Full wwPDB EM Validation Report ⓘ

May 6, 2025 – 05:50 PM EDT

PDB ID	:	8UGR / pdb_00008ugr
EMDB ID	:	EMD-42233
Title	:	In-situ structure of typeX supercomplex in respiratory chain (composite)
Authors	:	Zheng, W.; Zhang, K.; Zhu, J.
Deposited on	:	2023-10-06
Resolution	:	6.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

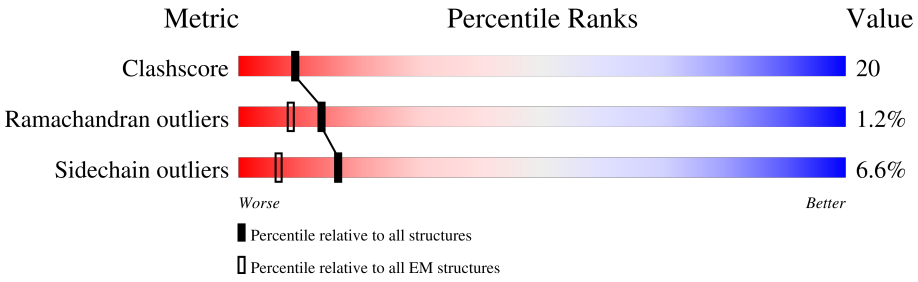
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	115	27% 54% 16%
1	5A	115	18% 57% 38% 5%
2	1B	258	22% 26% 9% 40%
2	5B	258	39% 19% 40%
3	1C	264	61% 18% 21%
3	5C	264	12% 61% 17% 21%
4	1D	466	64% 27% 8%
4	5D	466	11% 65% 26% 8%

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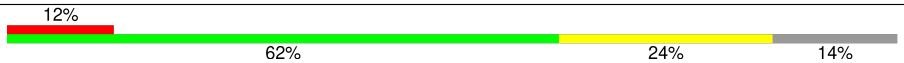
Mol	Chain	Length	Quality of chain
5	1E	249	
5	5E	249	
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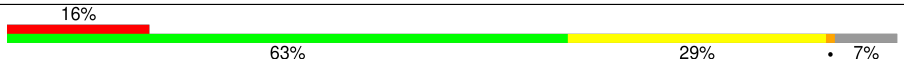
6	5F	464	
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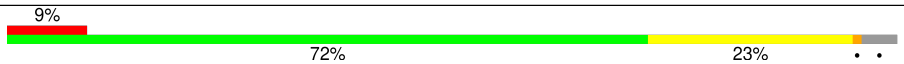
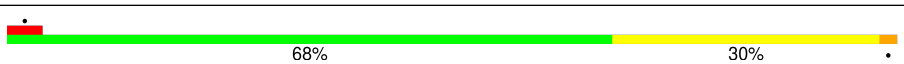
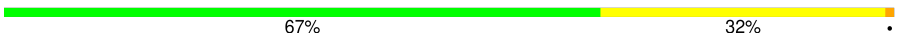
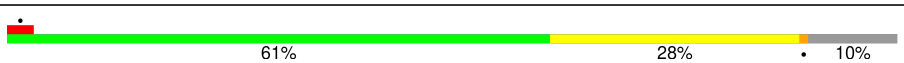
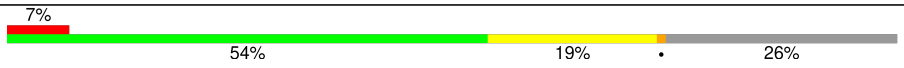
7	5G	727	
8	1H	318	
8	5H	318	
9	1I	239	
9	5I	239	
10	1J	175	
10	5J	175	
11	1K	98	
11	5K	98	
12	1L	606	
12	5L	606	
13	1M	459	
13	5M	459	
14	1N	347	
14	5N	347	
15	1O	357	
15	5O	357	
16	1P	377	
16	5P	377	
17	1Q	175	

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Mol	Chain	Length	Quality of chain
17	5Q	175	15% 55% 18% 26%
18	1R	123	67% 11% 22%
18	5R	123	67% 10% 22%
19	1S	99	61% 26% 12%
19	5S	99	8% 62% 25% 12%
20	1T	156	35% 19% 46%
20	1U	156	35% 19% 45%
20	5T	156	6% 34% 20% 46%
20	5U	156	5% 37% 18% 45%
21	1V	116	72% 27%
21	5V	116	14% 72% 26%
22	1W	128	70% 19% 10%
22	5W	128	9% 70% 19% 10%
23	1X	172	75% 23%
23	5X	172	74% 23%
24	1Y	141	67% 29%
24	5Y	141	68% 28%
25	1Z	144	69% 28%
25	5Z	144	68% 29%
26	1a	70	70% 30%
26	5a	70	73% 27%
27	1b	84	75% 20%
27	5b	84	75% 20%
28	1c	76	46% 18% 36%
28	5c	76	47% 17% 36%

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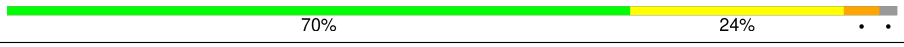
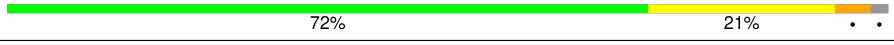
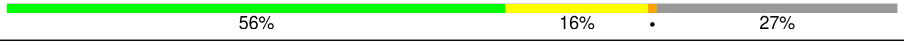
Mol	Chain	Length	Quality of chain
29	1d	122	
29	5d	122	
30	1e	106	
30	5e	106	
31	1f	58	
31	5f	58	
32	1g	154	
32	5g	154	
33	1h	189	
33	5h	189	
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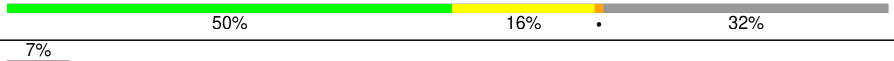
34	5i	128	
35	1j	105	
35	5j	105	
36	1k	98	
36	5k	98	
37	1l	186	
37	5l	186	
38	1m	129	
38	5m	129	
39	1n	179	
39	5n	179	
40	1o	136	
40	5o	136	
41	1p	176	

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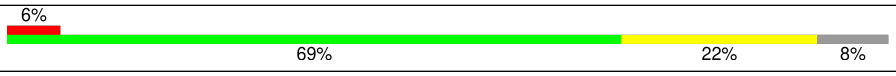
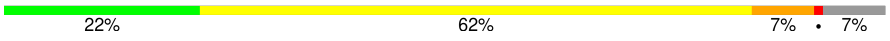
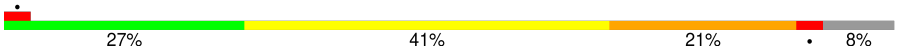
Mol	Chain	Length	Quality of chain
41	5p	176	
42	1q	145	
42	5q	145	
43	1r	113	
43	5r	113	
44	1s	471	
44	5s	471	
45	3A	480	
45	3N	480	
45	6A	480	
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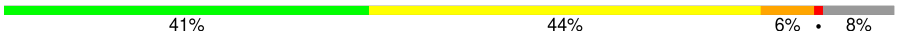
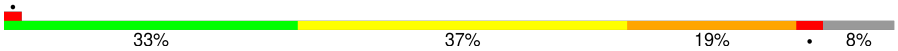
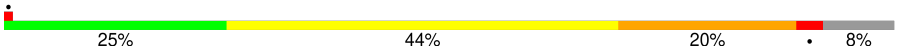
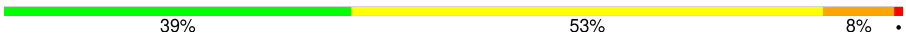
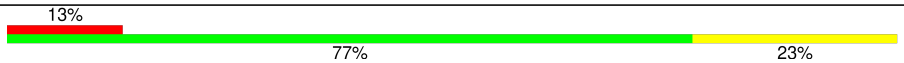
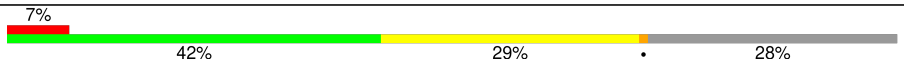
46	3B	453	
46	3O	453	
46	6B	453	
46	6O	453	
47	3C	379	
47	3P	379	
47	6C	379	
47	6P	379	
48	3D	326	
48	3Q	326	
48	6D	326	
48	6Q	326	
49	3E	274	
49	3I	274	

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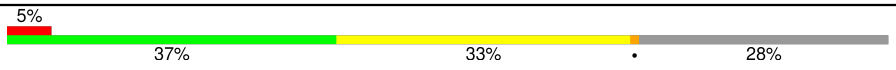
Mol	Chain	Length	Quality of chain
49	3R	274	
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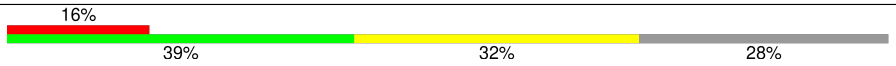
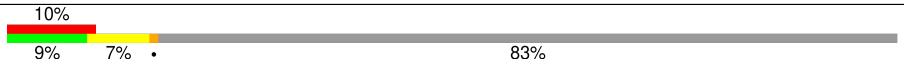
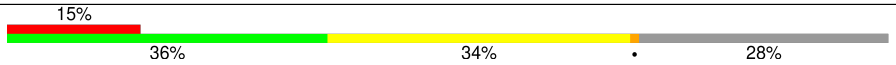
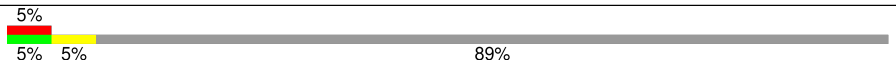
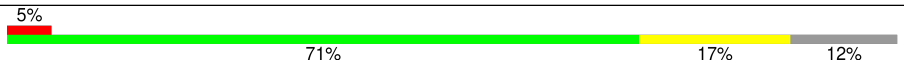
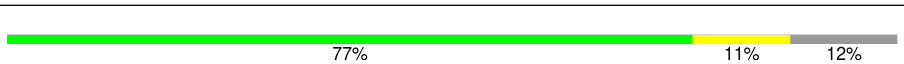
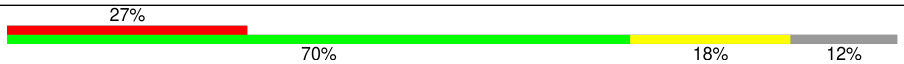
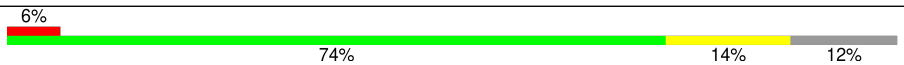
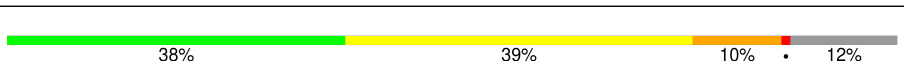
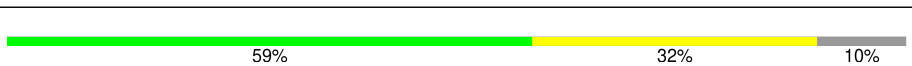
49	6E	274	
49	6I	274	
49	6R	274	
49	6V	274	
50	3F	111	
50	3S	111	
50	6F	111	
50	6S	111	
51	3G	82	
51	3T	82	
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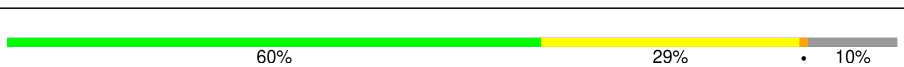
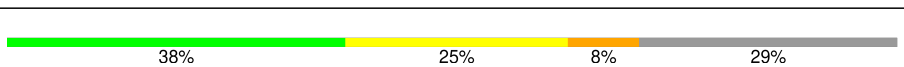
51	6T	82	
52	3H	91	
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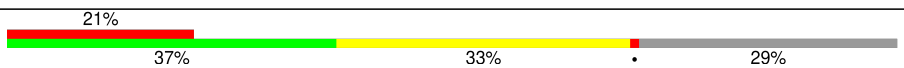
52	6H	91	
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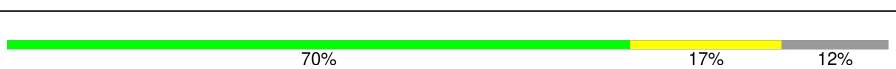
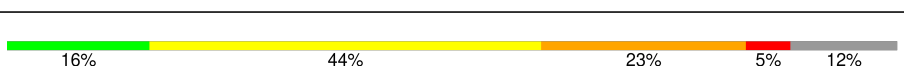
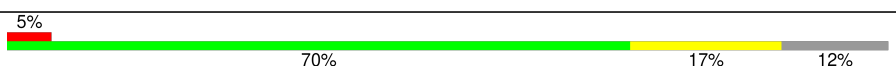
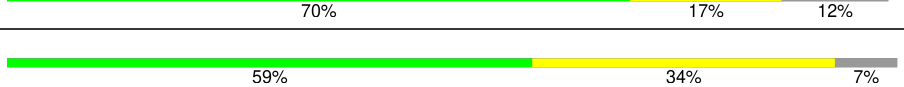
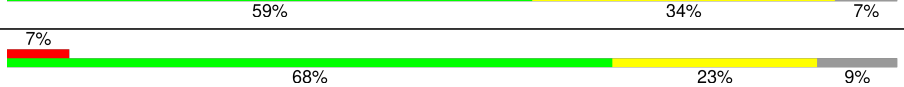
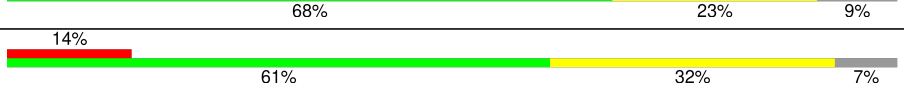
53	3J	64	
53	3W	64	
53	6J	64	
53	6W	64	
54	3X	56	
54	3Y	56	
54	6X	56	

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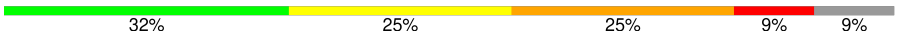
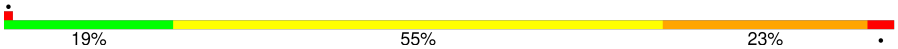
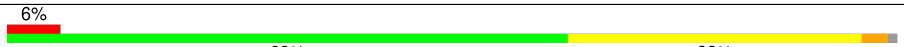
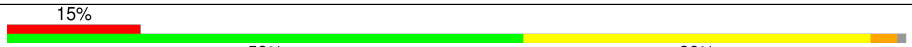
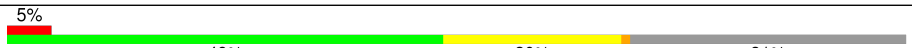
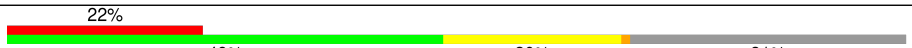
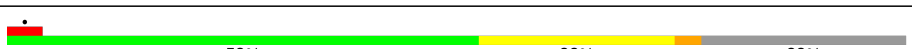
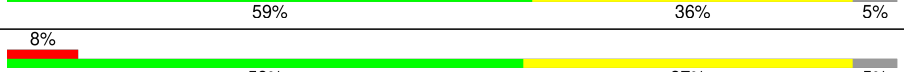
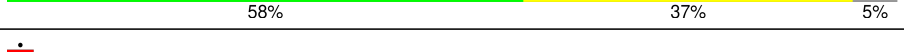
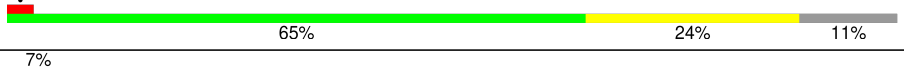
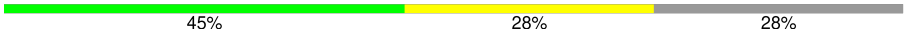
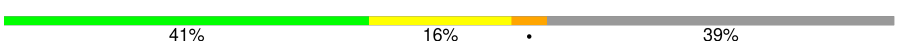
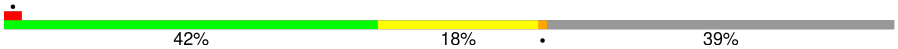
Mol	Chain	Length	Quality of chain
54	6Y	56	
55	4A	514	
55	8A	514	
56	4B	229	
56	8B	229	
57	4C	261	
57	8C	261	
58	4D	169	
58	8D	169	
59	4E	152	
59	8E	152	
60	4F	129	
60	8F	129	
61	4G	97	
61	8G	97	
62	4H	86	
62	8H	86	
63	4I	75	
63	8I	75	
64	4J	80	
64	8J	80	
65	4K	80	
65	8K	80	
66	4L	63	
66	8L	63	

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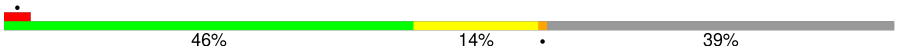
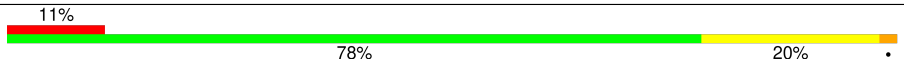
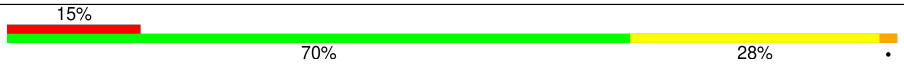
Mol	Chain	Length	Quality of chain
67	4M	70	
67	8M	70	
68	4N	82	
68	8N	82	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
70	SF4	1B	201	-	-	X	-
70	SF4	1F	502	-	-	X	-
70	SF4	5B	201	-	-	X	-
70	SF4	5F	502	-	-	X	-
72	FES	3E	301	-	-	X	-
72	FES	6E	301	-	-	X	-
75	CDL	8A	610	-	-	X	-
88	CUA	4B	302	-	-	X	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 233868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		
1	5A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		
2	5B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	209	Total	C	N	O	S	0	0
			1746	1128	299	317	2		
3	5C	209	Total	C	N	O	S	0	0
			1746	1128	299	317	2		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		
4	5D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		
5	5E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		
6	5F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		
7	5G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		
8	5H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		
9	5I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		
10	5J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		
11	5K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		
12	5L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		
13	5M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		
14	5N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	5O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		
16	5P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		
17	5Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		
18	5R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		
19	5S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		
20	5T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	5U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		
21	5V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		
22	5W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		
23	5X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		
24	5Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		
25	5Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		
26	5a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		
27	5b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	49	Total	C	N	O	0	0
			417	276	71	70		
28	5c	49	Total	C	N	O	0	0
			417	276	71	70		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		
29	5d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		
30	5e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		
31	5f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		
32	5g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		
33	5h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		
34	5i	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8
5i	0	ACE	-	acetylation	UNP A0A4X1UIV8

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		
35	5j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		
36	5k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		
37	5l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1m	128	Total	C	N	O	0	0
			1062	691	182	189		
38	5m	128	Total	C	N	O	0	0
			1062	691	182	189		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		
39	5n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		
40	5o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		
41	5p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		
42	5q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		
43	5r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		
44	5s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	3N	445	Total	C	N	O	S	0	0
			3415	2157	604	635	19		
45	6A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	6N	445	Total	C	N	O	S	0	0
			3415	2157	604	635	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3139	1965	556	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3132	1960	555	609	8		
46	6B	418	Total	C	N	O	S	0	0
			3139	1965	556	610	8		
46	6O	417	Total	C	N	O	S	0	0
			3132	1960	555	609	8		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		
47	6C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	6P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 48 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		
48	6D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	6Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		
49	6E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	6R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	6V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	6S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3G	72	Total	C	N	O	S	0	0
			616	403	114	97	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	6G	72	Total	C	N	O	S	0	0
			616	403	114	97	2		
51	6T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	6H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	6U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

- Molecule 53 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	3J	56	Total	C	N	O	0	0
			464	305	82	77		
53	3W	56	Total	C	N	O	0	0
			464	305	82	77		
53	6J	56	Total	C	N	O	0	0
			464	305	82	77		
53	6W	56	Total	C	N	O	0	0
			464	305	82	77		

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		
54	6X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	6Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	513	Total	C	N	O	S	0	0
			4016	2687	624	674	31		
55	8A	513	Total	C	N	O	S	0	0
			4016	2687	624	674	31		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		
56	8B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		
57	8C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		
58	8D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	4E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		
59	8E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		
60	8F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		
61	8G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		
62	8H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		
63	8I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		
64	8J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		
65	8K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		
66	8L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

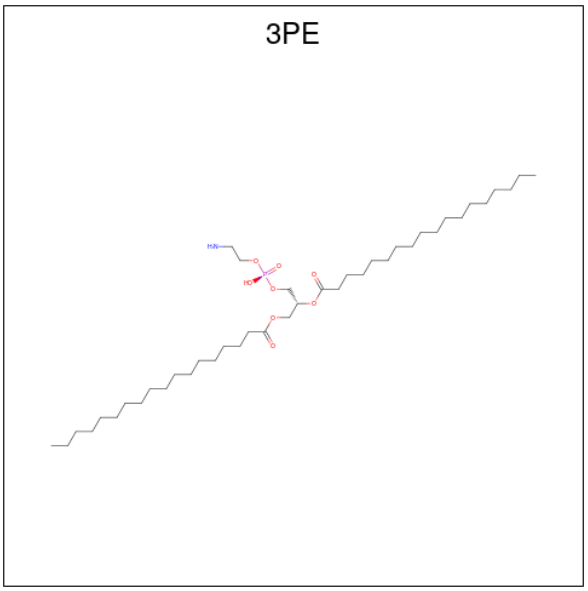
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		
67	8M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		
68	8N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1J	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	1M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1M	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	1N	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			41	31	1	8	1	

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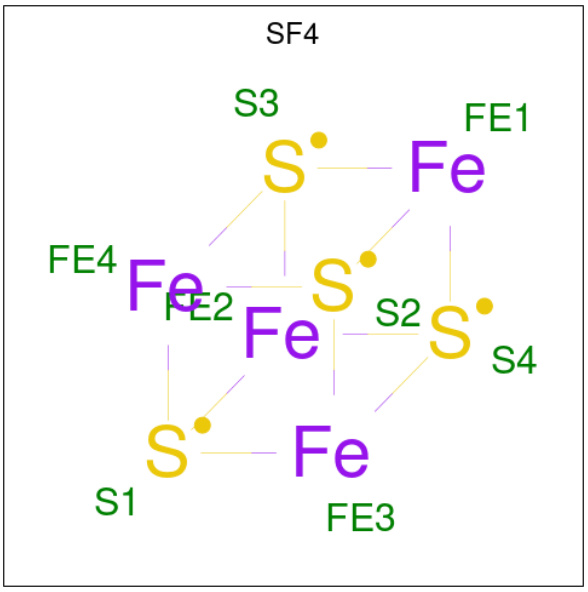
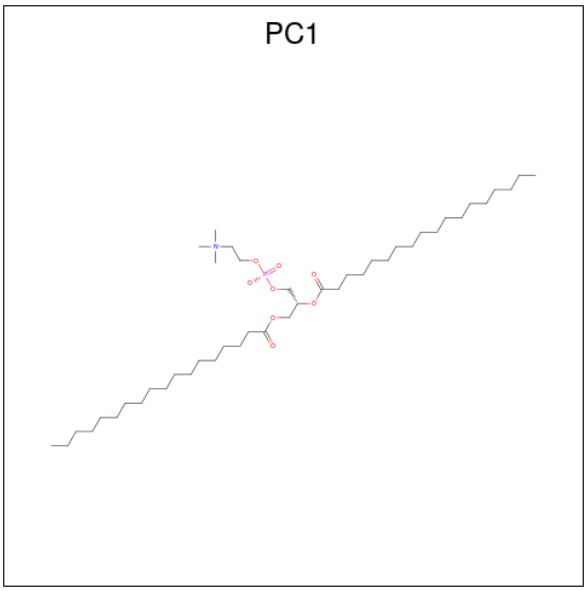
Mol	Chain	Residues	Atoms					AltConf
69	1d	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1j	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	5A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	5J	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	5L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	5L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	5L	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	5M	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	5M	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	5N	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	5N	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			30	20	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			27	17	1	8	1	
69	5Y	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	5d	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	5j	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 70 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
70	1B	1	Total Fe S 8 4 4	0
70	1F	1	Total Fe S 8 4 4	0
70	1G	1	Total Fe S 8 4 4	0
70	1G	1	Total Fe S 8 4 4	0
70	1I	1	Total Fe S 8 4 4	0
70	1I	1	Total Fe S 8 4 4	0
70	5B	1	Total Fe S 8 4 4	0
70	5F	1	Total Fe S 8 4 4	0
70	5G	1	Total Fe S 8 4 4	0
70	5G	1	Total Fe S 8 4 4	0
70	5I	1	Total Fe S 8 4 4	0
70	5I	1	Total Fe S 8 4 4	0

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
71	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
71	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
71	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
71	1m	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	5A	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	5B	1	Total	C	N	O	P	0
			46	36	1	8	1	
71	5H	1	Total	C	N	O	P	0
			48	38	1	8	1	
71	5I	1	Total	C	N	O	P	0
			54	44	1	8	1	

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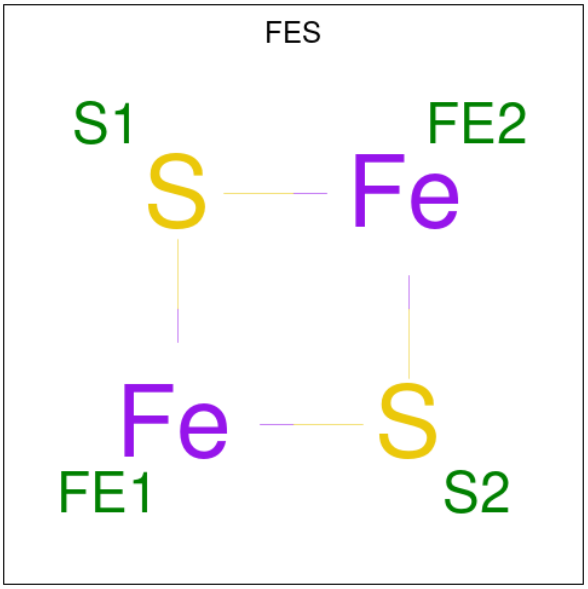
Mol	Chain	Residues	Atoms					AltConf
71	5I	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	5M	1	Total	C	N	O	P	0
			44	34	1	8	1	
71	5P	1	Total	C	N	O	P	0
			33	23	1	8	1	
71	5Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
71	5h	1	Total	C	N	O	P	0
			47	37	1	8	1	
71	5m	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
72	1E	1	Total	Fe	S	0
			4	2	2	
72	1G	1	Total	Fe	S	0
			4	2	2	
72	3E	1	Total	Fe	S	0
			4	2	2	
72	3R	1	Total	Fe	S	0
			4	2	2	
72	5E	1	Total	Fe	S	0
			4	2	2	

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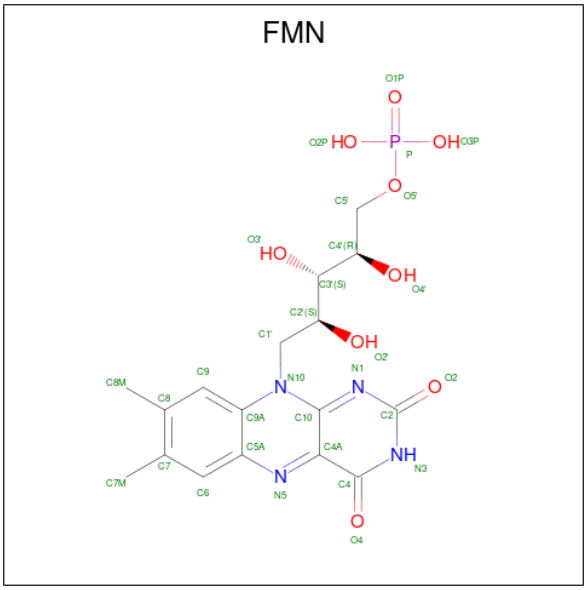
Mol	Chain	Residues	Atoms	AltConf
72	5G	1	Total Fe S 4 2 2	0
72	6E	1	Total Fe S 4 2 2	0
72	6R	1	Total Fe S 4 2 2	0

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

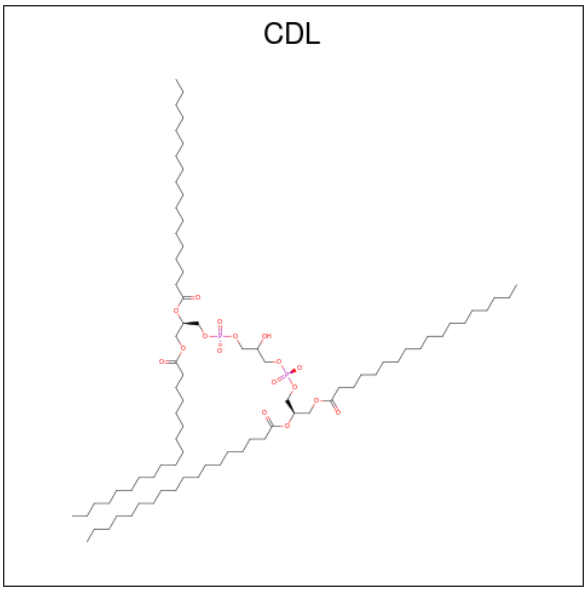


Mol	Chain	Residues	Atoms	AltConf
73	1F	1	Total C N O P 31 17 4 9 1	0
73	5F	1	Total C N O P 31 17 4 9 1	0

- Molecule 74 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
74	1G	1	Total K 1 1	0
74	5G	1	Total K 1 1	0

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
75	1L	1	Total	C	O	P	0
			76	57	17	2	
75	1N	1	Total	C	O	P	0
			62	43	17	2	
75	1X	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			65	46	17	2	
75	1i	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	5L	1	Total	C	O	P	0
			76	57	17	2	
75	5N	1	Total	C	O	P	0
			62	43	17	2	
75	5X	1	Total	C	O	P	0
			86	67	17	2	
75	5d	1	Total	C	O	P	0
			65	46	17	2	
75	5i	1	Total	C	O	P	0
			80	61	17	2	
75	5q	1	Total	C	O	P	0
			61	42	17	2	

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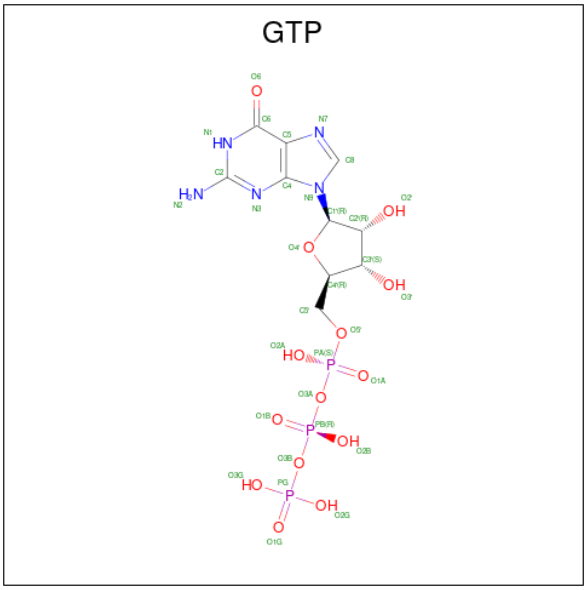
Mol	Chain	Residues	Atoms				AltConf
75	8A	1	Total	C	O	P	0
			100	81	17	2	
75	8B	1	Total	C	O	P	0
			100	81	17	2	
75	8D	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 76 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

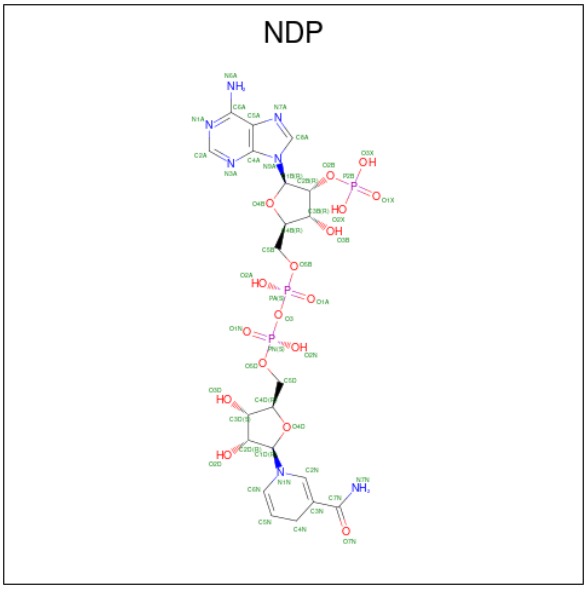


Mol	Chain	Residues	Atoms					AltConf
76	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	
76	5O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 77 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
77	1O	1	Total	Mg	0
			1	1	
77	4A	1	Total	Mg	0
			1	1	
77	5O	1	Total	Mg	0
			1	1	
77	8A	1	Total	Mg	0
			1	1	

- Molecule 78 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

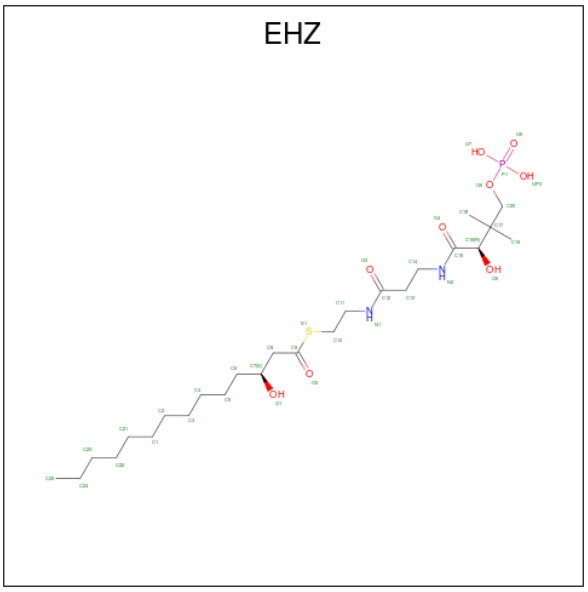


Mol	Chain	Residues	Atoms					AltConf
78	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	
78	5P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 79 is ZINC ION (CCD ID: ZN) (formula: Zn).

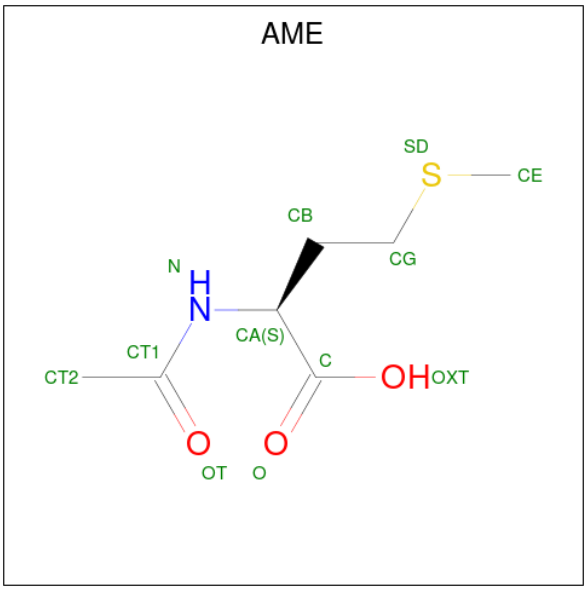
Mol	Chain	Residues	Atoms		AltConf
79	1R	1	Total	Zn	0
			1	1	
79	4F	1	Total	Zn	0
			1	1	
79	5R	1	Total	Zn	0
			1	1	
79	8F	1	Total	Zn	0
			1	1	

- Molecule 80 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



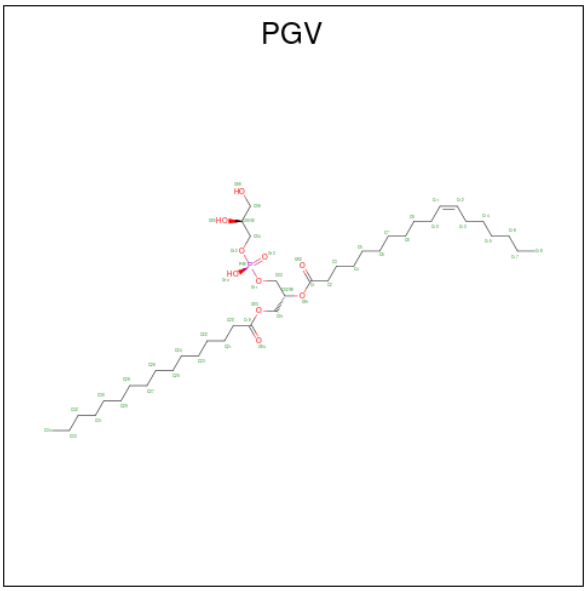
Mol	Chain	Residues	Atoms						AltConf
80	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	5T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
80	5n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 81 is N-ACETYLMETHIONINE (CCD ID: AME) (formula: $C_7H_{13}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
81	1h	1	Total	C	N	O	S	0
			11	7	1	2	1	
81	5h	1	Total	C	N	O	S	0
			11	7	1	2	1	

- Molecule 82 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
82	1p	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4A	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	
82	4C	1	Total	C	O	P	0
			51	40	10	1	

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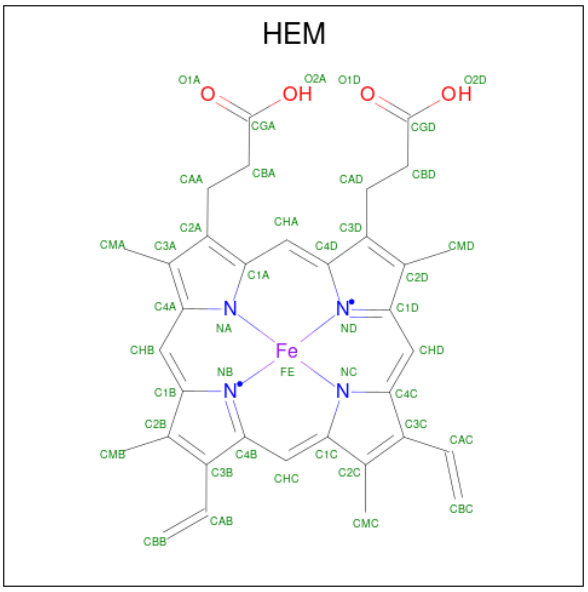
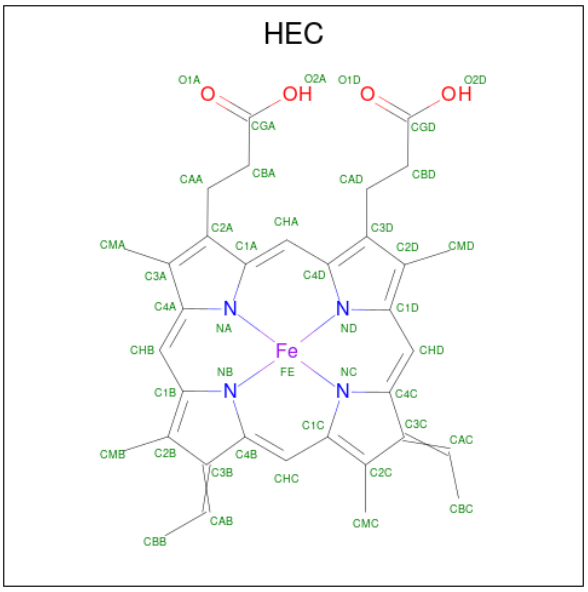
Mol	Chain	Residues	Atoms				AltConf
82	4C	1	Total	C	O	P	0
			51	40	10	1	
82	4G	1	Total	C	O	P	0
			51	40	10	1	
82	4J	1	Total	C	O	P	0
			51	40	10	1	
82	4K	1	Total	C	O	P	0
			51	40	10	1	
82	4L	1	Total	C	O	P	0
			51	40	10	1	
82	8A	1	Total	C	O	P	0
			51	40	10	1	
82	8A	1	Total	C	O	P	0
			51	40	10	1	
82	8A	1	Total	C	O	P	0
			51	40	10	1	
82	8A	1	Total	C	O	P	0
			51	40	10	1	
82	8B	1	Total	C	O	P	0
			51	40	10	1	
82	8C	1	Total	C	O	P	0
			51	40	10	1	
82	8C	1	Total	C	O	P	0
			51	40	10	1	
82	8C	1	Total	C	O	P	0
			51	40	10	1	
82	8C	1	Total	C	O	P	0
			51	40	10	1	
82	8C	1	Total	C	O	P	0
			51	40	10	1	
82	8G	1	Total	C	O	P	0
			51	40	10	1	
82	8J	1	Total	C	O	P	0
			51	40	10	1	
82	8K	1	Total	C	O	P	0
			51	40	10	1	
82	8L	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 83 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



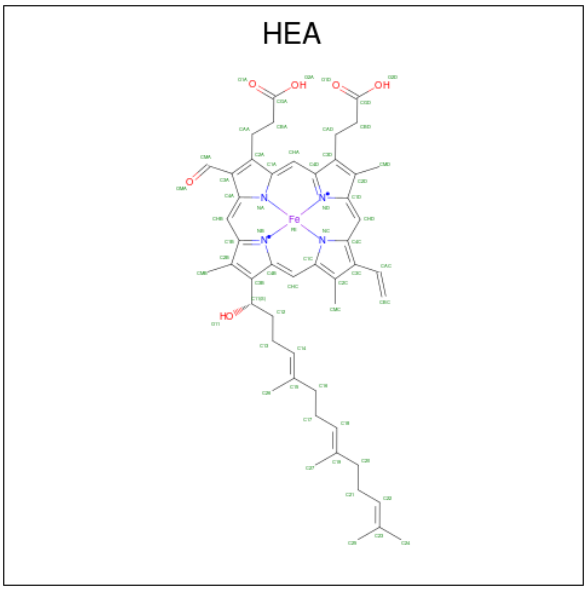
Mol	Chain	Residues	Atoms					AltConf
83	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	3C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	3P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	6C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	6C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	6P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
83	6P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 84 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
84	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
84	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
84	6D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
84	6Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 85 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
85	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
85	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
85	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
85	8A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

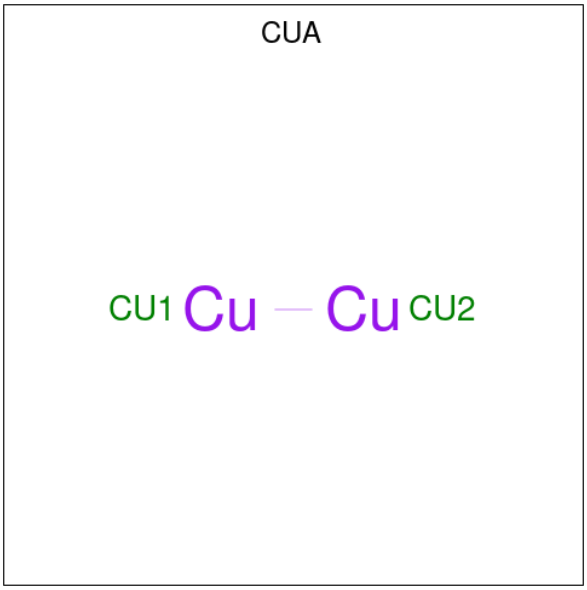
- Molecule 86 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
86	4A	1	Total	Cu	0
			1	1	
86	8A	1	Total	Cu	0
			1	1	

- Molecule 87 is SODIUM ION (CCD ID: NA) (formula: Na).

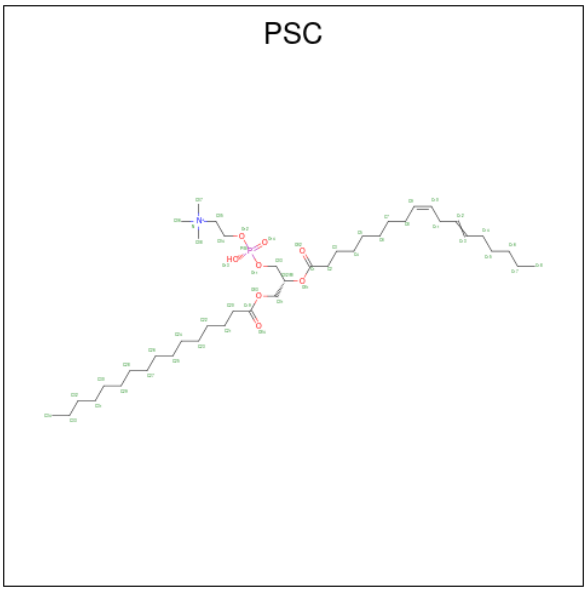
Mol	Chain	Residues	Atoms		AltConf
87	4A	1	Total	Na	0
			1	1	
87	8A	1	Total	Na	0
			1	1	

- Molecule 88 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



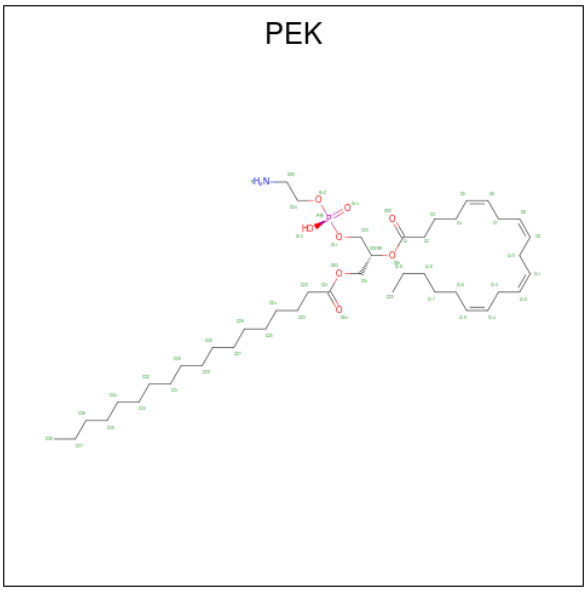
Mol	Chain	Residues	Atoms	AltConf
88	4B	1	Total Cu 2 2	0
88	8B	1	Total Cu 2 2	0

- Molecule 89 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



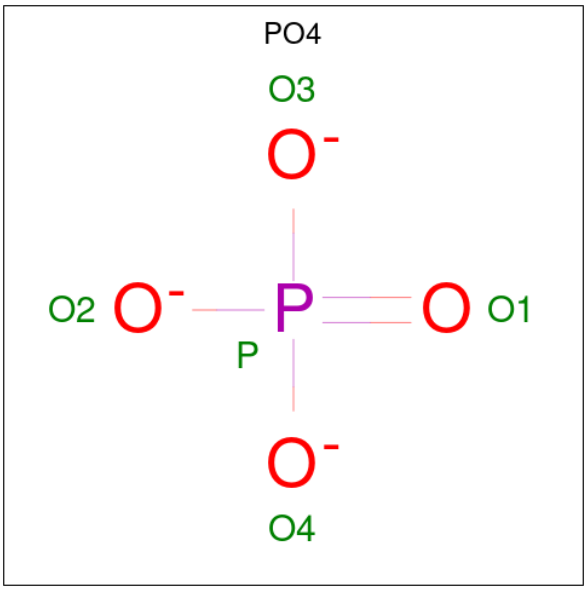
Mol	Chain	Residues	Atoms	AltConf
89	4B	1	Total C N O P 52 42 1 8 1	0
89	8A	1	Total C N O P 52 42 1 8 1	0

- Molecule 90 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
90	4C	1	Total	C	N	O	P	0
			53	43	1	8	1	
90	4C	1	Total	C	N	O	P	0
			52	42	1	8	1	
90	8C	1	Total	C	N	O	P	0
			53	43	1	8	1	
90	8C	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 91 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



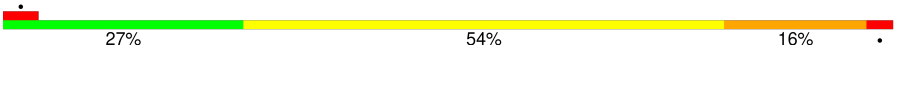
Mol	Chain	Residues	Atoms	AltConf
91	4H	1	Total O P 5 4 1	0
91	8H	1	Total O P 5 4 1	0

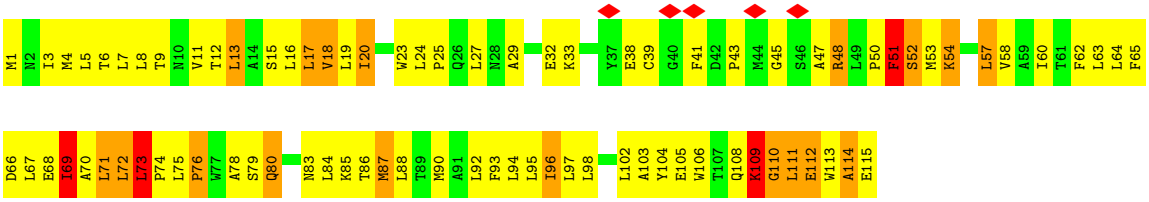
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

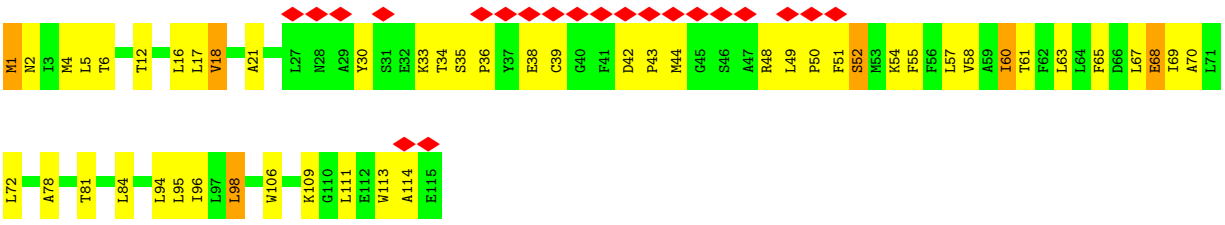
Chain 1A:





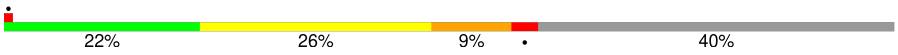
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

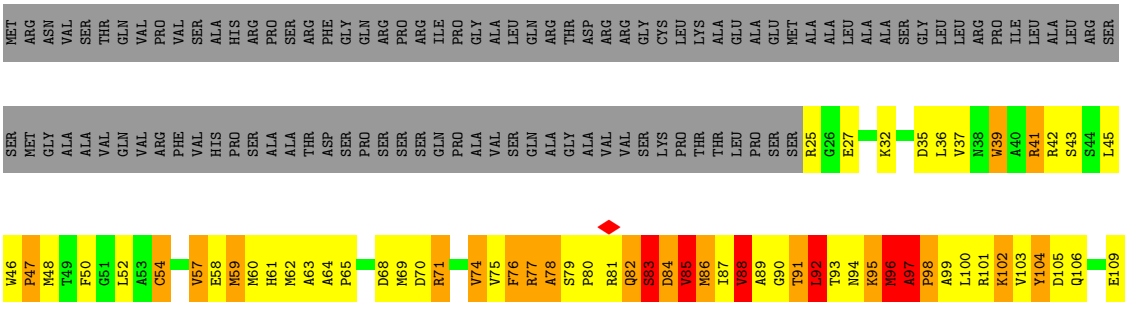
Chain 5A:

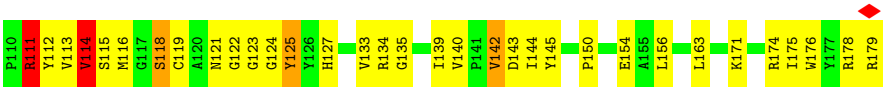


• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 1B:

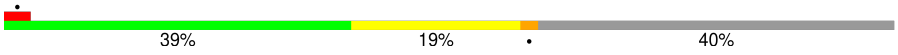


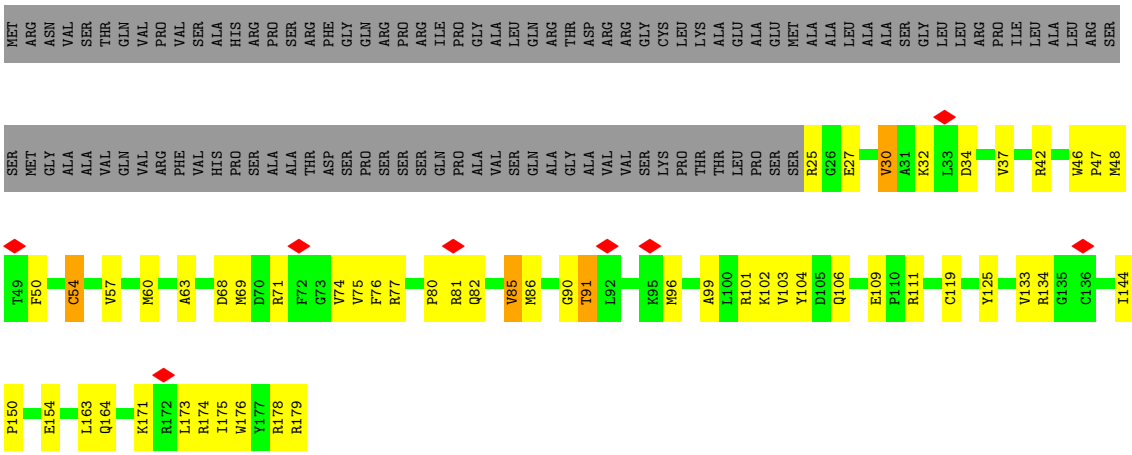




• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

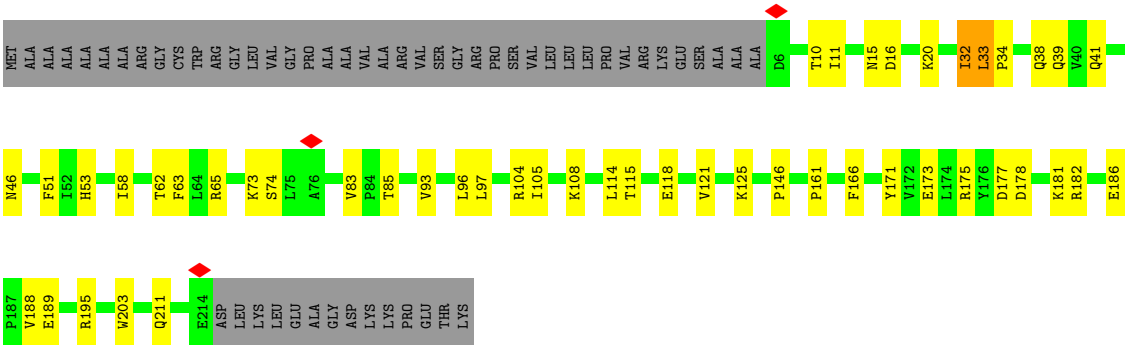
Chain 5B:





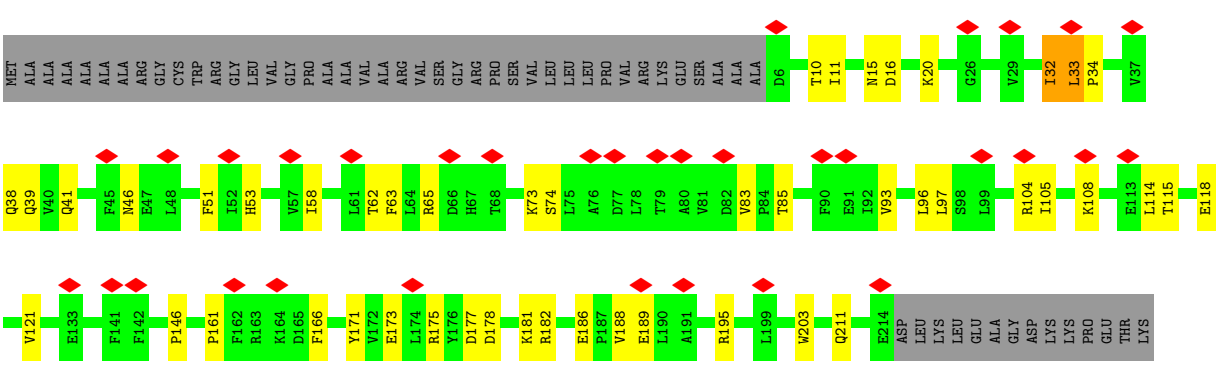
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain 1C:



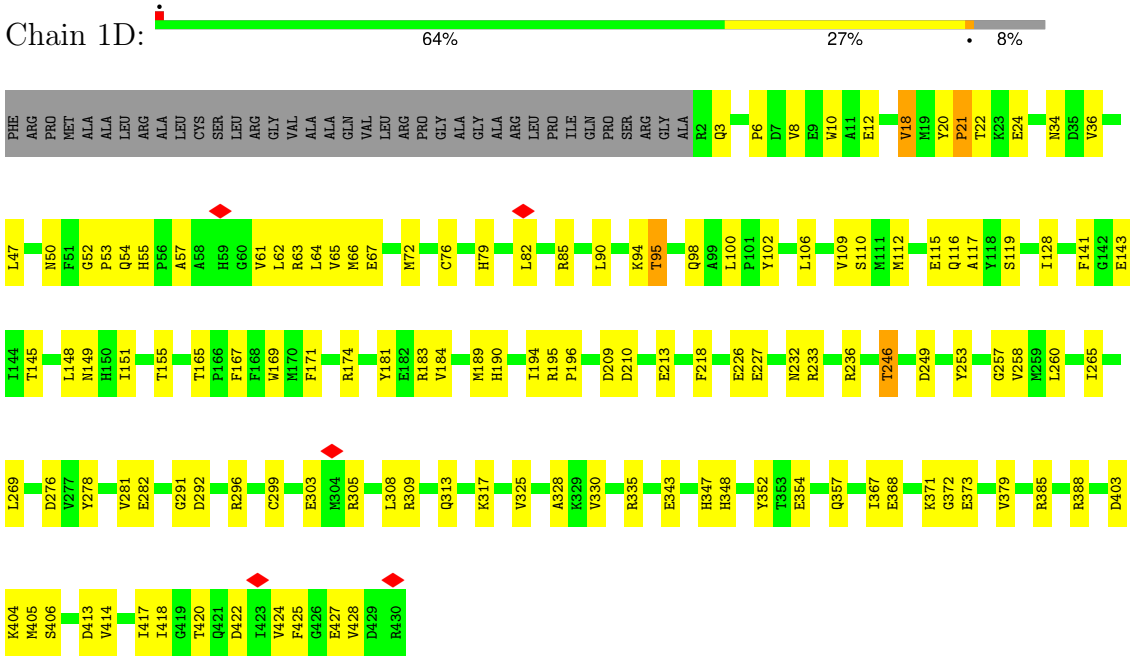
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain 5C:



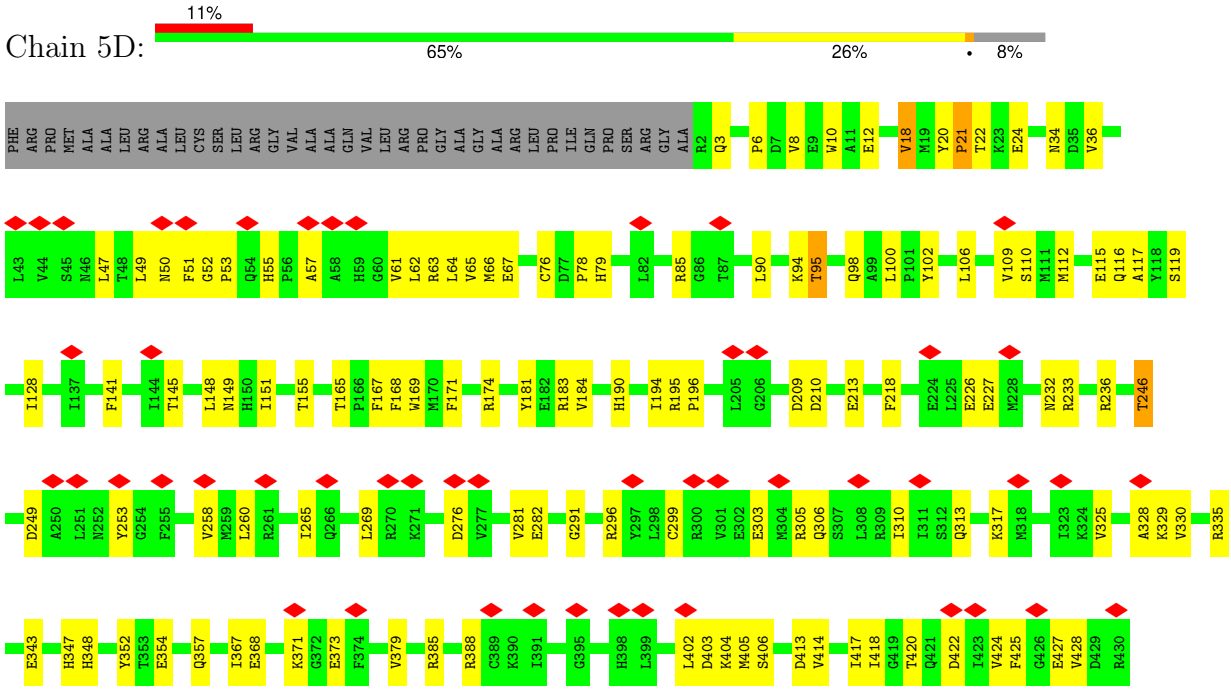
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D:



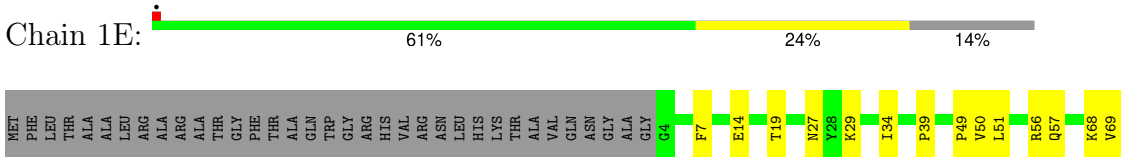
• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

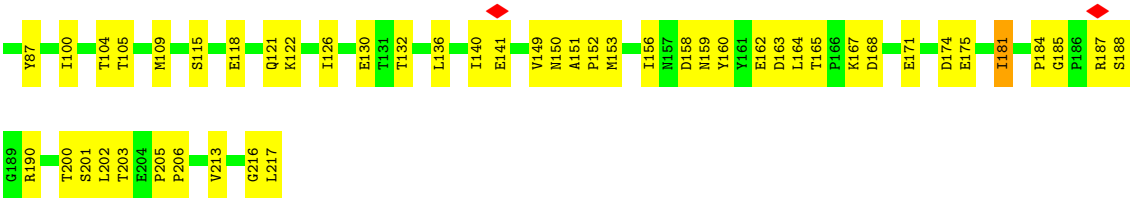
Chain 5D:



• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

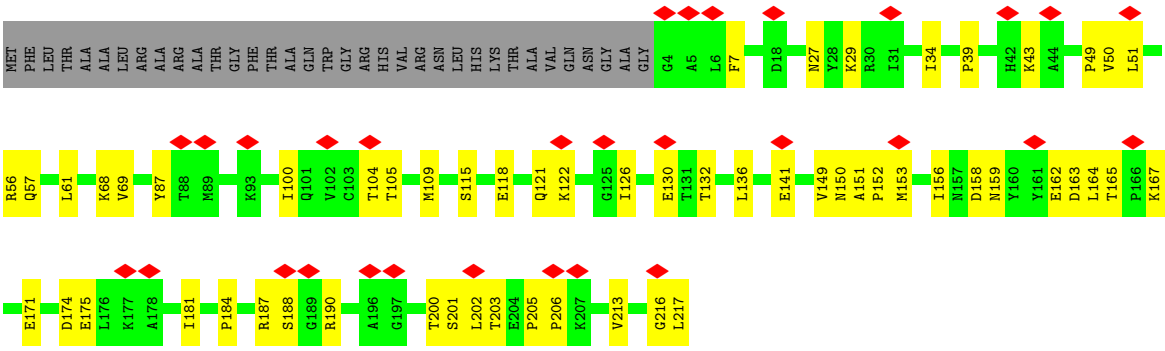
Chain 1E:





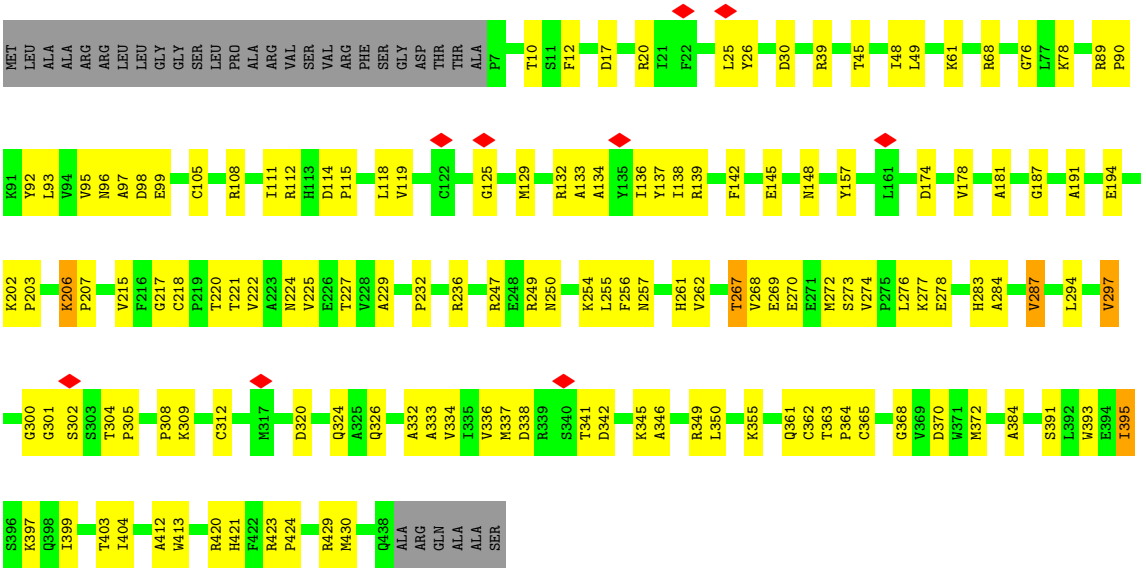
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 5E:



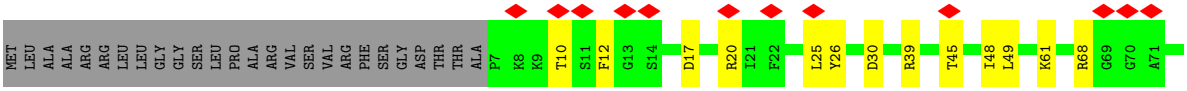
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

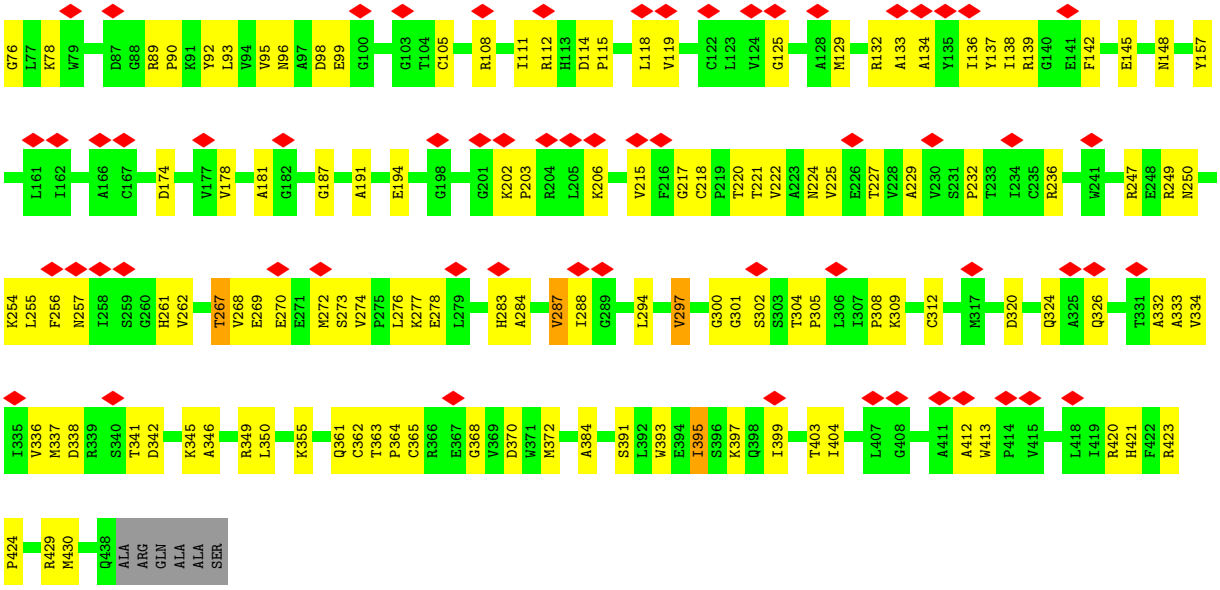
Chain 1F:



• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

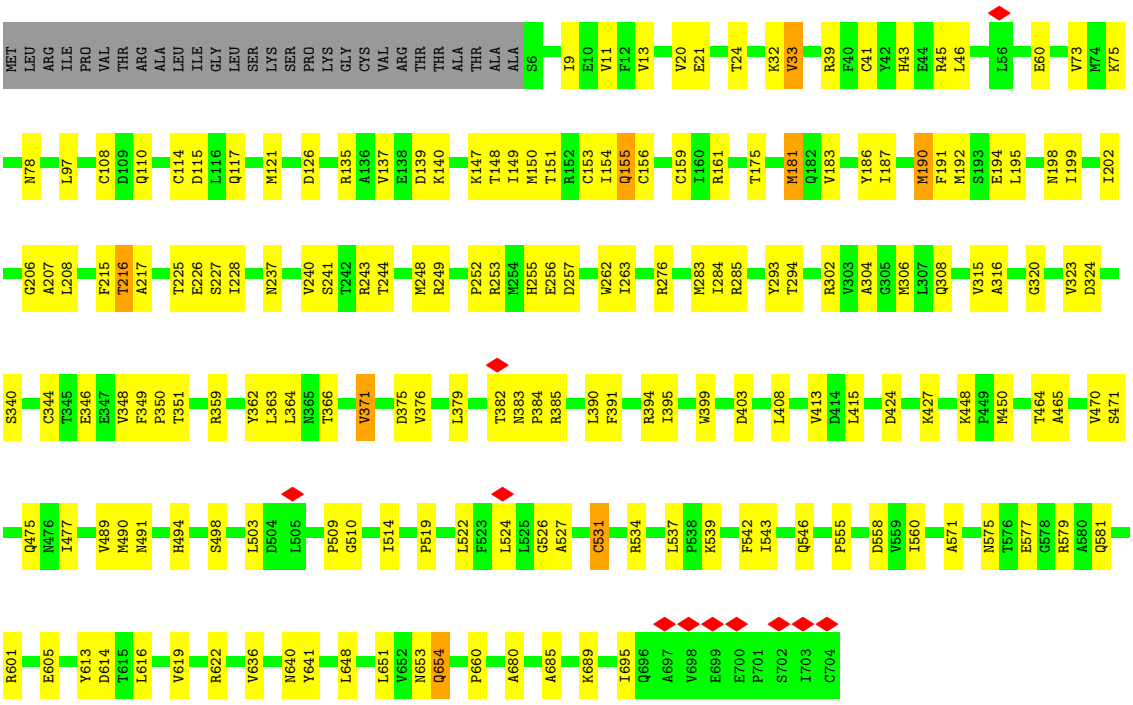
Chain 5F:





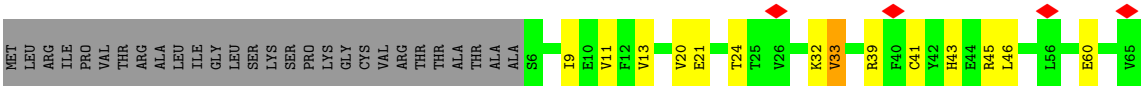
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

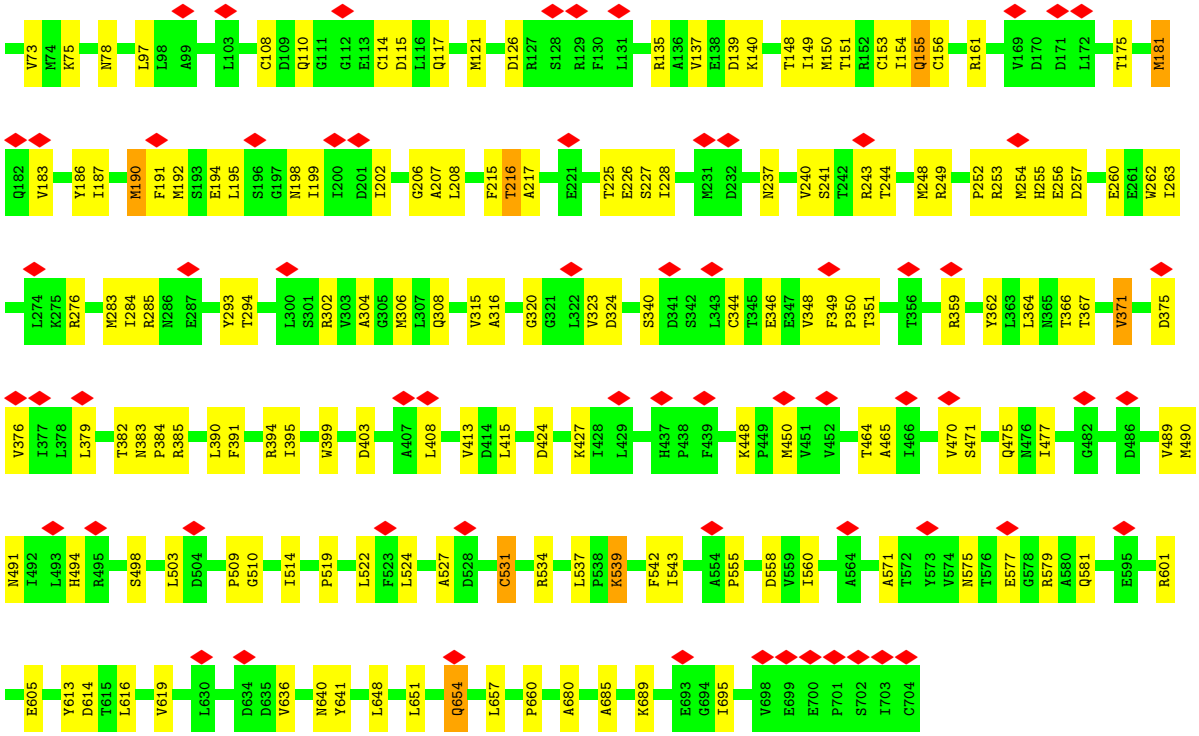
Chain 1G:



• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

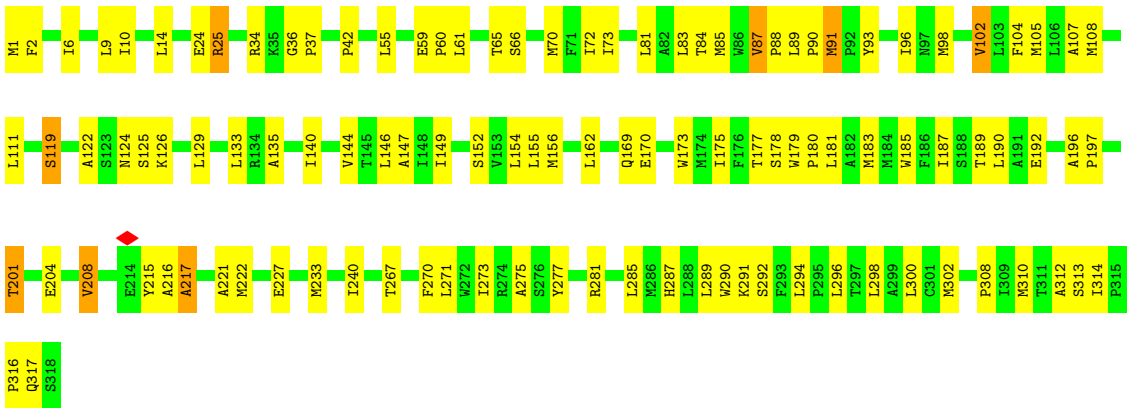
Chain 5G:





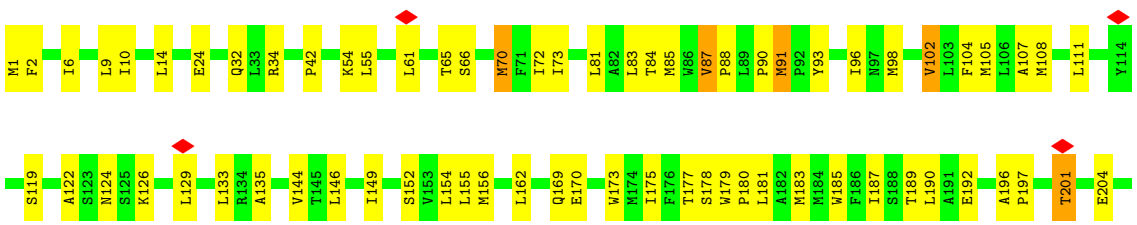
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H:



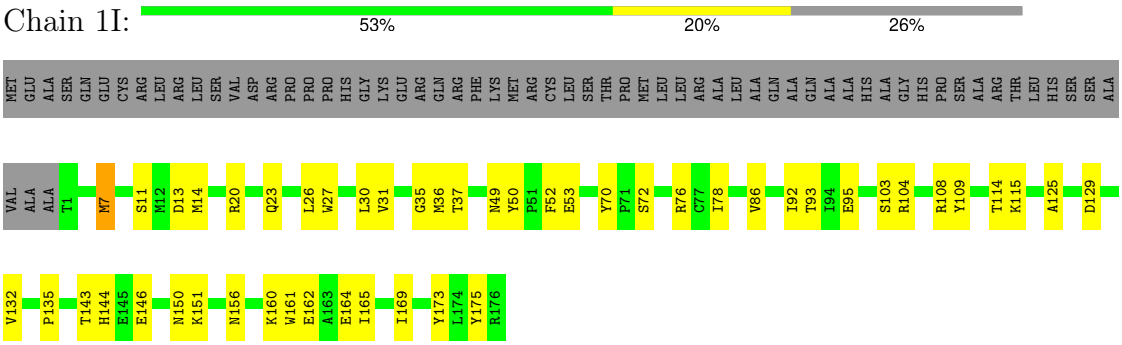
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 5H:



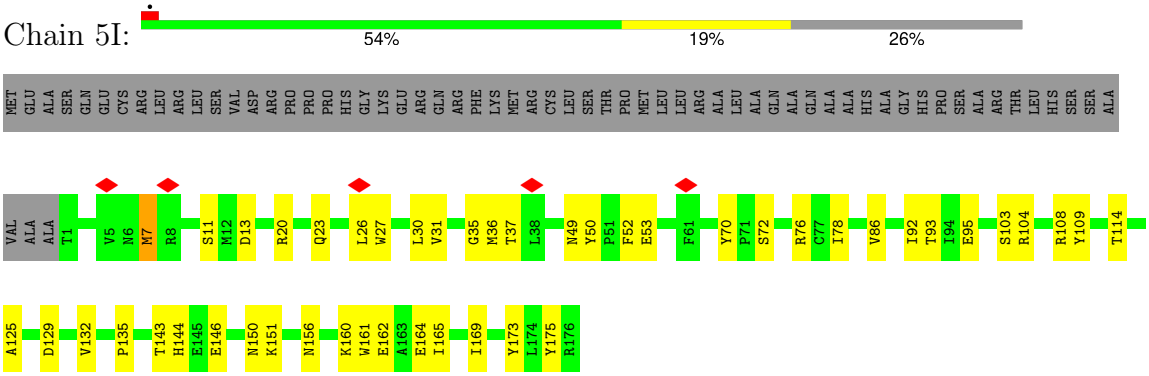
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I:



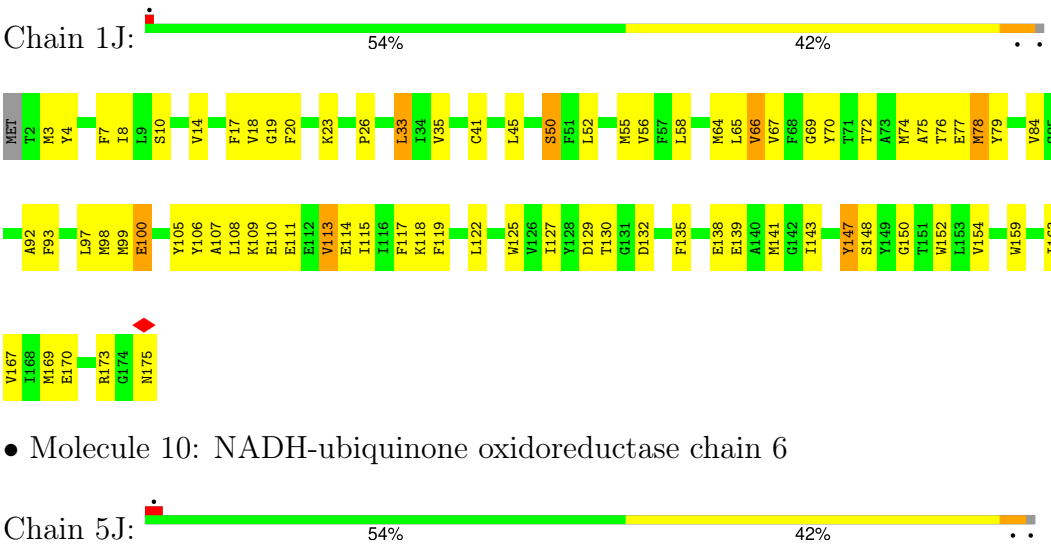
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 5I:



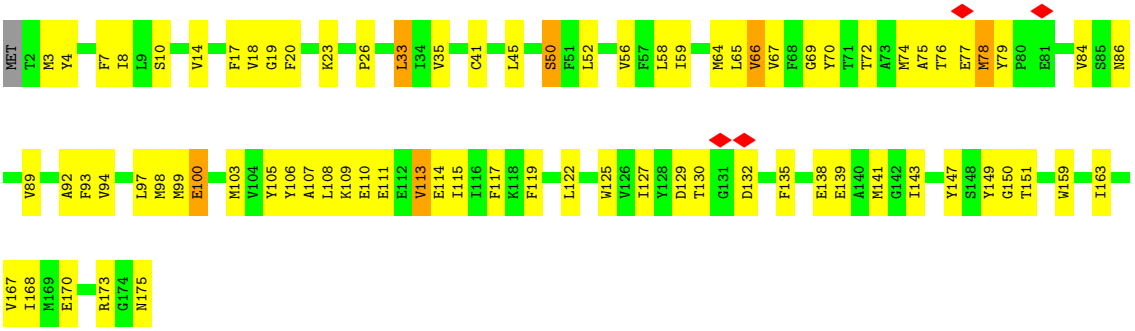
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J:



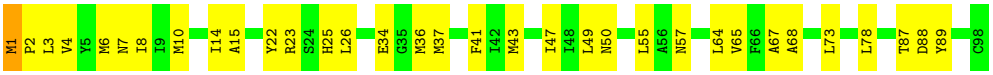
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 5J:



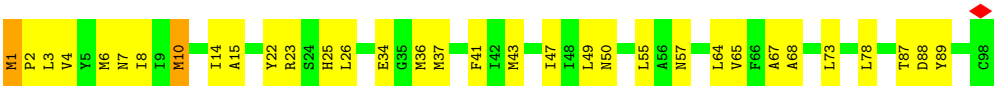
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:



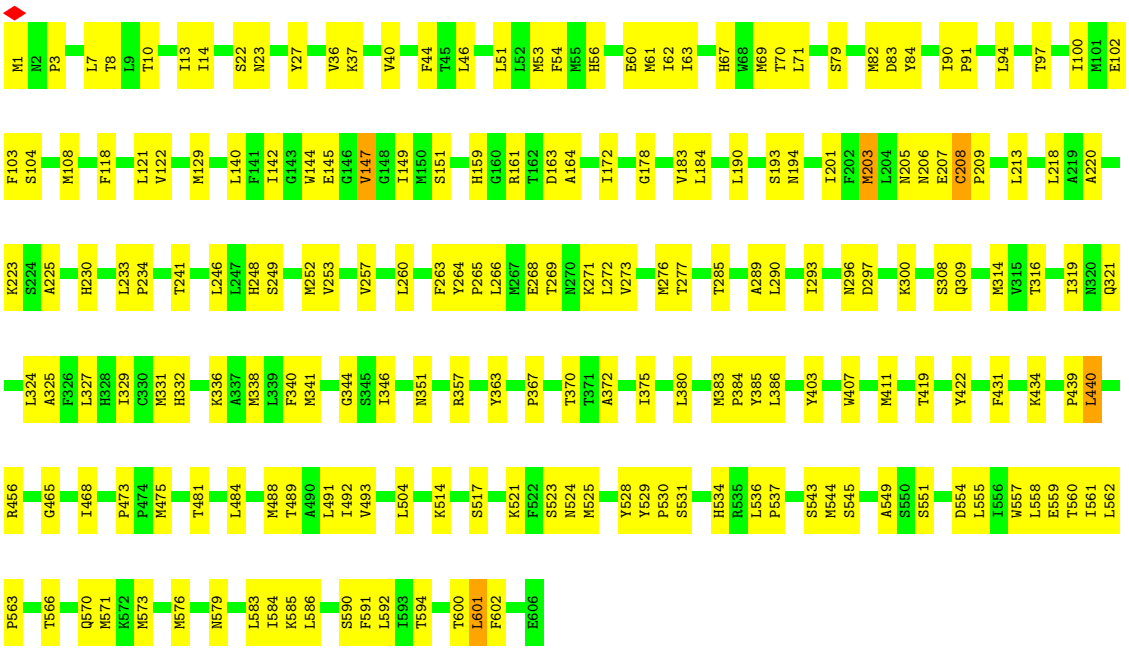
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 5K:



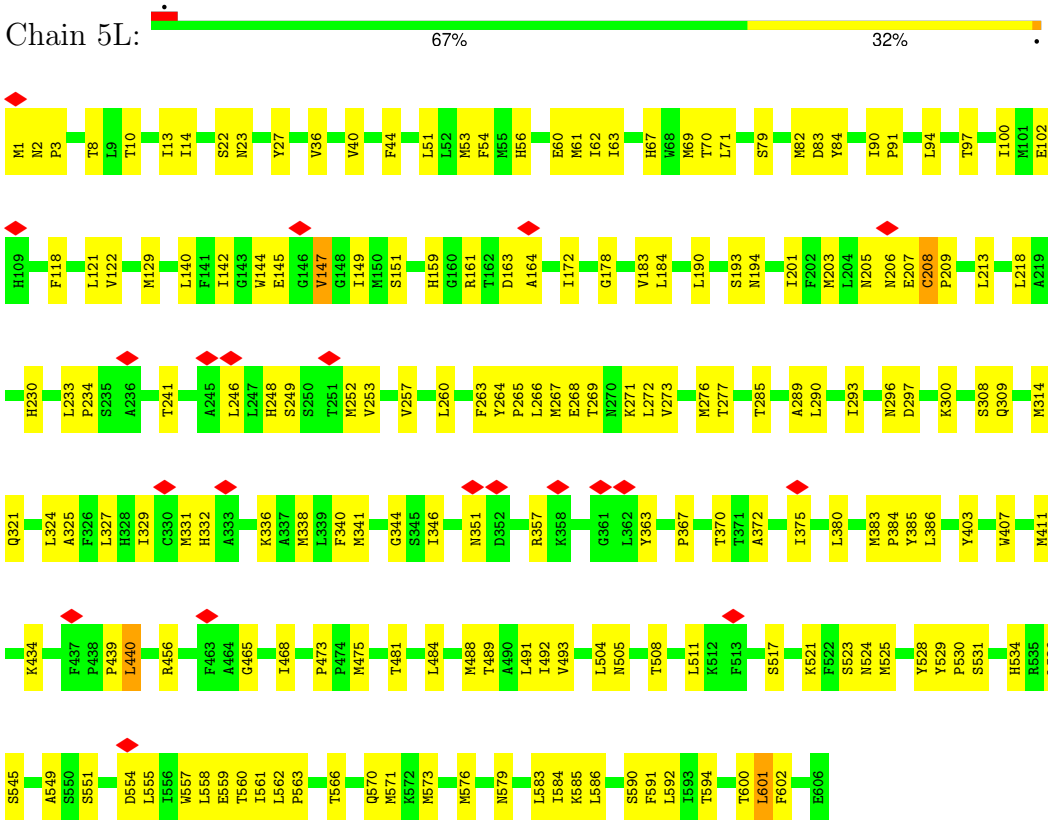
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 1L:



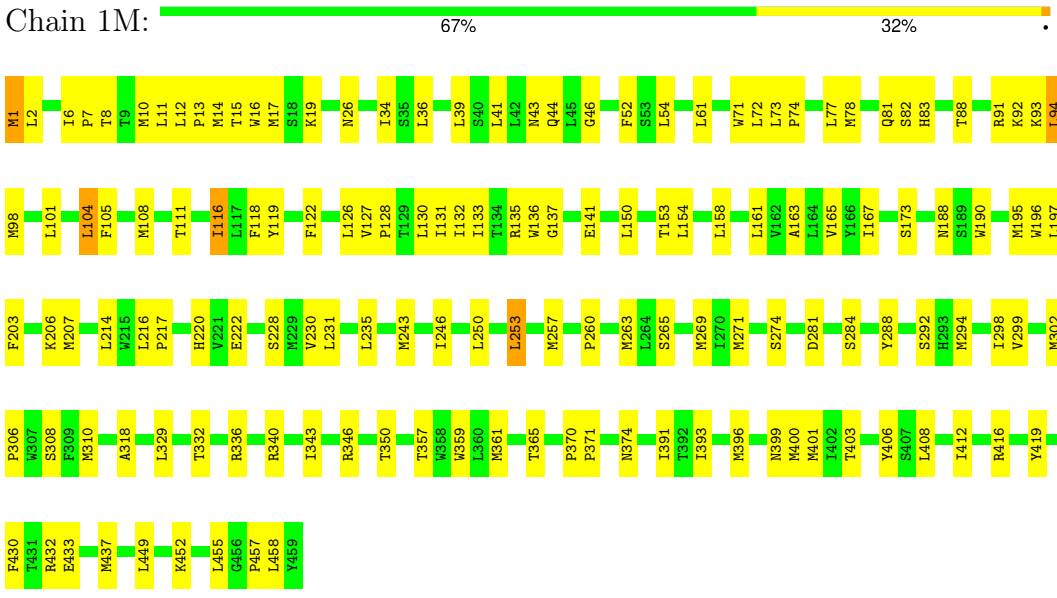
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain 5L:



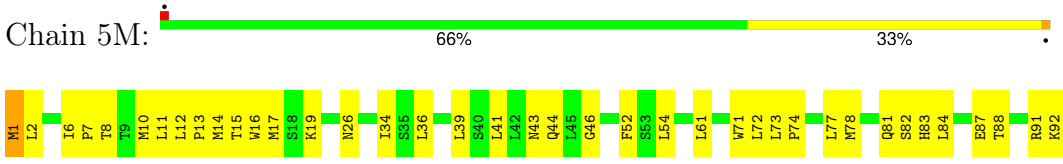
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

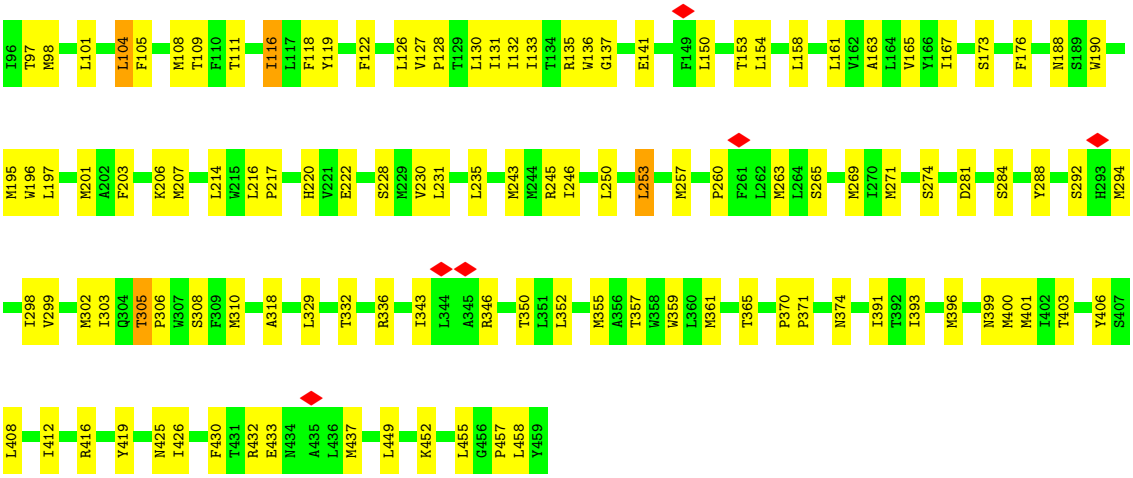
Chain 1M:



• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

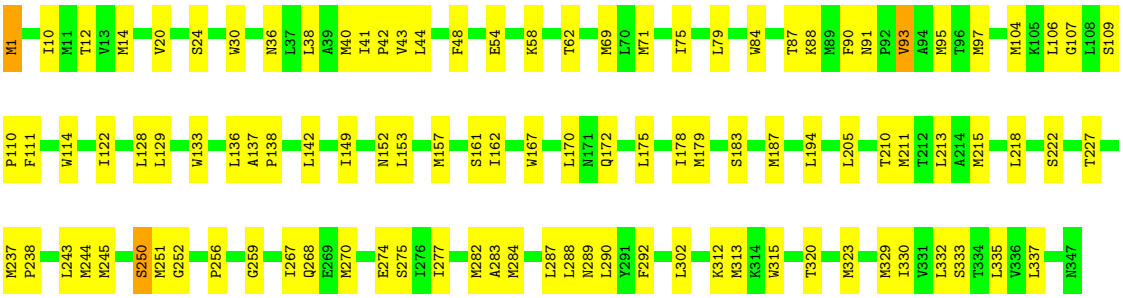
Chain 5M:





• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N:

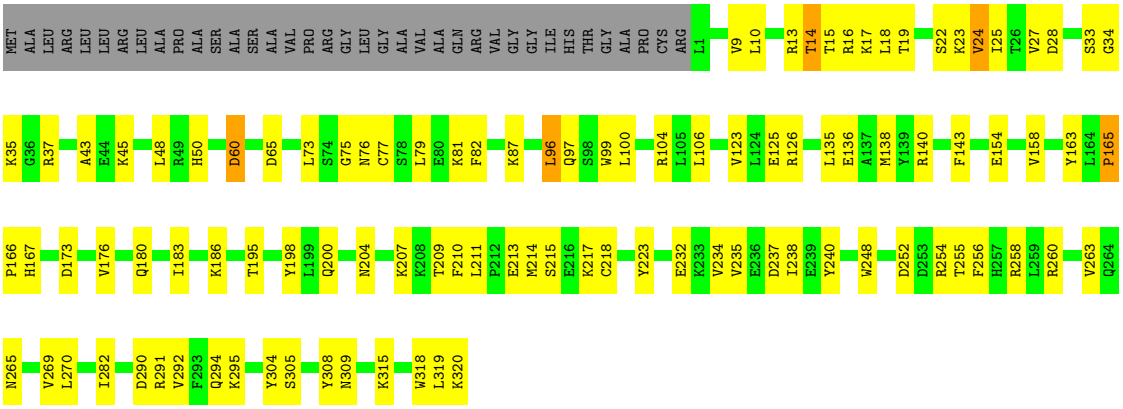


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 5N:

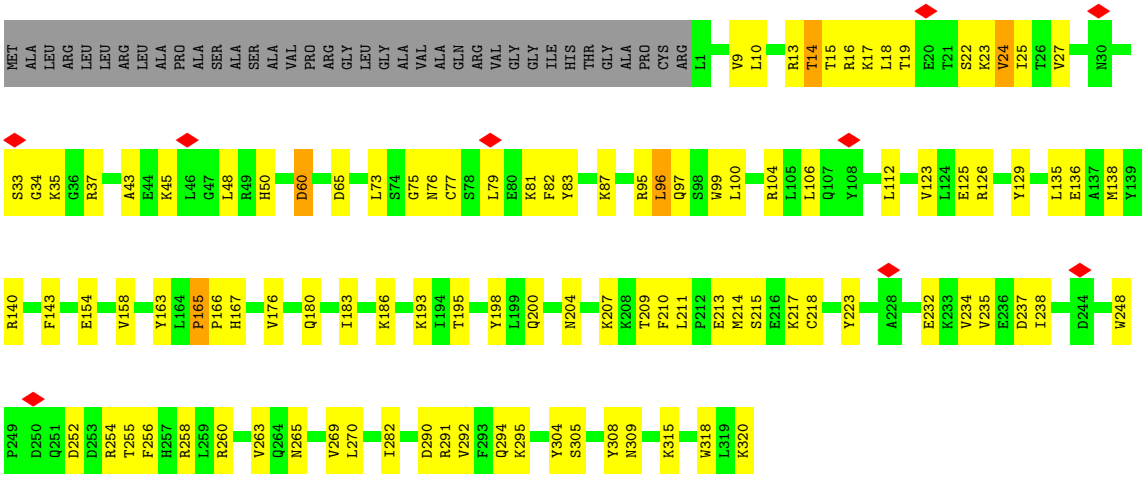
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O:



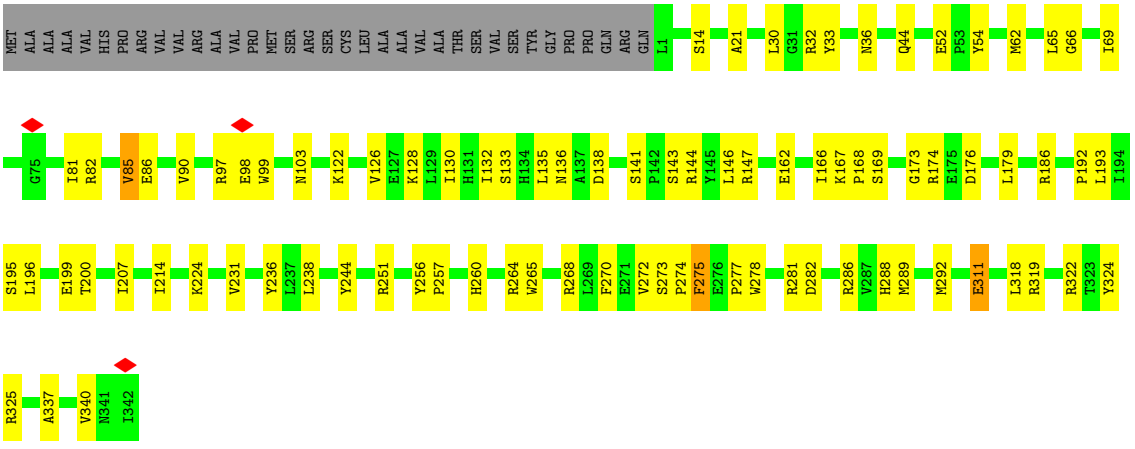
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 5O:



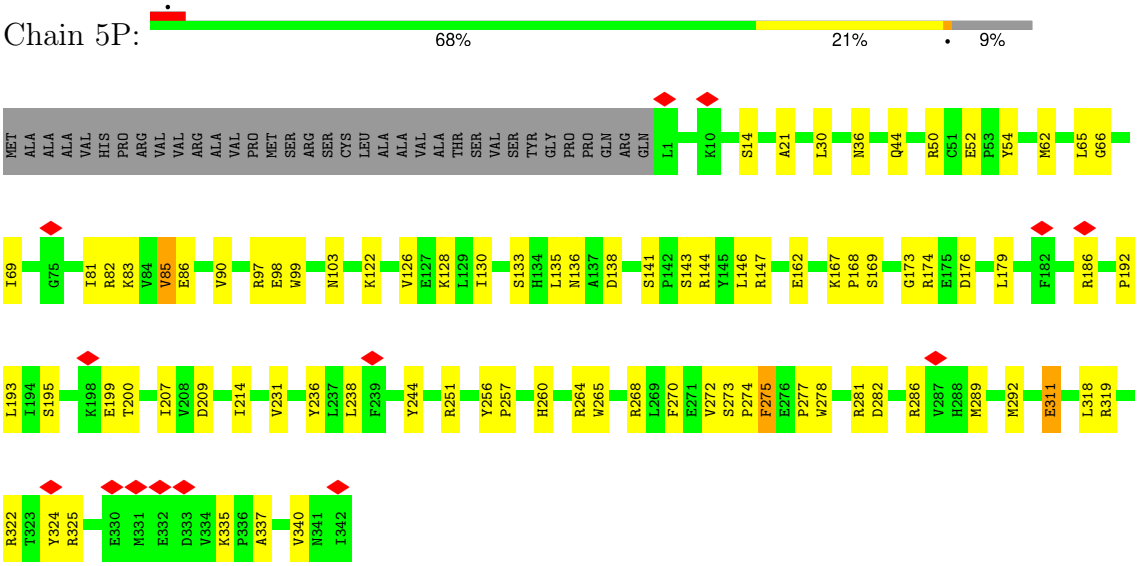
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:



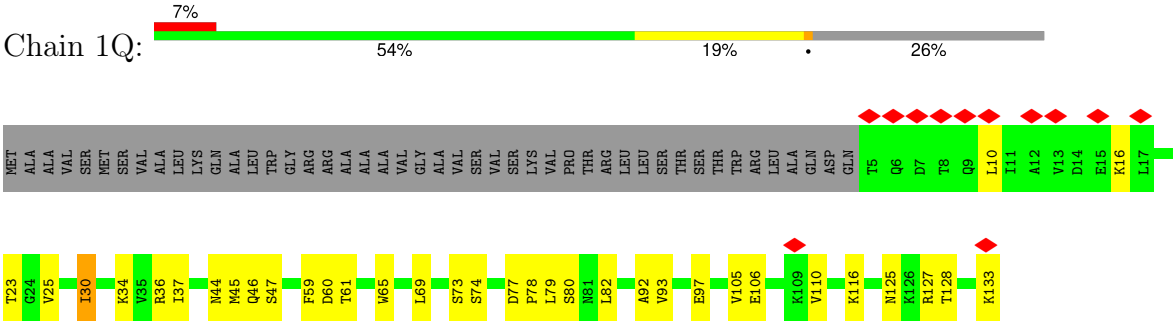
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 5P:



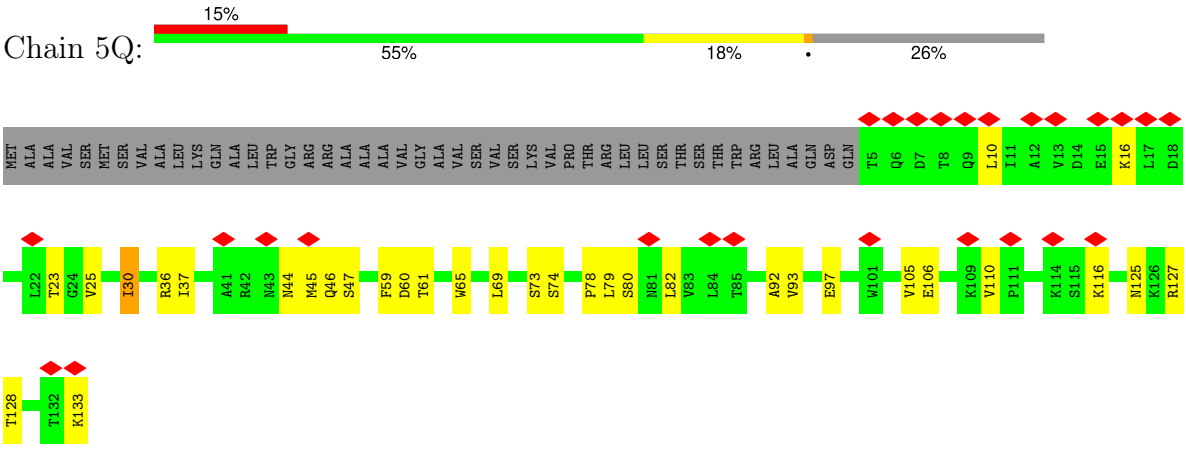
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q:



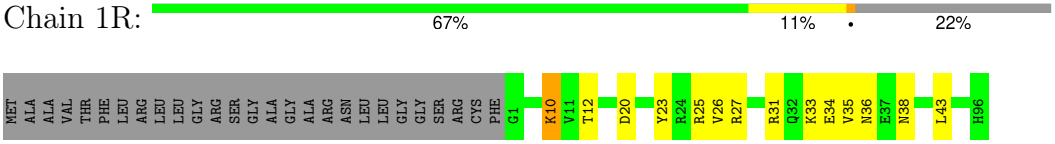
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 5Q:



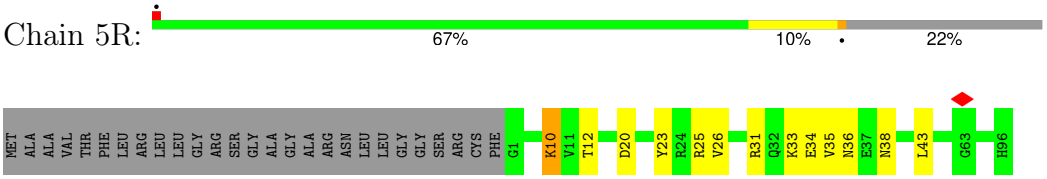
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:



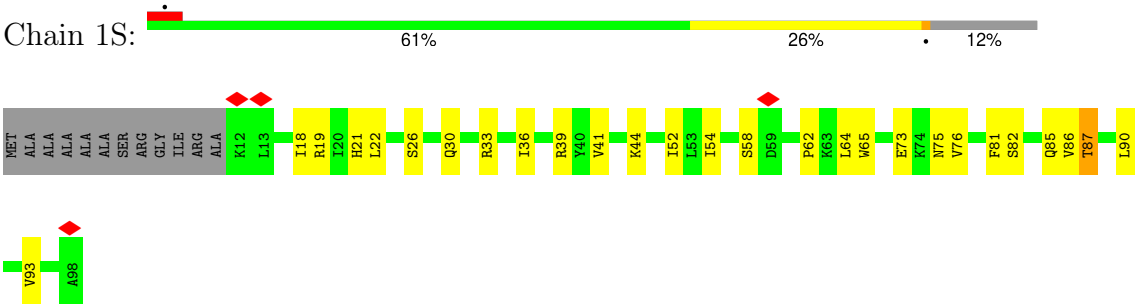
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 5R:



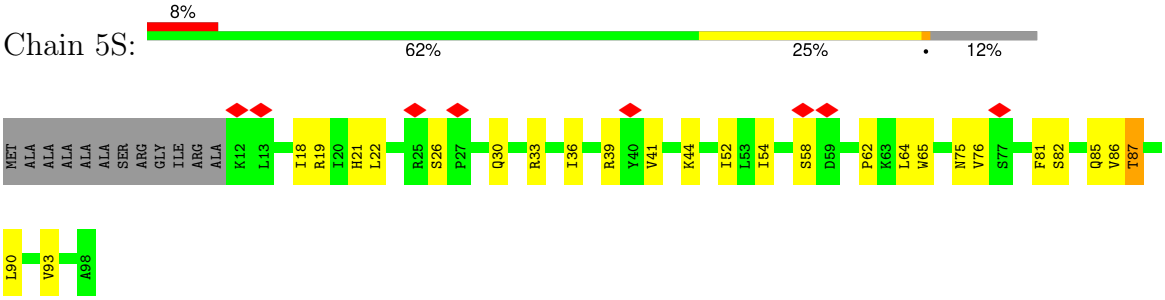
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S:



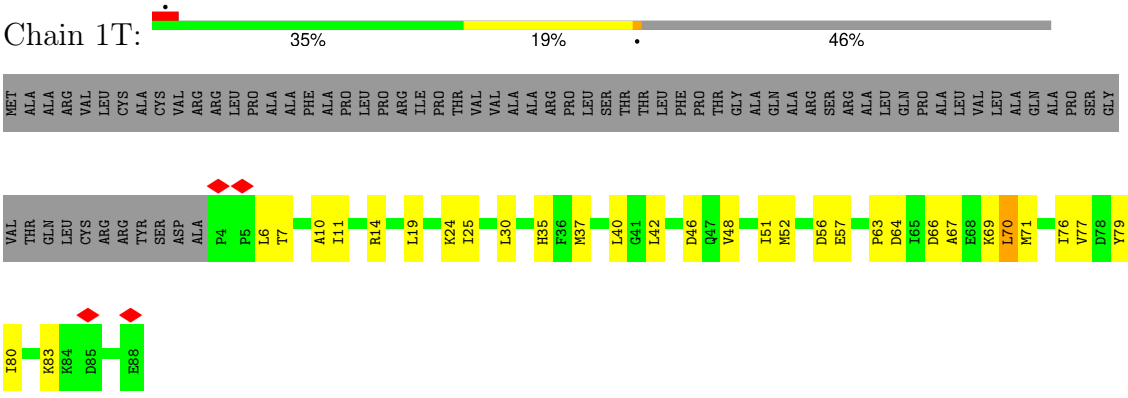
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 5S:



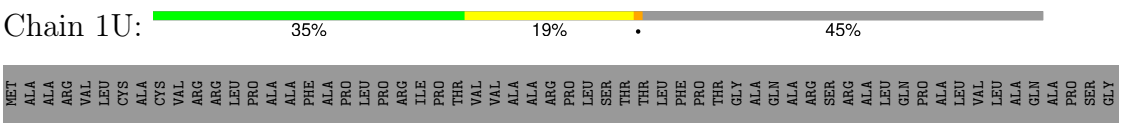
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1T:



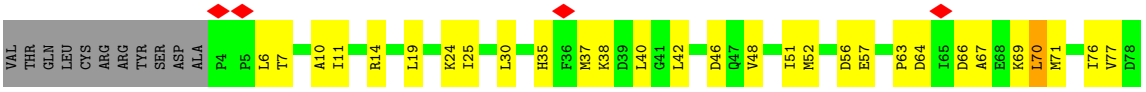
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

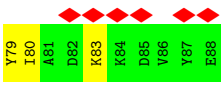
Chain 1U:



• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

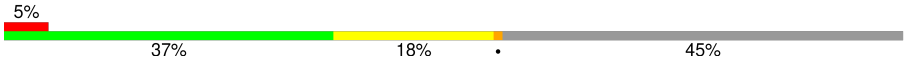
Chain 5T:

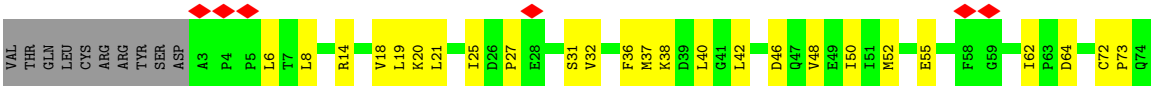


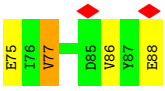


• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 5U:





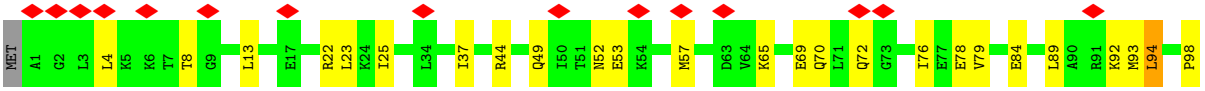


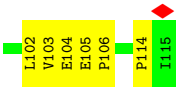
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V:

• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

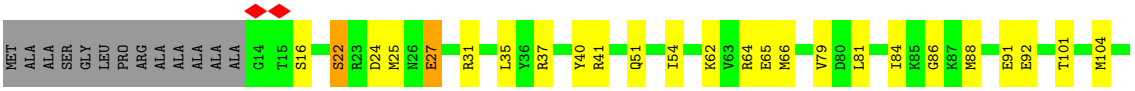
Chain 5V:





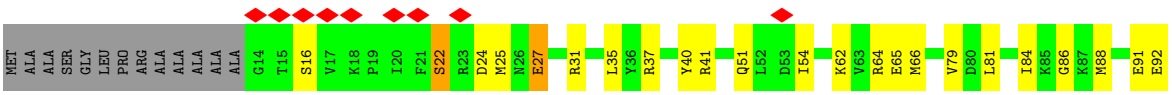
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

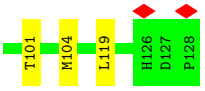
Chain 1W:



• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

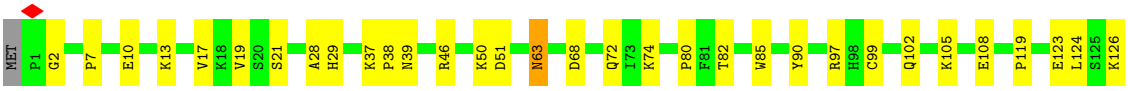
Chain 5W:





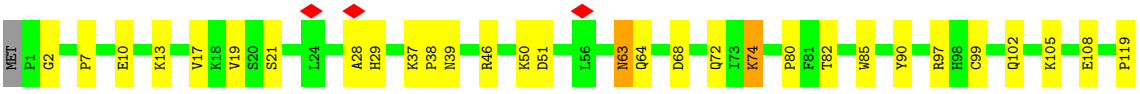
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 1X:



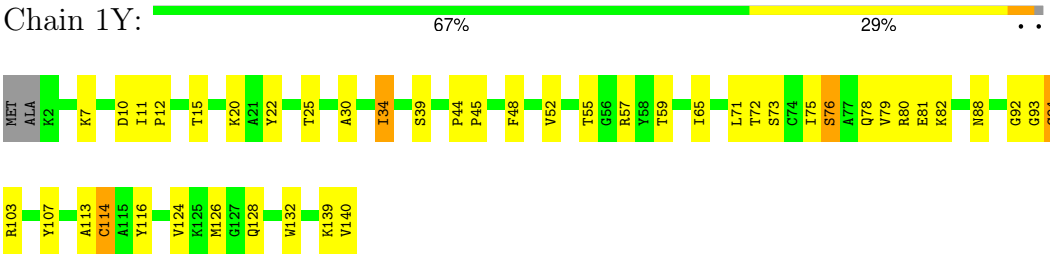
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 5X:



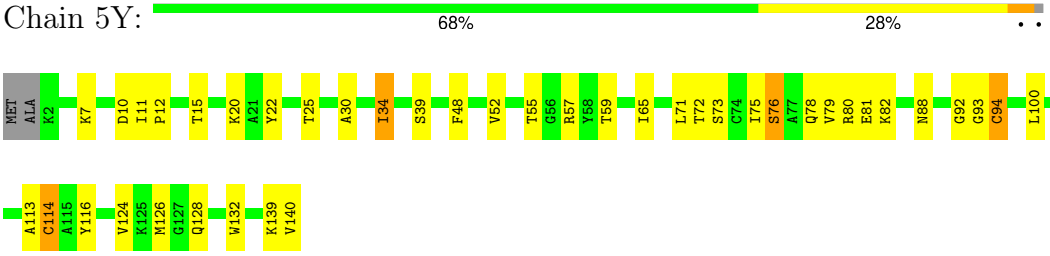
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y:



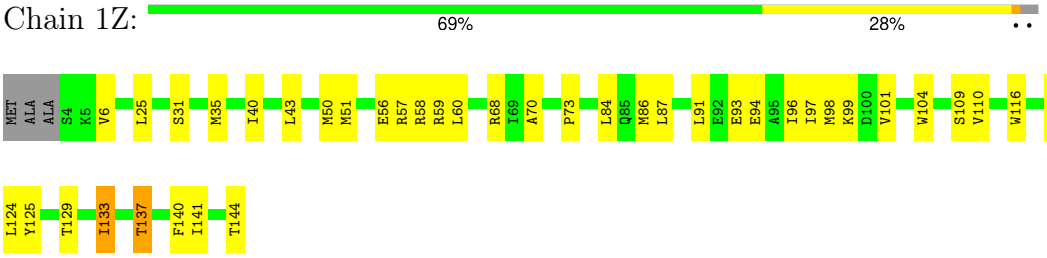
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 5Y:



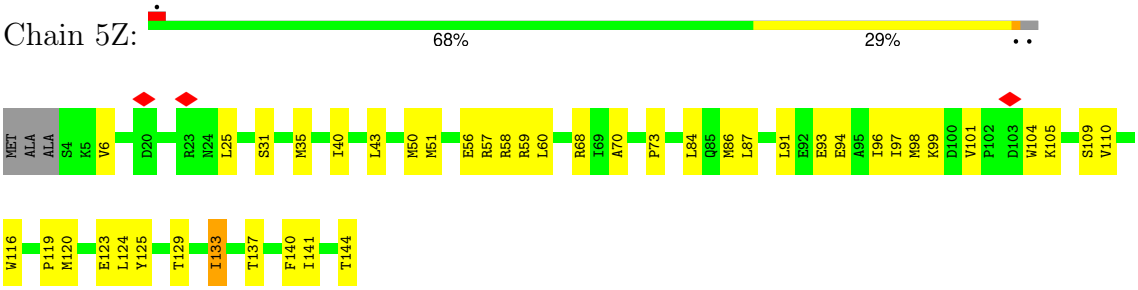
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z:



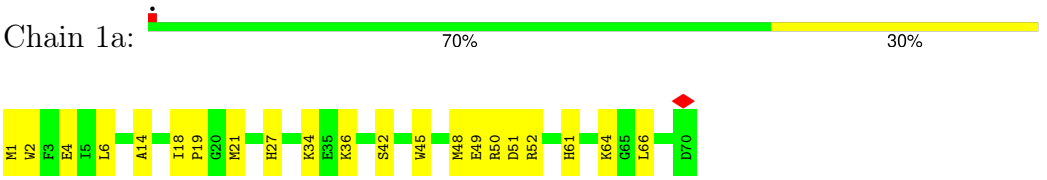
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 5Z:



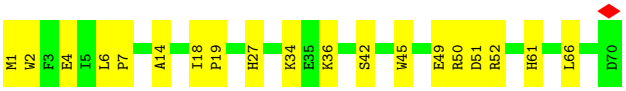
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a:



• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 5a:

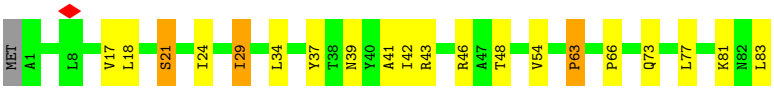


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b:

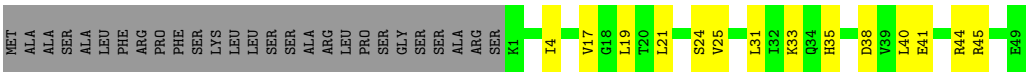
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 5b:



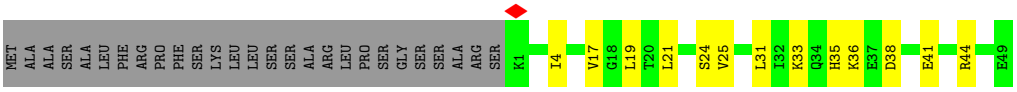
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 1c:



• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 5c:



• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

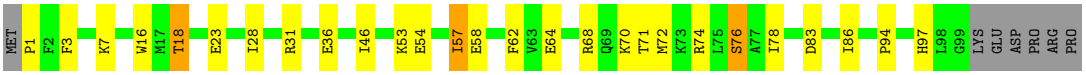
Chain 1d:

• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 5d:

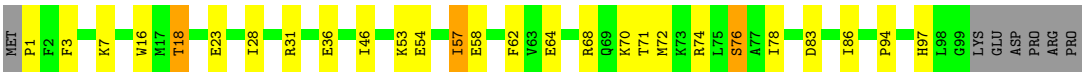
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:



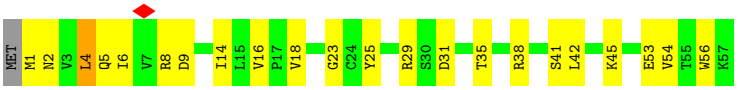
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 5e:



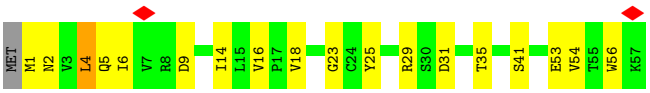
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain 1f:



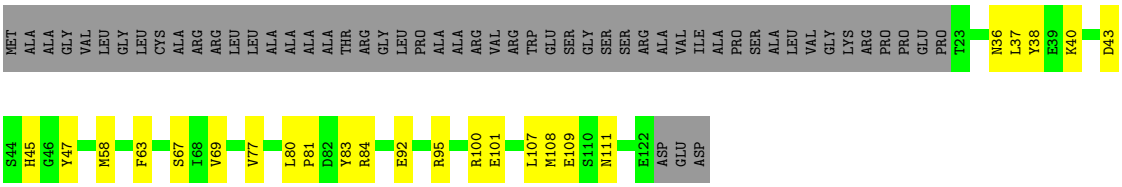
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain 5f:



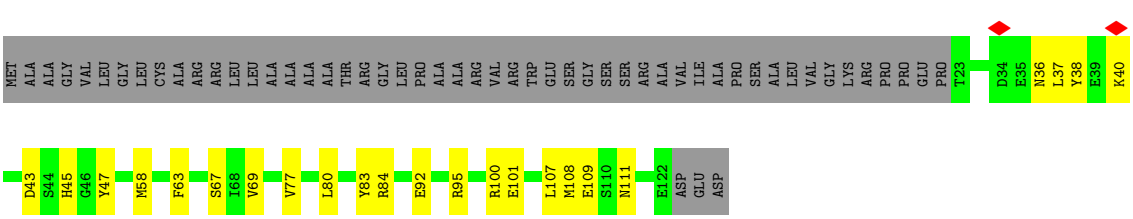
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 1g:



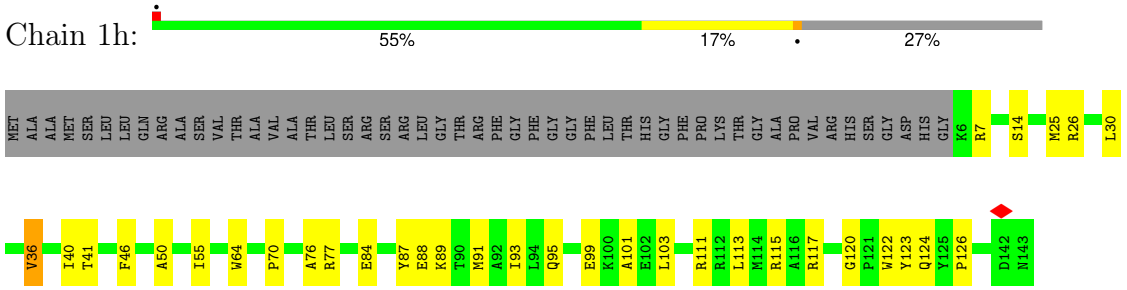
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain 5g:



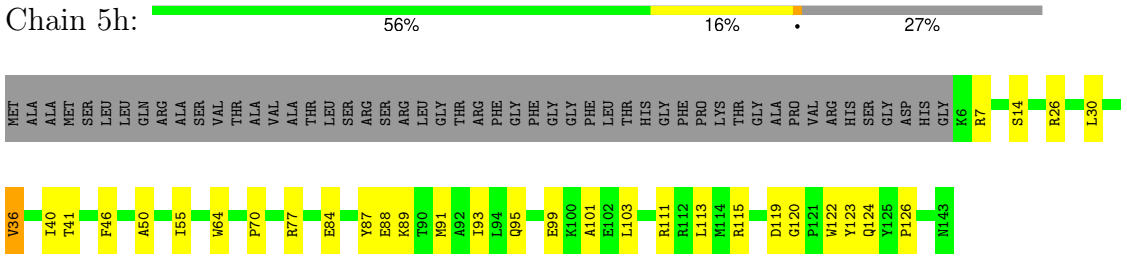
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:



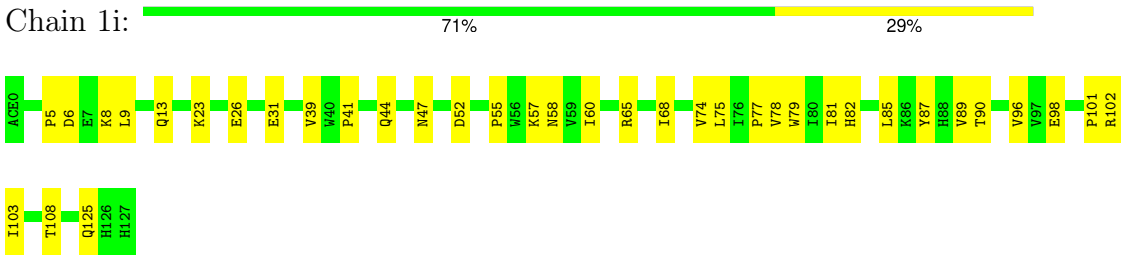
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 5h:



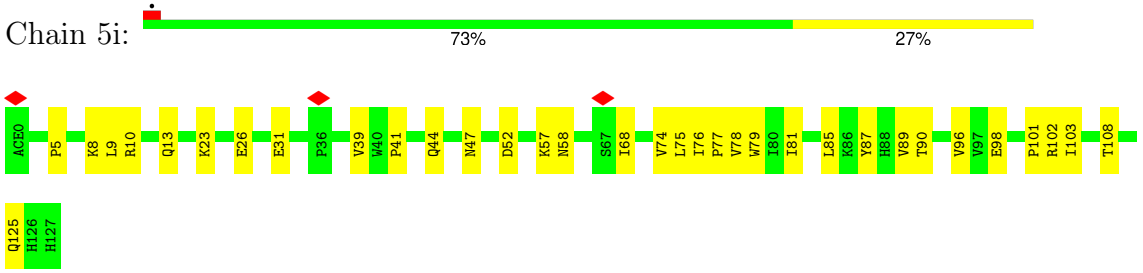
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:



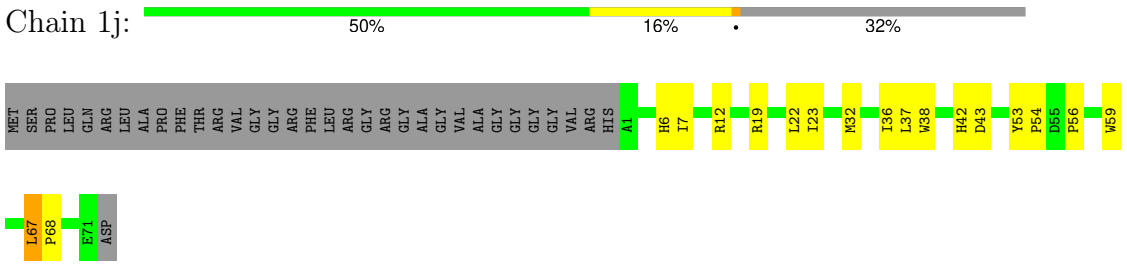
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 5i:



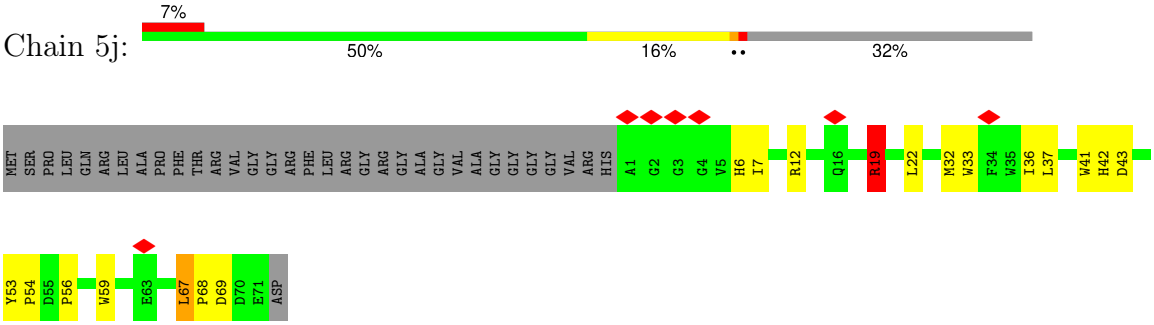
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



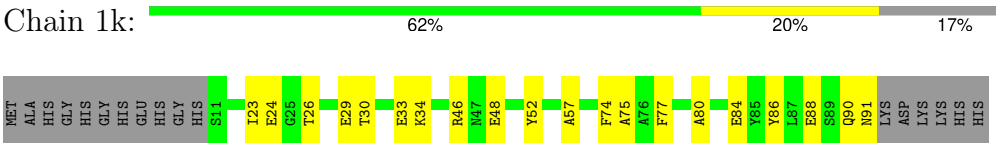
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 5j:



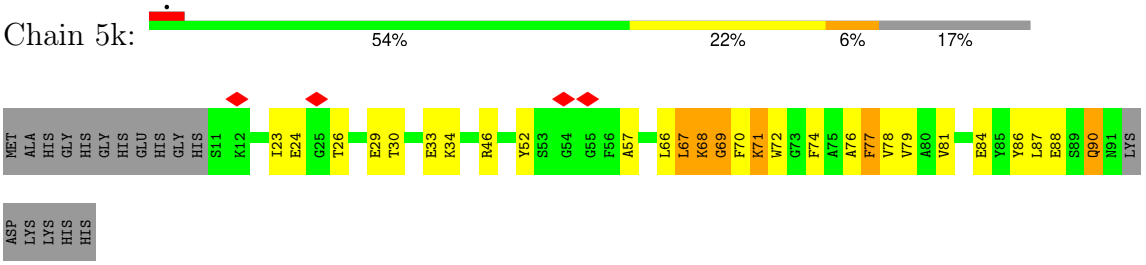
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k:



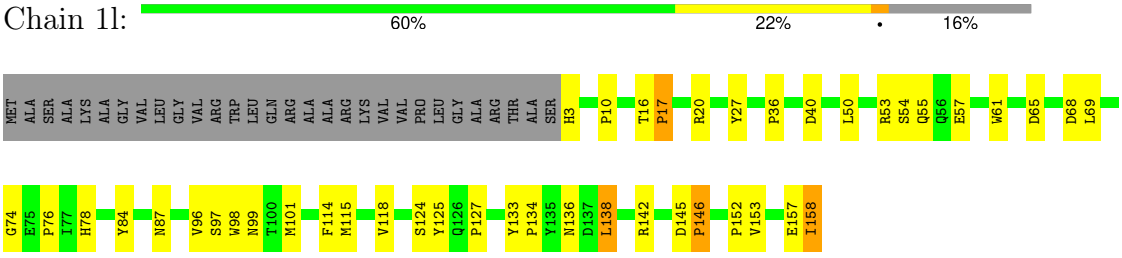
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 5k:



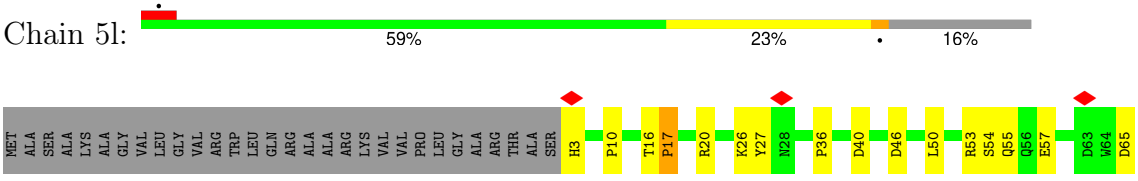
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

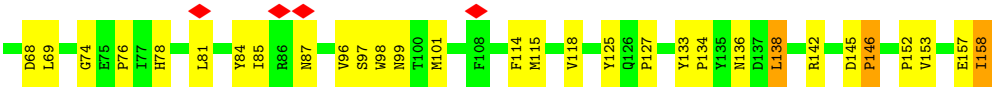
Chain 1l:



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

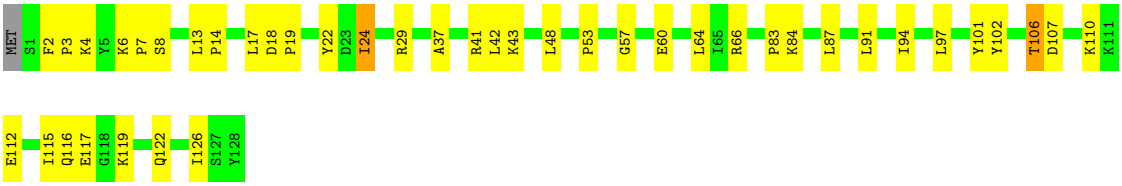
Chain 5l:





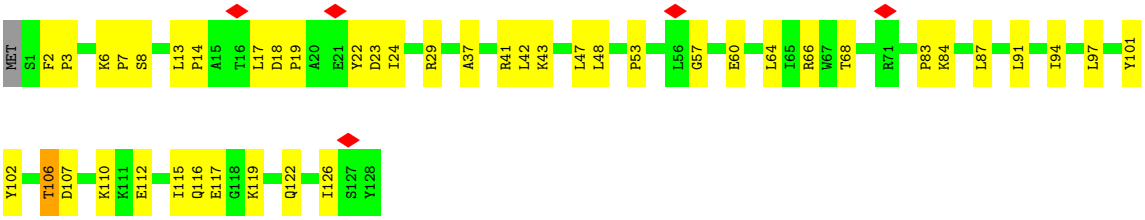
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m:



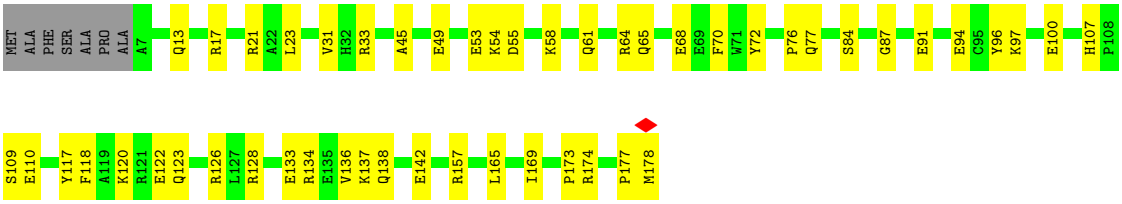
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 5m:



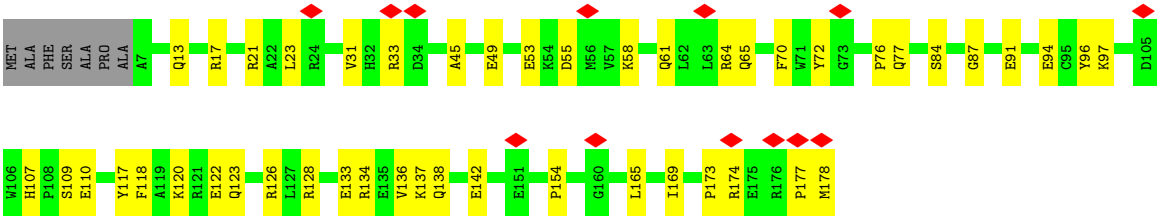
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n:



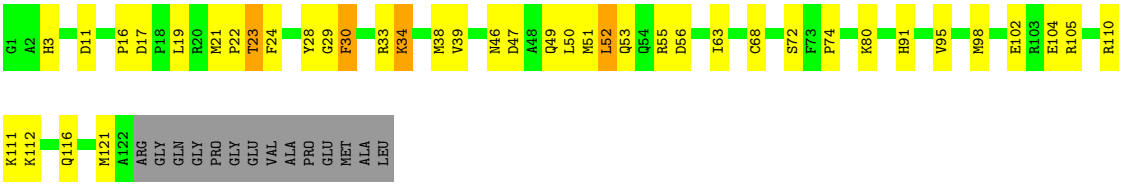
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 5n:



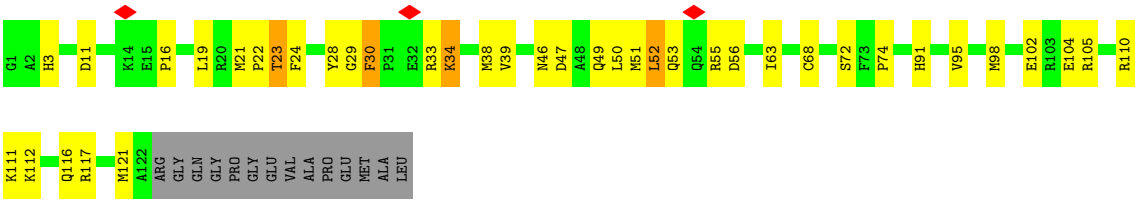
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:



• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 5o:



• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

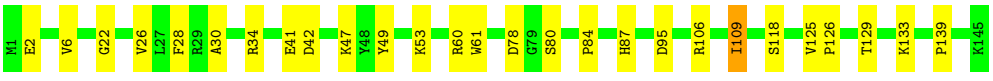
Chain 1p:

• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 5p:

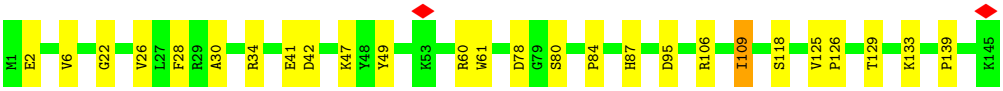
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 1q:



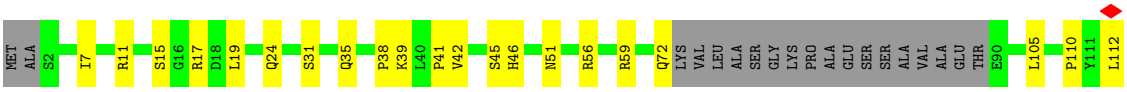
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain 5q:



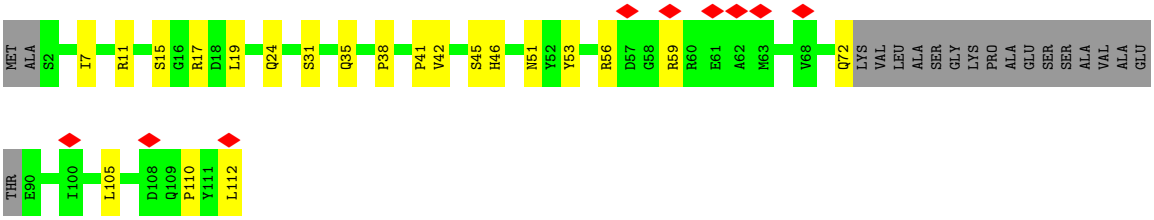
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain 1r:



• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain 5r:

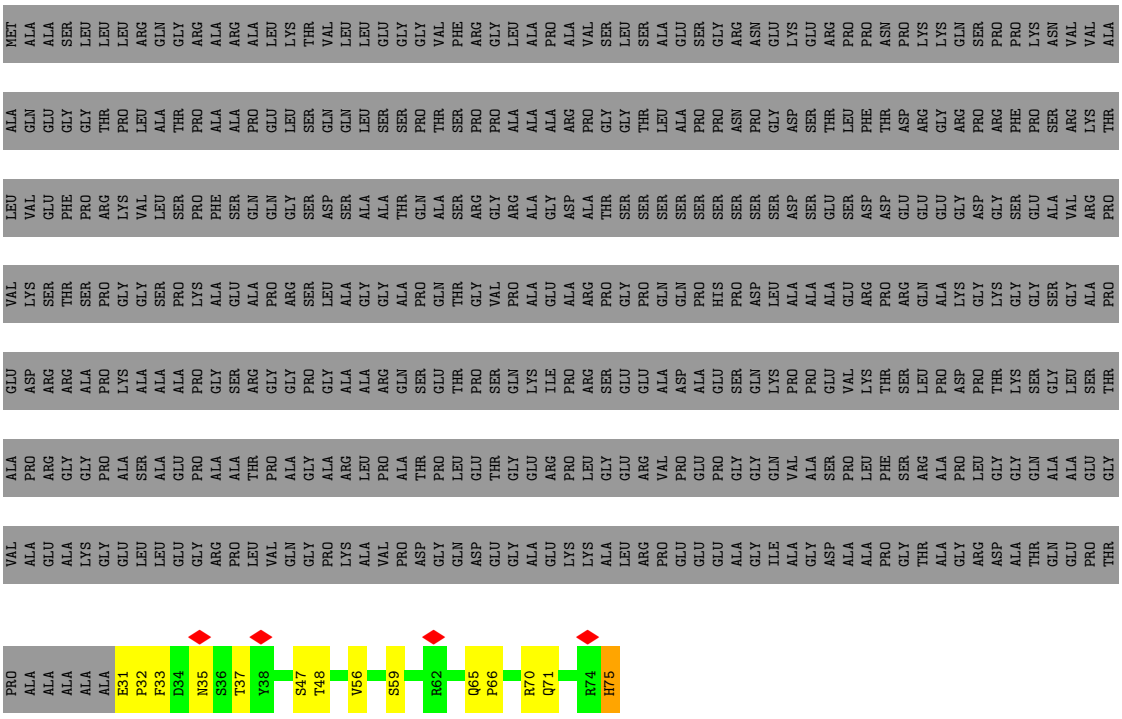


• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain 1s:

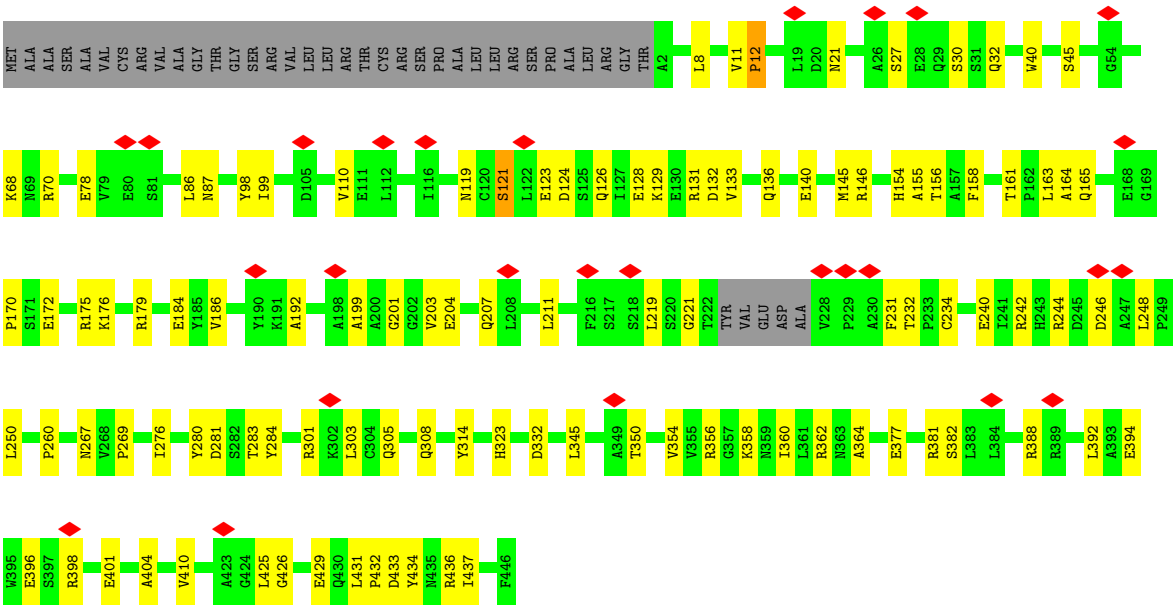
• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain 5s:



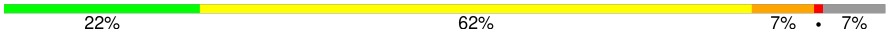
• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

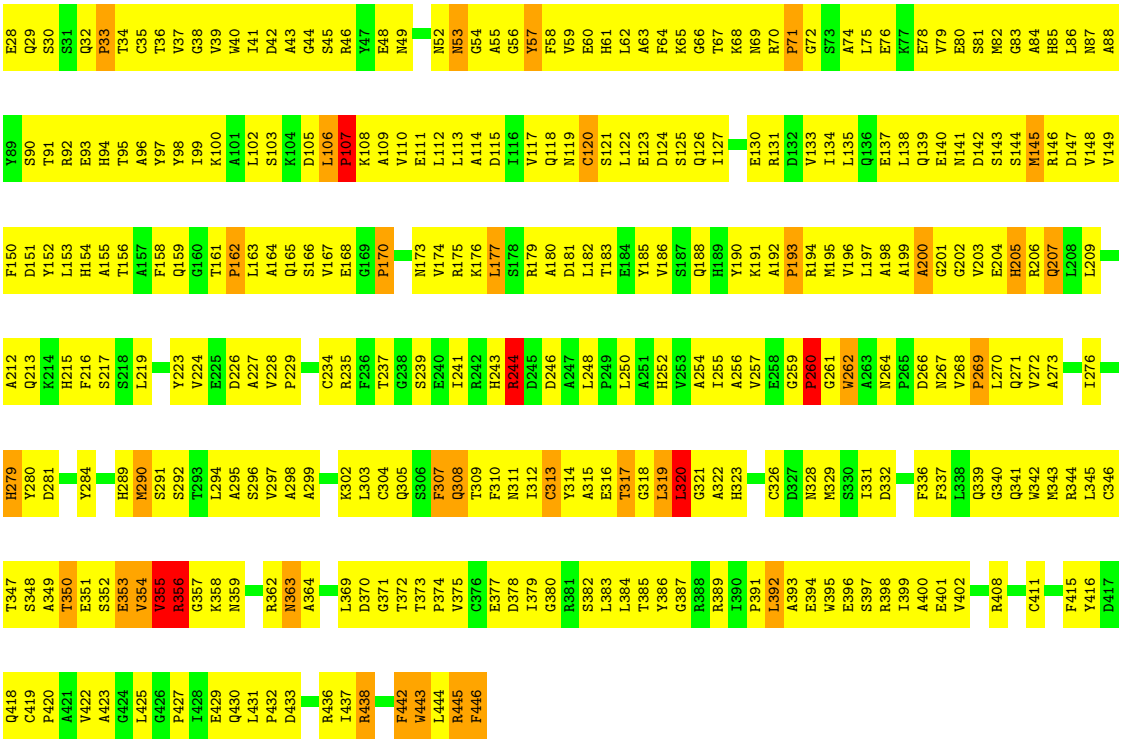
Chain 3A:



• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

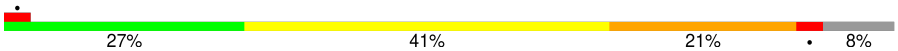
Chain 3N:

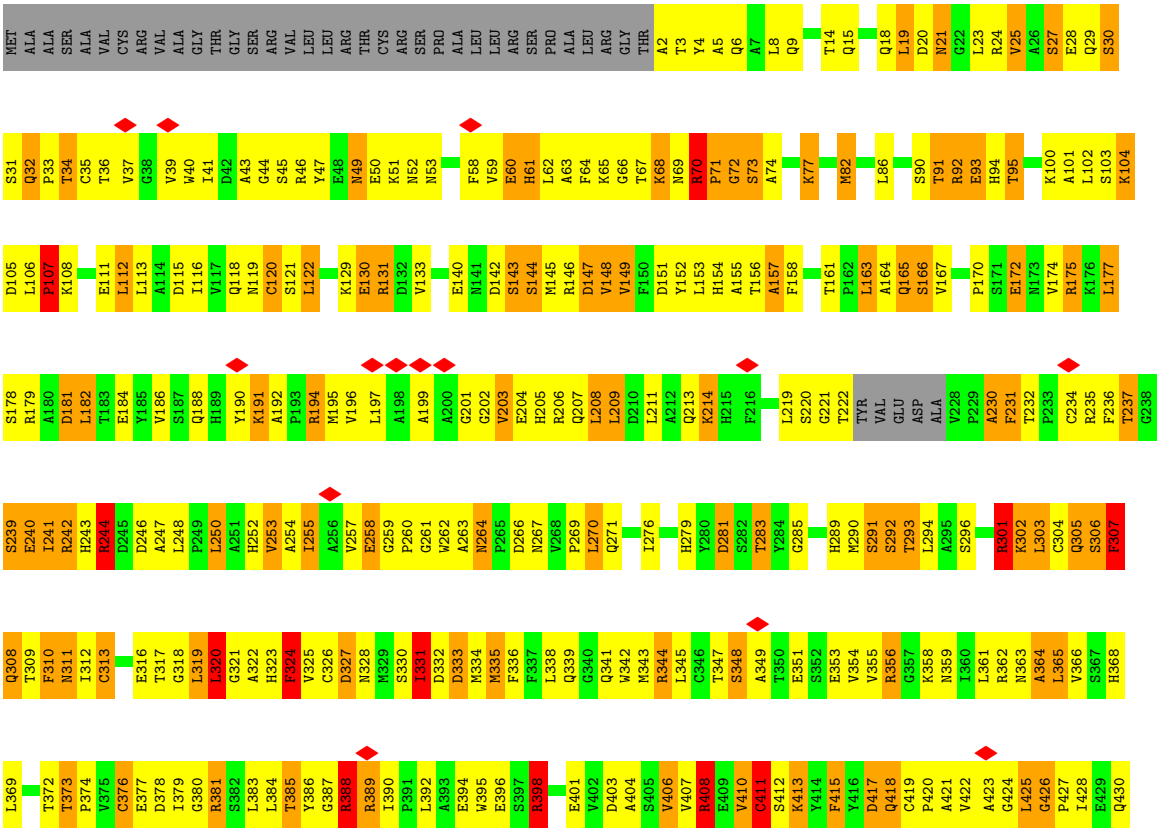


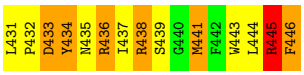


• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 6A:

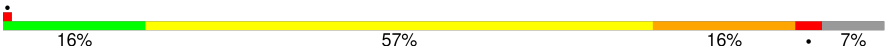


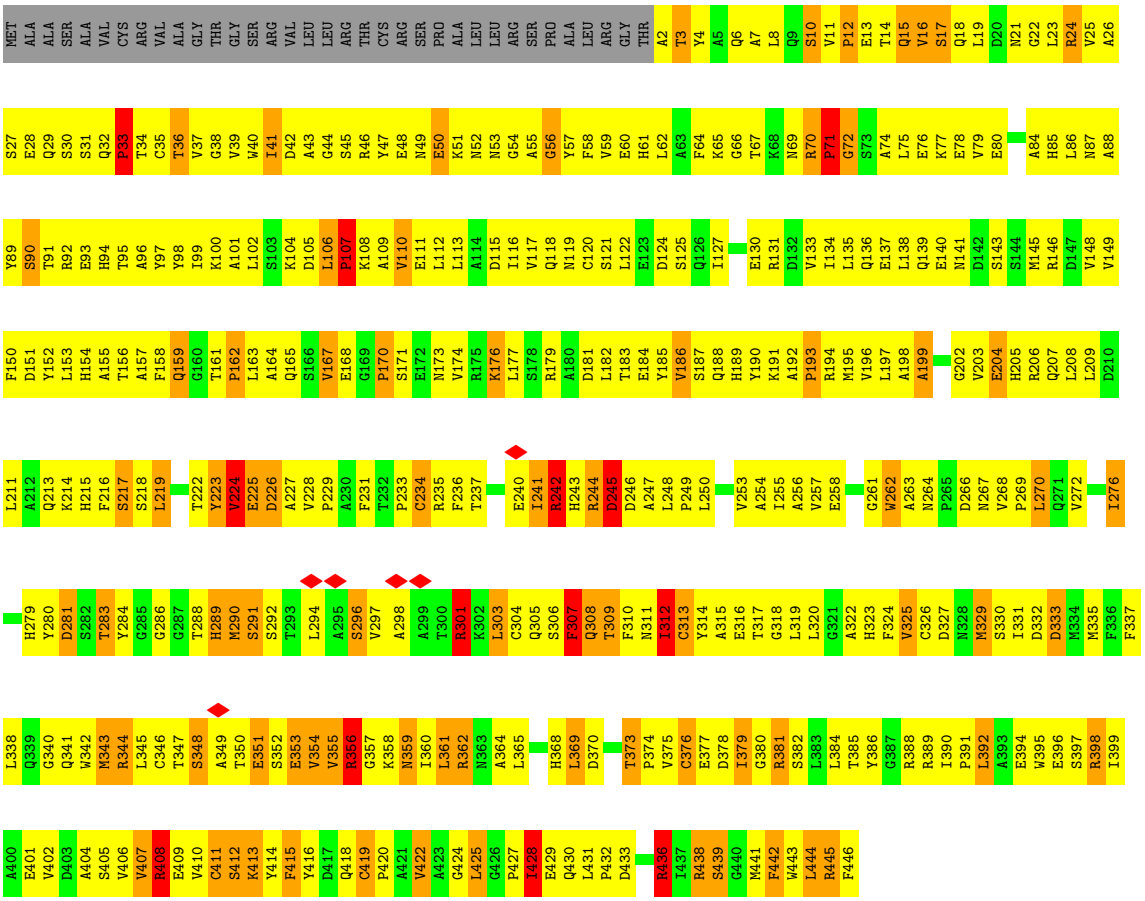




• Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

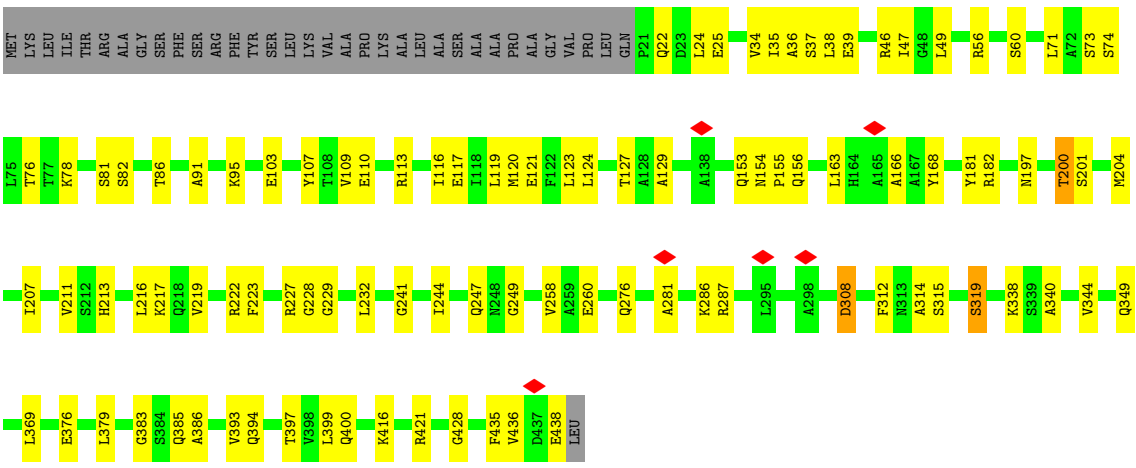
Chain 6N:





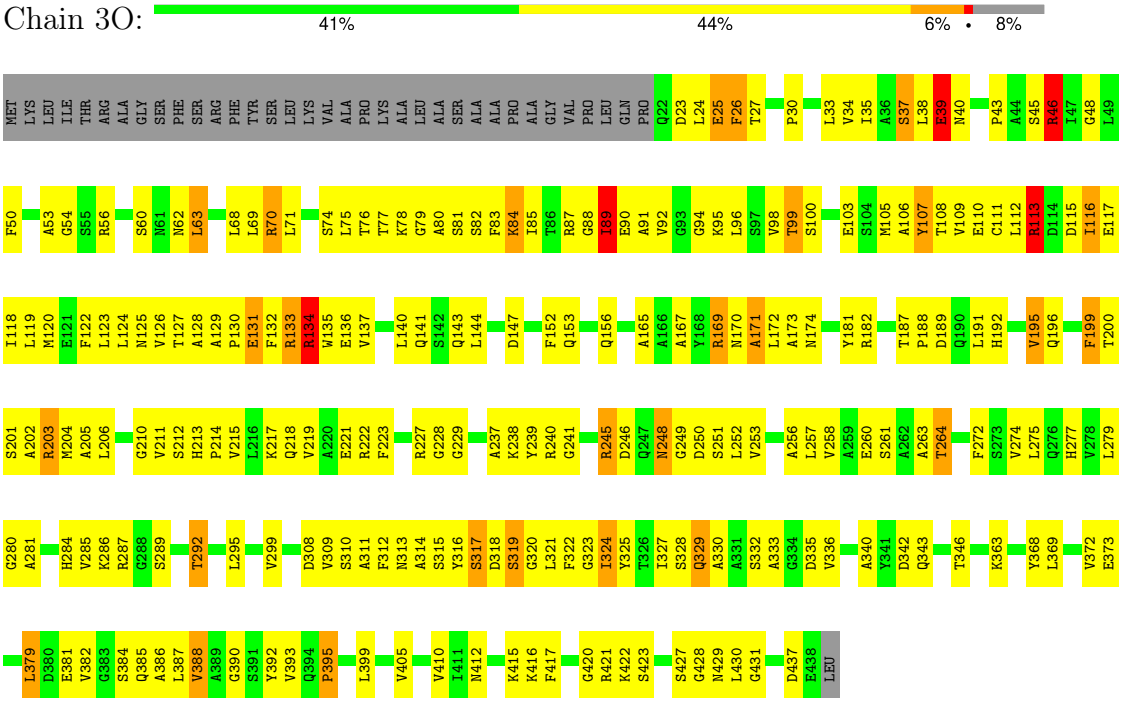
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B:



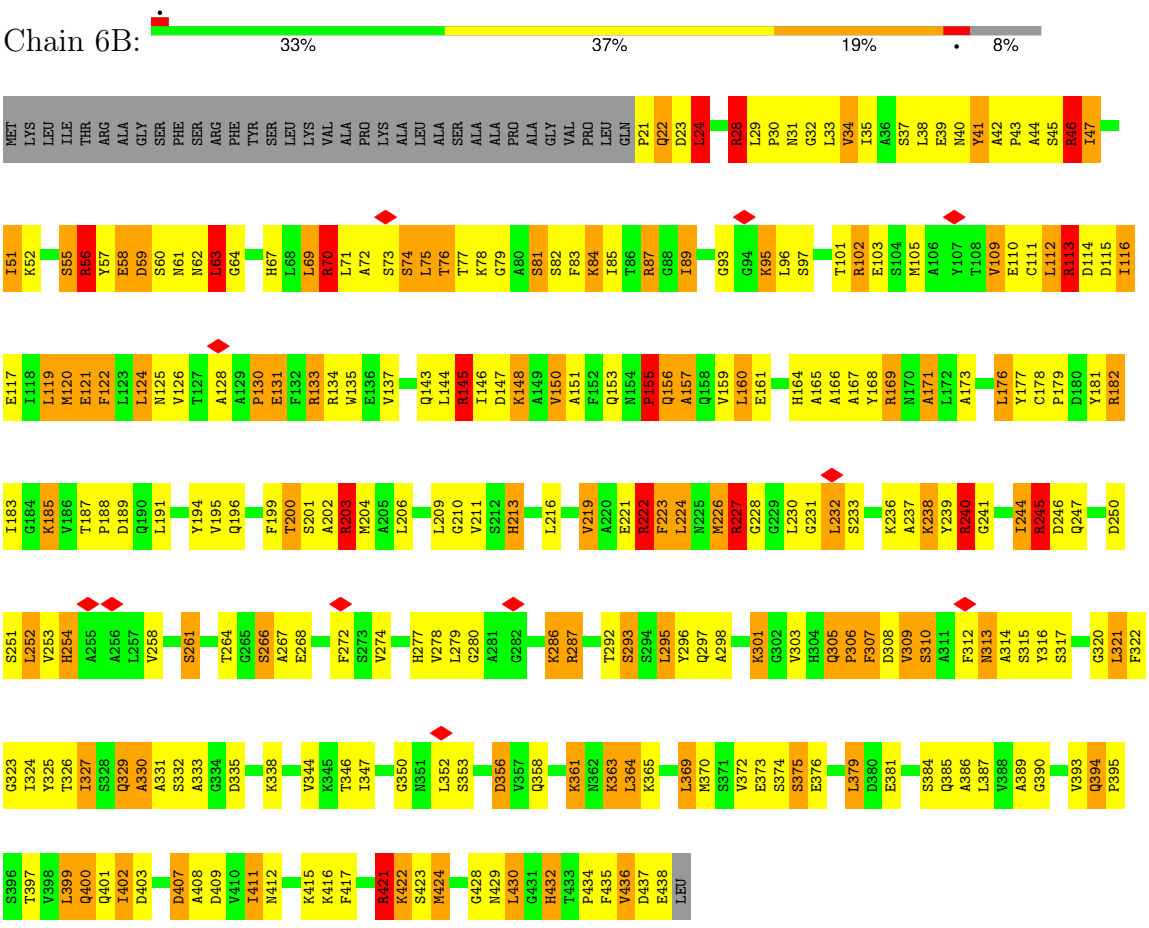
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O:



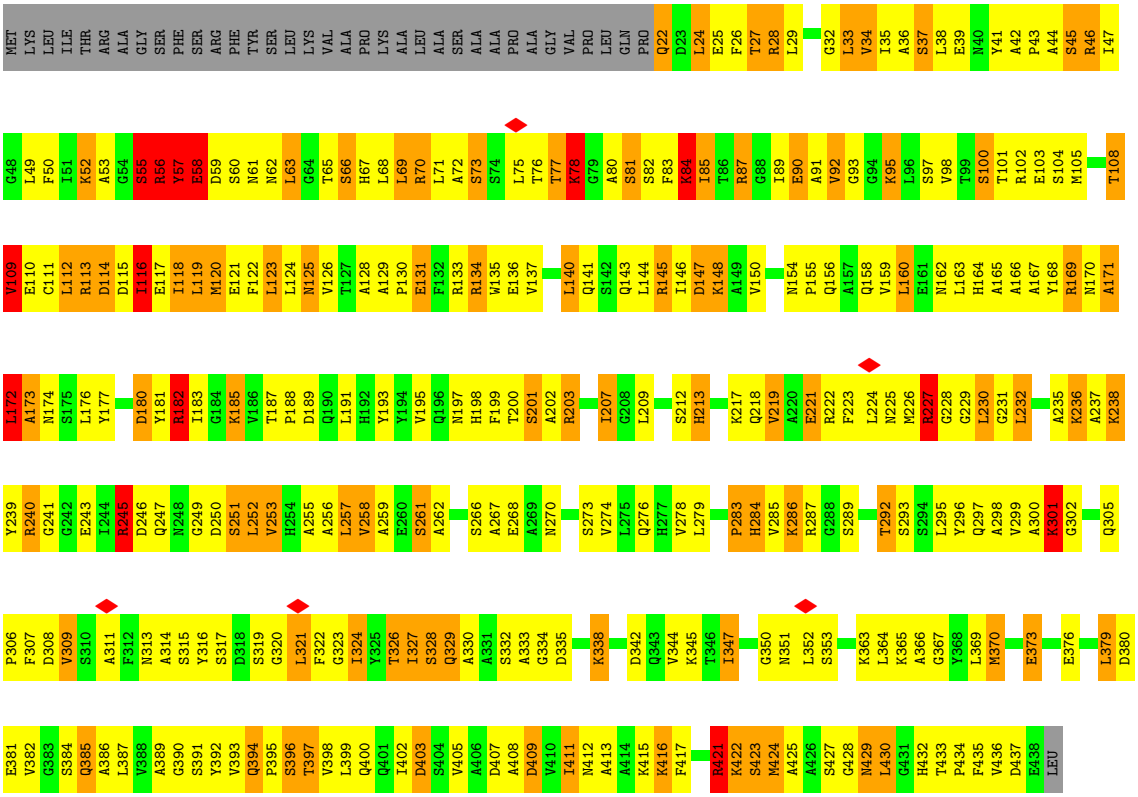
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 6B:



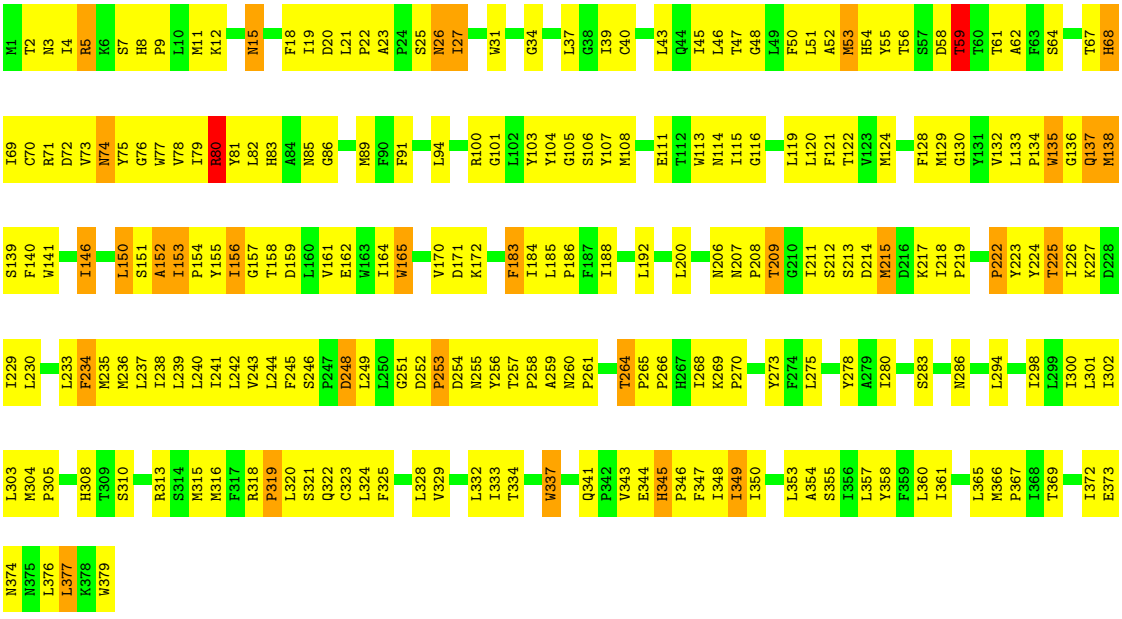
• Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 6O:



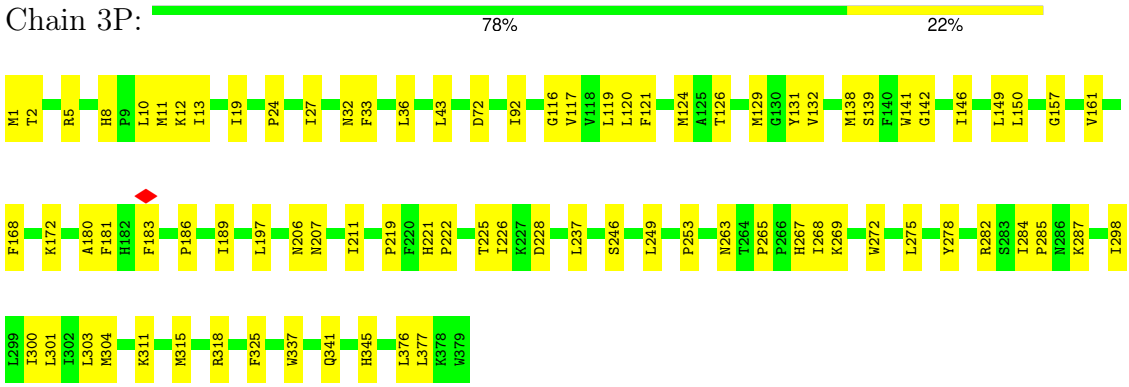
• Molecule 47: Cytochrome b

Chain 3C:



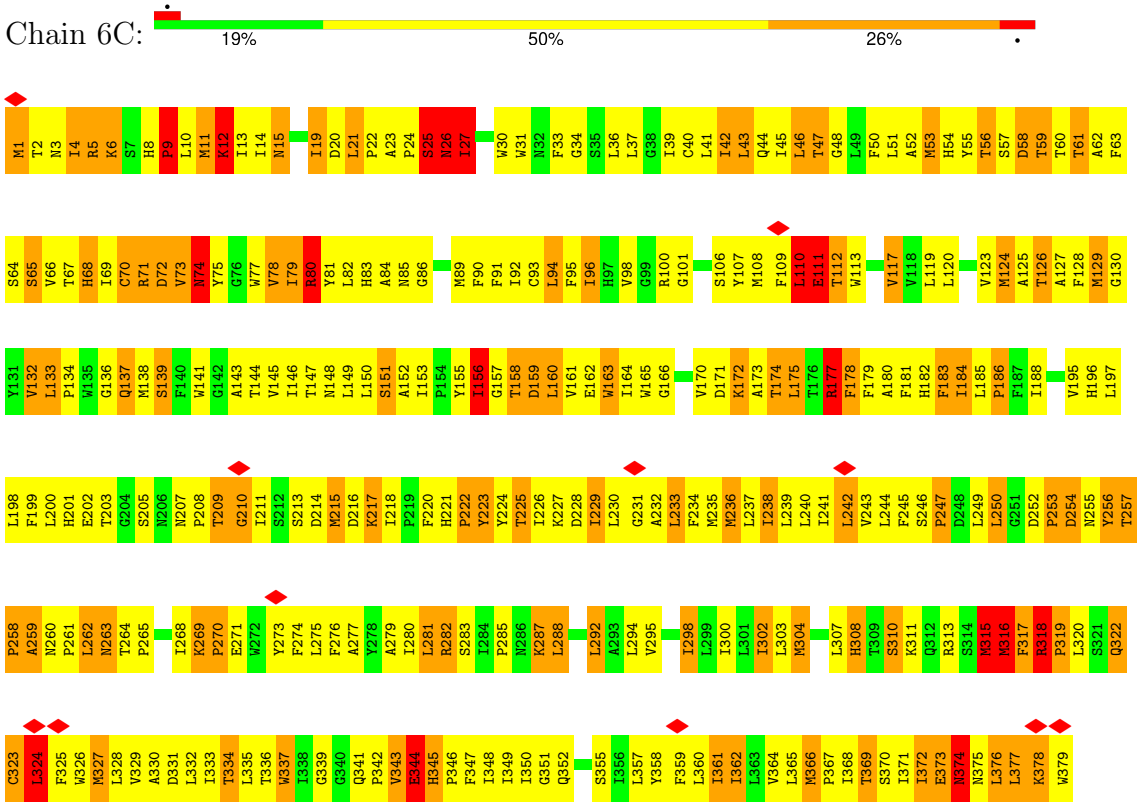
• Molecule 47: Cytochrome b

Chain 3P:



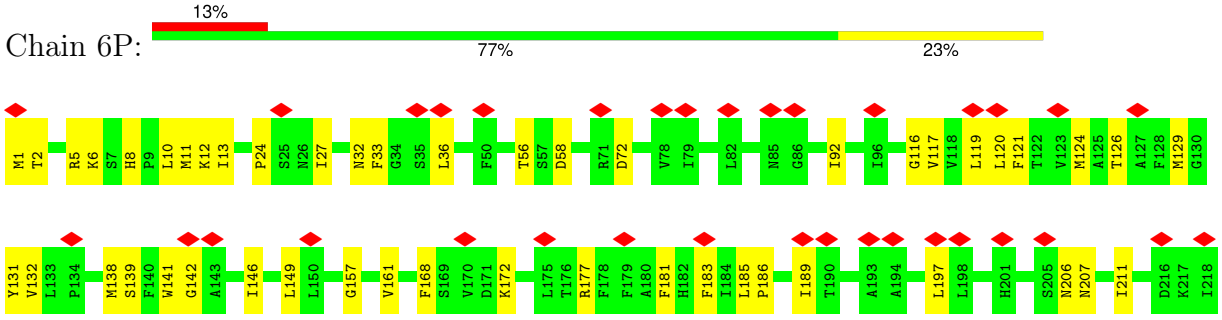
• Molecule 47: Cytochrome b

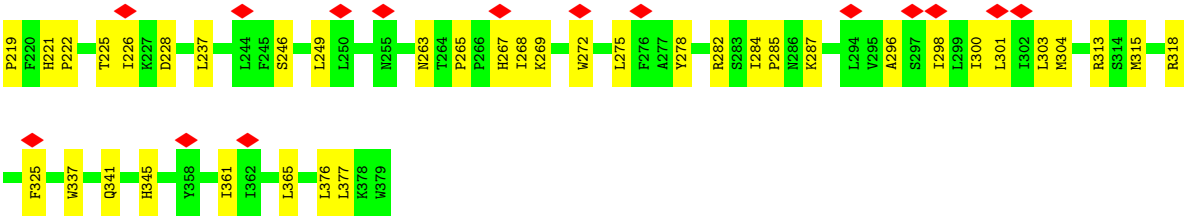
Chain 6C:



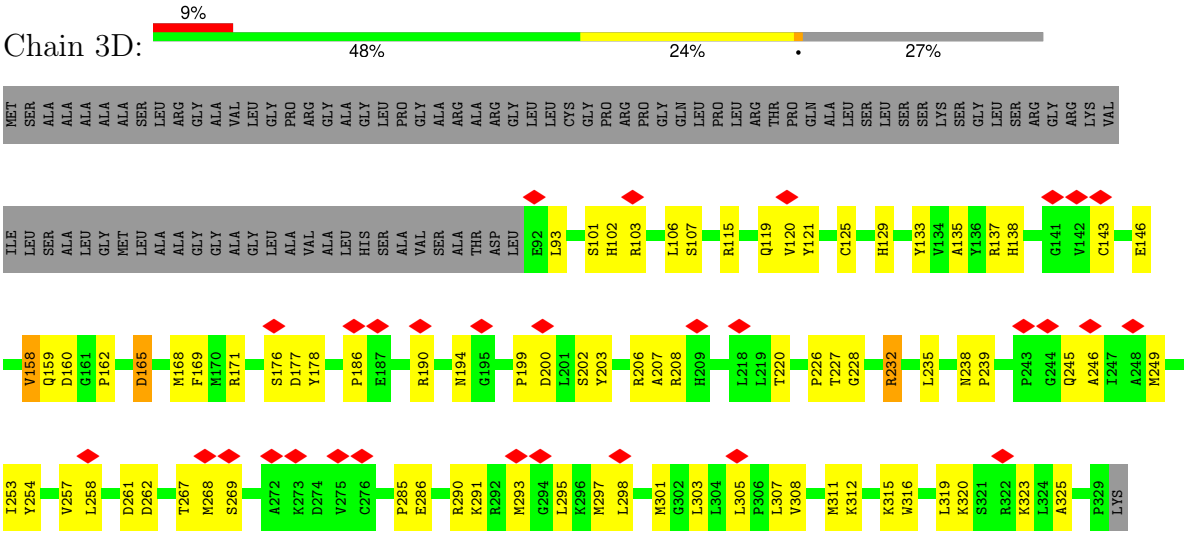
• Molecule 47: Cytochrome b

Chain 6P:

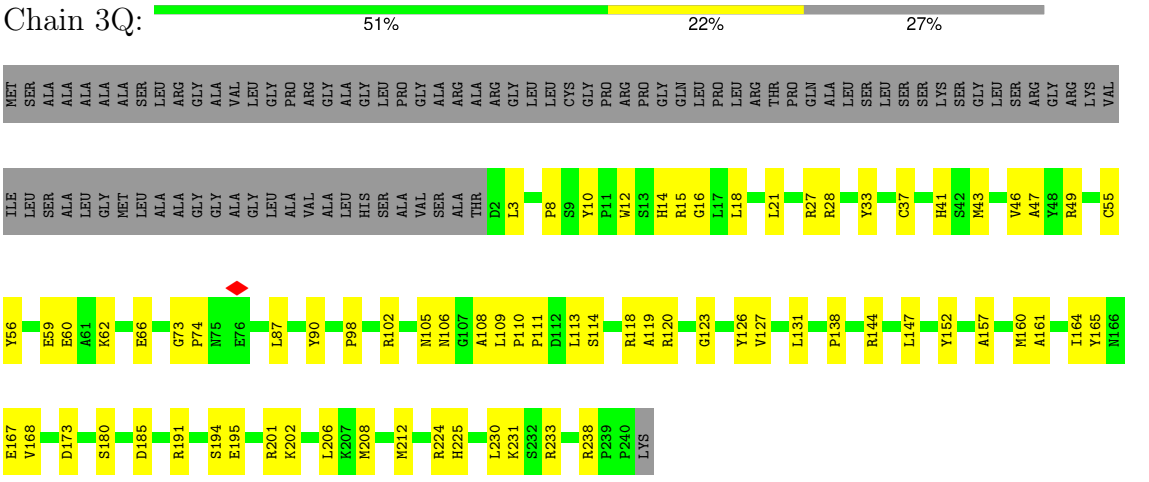




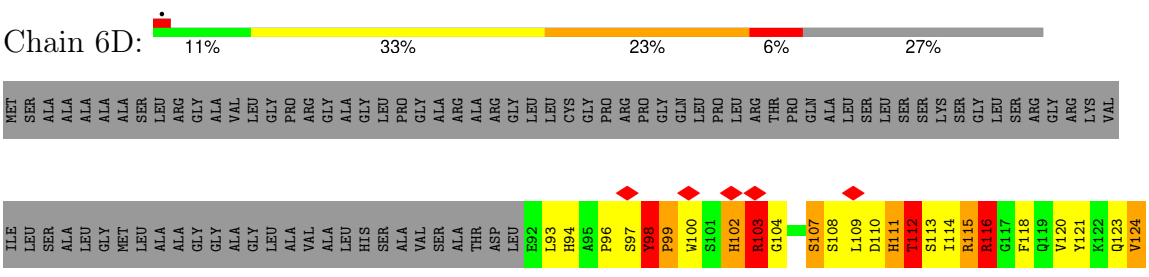
• Molecule 48: Cytochrome c1

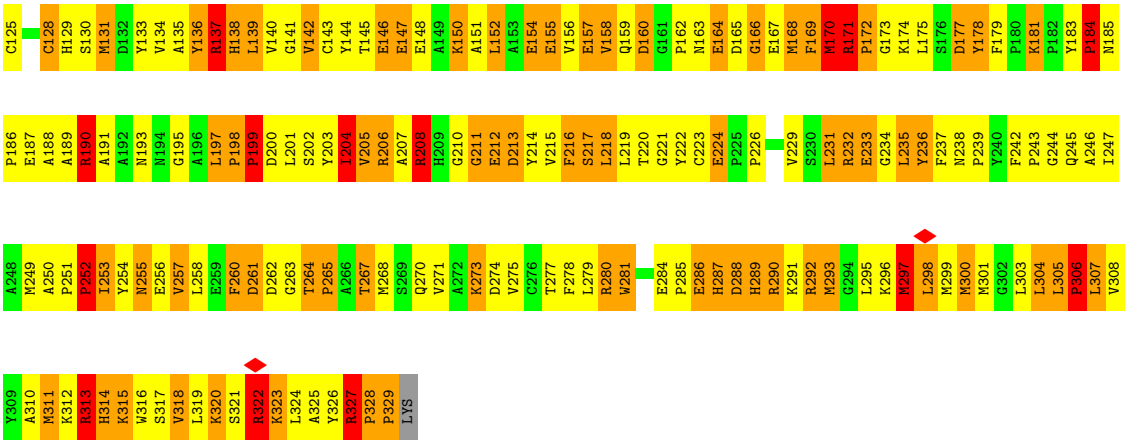


• Molecule 48: Cytochrome c1



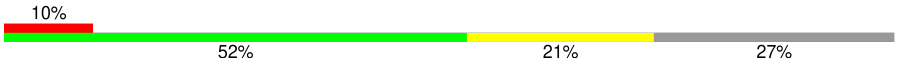
• Molecule 48: Cytochrome c1

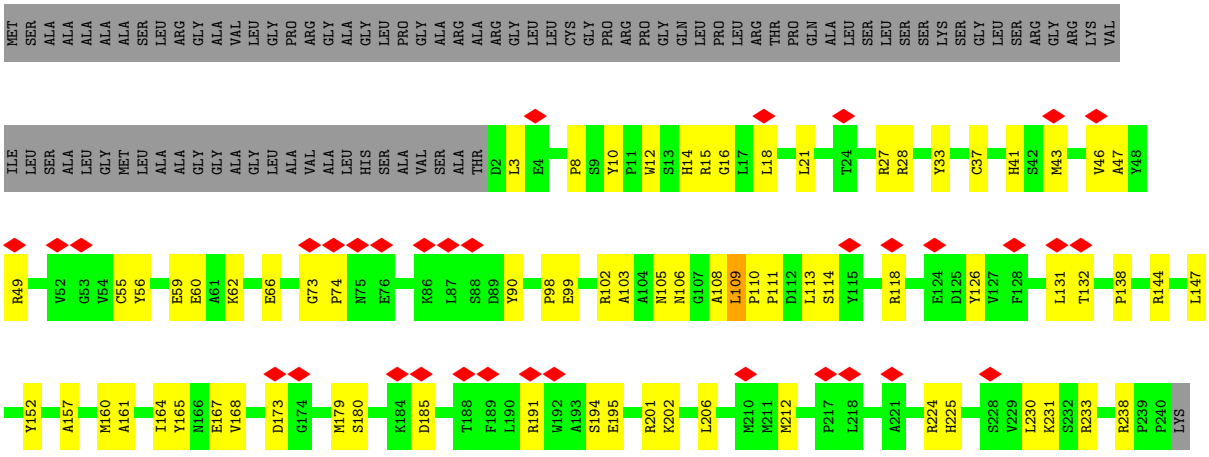




• Molecule 48: Cytochrome c1

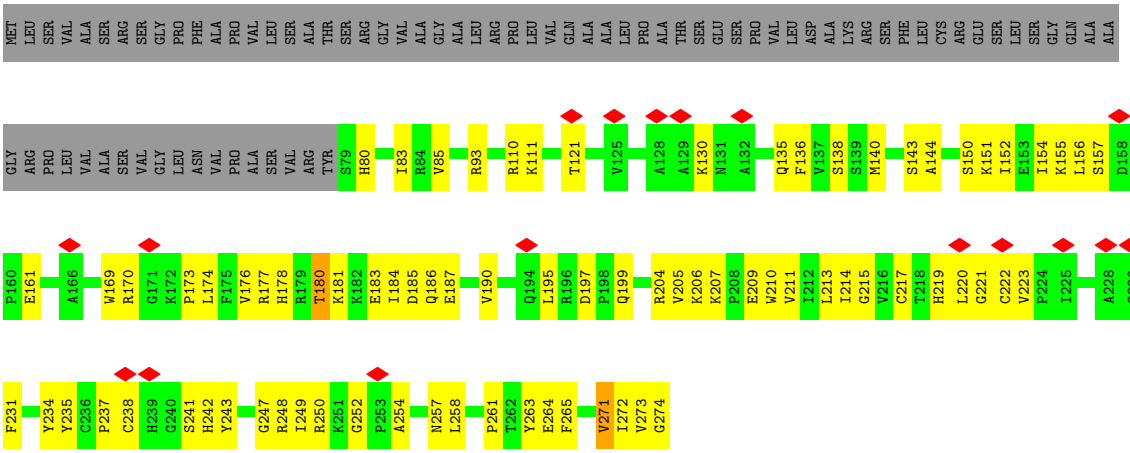
Chain 6Q:





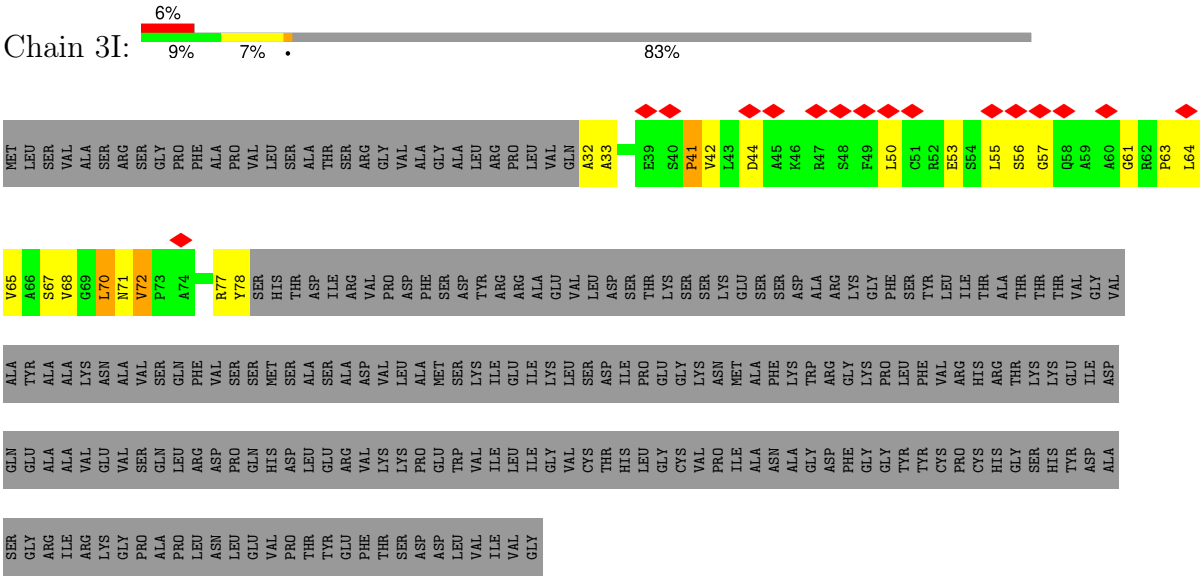
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3E:



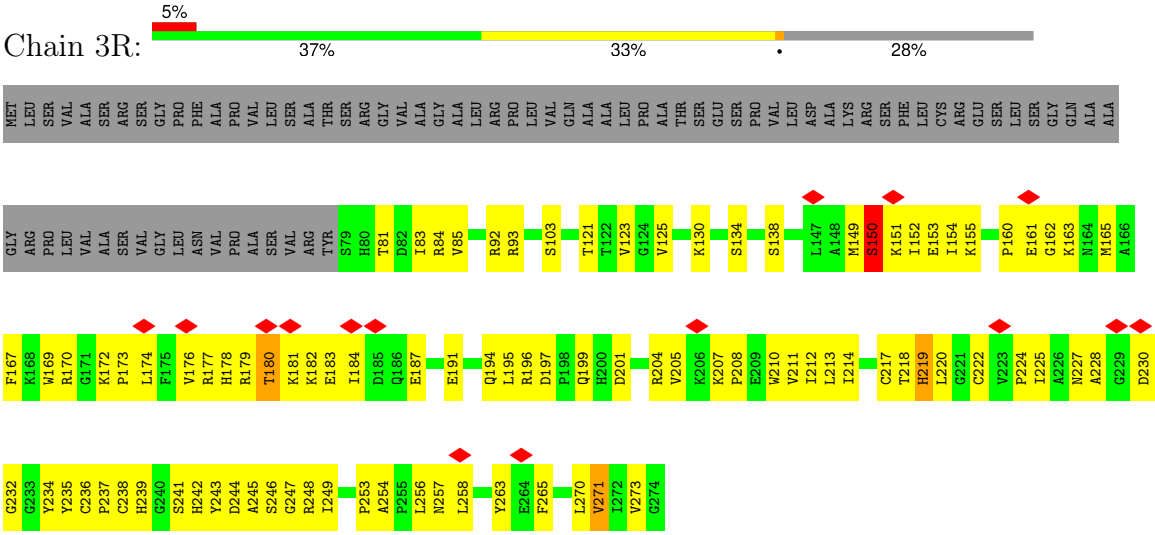
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3I:



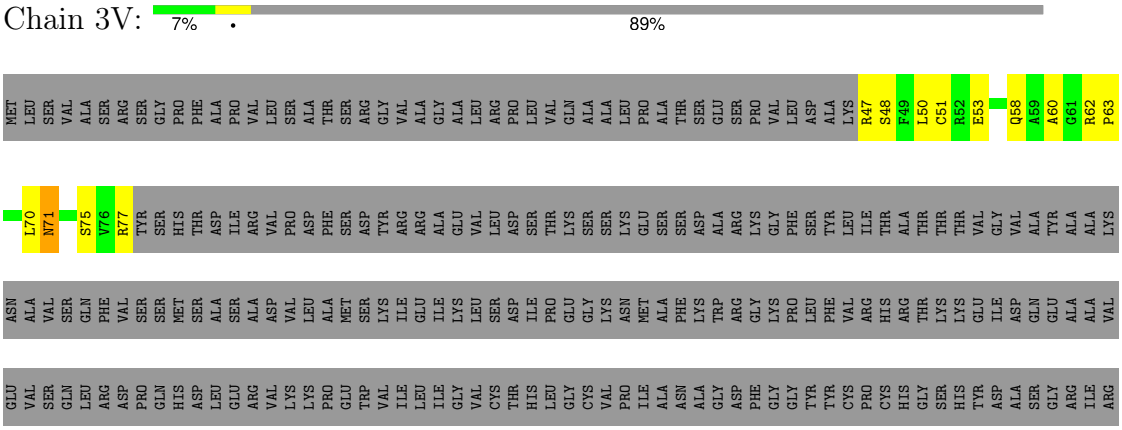
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3R:



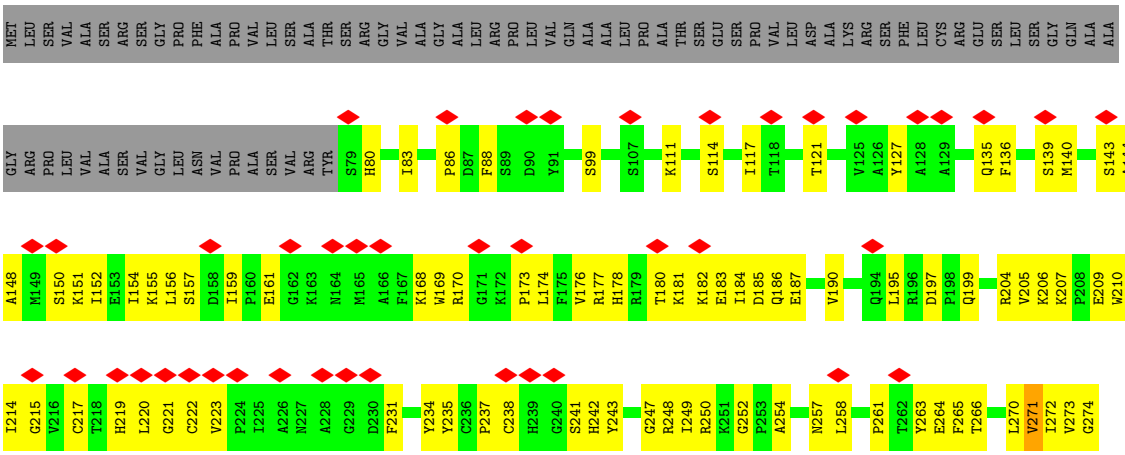
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3V:



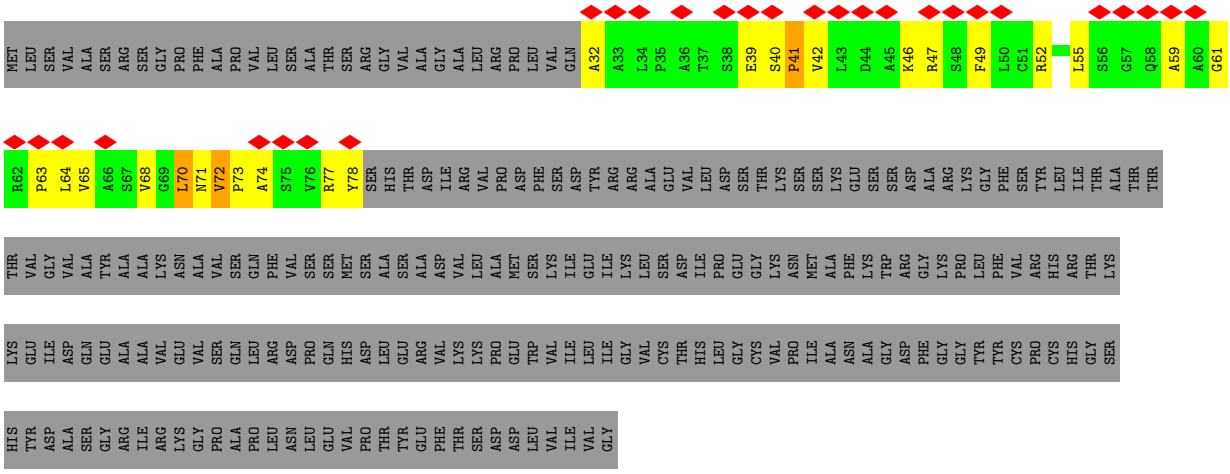
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 6E:



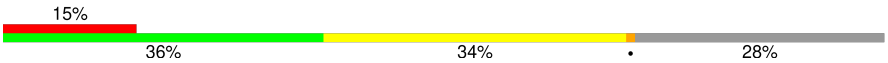
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

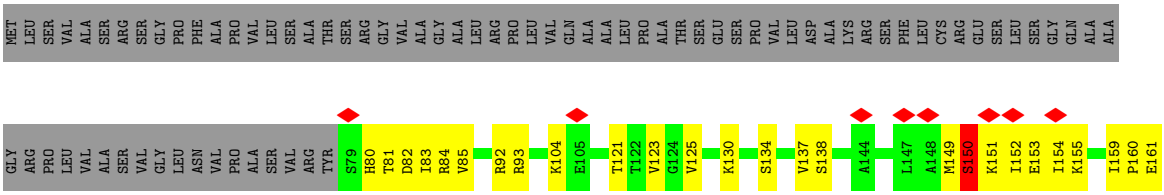
Chain 6I:

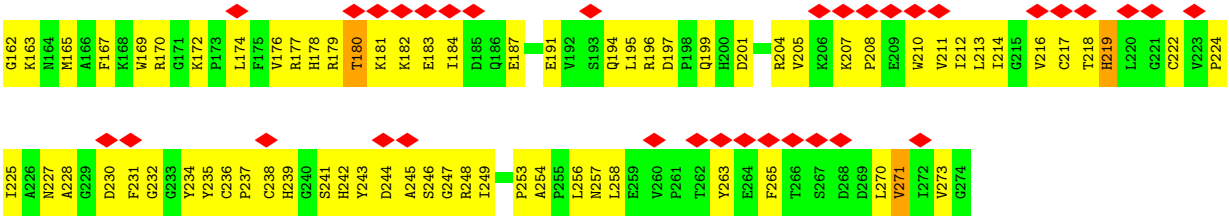


• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 6R:

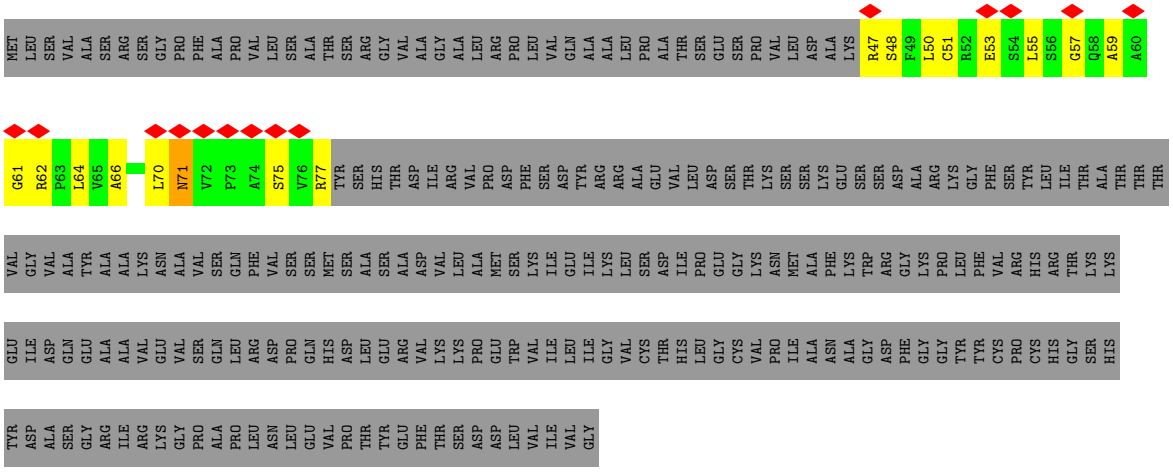






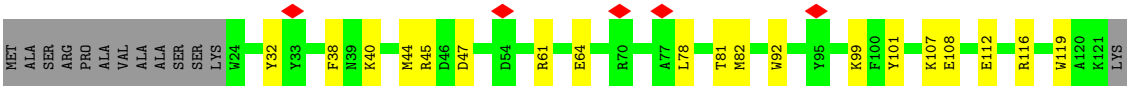
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 6V:



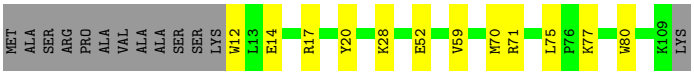
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3F:



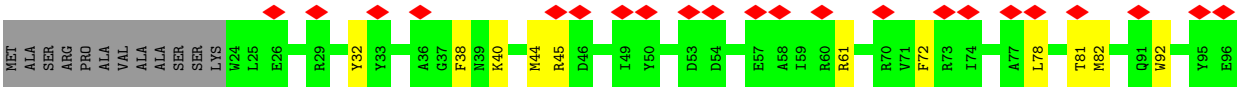
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3S:



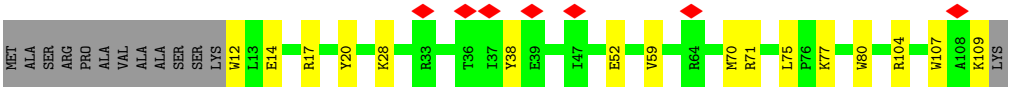
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 6F:



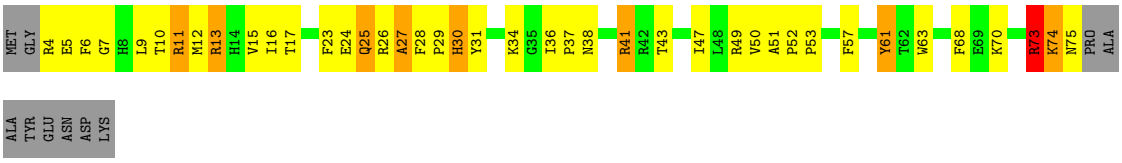
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 6S:



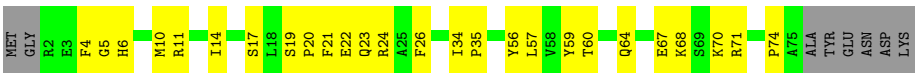
• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3G:



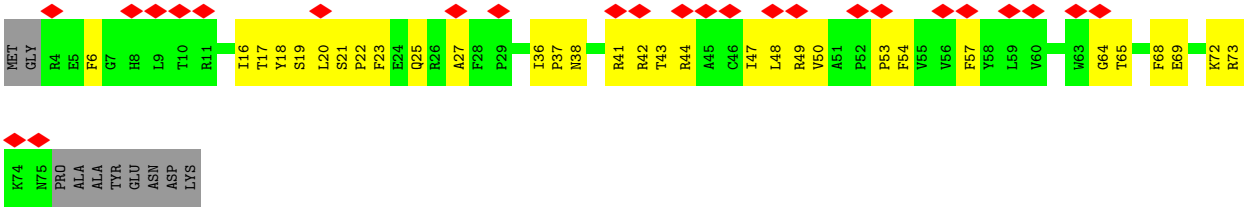
• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3T:



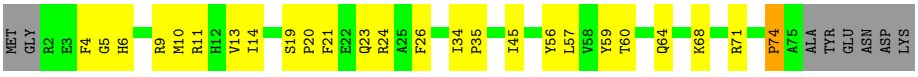
• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 6G:



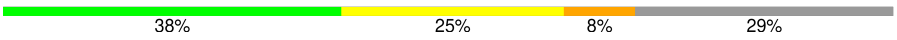
• Molecule 51: Cytochrome b-c1 complex subunit 8

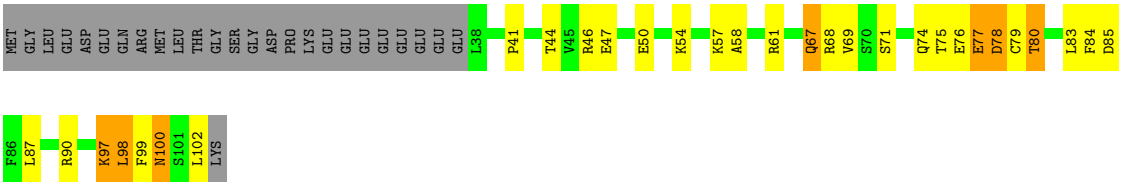
Chain 6T:



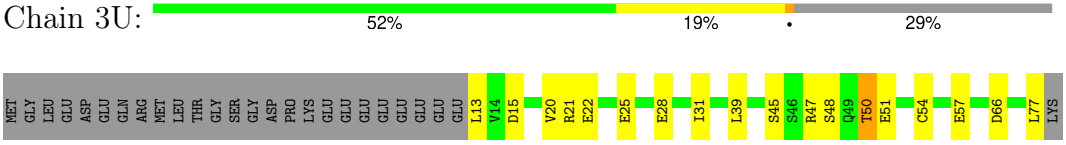
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H:

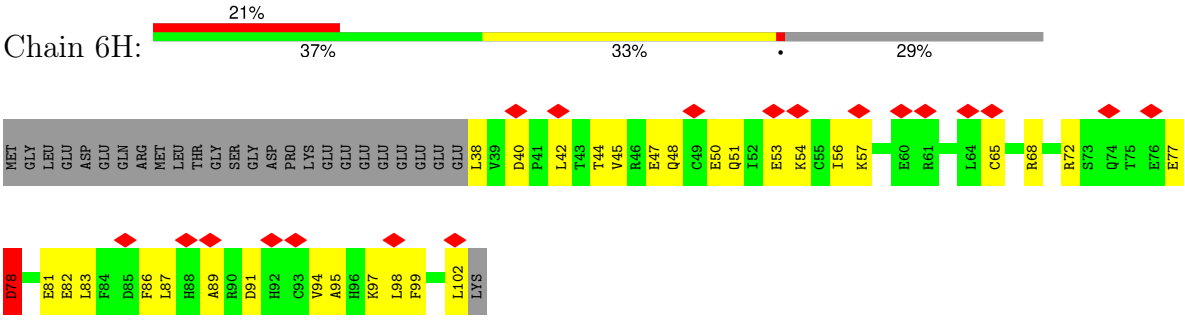




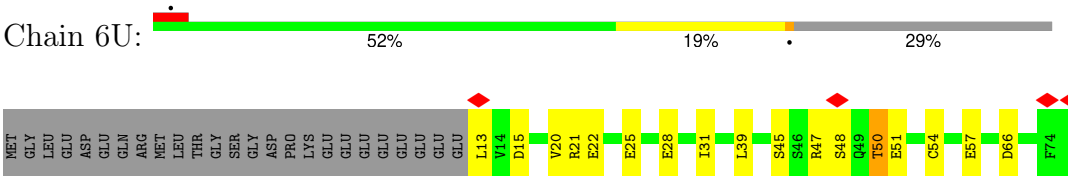
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



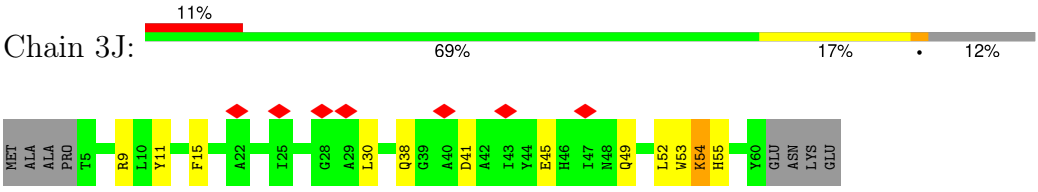
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



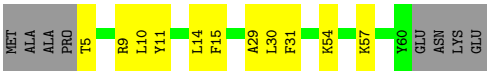
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial



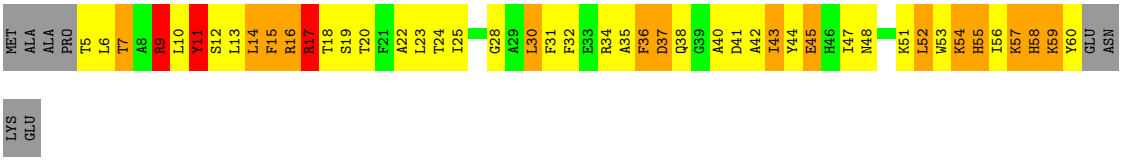
• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

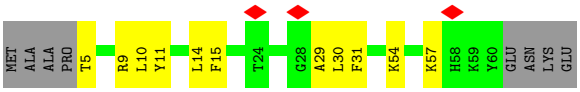


• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



• Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 6W:

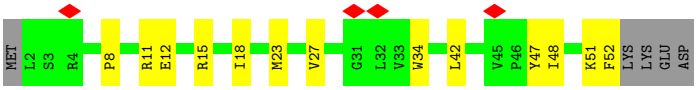


• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X:

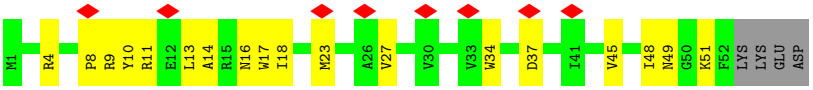
• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y:



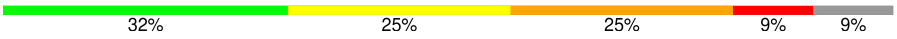
• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 6X:



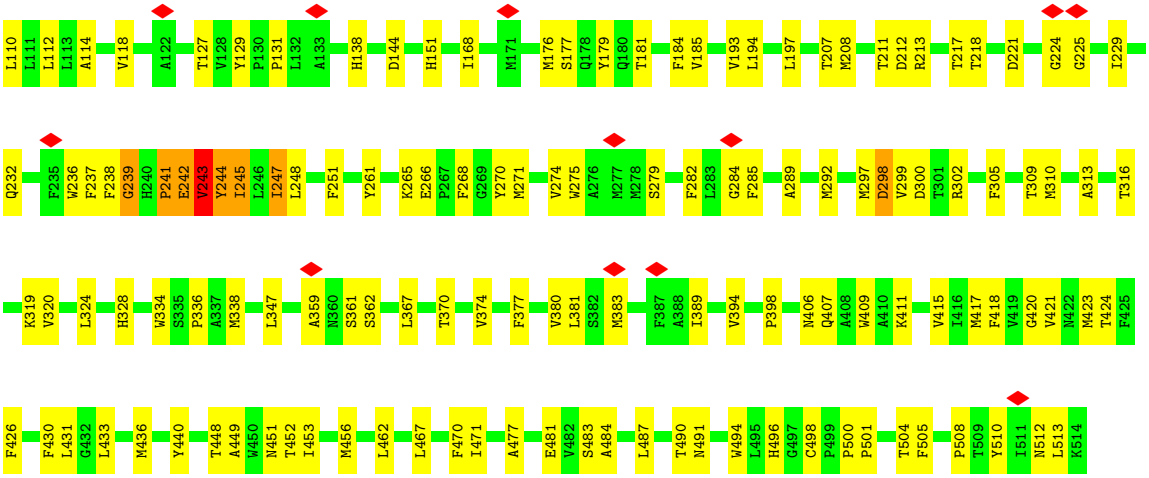
• Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 6Y:



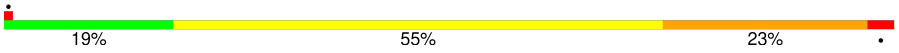
• Molecule 55: Cytochrome c oxidase subunit 1

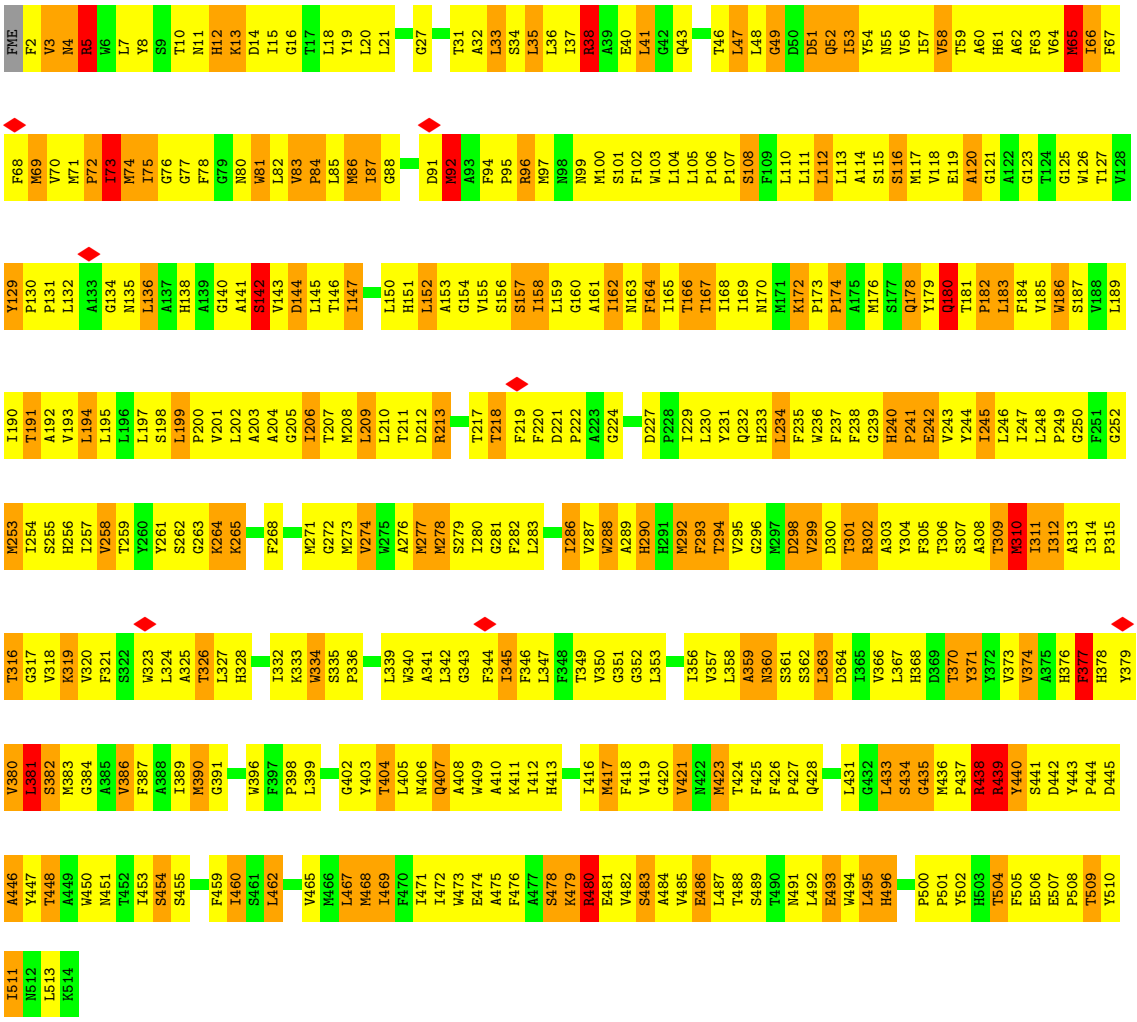
Chain 4A:



• Molecule 55: Cytochrome c oxidase subunit 1

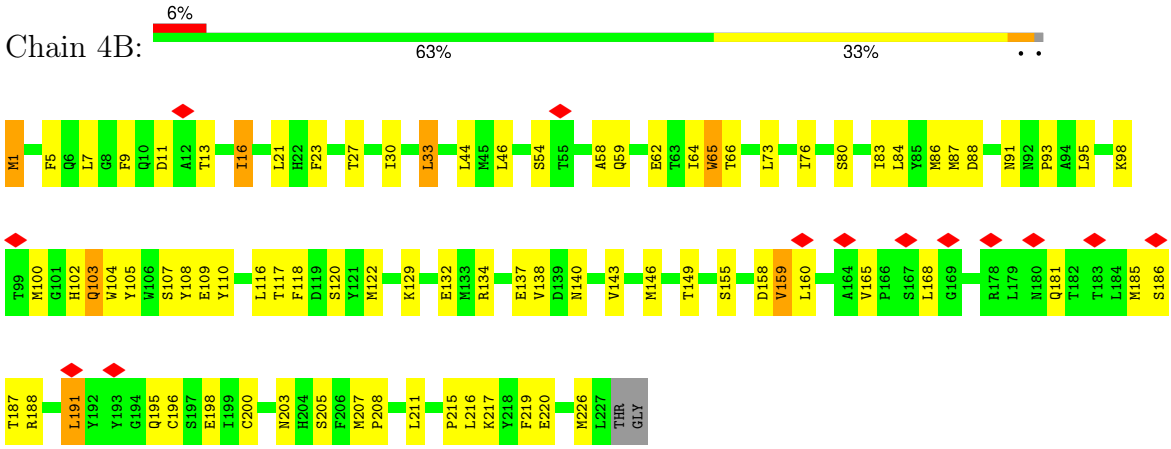
Chain 8A:





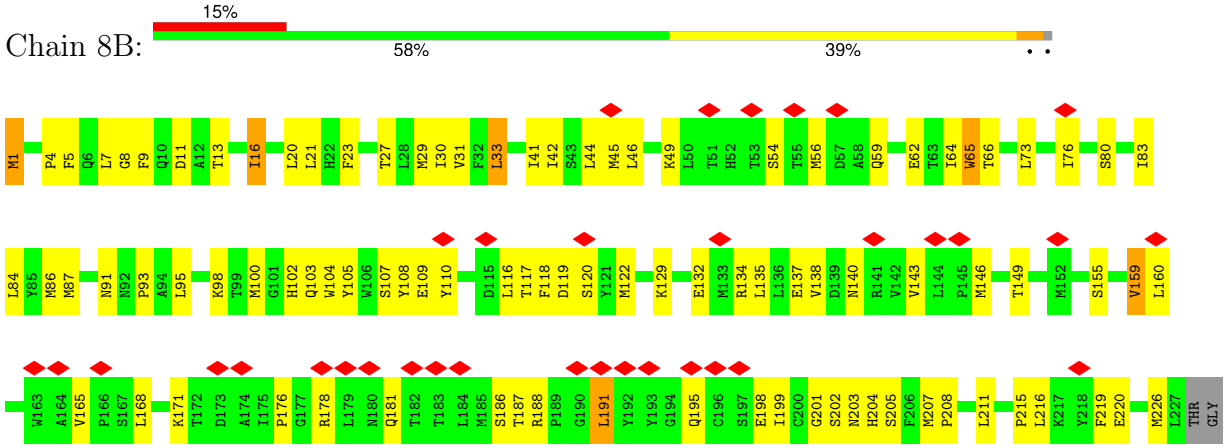
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B:



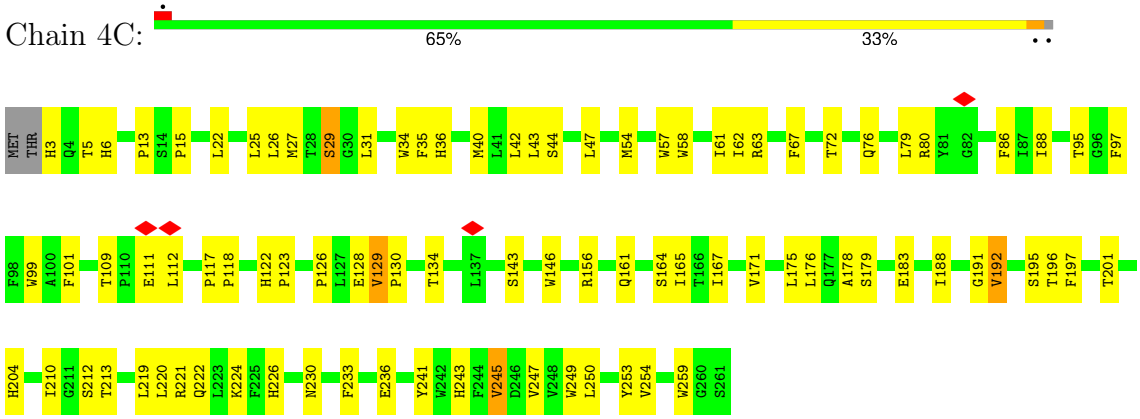
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 8B:



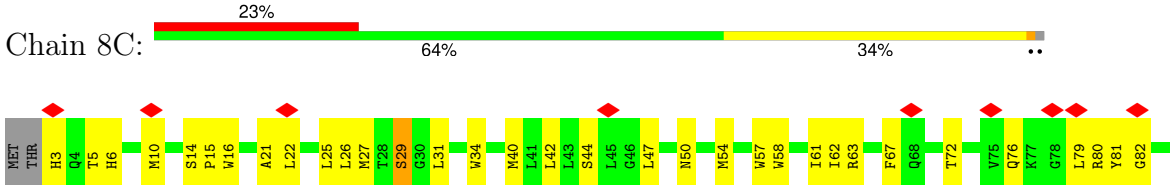
• Molecule 57: Cytochrome c oxidase subunit 3

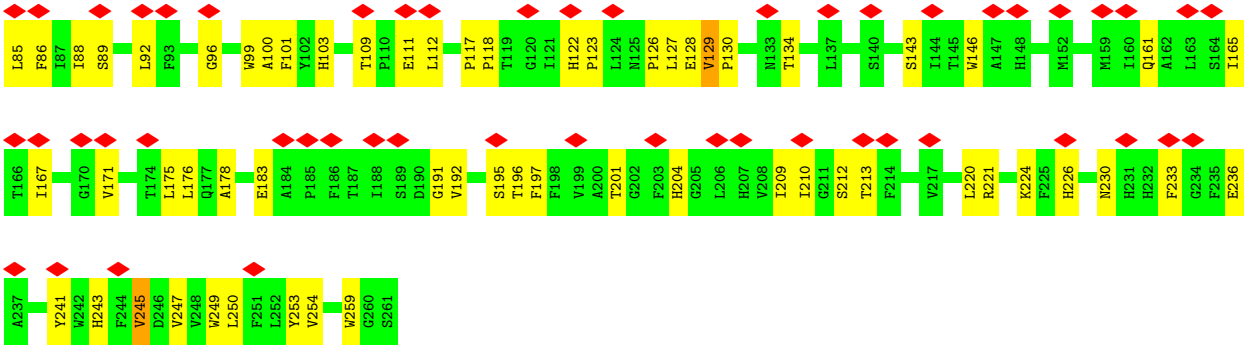
Chain 4C:



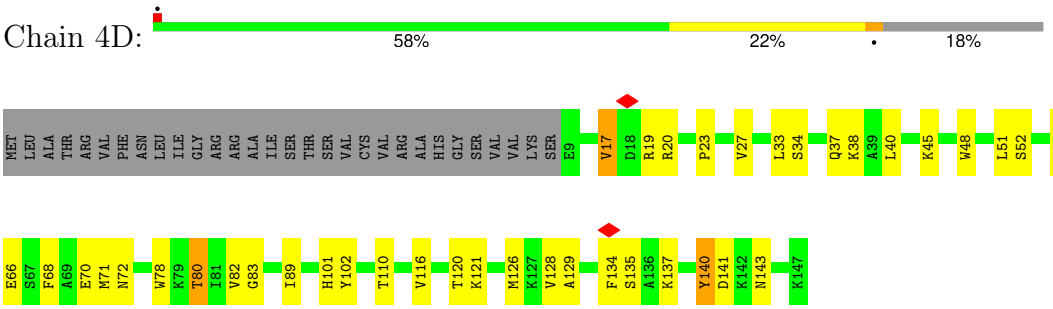
• Molecule 57: Cytochrome c oxidase subunit 3

Chain 8C:

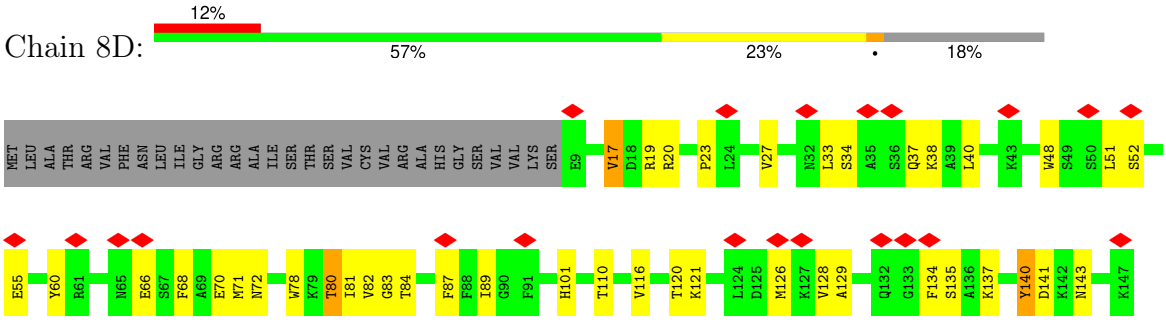




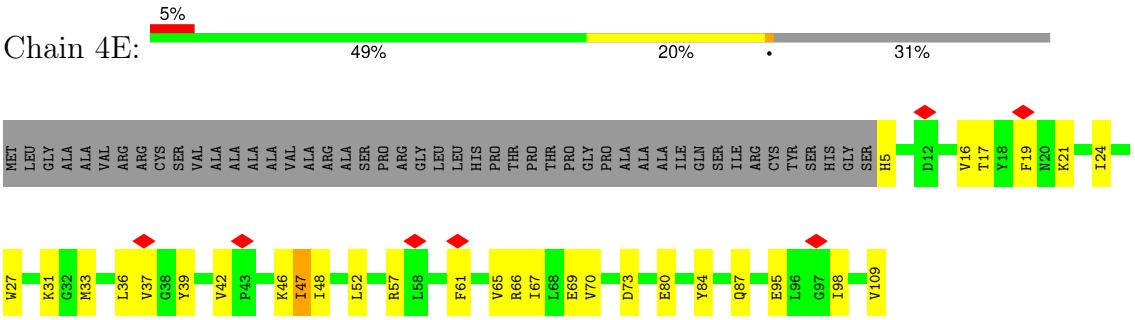
• Molecule 58: Cytochrome c oxidase subunit 4



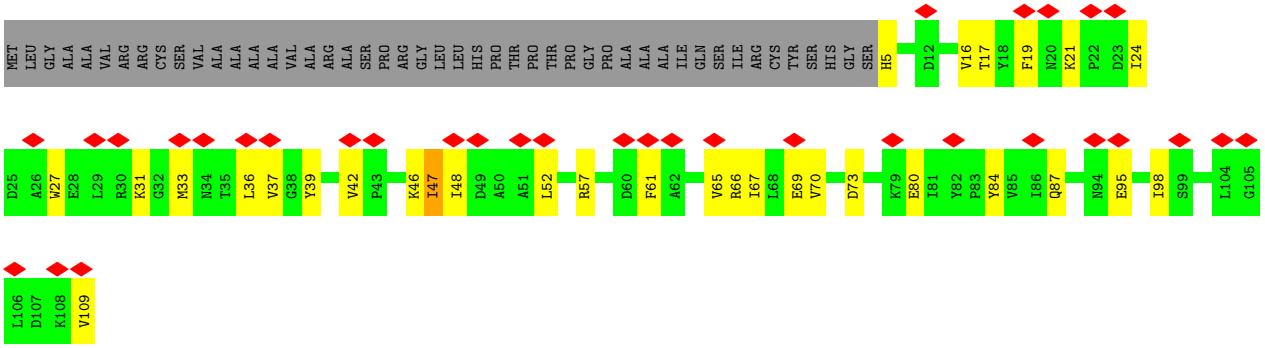
• Molecule 58: Cytochrome c oxidase subunit 4



• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

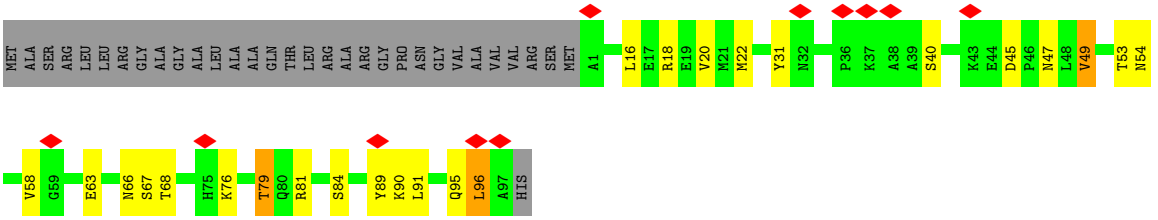


• Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial



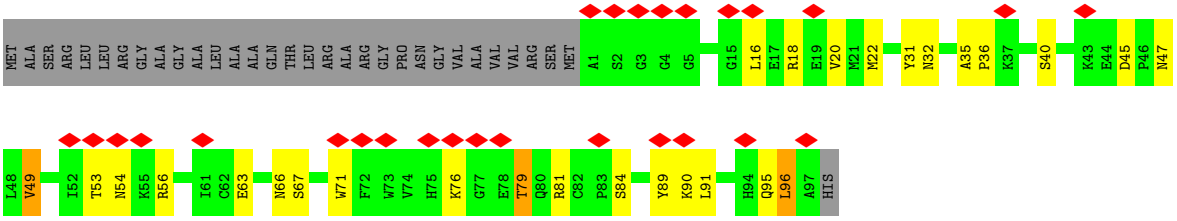
• Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 4F:



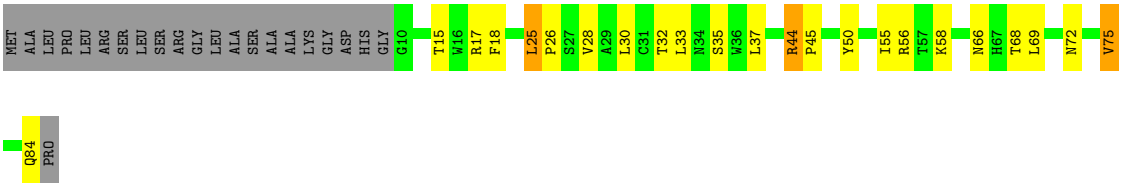
• Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 8F:



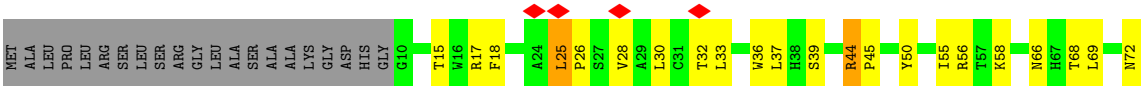
• Molecule 61: Cytochrome c oxidase subunit 6A2

Chain 4G:



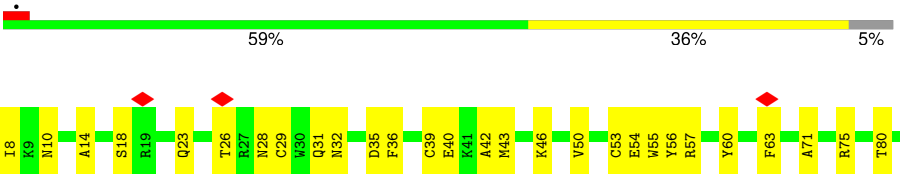
• Molecule 61: Cytochrome c oxidase subunit 6A2

Chain 8G:



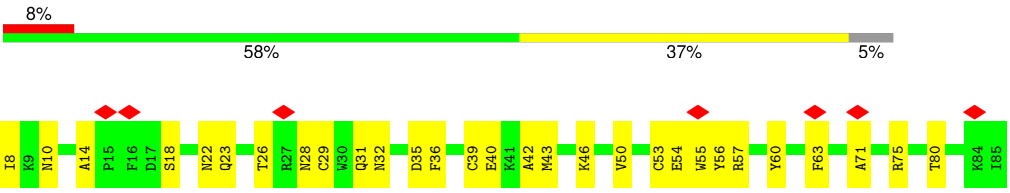
• Molecule 62: Cytochrome c oxidase subunit 6B1

Chain 4H:



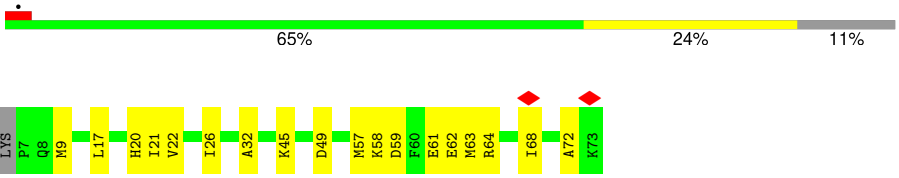
• Molecule 62: Cytochrome c oxidase subunit 6B1

Chain 8H:



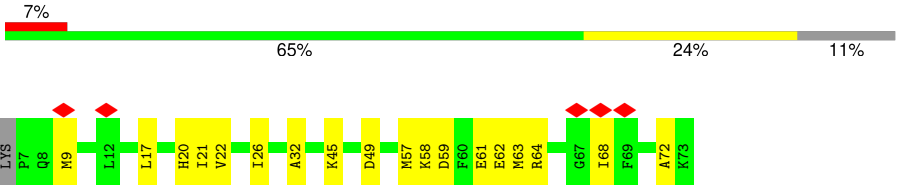
• Molecule 63: Cytochrome c oxidase subunit 6C

Chain 4I:



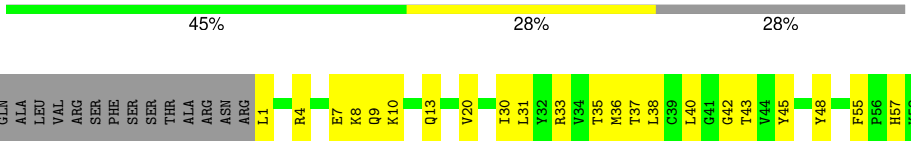
• Molecule 63: Cytochrome c oxidase subunit 6C

Chain 8I:



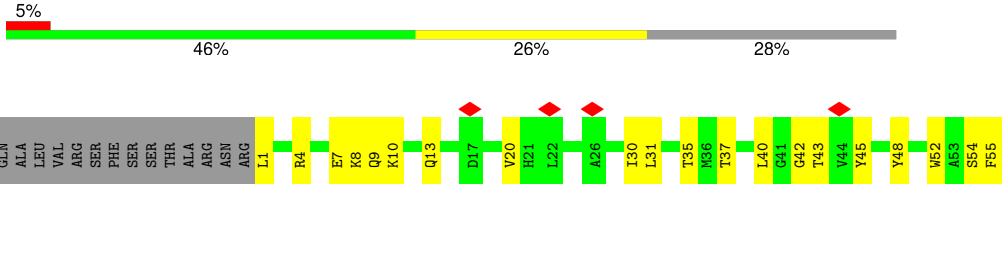
• Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 4J:



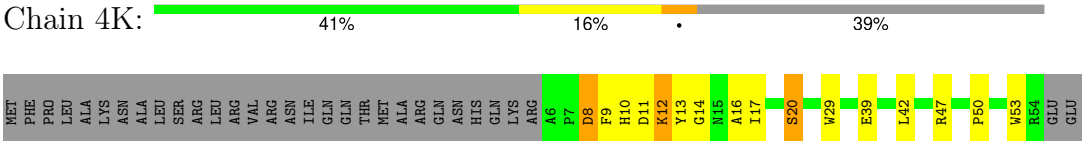
• Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 8J:



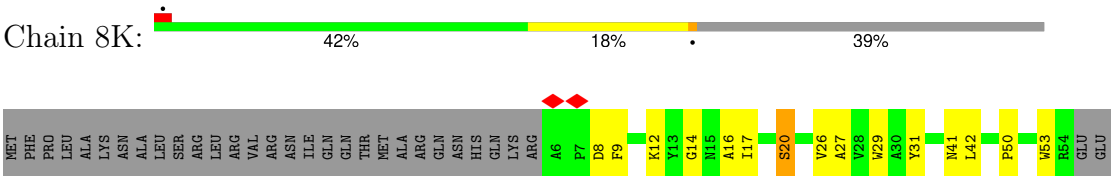
• Molecule 65: Cytochrome c oxidase subunit 7B

Chain 4K:



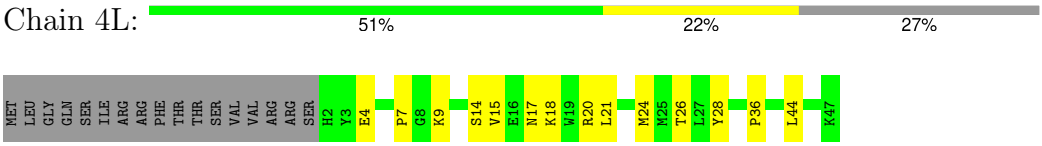
• Molecule 65: Cytochrome c oxidase subunit 7B

Chain 8K:



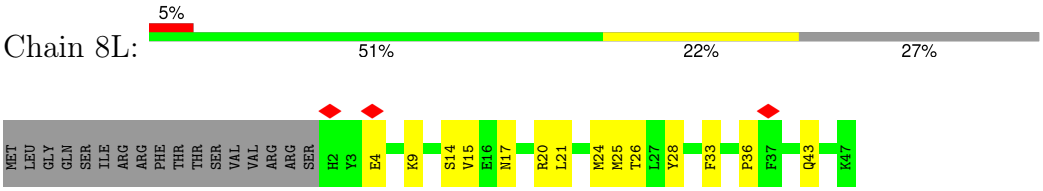
• Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 4L:



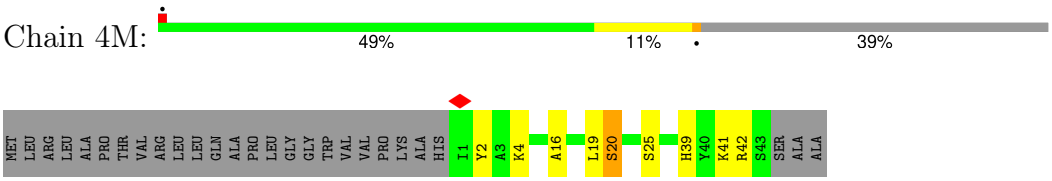
• Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 8L:



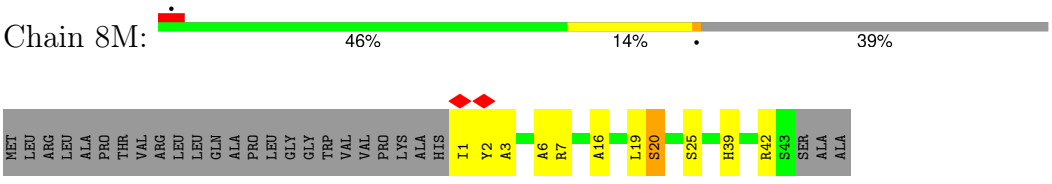
• Molecule 67: Cytochrome c oxidase subunit 8

Chain 4M:



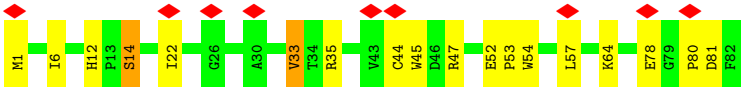
• Molecule 67: Cytochrome c oxidase subunit 8

Chain 8M:

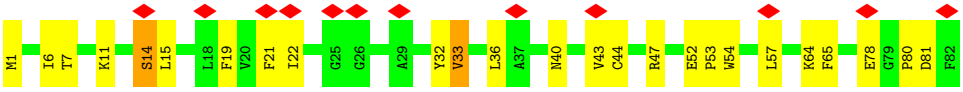


• Molecule 68: Cytochrome c oxidase subunit NDUFA4

Chain 4N:



• Molecule 68: Cytochrome c oxidase subunit NDUFA4



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.533	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	798.72, 798.72, 798.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, NA, PO4, ZN, CUA, CDL, FES, FME, NDP, FMN, MG, HEA, CU, PGV, HEC, EHZ, HEM, PSC, PC1, PEK, SF4, ACE, 3PE, GTP, AME

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.87	0/930	1.17	2/1271 (0.2%)
1	5A	0.20	0/930	0.42	0/1271
2	1B	2.15	4/1270 (0.3%)	2.56	17/1713 (1.0%)
2	5B	0.16	0/1273	0.32	0/1722
3	1C	0.13	0/1797	0.33	0/2447
3	5C	0.13	0/1797	0.33	0/2447
4	1D	0.95	1/3545 (0.0%)	0.54	3/4806 (0.1%)
4	5D	0.95	1/3545 (0.0%)	0.53	3/4806 (0.1%)
5	1E	0.14	0/1698	0.35	0/2311
5	5E	0.15	0/1698	0.35	0/2311
6	1F	0.15	0/3401	0.32	0/4595
6	5F	0.15	0/3401	0.32	0/4595
7	1G	0.14	0/5451	0.32	1/7387 (0.0%)
7	5G	0.14	0/5451	0.32	0/7387
8	1H	0.25	0/2566	0.45	0/3509
8	5H	0.17	0/2566	0.37	0/3509
9	1I	0.12	0/1443	0.29	0/1952
9	5I	0.12	0/1443	0.29	0/1952
10	1J	0.27	0/1364	0.54	1/1850 (0.1%)
10	5J	0.25	0/1364	0.50	0/1850
11	1K	0.19	0/751	0.34	0/1018
11	5K	0.19	0/751	0.34	0/1018
12	1L	0.16	0/4939	0.35	0/6718
12	5L	0.16	0/4939	0.35	0/6718
13	1M	0.16	0/3713	0.35	0/5063
13	5M	0.16	0/3713	0.35	0/5063
14	1N	0.16	0/2765	0.35	0/3758
14	5N	0.17	0/2765	0.35	0/3758
15	1O	0.22	1/2650 (0.0%)	0.54	4/3588 (0.1%)
15	5O	0.22	1/2650 (0.0%)	0.54	4/3588 (0.1%)
16	1P	0.15	0/2828	0.33	0/3834

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	5P	0.15	0/2828	0.33	0/3834
17	1Q	0.14	0/1070	0.32	0/1446
17	5Q	0.15	0/1070	0.32	0/1446
18	1R	0.12	0/755	0.29	0/1018
18	5R	0.12	0/755	0.29	0/1018
19	1S	0.16	0/711	0.36	0/956
19	5S	0.16	0/711	0.36	0/956
20	1T	0.14	0/701	0.30	0/946
20	1U	0.13	0/706	0.28	0/954
20	5T	0.14	0/701	0.30	0/946
20	5U	0.14	0/706	0.28	0/954
21	1V	0.17	0/946	0.31	0/1281
21	5V	0.17	0/946	0.31	0/1281
22	1W	0.17	0/995	0.30	0/1340
22	5W	0.17	0/995	0.30	0/1340
23	1X	0.13	0/1436	0.34	0/1938
23	5X	0.14	0/1436	0.34	0/1938
24	1Y	0.28	1/1037 (0.1%)	0.45	3/1404 (0.2%)
24	5Y	0.28	1/1037 (0.1%)	0.45	3/1404 (0.2%)
25	1Z	0.16	0/1199	0.30	0/1617
25	5Z	0.16	0/1199	0.30	0/1617
26	1a	0.14	0/577	0.31	0/777
26	5a	0.14	0/577	0.31	0/777
27	1b	1.41	4/664 (0.6%)	1.48	7/912 (0.8%)
27	5b	1.41	4/664 (0.6%)	1.49	7/912 (0.8%)
28	1c	0.13	0/430	0.31	0/581
28	5c	0.14	0/430	0.31	0/581
29	1d	0.13	0/1016	0.25	0/1374
29	5d	0.13	0/1016	0.25	0/1374
30	1e	0.15	0/836	0.34	0/1118
30	5e	0.15	0/836	0.34	0/1118
31	1f	0.14	0/499	0.35	0/673
31	5f	0.15	0/499	0.35	0/673
32	1g	0.13	0/858	0.33	0/1165
32	5g	0.13	0/858	0.34	0/1165
33	1h	0.14	0/1184	0.32	0/1603
33	5h	0.14	0/1184	0.32	0/1603
34	1i	0.14	0/1138	0.33	0/1551
34	5i	0.15	0/1138	0.33	0/1551
35	1j	0.12	0/627	0.28	0/858
35	5j	0.19	0/627	0.41	0/858
36	1k	0.44	0/668	0.67	1/903 (0.1%)
36	5k	0.68	1/668 (0.1%)	0.98	5/903 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	1l	2.70	2/1365 (0.1%)	1.26	11/1867 (0.6%)
37	5l	2.70	2/1365 (0.1%)	1.26	11/1867 (0.6%)
38	1m	0.72	1/1092 (0.1%)	0.48	1/1481 (0.1%)
38	5m	0.72	1/1092 (0.1%)	0.48	1/1481 (0.1%)
39	1n	0.15	0/1549	0.33	0/2098
39	5n	0.15	0/1549	0.33	0/2098
40	1o	0.13	0/1069	0.28	0/1430
40	5o	0.13	0/1069	0.28	0/1430
41	1p	0.17	0/1481	0.33	0/1997
41	5p	0.17	0/1481	0.33	0/1997
42	1q	0.12	0/1253	0.27	0/1704
42	5q	0.12	0/1253	0.27	0/1704
43	1r	0.12	0/777	0.27	0/1051
43	5r	0.13	0/777	0.26	0/1051
44	1s	0.13	0/394	0.30	0/533
44	5s	0.13	0/394	0.30	0/533
45	3A	0.29	1/3481 (0.0%)	0.56	4/4722 (0.1%)
45	3N	0.91	0/3487	1.29	17/4711 (0.4%)
45	6A	0.96	0/3481	1.17	3/4722 (0.1%)
45	6N	0.93	0/3487	1.21	14/4711 (0.3%)
46	3B	0.17	0/3192	0.33	0/4322
46	3O	0.97	0/3184	1.21	2/4311 (0.0%)
46	6B	0.98	0/3192	1.19	1/4322 (0.0%)
46	6O	0.96	0/3184	1.20	4/4311 (0.1%)
47	3C	0.91	0/3123	1.22	2/4269 (0.0%)
47	3P	0.18	0/3122	0.35	0/4269
47	6C	0.91	0/3123	1.18	6/4269 (0.1%)
47	6P	0.18	0/3122	0.36	0/4269
48	3D	0.27	0/1946	0.44	0/2641
48	3Q	1.95	2/1962 (0.1%)	1.07	5/2663 (0.2%)
48	6D	0.93	0/1946	1.22	8/2641 (0.3%)
48	6Q	1.95	2/1962 (0.1%)	1.07	4/2663 (0.2%)
49	3E	0.22	0/1551	0.42	0/2098
49	3I	1.38	4/342 (1.2%)	1.72	5/465 (1.1%)
49	3R	0.17	0/1551	0.40	0/2098
49	3V	0.17	0/225	0.34	0/303
49	6E	0.22	0/1551	0.42	0/2098
49	6I	1.38	4/342 (1.2%)	1.71	5/465 (1.1%)
49	6R	0.18	0/1551	0.40	0/2098
49	6V	0.17	0/225	0.34	0/303
50	3F	0.17	0/888	0.32	0/1193
50	3S	0.14	0/888	0.27	0/1193
50	6F	0.17	0/888	0.33	0/1193

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
50	6S	0.14	0/888	0.27	0/1193
51	3G	0.92	0/636	1.20	0/859
51	3T	0.62	3/649 (0.5%)	1.52	4/878 (0.5%)
51	6G	0.22	0/636	0.41	0/859
51	6T	0.61	3/649 (0.5%)	1.52	4/878 (0.5%)
52	3H	0.90	0/539	1.27	0/724
52	3U	0.24	0/539	0.44	0/724
52	6H	0.44	0/539	0.59	0/724
52	6U	0.23	0/539	0.44	0/724
53	3J	0.19	0/476	0.44	0/641
53	3W	0.19	0/476	0.32	0/641
53	6J	0.88	0/476	1.16	0/641
53	6W	0.19	0/476	0.32	0/641
54	3X	0.16	0/445	0.32	0/608
54	3Y	0.17	0/437	0.37	0/598
54	6X	0.16	0/445	0.33	0/608
54	6Y	0.89	0/437	1.09	0/598
55	4A	0.32	1/4156 (0.0%)	0.66	7/5679 (0.1%)
55	8A	0.88	0/4156	1.26	7/5679 (0.1%)
56	4B	0.32	0/1865	0.51	0/2544
56	8B	0.32	0/1865	0.50	0/2544
57	4C	0.20	0/2179	0.34	0/2981
57	8C	0.21	0/2179	0.34	0/2981
58	4D	0.19	0/1197	0.32	0/1617
58	8D	0.19	0/1197	0.32	0/1617
59	4E	0.20	0/871	0.40	1/1182 (0.1%)
59	8E	0.20	0/871	0.40	1/1182 (0.1%)
60	4F	0.23	0/749	0.40	0/1016
60	8F	0.23	0/749	0.40	0/1016
61	4G	0.18	0/644	0.34	0/881
61	8G	0.18	0/644	0.34	0/881
62	4H	0.30	0/708	0.47	0/956
62	8H	0.30	0/708	0.47	0/956
63	4I	0.20	0/563	0.35	0/748
63	8I	0.20	0/563	0.35	0/748
64	4J	0.20	0/466	0.34	0/631
64	8J	0.20	0/466	0.34	0/631
65	4K	0.40	0/396	0.54	0/543
65	8K	0.18	0/396	0.34	0/543
66	4L	0.21	0/394	0.36	0/528
66	8L	0.22	0/394	0.36	0/528
67	4M	0.18	0/349	0.32	0/477
67	8M	0.18	0/349	0.32	0/477

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
68	4N	0.19	0/680	0.41	0/921
68	8N	0.19	0/680	0.41	0/921
All	All	0.62	45/233003 (0.0%)	0.67	189/316071 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1B	0	6
6	1F	0	1
6	5F	0	1
8	1H	0	2
8	5H	0	1
35	5j	0	1
45	3N	0	7
45	6A	0	17
45	6N	0	10
46	3O	0	8
46	6B	0	17
46	6O	0	15
47	3C	0	2
47	6C	0	8
48	3D	0	1
48	6D	0	13
51	3G	0	5
52	3H	0	1
52	6H	0	1
53	6J	0	4
54	6Y	0	5
55	8A	0	8
58	4D	0	1
58	8D	0	1
All	All	0	136

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	3Q	74	PRO	N-CD	85.76	2.67	1.47
48	6Q	74	PRO	N-CD	85.70	2.67	1.47
37	5l	17	PRO	N-CD	76.92	2.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1l	17	PRO	N-CD	76.83	2.55	1.47
37	5l	146	PRO	N-CD	63.31	2.36	1.47
37	1l	146	PRO	N-CD	63.30	2.36	1.47
4	5D	21	PRO	N-CD	55.76	2.25	1.47
4	1D	21	PRO	N-CD	55.69	2.25	1.47
2	1B	57	VAL	C-N	44.64	1.94	1.33
2	1B	92	LEU	C-N	-40.54	0.77	1.33
2	1B	95	LYS	C-N	40.02	1.89	1.33
27	5b	63	PRO	N-CD	28.68	1.87	1.47
27	1b	63	PRO	N-CD	28.57	1.87	1.47
38	1m	19	PRO	N-CD	-22.99	1.15	1.47
38	5m	19	PRO	N-CD	-22.92	1.15	1.47
49	6I	41	PRO	CG-CD	-15.69	0.97	1.50
49	3I	41	PRO	CG-CD	-15.67	0.97	1.50
49	6I	41	PRO	CB-CG	14.81	2.23	1.49
49	3I	41	PRO	CB-CG	14.80	2.23	1.49
27	1b	63	PRO	CA-CB	-13.77	1.34	1.54
27	5b	63	PRO	CA-CB	-13.69	1.35	1.54
27	1b	63	PRO	CG-CD	-13.25	1.05	1.50
27	5b	63	PRO	CG-CD	-13.24	1.05	1.50
45	3A	12	PRO	CG-CD	-11.56	1.11	1.50
51	3T	74	PRO	CG-CD	-10.36	1.15	1.50
51	6T	74	PRO	CG-CD	-10.35	1.15	1.50
55	4A	501	PRO	CB-CG	-10.32	0.98	1.49
27	1b	63	PRO	CB-CG	9.92	1.99	1.49
27	5b	63	PRO	CB-CG	9.90	1.99	1.49
49	6I	41	PRO	CA-CB	-8.42	1.41	1.53
49	3I	41	PRO	CA-CB	-8.41	1.41	1.53
49	3I	41	PRO	N-CD	7.87	1.58	1.47
49	6I	41	PRO	N-CD	7.71	1.58	1.47
51	6T	74	PRO	CB-CG	6.51	1.82	1.49
51	3T	74	PRO	CB-CG	6.49	1.82	1.49
36	5k	68	LYS	C-O	6.48	1.31	1.24
15	1O	165	PRO	N-CD	6.32	1.56	1.47
15	5O	165	PRO	N-CD	6.30	1.56	1.47
48	3Q	74	PRO	CG-CD	-5.85	1.30	1.50
48	6Q	74	PRO	CG-CD	-5.84	1.30	1.50
24	1Y	114	CYS	CB-SG	5.52	1.99	1.81
24	5Y	114	CYS	CB-SG	5.50	1.99	1.81
51	3T	74	PRO	CA-CB	-5.26	1.46	1.53
2	1B	97	ALA	C-O	-5.25	1.17	1.24
51	6T	74	PRO	CA-CB	-5.15	1.46	1.53

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	6Q	74	PRO	N-CD-CG	-47.94	31.30	103.20
48	3Q	74	PRO	N-CD-CG	-47.91	31.34	103.20
2	1B	95	LYS	CA-C-N	-42.09	41.14	121.54
2	1B	95	LYS	C-N-CA	-42.09	41.14	121.54
51	6T	74	PRO	N-CD-CG	-37.36	47.16	103.20
51	3T	74	PRO	N-CD-CG	-37.32	47.22	103.20
2	1B	96	MET	CA-C-N	-35.95	34.09	121.80
2	1B	96	MET	C-N-CA	-35.95	34.09	121.80
37	5l	17	PRO	N-CD-CG	-34.72	51.12	103.20
37	1l	17	PRO	N-CD-CG	-34.69	51.17	103.20
27	5b	63	PRO	N-CD-CG	-34.48	51.47	103.20
27	1b	63	PRO	N-CD-CG	-34.44	51.54	103.20
2	1B	57	VAL	CA-C-N	-32.23	60.64	122.53
2	1B	57	VAL	C-N-CA	-32.23	60.64	122.53
37	5l	146	PRO	N-CD-CG	-30.38	57.63	103.20
37	1l	146	PRO	N-CD-CG	-30.37	57.65	103.20
4	5D	21	PRO	N-CD-CG	-25.67	64.70	103.20
4	1D	21	PRO	N-CD-CG	-25.64	64.74	103.20
55	4A	501	PRO	CB-CG-CD	23.08	179.97	106.10
2	1B	96	MET	O-C-N	22.89	153.04	122.59
45	3A	12	PRO	N-CD-CG	-22.01	70.18	103.20
55	4A	501	PRO	N-CD-CG	-20.50	72.46	103.20
15	5O	165	PRO	N-CD-CG	-20.24	72.84	103.20
15	1O	165	PRO	N-CD-CG	-20.23	72.85	103.20
49	3I	41	PRO	N-CD-CG	-18.75	75.08	103.20
49	6I	41	PRO	N-CD-CG	-18.63	75.25	103.20
55	4A	501	PRO	CA-CB-CG	-18.48	69.38	104.50
49	6I	41	PRO	CA-CB-CG	-17.03	72.14	104.50
49	3I	41	PRO	CA-CB-CG	-17.02	72.17	104.50
45	3A	12	PRO	CA-CB-CG	-16.99	72.21	104.50
51	6T	74	PRO	CA-CB-CG	-16.47	73.20	104.50
51	3T	74	PRO	CA-CB-CG	-16.42	73.30	104.50
48	3Q	74	PRO	CA-N-CD	-15.52	90.28	112.00
49	3I	41	PRO	N-CA-CB	-15.51	86.96	103.25
48	6Q	74	PRO	CA-N-CD	-15.51	90.29	112.00
49	6I	41	PRO	N-CA-CB	-15.44	87.04	103.25
49	6I	41	PRO	CB-CG-CD	-14.99	58.12	106.10
49	3I	41	PRO	CB-CG-CD	-14.99	58.14	106.10
27	5b	63	PRO	CA-CB-CG	-14.80	76.37	104.50
27	1b	63	PRO	CA-CB-CG	-14.80	76.38	104.50
37	1l	17	PRO	CA-N-CD	-14.11	92.25	112.00
37	5l	17	PRO	CA-N-CD	-14.10	92.27	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1B	57	VAL	O-C-N	14.02	140.91	122.26
2	1B	104	TYR	CA-C-O	12.77	125.35	117.94
27	1b	63	PRO	N-CA-CB	-12.76	87.67	102.60
2	1B	95	LYS	O-C-N	12.75	139.51	122.43
27	5b	63	PRO	N-CA-CB	-12.74	87.69	102.60
15	5O	165	PRO	CA-CB-CG	-12.58	80.61	104.50
15	1O	165	PRO	CA-CB-CG	-12.56	80.63	104.50
37	5l	146	PRO	CA-N-CD	-12.20	94.91	112.00
37	1l	146	PRO	CA-N-CD	-12.19	94.94	112.00
2	1B	92	LEU	CA-C-N	-12.18	101.25	123.05
2	1B	92	LEU	C-N-CA	-12.18	101.25	123.05
48	6Q	74	PRO	CA-CB-CG	-11.71	82.25	104.50
55	8A	377	PHE	CA-CB-CG	11.70	125.50	113.80
48	3Q	74	PRO	CA-CB-CG	-11.68	82.31	104.50
51	3T	74	PRO	N-CA-CB	-11.64	91.02	103.25
51	6T	74	PRO	N-CA-CB	-11.59	91.08	103.25
45	6N	70	ARG	C-N-CD	-11.28	78.75	125.00
2	1B	97	ALA	C-N-CD	-11.16	79.23	125.00
4	5D	21	PRO	CA-N-CD	-11.15	96.38	112.00
4	1D	21	PRO	CA-N-CD	-11.12	96.44	112.00
27	5b	63	PRO	CB-CG-CD	-10.51	72.48	106.10
27	1b	63	PRO	CB-CG-CD	-10.48	72.56	106.10
38	1m	19	PRO	N-CD-CG	9.75	117.83	103.20
38	5m	19	PRO	N-CD-CG	9.74	117.82	103.20
45	3N	356	ARG	N-CA-C	-9.70	99.60	111.33
45	6N	71	PRO	CA-N-CD	-9.52	98.68	112.00
45	6N	33	PRO	CA-N-CD	-9.44	98.79	112.00
45	6N	12	PRO	CA-N-CD	-9.23	99.07	112.00
45	3N	107	PRO	CA-N-CD	-9.22	99.09	112.00
45	6N	107	PRO	CA-N-CD	-9.17	99.16	112.00
45	3N	170	PRO	CA-N-CD	-9.10	99.27	112.00
45	6N	170	PRO	CA-N-CD	-9.06	99.32	112.00
45	3N	33	PRO	CA-N-CD	-8.98	99.42	112.00
45	3N	12	PRO	CA-N-CD	-8.88	99.56	112.00
45	6N	193	PRO	CA-N-CD	-8.81	99.66	112.00
45	3N	193	PRO	CA-N-CD	-8.78	99.70	112.00
45	3N	162	PRO	CA-N-CD	-8.77	99.72	112.00
45	6N	106	LEU	C-N-CD	-8.72	89.23	125.00
45	3N	71	PRO	CA-N-CD	-8.69	99.83	112.00
45	3N	106	LEU	C-N-CD	-8.55	89.95	125.00
46	6O	56	ARG	N-CA-CB	-8.45	95.95	110.32
27	1b	63	PRO	CB-CA-C	8.43	121.99	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	5b	63	PRO	CB-CA-C	8.43	121.98	110.52
47	6C	247	PRO	N-CA-C	-8.39	103.94	114.68
27	5b	63	PRO	CA-N-CD	-8.35	100.32	112.00
27	1b	63	PRO	CA-N-CD	-8.30	100.38	112.00
36	5k	67	LEU	N-CA-C	8.15	121.31	110.88
45	6N	162	PRO	CA-N-CD	-8.11	100.65	112.00
37	5l	17	PRO	CA-CB-CG	-7.90	89.49	104.50
37	1l	17	PRO	CA-CB-CG	-7.90	89.50	104.50
49	6I	41	PRO	CA-N-CD	-7.85	101.01	112.00
49	3I	41	PRO	CA-N-CD	-7.84	101.03	112.00
55	4A	238	PHE	N-CA-C	-7.76	103.95	113.41
37	5l	146	PRO	CA-CB-CG	-7.60	90.07	104.50
37	1l	146	PRO	CA-CB-CG	-7.59	90.07	104.50
48	6D	328	PRO	N-CA-C	-7.49	101.56	110.70
51	3T	74	PRO	CB-CG-CD	-7.28	82.80	106.10
51	6T	74	PRO	CB-CG-CD	-7.27	82.84	106.10
36	5k	78	VAL	N-CA-C	-7.25	103.22	110.62
45	3N	355	VAL	N-CA-C	-7.25	103.90	111.58
45	3N	226	ASP	N-CA-C	-7.24	104.42	113.18
55	8A	377	PHE	CB-CA-C	7.24	122.77	110.74
46	6O	56	ARG	CA-C-N	-7.19	107.80	121.54
46	6O	56	ARG	C-N-CA	-7.19	107.80	121.54
45	3N	260	PRO	N-CA-CB	-6.91	96.00	103.25
46	6B	155	PRO	N-CA-CB	-6.80	96.11	103.25
55	8A	180	GLN	N-CA-C	-6.72	103.27	113.89
36	5k	69	GLY	N-CA-C	-6.60	104.59	113.24
55	8A	92	MET	CB-CA-C	-6.58	106.17	114.40
24	5Y	94	CYS	CA-CB-SG	6.51	129.38	114.40
24	1Y	94	CYS	CA-CB-SG	6.51	129.36	114.40
36	5k	67	LEU	N-CA-CB	-6.48	101.92	111.51
55	4A	501	PRO	CA-N-CD	-6.47	102.94	112.00
4	1D	21	PRO	CA-CB-CG	-6.41	92.32	104.50
4	5D	21	PRO	CA-CB-CG	-6.40	92.34	104.50
55	8A	129	TYR	CB-CA-C	6.39	116.49	110.17
45	3N	354	VAL	N-CA-C	-6.36	103.14	111.09
36	5k	68	LYS	N-CA-C	-6.35	103.88	111.69
15	5O	165	PRO	N-CA-CB	-6.28	96.99	103.08
15	1O	165	PRO	N-CA-CB	-6.23	97.04	103.08
46	6O	55	SER	O-C-N	6.22	130.86	122.59
47	6C	82	LEU	N-CA-C	-6.20	104.44	111.07
45	6N	162	PRO	N-CA-C	-6.10	105.41	113.65
24	1Y	93	GLY	CA-C-N	-6.01	110.87	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	1Y	93	GLY	C-N-CA	-6.01	110.87	122.06
24	5Y	93	GLY	CA-C-N	-6.00	110.91	122.06
24	5Y	93	GLY	C-N-CA	-6.00	110.91	122.06
48	3Q	73	GLY	C-N-CD	5.96	149.43	125.00
48	6Q	73	GLY	C-N-CD	5.96	149.43	125.00
48	6D	138	HIS	N-CA-C	-5.92	104.91	111.36
45	3N	392	LEU	N-CA-C	-5.85	104.91	111.28
46	3O	395	PRO	N-CA-C	-5.82	105.44	113.53
55	4A	244	TYR	N-CA-C	-5.79	104.89	111.14
36	1k	75	ALA	N-CA-C	-5.78	104.98	111.28
48	6D	199	PRO	N-CA-C	5.78	124.37	112.47
45	3N	353	GLU	N-CA-C	-5.72	106.30	113.28
27	1b	63	PRO	N-CA-C	5.71	120.61	114.68
47	6C	81	TYR	CB-CA-C	5.70	122.01	110.38
2	1B	97	ALA	CA-C-O	5.64	127.89	120.16
1	1A	69	ILE	N-CA-C	-5.63	105.01	110.42
27	5b	63	PRO	N-CA-C	5.63	120.54	114.68
48	6D	98	TYR	CA-CB-CG	5.62	124.01	113.90
45	3N	57	TYR	N-CA-C	-5.61	105.07	111.07
37	1l	16	THR	C-N-CD	5.61	147.99	125.00
37	5l	16	THR	C-N-CD	5.58	147.88	125.00
46	3O	30	PRO	N-CA-C	-5.51	106.67	113.84
45	3A	12	PRO	CA-N-CD	-5.51	104.29	112.00
45	3A	12	PRO	N-CA-CB	-5.51	98.21	103.39
47	3C	265	PRO	N-CA-CB	-5.51	97.74	103.08
10	1J	147	TYR	N-CA-C	-5.48	106.09	112.89
45	6A	307	PHE	CA-CB-CG	5.44	119.24	113.80
45	6N	307	PHE	CA-CB-CG	5.38	119.18	113.80
2	1B	41	ARG	N-CA-C	-5.35	105.45	111.28
1	1A	67	LEU	N-CA-C	-5.29	105.69	111.82
55	4A	245	ILE	N-CA-C	-5.28	104.81	110.36
55	8A	51	ASP	CA-CB-CG	5.28	117.88	112.60
48	6D	112	THR	N-CA-C	-5.28	105.69	111.82
48	6D	198	PRO	N-CA-C	-5.28	104.27	110.70
47	3C	183	PHE	N-CA-CB	-5.26	102.24	109.91
2	1B	47	PRO	N-CA-C	5.25	118.85	110.40
37	1l	17	PRO	N-CA-CB	-5.23	98.25	103.48
37	5l	17	PRO	CB-CG-CD	-5.22	89.39	106.10
37	1l	17	PRO	CB-CG-CD	-5.22	89.40	106.10
45	6N	354	VAL	N-CA-C	-5.21	105.41	110.42
37	5l	17	PRO	N-CA-CB	-5.21	98.27	103.48
48	6D	136	TYR	N-CA-C	-5.14	106.52	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1B	86	MET	CG-SD-CE	-5.14	89.59	100.90
15	5O	165	PRO	CA-N-CD	-5.12	104.83	112.00
45	6N	214	LYS	N-CA-C	-5.12	107.70	114.31
45	6A	310	PHE	CA-CB-CG	5.10	118.90	113.80
47	6C	261	PRO	N-CA-C	-5.10	109.38	114.68
15	1O	165	PRO	CA-N-CD	-5.09	104.87	112.00
47	6C	210	GLY	N-CA-C	-5.09	108.22	115.30
37	5l	145	ASP	C-N-CD	5.07	145.80	125.00
48	3Q	74	PRO	N-CA-CB	-5.07	98.80	103.31
45	6A	324	PHE	CA-CB-CG	5.07	118.87	113.80
55	8A	274	VAL	N-CA-CB	5.07	116.48	110.55
37	1l	145	ASP	C-N-CD	5.07	145.77	125.00
45	3N	205	HIS	N-CA-C	-5.06	105.20	111.33
59	4E	46	LYS	N-CA-C	-5.05	106.47	113.18
47	6C	183	PHE	CA-CB-CG	-5.05	108.75	113.80
59	8E	46	LYS	N-CA-C	-5.03	106.49	113.18
48	6D	252	PRO	N-CA-CB	-5.03	97.97	103.25
37	5l	146	PRO	CB-CG-CD	-5.03	90.02	106.10
37	1l	146	PRO	CB-CG-CD	-5.02	90.03	106.10
7	1G	653	ASN	CB-CA-C	-5.01	110.42	117.23
45	6N	233	PRO	N-CA-C	-5.00	102.16	112.47

There are no chirality outliers.

All (136) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	111	ARG	Sidechain
2	1B	71	ARG	Sidechain
2	1B	77	ARG	Sidechain
2	1B	81	ARG	Sidechain
2	1B	92	LEU	Mainchain
2	1B	96	MET	Mainchain
6	1F	206	LYS	Peptide
8	1H	25	ARG	Sidechain
8	1H	91	MET	Peptide
47	3C	5	ARG	Sidechain
47	3C	80	ARG	Sidechain
48	3D	232	ARG	Sidechain
51	3G	11	ARG	Sidechain
51	3G	13	ARG	Sidechain
51	3G	4	ARG	Sidechain
51	3G	41	ARG	Sidechain

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Mol	Chain	Res	Type	Group
51	3G	73	ARG	Sidechain
52	3H	77	GLU	Peptide
45	3N	206	ARG	Mainchain
45	3N	207	GLN	Mainchain
45	3N	244	ARG	Sidechain
45	3N	356	ARG	Sidechain
45	3N	389	ARG	Sidechain
45	3N	408	ARG	Sidechain
45	3N	438	ARG	Sidechain
46	3O	113	ARG	Sidechain
46	3O	133	ARG	Sidechain
46	3O	134	ARG	Sidechain
46	3O	169	ARG	Sidechain
46	3O	203	ARG	Sidechain
46	3O	245	ARG	Sidechain
46	3O	46	ARG	Sidechain
46	3O	70	ARG	Sidechain
58	4D	140	TYR	Peptide
6	5F	206	LYS	Peptide
8	5H	91	MET	Peptide
35	5j	19	ARG	Sidechain
45	6A	131	ARG	Sidechain
45	6A	175	ARG	Sidechain
45	6A	194	ARG	Sidechain
45	6A	24	ARG	Sidechain
45	6A	242	ARG	Sidechain
45	6A	244	ARG	Sidechain
45	6A	301	ARG	Sidechain
45	6A	356	ARG	Sidechain
45	6A	381	ARG	Sidechain
45	6A	388	ARG	Sidechain
45	6A	389	ARG	Sidechain
45	6A	398	ARG	Sidechain
45	6A	408	ARG	Sidechain
45	6A	436	ARG	Sidechain
45	6A	445	ARG	Sidechain
45	6A	70	ARG	Sidechain
45	6A	92	ARG	Sidechain
46	6B	113	ARG	Sidechain
46	6B	133	ARG	Sidechain
46	6B	134	ARG	Sidechain
46	6B	145	ARG	Sidechain

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Mol	Chain	Res	Type	Group
46	6B	169	ARG	Sidechain
46	6B	203	ARG	Sidechain
46	6B	222	ARG	Sidechain
46	6B	227	ARG	Sidechain
46	6B	240	ARG	Sidechain
46	6B	245	ARG	Sidechain
46	6B	28	ARG	Sidechain
46	6B	287	ARG	Sidechain
46	6B	421	ARG	Sidechain
46	6B	46	ARG	Sidechain
46	6B	56	ARG	Sidechain
46	6B	70	ARG	Sidechain
46	6B	87	ARG	Sidechain
47	6C	177	ARG	Sidechain
47	6C	282	ARG	Sidechain
47	6C	313	ARG	Sidechain
47	6C	318	ARG	Sidechain
47	6C	345	HIS	Peptide
47	6C	5	ARG	Sidechain
47	6C	71	ARG	Sidechain
47	6C	80	ARG	Sidechain
48	6D	103	ARG	Sidechain
48	6D	115	ARG	Sidechain
48	6D	116	ARG	Sidechain
48	6D	137	ARG	Sidechain
48	6D	171	ARG	Sidechain
48	6D	190	ARG	Sidechain
48	6D	206	ARG	Sidechain
48	6D	208	ARG	Sidechain
48	6D	280	ARG	Sidechain
48	6D	290	ARG	Sidechain
48	6D	313	ARG	Sidechain
48	6D	322	ARG	Sidechain
48	6D	327	ARG	Sidechain
52	6H	72	ARG	Sidechain
53	6J	16	ARG	Sidechain
53	6J	17	ARG	Sidechain
53	6J	34	ARG	Sidechain
53	6J	9	ARG	Sidechain
45	6N	235	ARG	Sidechain
45	6N	242	ARG	Sidechain
45	6N	244	ARG	Sidechain

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Mol	Chain	Res	Type	Group
45	6N	301	ARG	Sidechain
45	6N	344	ARG	Sidechain
45	6N	356	ARG	Sidechain
45	6N	362	ARG	Sidechain
45	6N	398	ARG	Sidechain
45	6N	408	ARG	Sidechain
45	6N	436	ARG	Sidechain
46	6O	102	ARG	Sidechain
46	6O	113	ARG	Sidechain
46	6O	134	ARG	Sidechain
46	6O	145	ARG	Sidechain
46	6O	169	ARG	Sidechain
46	6O	182	ARG	Sidechain
46	6O	203	ARG	Sidechain
46	6O	222	ARG	Sidechain
46	6O	227	ARG	Sidechain
46	6O	245	ARG	Sidechain
46	6O	28	ARG	Sidechain
46	6O	421	ARG	Sidechain
46	6O	46	ARG	Sidechain
46	6O	55	SER	Mainchain
46	6O	56	ARG	Sidechain
54	6Y	11	ARG	Sidechain
54	6Y	15	ARG	Sidechain
54	6Y	39	ARG	Sidechain
54	6Y	4	ARG	Sidechain
54	6Y	9	ARG	Sidechain
55	8A	213	ARG	Sidechain
55	8A	302	ARG	Sidechain
55	8A	38	ARG	Sidechain
55	8A	438	ARG	Sidechain
55	8A	439	ARG	Sidechain
55	8A	480	ARG	Sidechain
55	8A	5	ARG	Sidechain
55	8A	96	ARG	Sidechain
58	8D	140	TYR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	949	67	0
1	5A	916	0	950	49	0
2	1B	1242	0	1241	201	0
2	5B	1242	0	1249	39	0
3	1C	1746	0	1697	35	0
3	5C	1746	0	1697	34	0
4	1D	3452	0	3389	121	0
4	5D	3452	0	3389	93	0
5	1E	1658	0	1662	42	0
5	5E	1658	0	1662	41	0
6	1F	3325	0	3288	94	0
6	5F	3325	0	3288	91	0
7	1G	5362	0	5388	127	0
7	5G	5362	0	5388	123	0
8	1H	2504	0	2602	93	0
8	5H	2504	0	2602	86	0
9	1I	1412	0	1366	48	0
9	5I	1412	0	1366	43	0
10	1J	1329	0	1326	88	0
10	5J	1329	0	1326	90	0
11	1K	750	0	798	41	0
11	5K	750	0	798	39	0
12	1L	4818	0	4956	160	0
12	5L	4818	0	4956	159	0
13	1M	3632	0	3836	136	0
13	5M	3632	0	3836	138	0
14	1N	2712	0	2872	84	0
14	5N	2712	0	2872	85	0
15	1O	2590	0	2556	70	0
15	5O	2590	0	2556	72	0
16	1P	2751	0	2776	60	0
16	5P	2751	0	2776	60	0
17	1Q	1047	0	1042	31	0
17	5Q	1047	0	1042	31	0
18	1R	741	0	704	11	0
18	5R	741	0	704	10	0
19	1S	700	0	719	18	0
19	5S	700	0	719	16	0
20	1T	689	0	687	25	0
20	1U	694	0	691	17	0
20	5T	689	0	687	25	0
20	5U	694	0	691	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	1V	927	0	972	25	0
21	5V	927	0	972	25	0
22	1W	971	0	975	23	0
22	5W	971	0	975	24	0
23	1X	1398	0	1378	34	0
23	5X	1398	0	1378	31	0
24	1Y	1016	0	1020	41	0
24	5Y	1016	0	1020	38	0
25	1Z	1168	0	1161	42	0
25	5Z	1168	0	1161	40	0
26	1a	562	0	557	18	0
26	5a	562	0	557	17	0
27	1b	643	0	645	14	0
27	5b	643	0	645	15	0
28	1c	417	0	425	10	0
28	5c	417	0	425	9	0
29	1d	985	0	978	36	0
29	5d	985	0	978	34	0
30	1e	816	0	823	33	0
30	5e	816	0	823	33	0
31	1f	487	0	498	17	0
31	5f	487	0	498	14	0
32	1g	835	0	795	26	0
32	5g	835	0	795	25	0
33	1h	1151	0	1164	29	0
33	5h	1151	0	1164	27	0
34	1i	1100	0	1107	29	0
34	5i	1100	0	1107	25	0
35	1j	601	0	546	29	0
35	5j	601	0	546	35	0
36	1k	649	0	626	21	0
36	5k	649	0	626	46	0
37	1l	1310	0	1204	42	0
37	5l	1310	0	1204	41	0
38	1m	1062	0	1075	44	0
38	5m	1062	0	1075	49	0
39	1n	1495	0	1434	52	0
39	5n	1495	0	1434	51	0
40	1o	1045	0	1016	38	0
40	5o	1045	0	1016	35	0
41	1p	1449	0	1416	42	0
41	5p	1449	0	1416	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	1q	1212	0	1174	20	0
42	5q	1212	0	1174	19	0
43	1r	759	0	783	16	0
43	5r	759	0	783	14	0
44	1s	382	0	351	11	0
44	5s	382	0	351	12	0
45	3A	3411	0	3309	70	0
45	3N	3415	0	3331	767	0
45	6A	3411	0	3309	235	0
45	6N	3415	0	3326	836	0
46	3B	3139	0	3118	89	0
46	3O	3132	0	3110	233	0
46	6B	3139	0	3118	192	0
46	6O	3132	0	3110	278	0
47	3C	3025	0	3090	339	0
47	3P	3024	0	3090	76	0
47	6C	3025	0	3090	322	0
47	6P	3024	0	3090	77	0
48	3D	1888	0	1834	112	0
48	3Q	1904	0	1849	65	0
48	6D	1888	0	1832	230	0
48	6Q	1904	0	1849	62	0
49	3E	1518	0	1498	104	0
49	3I	337	0	347	29	0
49	3R	1518	0	1498	105	0
49	3V	223	0	233	24	0
49	6E	1518	0	1498	113	0
49	6I	337	0	347	33	0
49	6R	1518	0	1498	97	0
49	6V	223	0	233	27	0
50	3F	868	0	857	35	0
50	3S	868	0	857	11	0
50	6F	868	0	857	29	0
50	6S	868	0	857	15	0
51	3G	616	0	620	53	0
51	3T	628	0	634	26	0
51	6G	616	0	622	53	0
51	6T	628	0	634	29	0
52	3H	533	0	513	29	0
52	3U	533	0	513	13	0
52	6H	533	0	513	40	0
52	6U	533	0	513	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	3J	464	0	467	9	0
53	3W	464	0	467	7	0
53	6J	464	0	467	42	0
53	6W	464	0	467	8	0
54	3X	429	0	430	15	0
54	3Y	421	0	418	10	0
54	6X	429	0	430	17	0
54	6Y	421	0	418	31	0
55	4A	4016	0	3994	148	0
55	8A	4016	0	3994	501	0
56	4B	1828	0	1837	68	0
56	8B	1828	0	1836	93	0
57	4C	2096	0	2027	83	0
57	8C	2096	0	2027	110	0
58	4D	1163	0	1143	37	0
58	8D	1163	0	1143	36	0
59	4E	852	0	845	20	0
59	8E	852	0	845	19	0
60	4F	734	0	718	18	0
60	8F	734	0	718	29	0
61	4G	617	0	585	17	0
61	8G	617	0	585	21	0
62	4H	687	0	647	26	0
62	8H	687	0	647	30	0
63	4I	550	0	560	16	0
63	8I	550	0	560	16	0
64	4J	456	0	459	23	0
64	8J	456	0	459	24	0
65	4K	383	0	366	16	0
65	8K	383	0	366	25	0
66	4L	381	0	380	12	0
66	8L	381	0	380	13	0
67	4M	338	0	345	9	0
67	8M	338	0	345	14	0
68	4N	660	0	664	17	0
68	8N	660	0	664	29	0
69	1A	47	0	71	4	0
69	1J	44	0	62	5	0
69	1L	122	0	172	8	0
69	1M	95	0	141	12	0
69	1N	100	0	157	19	0
69	1Y	171	0	218	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	1d	48	0	73	11	0
69	1j	44	0	65	0	0
69	5A	47	0	71	2	0
69	5J	44	0	62	5	0
69	5L	122	0	172	7	0
69	5M	95	0	141	13	0
69	5N	100	0	157	20	0
69	5Y	171	0	218	17	0
69	5d	48	0	73	12	0
69	5j	44	0	65	0	0
70	1B	8	0	0	5	0
70	1F	8	0	0	2	0
70	1G	16	0	0	1	0
70	1I	16	0	0	0	0
70	5B	8	0	0	2	0
70	5F	8	0	0	2	0
70	5G	16	0	0	1	0
70	5I	16	0	0	0	0
71	1B	46	0	66	3	0
71	1H	48	0	73	7	0
71	1I	98	0	150	11	0
71	1J	35	0	44	4	0
71	1M	44	0	65	8	0
71	1P	33	0	40	5	0
71	1Y	35	0	44	3	0
71	1h	47	0	71	3	0
71	1m	46	0	66	5	0
71	5A	35	0	44	1	0
71	5B	46	0	66	2	0
71	5H	48	0	73	5	0
71	5I	98	0	150	11	0
71	5M	44	0	65	8	0
71	5P	33	0	40	2	0
71	5Y	35	0	44	3	0
71	5h	47	0	71	3	0
71	5m	46	0	66	5	0
72	1E	4	0	0	1	0
72	1G	4	0	0	1	0
72	3E	4	0	0	4	0
72	3R	4	0	0	1	0
72	5E	4	0	0	1	0
72	5G	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	6E	4	0	0	4	0
72	6R	4	0	0	1	0
73	1F	31	0	19	2	0
73	5F	31	0	19	1	0
74	1G	1	0	0	0	0
74	5G	1	0	0	0	0
75	1L	76	0	99	3	0
75	1N	62	0	68	4	0
75	1X	86	0	125	12	0
75	1d	65	0	77	7	0
75	1i	80	0	104	8	0
75	1q	61	0	66	5	0
75	4B	100	0	156	6	0
75	4C	100	0	156	18	0
75	5L	76	0	99	2	0
75	5N	62	0	68	4	0
75	5X	86	0	125	13	0
75	5d	65	0	77	7	0
75	5i	80	0	104	9	0
75	5q	61	0	66	5	0
75	8A	100	0	156	28	0
75	8B	100	0	156	7	0
75	8D	100	0	156	19	0
76	1O	32	0	12	4	0
76	5O	32	0	12	5	0
77	1O	1	0	0	0	0
77	4A	1	0	0	0	0
77	5O	1	0	0	0	0
77	8A	1	0	0	0	0
78	1P	48	0	26	1	0
78	5P	48	0	26	1	0
79	1R	1	0	0	0	0
79	4F	1	0	0	0	0
79	5R	1	0	0	0	0
79	8F	1	0	0	0	0
80	1T	37	0	0	1	0
80	1n	37	0	0	1	0
80	5T	37	0	0	1	0
80	5n	37	0	0	1	0
81	1h	11	0	12	3	0
81	5h	11	0	12	3	0
82	1p	51	0	76	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
82	4A	204	0	304	30	0
82	4C	255	0	380	33	0
82	4G	51	0	76	8	0
82	4J	51	0	76	11	0
82	4K	51	0	76	7	0
82	4L	51	0	76	12	0
82	8A	204	0	304	46	0
82	8B	51	0	76	10	0
82	8C	255	0	380	39	0
82	8G	51	0	76	12	0
82	8J	51	0	76	11	0
82	8K	51	0	76	9	0
82	8L	51	0	76	7	0
83	3C	86	0	60	11	0
83	3P	86	0	60	6	0
83	6C	86	0	60	16	0
83	6P	86	0	60	6	0
84	3D	42	0	32	2	0
84	3Q	43	0	32	2	0
84	6D	42	0	32	5	0
84	6Q	43	0	32	2	0
85	4A	120	0	108	8	0
85	8A	120	0	108	16	0
86	4A	1	0	0	0	0
86	8A	1	0	0	0	0
87	4A	1	0	0	0	0
87	8A	1	0	0	0	0
88	4B	2	0	0	3	0
88	8B	2	0	0	0	0
89	4B	52	0	80	7	0
89	8A	52	0	80	7	0
90	4C	105	0	149	7	0
90	8C	105	0	149	9	0
91	4H	5	0	0	0	0
91	8H	5	0	0	0	0
All	All	233868	0	234967	9307	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (9307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:95:LYS:HG2	2:1B:96:MET:SD	1.25	1.68
45:3N:150:PHE:HE1	45:3N:310:PHE:CZ	1.11	1.66
45:6N:148:VAL:HG12	45:6N:152:TYR:CE2	1.17	1.65
45:3N:64:PHE:CE1	45:3N:86:LEU:HD13	1.24	1.63
2:1B:96:MET:HG3	4:1D:82:LEU:CD2	1.26	1.61
47:3C:154:PRO:HA	47:3C:158:THR:CB	1.23	1.57
45:6N:4:TYR:CZ	46:6O:112:LEU:HD13	1.36	1.57
45:6N:86:LEU:CD2	45:6N:99:ILE:HG12	1.32	1.57
49:6E:249:ILE:CG2	49:6E:257:ASN:HD22	1.19	1.56
45:6N:127:ILE:CD1	45:6N:179:ARG:CG	1.76	1.56
45:3N:148:VAL:HG12	45:3N:152:TYR:CE2	1.39	1.55
2:1B:92:LEU:C	2:1B:93:THR:CA	1.77	1.55
45:6N:25:VAL:CG1	45:6N:209:LEU:HD23	1.22	1.55
2:1B:57:VAL:C	2:1B:58:GLU:HA	1.18	1.54
45:6N:34:THR:HG22	45:6N:102:LEU:CD2	1.10	1.53
45:3N:29:GLN:HE21	45:3N:204:GLU:CA	1.22	1.53
45:6N:66:GLY:HA2	45:6N:75:LEU:CD1	1.11	1.53
45:3N:18:GLN:HE21	45:3N:24:ARG:CG	1.19	1.52
45:3N:25:VAL:CG2	45:3N:197:LEU:HD12	1.38	1.52
2:1B:57:VAL:C	2:1B:58:GLU:CA	1.76	1.51
49:3E:249:ILE:CG2	49:3E:257:ASN:HD22	1.19	1.51
45:3N:64:PHE:CZ	45:3N:86:LEU:HB3	1.47	1.50
45:3N:62:LEU:HD23	45:3N:65:LYS:CD	1.39	1.50
45:3N:64:PHE:CE1	45:3N:86:LEU:CD1	1.93	1.49
45:6N:185:TYR:HB3	45:6N:189:HIS:CD2	1.46	1.49
45:6N:66:GLY:CA	45:6N:75:LEU:HD12	1.03	1.49
45:3N:150:PHE:CE1	45:3N:310:PHE:CZ	2.00	1.46
2:1B:96:MET:CG	4:1D:82:LEU:CD2	1.94	1.46
2:1B:61:HIS:CE1	4:1D:171:PHE:CE2	2.04	1.45
45:3N:52:ASN:CG	45:3N:185:TYR:HE1	1.19	1.45
2:1B:95:LYS:CG	2:1B:96:MET:SD	2.05	1.44
45:3N:64:PHE:CD1	45:3N:86:LEU:HD13	1.49	1.44
45:3N:52:ASN:CG	45:3N:185:TYR:CE1	1.91	1.44
45:6N:58:PHE:CD1	45:6N:134:ILE:CD1	2.01	1.44
45:6N:148:VAL:CG1	45:6N:152:TYR:CE2	1.98	1.43
45:3N:18:GLN:NE2	45:3N:24:ARG:HG2	1.12	1.42
2:1B:61:HIS:ND1	4:1D:171:PHE:CD2	1.76	1.42
45:6N:127:ILE:CD1	45:6N:179:ARG:HG2	0.94	1.41
2:1B:96:MET:CG	4:1D:82:LEU:HD23	1.49	1.41
45:6N:105:ASP:C	45:6N:107:PRO:HD3	1.41	1.41
45:3N:29:GLN:NE2	45:3N:204:GLU:HA	1.36	1.39
45:6N:71:PRO:CD	45:6N:74:ALA:HB3	1.53	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:52:ASN:OD1	45:3N:185:TYR:CE1	1.71	1.39
45:3N:92:ARG:CZ	45:3N:165:GLN:O	1.70	1.38
2:1B:101:ARG:CD	2:1B:139:ILE:HG22	1.50	1.38
2:1B:92:LEU:CA	2:1B:93:THR:N	1.88	1.37
45:6N:105:ASP:O	45:6N:107:PRO:CD	1.72	1.36
38:1m:22:TYR:HB3	39:1n:64:ARG:NH2	1.39	1.35
38:5m:22:TYR:HB3	39:5n:64:ARG:NH2	1.39	1.35
45:6N:127:ILE:HD12	45:6N:179:ARG:CG	1.43	1.35
47:3C:154:PRO:CA	47:3C:158:THR:HB	1.57	1.34
45:6N:34:THR:CG2	45:6N:102:LEU:CD2	2.05	1.34
45:6N:33:PRO:HD2	46:6O:373:GLU:OE2	1.19	1.34
45:3N:52:ASN:OD1	45:3N:185:TYR:CZ	1.81	1.34
45:6N:148:VAL:CG1	45:6N:152:TYR:HE2	1.37	1.34
46:3O:24:LEU:HD21	46:3O:26:PHE:CD2	1.62	1.33
45:3N:159:GLN:CD	49:3R:85:VAL:HG11	1.50	1.33
2:1B:58:GLU:O	2:1B:61:HIS:N	1.61	1.33
45:3N:87:ASN:ND2	45:3N:100:LYS:HE3	1.43	1.33
45:6N:40:TRP:CZ2	45:6N:377:GLU:CA	1.77	1.33
45:6N:34:THR:CG2	45:6N:102:LEU:HD23	1.57	1.33
2:1B:60:MET:C	2:1B:61:HIS:HA	1.52	1.32
45:3N:118:GLN:NE2	45:3N:219:LEU:HD23	1.40	1.32
45:6N:42:ASP:OD2	45:6N:384:LEU:CD2	1.76	1.32
45:6N:118:GLN:HG3	45:6N:219:LEU:CD2	1.57	1.31
45:6N:40:TRP:HZ2	45:6N:377:GLU:CA	1.05	1.31
45:6N:4:TYR:CE1	46:6O:112:LEU:HD13	1.65	1.31
45:3N:62:LEU:CD2	45:3N:65:LYS:HD2	1.59	1.31
45:6N:105:ASP:O	45:6N:107:PRO:HD2	1.18	1.30
45:3N:60:GLU:HA	45:3N:97:TYR:OH	1.32	1.30
45:6N:40:TRP:CD1	45:6N:380:GLY:HA3	1.67	1.30
45:6N:186:VAL:HG13	45:6N:190:TYR:CD2	1.66	1.29
45:6N:87:ASN:ND2	45:6N:100:LYS:HE3	1.44	1.29
45:3N:25:VAL:HG22	45:3N:197:LEU:CD1	1.65	1.27
2:1B:57:VAL:O	2:1B:58:GLU:HA	1.32	1.27
45:6N:170:PRO:HG2	45:6N:173:ASN:CB	1.65	1.27
45:6N:4:TYR:OH	46:6O:112:LEU:HB3	1.35	1.27
45:6N:86:LEU:HD23	45:6N:99:ILE:CG1	1.64	1.26
45:3N:80:GLU:OE1	46:3O:292:THR:HG23	1.32	1.26
45:6N:118:GLN:CG	45:6N:219:LEU:CD2	2.12	1.26
45:6N:41:ILE:HD12	45:6N:97:TYR:CD2	1.69	1.26
45:6N:127:ILE:HD12	45:6N:179:ARG:CD	1.64	1.26
49:6E:249:ILE:HG22	49:6E:257:ASN:ND2	0.95	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:249:ILE:HG22	49:3E:257:ASN:ND2	0.95	1.25
45:3N:150:PHE:HE1	45:3N:310:PHE:CE2	1.53	1.25
45:6N:58:PHE:CE1	45:6N:134:ILE:CD1	2.20	1.25
2:1B:100:LEU:HG	2:1B:104:TYR:CE2	1.71	1.25
45:6N:29:GLN:HG2	45:6N:204:GLU:N	1.51	1.25
45:6N:42:ASP:OD2	45:6N:384:LEU:HD22	1.12	1.25
45:6N:25:VAL:CG1	45:6N:209:LEU:CD2	2.14	1.24
45:6N:42:ASP:OD1	45:6N:384:LEU:HD13	1.33	1.24
62:8H:39:CYS:SG	62:8H:53:CYS:HB3	1.77	1.24
2:1B:57:VAL:C	2:1B:58:GLU:N	1.93	1.23
49:3E:249:ILE:CG2	49:3E:257:ASN:ND2	1.83	1.23
45:3N:60:GLU:OE2	45:3N:90:SER:CB	1.84	1.23
45:6N:40:TRP:CZ2	45:6N:377:GLU:C	2.13	1.23
45:6N:86:LEU:CD2	45:6N:99:ILE:CG1	2.15	1.23
62:4H:39:CYS:SG	62:4H:53:CYS:HB3	1.77	1.23
45:6N:40:TRP:HZ2	45:6N:377:GLU:C	1.44	1.23
45:3N:148:VAL:CG1	45:3N:152:TYR:CE2	2.22	1.23
49:6E:249:ILE:CG2	49:6E:257:ASN:ND2	1.83	1.23
46:3B:95:LYS:NZ	49:3I:71:ASN:OD1	1.71	1.22
45:6N:58:PHE:CD1	45:6N:134:ILE:HD12	1.69	1.22
45:6N:118:GLN:CG	45:6N:219:LEU:HD23	1.65	1.22
2:1B:101:ARG:O	2:1B:103:VAL:N	1.71	1.22
45:3N:64:PHE:CE1	45:3N:86:LEU:HB3	1.73	1.22
45:6N:66:GLY:C	45:6N:75:LEU:HD11	1.65	1.22
45:3N:158:PHE:CE1	45:3N:163:LEU:HD13	1.73	1.22
48:6D:162:PRO:HA	48:6D:166:GLY:CA	1.69	1.21
45:6N:118:GLN:NE2	45:6N:218:SER:OG	1.72	1.21
45:3N:140:GLU:OE2	49:3V:50:LEU:N	1.69	1.21
2:1B:100:LEU:O	2:1B:104:TYR:CD2	1.93	1.21
48:6D:162:PRO:CA	48:6D:166:GLY:HA2	1.71	1.21
45:6N:67:THR:N	45:6N:75:LEU:HD11	1.52	1.21
45:6N:170:PRO:CG	45:6N:173:ASN:HB2	1.70	1.21
45:3N:64:PHE:CE1	45:3N:86:LEU:CB	2.24	1.20
45:6N:99:ILE:CD1	45:6N:113:LEU:HD21	1.71	1.20
45:3N:41:ILE:HG12	45:3N:195:MET:SD	1.80	1.20
27:5b:63:PRO:CB	27:5b:63:PRO:CD	1.95	1.20
45:3N:52:ASN:CB	45:3N:185:TYR:HE1	1.54	1.19
27:1b:63:PRO:CD	27:1b:63:PRO:CB	1.95	1.19
45:3N:69:ASN:ND2	45:3N:119:ASN:HD21	1.38	1.19
45:6N:156:THR:HA	45:6N:159:GLN:CG	1.73	1.19
45:3N:64:PHE:CD1	45:3N:86:LEU:CD1	2.12	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:65:LYS:HZ1	45:6N:130:GLU:HG3	1.06	1.18
2:1B:60:MET:C	2:1B:61:HIS:CA	2.16	1.18
2:1B:61:HIS:ND1	4:1D:171:PHE:CE2	2.02	1.18
2:1B:92:LEU:O	2:1B:93:THR:HA	1.37	1.18
45:6N:151:ASP:HA	45:6N:154:HIS:CD2	1.79	1.17
45:3N:25:VAL:CG2	45:3N:197:LEU:CD1	2.18	1.17
45:6N:29:GLN:HG2	45:6N:203:VAL:C	1.70	1.17
45:6N:185:TYR:CB	45:6N:189:HIS:CD2	2.28	1.17
2:1B:61:HIS:CE1	4:1D:171:PHE:CD2	2.29	1.17
45:3N:35:CYS:HA	45:3N:201:GLY:HA3	1.24	1.16
45:6N:66:GLY:CA	45:6N:75:LEU:CD1	1.84	1.16
45:6N:118:GLN:NE2	45:6N:219:LEU:H	1.42	1.16
2:1B:92:LEU:O	2:1B:93:THR:N	1.77	1.16
45:6A:383:LEU:HA	45:6A:387:GLY:HA2	1.18	1.16
46:6B:315:SER:HA	46:6B:320:GLY:HA2	1.17	1.16
45:3N:127:ILE:CD1	45:3N:179:ARG:HG2	1.73	1.16
27:5b:63:PRO:CB	27:5b:63:PRO:HD3	1.72	1.16
45:6A:444:LEU:HD12	45:6A:445:ARG:NH2	1.57	1.16
45:6N:38:GLY:HA3	45:6N:98:TYR:HA	1.18	1.16
45:6N:87:ASN:HD21	45:6N:100:LYS:CE	1.57	1.16
2:1B:101:ARG:CG	2:1B:139:ILE:HG22	1.76	1.15
45:6N:162:PRO:HD2	45:6N:163:LEU:H	1.02	1.15
45:6N:185:TYR:HB3	45:6N:189:HIS:NE2	1.59	1.15
45:6N:90:SER:HA	45:6N:95:THR:HA	1.15	1.15
45:6N:156:THR:HA	45:6N:159:GLN:HG3	1.24	1.15
45:3N:34:THR:HG22	45:3N:102:LEU:HD23	1.18	1.15
47:3C:154:PRO:CA	47:3C:158:THR:CB	2.20	1.14
45:6N:45:SER:HA	45:6N:167:VAL:HG21	1.24	1.14
45:3N:70:ARG:CZ	45:3N:78:GLU:OE1	1.94	1.14
45:6N:58:PHE:CE1	45:6N:134:ILE:HD13	1.79	1.14
45:6N:66:GLY:C	45:6N:75:LEU:CD1	2.19	1.14
45:3N:64:PHE:CZ	45:3N:86:LEU:CB	2.31	1.14
45:3N:60:GLU:CD	45:3N:90:SER:HB3	1.72	1.14
2:1B:100:LEU:CD2	2:1B:104:TYR:HE2	1.60	1.13
45:6N:4:TYR:CZ	46:6O:112:LEU:CD1	2.29	1.13
45:6N:105:ASP:C	45:6N:107:PRO:CD	2.15	1.13
45:3N:34:THR:HG22	45:3N:102:LEU:CD2	1.77	1.13
45:6N:40:TRP:CE2	45:6N:377:GLU:HA	1.83	1.13
2:1B:101:ARG:NE	2:1B:139:ILE:CG2	1.95	1.13
45:3N:313:CYS:HA	45:3N:318:GLY:CA	1.79	1.13
45:6N:58:PHE:CD1	45:6N:134:ILE:HD13	1.81	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:58:PHE:CZ	45:6N:174:VAL:HG22	1.81	1.13
45:3N:148:VAL:CG1	45:3N:152:TYR:HE2	1.57	1.12
45:6N:151:ASP:CA	45:6N:154:HIS:HD2	1.61	1.12
46:3B:154:ASN:ND2	46:3B:156:GLN:OE1	1.81	1.12
45:3N:36:THR:HG23	45:3N:372:THR:HB	1.24	1.12
45:6N:42:ASP:CG	45:6N:384:LEU:HD13	1.74	1.11
45:6N:71:PRO:HD3	45:6N:74:ALA:CB	1.80	1.11
45:3N:36:THR:CG2	45:3N:372:THR:HB	1.80	1.11
45:3N:70:ARG:HD2	45:3N:75:LEU:HD23	1.30	1.11
45:3N:170:PRO:HG2	45:3N:173:ASN:ND2	1.63	1.11
45:6N:304:CYS:HA	45:6N:326:CYS:HA	1.30	1.11
45:3N:193:PRO:HD2	45:3N:194:ARG:H	1.13	1.11
45:3N:150:PHE:CE1	45:3N:310:PHE:CE2	2.34	1.10
46:3O:39:GLU:HA	46:3O:210:GLY:HA2	1.19	1.10
45:6N:170:PRO:HG2	45:6N:173:ASN:HB2	1.14	1.10
45:3N:110:VAL:HG13	45:3N:216:PHE:CE2	1.86	1.10
46:3O:386:ALA:HA	46:3O:390:GLY:CA	1.80	1.10
2:1B:92:LEU:O	2:1B:93:THR:CA	1.86	1.10
45:6N:62:LEU:HD21	45:6N:127:ILE:HG13	1.34	1.10
2:1B:101:ARG:HD3	2:1B:140:VAL:CG1	1.81	1.10
45:3N:29:GLN:HE22	45:3N:204:GLU:CG	1.64	1.10
45:6A:309:THR:HA	45:6A:322:ALA:HA	1.21	1.10
45:3N:60:GLU:OE2	45:3N:90:SER:HB3	0.92	1.09
45:6A:34:THR:HA	45:6A:102:LEU:HA	1.11	1.09
45:6N:99:ILE:HD12	45:6N:113:LEU:HD21	1.29	1.09
45:6N:127:ILE:HD11	45:6N:179:ARG:HG2	1.11	1.09
45:6N:170:PRO:HG2	45:6N:173:ASN:CG	1.75	1.09
48:6D:157:GLU:HA	48:6D:172:PRO:HA	1.15	1.09
45:6N:127:ILE:HD12	45:6N:179:ARG:NE	1.67	1.09
45:3N:18:GLN:HG2	45:3N:24:ARG:HA	1.32	1.09
45:3N:29:GLN:NE2	45:3N:204:GLU:CA	2.01	1.09
45:6N:25:VAL:HG12	45:6N:209:LEU:HD23	1.27	1.09
45:6N:58:PHE:CE1	45:6N:174:VAL:HG13	1.88	1.09
45:3N:25:VAL:HG23	45:3N:197:LEU:HD12	1.24	1.08
10:5J:78:MET:HE2	10:5J:79:TYR:N	1.67	1.08
45:6N:156:THR:CA	45:6N:159:GLN:HG3	1.83	1.08
10:1J:78:MET:HE2	10:1J:79:TYR:N	1.67	1.08
45:3N:29:GLN:HG2	45:3N:203:VAL:O	1.50	1.08
65:8K:27:ALA:O	65:8K:31:TYR:CD2	2.04	1.08
2:1B:101:ARG:HD3	2:1B:140:VAL:HG12	1.35	1.08
38:1m:22:TYR:HB3	39:1n:64:ARG:CZ	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:58:PHE:CE1	45:6N:134:ILE:HD12	1.86	1.08
45:6N:70:ARG:HB2	45:6N:75:LEU:CD2	1.84	1.08
45:6A:66:GLY:HA3	45:6A:72:GLY:HA2	1.09	1.08
45:6N:34:THR:HA	45:6N:102:LEU:HA	1.34	1.08
45:6N:37:VAL:HG12	45:6N:38:GLY:H	1.16	1.08
45:6N:193:PRO:HD2	45:6N:194:ARG:H	1.13	1.08
45:6A:311:ASN:HA	45:6A:320:LEU:HA	1.22	1.08
55:8A:508:PRO:O	55:8A:509:THR:O	1.71	1.07
65:8K:27:ALA:O	65:8K:31:TYR:HD2	1.32	1.07
45:3N:42:ASP:HA	45:3N:94:HIS:ND1	1.45	1.07
47:6C:137:GLN:HA	47:6C:259:ALA:HA	1.37	1.07
2:1B:103:VAL:N	2:1B:104:TYR:N	1.86	1.07
45:3N:70:ARG:CD	45:3N:75:LEU:HD23	1.84	1.07
45:6N:40:TRP:CZ2	45:6N:377:GLU:HA	1.51	1.07
45:6N:65:LYS:NZ	45:6N:130:GLU:HG3	1.67	1.07
45:3N:34:THR:HA	45:3N:102:LEU:HA	1.31	1.07
38:5m:22:TYR:HB3	39:5n:64:ARG:CZ	1.83	1.07
48:6D:252:PRO:HB3	84:6D:501:HEC:HHC	1.36	1.07
45:6N:127:ILE:HD13	45:6N:179:ARG:HG2	1.08	1.07
45:6N:151:ASP:HA	45:6N:154:HIS:HD2	0.95	1.07
45:3N:110:VAL:HG13	45:3N:216:PHE:HE2	1.18	1.06
46:3O:386:ALA:CA	46:3O:390:GLY:HA2	1.85	1.06
45:6N:170:PRO:CG	45:6N:173:ASN:HD22	1.65	1.06
2:1B:61:HIS:CE1	4:1D:174:ARG:HE	1.73	1.06
45:3N:4:TYR:OH	46:3O:112:LEU:HB3	1.55	1.06
45:3N:69:ASN:ND2	45:3N:119:ASN:ND2	2.01	1.06
45:6N:4:TYR:HE2	46:6O:114:ASP:HB2	1.19	1.06
45:6N:71:PRO:HD3	45:6N:74:ALA:HB3	1.08	1.06
45:6N:170:PRO:HG2	45:6N:173:ASN:ND2	1.69	1.06
12:1L:559:GLU:OE2	13:1M:214:LEU:HD23	1.55	1.06
45:3N:158:PHE:CE1	45:3N:163:LEU:CD1	2.37	1.06
45:6N:66:GLY:CA	45:6N:72:GLY:HA2	1.85	1.06
45:6N:33:PRO:CD	46:6O:373:GLU:OE2	2.04	1.06
45:3N:29:GLN:HE22	45:3N:204:GLU:HG2	0.94	1.05
45:6N:4:TYR:OH	46:6O:112:LEU:CB	2.03	1.05
45:6N:71:PRO:CD	45:6N:74:ALA:CB	2.34	1.05
2:1B:96:MET:HG2	4:1D:82:LEU:HD23	1.37	1.05
45:3N:64:PHE:CE1	45:3N:86:LEU:CG	2.39	1.05
45:3N:353:GLU:HA	45:3N:356:ARG:HB3	1.31	1.05
46:6O:313:ASN:HA	46:6O:322:PHE:HA	1.31	1.05
2:1B:101:ARG:CD	2:1B:140:VAL:HG13	1.87	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:18:GLN:NE2	45:3N:24:ARG:CG	1.93	1.05
45:3N:133:VAL:HG13	49:3V:51:CYS:SG	1.96	1.05
2:1B:97:ALA:O	2:1B:99:ALA:N	1.88	1.04
45:3N:58:PHE:HA	45:3N:61:HIS:HD2	1.08	1.04
12:5L:559:GLU:OE2	13:5M:214:LEU:HD23	1.55	1.04
45:3N:159:GLN:CG	49:3R:85:VAL:HG11	1.88	1.04
45:6N:309:THR:HA	45:6N:322:ALA:HA	1.35	1.04
45:3N:80:GLU:OE1	46:3O:292:THR:CG2	2.05	1.04
45:6N:40:TRP:NE1	45:6N:377:GLU:O	1.91	1.04
45:6N:66:GLY:HA3	45:6N:72:GLY:HA2	1.04	1.04
45:6N:118:GLN:HE21	45:6N:219:LEU:N	1.54	1.04
45:3N:14:THR:HG22	45:3N:28:GLU:HG3	1.07	1.03
45:6N:16:VAL:HA	45:6N:26:ALA:HA	1.37	1.03
27:1b:63:PRO:CB	27:1b:63:PRO:HD3	1.72	1.03
45:6N:34:THR:HG22	45:6N:102:LEU:HD21	1.39	1.03
45:6N:118:GLN:HG2	45:6N:219:LEU:HD23	1.07	1.03
45:3N:58:PHE:HA	45:3N:61:HIS:CD2	1.92	1.03
45:6A:66:GLY:CA	45:6A:72:GLY:HA2	1.89	1.03
45:3N:313:CYS:CA	45:3N:318:GLY:HA2	1.89	1.03
45:3N:29:GLN:NE2	45:3N:204:GLU:CG	2.20	1.02
45:3N:29:GLN:HG2	45:3N:203:VAL:C	1.84	1.02
46:3O:24:LEU:CD2	46:3O:26:PHE:HD2	1.71	1.02
45:6N:170:PRO:HG3	45:6N:173:ASN:HD22	1.20	1.02
2:1B:101:ARG:NE	2:1B:139:ILE:HG22	1.32	1.02
2:1B:101:ARG:HG3	2:1B:139:ILE:CG2	1.90	1.02
45:3N:14:THR:CG2	45:3N:28:GLU:HG3	1.89	1.02
45:6N:40:TRP:CE2	45:6N:377:GLU:O	2.12	1.02
45:6N:158:PHE:CZ	45:6N:236:PHE:CD1	2.41	1.02
2:1B:119:CYS:SG	70:1B:201:SF4:FE4	1.51	1.02
2:1B:100:LEU:CG	2:1B:104:TYR:HE2	1.72	1.01
45:3N:159:GLN:NE2	49:3R:85:VAL:HG11	1.76	1.01
45:3N:170:PRO:CG	45:3N:173:ASN:HD22	1.73	1.01
45:6N:4:TYR:HH	46:6O:112:LEU:HB3	1.03	1.01
45:6N:170:PRO:CD	45:6N:173:ASN:HB2	1.88	1.01
45:3N:29:GLN:NE2	45:3N:204:GLU:HG2	1.74	1.01
45:3N:64:PHE:HE1	45:3N:86:LEU:CG	1.74	1.01
49:3E:151:LYS:HG3	49:3E:152:ILE:HD13	1.43	1.01
45:6N:27:SER:HB2	45:6N:208:LEU:HD12	1.41	1.01
45:6N:118:GLN:HG3	45:6N:219:LEU:HD21	1.04	1.01
45:6N:186:VAL:HG13	45:6N:190:TYR:HD2	1.25	1.01
45:3N:64:PHE:HE1	45:3N:86:LEU:CD1	1.51	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6A:66:GLY:HA3	45:6A:72:GLY:CA	1.91	1.01
45:6N:158:PHE:CE2	45:6N:236:PHE:HD1	1.78	1.01
46:6B:376:GLU:OE1	46:6B:379:LEU:CD2	2.08	1.00
46:3B:120:MET:HE3	46:3B:219:VAL:HG21	1.43	1.00
45:3N:118:GLN:NE2	45:3N:219:LEU:CD2	2.24	1.00
45:3N:162:PRO:HD2	45:3N:163:LEU:H	1.24	1.00
45:6N:4:TYR:CD2	46:6O:114:ASP:OD2	2.15	1.00
39:1n:55:ASP:HB3	39:1n:58:LYS:HE2	1.40	1.00
45:6N:4:TYR:CE2	46:6O:114:ASP:CG	2.40	1.00
45:3N:127:ILE:HD12	45:3N:179:ARG:CG	1.92	1.00
45:6N:140:GLU:OE2	49:6V:50:LEU:N	1.95	1.00
45:6N:66:GLY:HA3	45:6N:72:GLY:CA	1.91	0.99
45:3N:14:THR:HG22	45:3N:28:GLU:CG	1.90	0.99
49:6E:151:LYS:HG3	49:6E:152:ILE:HD13	1.43	0.99
45:3N:159:GLN:NE2	49:3R:85:VAL:CG1	2.25	0.99
45:3N:41:ILE:HD11	45:3N:195:MET:HE1	1.40	0.99
45:3N:64:PHE:HZ	45:3N:86:LEU:HB3	1.24	0.99
39:5n:55:ASP:HB3	39:5n:58:LYS:HE2	1.40	0.99
45:3N:118:GLN:HE21	45:3N:219:LEU:HD23	0.83	0.99
62:4H:14:ALA:HB3	62:4H:63:PHE:HE1	1.28	0.98
45:3N:158:PHE:CD1	45:3N:163:LEU:HD12	1.98	0.98
46:3O:315:SER:HA	46:3O:320:GLY:HA2	1.44	0.98
45:6N:66:GLY:HA2	45:6N:75:LEU:CG	1.92	0.98
45:6N:99:ILE:HD12	45:6N:113:LEU:CD2	1.92	0.98
45:6N:29:GLN:CG	45:6N:203:VAL:C	2.35	0.98
45:3N:170:PRO:CG	45:3N:173:ASN:ND2	2.26	0.98
45:3N:186:VAL:HA	45:3N:190:TYR:HD2	1.27	0.98
45:6N:4:TYR:HE2	46:6O:114:ASP:CB	1.76	0.97
45:6N:37:VAL:HG12	45:6N:38:GLY:N	1.76	0.97
4:1D:21:PRO:CD	4:1D:21:PRO:N	2.25	0.97
45:3N:309:THR:HA	45:3N:322:ALA:HA	1.41	0.97
21:1V:65:LYS:O	21:1V:69:GLU:OE2	1.82	0.97
45:3N:42:ASP:CA	45:3N:94:HIS:ND1	2.16	0.97
45:6N:170:PRO:CG	45:6N:173:ASN:ND2	2.23	0.97
2:1B:100:LEU:CG	2:1B:104:TYR:CE2	2.43	0.97
45:6N:58:PHE:HZ	45:6N:174:VAL:HG22	1.15	0.97
45:3N:92:ARG:NE	45:3N:165:GLN:O	1.97	0.97
2:1B:100:LEU:HD23	2:1B:101:ARG:HG2	1.43	0.97
45:3N:70:ARG:HD2	45:3N:75:LEU:CD2	1.94	0.97
45:3N:79:VAL:HG22	45:3N:112:LEU:HD13	1.43	0.97
45:3N:118:GLN:HE21	45:3N:219:LEU:CD2	1.77	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:508:PRO:O	60:8F:56:ARG:NH2	1.98	0.97
21:5V:65:LYS:O	21:5V:69:GLU:OE2	1.82	0.97
41:5p:166:ARG:HG2	41:5p:170:LYS:HE2	1.47	0.97
45:6N:99:ILE:CD1	45:6N:113:LEU:CD2	2.43	0.97
30:1e:53:LYS:HE3	30:1e:54:GLU:HG3	1.45	0.97
38:1m:22:TYR:CB	39:1n:64:ARG:NH2	2.28	0.96
41:1p:166:ARG:HG2	41:1p:170:LYS:HE2	1.47	0.96
45:3N:35:CYS:SG	45:3N:203:VAL:HG23	2.05	0.96
38:5m:22:TYR:CB	39:5n:64:ARG:NH2	2.28	0.96
45:3N:92:ARG:CZ	45:3N:165:GLN:C	2.38	0.96
45:3N:46:ARG:NE	45:3N:163:LEU:CD2	2.28	0.96
45:3N:140:GLU:CD	49:3V:50:LEU:H	1.71	0.96
2:1B:58:GLU:O	2:1B:60:MET:N	1.98	0.96
45:6N:29:GLN:CG	45:6N:204:GLU:N	2.26	0.96
45:3N:24:ARG:HD2	45:3N:196:VAL:HG22	1.48	0.96
45:6A:444:LEU:HD12	45:6A:445:ARG:HH22	1.29	0.96
55:8A:4:ASN:HA	55:8A:8:TYR:HB2	1.46	0.96
46:6O:213:HIS:HB3	46:6O:217:LYS:HZ2	1.29	0.95
62:8H:39:CYS:SG	62:8H:53:CYS:CB	2.54	0.95
2:1B:61:HIS:HE1	4:1D:171:PHE:CE2	1.75	0.95
38:1m:22:TYR:HB3	39:1n:64:ARG:HH21	1.19	0.95
45:3N:87:ASN:HD22	45:3N:100:LYS:HE3	1.22	0.95
45:3N:52:ASN:OD1	45:3N:185:TYR:OH	1.82	0.95
53:6J:59:LYS:NZ	53:6J:60:TYR:HB3	1.81	0.95
45:3N:29:GLN:HE21	45:3N:204:GLU:HA	0.80	0.95
45:3N:313:CYS:HA	45:3N:318:GLY:HA2	0.96	0.95
45:6N:40:TRP:HD1	45:6N:380:GLY:HA3	1.31	0.95
45:6N:158:PHE:CZ	45:6N:236:PHE:HD1	1.68	0.95
2:1B:119:CYS:HA	2:1B:123:GLY:HA2	1.47	0.95
45:6N:13:GLU:O	45:6N:28:GLU:HG2	1.66	0.95
45:6N:185:TYR:HD1	45:6N:189:HIS:HE2	1.12	0.95
2:1B:100:LEU:CD2	2:1B:104:TYR:CE2	2.50	0.95
45:6N:25:VAL:HG11	45:6N:209:LEU:CD2	1.84	0.95
48:6D:157:GLU:HA	48:6D:172:PRO:CA	1.97	0.95
45:6N:15:GLN:HB2	45:6N:205:HIS:ND1	1.82	0.95
45:6N:25:VAL:HG11	45:6N:209:LEU:HD23	0.96	0.95
46:3B:95:LYS:NZ	49:3I:70:LEU:O	2.00	0.94
45:3N:87:ASN:ND2	45:3N:100:LYS:CE	2.29	0.94
47:3C:244:LEU:HA	48:3D:290:ARG:HG2	1.46	0.94
62:4H:39:CYS:SG	62:4H:53:CYS:CB	2.54	0.94
45:6N:4:TYR:CE2	46:6O:114:ASP:HB2	2.01	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:257:LEU:HD11	46:3O:422:LYS:HB3	1.48	0.94
30:5e:53:LYS:HE3	30:5e:54:GLU:HG3	1.46	0.94
45:6N:436:ARG:HD3	47:6P:222:PRO:HD3	1.48	0.94
45:6N:122:LEU:HD13	45:6N:183:THR:HG22	1.49	0.94
45:6N:185:TYR:C	45:6N:189:HIS:HD2	1.75	0.94
45:3N:158:PHE:CD1	45:3N:163:LEU:CD1	2.50	0.94
45:6N:58:PHE:HZ	45:6N:174:VAL:CG2	1.80	0.94
45:6N:90:SER:CA	45:6N:95:THR:HA	1.96	0.94
2:1B:96:MET:CG	4:1D:82:LEU:HD22	1.81	0.94
45:6N:349:ALA:HB2	45:6N:408:ARG:HB2	1.49	0.94
2:1B:52:LEU:HD13	2:1B:92:LEU:HD23	1.48	0.94
45:3N:40:TRP:CZ2	45:3N:377:GLU:HG3	2.02	0.94
45:3N:350:THR:HB	54:3X:9:ARG:HD2	1.50	0.94
45:6A:307:PHE:HA	45:6A:324:PHE:HA	1.46	0.94
45:6N:4:TYR:CE1	46:6O:112:LEU:CD1	2.49	0.94
62:8H:14:ALA:HB3	62:8H:63:PHE:HE1	1.28	0.94
45:3N:159:GLN:HG2	49:3R:85:VAL:HG21	1.50	0.94
45:6N:111:GLU:OE2	45:6N:215:HIS:CE1	2.12	0.93
39:5n:118:PHE:O	39:5n:122:GLU:HG2	1.69	0.93
39:1n:118:PHE:O	39:1n:122:GLU:HG2	1.69	0.93
45:3N:61:HIS:CE1	45:3N:134:ILE:HG12	2.04	0.93
2:1B:101:ARG:CD	2:1B:140:VAL:CG1	2.46	0.93
46:3B:95:LYS:HD2	49:3I:32:ALA:HB2	1.50	0.93
45:6N:69:ASN:ND2	45:6N:119:ASN:HD22	1.66	0.93
45:6N:162:PRO:HD2	45:6N:163:LEU:N	1.80	0.93
46:3O:78:LYS:HB2	46:3O:129:ALA:HB1	1.50	0.93
45:6N:34:THR:HG22	45:6N:102:LEU:HD22	1.47	0.93
2:1B:96:MET:HG3	4:1D:82:LEU:HD22	0.95	0.93
45:6N:148:VAL:O	45:6N:152:TYR:CD2	2.22	0.93
56:4B:196:CYS:HG	88:4B:302:CUA:CU2	0.70	0.93
45:6N:127:ILE:HD13	45:6N:179:ARG:CG	1.66	0.93
45:3N:36:THR:OG1	45:3N:200:ALA:HB3	1.68	0.92
45:6A:155:ALA:HA	45:6A:164:ALA:HA	1.51	0.92
48:6D:113:SER:HB3	48:6D:274:ASP:HA	1.48	0.92
45:3N:71:PRO:HD2	45:3N:72:GLY:H	1.32	0.92
55:8A:488:THR:HA	55:8A:491:ASN:HB2	1.50	0.92
4:5D:21:PRO:N	4:5D:21:PRO:CD	2.25	0.92
47:3C:154:PRO:HA	47:3C:158:THR:OG1	1.68	0.92
45:3N:127:ILE:HD12	45:3N:179:ARG:HG2	1.51	0.92
45:6N:185:TYR:HB3	45:6N:189:HIS:HD2	1.29	0.92
45:3N:133:VAL:HG11	49:3V:53:GLU:HG3	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:57:TYR:CE2	45:3N:167:VAL:CG1	2.20	0.92
49:6E:155:LYS:HZ1	49:6E:176:VAL:HG11	1.34	0.92
2:1B:102:LYS:C	2:1B:104:TYR:N	2.27	0.92
2:1B:100:LEU:O	2:1B:104:TYR:N	1.96	0.91
45:3N:159:GLN:CD	49:3R:85:VAL:CG1	2.41	0.91
45:3N:127:ILE:CD1	45:3N:179:ARG:CG	2.46	0.91
38:5m:22:TYR:HB3	39:5n:64:ARG:HH21	1.19	0.91
45:6N:162:PRO:CD	45:6N:163:LEU:H	1.83	0.91
45:3N:35:CYS:CA	45:3N:201:GLY:HA3	2.00	0.91
45:3N:40:TRP:HZ2	45:3N:377:GLU:HG3	1.33	0.91
46:3O:39:GLU:HA	46:3O:210:GLY:CA	2.00	0.91
45:6N:37:VAL:CG1	45:6N:38:GLY:H	1.84	0.91
45:3N:191:LYS:HD3	45:3N:223:TYR:OH	1.67	0.91
45:6N:58:PHE:CZ	45:6N:134:ILE:HG21	2.04	0.91
2:1B:94:ASN:O	2:1B:97:ALA:HB3	1.71	0.91
47:3C:137:GLN:HG2	47:3C:260:ASN:H	1.35	0.90
45:6N:65:LYS:HE3	45:6N:130:GLU:OE2	1.71	0.90
45:3N:64:PHE:CD1	45:3N:86:LEU:HD12	2.03	0.90
45:3N:58:PHE:CA	45:3N:61:HIS:HD2	1.84	0.90
45:6N:106:LEU:N	45:6N:107:PRO:HD3	1.86	0.90
45:6N:185:TYR:C	45:6N:189:HIS:CD2	2.50	0.90
45:3N:44:GLY:HA3	45:3N:92:ARG:HA	1.52	0.90
12:5L:484:LEU:HD13	12:5L:488:MET:HE2	1.54	0.90
45:6N:70:ARG:HB2	45:6N:75:LEU:HD23	1.50	0.90
38:1m:22:TYR:CB	39:1n:64:ARG:HH21	1.85	0.90
45:6N:71:PRO:HD2	45:6N:74:ALA:HB3	1.51	0.89
45:6N:181:ASP:HB3	45:6N:185:TYR:HE2	1.34	0.89
56:4B:200:CYS:HG	88:4B:302:CUA:CU1	0.61	0.89
45:6N:64:PHE:HZ	45:6N:88:ALA:HB3	1.38	0.89
45:3N:193:PRO:HD2	45:3N:194:ARG:N	1.86	0.89
45:3N:8:LEU:HD13	45:3N:393:ALA:HA	1.52	0.89
2:1B:68:ASP:HB3	2:1B:71:ARG:HB2	1.53	0.89
45:6N:42:ASP:OD1	45:6N:384:LEU:CD1	2.20	0.89
2:1B:101:ARG:HG3	2:1B:139:ILE:HG22	1.50	0.89
48:6D:111:HIS:HA	48:6D:114:ILE:HG13	1.54	0.89
47:3C:71:ARG:HG2	48:3D:285:PRO:HG2	1.53	0.89
45:3N:46:ARG:HE	45:3N:163:LEU:CD2	1.86	0.89
38:5m:22:TYR:CB	39:5n:64:ARG:HH21	1.85	0.89
45:3N:92:ARG:NH1	45:3N:165:GLN:O	2.05	0.89
49:6R:219:HIS:CD2	49:6R:239:HIS:CE1	2.61	0.89
2:1B:52:LEU:HD13	2:1B:92:LEU:CD2	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:127:ILE:HD11	45:3N:179:ARG:HG2	1.54	0.88
45:6N:159:GLN:HE22	45:6N:241:ILE:HG13	1.37	0.88
55:8A:103:TRP:HB3	57:8C:21:ALA:HB2	1.55	0.88
45:3N:87:ASN:HD21	45:3N:100:LYS:HE3	1.30	0.88
45:6N:118:GLN:CG	45:6N:219:LEU:HD21	1.91	0.88
12:1L:600:THR:HG22	12:1L:601:LEU:H	1.37	0.88
32:1g:37:LEU:HD22	32:1g:40:LYS:HZ1	1.38	0.88
46:6B:376:GLU:OE1	46:6B:379:LEU:HD23	1.73	0.88
45:6N:27:SER:O	45:6N:205:HIS:CE1	2.25	0.88
45:3N:156:THR:HG21	45:3N:423:ALA:HB2	1.55	0.88
47:6C:324:LEU:HD13	47:6C:366:MET:HA	1.53	0.88
45:6N:25:VAL:CB	45:6N:209:LEU:HD23	2.04	0.88
12:1L:484:LEU:HD13	12:1L:488:MET:HE2	1.54	0.88
49:3R:219:HIS:CD2	49:3R:239:HIS:CE1	2.61	0.88
82:4C:302:PGV:H21	82:4C:302:PGV:H92	1.56	0.88
48:6D:135:ALA:HA	48:6D:178:TYR:HA	1.56	0.88
45:6N:41:ILE:O	45:6N:95:THR:OG1	1.90	0.88
2:1B:36:LEU:HA	2:1B:39:TRP:HB2	1.54	0.88
2:1B:94:ASN:O	2:1B:97:ALA:CB	2.21	0.88
12:5L:600:THR:HG22	12:5L:601:LEU:H	1.37	0.88
52:6H:97:LYS:O	52:6H:97:LYS:HD3	1.73	0.88
45:6N:193:PRO:HD2	45:6N:194:ARG:N	1.88	0.88
45:3N:191:LYS:CD	45:3N:223:TYR:OH	2.22	0.88
14:1N:238:PRO:HB2	69:1N:902:3PE:H31	1.54	0.88
45:3N:86:LEU:HD23	45:3N:99:ILE:HG12	1.56	0.88
52:3H:54:LYS:HA	52:3H:57:LYS:HE2	1.54	0.88
45:3N:36:THR:CG2	45:3N:372:THR:CB	2.53	0.88
45:3N:445:ARG:HE	45:3N:445:ARG:H	1.22	0.88
46:6O:180:ASP:HA	46:6O:183:ILE:HD12	1.56	0.88
41:1p:166:ARG:O	41:1p:170:LYS:CD	2.22	0.87
41:5p:166:ARG:O	41:5p:170:LYS:CD	2.22	0.87
45:6N:42:ASP:OD2	45:6N:384:LEU:CD1	2.23	0.87
55:8A:52:GLN:H	56:8B:202:SER:HA	1.37	0.87
36:5k:68:LYS:O	36:5k:72:TRP:HD1	1.57	0.87
46:6B:315:SER:HA	46:6B:320:GLY:CA	2.02	0.87
45:6A:363:ASN:HA	46:6B:112:LEU:HD21	1.55	0.87
2:1B:92:LEU:C	2:1B:93:THR:N	0.77	0.87
50:3F:119:TRP:HZ3	46:3O:91:ALA:HB3	1.39	0.87
45:3N:170:PRO:HG2	45:3N:173:ASN:CG	1.98	0.87
55:8A:64:VAL:HA	55:8A:68:PHE:HB2	1.54	0.87
45:6N:118:GLN:HE21	45:6N:219:LEU:H	0.94	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6D:129:HIS:HB2	48:6D:201:LEU:HG	1.56	0.87
49:6E:151:LYS:HG3	49:6E:152:ILE:CD1	2.05	0.87
45:6N:14:THR:HG22	45:6N:28:GLU:CG	2.04	0.87
52:3H:58:ALA:HA	52:3H:61:ARG:HE	1.40	0.87
45:3N:34:THR:CG2	45:3N:102:LEU:HD23	2.05	0.87
45:3N:152:TYR:O	45:3N:156:THR:HG23	1.74	0.87
45:6N:133:VAL:HG13	49:6V:51:CYS:SG	2.15	0.87
45:6N:148:VAL:CG1	45:6N:152:TYR:CZ	2.57	0.87
45:6N:350:THR:HB	54:6X:9:ARG:HD2	1.55	0.87
45:3N:72:GLY:HA2	45:3N:75:LEU:HD12	1.57	0.86
46:3O:37:SER:HB2	46:3O:211:VAL:HG13	1.56	0.86
49:3E:151:LYS:HG3	49:3E:152:ILE:CD1	2.05	0.86
45:3N:23:LEU:HD21	45:3N:219:LEU:HD12	1.57	0.86
14:5N:238:PRO:HB2	69:5N:902:3PE:H31	1.54	0.86
2:1B:61:HIS:ND1	4:1D:171:PHE:HD2	1.34	0.86
45:3N:83:GLY:HA2	46:3O:284:HIS:HE1	1.39	0.86
35:5j:37:LEU:HD13	36:5k:77:PHE:HB3	1.57	0.86
45:6N:87:ASN:HD21	45:6N:100:LYS:HE3	0.71	0.86
55:8A:179:TYR:HA	55:8A:186:TRP:HE1	1.39	0.86
13:1M:305:THR:HG22	13:1M:308:SER:H	1.40	0.86
45:3N:29:GLN:HE21	45:3N:204:GLU:N	1.74	0.86
45:3N:58:PHE:CZ	45:3N:174:VAL:HG13	2.09	0.86
13:5M:305:THR:HG22	13:5M:308:SER:H	1.40	0.86
47:6C:24:PRO:HA	47:6C:217:LYS:HA	1.58	0.86
45:6N:67:THR:N	45:6N:75:LEU:CD1	2.35	0.86
45:6N:70:ARG:CB	45:6N:75:LEU:HD23	2.06	0.86
45:3N:150:PHE:CE1	45:3N:310:PHE:HZ	1.61	0.86
56:4B:200:CYS:SG	88:4B:302:CUA:CU2	1.66	0.86
45:6N:19:LEU:HD12	45:6N:23:LEU:HD12	1.58	0.86
45:6N:58:PHE:HA	45:6N:61:HIS:HD2	1.40	0.86
6:5F:93:LEU:HD13	6:5F:129:MET:HE1	1.57	0.86
45:6N:118:GLN:NE2	45:6N:219:LEU:N	2.17	0.86
12:1L:484:LEU:HD12	82:4J:101:PGV:H011	1.58	0.86
24:1Y:94:CYS:HB2	24:1Y:114:CYS:CA	2.06	0.86
24:5Y:94:CYS:HB2	24:5Y:114:CYS:CA	2.06	0.86
45:6N:58:PHE:CZ	45:6N:174:VAL:HG13	2.10	0.86
55:8A:169:ILE:HG23	75:8A:610:CDL:HA62	1.57	0.86
32:5g:37:LEU:HD22	32:5g:40:LYS:HZ1	1.38	0.86
45:3N:52:ASN:CB	45:3N:185:TYR:CE1	2.45	0.85
45:6N:66:GLY:N	45:6N:75:LEU:HD12	1.91	0.85
45:3N:260:PRO:HB2	45:3N:264:ASN:HB3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:4:TYR:CE2	46:6O:114:ASP:OD2	2.29	0.85
45:6N:25:VAL:HG11	45:6N:209:LEU:HA	1.55	0.85
45:6N:93:GLU:OE1	45:6N:315:ALA:HB2	1.74	0.85
45:6N:261:GLY:HA2	45:6N:317:THR:HA	1.57	0.85
2:1B:60:MET:O	2:1B:61:HIS:HA	1.76	0.85
45:6N:35:CYS:SG	45:6N:202:GLY:N	2.49	0.85
45:6N:42:ASP:CG	45:6N:384:LEU:CD1	2.49	0.85
46:3O:24:LEU:CD2	46:3O:26:PHE:CD2	2.50	0.85
47:6C:344:GLU:HB3	51:6G:68:PHE:CE1	2.12	0.85
45:6N:40:TRP:CD1	45:6N:380:GLY:CA	2.58	0.85
49:3E:155:LYS:HZ1	49:3E:176:VAL:HG11	1.42	0.85
45:6A:34:THR:HA	45:6A:102:LEU:CA	2.04	0.85
55:8A:194:LEU:HB3	55:8A:245:ILE:HD11	1.59	0.85
45:3N:76:GLU:CD	46:3O:289:SER:OG	2.20	0.85
45:3N:87:ASN:HD21	45:3N:100:LYS:CE	1.85	0.85
45:6N:52:ASN:HA	45:6N:185:TYR:CZ	2.08	0.85
45:6N:170:PRO:HD2	45:6N:173:ASN:HB2	1.59	0.85
2:1B:52:LEU:CD1	2:1B:92:LEU:HD21	2.07	0.85
12:5L:484:LEU:CD1	12:5L:488:MET:HE2	2.07	0.85
45:6N:62:LEU:HD21	45:6N:127:ILE:CG1	2.07	0.85
2:1B:47:PRO:HB3	2:1B:85:VAL:HG23	1.59	0.85
12:1L:484:LEU:CD1	12:1L:488:MET:HE2	2.07	0.85
46:6B:313:ASN:HA	46:6B:322:PHE:HA	1.56	0.85
55:8A:82:LEU:HB3	55:8A:86:MET:HG3	1.58	0.85
47:3C:377:LEU:HD11	50:3F:38:PHE:HE2	1.40	0.84
46:6B:277:HIS:HB3	46:6B:363:LYS:HD3	1.59	0.84
45:6N:29:GLN:HG3	45:6N:203:VAL:O	1.77	0.84
45:6N:41:ILE:CD1	45:6N:97:TYR:CD2	2.59	0.84
45:3N:64:PHE:HD1	45:3N:86:LEU:CD1	1.90	0.84
47:6C:19:ILE:HG23	47:6C:221:HIS:HB2	1.58	0.84
45:6N:156:THR:HA	45:6N:159:GLN:CD	2.02	0.84
45:3N:18:GLN:CG	45:3N:24:ARG:HA	2.08	0.84
46:3O:96:LEU:HG	49:3V:70:LEU:HB2	1.59	0.84
7:5G:139:ASP:OD1	7:5G:149:ILE:HA	1.76	0.84
45:6A:383:LEU:CA	45:6A:387:GLY:HA2	2.06	0.84
45:6N:42:ASP:OD2	45:6N:384:LEU:CG	2.24	0.84
45:6N:86:LEU:CD2	45:6N:99:ILE:CD1	2.56	0.84
46:6B:312:PHE:HA	49:6I:61:GLY:HA2	1.58	0.84
45:6N:245:ASP:HA	51:6T:11:ARG:HA	1.60	0.84
7:1G:110:GLN:HG3	7:1G:114:CYS:HA	1.58	0.84
45:3N:62:LEU:HD23	45:3N:65:LYS:CE	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:62:LEU:CD2	45:3N:65:LYS:CD	2.30	0.84
45:6N:127:ILE:HD12	45:6N:179:ARG:HE	1.42	0.84
46:6B:29:LEU:HB2	46:6B:33:LEU:HB3	1.59	0.84
45:6N:25:VAL:CB	45:6N:209:LEU:CD2	2.55	0.84
45:6N:18:GLN:HG2	45:6N:24:ARG:CG	2.08	0.84
45:6N:40:TRP:CZ2	45:6N:377:GLU:O	2.28	0.84
7:1G:139:ASP:OD1	7:1G:149:ILE:HA	1.76	0.84
12:1L:559:GLU:OE2	13:1M:214:LEU:CD2	2.25	0.84
35:1j:23:ILE:HG21	65:8K:16:ALA:HB2	1.60	0.84
47:3C:52:ALA:HA	47:3C:55:TYR:HB3	1.59	0.84
45:3N:41:ILE:CG1	45:3N:195:MET:SD	2.64	0.84
45:6N:60:GLU:O	45:6N:64:PHE:CD2	2.31	0.84
2:1B:95:LYS:CB	2:1B:96:MET:SD	2.56	0.83
2:1B:101:ARG:NE	2:1B:140:VAL:HG13	1.92	0.83
6:1F:125:GLY:C	6:1F:129:MET:HE3	2.02	0.83
45:3N:35:CYS:SG	45:3N:202:GLY:N	2.51	0.83
45:6N:80:GLU:OE1	46:6O:292:THR:HG23	1.76	0.83
45:6N:38:GLY:CA	45:6N:98:TYR:HA	2.07	0.83
24:1Y:81:GLU:N	24:1Y:81:GLU:OE2	2.11	0.83
45:3N:162:PRO:HD2	45:3N:163:LEU:N	1.91	0.83
45:6N:242:ARG:HA	45:6N:424:GLY:HA3	1.60	0.83
6:1F:93:LEU:HD13	6:1F:129:MET:HE1	1.57	0.83
47:3C:26:ASN:HA	50:3F:82:MET:HA	1.60	0.83
62:4H:14:ALA:HB3	62:4H:63:PHE:CE1	2.14	0.83
24:5Y:81:GLU:N	24:5Y:81:GLU:OE2	2.11	0.83
45:6N:153:LEU:HA	45:6N:156:THR:OG1	1.78	0.83
45:3N:181:ASP:HB3	45:3N:185:TYR:HE2	1.39	0.83
7:5G:110:GLN:HG3	7:5G:114:CYS:HA	1.58	0.83
45:6N:14:THR:HG22	45:6N:28:GLU:CD	2.03	0.83
45:6N:185:TYR:CA	45:6N:189:HIS:CD2	2.60	0.83
12:5L:559:GLU:OE2	13:5M:214:LEU:CD2	2.25	0.83
45:6N:39:VAL:HG11	45:6N:195:MET:HE3	1.60	0.83
45:6N:134:ILE:HA	45:6N:137:GLU:HB2	1.60	0.83
48:6Q:10:TYR:O	48:6Q:15:ARG:NH1	2.12	0.83
49:6R:205:VAL:HB	49:6R:211:VAL:HG23	1.61	0.83
2:1B:96:MET:SD	4:1D:82:LEU:HD23	2.18	0.83
53:6J:44:TYR:HA	53:6J:47:ILE:HB	1.60	0.83
45:3N:181:ASP:HB3	45:3N:185:TYR:CE2	2.14	0.83
45:6N:14:THR:HG22	45:6N:28:GLU:HG3	1.58	0.83
6:5F:125:GLY:C	6:5F:129:MET:HE3	2.02	0.83
47:3C:121:PHE:HA	47:3C:124:MET:HE2	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3Q:10:TYR:O	48:3Q:15:ARG:NH1	2.12	0.82
46:6B:113:ARG:HH22	46:6B:210:GLY:HA3	1.44	0.82
45:6N:46:ARG:HD3	45:6N:231:PHE:CE1	2.13	0.82
46:6O:213:HIS:HB3	46:6O:217:LYS:NZ	1.94	0.82
24:1Y:80:ARG:C	24:1Y:81:GLU:OE2	2.22	0.82
47:3C:153:ILE:HB	47:3C:156:ILE:HB	1.60	0.82
47:3C:377:LEU:HB3	47:3C:379:TRP:CD1	2.14	0.82
45:6N:19:LEU:HD12	45:6N:23:LEU:CD1	2.08	0.82
2:1B:52:LEU:HD11	2:1B:92:LEU:HD21	1.61	0.82
2:1B:101:ARG:CG	2:1B:139:ILE:CG2	2.50	0.82
45:3N:193:PRO:CD	45:3N:194:ARG:H	1.92	0.82
36:5k:68:LYS:O	36:5k:72:TRP:CD1	2.31	0.82
45:6N:127:ILE:HD13	45:6N:179:ARG:HG3	1.60	0.82
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	1.61	0.82
47:3C:53:MET:HG2	49:3E:140:MET:HG2	1.60	0.82
45:3N:29:GLN:CG	45:3N:203:VAL:O	2.27	0.82
64:4J:4:ARG:HH12	64:4J:8:LYS:HZ3	1.22	0.82
45:3N:18:GLN:HG2	45:3N:24:ARG:CA	2.08	0.82
46:3O:201:SER:H	46:3O:228:GLY:HA2	1.44	0.82
47:6C:344:GLU:HB3	51:6G:68:PHE:HE1	1.43	0.82
45:6N:15:GLN:HG3	45:6N:205:HIS:CE1	2.14	0.82
45:6N:18:GLN:HE21	45:6N:24:ARG:HE	1.26	0.82
45:6N:25:VAL:HB	45:6N:209:LEU:CD2	2.09	0.82
64:8J:4:ARG:HH12	64:8J:8:LYS:HZ3	1.24	0.82
47:3C:344:GLU:HB3	51:3G:68:PHE:HE2	1.43	0.82
45:3N:62:LEU:HA	45:3N:65:LYS:HD2	1.60	0.82
45:6N:90:SER:HA	45:6N:95:THR:CA	2.04	0.82
41:1p:166:ARG:O	41:1p:170:LYS:HD2	1.80	0.82
24:5Y:80:ARG:C	24:5Y:81:GLU:OE2	2.22	0.82
45:6N:42:ASP:OD2	45:6N:384:LEU:HD13	1.77	0.82
45:6N:281:ASP:HA	45:6N:306:SER:HA	1.62	0.82
45:6N:151:ASP:OD2	45:6N:168:GLU:OE2	1.98	0.82
55:8A:131:PRO:HG2	56:8B:176:PRO:HG2	1.59	0.82
45:3N:153:LEU:HD23	45:3N:423:ALA:HB3	1.59	0.82
33:5h:7:ARG:NH2	34:5i:31:GLU:O	2.12	0.81
62:8H:14:ALA:HB3	62:8H:63:PHE:CE1	2.14	0.81
1:1A:45:GLY:HA2	8:1H:126:LYS:HG3	1.60	0.81
41:1p:170:LYS:HD2	41:1p:170:LYS:H	1.45	0.81
47:3P:5:ARG:HG3	47:3P:11:MET:CE	2.10	0.81
49:3R:205:VAL:HB	49:3R:211:VAL:HG23	1.61	0.81
39:5n:55:ASP:CB	39:5n:58:LYS:HE2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:86:LEU:HD22	45:6N:99:ILE:HG12	1.57	0.81
47:6P:5:ARG:HG3	47:6P:11:MET:CE	2.10	0.81
46:3B:60:SER:HB3	46:3O:431:GLY:HA3	1.62	0.81
1:5A:18:VAL:HG23	8:5H:222:MET:HE1	1.61	0.81
11:5K:37:MET:HE1	11:5K:64:LEU:HA	1.63	0.81
41:5p:170:LYS:H	41:5p:170:LYS:HD2	1.45	0.81
48:6D:136:TYR:HA	48:6D:139:LEU:HB2	1.62	0.81
45:3N:353:GLU:HA	45:3N:356:ARG:CB	2.10	0.81
55:4A:436:MET:HE1	55:4A:451:ASN:HD21	1.44	0.81
1:5A:58:VAL:HG21	8:5H:286:MET:HE1	1.62	0.81
45:6N:127:ILE:CD1	45:6N:179:ARG:HG3	2.03	0.81
2:1B:52:LEU:CD1	2:1B:92:LEU:CD2	2.58	0.81
37:1l:146:PRO:CD	37:1l:146:PRO:N	2.36	0.81
45:3N:59:VAL:HG11	45:3N:190:TYR:CE2	2.15	0.81
51:3T:64:GLN:O	51:3T:68:LYS:HG3	1.81	0.81
45:6N:188:GLN:NE2	45:6N:229:PRO:HG3	1.96	0.81
45:6N:244:ARG:HG2	51:6T:10:MET:HB3	1.63	0.81
2:1B:104:TYR:HB3	2:1B:111:ARG:HH22	1.45	0.81
46:3O:386:ALA:HA	46:3O:390:GLY:HA2	0.88	0.81
45:6N:29:GLN:CG	45:6N:204:GLU:CA	2.29	0.81
33:1h:7:ARG:NH2	34:1i:31:GLU:O	2.13	0.81
39:1n:55:ASP:CB	39:1n:58:LYS:HE2	2.10	0.81
49:3I:64:LEU:HA	49:3I:77:ARG:O	1.81	0.81
45:3N:115:ASP:OD1	45:3N:119:ASN:ND2	2.14	0.81
51:6T:64:GLN:O	51:6T:68:LYS:HG3	1.81	0.81
45:3N:23:LEU:HD13	45:3N:197:LEU:HD11	1.63	0.81
45:6N:185:TYR:CB	45:6N:189:HIS:NE2	2.36	0.81
29:1d:63:LEU:HD23	75:1d:202:CDL:HA62	1.63	0.80
7:5G:190:MET:HG3	7:5G:695:ILE:HD13	1.63	0.80
45:6N:135:LEU:HD23	45:6N:138:LEU:HD12	1.62	0.80
45:3N:54:GLY:HA2	45:3N:57:TYR:HD2	1.44	0.80
41:5p:166:ARG:O	41:5p:170:LYS:HD2	1.80	0.80
55:8A:506:GLU:HA	57:8C:6:HIS:CD2	2.17	0.80
45:3N:29:GLN:NE2	45:3N:204:GLU:CB	2.44	0.80
45:3N:351:GLU:HA	45:3N:354:VAL:HB	1.61	0.80
12:5L:161:ARG:HG2	12:5L:164:ALA:H	1.46	0.80
11:1K:37:MET:HE1	11:1K:64:LEU:HA	1.63	0.80
45:3N:17:SER:CB	45:3N:209:LEU:HD11	2.06	0.80
53:6J:59:LYS:HZ2	53:6J:60:TYR:HB3	1.44	0.80
45:6N:45:SER:CA	45:6N:167:VAL:HG21	2.11	0.80
2:1B:61:HIS:CE1	4:1D:171:PHE:HE2	1.92	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:71:PRO:HD2	45:3N:72:GLY:N	1.95	0.80
45:3N:151:ASP:HA	45:3N:154:HIS:HD2	1.45	0.80
7:5G:477:ILE:HD11	7:5G:489:VAL:HG11	1.61	0.80
37:5l:146:PRO:CD	37:5l:146:PRO:N	2.36	0.80
45:6N:58:PHE:HE1	45:6N:174:VAL:HG13	1.44	0.80
49:6R:213:LEU:HD23	49:6R:258:LEU:HB2	1.63	0.80
6:5F:112:ARG:HB3	6:5F:145:GLU:HG3	1.63	0.80
55:8A:506:GLU:HA	57:8C:6:HIS:HD2	1.45	0.80
49:3R:232:GLY:HA3	49:3R:244:ASP:HA	1.63	0.80
55:4A:131:PRO:HG2	56:4B:159:VAL:HA	1.64	0.80
55:4A:436:MET:HE1	55:4A:451:ASN:ND2	1.96	0.80
45:6N:14:THR:CG2	45:6N:28:GLU:OE2	2.29	0.80
45:3N:13:GLU:O	45:3N:28:GLU:HG2	1.81	0.80
46:3O:85:ILE:HG23	46:3O:122:PHE:HB3	1.62	0.80
45:6N:65:LYS:NZ	45:6N:130:GLU:CG	2.45	0.80
45:6N:124:ASP:HA	45:6N:127:ILE:HD12	1.64	0.80
49:6R:232:GLY:HA3	49:6R:244:ASP:HA	1.63	0.80
47:3C:150:LEU:HD11	47:3C:164:ILE:HD12	1.63	0.79
45:3N:25:VAL:HG22	45:3N:197:LEU:HD13	1.63	0.79
45:3N:148:VAL:HG12	45:3N:152:TYR:CD2	2.16	0.79
8:5H:146:LEU:HD11	8:5H:192:GLU:HG3	1.63	0.79
45:6N:60:GLU:OE1	46:6O:286:LYS:NZ	2.14	0.79
7:1G:190:MET:HG3	7:1G:695:ILE:HD13	1.64	0.79
49:3E:237:PRO:HB2	48:3Q:144:ARG:HD3	1.64	0.79
45:3N:19:LEU:HD12	45:3N:23:LEU:HD12	1.64	0.79
12:1L:524:ASN:HD21	39:1n:77:GLN:HG2	1.47	0.79
29:5d:63:LEU:HD23	75:5d:202:CDL:HA62	1.63	0.79
12:5L:60:GLU:HG2	12:5L:83:ASP:HA	1.65	0.79
41:5p:166:ARG:HG2	41:5p:170:LYS:CE	2.13	0.79
3:1C:93:VAL:HG22	3:1C:108:LYS:HG2	1.65	0.79
49:3R:213:LEU:HD23	49:3R:258:LEU:HB2	1.63	0.79
45:6N:136:GLN:OE1	49:6V:51:CYS:HB3	1.83	0.79
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	1.63	0.79
49:3E:151:LYS:O	49:3E:152:ILE:HD12	1.83	0.79
46:3O:39:GLU:CA	46:3O:210:GLY:HA2	2.10	0.79
41:5p:170:LYS:HD2	41:5p:170:LYS:N	1.97	0.79
13:1M:101:LEU:HD22	75:1X:201:CDL:H471	1.64	0.79
49:3E:223:VAL:HG12	49:3E:238:CYS:HB2	1.65	0.79
13:5M:101:LEU:HD22	75:5X:201:CDL:H471	1.64	0.79
45:6N:140:GLU:HA	49:6V:48:SER:HB2	1.63	0.79
45:6N:184:GLU:O	45:6N:187:SER:OG	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:166:SER:OG	49:3R:81:THR:HG22	1.83	0.79
45:3N:186:VAL:HA	45:3N:190:TYR:CD2	2.14	0.79
21:5V:49:GLN:O	21:5V:53:GLU:OE2	2.01	0.79
45:6N:38:GLY:HA3	45:6N:98:TYR:CA	2.08	0.79
45:6N:186:VAL:CG1	45:6N:190:TYR:CD2	2.60	0.79
55:4A:336:PRO:HB2	55:4A:394:VAL:HG11	1.65	0.79
1:5A:21:ALA:HB1	8:5H:218:GLY:HA3	1.65	0.79
8:1H:146:LEU:HD11	8:1H:192:GLU:HG3	1.63	0.79
21:1V:49:GLN:O	21:1V:53:GLU:OE2	2.01	0.79
41:1p:170:LYS:HD2	41:1p:170:LYS:N	1.96	0.79
45:3N:69:ASN:CG	45:3N:119:ASN:ND2	2.41	0.79
45:6N:18:GLN:NE2	45:6N:24:ARG:HE	1.81	0.79
12:5L:524:ASN:HD21	39:5n:77:GLN:HG2	1.47	0.78
49:6E:237:PRO:HB2	48:6Q:144:ARG:HD3	1.64	0.78
45:6N:148:VAL:O	45:6N:152:TYR:HD2	1.66	0.78
55:8A:311:ILE:HA	55:8A:314:ILE:HD12	1.64	0.78
56:4B:30:ILE:HG21	56:4B:76:ILE:HD11	1.64	0.78
4:5D:371:LYS:HE2	4:5D:424:VAL:HG23	1.65	0.78
45:6N:100:LYS:HB3	46:6O:370:MET:HE1	1.65	0.78
41:1p:166:ARG:HG2	41:1p:170:LYS:CE	2.13	0.78
45:3N:110:VAL:CG1	45:3N:216:PHE:CE2	2.66	0.78
57:4C:67:PHE:O	64:4J:13:GLN:NE2	2.16	0.78
12:1L:161:ARG:HG2	12:1L:164:ALA:H	1.46	0.78
45:3N:45:SER:OG	45:3N:92:ARG:HD3	1.84	0.78
49:6I:64:LEU:HA	49:6I:77:ARG:O	1.81	0.78
45:6N:111:GLU:OE2	45:6N:215:HIS:HE1	1.66	0.78
56:8B:30:ILE:HG21	56:8B:76:ILE:HD11	1.64	0.78
2:1B:71:ARG:HB3	8:1H:36:GLY:H	1.47	0.78
45:3N:46:ARG:NH2	45:3N:314:TYR:CG	2.52	0.78
45:3N:356:ARG:HB2	46:3O:91:ALA:HA	1.65	0.78
45:6N:25:VAL:HG12	45:6N:209:LEU:CD2	1.99	0.78
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.49	0.78
46:3O:83:PHE:CE2	46:3O:87:ARG:HG3	2.19	0.78
46:6B:307:PHE:H	49:6I:52:ARG:HG3	1.49	0.78
6:1F:125:GLY:O	6:1F:129:MET:HE3	1.83	0.78
46:3B:124:LEU:HD12	46:3B:223:PHE:HB2	1.65	0.78
38:5m:37:ALA:O	38:5m:41:ARG:HD3	1.83	0.78
12:1L:60:GLU:HG2	12:1L:83:ASP:HA	1.65	0.78
45:6N:39:VAL:HG12	45:6N:41:ILE:H	1.49	0.78
45:3N:70:ARG:NE	45:3N:78:GLU:OE1	2.16	0.78
49:6E:151:LYS:O	49:6E:152:ILE:HD12	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:86:LEU:HD21	45:6N:99:ILE:CD1	2.14	0.78
45:3N:35:CYS:HA	45:3N:201:GLY:CA	2.12	0.78
45:3N:62:LEU:HD23	45:3N:65:LYS:HD2	0.78	0.77
49:6E:261:PRO:HB2	49:6E:273:VAL:HG11	1.67	0.77
45:6N:4:TYR:HD2	46:6O:114:ASP:OD2	1.63	0.77
56:8B:132:GLU:HB3	56:8B:137:GLU:HG3	1.66	0.77
46:3B:241:GLY:HA3	46:3B:421:ARG:HD3	1.65	0.77
45:3N:86:LEU:CD2	45:3N:99:ILE:HG12	2.14	0.77
7:5G:349:PHE:H	7:5G:509:PRO:HB2	1.49	0.77
45:6N:85:HIS:HB2	45:6N:100:LYS:HB2	1.65	0.77
55:8A:165:ILE:HG21	75:8A:610:CDL:H332	1.66	0.77
2:1B:96:MET:HG3	4:1D:82:LEU:HD21	1.61	0.77
45:3N:133:VAL:HG13	49:3V:51:CYS:CB	2.14	0.77
49:3R:195:LEU:HB3	49:3R:248:ARG:HH21	1.47	0.77
47:6C:240:LEU:HA	47:6C:243:VAL:HB	1.65	0.77
49:6E:249:ILE:HG22	49:6E:257:ASN:HD21	1.43	0.77
45:6N:4:TYR:CE2	46:6O:112:LEU:HD13	2.15	0.77
49:6R:172:LYS:HD3	49:6R:214:ILE:HG21	1.67	0.77
45:6N:49:ASN:H	45:6N:52:ASN:HB2	1.49	0.77
49:6R:195:LEU:HB3	49:6R:248:ARG:HH21	1.47	0.77
4:1D:371:LYS:HE2	4:1D:424:VAL:HG23	1.65	0.77
16:1P:319:ARG:HA	16:1P:322:ARG:HD2	1.67	0.77
57:4C:109:THR:HG22	57:4C:111:GLU:H	1.50	0.77
46:6B:306:PRO:HA	49:6I:52:ARG:HB2	1.67	0.77
47:6C:65:SER:HA	47:6C:68:HIS:HB3	1.64	0.77
45:6N:93:GLU:OE1	45:6N:315:ALA:CB	2.31	0.77
55:8A:55:ASN:HB3	56:8B:199:ILE:HD11	1.65	0.77
8:1H:88:PRO:HB3	8:1H:98:MET:HE3	1.65	0.77
47:3C:154:PRO:C	47:3C:158:THR:HB	2.09	0.77
45:6N:14:THR:CG2	45:6N:389:ARG:NH2	2.47	0.77
45:6N:193:PRO:CD	45:6N:194:ARG:H	1.94	0.77
57:8C:67:PHE:O	64:8J:13:GLN:NE2	2.16	0.77
10:1J:99:MET:HE1	69:1J:202:3PE:H3E2	1.66	0.77
22:1W:25:MET:HE1	22:1W:79:VAL:HG21	1.66	0.77
47:3C:319:PRO:HA	51:3G:49:ARG:HH12	1.50	0.77
49:3E:261:PRO:HB2	49:3E:273:VAL:HG11	1.67	0.77
46:6O:250:ASP:HB2	46:6O:428:GLY:HA3	1.66	0.77
51:3G:28:PHE:HB3	51:3G:31:TYR:HB2	1.66	0.77
45:6N:16:VAL:HG12	45:6N:17:SER:N	2.00	0.77
45:6N:156:THR:CA	45:6N:159:GLN:CG	2.52	0.77
45:6N:186:VAL:HG22	45:6N:190:TYR:HE2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:256:ALA:HB2	45:6N:310:PHE:HE1	1.50	0.77
57:8C:109:THR:HG22	57:8C:111:GLU:H	1.50	0.77
2:1B:100:LEU:O	2:1B:101:ARG:O	1.86	0.77
1:1A:57:LEU:O	1:1A:60:ILE:HG22	1.85	0.77
10:1J:78:MET:HE1	10:1J:79:TYR:O	1.84	0.77
25:5Z:120:MET:HE3	30:5e:68:ARG:HG3	1.67	0.77
46:6O:56:ARG:O	46:6O:57:TYR:C	2.26	0.77
25:1Z:120:MET:HE3	30:1e:68:ARG:HG3	1.67	0.76
10:5J:78:MET:HE1	10:5J:79:TYR:O	1.85	0.76
15:5O:213:GLU:HG3	15:5O:214:MET:HE3	1.68	0.76
46:3B:47:ILE:HD11	46:3B:211:VAL:HG11	1.66	0.76
49:3E:249:ILE:HG22	49:3E:257:ASN:HD21	1.43	0.76
45:3N:46:ARG:HE	45:3N:163:LEU:HD23	1.48	0.76
45:3N:311:ASN:HA	45:3N:320:LEU:HA	1.67	0.76
55:4A:237:PHE:O	55:4A:241:PRO:HG2	1.86	0.76
6:5F:125:GLY:O	6:5F:129:MET:HE3	1.83	0.76
49:6E:223:VAL:HG12	49:6E:238:CYS:HB2	1.65	0.76
38:1m:37:ALA:O	38:1m:41:ARG:HD3	1.83	0.76
8:5H:88:PRO:HB3	8:5H:98:MET:HE3	1.65	0.76
46:6B:315:SER:CA	46:6B:320:GLY:HA2	2.07	0.76
45:3N:27:SER:HB2	45:3N:200:ALA:HA	1.66	0.76
46:3O:100:SER:HA	46:3O:105:MET:HA	1.68	0.76
45:6N:14:THR:HG23	45:6N:389:ARG:NH2	2.00	0.76
45:6N:45:SER:HA	45:6N:167:VAL:CG2	2.09	0.76
45:6N:48:GLU:O	45:6N:49:ASN:OD1	2.04	0.76
58:8D:84:THR:HG21	82:8K:101:PGV:H52	1.65	0.76
45:3N:58:PHE:HZ	45:3N:174:VAL:HG13	1.50	0.76
45:3N:76:GLU:OE2	46:3O:289:SER:OG	2.03	0.76
46:3O:75:LEU:HD22	46:3O:136:GLU:HB3	1.67	0.76
3:5C:93:VAL:HG22	3:5C:108:LYS:HG2	1.65	0.76
23:5X:152:GLU:OE1	23:5X:152:GLU:N	2.16	0.76
7:1G:150:MET:HE2	7:1G:150:MET:HA	1.68	0.76
47:3C:71:ARG:HH12	48:3D:202:SER:HB3	1.49	0.76
45:3N:61:HIS:HB3	45:3N:130:GLU:OE1	1.85	0.76
49:3R:224:PRO:HA	49:3R:237:PRO:HD3	1.67	0.76
10:5J:99:MET:HE1	69:5J:201:3PE:H3E2	1.66	0.76
46:6B:44:ALA:HA	46:6B:112:LEU:HA	1.66	0.76
23:1X:152:GLU:OE1	23:1X:152:GLU:N	2.16	0.76
45:3N:76:GLU:OE1	46:3O:289:SER:OG	2.03	0.76
45:3N:159:GLN:HG2	49:3R:85:VAL:CG2	2.15	0.76
6:5F:17:ASP:OD1	6:5F:20:ARG:NH1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6D:93:LEU:HD22	52:6H:87:LEU:HD13	1.68	0.76
48:6D:98:TYR:CD2	52:6H:95:ALA:HA	2.21	0.76
45:6N:311:ASN:HA	45:6N:320:LEU:HA	1.67	0.76
55:8A:465:VAL:HG22	85:8A:605:HEA:H162	1.68	0.76
6:1F:17:ASP:OD1	6:1F:20:ARG:NH1	2.19	0.76
7:5G:324:ASP:HB3	7:5G:571:ALA:HB1	1.68	0.76
45:6N:109:ALA:HA	45:6N:112:LEU:HD12	1.67	0.76
55:8A:424:THR:HA	55:8A:454:SER:HA	1.68	0.76
45:3N:133:VAL:CG1	49:3V:51:CYS:SG	2.74	0.76
57:4C:62:ILE:HG13	82:4C:305:PGV:H21	1.68	0.76
45:6A:311:ASN:HA	45:6A:320:LEU:CA	2.10	0.76
45:6N:69:ASN:ND2	45:6N:119:ASN:ND2	2.34	0.76
45:6N:69:ASN:HD22	45:6N:115:ASP:CG	1.93	0.76
46:6O:201:SER:HB2	46:6O:228:GLY:HA2	1.67	0.76
2:1B:114:VAL:HG13	2:1B:144:ILE:HB	1.68	0.76
37:1l:136:ASN:HD21	37:1l:152:PRO:HA	1.50	0.76
56:4B:132:GLU:HB3	56:4B:137:GLU:HG3	1.66	0.76
58:4D:102:TYR:CE2	36:5k:90:GLN:HB3	2.21	0.76
1:5A:43:PRO:C	1:5A:44:MET:HE2	2.11	0.76
16:5P:319:ARG:HA	16:5P:322:ARG:HD2	1.67	0.76
45:6N:70:ARG:O	45:6N:75:LEU:HG	1.87	0.76
53:3J:41:ASP:O	53:3J:45:GLU:HG3	1.85	0.75
45:3N:60:GLU:CA	45:3N:97:TYR:OH	2.26	0.75
56:4B:120:SER:OG	56:4B:140:ASN:O	2.04	0.75
45:6A:263:ALA:HB2	45:6A:386:TYR:HB3	1.68	0.75
47:6C:150:LEU:HB3	47:6C:161:VAL:HG22	1.67	0.75
52:6H:54:LYS:HG2	52:6H:89:ALA:HB1	1.68	0.75
45:3N:25:VAL:HG22	45:3N:197:LEU:HD12	1.20	0.75
45:3N:92:ARG:NH1	45:3N:163:LEU:O	2.19	0.75
22:5W:25:MET:HE1	22:5W:79:VAL:HG21	1.66	0.75
5:1E:105:THR:OG1	72:1E:301:FES:S2	2.45	0.75
45:3N:44:GLY:HA3	45:3N:92:ARG:CA	2.16	0.75
45:3N:63:ALA:HB2	45:3N:97:TYR:CZ	2.20	0.75
45:3N:158:PHE:HD1	45:3N:163:LEU:HD12	1.51	0.75
47:6C:326:TRP:HB3	51:6G:54:PHE:HE2	1.51	0.75
45:6N:127:ILE:O	45:6N:131:ARG:HG3	1.86	0.75
55:8A:116:SER:HA	55:8A:121:GLY:CA	2.16	0.75
55:8A:289:ALA:HA	55:8A:292:MET:HG3	1.68	0.75
45:3N:57:TYR:CE2	45:3N:167:VAL:HG12	1.54	0.75
55:8A:279:SER:HB3	68:8N:22:ILE:HG12	1.67	0.75
56:8B:120:SER:OG	56:8B:140:ASN:O	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:115:SER:OG	2:1B:145:TYR:HA	1.86	0.75
7:1G:324:ASP:HB3	7:1G:571:ALA:HB1	1.68	0.75
49:3R:172:LYS:HD3	49:3R:214:ILE:HG21	1.67	0.75
4:5D:66:MET:HE3	4:5D:76:CYS:SG	2.27	0.75
45:6A:14:THR:HA	45:6A:28:GLU:HA	1.67	0.75
45:6N:145:MET:HE1	45:6N:248:LEU:HD13	1.66	0.75
55:8A:37:ILE:HA	55:8A:54:TYR:HE1	1.52	0.75
4:1D:66:MET:HE3	4:1D:76:CYS:SG	2.27	0.75
46:3B:166:ALA:HB2	46:3B:244:ILE:HG13	1.66	0.75
82:4A:601:PGV:H62	64:4J:40:LEU:HD11	1.68	0.75
47:6C:350:ILE:HD11	51:6G:64:GLY:HA3	1.69	0.75
57:8C:62:ILE:HG13	82:8C:305:PGV:H21	1.68	0.75
2:1B:101:ARG:HG3	2:1B:139:ILE:HG21	1.67	0.75
45:3N:17:SER:CB	45:3N:209:LEU:CD1	2.59	0.75
45:3N:363:ASN:HD21	46:3O:112:LEU:HD11	1.50	0.75
55:4A:244:TYR:HA	55:4A:247:ILE:HG22	1.69	0.75
37:5l:136:ASN:HD21	37:5l:152:PRO:HA	1.51	0.75
45:6N:27:SER:O	45:6N:205:HIS:ND1	2.19	0.75
45:6N:70:ARG:HB2	45:6N:75:LEU:HD21	1.68	0.75
47:3C:244:LEU:HA	48:3D:290:ARG:CG	2.16	0.75
45:3N:46:ARG:NE	45:3N:163:LEU:HD23	2.02	0.75
45:3N:111:GLU:HG2	45:3N:215:HIS:CE1	2.21	0.75
13:5M:10:MET:HE2	13:5M:10:MET:HA	1.68	0.75
46:6B:168:TYR:HA	46:6B:239:TYR:HA	1.67	0.75
47:3C:154:PRO:CA	47:3C:158:THR:OG1	2.31	0.75
90:8C:307:PEK:H9	90:8C:307:PEK:H311	1.69	0.75
45:3N:62:LEU:HA	45:3N:65:LYS:CD	2.16	0.74
46:3O:24:LEU:HD21	46:3O:26:PHE:HD2	1.00	0.74
55:4A:138:HIS:O	55:4A:213:ARG:NH2	2.20	0.74
55:4A:179:TYR:OH	82:4A:603:PGV:O02	2.05	0.74
5:5E:105:THR:OG1	72:5E:301:FES:S2	2.45	0.74
45:6A:435:ASN:HA	48:6D:315:LYS:NZ	2.00	0.74
48:6D:159:GLN:HG2	48:6D:170:MET:HG2	1.69	0.74
45:6N:60:GLU:O	45:6N:64:PHE:HD2	1.70	0.74
49:6R:224:PRO:HA	49:6R:237:PRO:HD3	1.67	0.74
55:8A:190:ILE:HD13	55:8A:277:MET:HB3	1.69	0.74
51:3G:52:PRO:HB2	51:3G:53:PRO:HD3	1.69	0.74
49:3I:32:ALA:HA	49:3I:71:ASN:ND2	2.02	0.74
45:3N:41:ILE:HG21	45:3N:190:TYR:CD1	2.21	0.74
49:6I:32:ALA:HA	49:6I:71:ASN:ND2	2.02	0.74
45:6N:16:VAL:HA	45:6N:26:ALA:CA	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:156:THR:HG22	45:6N:159:GLN:NE2	2.01	0.74
45:6N:313:CYS:HA	45:6N:318:GLY:HA2	1.68	0.74
49:3R:204:ARG:NH1	49:3R:246:SER:O	2.20	0.74
7:5G:150:MET:HE2	7:5G:150:MET:HA	1.67	0.74
48:6D:311:MET:HA	48:6D:314:HIS:HB3	1.69	0.74
45:6N:4:TYR:HE2	46:6O:114:ASP:CG	1.88	0.74
55:8A:381:LEU:HD13	85:8A:605:HEA:HAC	1.68	0.74
15:1O:213:GLU:HG3	15:1O:214:MET:HE3	1.68	0.74
45:3N:159:GLN:NE2	49:3R:85:VAL:HG13	2.01	0.74
45:3N:399:ILE:HA	45:3N:402:VAL:HG23	1.69	0.74
12:5L:297:ASP:HB3	12:5L:300:LYS:HB2	1.69	0.74
45:6N:4:TYR:CE2	46:6O:114:ASP:CB	2.60	0.74
45:6N:151:ASP:CA	45:6N:154:HIS:CD2	2.53	0.74
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	1.69	0.74
42:1q:106:ARG:HB2	42:1q:109:ILE:HG13	1.69	0.74
47:3C:344:GLU:HB3	51:3G:68:PHE:CE2	2.22	0.74
45:3N:30:SER:OG	45:3N:202:GLY:N	2.21	0.74
45:6A:443:TRP:HB3	45:6A:446:PHE:HB2	1.67	0.74
14:1N:128:LEU:HD13	75:1N:903:CDL:HA61	1.70	0.74
9:5I:156:ASN:ND2	18:5R:34:GLU:OE2	2.21	0.74
13:1M:10:MET:HE2	13:1M:10:MET:HA	1.68	0.74
90:4C:307:PEK:H9	90:4C:307:PEK:H311	1.69	0.74
10:5J:77:GLU:HB3	11:5K:25:HIS:CD2	2.23	0.74
47:6C:119:LEU:HB3	83:6C:502:HEM:HBB2	1.68	0.74
1:1A:4:MET:HA	1:1A:7:LEU:HD12	1.70	0.74
15:1O:25:ILE:HB	15:1O:123:VAL:HG12	1.68	0.74
45:3A:32:GLN:NE2	45:3A:201:GLY:HA2	2.03	0.74
50:6F:44:MET:HE2	50:6F:99:LYS:H	1.51	0.74
45:6N:4:TYR:HA	45:6N:7:ALA:HB3	1.68	0.74
45:6N:261:GLY:HA2	45:6N:317:THR:CA	2.17	0.74
55:8A:325:ALA:HA	89:8A:611:PSC:H61	1.70	0.74
45:6N:18:GLN:CG	45:6N:24:ARG:HG2	2.17	0.74
9:1I:156:ASN:ND2	18:1R:34:GLU:OE2	2.21	0.74
45:3N:23:LEU:HD21	45:3N:219:LEU:CD1	2.18	0.74
62:4H:39:CYS:HG	62:4H:53:CYS:CB	1.99	0.74
46:6B:124:LEU:HD11	46:6B:224:LEU:HG	1.70	0.74
45:3N:25:VAL:HA	45:3N:197:LEU:HB2	1.69	0.73
58:4D:101:HIS:CD2	36:5k:90:GLN:HB2	2.23	0.73
37:5l:134:PRO:HG3	40:5o:38:MET:HE2	1.70	0.73
46:3O:117:GLU:HA	46:3O:120:MET:HE2	1.67	0.73
2:5B:25:ARG:HG2	2:5B:27:GLU:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5Y:94:CYS:HB2	24:5Y:114:CYS:HA	1.70	0.73
45:6A:311:ASN:CA	45:6A:320:LEU:HA	2.12	0.73
63:8I:45:LYS:O	63:8I:49:ASP:OD1	2.06	0.73
2:1B:60:MET:C	2:1B:61:HIS:N	2.47	0.73
47:3C:240:LEU:HA	47:3C:243:VAL:HB	1.70	0.73
6:5F:92:TYR:HB2	6:5F:220:THR:HG22	1.71	0.73
45:6N:64:PHE:CD2	46:6O:287:ARG:NH2	2.56	0.73
45:6N:104:LYS:O	45:6N:107:PRO:HG3	1.88	0.73
46:6O:95:LYS:HZ1	49:6V:70:LEU:HB3	1.53	0.73
48:3Q:12:TRP:HD1	48:3Q:15:ARG:HH12	1.37	0.73
45:6N:185:TYR:HD1	45:6N:189:HIS:NE2	1.85	0.73
4:5D:52:GLY:H	4:5D:53:PRO:HD3	1.54	0.73
42:5q:106:ARG:HB2	42:5q:109:ILE:HG13	1.69	0.73
46:6O:76:THR:HB	46:6O:133:ARG:HD2	1.69	0.73
2:1B:61:HIS:CE1	4:1D:174:ARG:NE	2.53	0.73
37:1l:134:PRO:HG3	40:1o:38:MET:HE2	1.70	0.73
48:3D:235:LEU:HD11	49:3R:238:CYS:HA	1.71	0.73
45:3N:41:ILE:HD11	45:3N:195:MET:CE	2.18	0.73
45:3N:59:VAL:HG11	45:3N:190:TYR:CZ	2.23	0.73
45:3N:111:GLU:CG	45:3N:215:HIS:CE1	2.71	0.73
45:3N:170:PRO:HG3	45:3N:173:ASN:HD22	1.51	0.73
46:3O:248:ASN:HD21	46:3O:427:SER:HB2	1.52	0.73
2:5B:48:MET:HE2	2:5B:80:PRO:HB3	1.70	0.73
14:5N:128:LEU:HD13	75:5N:903:CDL:HA61	1.70	0.73
45:6N:14:THR:HG22	45:6N:28:GLU:OE2	1.87	0.73
49:6R:204:ARG:NH1	49:6R:246:SER:O	2.20	0.73
62:8H:39:CYS:HG	62:8H:53:CYS:CB	1.97	0.73
2:1B:101:ARG:CD	2:1B:139:ILE:CG2	2.46	0.73
10:1J:77:GLU:HB3	11:1K:25:HIS:CD2	2.23	0.73
50:3F:44:MET:HE2	50:3F:99:LYS:H	1.51	0.73
63:4I:45:LYS:O	63:4I:49:ASP:OD1	2.06	0.73
45:6A:253:VAL:HA	45:6A:424:GLY:HA2	1.70	0.73
45:6N:65:LYS:CE	45:6N:130:GLU:OE2	2.37	0.73
75:8A:610:CDL:H191	75:8A:610:CDL:H322	1.70	0.73
4:1D:52:GLY:H	4:1D:53:PRO:HD3	1.54	0.73
41:1p:23:THR:HG22	41:1p:25:LEU:H	1.54	0.73
45:3N:353:GLU:CA	45:3N:356:ARG:HB3	2.17	0.73
45:6A:435:ASN:HA	48:6D:315:LYS:HZ2	1.54	0.73
46:6O:169:ARG:HG3	46:6O:238:LYS:HB3	1.71	0.73
45:3A:204:GLU:HG2	45:3A:207:GLN:H	1.54	0.73
47:3C:237:LEU:N	48:3D:301:MET:HE3	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3F:119:TRP:CZ3	46:3O:91:ALA:HB3	2.23	0.73
15:5O:25:ILE:HB	15:5O:123:VAL:HG12	1.68	0.73
45:6N:159:GLN:HE22	45:6N:241:ILE:CG1	2.02	0.73
18:5R:20:ASP:O	18:5R:25:ARG:NH2	2.22	0.73
37:5l:136:ASN:ND2	37:5l:152:PRO:HA	2.04	0.73
45:6N:41:ILE:O	45:6N:41:ILE:HG22	1.89	0.73
46:6O:78:LYS:HB2	46:6O:129:ALA:HB1	1.69	0.73
2:1B:85:VAL:HG12	2:1B:112:TYR:HB2	1.71	0.72
2:1B:100:LEU:HD21	2:1B:104:TYR:HE2	1.50	0.72
4:1D:8:VAL:O	4:1D:12:GLU:HG2	1.88	0.72
4:5D:8:VAL:O	4:5D:12:GLU:HG2	1.88	0.72
7:5G:371:VAL:HG12	7:5G:450:MET:HE1	1.71	0.72
13:5M:306:PRO:HA	13:5M:458:LEU:HD13	1.71	0.72
47:6C:366:MET:HB3	47:6C:367:PRO:HD3	1.71	0.72
45:3N:156:THR:HG22	45:3N:241:ILE:HB	1.69	0.72
46:6B:325:TYR:HB3	49:6I:59:ALA:HB1	1.69	0.72
45:6N:118:GLN:NE2	45:6N:219:LEU:HG	2.04	0.72
82:8A:601:PGV:H62	64:8J:40:LEU:HD11	1.69	0.72
47:3C:154:PRO:HA	47:3C:158:THR:HB	0.74	0.72
45:3N:191:LYS:C	45:3N:193:PRO:CD	2.62	0.72
45:3N:354:VAL:O	45:3N:358:LYS:N	2.22	0.72
46:3O:78:LYS:HD3	46:3O:131:GLU:HG3	1.69	0.72
55:4A:436:MET:CE	55:4A:451:ASN:HD21	2.02	0.72
14:5N:69:MET:HE1	14:5N:104:MET:HE3	1.72	0.72
2:1B:45:LEU:HD22	2:1B:85:VAL:HG22	1.71	0.72
41:5p:23:THR:HG22	41:5p:25:LEU:H	1.54	0.72
46:6B:310:SER:HB3	49:6I:59:ALA:HB3	1.70	0.72
48:6Q:12:TRP:HD1	48:6Q:15:ARG:HH12	1.37	0.72
55:8A:233:HIS:HB3	57:8C:99:TRP:CZ2	2.24	0.72
45:3N:29:GLN:HE21	45:3N:204:GLU:CB	2.00	0.72
55:4A:361:SER:OG	56:4B:84:LEU:HD13	1.90	0.72
45:6N:99:ILE:HD11	45:6N:113:LEU:CD2	2.18	0.72
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.71	0.72
18:1R:20:ASP:O	18:1R:25:ARG:NH2	2.22	0.72
45:3N:191:LYS:C	45:3N:193:PRO:HD3	2.14	0.72
1:5A:44:MET:HE3	4:5D:51:PHE:HE2	1.55	0.72
45:6N:25:VAL:HG12	45:6N:25:VAL:O	1.90	0.72
75:4C:308:CDL:H191	75:4C:308:CDL:H322	1.70	0.72
47:6C:246:SER:HB2	47:6C:249:LEU:HB3	1.70	0.72
45:6N:51:LYS:C	45:6N:185:TYR:OH	2.33	0.72
45:6N:107:PRO:HD2	45:6N:108:LYS:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:371:VAL:HG12	7:1G:450:MET:HE1	1.71	0.72
40:1o:102:GLU:OE1	40:1o:105:ARG:HD3	1.90	0.72
58:4D:101:HIS:HD2	36:5k:90:GLN:HB2	1.55	0.72
12:5L:434:LYS:HE2	36:5k:52:TYR:HA	1.72	0.72
45:6N:36:THR:HA	45:6N:101:ALA:H	1.54	0.72
45:6N:42:ASP:OD1	45:6N:94:HIS:ND1	2.19	0.72
45:6N:186:VAL:CG1	45:6N:190:TYR:HD2	2.00	0.72
55:8A:292:MET:HE2	55:8A:295:VAL:HG11	1.69	0.72
19:1S:22:LEU:HD23	19:1S:22:LEU:H	1.55	0.72
45:3N:33:PRO:HG2	46:3O:369:LEU:HD13	1.71	0.72
45:3N:59:VAL:HG11	45:3N:190:TYR:OH	1.90	0.72
46:3O:89:ILE:HG22	46:3O:94:GLY:HA3	1.70	0.72
12:5L:62:ILE:HG12	41:5p:114:GLN:HG2	1.71	0.72
19:5S:22:LEU:HD23	19:5S:22:LEU:H	1.55	0.72
37:5l:133:TYR:HB3	37:5l:138:LEU:HD13	1.71	0.72
45:3N:170:PRO:HG2	45:3N:173:ASN:CB	2.20	0.72
55:4A:176:MET:HE3	55:4A:181:THR:HG22	1.71	0.72
55:4A:347:LEU:HD13	55:4A:383:MET:HG2	1.72	0.72
12:5L:207:GLU:HG3	12:5L:266:LEU:HA	1.71	0.72
45:6A:313:CYS:HA	45:6A:318:GLY:HA2	1.70	0.72
48:6D:218:LEU:HD21	48:6D:249:MET:HE1	1.72	0.72
45:6N:34:THR:HG22	45:6N:102:LEU:HD23	0.72	0.72
12:1L:207:GLU:HG3	12:1L:266:LEU:HA	1.71	0.71
12:1L:434:LYS:HE2	36:1k:52:TYR:HA	1.72	0.71
45:3N:170:PRO:HD2	45:3N:173:ASN:HB2	1.71	0.71
45:6N:156:THR:HG22	45:6N:159:GLN:HE21	1.54	0.71
45:6N:181:ASP:C	45:6N:185:TYR:HD2	1.98	0.71
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.71	0.71
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.70	0.71
6:1F:92:TYR:HB2	6:1F:220:THR:HG22	1.71	0.71
37:1l:136:ASN:ND2	37:1l:152:PRO:HA	2.04	0.71
55:4A:131:PRO:HB2	56:4B:159:VAL:HG12	1.71	0.71
45:6N:162:PRO:CD	45:6N:163:LEU:N	2.46	0.71
45:6N:216:PHE:HD1	45:6N:219:LEU:HD11	1.55	0.71
55:8A:183:LEU:HD11	55:8A:273:MET:HB2	1.72	0.71
24:1Y:94:CYS:HB2	24:1Y:114:CYS:HA	1.70	0.71
4:5D:328:ALA:HB3	7:5G:126:ASP:HB2	1.71	0.71
48:6D:253:ILE:HB	48:6D:268:MET:HB2	1.73	0.71
45:6N:46:ARG:HD3	45:6N:231:PHE:CZ	2.25	0.71
56:8B:44:LEU:HD21	63:8I:20:HIS:HB3	1.70	0.71
75:8D:201:CDL:H782	75:8D:201:CDL:H231	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:77:TRP:CD2	48:3D:286:GLU:HB2	2.25	0.71
47:3C:377:LEU:HB2	50:3F:32:TYR:HE2	1.55	0.71
45:3N:191:LYS:O	45:3N:193:PRO:HD2	1.91	0.71
56:4B:44:LEU:HD21	63:4I:20:HIS:HB3	1.70	0.71
45:6N:2:ALA:HA	45:6N:6:GLN:OE1	1.89	0.71
8:1H:152:SER:HA	8:1H:155:LEU:HD12	1.73	0.71
47:3C:240:LEU:HB2	48:3D:297:MET:HG3	1.73	0.71
45:3N:44:GLY:CA	45:3N:92:ARG:HA	2.20	0.71
45:3N:70:ARG:HD3	45:3N:75:LEU:HD23	1.71	0.71
8:5H:152:SER:HA	8:5H:155:LEU:HD12	1.73	0.71
40:5o:102:GLU:OE1	40:5o:105:ARG:HD3	1.90	0.71
49:6E:249:ILE:CG2	49:6E:257:ASN:HD21	1.99	0.71
55:8A:72:PRO:HA	55:8A:76:GLY:HA3	1.71	0.71
2:1B:92:LEU:HA	2:1B:93:THR:N	2.04	0.71
37:1l:133:TYR:HB3	37:1l:138:LEU:HD13	1.71	0.71
45:3N:158:PHE:HE1	45:3N:163:LEU:HD13	1.54	0.71
45:3N:255:ILE:HD11	45:3N:420:PRO:HG2	1.71	0.71
49:3R:176:VAL:HG22	49:3R:212:ILE:HG13	1.72	0.71
55:4A:242:GLU:O	55:4A:244:TYR:N	2.24	0.71
4:5D:269:LEU:HB2	4:5D:368:GLU:HB2	1.71	0.71
7:5G:366:THR:HB	7:5G:450:MET:HE3	1.73	0.71
8:5H:32:GLN:OE1	8:5H:34:ARG:NH1	2.24	0.71
45:6N:185:TYR:CA	45:6N:189:HIS:HD2	2.02	0.71
55:8A:46:THR:HB	55:8A:49:GLY:HA2	1.73	0.71
55:8A:200:PRO:HB2	57:8C:92:LEU:HB3	1.73	0.71
46:3B:397:THR:HA	46:3B:400:GLN:HE21	1.55	0.71
8:5H:149:ILE:HG21	8:5H:185:TRP:HB2	1.71	0.71
45:6A:254:ALA:HB2	45:6A:323:HIS:HD2	1.55	0.71
45:6N:150:PHE:C	45:6N:154:HIS:CD2	2.69	0.71
45:6N:191:LYS:C	45:6N:193:PRO:HD3	2.16	0.71
45:6N:156:THR:C	45:6N:159:GLN:HG3	2.16	0.71
49:6R:199:GLN:HB2	49:6R:248:ARG:HD3	1.72	0.71
45:6N:165:GLN:O	45:6N:167:VAL:HG23	1.90	0.71
46:6O:60:SER:HA	46:6O:63:LEU:HG	1.71	0.71
47:3C:59:THR:HG23	47:3C:172:LYS:HB2	1.73	0.70
12:5L:8:THR:HB	12:5L:82:MET:HE3	1.73	0.70
14:5N:210:THR:HG23	14:5N:329:MET:HE3	1.73	0.70
47:6C:56:THR:HG23	47:6C:65:SER:HB2	1.73	0.70
45:6N:34:THR:CB	45:6N:102:LEU:HD23	2.20	0.70
45:6N:43:ALA:HB3	45:6N:95:THR:HG21	1.72	0.70
45:6N:170:PRO:CG	45:6N:173:ASN:CB	2.46	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:69:MET:HE1	14:1N:104:MET:HE3	1.72	0.70
49:3V:62:ARG:HB2	49:3V:77:ARG:HH12	1.56	0.70
3:5C:189:GLU:HG2	16:5P:14:SER:HB2	1.73	0.70
6:5F:365:CYS:HB3	70:5F:502:SF4:S3	2.31	0.70
10:5J:78:MET:CE	10:5J:79:TYR:O	2.39	0.70
45:6N:70:ARG:CB	45:6N:75:LEU:CD2	2.65	0.70
45:6N:191:LYS:C	45:6N:193:PRO:CD	2.64	0.70
46:6O:376:GLU:OE1	46:6O:379:LEU:CD2	2.38	0.70
6:1F:365:CYS:HB3	70:1F:502:SF4:S3	2.31	0.70
12:1L:62:ILE:HG12	41:1p:114:GLN:HG2	1.71	0.70
47:3C:226:ILE:HD11	48:3D:308:VAL:HG13	1.73	0.70
45:3N:64:PHE:HE1	45:3N:86:LEU:HD13	0.98	0.70
45:3N:170:PRO:HG2	45:3N:173:ASN:HB2	1.72	0.70
45:6N:148:VAL:HG13	45:6N:152:TYR:CE2	2.21	0.70
2:1B:71:ARG:HE	8:1H:36:GLY:HA2	1.57	0.70
10:1J:78:MET:CE	10:1J:79:TYR:O	2.39	0.70
69:1M:503:3PE:H342	71:1Y:201:PC1:H231	1.73	0.70
24:1Y:124:VAL:HA	69:1Y:203:3PE:H251	1.74	0.70
45:3N:429:GLU:HB3	51:3T:5:GLY:HA2	1.72	0.70
7:5G:283:MET:HB2	7:5G:560:ILE:HB	1.73	0.70
69:5M:503:3PE:H342	71:5Y:201:PC1:H231	1.73	0.70
22:5W:22:SER:HB3	22:5W:27:GLU:HB2	1.73	0.70
25:5Z:120:MET:HG3	25:5Z:123:GLU:HG2	1.74	0.70
35:5j:67:LEU:HD22	40:5o:29:GLY:HA2	1.73	0.70
36:5k:67:LEU:HB3	36:5k:70:PHE:HB3	1.73	0.70
13:1M:306:PRO:HA	13:1M:458:LEU:HD13	1.71	0.70
16:1P:270:PHE:HA	71:1P:401:PC1:H331	1.73	0.70
47:3C:213:SER:HA	50:3F:78:LEU:HD13	1.74	0.70
47:3C:324:LEU:HD13	47:3C:366:MET:HA	1.72	0.70
49:3E:223:VAL:HG11	48:3Q:144:ARG:NH1	2.07	0.70
49:3R:199:GLN:HB2	49:3R:248:ARG:HD3	1.72	0.70
10:5J:132:ASP:OD1	26:5a:42:SER:OG	2.09	0.70
25:5Z:98:MET:HE2	30:5e:78:ILE:HA	1.74	0.70
49:6V:62:ARG:HB2	49:6V:77:ARG:HH12	1.56	0.70
47:3C:226:ILE:HG12	48:3D:311:MET:CB	2.22	0.70
45:3N:66:GLY:HA2	45:3N:75:LEU:HD12	1.73	0.70
45:6N:18:GLN:HG2	45:6N:24:ARG:HG3	1.71	0.70
45:6N:159:GLN:NE2	45:6N:241:ILE:HG13	2.05	0.70
45:6N:348:SER:HB3	54:6X:17:TRP:HE1	1.55	0.70
62:4H:39:CYS:CB	62:4H:53:CYS:HB3	2.22	0.70
49:6E:223:VAL:HG11	48:6Q:144:ARG:NH1	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:43:ALA:HB3	45:6N:95:THR:CG2	2.20	0.70
7:1G:283:MET:HB2	7:1G:560:ILE:HB	1.74	0.70
7:1G:302:ARG:HH11	7:1G:302:ARG:HB2	1.56	0.70
7:1G:366:THR:HB	7:1G:450:MET:HE3	1.73	0.70
49:3R:196:ARG:NH2	49:3R:254:ALA:O	2.24	0.70
58:4D:60:TYR:OH	59:4E:69:GLU:OE1	2.07	0.70
36:5k:66:LEU:HB2	36:5k:67:LEU:HD12	1.73	0.70
46:6B:202:ALA:H	46:6B:228:GLY:HA2	1.55	0.70
48:6D:136:TYR:HB2	48:6D:175:LEU:HA	1.73	0.70
2:1B:100:LEU:O	2:1B:104:TYR:CG	2.44	0.70
12:1L:8:THR:HB	12:1L:82:MET:HE3	1.73	0.70
22:1W:22:SER:HB3	22:1W:27:GLU:HB2	1.73	0.70
25:1Z:98:MET:HE2	30:1e:78:ILE:HA	1.74	0.70
45:3N:36:THR:HG21	45:3N:372:THR:C	2.16	0.70
45:3N:71:PRO:CD	45:3N:72:GLY:H	2.05	0.70
46:3O:76:THR:HG23	46:3O:81:SER:HA	1.74	0.70
48:3Q:144:ARG:HE	48:3Q:147:LEU:HG	1.56	0.70
82:4G:101:PGV:H241	82:4G:101:PGV:H012	1.73	0.70
71:5M:502:PC1:H322	75:5i:201:CDL:H111	1.73	0.70
45:6N:136:GLN:OE1	49:6V:51:CYS:CB	2.39	0.70
49:6R:176:VAL:HG22	49:6R:212:ILE:HG13	1.72	0.70
50:6S:109:LYS:HG3	54:6Y:4:ARG:HH11	1.57	0.70
8:1H:196:ALA:HB3	8:1H:197:PRO:HD3	1.73	0.70
14:1N:210:THR:HG23	14:1N:329:MET:HE3	1.73	0.70
46:3B:154:ASN:C	46:3B:154:ASN:HD22	1.99	0.70
45:3N:55:ALA:CB	45:3N:185:TYR:CD1	2.74	0.70
45:3N:115:ASP:CG	45:3N:119:ASN:HD22	1.99	0.70
45:3N:159:GLN:HG2	49:3R:85:VAL:HG11	1.73	0.70
27:5b:63:PRO:CD	27:5b:63:PRO:HB3	2.19	0.70
41:5p:166:ARG:O	41:5p:170:LYS:HD3	1.91	0.70
45:3N:63:ALA:CB	45:3N:97:TYR:CE1	2.74	0.69
45:3N:141:ASN:HB3	45:3N:168:GLU:OE2	1.91	0.69
53:6J:59:LYS:HZ3	53:6J:60:TYR:HB3	1.56	0.69
45:6N:185:TYR:CB	45:6N:189:HIS:HE2	2.02	0.69
48:6Q:144:ARG:HE	48:6Q:147:LEU:HG	1.56	0.69
25:1Z:120:MET:HG3	25:1Z:123:GLU:HG2	1.74	0.69
45:3N:45:SER:HA	45:3N:48:GLU:HB2	1.74	0.69
46:3O:258:VAL:HG12	46:3O:323:GLY:HA3	1.74	0.69
46:3O:277:HIS:HA	46:3O:281:ALA:HB2	1.73	0.69
54:3X:14:ALA:O	54:3X:18:ILE:HG12	1.92	0.69
45:6N:122:LEU:CD1	45:6N:183:THR:HG22	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:196:ALA:HB3	8:5H:197:PRO:HD3	1.72	0.69
45:6N:71:PRO:HD2	45:6N:72:GLY:H	1.56	0.69
47:3C:226:ILE:CD1	48:3D:308:VAL:HG13	2.23	0.69
45:3N:60:GLU:O	46:3O:287:ARG:NH2	2.25	0.69
45:3N:159:GLN:HG2	49:3R:85:VAL:CB	2.22	0.69
57:4C:47:LEU:HD22	82:4C:302:PGV:H142	1.72	0.69
7:5G:302:ARG:HB2	7:5G:302:ARG:HH11	1.56	0.69
45:6N:141:ASN:HA	49:6V:47:ARG:HH21	1.56	0.69
47:6P:221:HIS:O	47:6P:225:THR:OG1	2.08	0.69
7:1G:465:ALA:HB2	7:1G:654:GLN:HG3	1.75	0.69
71:1M:502:PC1:H322	75:1i:201:CDL:H111	1.73	0.69
39:1n:134:ARG:HH11	39:1n:137:LYS:HD2	1.58	0.69
49:3E:155:LYS:HE3	49:3E:176:VAL:HG21	1.75	0.69
47:3P:120:LEU:HG	47:3P:124:MET:HE2	1.74	0.69
54:3Y:8:PRO:O	54:3Y:12:GLU:HG3	1.92	0.69
45:6N:10:SER:O	45:6N:11:VAL:HG23	1.92	0.69
45:6N:40:TRP:CE2	45:6N:377:GLU:CA	2.51	0.69
49:6R:196:ARG:NH2	49:6R:254:ALA:O	2.24	0.69
56:8B:104:TRP:HA	56:8B:207:MET:SD	2.32	0.69
35:1j:38:TRP:CZ3	36:1k:80:ALA:HB1	2.27	0.69
48:6D:237:PHE:HA	48:6D:246:ALA:HA	1.75	0.69
53:6W:11:TYR:HA	53:6W:15:PHE:HB2	1.75	0.69
55:8A:413:HIS:HD2	55:8A:467:LEU:HB3	1.58	0.69
46:3B:121:GLU:OE1	46:3B:222:ARG:NH1	2.23	0.69
55:4A:129:TYR:OH	55:4A:236:TRP:NE1	2.25	0.69
48:6D:93:LEU:HD23	48:6D:239:PRO:HB2	1.74	0.69
48:6D:317:SER:HB3	51:6G:25:GLN:HG3	1.75	0.69
45:6N:58:PHE:CZ	45:6N:174:VAL:CG2	2.63	0.69
45:6N:61:HIS:CD2	45:6N:134:ILE:HD11	2.27	0.69
45:6N:110:VAL:HG13	45:6N:216:PHE:CE2	2.27	0.69
47:6P:124:MET:HE1	47:6P:298:ILE:HD13	1.75	0.69
54:6X:14:ALA:O	54:6X:18:ILE:HG12	1.93	0.69
58:8D:78:TRP:HE1	75:8D:201:CDL:H631	1.56	0.69
10:1J:132:ASP:OD1	26:1a:42:SER:OG	2.09	0.69
26:1a:49:GLU:OE1	26:1a:52:ARG:NH2	2.25	0.69
35:1j:67:LEU:HD22	40:1o:29:GLY:HA2	1.74	0.69
41:1p:166:ARG:O	41:1p:170:LYS:HD3	1.91	0.69
47:3C:319:PRO:HA	51:3G:49:ARG:NH1	2.08	0.69
49:3E:110:ARG:HD2	51:3G:23:PHE:O	1.93	0.69
45:3N:58:PHE:HZ	45:3N:174:VAL:HA	1.58	0.69
55:4A:33:LEU:HB3	55:4A:61:HIS:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:4C:308:CDL:H581	75:4C:308:CDL:H761	1.75	0.69
24:5Y:124:VAL:HA	69:5Y:203:3PE:H251	1.74	0.69
49:6E:155:LYS:HE3	49:6E:176:VAL:HG21	1.74	0.69
45:6N:86:LEU:HD23	45:6N:99:ILE:HG12	0.70	0.69
45:6N:181:ASP:C	45:6N:185:TYR:CD2	2.71	0.69
45:6N:353:GLU:HA	45:6N:356:ARG:HB3	1.73	0.69
55:8A:336:PRO:HB3	55:8A:411:LYS:HG3	1.73	0.69
12:1L:118:PHE:O	12:1L:122:VAL:HG23	1.93	0.69
47:3P:221:HIS:O	47:3P:225:THR:OG1	2.08	0.69
10:5J:78:MET:HG2	11:5K:89:TYR:OH	1.93	0.69
35:5j:37:LEU:HB3	36:5k:77:PHE:CG	2.28	0.69
48:6D:157:GLU:CA	48:6D:172:PRO:HA	2.08	0.69
62:8H:39:CYS:CB	62:8H:53:CYS:HB3	2.22	0.69
45:3N:61:HIS:HA	46:3O:287:ARG:CZ	2.23	0.69
45:3N:118:GLN:CD	45:3N:219:LEU:HD23	2.16	0.69
45:3N:127:ILE:HD12	45:3N:179:ARG:HE	1.58	0.69
53:3W:11:TYR:HA	53:3W:15:PHE:HB2	1.75	0.69
12:5L:118:PHE:O	12:5L:122:VAL:HG23	1.93	0.69
13:5M:271:MET:HA	13:5M:271:MET:HE2	1.75	0.69
45:6A:2:ALA:HB2	46:6B:41:TYR:HB3	1.75	0.69
45:6A:417:ASP:HA	45:6A:441:MET:HB3	1.75	0.69
3:1C:189:GLU:HG2	16:1P:14:SER:HB2	1.73	0.68
47:3C:227:LYS:HA	48:3D:312:LYS:HG3	1.74	0.68
45:3N:193:PRO:CD	45:3N:194:ARG:N	2.53	0.68
64:4J:40:LEU:HD12	82:4J:101:PGV:H152	1.74	0.68
26:5a:49:GLU:OE1	26:5a:52:ARG:NH2	2.25	0.68
47:6C:224:TYR:HA	47:6C:227:LYS:HB3	1.73	0.68
53:6J:17:ARG:HB3	53:6J:20:THR:HB	1.73	0.68
45:6N:181:ASP:HB3	45:6N:185:TYR:CE2	2.24	0.68
45:6N:216:PHE:HB3	45:6N:219:LEU:HD12	1.75	0.68
55:8A:431:LEU:HD21	55:8A:450:TRP:HB2	1.74	0.68
8:1H:104:PHE:HE1	71:1H:401:PC1:H342	1.58	0.68
12:1L:161:ARG:NH2	39:1n:87:GLY:O	2.26	0.68
10:1J:78:MET:HG2	11:1K:89:TYR:OH	1.93	0.68
47:3C:224:TYR:HA	47:3C:227:LYS:HB3	1.75	0.68
45:3N:33:PRO:HD2	45:3N:34:THR:N	2.08	0.68
45:3N:296:SER:C	47:3P:1:MET:HE1	2.18	0.68
45:3N:431:LEU:HD12	45:3N:432:PRO:HD2	1.74	0.68
46:3O:23:ASP:HB3	46:3O:25:GLU:OE2	1.94	0.68
55:4A:243:VAL:HB	85:4A:606:HEA:C3C	2.23	0.68
16:5P:138:ASP:HB3	16:5P:141:SER:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6B:45:SER:HB2	46:6B:116:ILE:HG21	1.75	0.68
46:6B:46:ARG:HA	46:6B:110:GLU:HA	1.75	0.68
45:6N:107:PRO:HD2	45:6N:108:LYS:N	2.09	0.68
45:6N:410:VAL:HA	45:6N:413:LYS:HD2	1.74	0.68
55:8A:116:SER:HA	55:8A:121:GLY:HA3	1.74	0.68
16:1P:138:ASP:HB3	16:1P:141:SER:HB2	1.75	0.68
45:3N:33:PRO:HD2	45:3N:34:THR:H	1.58	0.68
45:3N:41:ILE:CD1	45:3N:195:MET:HE1	2.18	0.68
46:3O:245:ARG:HB3	46:3O:430:LEU:HD13	1.75	0.68
55:4A:431:LEU:HD22	55:4A:436:MET:SD	2.33	0.68
1:5A:55:PHE:HB2	10:5J:74:MET:HE1	1.74	0.68
48:6D:152:LEU:HA	48:6D:155:GLU:HB2	1.75	0.68
57:8C:99:TRP:HA	82:8C:303:PGV:H51	1.75	0.68
2:1B:58:GLU:O	2:1B:59:MET:C	2.37	0.68
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.26	0.68
47:3C:58:ASP:HA	47:3C:172:LYS:HE3	1.73	0.68
56:4B:100:MET:HE1	56:4B:155:SER:HB3	1.75	0.68
7:5G:465:ALA:HB2	7:5G:654:GLN:HG3	1.75	0.68
10:5J:129:ASP:HB3	30:5e:31:ARG:HE	1.58	0.68
45:6N:58:PHE:CZ	45:6N:134:ILE:HD13	2.27	0.68
45:6N:80:GLU:HA	46:6O:284:HIS:CE1	2.29	0.68
45:6N:106:LEU:HD11	45:6N:203:VAL:HG22	1.75	0.68
47:6P:120:LEU:HG	47:6P:124:MET:HE2	1.74	0.68
82:8C:302:PGV:H241	82:8C:302:PGV:H72	1.76	0.68
2:1B:71:ARG:HB3	8:1H:36:GLY:N	2.07	0.68
45:3N:170:PRO:CD	45:3N:173:ASN:HB2	2.24	0.68
34:5i:101:PRO:HD3	41:5p:14:ARG:HH22	1.59	0.68
46:6O:334:GLY:HA2	46:6O:434:PRO:HD3	1.76	0.68
55:8A:135:ASN:HD22	61:8G:58:LYS:HB2	1.57	0.68
82:8A:601:PGV:H05	82:8A:601:PGV:H31	1.74	0.68
2:1B:101:ARG:HE	2:1B:139:ILE:CG2	1.62	0.68
3:1C:195:ARG:NH2	9:1I:92:ILE:O	2.27	0.68
45:3A:250:LEU:HD12	49:3I:44:ASP:HB2	1.74	0.68
45:3N:52:ASN:HB3	45:3N:185:TYR:HE1	1.56	0.68
12:5L:439:PRO:HB3	35:5j:12:ARG:HG2	1.76	0.68
46:6B:165:ALA:HA	46:6B:173:ALA:HB1	1.74	0.68
55:8A:353:LEU:HB3	56:8B:31:VAL:HG22	1.76	0.68
1:1A:113:TRP:H	8:1H:287:HIS:HE1	1.42	0.68
45:3N:153:LEU:CD2	45:3N:423:ALA:HB3	2.24	0.68
45:3N:341:GLN:HB3	45:3N:344:ARG:HH21	1.58	0.68
46:3O:171:ALA:HB3	46:3O:237:ALA:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:6E:231:PHE:HE1	49:6E:242:HIS:HB3	1.59	0.68
75:8A:610:CDL:H581	75:8A:610:CDL:H761	1.75	0.68
34:1i:101:PRO:HD3	41:1p:14:ARG:HH22	1.59	0.68
45:3N:54:GLY:HA2	45:3N:57:TYR:CD2	2.28	0.68
3:5C:195:ARG:NH2	9:5I:92:ILE:O	2.27	0.68
48:6D:313:ARG:HA	48:6D:316:TRP:HB2	1.75	0.68
55:8A:162:ILE:HG23	57:8C:85:LEU:HB2	1.75	0.68
55:8A:459:PHE:HA	55:8A:462:LEU:HD23	1.76	0.68
2:1B:57:VAL:C	2:1B:58:GLU:C	2.62	0.67
6:1F:203:PRO:O	17:1Q:133:LYS:NZ	2.28	0.67
12:1L:439:PRO:HB3	35:1j:12:ARG:HG2	1.76	0.67
39:1n:61:GLN:O	39:1n:65:GLN:OE1	2.12	0.67
49:3E:93:ARG:NH2	51:3G:23:PHE:HA	2.09	0.67
47:3P:124:MET:HE1	47:3P:298:ILE:HD13	1.75	0.67
8:5H:104:PHE:HE1	71:5H:401:PC1:H342	1.58	0.67
47:6C:213:SER:HA	50:6F:78:LEU:HD13	1.76	0.67
55:8A:234:LEU:HA	55:8A:237:PHE:HB3	1.75	0.67
55:8A:412:ILE:HG13	58:8D:81:ILE:HG23	1.76	0.67
45:3N:353:GLU:O	45:3N:357:GLY:N	2.28	0.67
6:5F:30:ASP:O	6:5F:39:ARG:NH2	2.27	0.67
6:5F:203:PRO:O	17:5Q:133:LYS:NZ	2.28	0.67
19:5S:26:SER:O	19:5S:33:ARG:NH2	2.28	0.67
45:6N:216:PHE:HD1	45:6N:219:LEU:CD1	2.07	0.67
2:1B:96:MET:SD	4:1D:82:LEU:CD2	2.79	0.67
4:5D:149:ASN:OD1	4:5D:371:LYS:NZ	2.26	0.67
39:5n:134:ARG:HH11	39:5n:137:LYS:HD2	1.58	0.67
55:8A:115:SER:HB2	55:8A:142:SER:HA	1.76	0.67
30:1e:94:PRO:HD2	30:1e:97:HIS:HB2	1.77	0.67
48:3D:267:THR:HG21	52:3H:41:PRO:HD2	1.77	0.67
45:3N:58:PHE:CZ	45:3N:174:VAL:HA	2.30	0.67
57:4C:95:THR:HG23	82:4C:303:PGV:H101	1.75	0.67
12:5L:161:ARG:NH2	39:5n:87:GLY:O	2.26	0.67
46:6B:171:ALA:HB3	46:6B:237:ALA:HB2	1.77	0.67
45:6N:86:LEU:HD22	45:6N:99:ILE:CG1	2.20	0.67
55:8A:147:ILE:HG21	55:8A:210:LEU:HB2	1.77	0.67
6:1F:257:ASN:ND2	6:1F:267:THR:OG1	2.28	0.67
10:1J:129:ASP:HB3	30:1e:31:ARG:HE	1.58	0.67
12:1L:351:ASN:O	12:1L:351:ASN:ND2	2.27	0.67
46:3B:227:ARG:HG3	46:3B:229:GLY:H	1.59	0.67
45:3N:62:LEU:HD23	45:3N:65:LYS:HD3	1.68	0.67
55:4A:86:MET:HE1	55:4A:184:PHE:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:5d:202:CDL:H321	75:5d:202:CDL:HB62	1.76	0.67
47:6C:186:PRO:HG2	83:6C:501:HEM:HMC1	1.77	0.67
45:6N:42:ASP:HA	45:6N:94:HIS:HA	1.75	0.67
21:1V:65:LYS:HD2	21:1V:69:GLU:OE1	1.94	0.67
47:3C:72:ASP:HB3	49:3E:144:ALA:HB3	1.74	0.67
45:3N:61:HIS:CD2	45:3N:134:ILE:HD11	2.29	0.67
56:4B:146:MET:HE2	56:4B:215:PRO:HG3	1.76	0.67
10:5J:173:ARG:NH1	14:5N:1:FME:O1	2.28	0.67
12:5L:545:SER:OG	13:5M:274:SER:O	2.13	0.67
22:5W:54:ILE:HG23	22:5W:104:MET:HE1	1.77	0.67
45:6N:62:LEU:HD12	45:6N:182:LEU:HD13	1.75	0.67
56:8B:100:MET:HE1	56:8B:155:SER:HB3	1.75	0.67
19:1S:26:SER:O	19:1S:33:ARG:NH2	2.28	0.67
49:3E:231:PHE:HE1	49:3E:242:HIS:HB3	1.59	0.67
45:3N:150:PHE:CZ	45:3N:310:PHE:CZ	2.80	0.67
1:5A:44:MET:HE3	4:5D:51:PHE:CE2	2.30	0.67
46:6O:131:GLU:HB3	46:6O:133:ARG:HG2	1.76	0.67
49:3E:151:LYS:C	49:3E:152:ILE:HD12	2.20	0.67
45:3N:92:ARG:HG3	45:3N:167:VAL:CG2	2.24	0.67
45:3N:442:PHE:HB2	45:3N:446:PHE:C	2.19	0.67
46:3O:128:ALA:HB3	46:3O:223:PHE:HE1	1.59	0.67
49:3R:149:MET:O	49:3R:151:LYS:N	2.28	0.67
34:5i:85:LEU:O	34:5i:90:THR:HG23	1.95	0.67
39:5n:61:GLN:O	39:5n:65:GLN:OE1	2.12	0.67
47:6C:46:LEU:HB3	49:6E:136:PHE:CE2	2.30	0.67
47:6C:54:HIS:CD2	47:6C:73:VAL:HG21	2.30	0.67
49:6E:213:LEU:HD13	49:6E:258:LEU:HB2	1.77	0.67
56:8B:146:MET:HE2	56:8B:215:PRO:HG3	1.76	0.67
10:5J:64:MET:HE1	11:5K:68:ALA:HA	1.76	0.67
12:5L:61:MET:HE2	34:5i:98:GLU:HG2	1.77	0.67
13:5M:207:MET:HE2	13:5M:298:ILE:HG13	1.77	0.67
25:5Z:86:MET:HE3	25:5Z:124:LEU:HG	1.77	0.67
45:6A:435:ASN:HB3	47:6C:222:PRO:HB3	1.77	0.67
48:6D:301:MET:HA	48:6D:304:LEU:HB2	1.77	0.67
48:6D:311:MET:HB3	49:6E:117:ILE:HG22	1.77	0.67
45:6N:307:PHE:HA	45:6N:324:PHE:HA	1.77	0.67
49:6R:236:CYS:SG	49:6R:239:HIS:HB2	2.35	0.67
58:8D:87:PHE:HB3	82:8K:101:PGV:H151	1.75	0.67
6:1F:30:ASP:O	6:1F:39:ARG:NH2	2.27	0.67
47:3C:226:ILE:HD12	47:3C:229:ILE:HB	1.77	0.67
55:4A:381:LEU:HD13	85:4A:605:HEA:HAC	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:534:ARG:NH2	7:5G:558:ASP:OD1	2.28	0.67
10:5J:170:GLU:OE2	10:5J:173:ARG:NH2	2.28	0.67
45:6N:185:TYR:CB	45:6N:189:HIS:HD2	1.83	0.67
2:1B:71:ARG:NE	8:1H:36:GLY:HA2	2.10	0.66
22:1W:54:ILE:HG23	22:1W:104:MET:HE1	1.77	0.66
45:3N:63:ALA:CB	45:3N:97:TYR:CZ	2.78	0.66
3:5C:211:GLN:NE2	21:5V:114:PRO:O	2.28	0.66
45:6N:70:ARG:HD2	45:6N:75:LEU:HD23	1.75	0.66
20:1U:46:ASP:O	20:1U:50:ILE:HG13	1.95	0.66
46:3B:153:GLN:HE22	49:3I:42:VAL:HA	1.59	0.66
47:3C:253:PRO:C	48:3D:207:ALA:HA	2.20	0.66
6:5F:257:ASN:ND2	6:5F:267:THR:OG1	2.28	0.66
7:5G:21:GLU:CD	7:5G:21:GLU:H	2.03	0.66
45:6N:19:LEU:HG	45:6N:25:VAL:HG23	1.77	0.66
45:6N:304:CYS:HA	45:6N:326:CYS:CA	2.18	0.66
45:6N:395:TRP:HA	45:6N:398:ARG:HD2	1.76	0.66
5:1E:29:LYS:HE2	44:1s:56:VAL:HG11	1.76	0.66
10:1J:64:MET:HE1	11:1K:68:ALA:HA	1.76	0.66
20:1U:72:CYS:HB3	20:1U:75:GLU:HG3	1.76	0.66
25:1Z:86:MET:HE3	25:1Z:124:LEU:HG	1.76	0.66
47:3C:158:THR:O	47:3C:161:VAL:HG12	1.95	0.66
46:6B:76:THR:HG23	46:6B:81:SER:HA	1.77	0.66
45:6N:62:LEU:CD1	45:6N:182:LEU:HD13	2.26	0.66
2:1B:58:GLU:C	2:1B:61:HIS:N	2.53	0.66
75:1d:202:CDL:H321	75:1d:202:CDL:HB62	1.76	0.66
35:1j:19:ARG:HG3	65:8K:12:LYS:HA	1.77	0.66
47:3C:150:LEU:HD13	47:3C:161:VAL:HA	1.77	0.66
45:3N:92:ARG:HG3	45:3N:167:VAL:HG23	1.76	0.66
12:5L:10:THR:O	12:5L:14:ILE:HG22	1.96	0.66
12:5L:351:ASN:O	12:5L:351:ASN:ND2	2.27	0.66
21:5V:65:LYS:HD2	21:5V:69:GLU:OE1	1.95	0.66
37:5l:54:SER:HA	37:5l:84:TYR:HB3	1.78	0.66
52:6H:81:GLU:H	52:6H:81:GLU:CD	2.03	0.66
45:6N:186:VAL:HG22	45:6N:190:TYR:CE2	2.29	0.66
1:1A:87:MET:N	1:1A:87:MET:SD	2.68	0.66
9:1I:53:GLU:OE2	42:1q:34:ARG:NH2	2.29	0.66
12:1L:545:SER:OG	13:1M:274:SER:O	2.13	0.66
35:1j:19:ARG:NH2	65:8K:12:LYS:HD2	2.10	0.66
47:3C:69:ILE:HA	47:3C:73:VAL:HG23	1.78	0.66
46:3O:256:ALA:HB2	46:3O:325:TYR:HA	1.78	0.66
35:5j:33:TRP:CG	36:5k:70:PHE:HA	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:6U:22:GLU:HA	52:6U:25:GLU:HG2	1.76	0.66
13:1M:167:ILE:HD11	13:1M:195:MET:HE3	1.78	0.66
34:1i:85:LEU:O	34:1i:90:THR:HG23	1.95	0.66
47:3C:58:ASP:O	47:3C:59:THR:C	2.38	0.66
47:3C:74:ASN:HD22	49:3E:138:SER:HB3	1.60	0.66
45:3N:122:LEU:HD13	45:3N:183:THR:HG22	1.78	0.66
45:3N:356:ARG:CB	46:3O:91:ALA:HA	2.26	0.66
1:5A:1:FME:H	1:5A:4:MET:HE2	1.60	0.66
69:5L:703:3PE:H281	75:5i:201:CDL:HB62	1.78	0.66
20:5U:46:ASP:O	20:5U:50:ILE:HG13	1.95	0.66
45:6N:67:THR:H	45:6N:75:LEU:HD11	1.60	0.66
45:6N:257:VAL:HG12	45:6N:420:PRO:HB3	1.77	0.66
48:6Q:147:LEU:HD13	48:6Q:157:ALA:HB1	1.78	0.66
49:6R:149:MET:O	49:6R:151:LYS:N	2.28	0.66
45:3N:155:ALA:HA	45:3N:164:ALA:HB1	1.77	0.66
45:3N:255:ILE:HB	45:3N:422:VAL:HG13	1.77	0.66
5:5E:29:LYS:HE2	44:5s:56:VAL:HG11	1.76	0.66
7:5G:283:MET:HE3	7:5G:293:TYR:CE1	2.31	0.66
69:5L:703:3PE:H262	75:5i:201:CDL:HB32	1.78	0.66
35:5j:33:TRP:CE2	36:5k:70:PHE:HB2	2.31	0.66
45:6N:60:GLU:HB3	45:6N:64:PHE:HE2	1.61	0.66
45:6N:173:ASN:O	45:6N:177:LEU:HG	1.95	0.66
46:6O:29:LEU:HG	46:6O:35:ILE:HD11	1.78	0.66
55:8A:377:PHE:HB2	85:8A:606:HEA:C3D	2.26	0.66
10:1J:170:GLU:OE2	10:1J:173:ARG:NH2	2.28	0.66
23:1X:137:PRO:HB2	23:1X:140:PRO:HG3	1.76	0.66
45:3N:328:ASN:HD21	51:3T:6:HIS:CD2	2.14	0.66
8:5H:129:LEU:O	8:5H:133:LEU:HD23	1.96	0.66
46:6B:252:LEU:HD11	49:6I:49:PHE:HB2	1.78	0.66
6:1F:93:LEU:O	6:1F:134:ALA:HA	1.95	0.66
13:1M:207:MET:HE2	13:1M:298:ILE:HG13	1.77	0.66
13:1M:271:MET:HE2	13:1M:271:MET:HA	1.75	0.66
49:3E:93:ARG:HG3	51:3G:24:GLU:C	2.21	0.66
45:3N:250:LEU:HD13	45:3N:305:GLN:HG3	1.78	0.66
9:5I:53:GLU:OE2	42:5q:34:ARG:NH2	2.29	0.66
23:5X:137:PRO:HB2	23:5X:140:PRO:HG3	1.76	0.66
45:6N:71:PRO:HD2	45:6N:72:GLY:N	2.09	0.66
45:6N:151:ASP:N	45:6N:154:HIS:HD2	1.94	0.66
75:8A:610:CDL:H212	75:8A:610:CDL:H311	1.78	0.66
2:1B:104:TYR:CD2	2:1B:140:VAL:HG11	2.31	0.66
7:1G:21:GLU:H	7:1G:21:GLU:CD	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:129:LEU:O	8:1H:133:LEU:HD23	1.96	0.66
27:1b:63:PRO:CD	27:1b:63:PRO:HB3	2.19	0.66
47:3C:226:ILE:HG12	48:3D:311:MET:HB2	1.78	0.66
48:3D:220:THR:HG22	48:3D:268:MET:HE3	1.76	0.66
46:3O:201:SER:N	46:3O:228:GLY:HA2	2.10	0.66
48:3Q:147:LEU:HD13	48:3Q:157:ALA:HB1	1.78	0.66
82:4C:302:PGV:H241	82:4C:302:PGV:H91	1.78	0.66
6:5F:96:ASN:ND2	6:5F:187:GLY:O	2.26	0.66
21:5V:105:GLU:HG3	21:5V:106:PRO:HD2	1.78	0.66
45:6N:15:GLN:CG	45:6N:205:HIS:CE1	2.78	0.66
12:1L:61:MET:HE2	34:1i:98:GLU:HG2	1.77	0.65
49:3R:236:CYS:SG	49:3R:239:HIS:HB2	2.35	0.65
55:4A:37:ILE:HD11	55:4A:58:VAL:HA	1.77	0.65
75:4C:308:CDL:H311	75:4C:308:CDL:H212	1.78	0.65
75:5X:201:CDL:H231	75:5X:201:CDL:H171	1.78	0.65
30:5e:94:PRO:HD2	30:5e:97:HIS:HB2	1.77	0.65
38:5m:14:PRO:HG2	38:5m:17:LEU:HB2	1.78	0.65
47:6C:127:ALA:HA	83:6C:501:HEM:HHB	1.76	0.65
47:6C:184:ILE:HB	47:6P:183:PHE:CE1	2.31	0.65
49:6E:151:LYS:C	49:6E:152:ILE:HD12	2.20	0.65
45:6N:168:GLU:HB2	49:6R:81:THR:HG21	1.77	0.65
56:8B:104:TRP:CD2	56:8B:203:ASN:HB2	2.30	0.65
2:1B:46:TRP:HB3	2:1B:75:VAL:HB	1.78	0.65
3:1C:211:GLN:NE2	21:1V:114:PRO:O	2.28	0.65
10:1J:173:ARG:NH1	14:1N:1:FME:O1	2.28	0.65
46:3B:95:LYS:CD	49:3I:32:ALA:HB2	2.26	0.65
45:3N:170:PRO:HG3	45:3N:173:ASN:ND2	2.10	0.65
52:3U:22:GLU:HA	52:3U:25:GLU:HG2	1.76	0.65
56:4B:16:ILE:HG12	56:4B:87:MET:HG3	1.77	0.65
21:1V:105:GLU:HG3	21:1V:106:PRO:HD2	1.78	0.65
46:3B:308:ASP:OD2	49:3I:55:LEU:O	2.14	0.65
65:4K:47:ARG:HH12	82:4K:101:PGV:H211	1.61	0.65
4:5D:335:ARG:NH2	9:5I:129:ASP:OD1	2.29	0.65
14:5N:218:LEU:HB3	14:5N:244:MET:HE2	1.79	0.65
40:5o:21:MET:HG3	40:5o:104:GLU:HG2	1.78	0.65
47:6C:26:ASN:HB2	47:6C:208:PRO:HD2	1.79	0.65
47:6C:326:TRP:HB3	51:6G:54:PHE:CE2	2.29	0.65
55:8A:158:ILE:HG21	82:8A:602:PGV:H331	1.78	0.65
55:8A:334:TRP:HZ2	82:8B:301:PGV:H242	1.62	0.65
57:8C:76:GLN:O	57:8C:80:ARG:HG3	1.97	0.65
29:1d:89:ASP:HB2	33:1h:122:TRP:CH2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:107:ASP:HA	38:1m:110:LYS:HE2	1.79	0.65
48:3D:101:SER:O	48:3D:107:SER:OG	2.12	0.65
6:5F:93:LEU:O	6:5F:134:ALA:HA	1.95	0.65
36:5k:30:THR:O	36:5k:34:LYS:HG2	1.97	0.65
46:6O:76:THR:HG23	46:6O:81:SER:HA	1.79	0.65
55:8A:298:ASP:HA	62:8H:22:ASN:ND2	2.12	0.65
55:8A:442:ASP:HB3	56:8B:135:LEU:HD21	1.78	0.65
56:8B:16:ILE:HG12	56:8B:87:MET:HG3	1.77	0.65
38:1m:14:PRO:HG2	38:1m:17:LEU:HB2	1.79	0.65
46:3O:165:ALA:HA	46:3O:173:ALA:HB1	1.78	0.65
46:3O:275:LEU:HD13	46:3O:410:VAL:HG13	1.78	0.65
14:5N:142:LEU:HB3	14:5N:194:LEU:HD21	1.78	0.65
29:5d:89:ASP:HB2	33:5h:122:TRP:CH2	2.31	0.65
45:6A:328:ASN:HB3	45:6A:427:PRO:HB2	1.77	0.65
47:6C:275:LEU:HB3	47:6C:336:THR:HA	1.77	0.65
45:6N:248:LEU:HB2	45:6N:427:PRO:HD3	1.78	0.65
82:8L:101:PGV:H211	82:8L:101:PGV:H251	1.78	0.65
6:1F:224:ASN:ND2	73:1F:501:FMN:O2	2.28	0.65
6:1F:372:MET:HG3	6:1F:395:ILE:HD11	1.79	0.65
7:1G:534:ARG:NH2	7:1G:558:ASP:OD1	2.28	0.65
11:1K:3:LEU:O	11:1K:7:ASN:ND2	2.30	0.65
69:1L:703:3PE:H281	75:1i:201:CDL:HB62	1.78	0.65
14:1N:142:LEU:HB3	14:1N:194:LEU:HD21	1.78	0.65
37:1l:157:GLU:N	40:1o:34:LYS:O	2.30	0.65
47:3C:379:TRP:CE3	50:3F:45:ARG:HD3	2.32	0.65
45:3N:148:VAL:O	45:3N:152:TYR:CD2	2.50	0.65
47:3P:149:LEU:HD23	47:3P:287:LYS:HZ2	1.61	0.65
71:5H:401:PC1:H153	25:5Z:141:ILE:HA	1.79	0.65
13:5M:167:ILE:HD11	13:5M:195:MET:HE3	1.78	0.65
14:5N:313:MET:HG2	15:5O:270:LEU:HD13	1.78	0.65
41:5p:72:ASP:OD1	41:5p:74:THR:OG1	2.12	0.65
47:6C:44:GLN:HB3	83:6C:501:HEM:HAB	1.77	0.65
45:6N:329:MET:HA	45:6N:430:GLN:HE22	1.61	0.65
46:6O:376:GLU:OE1	46:6O:379:LEU:HD23	1.95	0.65
55:8A:169:ILE:CG2	75:8A:610:CDL:HA62	2.26	0.65
71:1H:401:PC1:H153	25:1Z:141:ILE:HA	1.78	0.65
43:1r:11:ARG:HD3	43:1r:19:LEU:HD11	1.79	0.65
47:3C:234:PHE:N	48:3D:305:LEU:HD21	2.11	0.65
45:3N:260:PRO:HD2	45:3N:313:CYS:HB2	1.78	0.65
55:4A:297:MET:O	55:4A:302:ARG:NH1	2.30	0.65
12:5L:257:VAL:HG23	12:5L:329:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5U:72:CYS:HB3	20:5U:75:GLU:HG3	1.76	0.65
48:6D:163:ASN:H	48:6D:167:GLU:H	1.45	0.65
45:6N:4:TYR:HE1	46:6O:112:LEU:HD22	1.62	0.65
45:6N:29:GLN:CG	45:6N:203:VAL:O	2.40	0.65
55:8A:510:TYR:HE1	60:8F:47:ASN:HB3	1.61	0.65
19:1S:21:HIS:O	19:1S:62:PRO:HA	1.96	0.65
49:3E:213:LEU:HD13	49:3E:258:LEU:HB2	1.77	0.65
46:3O:78:LYS:HE2	46:3O:131:GLU:HA	1.78	0.65
7:5G:304:ALA:O	7:5G:308:GLN:HG2	1.97	0.65
12:5L:183:VAL:HG21	13:5M:400:MET:HE1	1.78	0.65
48:6D:146:GLU:O	48:6D:147:GLU:C	2.39	0.65
54:6Y:45:VAL:HB	54:6Y:48:ILE:HB	1.78	0.65
4:1D:335:ARG:NH2	9:1I:129:ASP:OD1	2.29	0.65
16:1P:179:LEU:H	16:1P:179:LEU:HD23	1.62	0.65
47:3C:361:ILE:HG12	47:3C:365:LEU:HD12	1.78	0.65
55:4A:241:PRO:HG3	55:4A:284:GLY:O	1.96	0.65
4:5D:50:ASN:HA	4:5D:65:VAL:HA	1.78	0.65
11:5K:3:LEU:O	11:5K:7:ASN:ND2	2.30	0.65
47:6C:334:THR:HA	47:6C:337:TRP:HE3	1.62	0.65
55:8A:106:PRO:HB2	55:8A:107:PRO:HD3	1.79	0.65
55:8A:141:ALA:O	55:8A:142:SER:C	2.40	0.65
12:1L:257:VAL:HG23	12:1L:329:ILE:HD11	1.78	0.65
14:1N:218:LEU:HB3	14:1N:244:MET:HE2	1.79	0.65
46:3O:169:ARG:HD2	46:3O:238:LYS:HB3	1.77	0.65
49:3R:243:TYR:HB3	49:3R:247:GLY:HA2	1.79	0.65
48:6D:289:HIS:HA	48:6D:292:ARG:HB3	1.79	0.65
45:6N:15:GLN:CB	45:6N:205:HIS:ND1	2.58	0.65
45:6N:27:SER:OG	45:6N:205:HIS:HA	1.97	0.65
45:6N:188:GLN:O	45:6N:191:LYS:HE3	1.96	0.65
55:8A:204:ALA:HB3	57:8C:96:GLY:HA3	1.79	0.65
7:1G:283:MET:HE3	7:1G:293:TYR:CE1	2.31	0.64
12:1L:10:THR:O	12:1L:14:ILE:HG22	1.95	0.64
41:1p:166:ARG:HA	41:1p:170:LYS:HZ3	1.62	0.64
46:3B:308:ASP:OD2	49:3I:56:SER:HA	1.97	0.64
47:3C:366:MET:HB2	47:3C:367:PRO:HD3	1.77	0.64
45:3N:158:PHE:CD1	45:3N:163:LEU:HB2	2.32	0.64
45:3N:162:PRO:CD	45:3N:163:LEU:N	2.58	0.64
55:4A:107:PRO:HB3	57:4C:25:LEU:HB2	1.80	0.64
5:5E:213:VAL:HA	5:5E:217:LEU:HD13	1.79	0.64
45:6N:71:PRO:CG	45:6N:74:ALA:CB	2.75	0.64
45:6N:382:SER:HB3	45:6N:389:ARG:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:66:ILE:HG22	55:8A:71:MET:HG3	1.79	0.64
55:8A:404:THR:HG21	67:8M:3:ALA:HB2	1.79	0.64
55:8A:507:GLU:HG2	60:8F:56:ARG:NE	2.11	0.64
58:8D:60:TYR:OH	59:8E:69:GLU:OE1	2.07	0.64
31:1f:25:TYR:OH	31:1f:29:ARG:NH1	2.30	0.64
47:3C:226:ILE:HD13	48:3D:311:MET:HE2	1.79	0.64
45:3N:52:ASN:O	45:3N:53:ASN:C	2.40	0.64
45:3N:71:PRO:CD	45:3N:72:GLY:N	2.60	0.64
45:3N:118:GLN:NE2	45:3N:219:LEU:HA	2.12	0.64
7:5G:46:LEU:O	17:5Q:116:LYS:NZ	2.29	0.64
71:5Y:201:PC1:H221	71:5Y:201:PC1:H331	1.78	0.64
6:1F:362:CYS:HB3	6:1F:404:ILE:HD12	1.79	0.64
7:1G:304:ALA:O	7:1G:308:GLN:HG2	1.97	0.64
16:1P:82:ARG:HE	16:1P:86:GLU:HG2	1.62	0.64
65:4K:16:ALA:O	65:4K:20:SER:OG	2.15	0.64
1:5A:69:ILE:HD11	8:5H:144:VAL:HG13	1.80	0.64
6:5F:362:CYS:HB3	6:5F:404:ILE:HD12	1.79	0.64
6:5F:372:MET:HG3	6:5F:395:ILE:HD11	1.79	0.64
45:6A:15:GLN:HB3	45:6A:205:HIS:HB3	1.80	0.64
48:6D:135:ALA:H	48:6D:138:HIS:HB2	1.62	0.64
53:6J:19:SER:HB2	54:6Y:23:MET:HE2	1.79	0.64
45:6N:86:LEU:HD12	46:6O:285:VAL:HG22	1.78	0.64
46:6O:245:ARG:HE	46:6O:430:LEU:HB3	1.62	0.64
1:1A:74:PRO:HB2	10:1J:147:TYR:HE2	1.62	0.64
2:1B:60:MET:C	2:1B:61:HIS:C	2.65	0.64
13:1M:6:ILE:HG12	75:1X:201:CDL:H652	1.79	0.64
14:1N:313:MET:HG2	15:1O:270:LEU:HD13	1.78	0.64
46:3B:394:GLN:OE1	46:3B:394:GLN:N	2.21	0.64
47:3C:136:GLY:HA2	47:3C:255:ASN:O	1.98	0.64
47:3C:334:THR:HG21	47:3C:354:ALA:HB3	1.79	0.64
45:3N:165:GLN:HA	49:3R:84:ARG:HH22	1.61	0.64
45:3N:373:THR:HB	45:3N:374:PRO:HD3	1.79	0.64
56:4B:102:HIS:O	56:4B:103:GLN:C	2.41	0.64
57:4C:76:GLN:O	57:4C:80:ARG:HG3	1.96	0.64
13:5M:6:ILE:HG12	75:5X:201:CDL:H652	1.79	0.64
47:6C:138:MET:HA	47:6C:265:PRO:HG3	1.79	0.64
55:8A:233:HIS:HB3	57:8C:99:TRP:HZ2	1.62	0.64
7:1G:579:ARG:HB2	7:1G:636:VAL:HG22	1.79	0.64
46:3B:49:LEU:HD21	46:3B:204:MET:HE2	1.80	0.64
47:3C:253:PRO:HA	48:3D:206:ARG:O	1.97	0.64
51:3G:70:LYS:HA	51:3G:73:ARG:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:57:TYR:CD2	45:3N:167:VAL:HG12	2.26	0.64
49:3R:162:GLY:H	49:3R:178:HIS:HB3	1.63	0.64
53:3W:10:LEU:HD12	53:3W:14:LEU:HD12	1.80	0.64
55:4A:436:MET:HE1	55:4A:451:ASN:CG	2.22	0.64
19:5S:21:HIS:O	19:5S:62:PRO:HA	1.96	0.64
45:6A:172:GLU:HA	45:6A:175:ARG:HD2	1.80	0.64
47:6C:89:MET:HG2	47:6C:239:LEU:HB2	1.78	0.64
45:6N:106:LEU:CD1	45:6N:203:VAL:HG22	2.27	0.64
45:6N:170:PRO:HG3	45:6N:173:ASN:ND2	1.98	0.64
45:6N:347:THR:HB	54:6X:17:TRP:CH2	2.33	0.64
47:6P:5:ARG:HG3	47:6P:11:MET:HE2	1.79	0.64
1:1A:75:LEU:HA	1:1A:78:ALA:HB3	1.80	0.64
4:1D:50:ASN:HA	4:1D:65:VAL:HA	1.78	0.64
12:1L:504:LEU:HG	64:4J:30:ILE:HD11	1.80	0.64
69:1L:703:3PE:H262	75:1i:201:CDL:HB32	1.78	0.64
71:1Y:201:PC1:H221	71:1Y:201:PC1:H331	1.78	0.64
36:1k:30:THR:O	36:1k:34:LYS:HG2	1.97	0.64
49:3E:223:VAL:HG11	48:3Q:144:ARG:CZ	2.28	0.64
45:3N:27:SER:N	45:3N:205:HIS:ND1	2.41	0.64
45:3N:133:VAL:HG11	49:3V:53:GLU:CG	2.24	0.64
45:3N:291:SER:HA	46:3O:87:ARG:CZ	2.27	0.64
47:3P:278:TYR:CE2	47:3P:282:ARG:HD3	2.33	0.64
55:4A:423:MET:HE2	55:4A:456:MET:HB2	1.79	0.64
82:4A:604:PGV:H211	82:4C:303:PGV:H62	1.79	0.64
75:5q:201:CDL:H331	75:5q:201:CDL:H172	1.80	0.64
43:5r:11:ARG:HD3	43:5r:19:LEU:HD11	1.79	0.64
45:6A:27:SER:HB2	45:6A:199:ALA:HB3	1.80	0.64
45:6N:87:ASN:ND2	45:6N:100:LYS:CE	2.35	0.64
45:6N:118:GLN:CD	45:6N:218:SER:OG	2.39	0.64
2:1B:61:HIS:O	2:1B:64:ALA:N	2.31	0.64
2:1B:109:GLU:OE1	16:1P:54:TYR:OH	2.16	0.64
12:1L:481:THR:OG1	40:1o:91:HIS:ND1	2.26	0.64
82:4L:101:PGV:H211	82:4L:101:PGV:H251	1.78	0.64
45:6N:349:ALA:HB3	54:6X:16:ASN:HD21	1.62	0.64
46:6O:46:ARG:HB3	46:6O:209:LEU:HB2	1.79	0.64
47:6P:278:TYR:CE2	47:6P:282:ARG:HD3	2.33	0.64
55:8A:205:GLY:HA2	55:8A:208:MET:SD	2.38	0.64
55:8A:327:LEU:HB3	56:8B:45:MET:HG3	1.78	0.64
75:1X:201:CDL:H231	75:1X:201:CDL:H171	1.78	0.64
47:3C:47:THR:HB	47:3C:83:HIS:HB2	1.80	0.64
47:3C:73:VAL:HB	47:3C:76:GLY:HA3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:44:GLY:HA3	45:3N:92:ARG:C	2.23	0.64
45:3N:68:LYS:H	45:3N:119:ASN:HB3	1.62	0.64
16:5P:82:ARG:HE	16:5P:86:GLU:HG2	1.61	0.64
37:5l:157:GLU:N	40:5o:34:LYS:O	2.30	0.64
47:6C:347:PHE:HE1	51:6G:65:THR:HA	1.61	0.64
45:6N:41:ILE:CG1	45:6N:195:MET:HE1	2.28	0.64
45:6N:151:ASP:N	45:6N:154:HIS:CD2	2.66	0.64
45:6N:279:HIS:HB2	45:6N:308:GLN:HA	1.80	0.64
55:8A:230:LEU:HD11	57:8C:100:ALA:HA	1.80	0.64
45:3N:29:GLN:CD	45:3N:204:GLU:HA	2.21	0.64
49:3R:160:PRO:HD2	49:3R:163:LYS:HB3	1.80	0.64
55:4A:279:SER:HB3	68:4N:22:ILE:HG12	1.79	0.64
7:5G:302:ARG:HB2	7:5G:302:ARG:NH1	2.13	0.64
45:6A:49:ASN:H	45:6A:52:ASN:HB2	1.63	0.64
45:6A:58:PHE:HB3	45:6A:182:LEU:HD21	1.79	0.64
47:6C:101:GLY:HA2	47:6C:106:SER:HB2	1.79	0.64
45:6N:158:PHE:CE2	45:6N:236:PHE:CD1	2.71	0.64
45:6N:430:GLN:HA	51:6T:4:PHE:HB3	1.79	0.64
82:8K:101:PGV:H272	67:8M:19:LEU:HD23	1.80	0.64
14:1N:175:LEU:O	14:1N:179:MET:HG2	1.98	0.64
45:3N:34:THR:CG2	45:3N:102:LEU:CD2	2.66	0.64
45:3N:279:HIS:HD1	45:3N:284:TYR:HE2	1.46	0.64
46:3O:79:GLY:HA3	46:3O:125:ASN:HB3	1.80	0.64
49:3R:219:HIS:NE2	49:3R:239:HIS:CE1	2.66	0.64
1:5A:12:THR:O	1:5A:16:LEU:HD12	1.98	0.64
20:5U:25:ILE:HG12	20:5U:40:LEU:HD13	1.80	0.64
45:6N:204:GLU:HB2	45:6N:207:GLN:OE1	1.98	0.64
49:6R:162:GLY:H	49:6R:178:HIS:HB3	1.62	0.64
2:1B:25:ARG:HD3	2:1B:27:GLU:HB3	1.79	0.63
7:1G:190:MET:HB3	7:1G:192:MET:HE3	1.79	0.63
35:1j:37:LEU:HD13	36:1k:77:PHE:HB2	1.79	0.63
45:3A:360:ILE:HG23	49:3I:33:ALA:HA	1.79	0.63
46:3B:200:THR:HB	46:3B:227:ARG:HG2	1.79	0.63
47:3C:8:HIS:HB3	47:3C:11:MET:HB2	1.79	0.63
47:3C:213:SER:HA	50:3F:78:LEU:CD1	2.28	0.63
1:5A:60:ILE:HG21	10:5J:168:ILE:HG21	1.79	0.63
7:5G:190:MET:HB3	7:5G:192:MET:HE3	1.79	0.63
46:6B:133:ARG:HH11	46:6B:135:TRP:HE1	1.46	0.63
48:6D:135:ALA:CA	48:6D:178:TYR:HA	2.27	0.63
49:6E:223:VAL:HG11	48:6Q:144:ARG:CZ	2.28	0.63
45:6N:18:GLN:HE21	45:6N:24:ARG:NE	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:135:LEU:HD23	45:6N:138:LEU:CD1	2.28	0.63
45:6N:323:HIS:HE1	45:6N:325:VAL:HG22	1.62	0.63
2:1B:61:HIS:HD1	4:1D:171:PHE:HD2	0.66	0.63
14:1N:270:MET:HB3	14:1N:275:SER:HB3	1.81	0.63
40:1o:21:MET:HG3	40:1o:104:GLU:HG2	1.78	0.63
45:3N:70:ARG:NH2	45:3N:78:GLU:OE1	2.30	0.63
45:3N:170:PRO:HD2	45:3N:170:PRO:O	1.96	0.63
49:3R:248:ARG:HD2	49:3R:257:ASN:HD22	1.63	0.63
57:4C:247:VAL:HG21	75:4C:308:CDL:H842	1.80	0.63
1:5A:33:LYS:HG2	8:5H:61:LEU:HD11	1.79	0.63
14:5N:175:LEU:O	14:5N:179:MET:HG2	1.98	0.63
37:5l:98:TRP:HA	37:5l:101:MET:HE3	1.80	0.63
45:6A:305:GLN:H	45:6A:326:CYS:HA	1.64	0.63
48:6D:317:SER:HA	48:6D:320:LYS:HD2	1.79	0.63
45:6N:18:GLN:HA	45:6N:24:ARG:HA	1.80	0.63
19:1S:64:LEU:HB3	19:1S:76:VAL:HG22	1.80	0.63
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.78	0.63
47:3C:107:TYR:HB2	47:3C:305:PRO:HG3	1.79	0.63
47:3C:334:THR:HA	51:3G:57:PHE:HZ	1.61	0.63
51:3G:36:ILE:HB	51:3G:37:PRO:HD3	1.79	0.63
45:3N:7:ALA:O	45:3N:10:SER:OG	2.12	0.63
45:3N:8:LEU:HD13	45:3N:393:ALA:CA	2.26	0.63
45:3N:192:ALA:HB2	45:3N:219:LEU:HB3	1.79	0.63
19:5S:64:LEU:HB3	19:5S:76:VAL:HG22	1.80	0.63
49:6R:219:HIS:NE2	49:6R:239:HIS:CE1	2.66	0.63
55:8A:349:THR:HA	85:8A:606:HEA:H162	1.80	0.63
85:8A:605:HEA:HHC	85:8A:605:HEA:H131	1.80	0.63
11:1K:37:MET:HE2	11:1K:67:ALA:HB3	1.81	0.63
64:4J:37:THR:HA	82:4J:101:PGV:H151	1.80	0.63
47:6C:6:LYS:HA	47:6C:12:LYS:HA	1.79	0.63
48:6D:159:GLN:HA	48:6D:170:MET:HA	1.81	0.63
45:6N:41:ILE:HD12	45:6N:97:TYR:HD2	1.53	0.63
45:6N:58:PHE:CG	45:6N:134:ILE:HD13	2.32	0.63
5:1E:100:ILE:HG13	5:1E:156:ILE:HD12	1.79	0.63
5:1E:213:VAL:HA	5:1E:217:LEU:HD13	1.79	0.63
12:1L:484:LEU:O	12:1L:484:LEU:HD22	1.98	0.63
35:1j:19:ARG:HE	65:8K:12:LYS:HG2	1.62	0.63
45:3N:61:HIS:HB3	45:3N:130:GLU:CD	2.23	0.63
45:3N:362:ARG:HG3	45:3N:399:ILE:HG21	1.80	0.63
46:3O:315:SER:CA	46:3O:320:GLY:HA2	2.25	0.63
48:3Q:118:ARG:HG3	48:3Q:194:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:50:ASN:HB2	4:5D:65:VAL:HG22	1.80	0.63
12:5L:484:LEU:HD22	12:5L:484:LEU:O	1.98	0.63
12:5L:504:LEU:HG	64:8J:30:ILE:HD11	1.80	0.63
45:3A:240:GLU:OE1	45:3A:242:ARG:NH1	2.32	0.63
46:3B:397:THR:HA	46:3B:400:GLN:NE2	2.12	0.63
47:3C:150:LEU:HB3	47:3C:161:VAL:HB	1.81	0.63
47:3C:212:SER:O	50:3F:78:LEU:HD11	1.99	0.63
45:3N:153:LEU:HD11	45:3N:254:ALA:HB3	1.81	0.63
6:5F:194:GLU:OE2	17:5Q:133:LYS:HE2	1.98	0.63
8:5H:81:LEU:HD21	8:5H:111:LEU:HD12	1.81	0.63
16:5P:179:LEU:HD23	16:5P:179:LEU:H	1.62	0.63
46:6B:314:ALA:HB3	46:6B:321:LEU:HB2	1.79	0.63
45:6N:99:ILE:HD11	45:6N:113:LEU:HD21	1.72	0.63
45:6N:136:GLN:HB3	49:6V:50:LEU:HB2	1.79	0.63
4:1D:50:ASN:HB2	4:1D:65:VAL:HG22	1.80	0.63
14:1N:1:FME:HCN	15:1O:258:ARG:HH11	1.64	0.63
14:1N:54:GLU:OE1	14:1N:58:LYS:NZ	2.32	0.63
31:1f:14:ILE:O	31:1f:18:VAL:HG22	1.99	0.63
45:3N:153:LEU:O	45:3N:156:THR:OG1	2.16	0.63
46:3O:316:TYR:O	46:3O:317:SER:C	2.42	0.63
47:3P:142:GLY:O	47:3P:146:ILE:HD12	1.99	0.63
2:5B:109:GLU:OE1	16:5P:54:TYR:OH	2.16	0.63
38:5m:107:ASP:HA	38:5m:110:LYS:HE2	1.79	0.63
47:6C:73:VAL:HG22	49:6E:143:SER:HB3	1.79	0.63
47:6C:260:ASN:HD22	47:6C:263:ASN:HD22	1.45	0.63
45:6N:268:VAL:HG21	45:6N:398:ARG:HD3	1.81	0.63
50:6S:52:GLU:OE2	51:6T:11:ARG:NH1	2.29	0.63
1:1A:106:TRP:CE2	8:1H:291:LYS:HD3	2.33	0.63
2:1B:100:LEU:O	2:1B:104:TYR:HD2	1.73	0.63
6:1F:194:GLU:OE2	17:1Q:133:LYS:HE2	1.98	0.63
45:3N:99:ILE:HD12	45:3N:113:LEU:HG	1.80	0.63
45:3N:392:LEU:HD23	45:3N:395:TRP:HD1	1.63	0.63
85:4A:605:HEA:H131	85:4A:605:HEA:HHC	1.80	0.63
38:5m:22:TYR:HB3	39:5n:64:ARG:NE	2.13	0.63
46:6O:386:ALA:HA	46:6O:390:GLY:HA2	1.79	0.63
49:6R:243:TYR:HB3	49:6R:247:GLY:HA2	1.79	0.63
13:1M:158:LEU:HD22	14:1N:283:ALA:HB1	1.81	0.63
14:1N:109:SER:HB2	14:1N:157:MET:HG2	1.81	0.63
28:1c:19:LEU:HB3	75:1d:202:CDL:H132	1.80	0.63
29:1d:43:LEU:HD23	69:1d:201:3PE:H371	1.81	0.63
47:3C:258:PRO:HG2	48:3D:200:ASP:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:310:SER:HA	47:3C:374:ASN:HD21	1.64	0.63
47:3C:347:PHE:H	51:3G:68:PHE:HE1	1.46	0.63
45:3N:158:PHE:CZ	45:3N:314:TYR:HE2	2.17	0.63
46:3O:250:ASP:H	46:3O:428:GLY:HA2	1.64	0.63
56:4B:216:LEU:O	56:4B:220:GLU:HG2	1.99	0.63
9:5I:78:ILE:C	9:5I:78:ILE:HD12	2.24	0.63
21:5V:69:GLU:O	21:5V:72:GLN:NE2	2.32	0.63
47:6C:8:HIS:HB3	47:6C:11:MET:HB2	1.80	0.63
52:6H:45:VAL:HG12	52:6H:94:VAL:HG22	1.80	0.63
45:6N:19:LEU:CD1	45:6N:23:LEU:HD12	2.27	0.63
55:8A:192:ALA:HA	55:8A:195:LEU:HD12	1.81	0.63
55:8A:193:VAL:HG22	75:8A:610:CDL:H351	1.81	0.63
55:8A:208:MET:HB3	55:8A:219:PHE:CG	2.33	0.63
59:8E:42:VAL:HB	63:8I:9:MET:HB3	1.81	0.63
6:1F:326:GLN:O	6:1F:420:ARG:NH2	2.32	0.62
7:1G:302:ARG:HB2	7:1G:302:ARG:NH1	2.13	0.62
13:1M:260:PRO:HG3	69:1M:503:3PE:H371	1.81	0.62
21:1V:69:GLU:O	21:1V:72:GLN:NE2	2.32	0.62
75:1X:201:CDL:H272	75:1X:201:CDL:H452	1.81	0.62
30:1e:23:GLU:OE1	30:1e:23:GLU:N	2.30	0.62
47:3C:242:LEU:HA	47:3C:246:SER:HB3	1.81	0.62
49:3E:238:CYS:HA	48:3Q:147:LEU:HD11	1.80	0.62
49:3E:263:TYR:HB2	49:3E:272:ILE:H	1.64	0.62
50:3F:116:ARG:HG2	46:3O:83:PHE:CE2	2.34	0.62
45:3N:18:GLN:NE2	45:3N:24:ARG:HG3	2.06	0.62
45:3N:40:TRP:CD1	45:3N:380:GLY:HA3	2.34	0.62
45:3N:352:SER:O	45:3N:356:ARG:N	2.28	0.62
47:3P:5:ARG:HG3	47:3P:11:MET:HE2	1.79	0.62
7:5G:579:ARG:HB2	7:5G:636:VAL:HG22	1.79	0.62
31:5f:25:TYR:OH	31:5f:29:ARG:NH1	2.30	0.62
45:6A:366:VAL:HG13	46:6B:43:PRO:HB2	1.81	0.62
46:6B:254:HIS:HA	46:6B:327:ILE:HA	1.81	0.62
45:6N:18:GLN:HG2	45:6N:24:ARG:HG2	1.78	0.62
45:6N:58:PHE:HD1	45:6N:134:ILE:HD12	1.53	0.62
45:6N:70:ARG:CD	45:6N:75:LEU:HD23	2.28	0.62
45:6N:301:ARG:HG3	45:6N:303:LEU:HG	1.80	0.62
46:6O:243:GLU:HG3	46:6O:424:MET:HB3	1.81	0.62
47:6P:207:ASN:ND2	47:6P:211:ILE:O	2.32	0.62
55:8A:158:ILE:HG12	57:8C:89:SER:HB3	1.81	0.62
1:1A:115:GLU:HG3	4:1D:72:MET:HG3	1.79	0.62
8:1H:81:LEU:HD21	8:1H:111:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:104:TYR:HB3	47:3C:206:ASN:HD21	1.64	0.62
45:3N:153:LEU:HD23	45:3N:423:ALA:CB	2.29	0.62
62:4H:14:ALA:CB	62:4H:63:PHE:HE1	2.09	0.62
14:5N:172:GLN:HB2	14:5N:178:ILE:HG13	1.81	0.62
45:6N:193:PRO:CD	45:6N:194:ARG:N	2.56	0.62
46:6O:241:GLY:HA2	46:6O:423:SER:HB3	1.80	0.62
47:6P:142:GLY:O	47:6P:146:ILE:HD12	1.99	0.62
48:6Q:118:ARG:HG3	48:6Q:194:SER:HB3	1.80	0.62
55:8A:159:LEU:HA	55:8A:162:ILE:HD12	1.81	0.62
7:1G:190:MET:HB3	7:1G:192:MET:CE	2.30	0.62
9:1I:78:ILE:C	9:1I:78:ILE:HD12	2.24	0.62
12:1L:183:VAL:HG21	13:1M:400:MET:HE1	1.78	0.62
34:1i:103:ILE:HB	40:1o:47:ASP:HB2	1.82	0.62
37:1l:10:PRO:HD3	38:1m:66:ARG:HG2	1.80	0.62
37:1l:98:TRP:HA	37:1l:101:MET:HE3	1.79	0.62
38:1m:22:TYR:HB3	39:1n:64:ARG:NE	2.13	0.62
45:3A:381:ARG:NH2	45:3A:382:SER:OG	2.32	0.62
47:3C:165:TRP:HE1	47:3C:170:VAL:HG22	1.65	0.62
45:3N:27:SER:HG	45:3N:205:HIS:CE1	2.13	0.62
45:3N:52:ASN:HB3	45:3N:185:TYR:CE1	2.31	0.62
45:3N:433:ASP:HB3	45:3N:436:ARG:HG2	1.80	0.62
46:3O:111:CYS:SG	46:3O:112:LEU:N	2.73	0.62
82:4C:302:PGV:H11	82:4C:302:PGV:H272	1.80	0.62
11:5K:73:LEU:HD22	14:5N:38:LEU:HD12	1.80	0.62
21:5V:8:THR:HG21	21:5V:13:LEU:HD23	1.81	0.62
48:6D:255:ASN:HA	52:6H:38:LEU:HD23	1.81	0.62
49:6E:263:TYR:HB2	49:6E:272:ILE:H	1.64	0.62
45:6N:246:ASP:HB2	51:6T:9:ARG:HG3	1.81	0.62
46:6O:47:ILE:HB	46:6O:109:VAL:HG23	1.81	0.62
49:6R:248:ARG:HD2	49:6R:257:ASN:HD22	1.64	0.62
55:8A:279:SER:CB	68:8N:22:ILE:HG12	2.29	0.62
56:8B:216:LEU:O	56:8B:220:GLU:HG2	1.99	0.62
9:1I:27:TRP:HB3	9:1I:30:LEU:HD12	1.81	0.62
15:1O:305:SER:O	15:1O:309:ASN:ND2	2.33	0.62
41:1p:72:ASP:OD1	41:1p:74:THR:OG1	2.12	0.62
42:1q:60:ARG:HH22	42:1q:95:ASP:HA	1.65	0.62
49:3E:93:ARG:HG2	51:3G:26:ARG:HA	1.82	0.62
50:3F:61:ARG:HG2	46:3O:135:TRP:CD1	2.35	0.62
45:3N:106:LEU:HD21	45:3N:203:VAL:HG21	1.80	0.62
46:3O:279:LEU:HB2	46:3O:311:ALA:HB2	1.82	0.62
13:5M:260:PRO:HG3	69:5M:503:3PE:H371	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5c:19:LEU:HB3	75:5d:202:CDL:H132	1.80	0.62
29:5d:2:MET:N	81:5h:201:AME:O	2.32	0.62
39:5n:96:TYR:HB3	39:5n:178:MET:HB3	1.82	0.62
47:6C:30:TRP:HB3	47:6C:100:ARG:HG3	1.82	0.62
47:6C:220:PHE:HA	47:6C:224:TYR:HB2	1.81	0.62
47:6C:334:THR:HB	51:6G:57:PHE:HE1	1.64	0.62
49:6E:238:CYS:HA	48:6Q:147:LEU:HD11	1.81	0.62
53:6W:10:LEU:HD12	53:6W:14:LEU:HD12	1.80	0.62
82:8B:301:PGV:H241	75:8D:201:CDL:H411	1.81	0.62
12:1L:385:TYR:OH	35:1j:43:ASP:O	2.16	0.62
21:1V:8:THR:HG21	21:1V:13:LEU:HD23	1.81	0.62
45:3A:132:ASP:O	45:3A:136:GLN:HG2	2.00	0.62
48:3D:239:PRO:HB3	52:3H:84:PHE:CE1	2.35	0.62
47:3P:207:ASN:ND2	47:3P:211:ILE:O	2.32	0.62
4:5D:115:GLU:HG3	4:5D:194:ILE:HB	1.82	0.62
14:5N:54:GLU:OE1	14:5N:58:LYS:NZ	2.32	0.62
30:5e:23:GLU:N	30:5e:23:GLU:OE1	2.30	0.62
47:6C:54:HIS:CE1	49:6E:139:SER:HB2	2.34	0.62
47:6C:358:TYR:HA	47:6C:361:ILE:HD12	1.80	0.62
52:6H:54:LYS:HA	52:6H:57:LYS:HE2	1.82	0.62
45:6N:41:ILE:HG12	45:6N:195:MET:HE1	1.79	0.62
55:8A:191:THR:HG23	55:8A:245:ILE:HG23	1.81	0.62
13:1M:17:MET:HE1	29:1d:54:VAL:HG21	1.82	0.62
29:1d:2:MET:N	81:1h:201:AME:O	2.32	0.62
47:3C:137:GLN:HB2	47:3C:257:THR:HB	1.80	0.62
45:3N:70:ARG:HB2	45:3N:75:LEU:HD21	1.82	0.62
45:3N:166:SER:OG	49:3R:81:THR:CG2	2.47	0.62
15:5O:34:GLY:HA2	15:5O:37:ARG:HD2	1.82	0.62
15:5O:305:SER:O	15:5O:309:ASN:ND2	2.33	0.62
31:5f:14:ILE:O	31:5f:18:VAL:HG22	1.99	0.62
48:6D:307:LEU:HA	48:6D:310:ALA:HB3	1.82	0.62
46:6O:56:ARG:C	46:6O:58:GLU:N	2.57	0.62
75:1L:702:CDL:H651	69:1L:703:3PE:H3A1	1.82	0.62
13:5M:158:LEU:HD22	14:5N:283:ALA:HB1	1.81	0.62
47:6C:236:MET:HA	47:6C:239:LEU:HB3	1.80	0.62
48:6D:100:TRP:HB2	48:6D:103:ARG:HD2	1.82	0.62
48:6D:318:VAL:HG23	51:6G:22:PRO:HD3	1.80	0.62
45:6N:309:THR:HA	45:6N:322:ALA:CA	2.20	0.62
49:6R:160:PRO:HD2	49:6R:163:LYS:HB3	1.80	0.62
55:8A:427:PRO:HB3	55:8A:450:TRP:HB3	1.81	0.62
7:1G:226:GLU:HG2	7:1G:253:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:561:ILE:HG23	71:1m:201:PC1:H291	1.82	0.62
16:1P:122:LYS:NZ	16:1P:162:GLU:OE1	2.33	0.62
47:3C:45:ILE:HA	83:3C:501:HEM:HMC2	1.80	0.62
47:3C:155:TYR:N	47:3C:158:THR:HB	2.13	0.62
45:3N:108:LYS:O	45:3N:109:ALA:C	2.43	0.62
45:3N:127:ILE:HD12	45:3N:179:ARG:HG3	1.82	0.62
45:3N:168:GLU:HB2	49:3R:81:THR:HG21	1.82	0.62
45:3N:268:VAL:HB	45:3N:269:PRO:HD3	1.80	0.62
2:5B:68:ASP:O	2:5B:71:ARG:HG2	2.00	0.62
5:5E:100:ILE:HG13	5:5E:156:ILE:HD12	1.80	0.62
75:5L:702:CDL:H651	69:5L:703:3PE:H3A1	1.82	0.62
42:5q:78:ASP:OD2	42:5q:80:SER:OG	2.17	0.62
46:6B:64:GLY:CA	46:6B:178:CYS:HA	2.30	0.62
47:6C:33:PHE:HA	47:6C:36:LEU:HG	1.80	0.62
45:6N:242:ARG:HA	45:6N:424:GLY:CA	2.29	0.62
20:1U:25:ILE:HG12	20:1U:40:LEU:HD13	1.80	0.62
75:1q:201:CDL:H172	75:1q:201:CDL:H331	1.80	0.62
45:3A:354:VAL:HG21	45:3A:404:ALA:HA	1.81	0.62
45:3N:297:VAL:HA	47:3P:1:MET:SD	2.39	0.62
46:3O:274:VAL:HG21	46:3O:405:VAL:HG11	1.81	0.62
52:3U:57:GLU:OE1	52:3U:57:GLU:N	2.32	0.62
1:5A:58:VAL:HG21	8:5H:286:MET:CE	2.30	0.62
47:6C:75:TYR:HE2	49:6E:135:GLN:HG2	1.65	0.62
47:6C:224:TYR:O	47:6C:225:THR:C	2.43	0.62
45:6N:19:LEU:HG	45:6N:25:VAL:CG2	2.30	0.62
52:6U:57:GLU:OE1	52:6U:57:GLU:N	2.32	0.62
55:8A:182:PRO:HB3	55:8A:256:HIS:HE1	1.65	0.62
55:8A:190:ILE:HG23	82:8A:603:PGV:H262	1.82	0.62
59:8E:16:VAL:HG23	59:8E:47:ILE:HG22	1.82	0.62
7:1G:382:THR:HG23	7:1G:384:PRO:HD3	1.82	0.62
11:1K:73:LEU:HD22	14:1N:38:LEU:HD12	1.81	0.62
14:1N:170:LEU:HD11	14:1N:288:LEU:HD22	1.82	0.62
14:1N:172:GLN:HB2	14:1N:178:ILE:HG13	1.81	0.62
45:3A:126:GLN:HA	45:3A:129:LYS:HD3	1.82	0.62
45:3A:172:GLU:OE1	45:3A:172:GLU:N	2.29	0.62
47:3C:51:LEU:HD13	83:3C:501:HEM:HBD1	1.82	0.62
45:3N:30:SER:N	45:3N:202:GLY:HA2	2.14	0.62
45:3N:42:ASP:HA	45:3N:94:HIS:CG	2.32	0.62
7:5G:226:GLU:HG2	7:5G:253:ARG:HD3	1.82	0.62
12:5L:561:ILE:HG23	71:5m:201:PC1:H291	1.82	0.62
2:1B:119:CYS:SG	70:1B:201:SF4:S3	2.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:46:LEU:O	17:1Q:116:LYS:NZ	2.30	0.61
39:1n:96:TYR:HB3	39:1n:178:MET:HB3	1.82	0.61
49:3E:150:SER:HB3	49:3E:170:ARG:HG3	1.82	0.61
45:3N:62:LEU:HA	45:3N:65:LYS:CG	2.30	0.61
45:3N:165:GLN:HA	49:3R:84:ARG:NH2	2.15	0.61
56:4B:13:THR:CG2	56:4B:168:LEU:HG	2.30	0.61
63:4I:22:VAL:O	63:4I:26:ILE:HG12	2.00	0.61
7:5G:382:THR:HG23	7:5G:384:PRO:HD3	1.82	0.61
11:5K:37:MET:HE2	11:5K:67:ALA:HB3	1.81	0.61
20:5U:20:LYS:HD2	20:5U:27:PRO:HB3	1.81	0.61
37:5l:10:PRO:HD3	38:5m:66:ARG:HG2	1.80	0.61
47:6C:129:MET:HG2	47:6C:182:HIS:HB2	1.82	0.61
45:6N:71:PRO:CG	45:6N:74:ALA:HB2	2.30	0.61
55:8A:184:PHE:HA	55:8A:252:GLY:HA3	1.81	0.61
55:8A:381:LEU:O	55:8A:382:SER:C	2.43	0.61
75:8A:610:CDL:H842	57:8C:247:VAL:HG21	1.80	0.61
56:8B:13:THR:CG2	56:8B:168:LEU:HG	2.30	0.61
62:8H:29:CYS:HB3	62:8H:63:PHE:HB3	1.82	0.61
42:1q:78:ASP:OD2	42:1q:80:SER:OG	2.17	0.61
45:3N:14:THR:CG2	45:3N:28:GLU:CG	2.65	0.61
47:3P:8:HIS:HB3	47:3P:11:MET:HB2	1.82	0.61
47:6C:24:PRO:HB3	47:6C:213:SER:HB2	1.81	0.61
48:6D:201:LEU:HA	48:6D:204:ILE:HB	1.82	0.61
45:6N:263:ALA:HB2	45:6N:386:TYR:HA	1.82	0.61
47:6P:8:HIS:HB3	47:6P:11:MET:HB2	1.82	0.61
55:8A:55:ASN:CB	56:8B:199:ILE:HD11	2.30	0.61
55:8A:197:LEU:HD11	75:8A:610:CDL:H382	1.82	0.61
65:8K:16:ALA:O	65:8K:20:SER:OG	2.15	0.61
2:1B:63:ALA:HB2	2:1B:69:MET:SD	2.39	0.61
4:1D:149:ASN:OD1	4:1D:371:LYS:NZ	2.26	0.61
46:3O:95:LYS:HA	49:3V:70:LEU:HD23	1.81	0.61
55:4A:62:ALA:HB2	85:4A:605:HEA:HBD1	1.82	0.61
57:4C:63:ARG:NH1	64:4J:20:VAL:O	2.34	0.61
59:4E:42:VAL:HB	63:4I:9:MET:HB3	1.81	0.61
7:5G:350:PRO:HB3	7:5G:464:THR:HG22	1.83	0.61
13:5M:281:ASP:HB3	13:5M:284:SER:HB3	1.82	0.61
14:5N:1:FME:HCN	15:5O:258:ARG:HH11	1.64	0.61
46:6B:156:GLN:O	46:6B:157:ALA:C	2.43	0.61
45:6N:80:GLU:HB3	46:6O:292:THR:HG21	1.82	0.61
47:3C:136:GLY:CA	47:3C:255:ASN:HA	2.31	0.61
45:3N:55:ALA:HB1	45:3N:185:TYR:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:159:GLN:CG	49:3R:85:VAL:HG21	2.26	0.61
45:3N:363:ASN:ND2	46:3O:112:LEU:HD11	2.15	0.61
46:3O:134:ARG:HH11	46:3O:134:ARG:HB2	1.64	0.61
47:3P:377:LEU:HG	50:3S:20:TYR:HE2	1.66	0.61
10:5J:159:TRP:HE1	14:5N:12:THR:HG23	1.65	0.61
16:5P:122:LYS:NZ	16:5P:162:GLU:OE1	2.33	0.61
46:6B:143:GLN:HA	46:6B:146:ILE:HD12	1.81	0.61
47:6C:39:ILE:HA	47:6C:42:ILE:HD12	1.82	0.61
47:6C:379:TRP:CE3	50:6F:45:ARG:HD3	2.35	0.61
48:6D:211:GLY:O	48:6D:212:GLU:C	2.44	0.61
63:8I:22:VAL:O	63:8I:26:ILE:HG12	2.00	0.61
3:1C:181:LYS:HD3	16:1P:174:ARG:HD2	1.83	0.61
14:1N:10:ILE:O	14:1N:14:MET:HG2	2.00	0.61
47:3C:72:ASP:CB	49:3E:144:ALA:HB3	2.30	0.61
45:3N:62:LEU:HD13	45:3N:122:LEU:HA	1.81	0.61
45:3N:176:LYS:O	45:3N:177:LEU:C	2.43	0.61
46:3O:24:LEU:CG	46:3O:26:PHE:HD2	2.11	0.61
55:4A:436:MET:HE1	55:4A:451:ASN:OD1	2.01	0.61
58:4D:102:TYR:HE2	36:5k:90:GLN:HB3	1.62	0.61
65:4K:8:ASP:H	65:4K:11:ASP:HB2	1.65	0.61
6:5F:326:GLN:O	6:5F:420:ARG:NH2	2.33	0.61
7:5G:140:LYS:O	7:5G:148:THR:OG1	2.18	0.61
7:5G:524:LEU:HG	7:5G:527:ALA:HB3	1.82	0.61
9:5I:27:TRP:HB3	9:5I:30:LEU:HD12	1.81	0.61
14:5N:289:ASN:HA	14:5N:292:PHE:CE2	2.36	0.61
29:5d:43:LEU:HD23	69:5d:201:3PE:H371	1.81	0.61
45:6N:57:TYR:O	45:6N:61:HIS:CD2	2.53	0.61
47:6P:267:HIS:HD2	47:6P:269:LYS:HG2	1.66	0.61
55:8A:72:PRO:O	55:8A:73:ILE:C	2.44	0.61
3:1C:173:GLU:HG3	3:1C:188:VAL:HG23	1.82	0.61
20:1U:20:LYS:HD2	20:1U:27:PRO:HB3	1.81	0.61
31:1f:53:GLU:HG2	31:1f:54:VAL:HG22	1.83	0.61
47:3C:132:VAL:HA	47:3C:139:SER:HB3	1.82	0.61
48:3D:106:LEU:HD22	48:3D:295:LEU:HB2	1.82	0.61
45:3N:363:ASN:H	45:3N:363:ASN:HD22	1.48	0.61
3:5C:173:GLU:HG3	3:5C:188:VAL:HG23	1.82	0.61
4:5D:282:GLU:O	4:5D:313:GLN:NE2	2.23	0.61
14:5N:109:SER:HB2	14:5N:157:MET:HG2	1.81	0.61
47:6C:330:ALA:HB1	51:6G:57:PHE:CB	2.31	0.61
46:3B:117:GLU:O	46:3B:121:GLU:HG2	2.01	0.61
45:3N:124:ASP:HB2	45:3N:179:ARG:CZ	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:239:SER:HB2	51:3T:17:SER:O	2.00	0.61
55:4A:236:TRP:HE3	55:4A:239:GLY:HA3	1.64	0.61
1:5A:61:THR:O	1:5A:65:PHE:HD1	1.84	0.61
7:5G:190:MET:HB3	7:5G:192:MET:CE	2.30	0.61
7:5G:379:LEU:HB2	7:5G:408:LEU:HD23	1.82	0.61
14:5N:270:MET:HB3	14:5N:275:SER:HB3	1.81	0.61
47:6C:45:ILE:HG12	47:6C:186:PRO:HB3	1.81	0.61
47:6C:330:ALA:HB2	51:6G:54:PHE:CD1	2.36	0.61
55:8A:374:VAL:HA	55:8A:377:PHE:CD2	2.36	0.61
57:8C:259:TRP:O	68:8N:47:ARG:NH2	2.34	0.61
6:1F:297:VAL:HG22	6:1F:336:VAL:HG22	1.83	0.61
7:1G:524:LEU:HG	7:1G:527:ALA:HB3	1.82	0.61
7:5G:315:VAL:O	7:5G:340:SER:OG	2.18	0.61
14:5N:170:LEU:HD11	14:5N:288:LEU:HD22	1.82	0.61
45:6A:131:ARG:HD3	45:6A:175:ARG:HA	1.83	0.61
45:6N:14:THR:HG23	45:6N:389:ARG:HH21	1.65	0.61
45:6N:14:THR:HG21	45:6N:389:ARG:NH2	2.16	0.61
45:6N:33:PRO:HD2	45:6N:34:THR:N	2.16	0.61
75:8A:610:CDL:H141	75:8A:610:CDL:H541	1.83	0.61
57:8C:165:ILE:HG12	82:8C:301:PGV:H11	1.82	0.61
75:8D:201:CDL:H561	75:8D:201:CDL:H402	1.82	0.61
62:8H:39:CYS:HG	62:8H:53:CYS:HG	1.48	0.61
7:1G:140:LYS:O	7:1G:148:THR:OG1	2.18	0.61
10:1J:4:TYR:O	10:1J:8:ILE:HD12	2.01	0.61
15:1O:34:GLY:HA2	15:1O:37:ARG:HD2	1.82	0.61
39:1n:134:ARG:NH2	39:1n:138:GLN:HB2	2.16	0.61
45:3N:170:PRO:CG	45:3N:173:ASN:HB2	2.30	0.61
45:3N:291:SER:HA	46:3O:87:ARG:NE	2.16	0.61
57:4C:165:ILE:HG12	82:4C:301:PGV:H11	1.83	0.61
10:5J:167:VAL:HG22	14:5N:42:PRO:HG2	1.82	0.61
75:5X:201:CDL:H272	75:5X:201:CDL:H452	1.81	0.61
47:6C:138:MET:O	47:6C:139:SER:C	2.42	0.61
45:6N:58:PHE:CZ	45:6N:174:VAL:CG1	2.83	0.61
47:6P:377:LEU:HG	50:6S:20:TYR:HE2	1.66	0.61
14:1N:69:MET:HE1	14:1N:104:MET:CE	2.31	0.61
46:3B:74:SER:O	46:3B:82:SER:OG	2.17	0.61
6:5F:137:TYR:HA	6:5F:178:VAL:HG23	1.83	0.61
35:5j:37:LEU:HB3	36:5k:77:PHE:CD2	2.36	0.61
47:6C:46:LEU:C	49:6E:136:PHE:HE2	2.09	0.61
48:6D:145:THR:H	48:6D:148:GLU:HB3	1.65	0.61
45:6N:46:ARG:CZ	45:6N:93:GLU:OE2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:68:GLU:HB3	1:1A:98:LEU:HG	1.83	0.60
2:1B:61:HIS:HE1	4:1D:174:ARG:HE	1.39	0.60
2:1B:113:VAL:HG11	2:1B:140:VAL:HG21	1.83	0.60
7:1G:379:LEU:HB2	7:1G:408:LEU:HD23	1.82	0.60
12:1L:419:THR:HA	12:1L:422:TYR:CE2	2.36	0.60
47:3C:379:TRP:CD2	50:3F:45:ARG:HD3	2.36	0.60
48:3D:257:VAL:HG13	48:3D:258:LEU:HD23	1.82	0.60
45:3N:41:ILE:HD13	45:3N:190:TYR:HD1	1.65	0.60
45:3N:358:LYS:HG2	45:3N:402:VAL:HB	1.83	0.60
59:4E:16:VAL:HG23	59:4E:47:ILE:HG22	1.82	0.60
13:5M:17:MET:HE1	29:5d:54:VAL:HG21	1.82	0.60
35:5j:33:TRP:CD1	36:5k:70:PHE:N	2.69	0.60
2:1B:175:ILE:HG23	2:1B:178:ARG:NH2	2.15	0.60
10:1J:159:TRP:HE1	14:1N:12:THR:HG23	1.65	0.60
48:3D:115:ARG:HB2	48:3D:143:CYS:HB2	1.83	0.60
56:4B:13:THR:O	56:4B:187:THR:HG23	2.00	0.60
58:4D:121:LYS:HE2	65:4K:50:PRO:HB2	1.82	0.60
3:5C:181:LYS:HD3	16:5P:174:ARG:HD2	1.83	0.60
14:5N:10:ILE:O	14:5N:14:MET:HG2	2.00	0.60
45:6A:61:HIS:HB3	45:6A:130:GLU:HG3	1.83	0.60
52:6H:97:LYS:HD3	52:6H:97:LYS:C	2.26	0.60
49:6R:235:TYR:HA	49:6R:242:HIS:HA	1.83	0.60
55:8A:334:TRP:CZ3	56:8B:46:LEU:HD13	2.36	0.60
56:8B:13:THR:O	56:8B:187:THR:HG23	2.00	0.60
56:8B:104:TRP:C	56:8B:207:MET:HG3	2.26	0.60
13:1M:281:ASP:HB3	13:1M:284:SER:HB3	1.82	0.60
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.36	0.60
42:1q:41:GLU:HG3	42:1q:47:LYS:HG3	1.83	0.60
47:3C:337:TRP:CD1	51:3G:61:TYR:HH	2.20	0.60
45:3N:17:SER:HB3	45:3N:209:LEU:HD11	1.83	0.60
45:3N:216:PHE:HD1	45:3N:219:LEU:HD11	1.65	0.60
55:4A:310:MET:HB3	56:4B:73:LEU:HD22	1.83	0.60
75:4C:308:CDL:H141	75:4C:308:CDL:H541	1.83	0.60
62:4H:7:LYS:NZ	68:4N:78:GLU:OE1	2.28	0.60
46:6B:46:ARG:HH11	46:6B:375:SER:HB2	1.66	0.60
48:6D:131:MET:HB3	48:6D:134:VAL:HB	1.83	0.60
52:6H:54:LYS:HG2	52:6H:89:ALA:CB	2.30	0.60
45:6N:135:LEU:HA	45:6N:138:LEU:HD12	1.83	0.60
45:6N:211:LEU:C	45:6N:215:HIS:HD2	2.09	0.60
55:8A:8:TYR:CZ	57:8C:15:PRO:HB3	2.37	0.60
58:8D:121:LYS:HE2	65:8K:50:PRO:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:260:PRO:HB2	45:3N:264:ASN:CB	2.28	0.60
58:4D:89:ILE:HG21	82:4K:101:PGV:H151	1.84	0.60
1:5A:95:LEU:HD13	8:5H:302:MET:HG3	1.83	0.60
2:5B:175:ILE:HG23	2:5B:178:ARG:NH2	2.15	0.60
45:6N:296:SER:C	47:6P:1:MET:HE1	2.26	0.60
46:6O:299:VAL:HG21	46:6O:309:VAL:HG11	1.84	0.60
55:8A:386:VAL:HG21	85:8A:605:HEA:H262	1.82	0.60
4:1D:115:GLU:HG3	4:1D:194:ILE:HB	1.82	0.60
10:1J:167:VAL:HG22	14:1N:42:PRO:HG2	1.82	0.60
49:3E:249:ILE:CG2	49:3E:257:ASN:HD21	1.99	0.60
45:3N:159:GLN:HG2	49:3R:85:VAL:CG1	2.32	0.60
45:3N:191:LYS:NZ	45:3N:229:PRO:HD2	2.17	0.60
82:4J:101:PGV:H51	82:4J:101:PGV:H231	1.83	0.60
6:5F:297:VAL:HG22	6:5F:336:VAL:HG22	1.83	0.60
12:5L:385:TYR:OH	35:5j:43:ASP:O	2.16	0.60
30:5e:72:MET:O	30:5e:76:SER:OG	2.20	0.60
38:5m:29:ARG:HG2	45:6N:227:ALA:HB2	1.82	0.60
47:6C:68:HIS:HA	47:6C:72:ASP:CG	2.27	0.60
49:6E:150:SER:HB3	49:6E:170:ARG:HG3	1.82	0.60
45:6N:216:PHE:O	45:6N:217:SER:C	2.44	0.60
45:6N:272:VAL:HG22	45:6N:361:LEU:HD22	1.83	0.60
46:6O:247:GLN:HA	46:6O:428:GLY:O	2.02	0.60
55:8A:194:LEU:CB	55:8A:245:ILE:HD11	2.30	0.60
57:8C:63:ARG:NH1	64:8J:20:VAL:O	2.34	0.60
47:3C:155:TYR:O	47:3C:159:ASP:HB2	2.01	0.60
49:3E:219:HIS:HB3	72:3E:301:FES:S2	2.42	0.60
45:3N:355:VAL:HA	45:3N:358:LYS:HB2	1.83	0.60
46:3O:109:VAL:HB	46:3O:119:LEU:HD11	1.84	0.60
55:4A:35:LEU:HD11	55:4A:462:LEU:HB2	1.83	0.60
57:4C:259:TRP:O	68:4N:47:ARG:NH2	2.34	0.60
39:5n:134:ARG:NH2	39:5n:138:GLN:HB2	2.16	0.60
42:5q:60:ARG:HH22	42:5q:95:ASP:HA	1.65	0.60
48:6D:93:LEU:HD11	52:6H:91:ASP:OD2	2.02	0.60
48:6D:235:LEU:O	48:6D:236:TYR:C	2.45	0.60
53:6J:54:LYS:HA	53:6J:57:LYS:HD2	1.82	0.60
55:8A:201:VAL:HG23	57:8C:92:LEU:HD12	1.84	0.60
55:8A:325:ALA:HB2	56:8B:65:TRP:HH2	1.66	0.60
64:8J:45:TYR:HE1	82:8J:101:PGV:H02	1.66	0.60
2:1B:58:GLU:C	2:1B:60:MET:N	2.58	0.60
2:1B:100:LEU:C	2:1B:104:TYR:CD2	2.77	0.60
4:1D:52:GLY:N	4:1D:53:PRO:HD3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:269:PRO:HB2	45:3A:410:VAL:HG11	1.83	0.60
53:3J:11:TYR:HA	53:3J:15:PHE:HB2	1.84	0.60
47:3P:267:HIS:HD2	47:3P:269:LYS:HG2	1.66	0.60
49:3R:236:CYS:HB2	49:3R:241:SER:O	2.01	0.60
10:5J:4:TYR:O	10:5J:8:ILE:HD12	2.02	0.60
12:5L:102:GLU:OE1	12:5L:456:ARG:NH2	2.35	0.60
16:5P:36:ASN:HA	16:5P:62:MET:HG2	1.83	0.60
16:5P:52:GLU:HG3	16:5P:54:TYR:H	1.66	0.60
34:5i:103:ILE:HB	40:5o:47:ASP:HB2	1.82	0.60
46:6B:75:LEU:O	46:6B:76:THR:C	2.43	0.60
46:6B:160:LEU:HD12	49:6I:64:LEU:HB3	1.84	0.60
46:6B:179:PRO:HG2	46:6B:182:ARG:HB2	1.83	0.60
46:6B:261:SER:HB3	46:6B:322:PHE:H	1.67	0.60
2:1B:101:ARG:C	2:1B:103:VAL:N	2.58	0.60
6:1F:137:TYR:HA	6:1F:178:VAL:HG23	1.83	0.60
45:3N:64:PHE:HD1	45:3N:86:LEU:HD13	1.43	0.60
45:3N:216:PHE:HB3	45:3N:219:LEU:HD12	1.84	0.60
62:4H:29:CYS:HB3	62:4H:63:PHE:HB3	1.82	0.60
45:6A:331:ILE:HG13	45:6A:430:GLN:HB3	1.83	0.60
46:6B:369:LEU:HD11	46:6B:399:LEU:HD11	1.82	0.60
45:6N:46:ARG:NH1	45:6N:315:ALA:HB3	2.16	0.60
45:6N:429:GLU:HB3	51:6T:5:GLY:HA2	1.83	0.60
62:8H:7:LYS:NZ	68:8N:78:GLU:OE1	2.28	0.60
2:1B:65:PRO:HA	2:1B:68:ASP:OD1	2.02	0.60
5:1E:56:ARG:NH1	5:1E:158:ASP:OD2	2.34	0.60
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.82	0.60
22:1W:88:MET:O	22:1W:92:GLU:HG3	2.01	0.60
46:3B:435:PHE:CE2	46:3O:240:ARG:HB2	2.36	0.60
47:3C:153:ILE:O	47:3C:157:GLY:N	2.34	0.60
45:3N:39:VAL:HG13	45:3N:196:VAL:O	2.01	0.60
45:3N:124:ASP:CB	45:3N:179:ARG:CZ	2.50	0.60
6:5F:224:ASN:ND2	73:5F:501:FMN:O2	2.28	0.60
12:5L:419:THR:HA	12:5L:422:TYR:CE2	2.35	0.60
48:6D:146:GLU:O	48:6D:150:LYS:N	2.32	0.60
52:6H:82:GLU:OE1	52:6H:82:GLU:N	2.35	0.60
45:6N:156:THR:HA	45:6N:159:GLN:NE2	2.17	0.60
45:6N:427:PRO:O	45:6N:428:ILE:C	2.45	0.60
46:6O:171:ALA:O	46:6O:172:LEU:C	2.45	0.60
46:6O:258:VAL:HA	46:6O:323:GLY:HA3	1.84	0.60
55:8A:193:VAL:HG21	82:8A:603:PGV:H231	1.84	0.60
2:1B:57:VAL:N	2:1B:58:GLU:N	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:36:ASN:HA	16:1P:62:MET:HG2	1.84	0.60
45:3N:61:HIS:CB	45:3N:130:GLU:OE1	2.50	0.60
55:4A:236:TRP:CE3	55:4A:239:GLY:HA3	2.36	0.60
1:5A:70:ALA:HB2	10:5J:59:ILE:HG13	1.83	0.60
10:5J:78:MET:HE2	10:5J:78:MET:C	2.27	0.60
45:6A:254:ALA:HB2	45:6A:323:HIS:CD2	2.36	0.60
45:6N:18:GLN:CG	45:6N:24:ARG:CG	2.77	0.60
45:6N:58:PHE:HA	45:6N:61:HIS:CD2	2.30	0.60
45:6N:150:PHE:O	45:6N:154:HIS:CD2	2.55	0.60
48:6Q:152:TYR:OH	52:6U:66:ASP:OD2	2.17	0.60
49:6R:180:THR:O	49:6R:182:LYS:N	2.35	0.60
55:8A:371:TYR:HB2	55:8A:436:MET:HB3	1.84	0.60
58:8D:135:SER:OG	58:8D:140:TYR:OH	2.20	0.60
7:1G:190:MET:SD	7:1G:190:MET:N	2.75	0.59
10:1J:148:SER:HB2	71:1J:201:PC1:H142	1.84	0.59
23:1X:7:PRO:HG2	25:1Z:84:LEU:HD13	1.84	0.59
47:3C:337:TRP:HD1	51:3G:61:TYR:HH	1.49	0.59
45:3N:40:TRP:HZ2	45:3N:377:GLU:CG	2.11	0.59
45:3N:69:ASN:ND2	45:3N:115:ASP:OD1	2.33	0.59
45:3N:82:MET:HB3	45:3N:105:ASP:OD2	2.01	0.59
45:3N:344:ARG:HG3	45:3N:348:SER:HB2	1.83	0.59
82:4C:302:PGV:H183	82:4C:305:PGV:H172	1.83	0.59
61:4G:44:ARG:HH12	61:4G:84:GLN:HB3	1.67	0.59
7:5G:199:ILE:HA	7:5G:202:ILE:HG12	1.83	0.59
13:5M:44:GLN:H	32:5g:83:TYR:HD1	1.50	0.59
39:5n:134:ARG:NH1	39:5n:137:LYS:HD2	2.16	0.59
45:6N:39:VAL:HG11	45:6N:195:MET:CE	2.29	0.59
55:8A:103:TRP:HB3	57:8C:21:ALA:CB	2.30	0.59
55:8A:358:LEU:O	55:8A:359:ALA:C	2.45	0.59
2:1B:94:ASN:O	2:1B:97:ALA:HB2	2.01	0.59
23:1X:136:LEU:HD23	23:1X:137:PRO:HD2	1.83	0.59
32:1g:100:ARG:NH1	32:1g:107:LEU:O	2.36	0.59
45:3N:170:PRO:O	45:3N:174:VAL:HG23	2.02	0.59
1:5A:54:LYS:HD2	1:5A:114:ALA:H	1.65	0.59
45:6N:52:ASN:N	45:6N:185:TYR:OH	2.35	0.59
45:6N:64:PHE:HZ	45:6N:88:ALA:CB	2.14	0.59
60:8F:49:VAL:HG22	60:8F:91:LEU:HD12	1.84	0.59
6:1F:215:VAL:HG12	6:1F:220:THR:HG21	1.84	0.59
17:1Q:93:VAL:HG12	17:1Q:97:GLU:OE1	2.02	0.59
47:3C:130:GLY:HA2	47:3C:133:LEU:HG	1.84	0.59
49:3E:220:LEU:HD12	47:3P:263:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:69:LEU:HB3	46:3O:105:MET:HE1	1.84	0.59
49:3R:153:GLU:O	49:3R:155:LYS:NZ	2.36	0.59
11:5K:55:LEU:HD13	30:5e:16:TRP:HE3	1.67	0.59
13:5M:220:HIS:CE1	13:5M:231:LEU:HB3	2.37	0.59
14:5N:69:MET:HE1	14:5N:104:MET:CE	2.31	0.59
46:6B:376:GLU:OE1	46:6B:379:LEU:HD22	1.98	0.59
47:6C:183:PHE:CE1	47:6P:183:PHE:HB3	2.37	0.59
49:6R:236:CYS:HB2	49:6R:241:SER:O	2.01	0.59
55:8A:508:PRO:C	55:8A:509:THR:O	2.41	0.59
2:1B:25:ARG:HG2	2:1B:27:GLU:H	1.67	0.59
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.37	0.59
30:1e:36:GLU:HG3	30:1e:62:PHE:CZ	2.38	0.59
30:1e:57:ILE:HG13	30:1e:58:GLU:N	2.17	0.59
33:1h:95:GLN:O	33:1h:99:GLU:HG3	2.03	0.59
47:3C:4:ILE:HA	47:3C:7:SER:HB3	1.83	0.59
47:3C:91:PHE:HZ	47:3C:124:MET:HA	1.66	0.59
45:3N:42:ASP:OD1	45:3N:384:LEU:HD13	2.01	0.59
45:3N:55:ALA:HB2	45:3N:185:TYR:CE1	2.37	0.59
55:4A:3:VAL:HG11	82:4A:601:PGV:H32	1.84	0.59
82:4A:601:PGV:H332	82:4A:601:PGV:H161	1.85	0.59
6:5F:215:VAL:HG12	6:5F:220:THR:HG21	1.83	0.59
31:5f:53:GLU:HG2	31:5f:54:VAL:HG22	1.83	0.59
45:6A:289:HIS:HB3	46:6B:83:PHE:HA	1.83	0.59
47:6C:269:LYS:HB2	47:6C:275:LEU:HD11	1.83	0.59
47:6C:319:PRO:HA	51:6G:49:ARG:NH1	2.17	0.59
45:6N:104:LYS:O	45:6N:107:PRO:CG	2.50	0.59
55:8A:232:GLN:HB3	55:8A:292:MET:HE3	1.84	0.59
55:8A:311:ILE:HG23	68:8N:21:PHE:HB3	1.85	0.59
90:8C:307:PEK:H131	90:8C:307:PEK:H42	1.84	0.59
15:1O:75:GLY:HA2	15:1O:99:TRP:CD2	2.38	0.59
23:1X:2:GLY:O	25:1Z:109:SER:N	2.32	0.59
45:3N:66:GLY:HA2	45:3N:75:LEU:CD1	2.32	0.59
45:3N:191:LYS:O	45:3N:193:PRO:CD	2.50	0.59
46:3O:68:LEU:HD13	46:3O:144:LEU:HD11	1.83	0.59
14:5N:335:LEU:HD23	69:5N:902:3PE:H2H2	1.85	0.59
49:6E:220:LEU:HD12	47:6P:263:ASN:HD21	1.67	0.59
45:6N:58:PHE:CE2	45:6N:174:VAL:HG22	2.33	0.59
45:6N:148:VAL:C	45:6N:152:TYR:CD2	2.80	0.59
46:6O:182:ARG:HA	46:6O:185:LYS:HB2	1.84	0.59
47:6P:300:ILE:HG13	47:6P:303:LEU:HD12	1.83	0.59
55:8A:296:GLY:O	56:8B:178:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:312:LYS:HE3	15:1O:76:ASN:HB2	1.84	0.59
39:1n:134:ARG:NH1	39:1n:137:LYS:HD2	2.16	0.59
45:3N:24:ARG:HB2	45:3N:196:VAL:HA	1.85	0.59
55:4A:297:MET:HA	82:4A:604:PGV:H042	1.83	0.59
82:4C:303:PGV:H61	82:4C:303:PGV:H262	1.85	0.59
90:4C:307:PEK:H42	90:4C:307:PEK:H131	1.84	0.59
14:5N:312:LYS:HE3	15:5O:76:ASN:HB2	1.84	0.59
30:5e:36:GLU:HG3	30:5e:62:PHE:CZ	2.38	0.59
32:5g:36:ASN:HD21	32:5g:38:TYR:HB2	1.68	0.59
47:6C:20:ASP:O	47:6C:21:LEU:C	2.45	0.59
45:6N:133:VAL:HG11	49:6V:53:GLU:HG3	1.84	0.59
55:8A:51:ASP:O	55:8A:52:GLN:C	2.46	0.59
12:1L:102:GLU:OE1	12:1L:456:ARG:NH2	2.35	0.59
18:1R:20:ASP:N	18:1R:20:ASP:OD1	2.35	0.59
45:3A:246:ASP:OD2	51:3G:11:ARG:HA	2.02	0.59
47:3C:138:MET:HG2	47:3C:254:ASP:HB2	1.84	0.59
49:3E:223:VAL:HG11	48:3Q:144:ARG:NH2	2.18	0.59
48:3Q:152:TYR:OH	52:3U:66:ASP:OD2	2.17	0.59
50:3S:52:GLU:OE2	51:3T:11:ARG:NH1	2.29	0.59
22:5W:88:MET:O	22:5W:92:GLU:HG3	2.01	0.59
32:5g:100:ARG:NH1	32:5g:107:LEU:O	2.36	0.59
33:5h:26:ARG:HD2	33:5h:30:LEU:HD12	1.85	0.59
40:5o:11:ASP:OD2	40:5o:112:LYS:NZ	2.36	0.59
49:6I:32:ALA:N	49:6I:71:ASN:OD1	2.36	0.59
46:6O:160:LEU:HD12	49:6V:64:LEU:HB2	1.84	0.59
55:8A:236:TRP:HD1	55:8A:292:MET:HG2	1.67	0.59
57:8C:204:HIS:NE2	57:8C:249:TRP:HB2	2.18	0.59
2:1B:35:ASP:O	2:1B:39:TRP:N	2.35	0.59
3:1C:41:GLN:HG2	3:1C:51:PHE:HE1	1.68	0.59
7:1G:199:ILE:HA	7:1G:202:ILE:HG12	1.83	0.59
71:1H:401:PC1:H2I3	10:1J:35:VAL:HG13	1.85	0.59
30:1e:72:MET:O	30:1e:76:SER:OG	2.20	0.59
45:3N:124:ASP:HA	45:3N:127:ILE:HB	1.83	0.59
45:3N:158:PHE:HE1	45:3N:163:LEU:CD1	2.09	0.59
47:3P:284:ILE:HD12	47:3P:285:PRO:CD	2.33	0.59
47:3P:300:ILE:HG13	47:3P:303:LEU:HD12	1.83	0.59
49:3R:235:TYR:HA	49:3R:242:HIS:HA	1.83	0.59
59:4E:21:LYS:HB2	59:4E:24:ILE:HB	1.85	0.59
59:4E:36:LEU:HA	59:4E:39:TYR:CE2	2.38	0.59
61:4G:72:ASN:HB3	61:4G:75:VAL:HG12	1.85	0.59
4:5D:425:PHE:HA	4:5D:428:VAL:HB	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5E:56:ARG:NH1	5:5E:158:ASP:OD2	2.34	0.59
13:5M:403:THR:HA	13:5M:406:TYR:CE2	2.37	0.59
15:5O:75:GLY:HA2	15:5O:99:TRP:CD2	2.37	0.59
45:6A:310:PHE:H	45:6A:321:GLY:C	2.11	0.59
47:6C:226:ILE:HA	47:6C:229:ILE:HG13	1.84	0.59
49:6E:219:HIS:HB3	72:6E:301:FES:S2	2.42	0.59
45:6N:4:TYR:OH	46:6O:112:LEU:HD13	1.98	0.59
45:6N:23:LEU:HD21	45:6N:192:ALA:HB1	1.84	0.59
54:6Y:48:ILE:HD12	54:6Y:51:LYS:HD3	1.85	0.59
55:8A:94:PHE:CZ	57:8C:82:GLY:HA3	2.37	0.59
55:8A:118:VAL:HA	64:8J:54:SER:HA	1.85	0.59
55:8A:147:ILE:HG23	55:8A:206:ILE:HG13	1.85	0.59
55:8A:218:THR:HG21	61:8G:55:ILE:HD12	1.85	0.59
55:8A:240:HIS:HD2	55:8A:244:TYR:CZ	2.20	0.59
62:8H:14:ALA:CB	62:8H:63:PHE:HE1	2.09	0.59
4:1D:425:PHE:HA	4:1D:428:VAL:HB	1.85	0.59
13:1M:39:LEU:HD21	71:1M:502:PC1:H291	1.85	0.59
13:1M:44:GLN:HB2	32:1g:83:TYR:HE1	1.68	0.59
35:1j:19:ARG:CZ	65:8K:12:LYS:HD2	2.32	0.59
39:1n:13:GLN:O	39:1n:17:ARG:HG2	2.03	0.59
46:3O:279:LEU:HB3	46:3O:295:LEU:HD11	1.85	0.59
49:3R:92:ARG:O	51:3T:24:ARG:NH1	2.36	0.59
4:5D:52:GLY:N	4:5D:53:PRO:HD3	2.17	0.59
42:5q:41:GLU:HG3	42:5q:47:LYS:HG3	1.83	0.59
46:6B:51:ILE:HG12	46:6B:204:MET:HG2	1.85	0.59
46:6B:258:VAL:HG12	46:6B:323:GLY:HA3	1.85	0.59
45:6N:118:GLN:HE21	45:6N:219:LEU:CA	2.15	0.59
45:6N:359:ASN:HA	45:6N:362:ARG:HD2	1.83	0.59
46:6O:171:ALA:HB3	46:6O:237:ALA:HB2	1.84	0.59
46:6O:247:GLN:HE22	46:6O:429:ASN:HA	1.67	0.59
66:8L:4:GLU:OE1	66:8L:9:LYS:HE3	2.03	0.59
22:1W:62:LYS:HD2	22:1W:66:MET:HE3	1.85	0.59
40:1o:68:CYS:O	40:1o:72:SER:OG	2.21	0.59
49:3E:169:TRP:HD1	49:3E:214:ILE:HD11	1.68	0.59
45:3N:119:ASN:O	45:3N:120:CYS:C	2.45	0.59
57:4C:204:HIS:NE2	57:4C:249:TRP:HB2	2.18	0.59
60:4F:49:VAL:HG22	60:4F:91:LEU:HD12	1.84	0.59
66:4L:4:GLU:OE1	66:4L:9:LYS:HE3	2.03	0.59
8:5H:187:ILE:HD11	71:5I:201:PC1:H271	1.85	0.59
12:5L:481:THR:OG1	40:5o:91:HIS:ND1	2.26	0.59
23:5X:7:PRO:HG2	25:5Z:84:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:5X:136:LEU:HD23	23:5X:137:PRO:HD2	1.83	0.59
24:5Y:79:VAL:O	24:5Y:81:GLU:OE2	2.20	0.59
33:5h:95:GLN:O	33:5h:99:GLU:HG3	2.03	0.59
39:5n:13:GLN:O	39:5n:17:ARG:HG2	2.03	0.59
40:5o:52:LEU:HA	40:5o:55:ARG:HD2	1.85	0.59
45:6A:3:THR:H	45:6A:6:GLN:HB2	1.67	0.59
48:6D:313:ARG:HB2	51:6G:27:ALA:HB1	1.84	0.59
55:8A:82:LEU:O	55:8A:83:VAL:C	2.45	0.59
2:1B:101:ARG:CG	2:1B:140:VAL:HG13	2.33	0.58
10:1J:78:MET:HE2	10:1J:78:MET:C	2.27	0.58
24:1Y:72:THR:O	24:1Y:76:SER:OG	2.21	0.58
24:1Y:75:ILE:HG12	51:3T:56:TYR:HE2	1.67	0.58
34:1i:74:VAL:O	34:1i:78:VAL:HG12	2.03	0.58
36:1k:90:GLN:HB2	58:8D:101:HIS:NE2	2.17	0.58
40:1o:11:ASP:OD2	40:1o:112:LYS:NZ	2.36	0.58
47:3C:137:GLN:HG2	47:3C:260:ASN:N	2.13	0.58
49:3E:130:LYS:NZ	54:3Y:34:TRP:O	2.31	0.58
46:3O:45:SER:HB2	46:3O:113:ARG:HB2	1.85	0.58
57:4C:126:PRO:O	57:4C:253:TYR:OH	2.18	0.58
5:5E:203:THR:O	44:5s:35:ASN:ND2	2.36	0.58
71:5H:401:PC1:H2I3	10:5J:35:VAL:HG13	1.85	0.58
45:6A:395:TRP:HA	45:6A:398:ARG:HD2	1.84	0.58
45:6N:4:TYR:OH	46:6O:112:LEU:CA	2.51	0.58
45:6N:170:PRO:HD2	45:6N:170:PRO:O	2.02	0.58
55:8A:94:PHE:HB2	55:8A:97:MET:HB3	1.85	0.58
5:1E:104:THR:HG21	5:1E:141:GLU:HG2	1.86	0.58
71:1H:401:PC1:O14	10:1J:50:SER:OG	2.18	0.58
16:1P:52:GLU:HG3	16:1P:54:TYR:H	1.66	0.58
49:3I:32:ALA:N	49:3I:72:VAL:HG23	2.18	0.58
45:3N:72:GLY:HA2	45:3N:75:LEU:CD1	2.32	0.58
45:3N:118:GLN:HE21	45:3N:219:LEU:HA	1.69	0.58
55:4A:177:SER:HA	82:4A:603:PGV:H05	1.85	0.58
13:5M:44:GLN:HB2	32:5g:83:TYR:HE1	1.68	0.58
13:5M:94:LEU:HD13	69:5N:902:3PE:H331	1.85	0.58
15:5O:200:GLN:NE2	15:5O:204:ASN:OD1	2.36	0.58
24:5Y:75:ILE:HG12	51:6T:56:TYR:HE2	1.67	0.58
48:6D:247:ILE:HG12	48:6D:249:MET:H	1.67	0.58
45:6N:15:GLN:HB2	45:6N:205:HIS:CG	2.37	0.58
45:6N:146:ARG:O	45:6N:150:PHE:HD2	1.86	0.58
45:6N:329:MET:HG2	51:6T:6:HIS:CE1	2.38	0.58
46:6O:27:THR:HB	46:6O:35:ILE:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:8E:36:LEU:HA	59:8E:39:TYR:CE2	2.38	0.58
8:1H:189:THR:HG22	8:1H:270:PHE:HZ	1.67	0.58
13:1M:190:TRP:CG	24:1Y:126:MET:HG2	2.38	0.58
33:1h:26:ARG:HD2	33:1h:30:LEU:HD12	1.85	0.58
47:3C:344:GLU:O	47:3C:347:PHE:HB2	2.03	0.58
48:3D:160:ASP:HB2	48:3D:171:ARG:HG2	1.85	0.58
45:3N:25:VAL:HG22	45:3N:197:LEU:CB	2.32	0.58
45:3N:259:GLY:HA3	45:3N:318:GLY:HA3	1.85	0.58
46:3O:124:LEU:HD13	46:3O:223:PHE:HB2	1.84	0.58
3:5C:41:GLN:HG2	3:5C:51:PHE:HE1	1.68	0.58
4:5D:24:GLU:OE2	12:5L:579:ASN:ND2	2.32	0.58
5:5E:201:SER:HB2	6:5F:26:TYR:HE2	1.68	0.58
13:5M:190:TRP:CG	24:5Y:126:MET:HG2	2.38	0.58
69:5M:503:3PE:H2C1	38:5m:97:LEU:HD13	1.84	0.58
14:5N:210:THR:HG22	14:5N:333:SER:HB3	1.85	0.58
17:5Q:93:VAL:HG12	17:5Q:97:GLU:OE1	2.02	0.58
46:6B:247:GLN:HE22	46:6B:429:ASN:HA	1.69	0.58
47:6C:319:PRO:HA	51:6G:49:ARG:HD3	1.85	0.58
49:6E:169:TRP:HD1	49:6E:214:ILE:HD11	1.68	0.58
45:6N:269:PRO:HB2	45:6N:410:VAL:HG21	1.84	0.58
65:8K:27:ALA:HB1	65:8K:31:TYR:HE2	1.67	0.58
2:1B:95:LYS:N	2:1B:96:MET:N	2.52	0.58
11:1K:55:LEU:HD13	30:1e:16:TRP:HE3	1.67	0.58
11:1K:87:THR:HG22	11:1K:89:TYR:H	1.68	0.58
69:1M:503:3PE:H2C1	38:1m:97:LEU:HD13	1.84	0.58
47:3C:209:THR:HG23	50:3F:81:THR:HG21	1.84	0.58
47:3C:218:ILE:HG21	48:3D:319:LEU:HD11	1.85	0.58
48:3D:227:THR:HG22	52:3H:69:VAL:CG1	2.33	0.58
49:3I:32:ALA:N	49:3I:71:ASN:OD1	2.36	0.58
45:3N:146:ARG:O	45:3N:150:PHE:CD2	2.57	0.58
55:4A:265:LYS:HG3	55:4A:490:THR:HG21	1.85	0.58
9:5I:156:ASN:OD1	18:5R:36:ASN:ND2	2.36	0.58
11:5K:87:THR:HG22	11:5K:89:TYR:H	1.68	0.58
40:5o:38:MET:HE1	40:5o:56:ASP:O	2.04	0.58
45:6A:248:LEU:HB2	45:6A:426:GLY:HA3	1.84	0.58
45:6A:435:ASN:HB3	47:6C:222:PRO:CB	2.33	0.58
47:6C:91:PHE:HZ	47:6C:124:MET:HA	1.69	0.58
47:6C:345:HIS:HB3	51:6G:68:PHE:HA	1.84	0.58
45:6N:19:LEU:HD21	45:6N:25:VAL:HG21	1.84	0.58
45:6N:60:GLU:C	46:6O:287:ARG:HH22	2.12	0.58
45:6N:80:GLU:CD	46:6O:292:THR:OG1	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:3:VAL:HG13	55:8A:7:LEU:HB2	1.84	0.58
55:8A:111:LEU:HB3	55:8A:145:LEU:HD22	1.84	0.58
55:8A:359:ALA:O	55:8A:360:ASN:C	2.46	0.58
2:1B:114:VAL:HG12	2:1B:115:SER:H	1.68	0.58
14:1N:335:LEU:HD23	69:1N:902:3PE:H2H2	1.85	0.58
24:1Y:79:VAL:O	24:1Y:81:GLU:OE2	2.20	0.58
35:1j:38:TRP:CE3	36:1k:80:ALA:HB1	2.38	0.58
45:3N:21:ASN:ND2	45:3N:217:SER:O	2.30	0.58
45:3N:133:VAL:HG13	49:3V:51:CYS:HB2	1.84	0.58
46:3O:368:TYR:HE2	46:3O:395:PRO:HB3	1.69	0.58
49:3R:180:THR:O	49:3R:182:LYS:N	2.35	0.58
1:5A:67:LEU:HD22	11:5K:65:VAL:HA	1.86	0.58
15:5O:60:ASP:N	15:5O:60:ASP:OD1	2.35	0.58
22:5W:62:LYS:HD2	22:5W:66:MET:HE3	1.85	0.58
45:6A:240:GLU:HG2	45:6A:242:ARG:HD2	1.85	0.58
45:6N:15:GLN:HB2	45:6N:205:HIS:HD1	1.65	0.58
45:6N:35:CYS:O	45:6N:37:VAL:HG23	2.03	0.58
49:6R:92:ARG:O	51:6T:24:ARG:NH1	2.36	0.58
55:8A:230:LEU:HB2	57:8C:103:HIS:CD2	2.38	0.58
6:1F:95:VAL:HG11	6:1F:118:LEU:HD11	1.85	0.58
7:1G:117:GLN:O	7:1G:121:MET:HG2	2.04	0.58
15:1O:200:GLN:NE2	15:1O:204:ASN:OD1	2.36	0.58
47:3C:91:PHE:HA	47:3C:94:LEU:HD12	1.86	0.58
5:5E:165:THR:OG1	5:5E:168:ASP:OD2	2.21	0.58
8:5H:189:THR:HG22	8:5H:270:PHE:HZ	1.68	0.58
47:6C:109:PHE:HB3	47:6C:112:THR:HG23	1.86	0.58
47:6C:162:GLU:HA	47:6C:165:TRP:HB2	1.86	0.58
45:6N:33:PRO:HD2	45:6N:34:THR:H	1.67	0.58
47:6P:284:ILE:HD12	47:6P:285:PRO:CD	2.33	0.58
56:8B:102:HIS:O	56:8B:103:GLN:C	2.46	0.58
59:8E:21:LYS:HB2	59:8E:24:ILE:HB	1.85	0.58
13:1M:433:GLU:O	13:1M:437:MET:HG2	2.04	0.58
45:3N:296:SER:HA	45:3N:299:ALA:HB3	1.85	0.58
45:6A:263:ALA:O	45:6A:264:ASN:C	2.46	0.58
45:6A:344:ARG:O	45:6A:348:SER:N	2.36	0.58
46:6O:52:LYS:HG2	46:6O:387:LEU:HD22	1.86	0.58
49:6R:153:GLU:O	49:6R:155:LYS:NZ	2.36	0.58
55:8A:218:THR:HA	55:8A:221:ASP:HB3	1.86	0.58
13:1M:220:HIS:CE1	13:1M:231:LEU:HB3	2.37	0.58
24:1Y:140:VAL:O	33:1h:115:ARG:NH1	2.37	0.58
45:3N:27:SER:OG	45:3N:205:HIS:ND1	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:57:TYR:C	45:3N:61:HIS:CD2	2.82	0.58
56:4B:104:TRP:HA	56:4B:207:MET:SD	2.43	0.58
64:4J:48:TYR:CE2	82:4J:101:PGV:H032	2.39	0.58
13:5M:39:LEU:HD21	71:5M:502:PC1:H291	1.85	0.58
16:5P:236:TYR:OH	16:5P:311:GLU:OE2	2.22	0.58
35:5j:37:LEU:CD1	36:5k:74:PHE:HA	2.34	0.58
47:6C:172:LYS:HD3	47:6P:56:THR:HG21	1.84	0.58
45:6N:99:ILE:CG1	45:6N:113:LEU:HD21	2.33	0.58
55:8A:301:THR:HG22	55:8A:305:PHE:HE2	1.69	0.58
55:8A:447:TYR:O	55:8A:448:THR:C	2.47	0.58
7:1G:283:MET:HE3	7:1G:293:TYR:CD1	2.39	0.58
12:1L:327:LEU:O	12:1L:331:MET:HG2	2.03	0.58
47:3C:68:HIS:O	47:3C:72:ASP:N	2.36	0.58
47:3C:377:LEU:HB2	50:3F:32:TYR:CE2	2.36	0.58
48:3D:226:PRO:HB2	52:3H:79:CYS:HB2	1.85	0.58
51:3G:50:VAL:O	51:3G:53:PRO:HD2	2.03	0.58
6:5F:95:VAL:HG11	6:5F:118:LEU:HD11	1.86	0.58
8:5H:91:MET:O	8:5H:93:TYR:N	2.37	0.58
12:5L:327:LEU:O	12:5L:331:MET:HG2	2.03	0.58
34:5i:74:VAL:O	34:5i:78:VAL:HG12	2.04	0.58
45:6A:241:ILE:HB	51:6G:18:TYR:HD1	1.69	0.58
47:6C:346:PRO:O	47:6C:347:PHE:C	2.46	0.58
48:6D:232:ARG:O	48:6D:233:GLU:C	2.47	0.58
55:8A:309:THR:O	55:8A:310:MET:C	2.45	0.58
55:8A:428:GLN:HA	55:8A:431:LEU:HG	1.85	0.58
62:8H:42:ALA:O	62:8H:46:LYS:HG2	2.04	0.58
5:1E:203:THR:O	44:1s:35:ASN:ND2	2.36	0.58
8:1H:187:ILE:HD11	71:1I:201:PC1:H271	1.85	0.58
45:3A:429:GLU:HG2	51:3G:7:GLY:H	1.69	0.58
47:3C:337:TRP:HB2	51:3G:61:TYR:HE2	1.68	0.58
54:3Y:51:LYS:HE3	54:3Y:52:PHE:CZ	2.39	0.58
7:5G:117:GLN:O	7:5G:121:MET:HG2	2.04	0.58
69:5J:201:3PE:H221	69:5Y:205:3PE:H321	1.86	0.58
16:5P:244:TYR:HB2	16:5P:337:ALA:HB2	1.86	0.58
33:5h:36:VAL:HA	71:5h:202:PC1:H2G2	1.86	0.58
45:6A:122:LEU:HD21	45:6A:182:LEU:HD22	1.84	0.58
49:6I:32:ALA:N	49:6I:72:VAL:HG23	2.19	0.58
45:6N:58:PHE:CG	45:6N:134:ILE:CD1	2.79	0.58
45:6N:218:SER:O	45:6N:219:LEU:C	2.47	0.58
45:6N:445:ARG:HE	45:6N:445:ARG:H	1.52	0.58
46:6O:24:LEU:HB2	46:6O:38:LEU:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6O:68:LEU:HD13	46:6O:144:LEU:HD11	1.84	0.58
49:6R:219:HIS:HB2	72:6R:301:FES:S1	2.44	0.58
55:8A:325:ALA:HB2	56:8B:65:TRP:CH2	2.39	0.58
12:1L:434:LYS:HE3	36:1k:57:ALA:HA	1.86	0.57
32:1g:36:ASN:HD21	32:1g:38:TYR:HB2	1.68	0.57
49:3E:264:GLU:H	49:3E:272:ILE:HG12	1.68	0.57
49:3I:32:ALA:HA	49:3I:71:ASN:HD21	1.68	0.57
45:3N:80:GLU:O	46:3O:363:LYS:NZ	2.35	0.57
45:3N:103:SER:O	45:3N:106:LEU:HG	2.03	0.57
45:3N:127:ILE:HD12	45:3N:179:ARG:NE	2.19	0.57
1:5A:1:FME:N	1:5A:4:MET:HE2	2.18	0.57
46:6B:292:THR:O	46:6B:293:SER:C	2.46	0.57
45:6N:4:TYR:OH	46:6O:112:LEU:C	2.47	0.57
46:6O:313:ASN:HB2	46:6O:322:PHE:HD1	1.69	0.57
49:6R:151:LYS:HG2	49:6R:152:ILE:HG12	1.85	0.57
61:8G:72:ASN:HB3	61:8G:75:VAL:HG12	1.85	0.57
82:8L:101:PGV:H301	82:8L:101:PGV:H81	1.86	0.57
4:1D:95:THR:HG22	4:1D:98:GLN:H	1.69	0.57
4:1D:406:SER:HB2	4:1D:414:VAL:HG22	1.86	0.57
6:1F:89:ARG:NH1	6:1F:217:GLY:O	2.37	0.57
47:3C:51:LEU:HG	47:3C:79:ILE:HG22	1.84	0.57
47:3C:240:LEU:CB	48:3D:297:MET:HG3	2.34	0.57
47:3C:377:LEU:HD11	50:3F:38:PHE:CE2	2.31	0.57
52:3H:80:THR:HG23	52:3H:84:PHE:CZ	2.38	0.57
45:3N:369:LEU:O	45:3N:370:ASP:C	2.45	0.57
46:3O:286:LYS:HG2	46:3O:287:ARG:HG3	1.86	0.57
49:3R:219:HIS:HB2	72:3R:301:FES:S1	2.44	0.57
55:4A:484:ALA:HB3	67:4M:2:TYR:HB2	1.86	0.57
6:5F:342:ASP:HB3	6:5F:345:LYS:HB3	1.86	0.57
46:6B:28:ARG:HA	46:6B:34:VAL:HA	1.85	0.57
46:6B:200:THR:HA	46:6B:226:MET:HG2	1.86	0.57
45:6N:46:ARG:HH12	45:6N:316:GLU:N	2.00	0.57
46:6O:124:LEU:HD21	46:6O:219:VAL:HG23	1.87	0.57
55:8A:13:LYS:HE3	55:8A:85:LEU:HD21	1.85	0.57
58:8D:23:PRO:O	59:8E:66:ARG:NH1	2.37	0.57
61:8G:44:ARG:HH12	61:8G:84:GLN:HB3	1.67	0.57
4:1D:3:GLN:NE2	13:1M:137:GLY:O	2.37	0.57
6:1F:342:ASP:HB3	6:1F:345:LYS:HB3	1.86	0.57
16:1P:236:TYR:OH	16:1P:311:GLU:OE2	2.22	0.57
47:3C:320:LEU:H	47:3C:320:LEU:HD12	1.67	0.57
49:3E:161:GLU:HA	49:3E:178:HIS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:37:VAL:HA	45:3N:199:ALA:CB	2.34	0.57
57:4C:164:SER:HB2	82:4C:301:PGV:H91	1.86	0.57
62:4H:42:ALA:O	62:4H:46:LYS:HG2	2.04	0.57
4:5D:3:GLN:NE2	13:5M:137:GLY:O	2.37	0.57
6:5F:89:ARG:NH1	6:5F:217:GLY:O	2.37	0.57
24:5Y:124:VAL:O	24:5Y:128:GLN:HG3	2.04	0.57
46:6B:58:GLU:HG2	46:6B:194:TYR:HE1	1.69	0.57
47:6C:39:ILE:HD13	47:6C:232:ALA:HA	1.85	0.57
47:6C:326:TRP:CG	51:6G:50:VAL:HG13	2.38	0.57
49:6E:150:SER:HB2	47:6P:168:PHE:CE1	2.39	0.57
57:8C:126:PRO:O	57:8C:253:TYR:OH	2.18	0.57
5:1E:201:SER:HB2	6:1F:26:TYR:HE2	1.68	0.57
7:1G:155:GLN:HG2	7:1G:181:MET:HE2	1.86	0.57
13:1M:94:LEU:HD13	69:1N:902:3PE:H331	1.86	0.57
40:1o:38:MET:HE1	40:1o:56:ASP:O	2.04	0.57
50:3F:116:ARG:HG2	46:3O:83:PHE:CD2	2.39	0.57
45:3N:158:PHE:CD1	45:3N:163:LEU:CB	2.87	0.57
46:3O:170:ASN:O	46:3O:172:LEU:N	2.38	0.57
56:4B:181:GLN:O	62:4H:23:GLN:NE2	2.25	0.57
58:4D:23:PRO:O	59:4E:66:ARG:NH1	2.37	0.57
6:5F:276:LEU:HD21	6:5F:297:VAL:HG11	1.86	0.57
6:5F:393:TRP:O	6:5F:397:LYS:HG2	2.04	0.57
46:6B:56:ARG:HG2	46:6B:103:GLU:HG2	1.87	0.57
48:6D:189:ALA:O	48:6D:190:ARG:C	2.46	0.57
48:6D:260:PHE:CZ	48:6D:271:VAL:HA	2.40	0.57
49:6E:223:VAL:HG11	48:6Q:144:ARG:NH2	2.18	0.57
45:6N:52:ASN:CA	45:6N:185:TYR:CZ	2.82	0.57
45:6N:192:ALA:N	45:6N:193:PRO:HD3	2.20	0.57
55:8A:173:PRO:O	55:8A:174:PRO:C	2.45	0.57
59:8E:84:TYR:HA	59:8E:87:GLN:HG2	1.86	0.57
7:1G:155:GLN:CG	7:1G:181:MET:HE2	2.35	0.57
47:3C:337:TRP:CD1	47:3C:341:GLN:HG2	2.39	0.57
45:3N:23:LEU:HB3	45:3N:197:LEU:CD1	2.35	0.57
45:3N:35:CYS:CB	45:3N:201:GLY:HA3	2.33	0.57
6:5F:39:ARG:NH1	6:5F:114:ASP:OD1	2.38	0.57
45:6A:14:THR:HA	45:6A:28:GLU:CA	2.34	0.57
48:6D:114:ILE:HG22	48:6D:143:CYS:SG	2.45	0.57
48:6D:321:SER:HB2	49:6E:88:PHE:CE1	2.39	0.57
53:6J:30:LEU:HD13	54:6Y:34:TRP:HD1	1.68	0.57
45:6N:43:ALA:C	45:6N:95:THR:HG23	2.28	0.57
48:6Q:105:ASN:HD21	48:6Q:110:PRO:HD3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:229:ILE:HA	55:8A:232:GLN:HB2	1.86	0.57
82:8A:602:PGV:H182	57:8C:27:MET:HB3	1.86	0.57
75:8D:201:CDL:H241	75:8D:201:CDL:H842	1.87	0.57
3:1C:58:ILE:HD13	3:1C:118:GLU:HB3	1.86	0.57
12:1L:383:MET:HE3	12:1L:384:PRO:HD2	1.85	0.57
14:1N:210:THR:HG22	14:1N:333:SER:HB3	1.85	0.57
16:1P:244:TYR:HB2	16:1P:337:ALA:HB2	1.86	0.57
47:3C:334:THR:HA	51:3G:57:PHE:CZ	2.39	0.57
45:3N:55:ALA:HB2	45:3N:185:TYR:CD1	2.40	0.57
45:3N:57:TYR:O	45:3N:61:HIS:CD2	2.57	0.57
46:3O:85:ILE:O	46:3O:89:ILE:HG13	2.05	0.57
49:3R:151:LYS:HG2	49:3R:152:ILE:HG12	1.85	0.57
30:5e:57:ILE:HG13	30:5e:58:GLU:N	2.17	0.57
46:6B:252:LEU:HD22	49:6I:55:LEU:HD22	1.87	0.57
47:6C:233:LEU:O	47:6C:234:PHE:C	2.47	0.57
47:6C:337:TRP:HH2	47:6C:350:ILE:HD13	1.67	0.57
49:6E:264:GLU:H	49:6E:272:ILE:HG12	1.68	0.57
45:6N:4:TYR:CE1	46:6O:112:LEU:HD22	2.38	0.57
45:6N:35:CYS:O	45:6N:36:THR:C	2.48	0.57
55:8A:229:ILE:HG22	57:8C:103:HIS:HE1	1.70	0.57
55:8A:274:VAL:HA	55:8A:277:MET:HE2	1.85	0.57
82:8A:603:PGV:H172	68:8N:19:PHE:HB3	1.86	0.57
1:1A:3:ILE:HG21	71:1H:401:PC1:H222	1.85	0.57
2:1B:57:VAL:CA	2:1B:58:GLU:N	2.65	0.57
3:1C:65:ARG:O	3:1C:73:LYS:NZ	2.37	0.57
4:1D:117:ALA:HB2	4:1D:367:ILE:HG12	1.85	0.57
6:1F:39:ARG:NH1	6:1F:114:ASP:OD1	2.38	0.57
6:1F:393:TRP:O	6:1F:397:LYS:HG2	2.04	0.57
13:1M:44:GLN:H	32:1g:83:TYR:HD1	1.50	0.57
47:3C:136:GLY:HA3	47:3C:255:ASN:HA	1.87	0.57
45:3N:351:GLU:O	45:3N:355:VAL:N	2.36	0.57
46:3O:71:LEU:HD12	46:3O:144:LEU:HD23	1.86	0.57
48:3Q:12:TRP:HD1	48:3Q:15:ARG:NH1	2.01	0.57
3:5C:58:ILE:HD13	3:5C:118:GLU:HB3	1.86	0.57
6:5F:78:LYS:NZ	6:5F:222:VAL:O	2.37	0.57
7:5G:115:ASP:OD1	17:5Q:46:GLN:NE2	2.38	0.57
12:5L:383:MET:HE3	12:5L:384:PRO:HD2	1.85	0.57
13:5M:433:GLU:O	13:5M:437:MET:HG2	2.04	0.57
19:5S:22:LEU:HD23	19:5S:22:LEU:N	2.20	0.57
39:5n:117:TYR:HA	39:5n:120:LYS:NZ	2.20	0.57
40:5o:21:MET:HG3	40:5o:104:GLU:CG	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6D:286:GLU:O	48:6D:287:HIS:C	2.47	0.57
45:6N:146:ARG:O	45:6N:150:PHE:CD2	2.57	0.57
55:8A:386:VAL:HA	55:8A:389:ILE:HD12	1.87	0.57
55:8A:469:ILE:HA	55:8A:472:ILE:HD12	1.85	0.57
2:1B:176:TRP:HA	2:1B:179:ARG:HD2	1.87	0.57
16:1P:136:ASN:HA	16:1P:292:MET:HE2	1.87	0.57
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.35	0.57
47:3C:77:TRP:CZ2	47:3C:78:VAL:HG22	2.40	0.57
47:3C:226:ILE:HG12	48:3D:311:MET:HB3	1.86	0.57
47:3C:346:PRO:O	47:3C:347:PHE:C	2.46	0.57
48:3Q:18:LEU:HD22	48:3Q:206:LEU:HB2	1.87	0.57
82:4L:101:PGV:H301	82:4L:101:PGV:H81	1.86	0.57
5:5E:104:THR:HG21	5:5E:141:GLU:HG2	1.86	0.57
6:5F:261:HIS:HD2	6:5F:337:MET:HA	1.69	0.57
16:5P:268:ARG:HG2	16:5P:281:ARG:HD2	1.87	0.57
17:5Q:23:THR:HG23	17:5Q:25:VAL:H	1.70	0.57
46:6B:296:TYR:HA	46:6B:307:PHE:HZ	1.69	0.57
45:6N:10:SER:O	45:6N:11:VAL:CG2	2.52	0.57
45:6N:156:THR:O	45:6N:159:GLN:HG3	2.05	0.57
55:8A:446:ALA:O	55:8A:447:TYR:C	2.48	0.57
6:1F:276:LEU:HD21	6:1F:297:VAL:HG11	1.86	0.57
8:1H:91:MET:O	8:1H:93:TYR:N	2.37	0.57
69:1J:202:3PE:H221	69:1Y:205:3PE:H321	1.86	0.57
71:1M:502:PC1:H341	75:1i:201:CDL:H311	1.87	0.57
15:1O:60:ASP:OD1	15:1O:60:ASP:N	2.35	0.57
40:1o:52:LEU:HA	40:1o:55:ARG:HD2	1.85	0.57
47:3C:244:LEU:HD21	48:3D:293:MET:HE2	1.86	0.57
45:3N:52:ASN:HA	45:3N:185:TYR:OH	2.05	0.57
45:3N:123:GLU:HA	45:3N:179:ARG:CZ	2.33	0.57
45:3N:182:LEU:HA	45:3N:185:TYR:HD2	1.69	0.57
45:3N:191:LYS:HZ1	45:3N:229:PRO:HD2	1.70	0.57
45:3N:297:VAL:HA	47:3P:1:MET:CE	2.35	0.57
4:5D:117:ALA:HB2	4:5D:367:ILE:HG12	1.85	0.57
7:5G:283:MET:HE3	7:5G:293:TYR:CD1	2.39	0.57
11:5K:41:PHE:CD2	11:5K:64:LEU:HD13	2.40	0.57
13:5M:396:MET:O	13:5M:400:MET:HG3	2.05	0.57
24:5Y:72:THR:O	24:5Y:76:SER:OG	2.21	0.57
45:6A:119:ASN:O	45:6A:120:CYS:C	2.48	0.57
46:6B:202:ALA:N	46:6B:228:GLY:HA2	2.19	0.57
46:6B:306:PRO:HB2	46:6B:329:GLN:HB2	1.86	0.57
45:6N:118:GLN:NE2	45:6N:216:PHE:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:145:MET:CE	45:6N:248:LEU:HD13	2.35	0.57
46:6O:315:SER:HA	46:6O:320:GLY:HA2	1.87	0.57
49:6R:165:MET:HG3	49:6R:167:PHE:CZ	2.40	0.57
54:6Y:48:ILE:HG23	54:6Y:51:LYS:HB3	1.86	0.57
82:8G:101:PGV:H012	82:8G:101:PGV:H232	1.86	0.57
69:1L:704:3PE:H31	69:1L:704:3PE:H231	1.86	0.57
16:1P:146:LEU:HD11	16:1P:289:MET:HE1	1.87	0.57
46:3B:154:ASN:HD22	46:3B:155:PRO:N	2.03	0.57
45:3N:145:MET:O	45:3N:149:VAL:HG23	2.03	0.57
45:3N:316:GLU:HG2	45:3N:317:THR:HG22	1.87	0.57
45:3N:341:GLN:O	45:3N:344:ARG:HB3	2.04	0.57
47:3P:301:LEU:HD23	47:3P:304:MET:HE3	1.87	0.57
62:4H:8:ILE:HD13	62:4H:54:GLU:HB3	1.87	0.57
12:5L:172:ILE:HG21	13:5M:408:LEU:HD12	1.87	0.57
15:5O:43:ALA:HB2	15:5O:123:VAL:HG21	1.87	0.57
45:6A:142:ASP:HA	49:6E:80:HIS:CE1	2.40	0.57
46:6B:148:LYS:HD2	46:6B:183:ILE:HD11	1.87	0.57
48:6D:328:PRO:O	48:6D:329:PRO:C	2.46	0.57
45:6N:65:LYS:CE	45:6N:130:GLU:HG3	2.34	0.57
4:1D:183:ARG:NH1	4:1D:210:ASP:OD2	2.29	0.56
4:1D:354:GLU:OE2	4:1D:357:GLN:NE2	2.38	0.56
17:1Q:23:THR:HG23	17:1Q:25:VAL:H	1.70	0.56
39:1n:107:HIS:ND1	39:1n:109:SER:OG	2.35	0.56
47:3C:50:PHE:O	47:3C:53:MET:HB2	2.05	0.56
49:3E:150:SER:HB2	47:3P:168:PHE:CE1	2.39	0.56
50:3F:116:ARG:HA	46:3O:83:PHE:CZ	2.39	0.56
55:4A:242:GLU:O	55:4A:245:ILE:N	2.38	0.56
10:5J:78:MET:HE2	10:5J:79:TYR:CA	2.35	0.56
39:5n:133:GLU:H	39:5n:133:GLU:CD	2.13	0.56
40:5o:51:MET:HE2	40:5o:53:GLN:HE21	1.70	0.56
45:6A:289:HIS:HA	46:6B:87:ARG:HH21	1.69	0.56
48:6Q:18:LEU:HD22	48:6Q:206:LEU:HB2	1.87	0.56
55:8A:280:ILE:HA	55:8A:283:LEU:HD12	1.87	0.56
55:8A:301:THR:HG22	55:8A:305:PHE:CE2	2.40	0.56
2:1B:52:LEU:HD13	2:1B:91:THR:O	2.05	0.56
2:1B:124:GLY:CA	9:1I:115:LYS:HA	2.34	0.56
3:1C:32:ILE:HG22	3:1C:33:LEU:HG	1.86	0.56
6:1F:391:SER:O	6:1F:395:ILE:HG23	2.05	0.56
10:1J:70:TYR:O	10:1J:74:MET:HG2	2.04	0.56
24:1Y:124:VAL:O	24:1Y:128:GLN:HG3	2.05	0.56
40:1o:21:MET:HG3	40:1o:104:GLU:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:58:ASP:HB3	47:3C:61:THR:OG1	2.05	0.56
47:3C:70:CYS:HA	47:3C:77:TRP:HA	1.88	0.56
47:3C:151:SER:O	47:3C:152:ALA:C	2.47	0.56
45:3N:261:GLY:O	45:3N:262:TRP:C	2.48	0.56
45:3N:266:ASP:O	45:3N:267:ASN:C	2.48	0.56
57:4C:122:HIS:CE1	61:4G:45:PRO:HB3	2.40	0.56
6:5F:270:GLU:OE1	6:5F:283:HIS:NE2	2.28	0.56
7:5G:155:GLN:CG	7:5G:181:MET:HE2	2.35	0.56
10:5J:70:TYR:O	10:5J:74:MET:HG2	2.04	0.56
12:5L:67:HIS:NE2	12:5L:70:THR:OG1	2.33	0.56
12:5L:434:LYS:HE3	36:5k:57:ALA:HA	1.86	0.56
71:5M:502:PC1:H341	75:5i:201:CDL:H311	1.87	0.56
15:5O:214:MET:HE2	15:5O:214:MET:HA	1.86	0.56
16:5P:136:ASN:HA	16:5P:292:MET:HE2	1.87	0.56
46:6B:95:LYS:HB3	46:6B:110:GLU:HB3	1.87	0.56
47:6C:377:LEU:HD11	50:6F:38:PHE:CE2	2.39	0.56
49:6E:161:GLU:HA	49:6E:178:HIS:HB3	1.86	0.56
45:6N:314:TYR:O	45:6N:315:ALA:C	2.48	0.56
46:6O:117:GLU:HA	46:6O:120:MET:HE2	1.87	0.56
48:6Q:105:ASN:ND2	48:6Q:108:ALA:O	2.31	0.56
58:8D:40:LEU:HD11	58:8D:55:GLU:HB3	1.87	0.56
4:1D:291:GLY:O	4:1D:296:ARG:NH2	2.38	0.56
8:1H:313:SER:HB3	25:1Z:51:MET:HA	1.87	0.56
10:1J:114:GLU:O	10:1J:114:GLU:HG3	2.05	0.56
11:1K:41:PHE:CD2	11:1K:64:LEU:HD13	2.40	0.56
12:1L:290:LEU:O	12:1L:523:SER:OG	2.23	0.56
69:1M:501:3PE:H352	69:1M:501:3PE:H282	1.87	0.56
15:1O:136:GLU:O	15:1O:140:ARG:HG2	2.06	0.56
19:1S:22:LEU:HD23	19:1S:22:LEU:N	2.20	0.56
24:1Y:72:THR:OG1	24:1Y:92:GLY:HA2	2.04	0.56
45:3A:170:PRO:HB2	45:3A:172:GLU:CD	2.30	0.56
47:3C:345:HIS:HA	47:3C:346:PRO:C	2.30	0.56
49:3E:242:HIS:O	49:3E:250:ARG:N	2.38	0.56
45:3N:41:ILE:CD1	45:3N:195:MET:SD	2.93	0.56
45:3N:67:THR:HA	45:3N:121:SER:N	2.20	0.56
45:3N:181:ASP:C	45:3N:185:TYR:CD2	2.83	0.56
46:3O:330:ALA:HB2	46:3O:429:ASN:HB3	1.86	0.56
57:4C:175:LEU:HD12	82:4G:101:PGV:H182	1.88	0.56
1:5A:106:TRP:CE2	8:5H:291:LYS:HD3	2.41	0.56
3:5C:32:ILE:HG22	3:5C:33:LEU:HG	1.86	0.56
4:5D:246:THR:HG22	4:5D:249:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5J:129:ASP:HB3	30:5e:31:ARG:HH21	1.70	0.56
15:5O:136:GLU:O	15:5O:140:ARG:HG2	2.06	0.56
46:6B:155:PRO:O	46:6B:156:GLN:C	2.47	0.56
46:6B:188:PRO:HA	46:6B:191:LEU:HD12	1.87	0.56
49:6E:242:HIS:O	49:6E:250:ARG:N	2.38	0.56
45:6N:34:THR:CG2	45:6N:102:LEU:HD22	2.19	0.56
45:6N:46:ARG:NE	45:6N:93:GLU:OE2	2.38	0.56
46:6O:327:ILE:HD11	49:6V:59:ALA:HA	1.88	0.56
48:6Q:12:TRP:HD1	48:6Q:15:ARG:NH1	2.01	0.56
55:8A:344:PHE:O	55:8A:345:ILE:C	2.48	0.56
55:8A:440:TYR:CZ	56:8B:205:SER:HA	2.40	0.56
57:8C:122:HIS:CE1	61:8G:45:PRO:HB3	2.40	0.56
5:1E:159:ASN:HB3	5:1E:184:PRO:HB3	1.88	0.56
6:1F:78:LYS:NZ	6:1F:222:VAL:O	2.37	0.56
6:1F:261:HIS:HD2	6:1F:337:MET:HA	1.69	0.56
9:1I:11:SER:O	9:1I:20:ARG:NH1	2.37	0.56
15:1O:81:LYS:HB3	15:1O:81:LYS:NZ	2.20	0.56
45:3N:64:PHE:HE1	45:3N:86:LEU:CD2	2.19	0.56
46:3O:46:ARG:HE	46:3O:379:LEU:HD22	1.70	0.56
47:3P:284:ILE:HD12	47:3P:285:PRO:HD2	1.87	0.56
63:4I:61:GLU:OE1	63:4I:64:ARG:NH1	2.39	0.56
7:5G:351:THR:HG23	7:5G:509:PRO:HG2	1.88	0.56
24:5Y:113:ALA:HA	71:5m:201:PC1:H381	1.88	0.56
45:6N:55:ALA:O	45:6N:56:GLY:C	2.48	0.56
45:6N:168:GLU:OE1	49:6R:80:HIS:CE1	2.59	0.56
45:6N:211:LEU:HB3	45:6N:215:HIS:HD2	1.70	0.56
54:6Y:39:ARG:O	54:6Y:40:LEU:C	2.48	0.56
2:1B:100:LEU:N	2:1B:101:ARG:N	2.53	0.56
39:1n:133:GLU:CD	39:1n:133:GLU:H	2.13	0.56
45:3N:216:PHE:CD1	45:3N:219:LEU:HD11	2.40	0.56
45:3N:419:CYS:N	45:3N:438:ARG:HE	2.03	0.56
45:3N:438:ARG:HH11	45:3N:442:PHE:HE2	1.54	0.56
55:4A:7:LEU:HD21	82:4A:601:PGV:H11	1.87	0.56
55:4A:51:ASP:OD2	56:4B:205:SER:OG	2.23	0.56
55:4A:282:PHE:HA	82:4A:603:PGV:H292	1.88	0.56
55:4A:452:THR:O	55:4A:456:MET:HG3	2.05	0.56
56:4B:9:PHE:HB2	56:4B:21:LEU:HD21	1.87	0.56
60:4F:63:GLU:O	60:4F:66:ASN:HB2	2.06	0.56
82:4K:101:PGV:H21	82:4K:101:PGV:H62	1.87	0.56
6:5F:391:SER:O	6:5F:395:ILE:HG23	2.05	0.56
7:5G:155:GLN:HG2	7:5G:181:MET:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:313:SER:HB3	25:5Z:51:MET:HA	1.86	0.56
10:5J:114:GLU:HG3	10:5J:114:GLU:O	2.05	0.56
12:5L:600:THR:HG22	12:5L:601:LEU:N	2.16	0.56
13:5M:203:PHE:O	13:5M:207:MET:HG2	2.05	0.56
15:5O:50:HIS:NE2	15:5O:125:GLU:OE1	2.38	0.56
23:5X:2:GLY:O	25:5Z:109:SER:N	2.32	0.56
41:5p:95:TYR:HB3	41:5p:96:LYS:NZ	2.21	0.56
45:6A:158:PHE:O	45:6A:164:ALA:HB2	2.05	0.56
47:6C:27:ILE:HB	47:6C:31:TRP:CG	2.41	0.56
47:6C:211:ILE:HB	50:6F:78:LEU:HD21	1.88	0.56
48:6D:231:LEU:HD13	48:6D:235:LEU:H	1.70	0.56
48:6D:312:LYS:HD3	48:6D:313:ARG:HG2	1.88	0.56
45:6N:211:LEU:HB3	45:6N:215:HIS:CD2	2.40	0.56
48:6Q:98:PRO:O	48:6Q:102:ARG:HG3	2.06	0.56
48:6Q:131:LEU:HB3	48:6Q:164:ILE:HD11	1.88	0.56
63:8I:61:GLU:OE1	63:8I:64:ARG:NH1	2.39	0.56
1:1A:69:ILE:HD12	8:1H:147:ALA:HB3	1.88	0.56
5:1E:165:THR:OG1	5:1E:168:ASP:OD2	2.21	0.56
6:1F:95:VAL:HB	6:1F:136:ILE:HG13	1.87	0.56
7:1G:385:ARG:HB2	7:1G:415:LEU:HD23	1.88	0.56
8:1H:173:TRP:HB3	8:1H:175:ILE:HG22	1.87	0.56
10:1J:78:MET:HE2	10:1J:79:TYR:CA	2.35	0.56
14:1N:136:LEU:HD23	14:1N:205:LEU:HD21	1.87	0.56
39:1n:117:TYR:HA	39:1n:120:LYS:NZ	2.20	0.56
45:3N:4:TYR:HH	46:3O:112:LEU:HB3	1.67	0.56
4:5D:66:MET:HE1	4:5D:414:VAL:HG21	1.88	0.56
4:5D:354:GLU:OE2	4:5D:357:GLN:NE2	2.38	0.56
6:5F:95:VAL:HB	6:5F:136:ILE:HG13	1.87	0.56
69:5L:704:3PE:H31	69:5L:704:3PE:H231	1.86	0.56
46:6B:64:GLY:HA3	46:6B:178:CYS:HA	1.88	0.56
47:6C:72:ASP:HB3	49:6E:144:ALA:HB3	1.87	0.56
82:8B:301:PGV:H252	75:8D:201:CDL:H272	1.88	0.56
57:8C:72:THR:O	57:8C:76:GLN:HG3	2.06	0.56
6:1F:300:GLY:O	6:1F:304:THR:OG1	2.23	0.56
9:1I:11:SER:OG	9:1I:13:ASP:OD2	2.24	0.56
10:1J:129:ASP:HB3	30:1e:31:ARG:HH21	1.70	0.56
13:1M:396:MET:O	13:1M:400:MET:HG3	2.05	0.56
15:1O:43:ALA:HB2	15:1O:123:VAL:HG21	1.87	0.56
46:3O:60:SER:HA	46:3O:63:LEU:HG	1.87	0.56
49:3R:165:MET:HG3	49:3R:167:PHE:CZ	2.40	0.56
54:3X:8:PRO:HA	54:3X:11:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5A:55:PHE:CB	10:5J:74:MET:HE1	2.36	0.56
7:5G:194:GLU:HG2	7:5G:195:LEU:HG	1.87	0.56
9:5I:35:GLY:HA3	71:5I:204:PC1:H331	1.88	0.56
13:5M:11:LEU:O	13:5M:15:THR:HG23	2.05	0.56
16:5P:169:SER:HB3	16:5P:231:VAL:HG12	1.87	0.56
20:5T:52:MET:HE1	22:5W:40:TYR:CD1	2.41	0.56
80:5n:201:EHZ:O1	80:5n:201:EHZ:S1	2.64	0.56
48:6D:111:HIS:CD2	53:6J:52:LEU:HA	2.40	0.56
54:6X:8:PRO:HA	54:6X:11:ARG:HE	1.70	0.56
55:8A:32:ALA:HB3	66:8L:36:PRO:HG2	1.87	0.56
55:8A:271:MET:HA	55:8A:274:VAL:HG22	1.88	0.56
57:8C:50:ASN:HB3	82:8C:302:PGV:H181	1.88	0.56
1:1A:69:ILE:HD11	8:1H:144:VAL:HA	1.88	0.56
4:1D:24:GLU:OE2	12:1L:579:ASN:ND2	2.32	0.56
33:1h:36:VAL:HA	71:1h:202:PC1:H2G2	1.86	0.56
40:1o:51:MET:HE2	40:1o:53:GLN:HE21	1.70	0.56
45:3A:86:LEU:HD13	45:3A:99:ILE:HG12	1.86	0.56
45:3N:21:ASN:CG	45:3N:219:LEU:O	2.49	0.56
48:3Q:105:ASN:HD21	48:3Q:110:PRO:HD3	1.70	0.56
55:4A:84:PRO:HG3	55:4A:92:MET:HE2	1.86	0.56
4:5D:95:THR:HG22	4:5D:98:GLN:H	1.69	0.56
4:5D:291:GLY:O	4:5D:296:ARG:NH2	2.38	0.56
4:5D:406:SER:HB2	4:5D:414:VAL:HG22	1.86	0.56
69:5M:501:3PE:H352	69:5M:501:3PE:H282	1.87	0.56
14:5N:136:LEU:HD23	14:5N:205:LEU:HD21	1.87	0.56
14:5N:252:GLY:HA3	14:5N:290:LEU:HD13	1.88	0.56
14:5N:335:LEU:HD11	69:5N:902:3PE:H2A1	1.88	0.56
46:6B:55:SER:HB3	46:6B:176:LEU:HD23	1.87	0.56
55:8A:339:LEU:HD22	75:8D:201:CDL:H112	1.88	0.56
55:8A:431:LEU:HD22	55:8A:447:TYR:HA	1.87	0.56
62:8H:8:ILE:HD13	62:8H:54:GLU:HB3	1.87	0.56
2:1B:100:LEU:HD23	2:1B:104:TYR:CE2	2.39	0.56
2:1B:119:CYS:HA	2:1B:123:GLY:CA	2.30	0.56
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	1.88	0.56
47:3C:377:LEU:HD22	50:3F:45:ARG:HG3	1.88	0.56
45:3N:28:GLU:HA	45:3N:205:HIS:HE2	1.70	0.56
45:3N:139:GLN:HB2	49:3V:50:LEU:HD12	1.87	0.56
45:3N:349:ALA:HB3	54:3X:16:ASN:HD21	1.69	0.56
57:4C:72:THR:O	57:4C:76:GLN:HG3	2.06	0.56
58:4D:40:LEU:HD11	58:4D:55:GLU:HB3	1.87	0.56
59:4E:84:TYR:HA	59:4E:87:GLN:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:4F:53:THR:HG22	60:4F:54:ASN:H	1.71	0.56
2:5B:176:TRP:HA	2:5B:179:ARG:HD2	1.87	0.56
16:5P:146:LEU:HD11	16:5P:289:MET:HE1	1.87	0.56
16:5P:282:ASP:OD1	16:5P:286:ARG:NE	2.33	0.56
40:5o:68:CYS:O	40:5o:72:SER:OG	2.21	0.56
45:6A:436:ARG:HD2	47:6C:221:HIS:HD2	1.71	0.56
49:6I:32:ALA:HA	49:6I:71:ASN:HD21	1.69	0.56
45:6N:185:TYR:CD1	45:6N:189:HIS:NE2	2.53	0.56
55:8A:218:THR:CG2	61:8G:55:ILE:HD12	2.36	0.56
55:8A:445:ASP:O	55:8A:447:TYR:N	2.39	0.56
65:8K:8:ASP:OD1	65:8K:8:ASP:N	2.39	0.56
12:1L:554:ASP:OD2	13:1M:288:TYR:OH	2.16	0.56
16:1P:200:THR:HB	16:1P:238:LEU:HB2	1.88	0.56
32:1g:92:GLU:OE2	32:1g:95:ARG:NH1	2.39	0.56
46:3B:197:ASN:HB3	46:3B:232:LEU:HB2	1.87	0.56
47:3C:67:THR:HG21	48:3D:133:TYR:CB	2.36	0.56
47:3C:361:ILE:HA	47:3C:365:LEU:HB2	1.86	0.56
45:3N:61:HIS:C	45:3N:65:LYS:HE3	2.31	0.56
45:3N:411:CYS:O	45:3N:415:PHE:HB2	2.06	0.56
15:5O:81:LYS:NZ	15:5O:81:LYS:HB3	2.20	0.56
31:5f:56:TRP:HE1	33:5h:88:GLU:HG3	1.71	0.56
35:5j:41:TRP:CD2	36:5k:81:VAL:HG22	2.41	0.56
36:5k:84:GLU:O	36:5k:88:GLU:HG2	2.05	0.56
48:6D:310:ALA:HB1	49:6E:117:ILE:HD13	1.87	0.56
45:6N:29:GLN:HA	45:6N:203:VAL:N	2.20	0.56
46:6O:395:PRO:O	46:6O:396:SER:C	2.49	0.56
48:6Q:180:SER:OG	52:6U:15:ASP:OD1	2.24	0.56
55:8A:70:VAL:HA	55:8A:73:ILE:HB	1.88	0.56
4:1D:282:GLU:O	4:1D:313:GLN:NE2	2.23	0.55
17:1Q:25:VAL:CG1	17:1Q:30:ILE:HG13	2.36	0.55
24:1Y:113:ALA:HA	71:1m:201:PC1:H381	1.87	0.55
26:1a:1:MET:O	26:1a:4:GLU:HG3	2.06	0.55
45:3N:337:PHE:HE1	47:3P:2:THR:HA	1.71	0.55
46:3O:316:TYR:HB2	46:3O:319:SER:HB3	1.87	0.55
75:4C:308:CDL:H473	68:4N:1:MET:HA	1.88	0.55
62:4H:57:ARG:HA	62:4H:60:TYR:CE2	2.41	0.55
1:5A:106:TRP:CZ2	8:5H:291:LYS:HD3	2.41	0.55
3:5C:65:ARG:O	3:5C:73:LYS:NZ	2.37	0.55
5:5E:159:ASN:HB3	5:5E:184:PRO:HB3	1.88	0.55
14:5N:84:TRP:HB2	30:5e:18:THR:HA	1.88	0.55
45:6A:191:LYS:HG2	45:6A:194:ARG:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6D:304:LEU:O	48:6D:305:LEU:C	2.49	0.55
45:6N:18:GLN:HA	45:6N:24:ARG:CA	2.36	0.55
47:6P:284:ILE:HD12	47:6P:285:PRO:HD2	1.87	0.55
47:6P:301:LEU:HD23	47:6P:304:MET:HE3	1.87	0.55
55:8A:132:LEU:HD13	56:8B:159:VAL:HG21	1.86	0.55
55:8A:406:ASN:HD21	82:8K:101:PGV:H22	1.70	0.55
56:8B:181:GLN:O	62:8H:23:GLN:NE2	2.25	0.55
8:1H:24:GLU:HA	8:1H:271:LEU:HD13	1.88	0.55
12:1L:10:THR:HA	12:1L:13:ILE:HG22	1.88	0.55
13:1M:11:LEU:O	13:1M:15:THR:HG23	2.05	0.55
14:1N:337:LEU:HD23	75:1X:201:CDL:H191	1.87	0.55
15:1O:27:VAL:HG12	15:1O:35:LYS:HG3	1.88	0.55
75:1X:201:CDL:H462	69:1d:201:3PE:H3D2	1.89	0.55
45:3A:192:ALA:HB2	45:3A:219:LEU:HB3	1.88	0.55
49:3E:195:LEU:HD13	49:3E:250:ARG:HA	1.88	0.55
49:3E:197:ASP:OD2	49:3E:257:ASN:ND2	2.40	0.55
48:3Q:98:PRO:O	48:3Q:102:ARG:HG3	2.06	0.55
24:5Y:72:THR:OG1	24:5Y:92:GLY:HA2	2.05	0.55
26:5a:1:MET:O	26:5a:4:GLU:HG3	2.06	0.55
32:5g:92:GLU:OE2	32:5g:95:ARG:NH1	2.39	0.55
36:5k:23:ILE:O	36:5k:26:THR:OG1	2.23	0.55
45:6N:106:LEU:O	45:6N:107:PRO:C	2.49	0.55
45:6N:145:MET:HE1	45:6N:248:LEU:CD1	2.35	0.55
48:6Q:16:GLY:O	48:6Q:202:LYS:NZ	2.38	0.55
48:6Q:43:MET:HG2	48:6Q:46:VAL:HB	1.88	0.55
55:8A:288:TRP:HH2	82:8A:604:PGV:H201	1.70	0.55
75:8B:302:CDL:H661	75:8B:302:CDL:H412	1.88	0.55
4:1D:148:LEU:HD23	4:1D:174:ARG:HG2	1.88	0.55
4:1D:246:THR:HG22	4:1D:249:ASP:H	1.71	0.55
9:1I:35:GLY:HA3	71:1I:204:PC1:H331	1.88	0.55
14:1N:84:TRP:HB2	30:1e:18:THR:HA	1.88	0.55
16:1P:169:SER:HB3	16:1P:231:VAL:HG12	1.87	0.55
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.71	0.55
41:1p:95:TYR:HB3	41:1p:96:LYS:NZ	2.20	0.55
45:3A:244:ARG:HG2	51:3G:12:MET:O	2.05	0.55
10:5J:127:ILE:O	30:5e:31:ARG:NH2	2.40	0.55
12:5L:290:LEU:O	12:5L:523:SER:OG	2.23	0.55
24:5Y:140:VAL:O	33:5h:115:ARG:NH1	2.37	0.55
34:5i:103:ILE:HD13	41:5p:17:PRO:HG3	1.88	0.55
47:6C:61:THR:O	47:6C:62:ALA:C	2.48	0.55
47:6C:257:THR:O	47:6C:258:PRO:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6D:171:ARG:O	48:6D:172:PRO:C	2.49	0.55
55:8A:373:VAL:O	55:8A:374:VAL:C	2.49	0.55
75:8A:610:CDL:H473	68:8N:1:MET:HA	1.88	0.55
63:8I:63:MET:HB3	63:8I:68:ILE:HD11	1.89	0.55
4:1D:66:MET:HE1	4:1D:414:VAL:HG21	1.88	0.55
5:1E:126:ILE:HG13	5:1E:130:GLU:HG3	1.89	0.55
9:1I:156:ASN:OD1	18:1R:36:ASN:ND2	2.36	0.55
14:1N:252:GLY:HA3	14:1N:290:LEU:HD13	1.88	0.55
16:1P:268:ARG:HG2	16:1P:281:ARG:HD2	1.87	0.55
34:1i:103:ILE:HD13	41:1p:17:PRO:HG3	1.88	0.55
45:3A:242:ARG:NH2	45:3A:431:LEU:O	2.39	0.55
47:3C:241:ILE:HA	48:3D:297:MET:HE1	1.89	0.55
45:3N:79:VAL:HG13	45:3N:84:ALA:HB3	1.87	0.55
45:3N:158:PHE:CG	45:3N:163:LEU:HB2	2.40	0.55
46:3O:100:SER:HA	46:3O:106:ALA:H	1.70	0.55
63:4I:63:MET:HB3	63:4I:68:ILE:HD11	1.89	0.55
64:4J:33:ARG:NH1	82:4J:101:PGV:H183	2.21	0.55
7:5G:385:ARG:HB2	7:5G:415:LEU:HD23	1.88	0.55
8:5H:65:THR:O	8:5H:124:ASN:ND2	2.37	0.55
17:5Q:25:VAL:CG1	17:5Q:30:ILE:HG13	2.36	0.55
45:6A:242:ARG:N	51:6G:17:THR:O	2.39	0.55
46:6B:148:LYS:HE3	46:6B:177:TYR:HB3	1.88	0.55
48:6D:317:SER:O	48:6D:318:VAL:C	2.49	0.55
45:6N:21:ASN:ND2	45:6N:219:LEU:O	2.39	0.55
45:6N:107:PRO:CD	45:6N:108:LYS:H	2.20	0.55
55:8A:399:LEU:HB2	55:8A:494:TRP:CZ2	2.42	0.55
62:8H:57:ARG:HA	62:8H:60:TYR:CE2	2.41	0.55
7:1G:115:ASP:OD1	17:1Q:46:GLN:NE2	2.38	0.55
10:1J:127:ILE:O	30:1e:31:ARG:NH2	2.40	0.55
24:1Y:7:LYS:O	24:1Y:11:ILE:HD13	2.06	0.55
25:1Z:125:TYR:HB3	25:1Z:133:ILE:HG22	1.88	0.55
45:3N:303:LEU:HD12	45:3N:337:PHE:HE2	1.72	0.55
1:5A:36:PRO:HB2	1:5A:43:PRO:HG2	1.89	0.55
14:5N:337:LEU:HD23	75:5X:201:CDL:H191	1.87	0.55
20:5T:46:ASP:OD1	22:5W:64:ARG:NH2	2.36	0.55
45:6A:417:ASP:O	49:6E:111:LYS:NZ	2.37	0.55
47:6C:362:ILE:HA	47:6C:366:MET:HB2	1.88	0.55
48:6D:99:PRO:HD2	52:6H:99:PHE:HB2	1.87	0.55
46:6O:71:LEU:HD12	46:6O:144:LEU:HD23	1.89	0.55
46:6O:188:PRO:HA	46:6O:191:LEU:HD12	1.88	0.55
55:8A:166:THR:HG23	57:8C:81:TYR:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:8F:63:GLU:O	60:8F:66:ASN:HB2	2.06	0.55
7:1G:194:GLU:HG2	7:1G:195:LEU:HG	1.87	0.55
12:1L:407:TRP:CD2	37:1l:115:MET:HB3	2.42	0.55
13:1M:203:PHE:O	13:1M:207:MET:HG2	2.05	0.55
17:1Q:25:VAL:HB	17:1Q:30:ILE:HD11	1.89	0.55
17:1Q:36:ARG:NH2	17:1Q:106:GLU:OE2	2.29	0.55
20:1T:52:MET:HE1	22:1W:40:TYR:CD1	2.41	0.55
36:1k:23:ILE:O	36:1k:26:THR:OG1	2.23	0.55
47:3C:319:PRO:O	51:3G:49:ARG:NH1	2.38	0.55
51:3G:28:PHE:HB3	51:3G:31:TYR:CB	2.36	0.55
62:4H:71:ALA:O	62:4H:75:ARG:HG3	2.06	0.55
6:5F:300:GLY:O	6:5F:304:THR:OG1	2.23	0.55
12:5L:331:MET:SD	12:5L:465:GLY:HA2	2.47	0.55
13:5M:195:MET:HG3	69:5M:501:3PE:H221	1.89	0.55
14:5N:36:ASN:O	14:5N:40:MET:HB2	2.07	0.55
16:5P:200:THR:HB	16:5P:238:LEU:HB2	1.88	0.55
46:6B:150:VAL:HG22	49:6I:42:VAL:HB	1.88	0.55
49:6E:197:ASP:OD2	49:6E:257:ASN:ND2	2.40	0.55
53:6J:48:ASN:HB3	53:6J:52:LEU:HD11	1.89	0.55
45:6N:159:GLN:CG	49:6R:85:VAL:HG21	2.36	0.55
45:6N:159:GLN:NE2	45:6N:241:ILE:CD1	2.70	0.55
45:6N:168:GLU:OE1	49:6R:80:HIS:NE2	2.39	0.55
45:6N:332:ASP:H	45:6N:430:GLN:HG2	1.71	0.55
45:6N:378:ASP:HA	45:6N:381:ARG:HE	1.71	0.55
55:8A:281:GLY:HA3	82:8A:603:PGV:H271	1.89	0.55
2:1B:82:GLN:O	2:1B:83:SER:C	2.49	0.55
7:1G:351:THR:HG23	7:1G:509:PRO:HG2	1.88	0.55
12:1L:67:HIS:NE2	12:1L:70:THR:OG1	2.33	0.55
15:1O:214:MET:HE2	15:1O:214:MET:HA	1.86	0.55
47:3C:184:ILE:HB	47:3P:183:PHE:CE1	2.41	0.55
47:3C:346:PRO:O	47:3C:350:ILE:HG13	2.07	0.55
82:4A:603:PGV:H131	68:4N:22:ILE:HG21	1.87	0.55
56:4B:160:LEU:HB3	56:4B:198:GLU:HG2	1.89	0.55
12:5L:10:THR:HA	12:5L:13:ILE:HG22	1.88	0.55
17:5Q:25:VAL:HB	17:5Q:30:ILE:HD11	1.89	0.55
75:5X:201:CDL:H462	69:5d:201:3PE:H3D2	1.89	0.55
24:5Y:7:LYS:O	24:5Y:11:ILE:HD13	2.06	0.55
35:5j:37:LEU:HD13	36:5k:74:PHE:HA	1.88	0.55
46:6B:206:LEU:HG	46:6B:216:LEU:HD13	1.89	0.55
46:6B:329:GLN:O	46:6B:330:ALA:C	2.49	0.55
52:6H:53:GLU:O	52:6H:57:LYS:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:155:ALA:O	45:6N:156:THR:C	2.49	0.55
55:8A:60:ALA:O	55:8A:61:HIS:C	2.50	0.55
62:8H:71:ALA:O	62:8H:75:ARG:HG3	2.06	0.55
2:1B:119:CYS:HG	70:1B:201:SF4:FE4	0.34	0.55
14:1N:36:ASN:O	14:1N:40:MET:HB2	2.07	0.55
31:1f:56:TRP:HE1	33:1h:88:GLU:HG3	1.71	0.55
36:1k:88:GLU:HA	36:1k:91:ASN:HD22	1.72	0.55
80:1n:201:EHZ:O1	80:1n:201:EHZ:S1	2.64	0.55
46:3B:25:GLU:HG2	46:3B:213:HIS:CD2	2.41	0.55
46:3B:109:VAL:HG13	46:3B:123:LEU:HD13	1.87	0.55
47:3C:233:LEU:HA	48:3D:301:MET:HE1	1.89	0.55
47:3C:253:PRO:O	48:3D:207:ALA:HA	2.06	0.55
47:3C:337:TRP:HD1	47:3C:341:GLN:HG2	1.70	0.55
45:3N:58:PHE:CA	45:3N:61:HIS:CD2	2.72	0.55
56:4B:7:LEU:HD21	75:4B:301:CDL:H782	1.89	0.55
57:4C:88:ILE:HG12	75:4C:308:CDL:H621	1.89	0.55
13:5M:97:THR:O	13:5M:101:LEU:HG	2.07	0.55
15:5O:165:PRO:O	15:5O:248:TRP:NE1	2.35	0.55
17:5Q:36:ARG:NH2	17:5Q:106:GLU:OE2	2.29	0.55
25:5Z:58:ARG:NH2	27:5b:48:THR:OG1	2.36	0.55
35:5j:42:HIS:HE1	36:5k:84:GLU:HG3	1.72	0.55
45:6A:40:TRP:CZ2	45:6A:377:GLU:HA	2.42	0.55
45:6A:142:ASP:HA	49:6E:80:HIS:ND1	2.21	0.55
48:6D:226:PRO:HG2	48:6D:229:VAL:HG21	1.89	0.55
45:6N:10:SER:C	45:6N:11:VAL:HG23	2.32	0.55
45:6N:14:THR:HG23	45:6N:28:GLU:OE2	2.03	0.55
45:6N:40:TRP:O	45:6N:41:ILE:C	2.49	0.55
45:6N:76:GLU:O	45:6N:77:LYS:C	2.50	0.55
47:6P:5:ARG:HG3	47:6P:11:MET:HE1	1.89	0.55
55:8A:491:ASN:HB3	55:8A:494:TRP:CD1	2.42	0.55
8:1H:9:LEU:HD12	26:1a:19:PRO:HB3	1.89	0.55
37:1l:17:PRO:CD	37:1l:17:PRO:N	2.55	0.55
44:1s:31:GLU:HG3	44:1s:32:PRO:HD3	1.89	0.55
48:3D:239:PRO:HB3	52:3H:84:PHE:CZ	2.41	0.55
45:3N:60:GLU:OE2	45:3N:90:SER:CA	2.54	0.55
46:3O:131:GLU:HB3	46:3O:133:ARG:HG3	1.88	0.55
49:3R:227:ASN:H	49:3R:234:TYR:HD1	1.54	0.55
55:4A:218:THR:HG21	61:4G:55:ILE:HD12	1.89	0.55
12:5L:357:ARG:HG2	39:5n:31:VAL:HG22	1.89	0.55
13:5M:425:ASN:ND2	38:5m:57:GLY:HA2	2.22	0.55
24:5Y:48:PHE:HA	69:5Y:205:3PE:H222	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:5l:17:PRO:CD	37:5l:17:PRO:N	2.55	0.55
48:6D:313:ARG:CB	51:6G:27:ALA:HB1	2.37	0.55
45:6N:19:LEU:HB2	45:6N:23:LEU:HB2	1.88	0.55
45:6N:113:LEU:HA	45:6N:116:ILE:HD12	1.89	0.55
45:6N:124:ASP:HA	45:6N:127:ILE:HB	1.88	0.55
49:6R:179:ARG:HH21	49:6R:184:ILE:HA	1.71	0.55
54:6X:37:ASP:OD1	54:6X:51:LYS:NZ	2.32	0.55
55:8A:97:MET:HE2	55:8A:163:ASN:HD22	1.72	0.55
6:1F:270:GLU:OE1	6:1F:283:HIS:NE2	2.28	0.55
13:1M:97:THR:O	13:1M:101:LEU:HG	2.07	0.55
47:3C:377:LEU:HD13	47:3C:379:TRP:HE1	1.72	0.55
45:3N:45:SER:OG	45:3N:92:ARG:CD	2.55	0.55
45:3N:69:ASN:HD22	45:3N:115:ASP:CG	2.15	0.55
45:3N:354:VAL:O	45:3N:358:LYS:HG3	2.06	0.55
55:4A:426:PHE:HZ	75:4B:301:CDL:H142	1.72	0.55
64:4J:36:MET:HG2	82:4J:101:PGV:H181	1.89	0.55
4:5D:148:LEU:HD23	4:5D:174:ARG:HG2	1.87	0.55
8:5H:9:LEU:HD12	26:5a:19:PRO:HB3	1.89	0.55
9:5I:31:VAL:HG12	71:5I:204:PC1:H321	1.89	0.55
10:5J:98:MET:HA	10:5J:98:MET:HE2	1.89	0.55
36:5k:68:LYS:O	36:5k:71:LYS:HG3	2.06	0.55
45:6A:59:VAL:O	45:6A:60:GLU:C	2.48	0.55
45:6A:67:THR:HA	45:6A:121:SER:H	1.72	0.55
45:6A:420:PRO:O	45:6A:421:ALA:C	2.50	0.55
47:6C:319:PRO:HG2	47:6C:373:GLU:HG2	1.89	0.55
49:6E:223:VAL:HG11	48:6Q:144:ARG:HH12	1.72	0.55
45:6N:311:ASN:O	45:6N:312:ILE:C	2.50	0.55
55:8A:83:VAL:HB	55:8A:84:PRO:HD3	1.88	0.55
4:1D:226:GLU:OE2	4:1D:305:ARG:NH2	2.32	0.54
7:1G:13:VAL:HB	7:1G:33:VAL:HG21	1.89	0.54
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	1.89	0.54
12:1L:357:ARG:HG2	39:1n:31:VAL:HG22	1.89	0.54
47:3C:223:TYR:HB3	48:3D:316:TRP:NE1	2.22	0.54
45:3N:342:TRP:O	45:3N:346:CYS:N	2.29	0.54
47:3P:157:GLY:O	47:3P:161:VAL:HG23	2.07	0.54
8:5H:173:TRP:HB3	8:5H:175:ILE:HG22	1.87	0.54
9:5I:11:SER:OG	9:5I:13:ASP:OD2	2.24	0.54
15:5O:27:VAL:HG12	15:5O:35:LYS:HG3	1.88	0.54
45:6A:252:HIS:H	45:6A:425:LEU:HB2	1.71	0.54
45:6A:269:PRO:HB2	45:6A:410:VAL:HG11	1.89	0.54
46:6B:37:SER:HB2	46:6B:211:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6D:137:ARG:HD2	49:6E:148:ALA:HB1	1.88	0.54
45:6N:18:GLN:HG3	45:6N:24:ARG:HG2	1.88	0.54
45:6N:65:LYS:HE3	45:6N:130:GLU:CG	2.38	0.54
45:6N:65:LYS:CE	45:6N:130:GLU:CG	2.85	0.54
45:6N:430:GLN:O	45:6N:431:LEU:C	2.50	0.54
46:6O:77:THR:HG21	46:6O:126:VAL:HA	1.88	0.54
46:6O:128:ALA:O	46:6O:129:ALA:C	2.51	0.54
55:8A:276:ALA:HB1	55:8A:315:PRO:HB3	1.88	0.54
56:8B:9:PHE:HB2	56:8B:21:LEU:HD21	1.87	0.54
56:8B:108:TYR:O	56:8B:117:THR:HA	2.07	0.54
6:1F:372:MET:HE1	6:1F:412:ALA:HA	1.89	0.54
12:1L:172:ILE:HG21	13:1M:408:LEU:HD12	1.87	0.54
15:1O:50:HIS:NE2	15:1O:125:GLU:OE1	2.38	0.54
24:1Y:48:PHE:HA	69:1Y:205:3PE:H222	1.88	0.54
46:3B:369:LEU:HD11	46:3B:399:LEU:HD11	1.88	0.54
47:3C:70:CYS:HA	47:3C:77:TRP:CA	2.37	0.54
47:3C:151:SER:HA	47:3C:158:THR:HA	1.90	0.54
47:3C:241:ILE:O	47:3C:245:PHE:N	2.40	0.54
49:3E:80:HIS:HA	49:3E:83:ILE:HD12	1.88	0.54
45:3N:41:ILE:HD13	45:3N:190:TYR:CD1	2.41	0.54
47:3P:138:MET:HE1	47:3P:268:ILE:HA	1.89	0.54
48:3Q:43:MET:HG2	48:3Q:46:VAL:HB	1.88	0.54
48:3Q:131:LEU:HB3	48:3Q:164:ILE:HD11	1.88	0.54
57:4C:212:SER:HB2	82:4C:304:PGV:H151	1.89	0.54
1:5A:38:GLU:HB2	1:5A:43:PRO:HG3	1.88	0.54
6:5F:372:MET:HE1	6:5F:412:ALA:HA	1.89	0.54
8:5H:24:GLU:HA	8:5H:271:LEU:HD13	1.88	0.54
14:5N:152:ASN:HB3	69:5Y:204:3PE:H322	1.89	0.54
40:5o:74:PRO:HG3	41:5p:28:PRO:HD3	1.88	0.54
46:6B:124:LEU:HG	46:6B:223:PHE:HB2	1.89	0.54
46:6B:358:GLN:HA	46:6B:361:LYS:HD3	1.88	0.54
47:6C:51:LEU:HA	47:6C:54:HIS:CE1	2.43	0.54
49:6E:195:LEU:HD13	49:6E:250:ARG:HA	1.88	0.54
51:6G:20:LEU:HD23	51:6G:25:GLN:HB3	1.89	0.54
45:6N:87:ASN:HB3	45:6N:89:TYR:HE2	1.70	0.54
46:6O:241:GLY:HA3	46:6O:421:ARG:HD3	1.89	0.54
48:6Q:105:ASN:ND2	48:6Q:110:PRO:HD3	2.23	0.54
1:1A:106:TRP:CZ2	8:1H:291:LYS:HD3	2.43	0.54
2:1B:47:PRO:HD3	2:1B:74:VAL:HG12	1.88	0.54
6:1F:262:VAL:HG11	6:1F:284:ALA:HB1	1.89	0.54
10:1J:64:MET:HE3	11:1K:34:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:331:MET:SD	12:1L:465:GLY:HA2	2.47	0.54
46:3B:35:ILE:HD12	46:3B:217:LYS:HG2	1.88	0.54
48:3D:121:TYR:HA	48:3D:125:CYS:SG	2.48	0.54
59:4E:52:LEU:HD22	59:4E:98:ILE:HD13	1.89	0.54
60:4F:18:ARG:O	60:4F:22:MET:HG2	2.06	0.54
11:5K:10:MET:HE1	11:5K:14:ILE:HD11	1.89	0.54
14:5N:162:ILE:HD13	14:5N:282:MET:HG2	1.89	0.54
15:5O:291:ARG:O	15:5O:295:LYS:HD2	2.08	0.54
21:5V:37:ILE:HG12	21:5V:94:LEU:HD13	1.89	0.54
46:6B:353:SER:HB3	46:6B:356:ASP:HB3	1.88	0.54
46:6B:432:HIS:CD2	46:6B:432:HIS:H	2.22	0.54
48:6D:96:PRO:HG2	52:6H:95:ALA:HB2	1.89	0.54
48:6D:114:ILE:HG23	48:6D:278:PHE:HA	1.88	0.54
45:6N:99:ILE:HD11	45:6N:113:LEU:HD23	1.90	0.54
45:6N:145:MET:O	45:6N:146:ARG:C	2.50	0.54
57:8C:175:LEU:HD21	82:8C:304:PGV:H302	1.89	0.54
57:8C:212:SER:HB2	82:8C:304:PGV:H151	1.89	0.54
60:8F:18:ARG:O	60:8F:22:MET:HG2	2.06	0.54
1:1A:94:LEU:O	1:1A:96:ILE:N	2.39	0.54
7:1G:243:ARG:HG2	7:1G:244:THR:HG23	1.90	0.54
8:1H:65:THR:O	8:1H:124:ASN:ND2	2.37	0.54
13:1M:153:THR:HG23	13:1M:206:LYS:HD2	1.90	0.54
13:1M:195:MET:HG3	69:1M:501:3PE:H221	1.88	0.54
13:1M:425:ASN:ND2	38:1m:57:GLY:HA2	2.22	0.54
14:1N:62:THR:HG21	14:1N:114:TRP:CD1	2.42	0.54
15:1O:291:ARG:O	15:1O:295:LYS:HD2	2.07	0.54
48:3D:129:HIS:HE1	48:3D:199:PRO:HD2	1.72	0.54
45:3N:59:VAL:CG1	45:3N:190:TYR:OH	2.56	0.54
45:3N:115:ASP:CG	45:3N:119:ASN:ND2	2.63	0.54
46:3O:239:TYR:HE2	46:3O:421:ARG:HD3	1.72	0.54
62:4H:31:GLN:NE2	62:4H:35:ASP:OD1	2.41	0.54
69:5A:201:3PE:H352	27:5b:18:LEU:HB3	1.90	0.54
71:5M:502:PC1:H251	32:5g:77:VAL:HG11	1.90	0.54
25:5Z:125:TYR:HB3	25:5Z:133:ILE:HG22	1.88	0.54
37:5l:20:ARG:NH2	37:5l:36:PRO:HD2	2.23	0.54
46:6B:364:LEU:HG	46:6B:402:ILE:HD13	1.89	0.54
47:6C:327:MET:HE2	47:6C:357:LEU:HD21	1.89	0.54
45:6N:118:GLN:HE21	45:6N:219:LEU:HG	1.72	0.54
46:6O:154:ASN:HD21	46:6O:156:GLN:HB2	1.72	0.54
12:1L:562:LEU:HB3	69:1N:901:3PE:H3B2	1.90	0.54
14:1N:24:SER:HB3	30:1e:1:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:162:ILE:HD13	14:1N:282:MET:HG2	1.89	0.54
20:1T:76:ILE:O	20:1T:80:ILE:HG12	2.08	0.54
37:1l:20:ARG:NH2	37:1l:36:PRO:HD2	2.22	0.54
39:1n:54:LYS:NZ	45:3N:20:ASP:HA	2.22	0.54
47:3C:104:TYR:CD1	47:3C:208:PRO:HA	2.43	0.54
45:3N:80:GLU:HB3	46:3O:363:LYS:HZ1	1.72	0.54
47:3P:5:ARG:HG3	47:3P:11:MET:HE1	1.89	0.54
1:5A:54:LYS:HE3	1:5A:113:TRP:HE3	1.71	0.54
14:5N:62:THR:HG21	14:5N:114:TRP:CD1	2.42	0.54
16:5P:173:GLY:H	16:5P:176:ASP:HB3	1.72	0.54
20:5T:76:ILE:O	20:5T:80:ILE:HG12	2.08	0.54
41:5p:166:ARG:HA	41:5p:170:LYS:HZ3	1.72	0.54
75:5q:201:CDL:H712	75:5q:201:CDL:H332	1.90	0.54
45:6A:161:THR:HG21	45:6A:235:ARG:H	1.73	0.54
47:6C:160:LEU:HA	47:6C:163:TRP:HB2	1.88	0.54
45:6N:165:GLN:HA	49:6R:84:ARG:HH22	1.73	0.54
55:8A:268:PHE:HB2	55:8A:326:THR:HG23	1.88	0.54
56:8B:7:LEU:HD21	75:8B:302:CDL:H782	1.89	0.54
10:1J:77:GLU:HB3	11:1K:25:HIS:NE2	2.23	0.54
21:1V:37:ILE:HG12	21:1V:94:LEU:HD13	1.89	0.54
45:3N:344:ARG:O	45:3N:348:SER:N	2.41	0.54
46:3O:68:LEU:HA	46:3O:144:LEU:HD21	1.88	0.54
48:3Q:105:ASN:ND2	48:3Q:110:PRO:HD3	2.23	0.54
49:3R:179:ARG:HH21	49:3R:184:ILE:HA	1.71	0.54
52:3U:47:ARG:HD2	52:3U:50:THR:HB	1.89	0.54
55:4A:52:GLN:O	55:4A:56:VAL:HG23	2.07	0.54
15:5O:104:ARG:NH2	76:5O:401:GTP:N7	2.56	0.54
18:5R:20:ASP:N	18:5R:20:ASP:OD1	2.36	0.54
38:5m:7:PRO:HB3	38:5m:13:LEU:HB2	1.90	0.54
47:6C:26:ASN:HA	50:6F:82:MET:HA	1.90	0.54
47:6C:184:ILE:O	47:6C:185:LEU:C	2.49	0.54
48:6D:211:GLY:O	48:6D:215:VAL:N	2.39	0.54
49:6E:80:HIS:HA	49:6E:83:ILE:HD12	1.88	0.54
49:6E:183:GLU:O	49:6E:187:GLU:HG2	2.08	0.54
49:6E:249:ILE:H	49:6E:257:ASN:ND2	2.05	0.54
45:6N:16:VAL:HG12	45:6N:17:SER:H	1.69	0.54
45:6N:69:ASN:HD21	45:6N:119:ASN:ND2	2.06	0.54
55:8A:258:VAL:O	55:8A:262:SER:N	2.39	0.54
55:8A:361:SER:O	55:8A:362:SER:C	2.50	0.54
55:8A:370:THR:HG23	56:8B:171:LYS:NZ	2.22	0.54
55:8A:382:SER:O	55:8A:386:VAL:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:479:LYS:HB3	67:8M:7:ARG:HB2	1.88	0.54
58:8D:89:ILE:HG22	65:8K:29:TRP:HE1	1.72	0.54
60:8F:53:THR:HG22	60:8F:54:ASN:H	1.71	0.54
1:1A:13:LEU:HD21	8:1H:14:LEU:HD11	1.90	0.54
2:1B:90:GLY:HA2	70:1B:201:SF4:S2	2.48	0.54
12:1L:316:THR:HA	12:1L:319:ILE:HG12	1.90	0.54
12:1L:407:TRP:CZ2	12:1L:411:MET:HE3	2.43	0.54
16:1P:282:ASP:OD1	16:1P:286:ARG:NE	2.33	0.54
20:1T:6:LEU:HD23	20:1T:6:LEU:H	1.73	0.54
39:1n:117:TYR:HA	39:1n:120:LYS:HZ1	1.73	0.54
47:3C:85:ASN:HB2	47:3C:243:VAL:HG22	1.89	0.54
45:3N:148:VAL:HG12	45:3N:152:TYR:HE2	0.84	0.54
54:3Y:11:ARG:HG3	54:3Y:15:ARG:NH1	2.23	0.54
4:5D:109:VAL:HG12	4:5D:149:ASN:HA	1.89	0.54
12:5L:407:TRP:CD2	37:5l:115:MET:HB3	2.42	0.54
12:5L:601:LEU:HD12	12:5L:602:PHE:CD1	2.43	0.54
13:5M:104:LEU:HD11	75:5X:201:CDL:H273	1.90	0.54
13:5M:153:THR:HG23	13:5M:206:LYS:HD2	1.90	0.54
36:5k:68:LYS:H	36:5k:68:LYS:HD3	1.73	0.54
45:6A:290:MET:O	45:6A:291:SER:C	2.51	0.54
46:6B:74:SER:HB2	49:6I:70:LEU:HD12	1.90	0.54
46:6B:307:PHE:H	49:6I:52:ARG:CG	2.19	0.54
50:6F:115:GLU:OE2	46:6O:84:LYS:HA	2.07	0.54
45:6N:107:PRO:CD	45:6N:108:LYS:N	2.70	0.54
47:6P:138:MET:HE1	47:6P:268:ILE:HA	1.90	0.54
47:6P:149:LEU:HD23	47:6P:287:LYS:HZ2	1.73	0.54
55:8A:396:TRP:HB3	55:8A:399:LEU:HB3	1.88	0.54
59:8E:52:LEU:HD22	59:8E:98:ILE:HD13	1.89	0.54
2:1B:61:HIS:HE1	4:1D:174:ARG:NE	2.00	0.54
4:1D:90:LEU:O	4:1D:94:LYS:HG2	2.08	0.54
11:1K:10:MET:HE1	11:1K:14:ILE:HD11	1.89	0.54
12:1L:601:LEU:HD12	12:1L:602:PHE:CD1	2.43	0.54
14:1N:40:MET:HE3	14:1N:44:LEU:HD21	1.90	0.54
16:1P:82:ARG:O	16:1P:86:GLU:HG3	2.08	0.54
38:1m:112:GLU:O	38:1m:116:GLN:HG2	2.08	0.54
45:3A:276:ILE:HG21	45:3A:345:LEU:HD21	1.89	0.54
47:3C:86:GLY:HA2	47:3C:239:LEU:HD11	1.90	0.54
1:5A:96:ILE:HD11	27:5b:29:ILE:HD11	1.90	0.54
5:5E:126:ILE:HG13	5:5E:130:GLU:HG3	1.89	0.54
71:5H:401:PC1:O14	10:5J:50:SER:OG	2.18	0.54
12:5L:316:THR:HA	12:5L:319:ILE:HG12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6B:62:ASN:O	46:6B:63:LEU:C	2.50	0.54
46:6B:307:PHE:O	49:6I:52:ARG:HG3	2.08	0.54
46:6B:412:ASN:HA	46:6B:415:LYS:HD2	1.90	0.54
47:6C:150:LEU:O	47:6C:151:SER:C	2.51	0.54
48:6D:252:PRO:HB2	84:6D:501:HEC:HAB	1.89	0.54
45:6N:58:PHE:CA	45:6N:61:HIS:HD2	2.18	0.54
45:6N:62:LEU:HD11	45:6N:182:LEU:CD1	2.37	0.54
45:6N:158:PHE:O	45:6N:159:GLN:C	2.51	0.54
55:8A:105:LEU:HB2	55:8A:106:PRO:HD3	1.88	0.54
55:8A:378:HIS:HD2	55:8A:382:SER:HB2	1.73	0.54
61:8G:56:ARG:NH2	61:8G:66:ASN:O	2.30	0.54
2:1B:85:VAL:HG11	2:1B:163:LEU:HD21	1.89	0.54
3:1C:175:ARG:NH1	3:1C:186:GLU:OE2	2.41	0.54
10:1J:98:MET:HE2	10:1J:98:MET:HA	1.89	0.54
12:1L:600:THR:HG22	12:1L:601:LEU:N	2.16	0.54
13:1M:104:LEU:HD11	75:1X:201:CDL:H273	1.90	0.54
14:1N:335:LEU:HD11	69:1N:902:3PE:H2A1	1.89	0.54
23:1X:80:PRO:HB3	23:1X:105:LYS:HG2	1.90	0.54
30:1e:83:ASP:HA	30:1e:86:ILE:HG22	1.90	0.54
47:3C:48:GLY:HA3	83:3C:501:HEM:C4C	2.43	0.54
47:3C:215:MET:SD	47:3C:215:MET:N	2.73	0.54
45:3N:62:LEU:HD23	45:3N:65:LYS:NZ	2.22	0.54
45:3N:262:TRP:CD2	45:3N:385:THR:HB	2.43	0.54
49:3R:150:SER:HB3	49:3R:170:ARG:H	1.73	0.54
55:4A:218:THR:HG22	55:4A:221:ASP:HB3	1.90	0.54
56:4B:33:LEU:HB2	63:4I:32:ALA:HB2	1.89	0.54
57:4C:213:THR:HB	82:4C:305:PGV:H11	1.90	0.54
16:5P:82:ARG:O	16:5P:86:GLU:HG3	2.08	0.54
23:5X:80:PRO:HB3	23:5X:105:LYS:HG2	1.90	0.54
38:5m:112:GLU:O	38:5m:116:GLN:HG2	2.07	0.54
48:6D:296:LYS:O	48:6D:297:MET:C	2.51	0.54
48:6Q:12:TRP:CD1	48:6Q:15:ARG:HH12	2.21	0.54
49:6R:227:ASN:H	49:6R:234:TYR:HD1	1.54	0.54
4:1D:109:VAL:HG12	4:1D:149:ASN:HA	1.89	0.54
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.43	0.54
14:1N:128:LEU:CD1	75:1N:903:CDL:HA61	2.38	0.54
15:1O:34:GLY:N	76:1O:401:GTP:O3G	2.41	0.54
46:3B:78:LYS:HB2	46:3B:129:ALA:HB1	1.89	0.54
48:3D:135:ALA:HA	48:3D:178:TYR:HA	1.90	0.54
45:3N:58:PHE:HZ	45:3N:174:VAL:CG1	2.19	0.54
45:3N:148:VAL:O	45:3N:152:TYR:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:268:VAL:O	45:3N:269:PRO:C	2.51	0.54
45:3N:311:ASN:HB2	45:3N:320:LEU:HD13	1.89	0.54
48:3Q:180:SER:OG	52:3U:15:ASP:OD1	2.24	0.54
55:4A:508:PRO:HG3	57:4C:6:HIS:HB3	1.89	0.54
2:5B:82:GLN:NE2	8:5H:215:TYR:O	2.41	0.54
10:5J:64:MET:HE3	11:5K:34:GLU:OE1	2.07	0.54
13:5M:196:TRP:CD1	13:5M:250:LEU:HB3	2.43	0.54
45:6A:279:HIS:HB3	45:6A:308:GLN:HA	1.90	0.54
46:6B:314:ALA:HB1	49:6I:63:PRO:HG3	1.90	0.54
45:6N:159:GLN:NE2	45:6N:241:ILE:HD11	2.22	0.54
45:6N:206:ARG:O	45:6N:207:GLN:C	2.51	0.54
46:6O:70:ARG:HA	46:6O:98:VAL:HG11	1.90	0.54
46:6O:100:SER:HB2	49:6V:66:ALA:HB3	1.90	0.54
48:6Q:126:TYR:OH	84:6Q:501:HEC:O2A	2.19	0.54
2:1B:59:MET:HE3	2:1B:76:PHE:HE1	1.72	0.53
2:1B:91:THR:HG22	2:1B:92:LEU:H	1.72	0.53
12:1L:194:ASN:ND2	38:1m:126:ILE:HD11	2.23	0.53
45:3A:133:VAL:HG11	49:3I:53:GLU:OE2	2.08	0.53
47:3C:320:LEU:HA	47:3C:323:CYS:SG	2.48	0.53
49:3E:223:VAL:HG11	48:3Q:144:ARG:HH12	1.72	0.53
49:3E:249:ILE:H	49:3E:257:ASN:ND2	2.06	0.53
45:3N:56:GLY:HA2	45:3N:59:VAL:HB	1.90	0.53
58:4D:135:SER:OG	58:4D:140:TYR:OH	2.20	0.53
1:5A:35:SER:O	2:5B:81:ARG:NH2	2.39	0.53
2:5B:90:GLY:HA2	70:5B:201:SF4:S2	2.48	0.53
12:5L:51:LEU:HD22	12:5L:91:PRO:HG2	1.89	0.53
38:5m:29:ARG:CG	45:6N:227:ALA:HB2	2.38	0.53
45:6N:343:MET:O	45:6N:344:ARG:C	2.51	0.53
55:8A:377:PHE:CD2	85:8A:606:HEA:HAD1	2.44	0.53
2:1B:36:LEU:CA	2:1B:39:TRP:HB2	2.34	0.53
10:1J:99:MET:HG3	10:1J:100:GLU:N	2.23	0.53
47:3C:337:TRP:CD1	47:3C:337:TRP:C	2.86	0.53
48:3D:137:ARG:HD3	48:3D:176:SER:HA	1.89	0.53
45:3N:38:GLY:HA3	45:3N:98:TYR:HA	1.89	0.53
45:3N:124:ASP:HA	45:3N:127:ILE:HD12	1.90	0.53
46:3O:34:VAL:HG11	46:3O:386:ALA:HB1	1.90	0.53
48:3Q:12:TRP:CD1	48:3Q:15:ARG:HH12	2.21	0.53
56:4B:23:PHE:CZ	56:4B:80:SER:HB2	2.43	0.53
75:4B:301:CDL:H412	75:4B:301:CDL:H661	1.88	0.53
1:5A:50:PRO:HB2	10:5J:74:MET:HA	1.90	0.53
3:5C:175:ARG:NH1	3:5C:186:GLU:OE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5J:78:MET:HE2	10:5J:79:TYR:H	1.67	0.53
13:5M:265:SER:OG	13:5M:299:VAL:HG23	2.09	0.53
46:6B:332:SER:O	46:6B:333:ALA:C	2.50	0.53
48:6D:201:LEU:O	48:6D:202:SER:C	2.51	0.53
48:6D:231:LEU:HB2	48:6D:235:LEU:HB2	1.90	0.53
53:6J:28:GLY:HA2	53:6J:31:PHE:HD1	1.72	0.53
45:6N:41:ILE:HG12	45:6N:195:MET:SD	2.48	0.53
52:6U:47:ARG:HD2	52:6U:50:THR:HB	1.89	0.53
55:8A:34:SER:HA	55:8A:37:ILE:HB	1.90	0.53
55:8A:426:PHE:HZ	75:8B:302:CDL:H112	1.72	0.53
57:8C:209:ILE:HG23	82:8C:304:PGV:H152	1.89	0.53
2:1B:61:HIS:ND1	4:1D:171:PHE:HE2	1.86	0.53
6:1F:308:PRO:HD3	6:1F:421:HIS:CD2	2.43	0.53
12:1L:100:ILE:HG21	12:1L:246:LEU:HB2	1.90	0.53
14:1N:152:ASN:HB3	69:1Y:204:3PE:H322	1.89	0.53
24:1Y:55:THR:O	24:1Y:59:THR:OG1	2.23	0.53
26:1a:34:LYS:NZ	26:1a:61:HIS:O	2.42	0.53
30:1e:68:ARG:HB3	30:1e:71:THR:HB	1.91	0.53
47:3C:135:TRP:HA	47:3C:135:TRP:CE3	2.44	0.53
49:3E:156:LEU:HG	49:3E:157:SER:H	1.72	0.53
49:3R:179:ARG:HD3	49:3R:211:VAL:HB	1.90	0.53
49:3R:225:ILE:HG12	49:3R:237:PRO:HG3	1.91	0.53
55:4A:266:GLU:HB3	60:4F:68:THR:HG21	1.90	0.53
57:4C:176:LEU:HD23	82:4G:101:PGV:H11	1.90	0.53
1:5A:44:MET:HE2	1:5A:44:MET:N	2.22	0.53
8:5H:311:THR:OG1	8:5H:313:SER:OG	2.27	0.53
9:5I:109:TYR:HB3	9:5I:151:LYS:HG3	1.90	0.53
69:5Y:206:3PE:H2C2	38:5m:94:ILE:HD11	1.91	0.53
46:6B:195:VAL:HG13	46:6B:199:PHE:HB2	1.89	0.53
46:6B:279:LEU:HB3	46:6B:295:LEU:HD11	1.89	0.53
45:6N:65:LYS:HZ2	45:6N:130:GLU:CD	2.16	0.53
45:6N:71:PRO:CD	45:6N:72:GLY:H	2.21	0.53
55:8A:433:LEU:HD22	56:8B:8:GLY:HA2	1.90	0.53
56:8B:33:LEU:HB2	63:8I:32:ALA:HB2	1.89	0.53
69:1N:902:3PE:H3I2	69:1N:902:3PE:H2E2	1.91	0.53
27:1b:42:ILE:HG22	27:1b:46:ARG:HD3	1.90	0.53
49:3E:195:LEU:HD11	49:3E:248:ARG:HD2	1.89	0.53
48:3Q:8:PRO:HG3	52:3U:66:ASP:HB3	1.90	0.53
55:4A:244:TYR:O	55:4A:248:LEU:N	2.40	0.53
89:4B:303:PSC:H251	63:4I:21:ILE:HG21	1.90	0.53
69:5A:201:3PE:H2F2	8:5H:302:MET:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6B:22:GLN:HE22	46:6B:39:GLU:HB3	1.72	0.53
47:6C:73:VAL:O	47:6C:74:ASN:C	2.51	0.53
49:6E:156:LEU:HG	49:6E:157:SER:H	1.73	0.53
45:6N:79:VAL:HG13	45:6N:84:ALA:HB3	1.90	0.53
46:6O:165:ALA:HA	46:6O:173:ALA:HA	1.89	0.53
55:8A:172:LYS:O	55:8A:173:PRO:C	2.50	0.53
56:8B:160:LEU:HB3	56:8B:198:GLU:HG2	1.89	0.53
1:1A:66:ASP:O	1:1A:69:ILE:HB	2.08	0.53
2:1B:124:GLY:HA3	9:1I:115:LYS:HA	1.90	0.53
9:1I:132:VAL:HG21	9:1I:165:ILE:HD12	1.90	0.53
13:1M:265:SER:OG	13:1M:299:VAL:HG23	2.09	0.53
15:1O:9:VAL:HG12	15:1O:10:LEU:HD23	1.91	0.53
47:3C:246:SER:OG	47:3C:249:LEU:HB3	2.08	0.53
47:3C:345:HIS:HB2	47:3C:349:ILE:H	1.72	0.53
53:3J:54:LYS:HG3	53:3J:55:HIS:N	2.23	0.53
45:3N:32:GLN:HE22	46:3O:373:GLU:HA	1.73	0.53
45:3N:57:TYR:CE1	45:3N:167:VAL:CG1	2.55	0.53
45:3N:118:GLN:HE22	45:3N:219:LEU:N	2.05	0.53
46:3O:172:LEU:C	46:3O:174:ASN:H	2.16	0.53
46:3O:381:GLU:HG3	46:3O:385:GLN:HE21	1.74	0.53
49:3R:219:HIS:CE1	49:3R:239:HIS:ND1	2.76	0.53
82:4A:604:PGV:H012	82:4C:303:PGV:H202	1.90	0.53
56:4B:108:TYR:O	56:4B:117:THR:HA	2.07	0.53
1:5A:54:LYS:HA	1:5A:57:LEU:HD12	1.90	0.53
6:5F:262:VAL:HG11	6:5F:284:ALA:HB1	1.89	0.53
7:5G:190:MET:SD	7:5G:190:MET:N	2.75	0.53
10:5J:77:GLU:HB3	11:5K:25:HIS:NE2	2.22	0.53
12:5L:194:ASN:ND2	38:5m:126:ILE:HD11	2.23	0.53
69:5M:503:3PE:H2A1	38:5m:97:LEU:HB3	1.91	0.53
14:5N:40:MET:HE3	14:5N:44:LEU:HD21	1.90	0.53
46:6B:277:HIS:HE1	46:6B:364:LEU:HD13	1.74	0.53
48:6D:110:ASP:OD1	53:6J:51:LYS:HA	2.08	0.53
48:6D:260:PHE:O	48:6D:261:ASP:C	2.51	0.53
45:6N:7:ALA:HB1	46:6O:43:PRO:HB3	1.90	0.53
45:6N:263:ALA:O	45:6N:264:ASN:C	2.52	0.53
46:6O:67:HIS:HE1	46:6O:144:LEU:HA	1.73	0.53
47:6P:157:GLY:O	47:6P:161:VAL:HG23	2.07	0.53
66:8L:28:TYR:HD2	82:8L:101:PGV:H302	1.73	0.53
7:1G:32:LYS:NZ	7:1G:32:LYS:HB3	2.23	0.53
13:1M:119:TYR:CZ	13:1M:161:LEU:HB2	2.44	0.53
71:1M:502:PC1:H251	32:1g:77:VAL:HG11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:7:PRO:HB3	38:1m:13:LEU:HB2	1.90	0.53
47:3C:334:THR:HG21	47:3C:354:ALA:CB	2.38	0.53
52:3H:97:LYS:O	52:3H:98:LEU:C	2.52	0.53
45:3N:355:VAL:O	45:3N:356:ARG:C	2.52	0.53
55:4A:362:SER:HA	56:4B:87:MET:HE1	1.89	0.53
4:5D:226:GLU:OE2	4:5D:305:ARG:NH2	2.32	0.53
7:5G:13:VAL:HB	7:5G:33:VAL:HG21	1.89	0.53
12:5L:407:TRP:CZ2	12:5L:411:MET:HE3	2.43	0.53
26:5a:34:LYS:NZ	26:5a:61:HIS:O	2.42	0.53
32:5g:43:ASP:OD1	39:5n:107:HIS:NE2	2.36	0.53
45:6A:330:SER:O	45:6A:331:ILE:C	2.52	0.53
47:6C:25:SER:O	47:6C:27:ILE:N	2.41	0.53
48:6D:308:VAL:HG22	49:6E:121:THR:HG23	1.91	0.53
49:6E:195:LEU:HD11	49:6E:248:ARG:HD2	1.90	0.53
45:6N:85:HIS:HA	46:6O:284:HIS:O	2.09	0.53
48:6Q:8:PRO:HG3	52:6U:66:ASP:HB3	1.90	0.53
55:8A:298:ASP:HA	62:8H:22:ASN:HD21	1.74	0.53
75:8A:610:CDL:H621	57:8C:88:ILE:HG12	1.89	0.53
62:8H:31:GLN:NE2	62:8H:35:ASP:OD1	2.41	0.53
75:1q:201:CDL:H332	75:1q:201:CDL:H712	1.90	0.53
47:3C:105:GLY:HA2	47:3C:107:TYR:CE2	2.44	0.53
47:3C:185:LEU:HB2	47:3C:186:PRO:HD3	1.90	0.53
47:3C:222:PRO:HB2	48:3D:315:LYS:HD2	1.91	0.53
49:3E:155:LYS:NZ	49:3E:176:VAL:HG11	2.18	0.53
45:3N:49:ASN:N	45:3N:52:ASN:HB2	2.24	0.53
58:4D:89:ILE:HG22	65:4K:29:TRP:HE1	1.72	0.53
4:5D:90:LEU:O	4:5D:94:LYS:HG2	2.08	0.53
7:5G:194:GLU:CD	7:5G:194:GLU:H	2.17	0.53
7:5G:226:GLU:OE1	17:5Q:36:ARG:NH2	2.30	0.53
14:5N:20:VAL:HG11	14:5N:137:ALA:HB1	1.90	0.53
14:5N:24:SER:HB3	30:5e:1:PRO:HD3	1.89	0.53
47:6C:147:THR:O	47:6C:148:ASN:C	2.52	0.53
47:6C:148:ASN:O	47:6C:149:LEU:C	2.51	0.53
45:6N:4:TYR:CD2	46:6O:114:ASP:CG	2.78	0.53
45:6N:65:LYS:HE3	45:6N:130:GLU:CD	2.31	0.53
46:6O:258:VAL:HG12	46:6O:323:GLY:HA3	1.91	0.53
55:8A:38:ARG:HA	55:8A:41:LEU:HD12	1.90	0.53
10:1J:129:ASP:N	30:1e:31:ARG:HH21	2.07	0.53
47:3C:78:VAL:HG13	48:3D:293:MET:HE1	1.91	0.53
47:3C:154:PRO:C	47:3C:156:ILE:H	2.16	0.53
47:3C:334:THR:OG1	51:3G:57:PHE:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:183:GLU:O	49:3E:187:GLU:HG2	2.08	0.53
48:3Q:27:ARG:HB2	48:3Q:55:CYS:HB2	1.91	0.53
57:4C:42:LEU:HD13	64:4J:45:TYR:HD2	1.74	0.53
15:5O:34:GLY:N	76:5O:401:GTP:O3G	2.41	0.53
20:5T:6:LEU:H	20:5T:6:LEU:HD23	1.73	0.53
30:5e:83:ASP:HA	30:5e:86:ILE:HG22	1.90	0.53
45:6A:239:SER:H	45:6A:421:ALA:HA	1.73	0.53
47:6C:109:PHE:O	47:6C:110:LEU:C	2.52	0.53
45:6N:15:GLN:H	45:6N:205:HIS:CE1	2.27	0.53
45:6N:58:PHE:CD1	45:6N:134:ILE:HD11	2.28	0.53
45:6N:87:ASN:HB3	45:6N:89:TYR:CE2	2.44	0.53
45:6N:161:THR:HB	45:6N:162:PRO:CD	2.39	0.53
49:6R:179:ARG:HD3	49:6R:211:VAL:HB	1.90	0.53
49:6R:219:HIS:HE1	49:6R:253:PRO:HD2	1.73	0.53
56:8B:1:FME:HE3	58:8D:128:VAL:HG22	1.91	0.53
57:8C:103:HIS:CD2	82:8C:303:PGV:H05	2.44	0.53
57:8C:213:THR:HB	82:8C:305:PGV:H11	1.90	0.53
7:1G:320:GLY:O	7:1G:498:SER:OG	2.27	0.53
9:1I:160:LYS:HG2	9:1I:161:TRP:CD1	2.43	0.53
13:1M:133:ILE:HD11	13:1M:231:LEU:HD11	1.90	0.53
15:1O:104:ARG:NH2	76:1O:401:GTP:N7	2.56	0.53
15:1O:234:VAL:O	15:1O:238:ILE:HG12	2.09	0.53
23:1X:82:THR:HA	23:1X:85:TRP:NE1	2.24	0.53
47:3C:234:PHE:O	47:3C:237:LEU:HB3	2.09	0.53
47:3C:334:THR:HG23	47:3C:337:TRP:CE3	2.44	0.53
48:3D:160:ASP:HB3	48:3D:169:PHE:CZ	2.44	0.53
55:4A:144:ASP:OD2	55:4A:213:ARG:NH1	2.42	0.53
56:4B:1:FME:HE3	58:4D:128:VAL:HG22	1.91	0.53
82:4K:101:PGV:H61	82:4K:101:PGV:H292	1.91	0.53
7:5G:217:ALA:HB2	7:5G:248:MET:HE2	1.91	0.53
8:5H:24:GLU:HB2	8:5H:271:LEU:HD22	1.90	0.53
25:5Z:93:GLU:O	25:5Z:97:ILE:HG13	2.09	0.53
47:6C:3:ASN:O	47:6C:4:ILE:C	2.51	0.53
47:6C:8:HIS:O	47:6C:9:PRO:C	2.51	0.53
47:6C:359:PHE:O	47:6C:360:LEU:C	2.50	0.53
47:6C:377:LEU:HB3	47:6C:379:TRP:CD1	2.44	0.53
45:6N:211:LEU:O	45:6N:215:HIS:CD2	2.62	0.53
45:6N:433:ASP:HB2	47:6P:219:PRO:HG3	1.91	0.53
52:6U:21:ARG:O	52:6U:25:GLU:HG2	2.09	0.53
55:8A:151:HIS:HB3	90:8C:307:PEK:H361	1.90	0.53
55:8A:296:GLY:HA2	62:8H:23:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:328:HIS:O	56:8B:56:MET:HE1	2.09	0.53
60:8F:79:THR:HG23	60:8F:90:LYS:HB2	1.91	0.53
2:1B:93:THR:O	2:1B:96:MET:N	2.42	0.53
9:1I:31:VAL:HG12	71:1I:204:PC1:H321	1.89	0.53
13:1M:165:VAL:HG21	14:1N:267:ILE:HG22	1.91	0.53
14:1N:20:VAL:HG11	14:1N:137:ALA:HB1	1.90	0.53
34:1i:44:GLN:HA	34:1i:47:ASN:OD1	2.09	0.53
45:3N:141:ASN:HA	49:3V:47:ARG:HH21	1.74	0.53
45:3N:158:PHE:CE1	45:3N:163:LEU:HD12	2.24	0.53
45:3N:290:MET:HE2	45:3N:290:MET:HA	1.91	0.53
45:3N:296:SER:O	47:3P:1:MET:HE1	2.09	0.53
66:4L:28:TYR:HD2	82:4L:101:PGV:H302	1.73	0.53
1:5A:33:LYS:HD3	8:5H:61:LEU:HD21	1.90	0.53
7:5G:243:ARG:HG2	7:5G:244:THR:HG23	1.90	0.53
12:5L:534:HIS:CD2	69:5L:701:3PE:H341	2.44	0.53
13:5M:104:LEU:HG	13:5M:108:MET:HE2	1.91	0.53
13:5M:133:ILE:HD11	13:5M:231:LEU:HD11	1.90	0.53
45:6A:30:SER:HB2	45:6A:201:GLY:HA2	1.90	0.53
47:6C:209:THR:HG23	50:6F:81:THR:HG21	1.91	0.53
52:6H:53:GLU:HA	52:6H:56:ILE:HD12	1.91	0.53
45:6N:186:VAL:HG13	45:6N:190:TYR:CE2	2.36	0.53
46:6O:143:GLN:HA	46:6O:146:ILE:HD12	1.90	0.53
49:6R:150:SER:HB3	49:6R:170:ARG:H	1.73	0.53
89:8A:611:PSC:H251	63:8I:21:ILE:HG21	1.90	0.53
57:8C:80:ARG:NH2	57:8C:236:GLU:OE1	2.42	0.53
4:1D:109:VAL:CG1	4:1D:149:ASN:HA	2.39	0.52
15:1O:165:PRO:O	15:1O:248:TRP:NE1	2.35	0.52
47:3C:257:THR:OG1	48:3D:207:ALA:HB1	2.09	0.52
45:3N:134:ILE:HA	45:3N:137:GLU:HB2	1.90	0.52
45:3N:268:VAL:HB	45:3N:269:PRO:CD	2.39	0.52
46:3O:77:THR:HG21	46:3O:126:VAL:HA	1.91	0.52
5:5E:151:ALA:HB1	5:5E:152:PRO:HD2	1.91	0.52
12:5L:591:PHE:CE1	14:5N:111:PHE:HA	2.44	0.52
15:5O:9:VAL:HG12	15:5O:10:LEU:HD23	1.90	0.52
15:5O:252:ASP:OD1	15:5O:252:ASP:N	2.42	0.52
46:6B:167:ALA:HA	46:6B:241:GLY:HA2	1.90	0.52
46:6B:277:HIS:CE1	46:6B:364:LEU:HD13	2.44	0.52
46:6B:313:ASN:HA	46:6B:322:PHE:CA	2.36	0.52
47:6C:350:ILE:HD11	51:6G:64:GLY:CA	2.38	0.52
53:6J:30:LEU:HD11	54:6Y:34:TRP:HA	1.91	0.52
45:6N:56:GLY:O	45:6N:60:GLU:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:65:LYS:NZ	45:6N:130:GLU:CD	2.67	0.52
46:6O:172:LEU:O	46:6O:173:ALA:C	2.52	0.52
46:6O:197:ASN:HA	46:6O:231:GLY:HA3	1.91	0.52
49:6R:219:HIS:CE1	49:6R:239:HIS:ND1	2.76	0.52
55:8A:34:SER:HB3	55:8A:61:HIS:NE2	2.24	0.52
4:1D:352:TYR:HD1	9:1I:86:VAL:HG21	1.74	0.52
5:1E:205:PRO:HG3	44:1s:33:PHE:HB3	1.91	0.52
25:1Z:93:GLU:O	25:1Z:97:ILE:HG13	2.09	0.52
40:1o:21:MET:HG2	40:1o:22:PRO:HA	1.91	0.52
48:3D:186:PRO:O	48:3D:190:ARG:HG3	2.09	0.52
50:3F:119:TRP:HZ2	46:3O:88:GLY:HA2	1.75	0.52
45:3N:395:TRP:HA	45:3N:398:ARG:HD2	1.90	0.52
48:3Q:16:GLY:O	48:3Q:202:LYS:NZ	2.38	0.52
48:3Q:62:LYS:O	48:3Q:66:GLU:HG3	2.09	0.52
1:5A:54:LYS:HD2	1:5A:114:ALA:N	2.23	0.52
4:5D:34:ASN:HB3	15:5O:158:VAL:HG13	1.90	0.52
15:5O:234:VAL:O	15:5O:238:ILE:HG12	2.09	0.52
45:6A:23:LEU:HD21	45:6A:197:LEU:HB2	1.91	0.52
46:6B:124:LEU:HD23	46:6B:219:VAL:HG12	1.90	0.52
47:6C:69:ILE:HG21	47:6C:80:ARG:HG3	1.90	0.52
47:6C:129:MET:O	47:6C:133:LEU:N	2.41	0.52
47:6C:136:GLY:O	47:6C:137:GLN:C	2.51	0.52
50:6F:61:ARG:HG2	46:6O:135:TRP:CD1	2.45	0.52
45:6N:41:ILE:HD12	45:6N:97:TYR:CG	2.37	0.52
45:6N:54:GLY:O	45:6N:58:PHE:HD2	1.92	0.52
45:6N:69:ASN:ND2	45:6N:115:ASP:OD2	2.30	0.52
45:6N:211:LEU:C	45:6N:215:HIS:CD2	2.88	0.52
46:6O:213:HIS:CB	46:6O:217:LYS:HZ2	2.13	0.52
49:6R:123:VAL:HG13	53:6W:29:ALA:HA	1.91	0.52
54:6X:4:ARG:NH1	54:6X:10:TYR:OH	2.42	0.52
55:8A:32:ALA:CB	66:8L:36:PRO:HG2	2.40	0.52
55:8A:232:GLN:CB	55:8A:292:MET:HE3	2.39	0.52
15:1O:256:PHE:O	15:1O:260:ARG:HG2	2.10	0.52
21:1V:89:LEU:O	21:1V:93:MET:HG2	2.09	0.52
29:1d:120:ARG:HD2	38:1m:115:ILE:HD13	1.92	0.52
45:3A:121:SER:HB3	45:3A:123:GLU:HG3	1.91	0.52
46:3B:37:SER:HB3	46:3B:216:LEU:HD12	1.91	0.52
47:3C:40:CYS:SG	47:3C:235:MET:SD	3.07	0.52
51:3G:74:LYS:NZ	51:3G:75:ASN:OD1	2.30	0.52
45:3N:30:SER:H	45:3N:202:GLY:HA2	1.74	0.52
45:3N:111:GLU:HG3	45:3N:215:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:159:GLN:HE21	49:3R:85:VAL:CG2	2.22	0.52
45:3N:235:ARG:HG3	49:3R:103:SER:HB3	1.90	0.52
49:3R:219:HIS:HE1	49:3R:253:PRO:HD2	1.74	0.52
54:3X:4:ARG:NH1	54:3X:10:TYR:OH	2.42	0.52
55:4A:500:PRO:HB2	55:4A:504:THR:HG21	1.89	0.52
4:5D:352:TYR:HD1	9:5I:86:VAL:HG21	1.74	0.52
7:5G:215:PHE:HB3	9:5I:104:ARG:HG3	1.91	0.52
7:5G:320:GLY:O	7:5G:498:SER:OG	2.27	0.52
7:5G:362:TYR:O	7:5G:494:HIS:NE2	2.32	0.52
13:5M:165:VAL:HG21	14:5N:267:ILE:HG22	1.91	0.52
14:5N:211:MET:HG3	14:5N:333:SER:HB2	1.92	0.52
27:5b:42:ILE:HG22	27:5b:46:ARG:HD3	1.90	0.52
30:5e:68:ARG:HB3	30:5e:71:THR:HB	1.91	0.52
39:5n:55:ASP:HB3	39:5n:58:LYS:CE	2.27	0.52
48:6D:235:LEU:HB3	48:6D:246:ALA:HB1	1.92	0.52
55:8A:378:HIS:O	55:8A:379:TYR:C	2.52	0.52
55:8A:383:MET:HE2	55:8A:421:VAL:HB	1.90	0.52
56:8B:23:PHE:CZ	56:8B:80:SER:HB2	2.43	0.52
58:8D:81:ILE:HD13	75:8D:201:CDL:H712	1.91	0.52
64:8J:40:LEU:HD12	82:8J:101:PGV:H151	1.90	0.52
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.44	0.52
23:1X:51:ASP:OD1	25:1Z:116:TRP:HB2	2.09	0.52
45:3N:58:PHE:HZ	45:3N:174:VAL:CA	2.21	0.52
45:3N:123:GLU:CA	45:3N:179:ARG:CZ	2.56	0.52
45:3N:161:THR:HG21	45:3N:235:ARG:H	1.74	0.52
52:3U:28:GLU:HA	52:3U:31:ILE:HB	1.90	0.52
55:4A:275:TRP:CE3	82:4A:603:PGV:H12	2.43	0.52
9:5I:11:SER:O	9:5I:20:ARG:NH1	2.37	0.52
9:5I:160:LYS:HG2	9:5I:161:TRP:CD1	2.43	0.52
10:5J:99:MET:HG3	10:5J:100:GLU:N	2.23	0.52
12:5L:100:ILE:HG21	12:5L:246:LEU:HB2	1.90	0.52
23:5X:82:THR:HA	23:5X:85:TRP:NE1	2.24	0.52
29:5d:64:TYR:CD1	75:5d:202:CDL:H331	2.44	0.52
39:5n:107:HIS:ND1	39:5n:109:SER:OG	2.35	0.52
44:5s:31:GLU:HG3	44:5s:32:PRO:HD3	1.89	0.52
45:6A:387:GLY:O	45:6A:388:ARG:C	2.52	0.52
48:6D:201:LEU:HB3	48:6D:279:LEU:HD22	1.92	0.52
51:6G:21:SER:O	51:6G:25:GLN:HG2	2.10	0.52
45:6N:34:THR:CG2	45:6N:102:LEU:HD21	2.12	0.52
51:6T:60:THR:O	51:6T:64:GLN:HG3	2.10	0.52
55:8A:129:TYR:HB3	56:8B:160:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:262:SER:O	55:8A:263:GLY:C	2.53	0.52
55:8A:398:PRO:O	55:8A:402:GLY:N	2.33	0.52
4:1D:34:ASN:HB3	15:1O:158:VAL:HG13	1.90	0.52
4:1D:227:GLU:OE2	43:1r:17:ARG:NH2	2.43	0.52
8:1H:24:GLU:HB2	8:1H:271:LEU:HD22	1.90	0.52
69:1M:503:3PE:H2A1	38:1m:97:LEU:HB3	1.91	0.52
14:1N:128:LEU:HD23	14:1N:128:LEU:C	2.35	0.52
38:1m:83:PRO:O	38:1m:87:LEU:HD13	2.09	0.52
47:3C:224:TYR:CD1	47:3C:227:LYS:HD3	2.45	0.52
45:3N:16:VAL:HG22	45:3N:26:ALA:HB2	1.90	0.52
45:3N:25:VAL:HG22	45:3N:197:LEU:HB2	1.92	0.52
45:3N:118:GLN:NE2	45:3N:219:LEU:CA	2.72	0.52
45:3N:140:GLU:HA	49:3V:48:SER:HB2	1.92	0.52
45:3N:151:ASP:HA	45:3N:154:HIS:CD2	2.35	0.52
45:3N:269:PRO:O	45:3N:273:ALA:N	2.35	0.52
46:3O:87:ARG:O	46:3O:90:GLU:HB2	2.09	0.52
52:3U:21:ARG:O	52:3U:25:GLU:HG2	2.09	0.52
56:4B:103:GLN:N	56:4B:158:ASP:OD2	2.42	0.52
75:4B:301:CDL:H162	75:4B:301:CDL:H442	1.91	0.52
59:4E:33:MET:O	59:4E:37:VAL:HG13	2.10	0.52
4:5D:109:VAL:CG1	4:5D:149:ASN:HA	2.39	0.52
6:5F:308:PRO:HD3	6:5F:421:HIS:CD2	2.43	0.52
14:5N:215:MET:HG3	14:5N:251:MET:SD	2.50	0.52
23:5X:51:ASP:OD1	25:5Z:116:TRP:HB2	2.09	0.52
45:6A:158:PHE:HB3	45:6A:234:CYS:HB3	1.91	0.52
47:6C:201:HIS:O	47:6C:202:GLU:C	2.53	0.52
45:6N:167:VAL:O	45:6N:168:GLU:C	2.53	0.52
52:6U:28:GLU:HA	52:6U:31:ILE:HB	1.90	0.52
57:8C:197:PHE:O	57:8C:201:THR:OG1	2.23	0.52
7:1G:215:PHE:HB3	9:1I:104:ARG:HG3	1.91	0.52
9:1I:109:TYR:HB3	9:1I:151:LYS:HG3	1.91	0.52
25:1Z:98:MET:SD	25:1Z:101:VAL:HG21	2.50	0.52
31:1f:41:SER:HB3	33:1h:88:GLU:OE1	2.10	0.52
45:3A:248:LEU:HD12	45:3A:426:GLY:HA2	1.90	0.52
47:3C:258:PRO:O	47:3C:259:ALA:C	2.52	0.52
49:3E:151:LYS:HZ2	49:3E:152:ILE:HD12	1.74	0.52
51:3G:38:ASN:O	51:3G:41:ARG:HG2	2.08	0.52
90:4C:307:PEK:O14	61:4G:68:THR:OG1	2.24	0.52
4:5D:227:GLU:OE2	43:5r:17:ARG:NH2	2.43	0.52
13:5M:44:GLN:HB2	32:5g:83:TYR:CE1	2.45	0.52
69:5N:902:3PE:H3I2	69:5N:902:3PE:H2E2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5S:81:PHE:CD2	19:5S:85:GLN:HG2	2.44	0.52
20:5T:25:ILE:HG23	20:5T:40:LEU:HD22	1.92	0.52
37:5l:96:VAL:O	37:5l:101:MET:HE2	2.10	0.52
40:5o:21:MET:HG2	40:5o:22:PRO:HA	1.91	0.52
46:6B:64:GLY:HA2	46:6B:178:CYS:HA	1.91	0.52
46:6B:77:THR:HG21	46:6B:126:VAL:HA	1.92	0.52
45:6N:276:ILE:HG13	45:6N:357:GLY:HA3	1.90	0.52
46:6O:261:SER:OG	46:6O:262:ALA:N	2.42	0.52
49:6R:217:CYS:HB2	49:6R:224:PRO:HD3	1.92	0.52
49:6R:225:ILE:HG12	49:6R:237:PRO:HG3	1.91	0.52
55:8A:181:THR:O	55:8A:182:PRO:C	2.53	0.52
1:1A:104:TYR:O	1:1A:105:GLU:C	2.50	0.52
8:1H:308:PRO:HB2	8:1H:314:ILE:HD13	1.91	0.52
71:1I:201:PC1:H3C1	27:1b:24:ILE:HD11	1.92	0.52
10:1J:107:ALA:HB1	11:1K:3:LEU:HD11	1.92	0.52
12:1L:534:HIS:CD2	69:1L:701:3PE:H341	2.44	0.52
16:1P:97:ARG:NH1	78:1P:402:NDP:O3X	2.42	0.52
29:1d:64:TYR:CD1	75:1d:202:CDL:H331	2.44	0.52
45:3N:63:ALA:HB2	45:3N:97:TYR:OH	2.09	0.52
45:3N:67:THR:HB	45:3N:119:ASN:CB	2.40	0.52
46:3O:212:SER:HB3	46:3O:215:VAL:HB	1.91	0.52
46:3O:260:GLU:HA	46:3O:320:GLY:O	2.10	0.52
4:5D:116:GLN:NE2	4:5D:276:ASP:OD2	2.36	0.52
8:5H:308:PRO:HB2	8:5H:314:ILE:HD13	1.91	0.52
12:5L:562:LEU:HB3	69:5N:901:3PE:H3B2	1.90	0.52
14:5N:128:LEU:C	14:5N:128:LEU:HD23	2.35	0.52
38:5m:83:PRO:O	38:5m:87:LEU:HD13	2.09	0.52
45:6A:430:GLN:O	45:6A:431:LEU:C	2.53	0.52
45:6A:438:ARG:HD2	45:6A:441:MET:HG2	1.91	0.52
47:6C:58:ASP:O	47:6C:59:THR:C	2.53	0.52
47:6C:283:SER:HB2	47:6C:348:ILE:O	2.10	0.52
47:6C:330:ALA:HA	47:6C:333:ILE:HD12	1.90	0.52
48:6D:159:GLN:H	48:6D:170:MET:HE2	1.75	0.52
45:6N:261:GLY:CA	45:6N:317:THR:HA	2.35	0.52
55:8A:198:SER:O	55:8A:199:LEU:C	2.52	0.52
56:8B:105:TYR:H	56:8B:207:MET:HE3	1.74	0.52
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.92	0.52
14:1N:215:MET:HG3	14:1N:251:MET:SD	2.50	0.52
19:1S:81:PHE:CD2	19:1S:85:GLN:HG2	2.44	0.52
28:1c:31:LEU:C	28:1c:31:LEU:HD13	2.34	0.52
32:1g:43:ASP:OD1	39:1n:107:HIS:NE2	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:102:TYR:O	38:1m:106:THR:OG1	2.27	0.52
45:3N:18:GLN:HE21	45:3N:24:ARG:HG2	0.38	0.52
45:3N:99:ILE:CD1	45:3N:113:LEU:HG	2.40	0.52
45:3N:308:GLN:HE21	45:3N:308:GLN:C	2.18	0.52
55:4A:268:PHE:HZ	56:4B:58:ALA:HB3	1.75	0.52
55:4A:467:LEU:O	55:4A:471:ILE:HG13	2.10	0.52
58:4D:101:HIS:HD2	36:5k:90:GLN:CB	2.22	0.52
7:5G:32:LYS:HB3	7:5G:32:LYS:NZ	2.23	0.52
9:5I:95:GLU:OE1	42:5q:133:LYS:NZ	2.43	0.52
9:5I:132:VAL:HG21	9:5I:165:ILE:HD12	1.90	0.52
41:5p:131:PHE:O	41:5p:135:SER:OG	2.24	0.52
45:6A:252:HIS:HB3	45:6A:323:HIS:NE2	2.24	0.52
45:6A:411:CYS:O	45:6A:415:PHE:N	2.43	0.52
45:6N:4:TYR:OH	46:6O:112:LEU:CD1	2.57	0.52
45:6N:70:ARG:O	45:6N:71:PRO:C	2.52	0.52
46:6O:329:GLN:O	46:6O:330:ALA:C	2.53	0.52
55:8A:283:LEU:HA	55:8A:286:ILE:HD13	1.91	0.52
75:8B:302:CDL:H442	75:8B:302:CDL:H162	1.91	0.52
58:8D:116:VAL:O	58:8D:120:THR:OG1	2.26	0.52
82:8L:101:PGV:H52	82:8L:101:PGV:H92	1.92	0.52
7:1G:194:GLU:H	7:1G:194:GLU:CD	2.17	0.52
7:1G:217:ALA:HB2	7:1G:248:MET:HE2	1.91	0.52
12:1L:184:LEU:HD13	13:1M:393:ILE:HG21	1.92	0.52
22:1W:24:ASP:OD1	22:1W:25:MET:N	2.43	0.52
28:1c:41:GLU:OE2	28:1c:44:ARG:NH1	2.43	0.52
47:3C:138:MET:SD	47:3C:268:ILE:HA	2.50	0.52
47:3C:323:CYS:SG	51:3G:49:ARG:HD3	2.49	0.52
46:3O:299:VAL:HG13	46:3O:336:VAL:HG22	1.92	0.52
48:3Q:33:TYR:HA	48:3Q:37:CYS:SG	2.50	0.52
3:5C:62:THR:HG21	21:5V:92:LYS:HE2	1.92	0.52
4:5D:6:PRO:HB3	4:5D:10:TRP:CD1	2.45	0.52
10:5J:129:ASP:CA	30:5e:31:ARG:HH21	2.23	0.52
21:5V:89:LEU:O	21:5V:93:MET:HG2	2.09	0.52
25:5Z:98:MET:SD	25:5Z:101:VAL:HG21	2.50	0.52
37:5l:55:GLN:NE2	37:5l:69:LEU:O	2.33	0.52
45:6A:248:LEU:HD12	45:6A:426:GLY:H	1.75	0.52
47:6C:110:LEU:O	47:6C:111:GLU:C	2.53	0.52
45:6N:71:PRO:CD	45:6N:72:GLY:N	2.72	0.52
45:6N:305:GLN:HB2	45:6N:325:VAL:HB	1.92	0.52
48:6Q:62:LYS:O	48:6Q:66:GLU:HG3	2.09	0.52
55:8A:360:ASN:HB2	55:8A:363:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:390:MET:HE1	85:8A:605:HEA:H261	1.92	0.52
10:1J:175:ASN:O	15:1O:254:ARG:NH2	2.39	0.52
15:1O:308:TYR:CE1	15:1O:320:LYS:HG3	2.45	0.52
69:1Y:206:3PE:H2C2	38:1m:94:ILE:HD11	1.91	0.52
32:1g:45:HIS:NE2	32:1g:58:MET:HE2	2.25	0.52
33:1h:46:PHE:O	41:1p:58:ASN:ND2	2.32	0.52
46:3B:227:ARG:HG3	46:3B:229:GLY:N	2.25	0.52
47:3C:61:THR:O	47:3C:62:ALA:C	2.52	0.52
47:3C:72:ASP:OD1	48:3D:137:ARG:NH1	2.41	0.52
47:3C:226:ILE:HG23	48:3D:312:LYS:HA	1.90	0.52
45:3N:61:HIS:CD2	45:3N:134:ILE:CD1	2.92	0.52
49:3R:123:VAL:HG13	53:3W:29:ALA:HA	1.91	0.52
51:3T:60:THR:O	51:3T:64:GLN:HG3	2.10	0.52
56:4B:104:TRP:CG	56:4B:203:ASN:HB2	2.44	0.52
1:5A:78:ALA:O	1:5A:81:THR:HG22	2.09	0.52
6:5F:365:CYS:HB2	70:5F:502:SF4:S2	2.49	0.52
10:5J:75:ALA:C	10:5J:77:GLU:H	2.18	0.52
13:5M:61:LEU:HB2	13:5M:457:PRO:HD3	1.93	0.52
29:5d:15:PRO:HG2	29:5d:81:TYR:CZ	2.45	0.52
36:5k:70:PHE:O	36:5k:71:LYS:C	2.53	0.52
45:6A:403:ASP:H	45:6A:406:VAL:HB	1.75	0.52
47:6C:326:TRP:O	47:6C:327:MET:C	2.52	0.52
48:6D:96:PRO:CG	52:6H:95:ALA:HB2	2.40	0.52
45:6N:40:TRP:NE1	45:6N:377:GLU:HA	2.23	0.52
45:6N:93:GLU:OE1	45:6N:315:ALA:N	2.36	0.52
46:6O:200:THR:HG22	46:6O:227:ARG:HG2	1.91	0.52
55:8A:368:HIS:N	56:8B:171:LYS:HD2	2.25	0.52
90:8C:307:PEK:O14	61:8G:68:THR:OG1	2.24	0.52
2:1B:58:GLU:OE2	4:1D:189:MET:HG3	2.10	0.51
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.45	0.51
4:1D:62:LEU:HB2	4:1D:425:PHE:CZ	2.45	0.51
7:1G:323:VAL:H	7:1G:498:SER:HB3	1.76	0.51
8:1H:170:GLU:OE1	23:1X:97:ARG:NH2	2.43	0.51
8:1H:267:THR:O	8:1H:271:LEU:HG	2.10	0.51
13:1M:130:LEU:HD22	13:1M:150:LEU:HD13	1.91	0.51
14:1N:243:LEU:HD23	69:1N:902:3PE:H262	1.92	0.51
16:1P:130:ILE:HG21	16:1P:214:ILE:HG23	1.92	0.51
23:1X:37:LYS:HB3	23:1X:38:PRO:HD3	1.92	0.51
32:1g:109:GLU:O	41:1p:141:ARG:NH1	2.35	0.51
37:1l:134:PRO:CG	40:1o:38:MET:HE2	2.40	0.51
47:3C:80:ARG:HD2	47:3C:81:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:57:TYR:CE1	45:3N:167:VAL:HG12	1.78	0.51
55:4A:25:TRP:HB2	82:4L:101:PGV:H281	1.92	0.51
60:4F:79:THR:HG23	60:4F:90:LYS:HB2	1.91	0.51
2:5B:77:ARG:NH2	2:5B:82:GLN:OE1	2.38	0.51
71:5I:201:PC1:H3C1	27:5b:24:ILE:HD11	1.92	0.51
15:5O:256:PHE:O	15:5O:260:ARG:HG2	2.10	0.51
25:5Z:129:THR:O	25:5Z:133:ILE:HG23	2.10	0.51
28:5c:31:LEU:HD13	28:5c:31:LEU:C	2.34	0.51
28:5c:41:GLU:OE2	28:5c:44:ARG:NH1	2.43	0.51
45:6A:164:ALA:O	45:6A:165:GLN:C	2.53	0.51
45:6A:410:VAL:HA	45:6A:413:LYS:HD2	1.91	0.51
47:6C:52:ALA:HA	47:6C:55:TYR:HB3	1.92	0.51
48:6D:98:TYR:HB2	52:6H:99:PHE:CD1	2.44	0.51
48:6D:162:PRO:HA	48:6D:166:GLY:HA2	0.76	0.51
48:6D:216:PHE:CZ	52:6H:102:LEU:HD13	2.45	0.51
53:6J:9:ARG:O	53:6J:10:LEU:C	2.53	0.51
54:6Y:38:TRP:O	54:6Y:39:ARG:C	2.52	0.51
1:1A:33:LYS:HG2	8:1H:61:LEU:HD21	1.92	0.51
5:1E:104:THR:O	6:1F:349:ARG:NE	2.43	0.51
10:1J:129:ASP:CA	30:1e:31:ARG:HH21	2.23	0.51
71:1M:502:PC1:H2D2	71:1M:502:PC1:H292	1.92	0.51
20:1T:25:ILE:HG23	20:1T:40:LEU:HD22	1.92	0.51
37:1l:96:VAL:O	37:1l:101:MET:HE2	2.10	0.51
45:3N:30:SER:H	45:3N:201:GLY:C	2.17	0.51
57:4C:86:PHE:HZ	82:4C:305:PGV:H301	1.76	0.51
57:4C:130:PRO:HB2	57:4C:253:TYR:HE1	1.76	0.51
7:5G:194:GLU:OE1	7:5G:194:GLU:N	2.37	0.51
8:5H:312:ALA:HA	27:5b:41:ALA:HB2	1.92	0.51
13:5M:173:SER:HB2	33:5h:101:ALA:HB2	1.93	0.51
15:5O:96:LEU:O	15:5O:100:LEU:HG	2.10	0.51
16:5P:66:GLY:HA3	17:5Q:69:LEU:HD13	1.93	0.51
34:5i:44:GLN:HA	34:5i:47:ASN:OD1	2.09	0.51
46:6B:69:LEU:HD22	46:6B:191:LEU:HD23	1.92	0.51
47:6C:231:GLY:O	47:6C:232:ALA:C	2.53	0.51
48:6D:109:LEU:HD22	48:6D:280:ARG:HB3	1.90	0.51
52:6H:45:VAL:HG22	52:6H:97:LYS:HD2	1.91	0.51
45:6N:64:PHE:CE2	46:6O:287:ARG:NH2	2.78	0.51
45:6N:67:THR:HA	45:6N:121:SER:H	1.75	0.51
55:8A:64:VAL:HG22	55:8A:112:LEU:HD21	1.90	0.51
55:8A:308:ALA:O	55:8A:309:THR:C	2.52	0.51
1:1A:50:PRO:HB2	10:1J:74:MET:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:62:THR:HG21	21:1V:92:LYS:HE2	1.92	0.51
7:1G:522:LEU:HD22	7:1G:537:LEU:HD11	1.93	0.51
10:1J:75:ALA:C	10:1J:77:GLU:H	2.18	0.51
12:1L:524:ASN:HD22	39:1n:76:PRO:HB2	1.76	0.51
49:3E:235:TYR:HA	49:3E:243:TYR:H	1.75	0.51
53:3W:30:LEU:HA	54:3X:34:TRP:CD1	2.45	0.51
53:3W:31:PHE:HA	54:3X:48:ILE:HD11	1.92	0.51
13:5M:408:LEU:O	13:5M:412:ILE:HG13	2.11	0.51
15:5O:79:LEU:HD11	76:5O:401:GTP:H1'	1.93	0.51
15:5O:308:TYR:CE1	15:5O:320:LYS:HG3	2.45	0.51
47:6C:23:ALA:HB3	47:6C:224:TYR:CE2	2.45	0.51
48:6D:99:PRO:C	52:6H:99:PHE:HD2	2.18	0.51
45:6N:52:ASN:O	45:6N:53:ASN:C	2.53	0.51
45:6N:127:ILE:CD1	45:6N:179:ARG:HE	2.19	0.51
45:6N:196:VAL:HG11	45:6N:380:GLY:HA2	1.92	0.51
45:6N:246:ASP:O	45:6N:247:ALA:C	2.53	0.51
48:6Q:27:ARG:HB2	48:6Q:55:CYS:HB2	1.91	0.51
49:6R:195:LEU:HD13	49:6R:248:ARG:HE	1.75	0.51
55:8A:64:VAL:O	55:8A:65:MET:C	2.52	0.51
55:8A:65:MET:O	55:8A:69:MET:HB3	2.11	0.51
57:8C:42:LEU:HD13	64:8J:45:TYR:HD2	1.74	0.51
1:1A:110:GLY:O	1:1A:111:LEU:C	2.54	0.51
14:1N:211:MET:HG3	14:1N:333:SER:HB2	1.92	0.51
16:1P:273:SER:HA	71:1P:401:PC1:H231	1.93	0.51
24:1Y:10:ASP:OD1	24:1Y:11:ILE:HD12	2.10	0.51
35:1j:38:TRP:HZ3	36:1k:80:ALA:HB1	1.71	0.51
45:3N:181:ASP:C	45:3N:185:TYR:HD2	2.18	0.51
45:3N:310:PHE:HE1	45:3N:323:HIS:H	1.58	0.51
45:3N:359:ASN:O	45:3N:362:ARG:HB2	2.09	0.51
49:3R:161:GLU:HA	49:3R:178:HIS:HB3	1.93	0.51
57:4C:210:ILE:HG12	82:4C:305:PGV:H141	1.93	0.51
8:5H:267:THR:O	8:5H:271:LEU:HG	2.10	0.51
12:5L:184:LEU:HD13	13:5M:393:ILE:HG21	1.92	0.51
13:5M:119:TYR:CZ	13:5M:161:LEU:HB2	2.44	0.51
38:5m:107:ASP:HA	38:5m:110:LYS:CE	2.40	0.51
45:6A:71:PRO:O	45:6A:72:GLY:C	2.54	0.51
45:6A:236:PHE:HB3	45:6A:258:GLU:CD	2.35	0.51
45:6N:94:HIS:O	45:6N:95:THR:CG2	2.58	0.51
54:6Y:5:PHE:O	54:6Y:6:LEU:C	2.52	0.51
55:8A:75:ILE:O	55:8A:76:GLY:C	2.53	0.51
6:1F:365:CYS:HB2	70:1F:502:SF4:S2	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:362:TYR:O	7:1G:494:HIS:NE2	2.32	0.51
8:1H:85:MET:HE3	8:1H:233:MET:HE2	1.93	0.51
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.92	0.51
14:1N:71:MET:O	14:1N:75:ILE:HG12	2.10	0.51
15:1O:79:LEU:HD11	76:1O:401:GTP:H1'	1.93	0.51
47:3C:59:THR:HG22	47:3C:135:TRP:HE1	1.75	0.51
45:3N:16:VAL:HA	45:3N:26:ALA:HB2	1.93	0.51
45:3N:260:PRO:O	45:3N:261:GLY:C	2.53	0.51
48:3Q:105:ASN:ND2	48:3Q:108:ALA:O	2.31	0.51
82:4A:604:PGV:H211	82:4C:303:PGV:H32	1.92	0.51
57:4C:5:THR:O	60:4F:31:TYR:HA	2.10	0.51
57:4C:80:ARG:NH2	57:4C:236:GLU:OE1	2.42	0.51
61:4G:28:VAL:O	61:4G:32:THR:OG1	2.28	0.51
65:4K:12:LYS:HD2	35:5j:19:ARG:HH21	1.75	0.51
5:5E:205:PRO:HG3	44:5s:33:PHE:HB3	1.91	0.51
16:5P:97:ARG:NH1	78:5P:402:NDP:O3X	2.42	0.51
22:5W:24:ASP:OD1	22:5W:25:MET:N	2.43	0.51
48:6D:135:ALA:HA	48:6D:178:TYR:CA	2.36	0.51
48:6D:326:TYR:HB2	50:6F:72:PHE:CZ	2.45	0.51
49:6E:235:TYR:HA	49:6E:243:TYR:H	1.75	0.51
45:6N:191:LYS:O	45:6N:193:PRO:HD2	2.10	0.51
45:6N:313:CYS:HA	45:6N:318:GLY:CA	2.37	0.51
46:6O:69:LEU:HD21	46:6O:195:VAL:HG23	1.92	0.51
46:6O:123:LEU:HA	46:6O:126:VAL:HB	1.91	0.51
46:6O:252:LEU:HA	46:6O:328:SER:C	2.35	0.51
55:8A:283:LEU:HD21	68:8N:22:ILE:HA	1.93	0.51
55:8A:328:HIS:CD2	63:8I:17:LEU:HD22	2.46	0.51
57:8C:241:TYR:O	57:8C:245:VAL:HG13	2.10	0.51
64:8J:48:TYR:CE2	82:8J:101:PGV:H032	2.45	0.51
14:1N:243:LEU:HD22	14:1N:330:ILE:HG21	1.93	0.51
15:1O:33:SER:N	76:1O:401:GTP:O3G	2.43	0.51
45:3A:301:ARG:HB2	45:3A:303:LEU:HG	1.93	0.51
47:3C:50:PHE:CD1	49:3E:136:PHE:HD2	2.28	0.51
47:3C:85:ASN:HD22	47:3C:243:VAL:HA	1.76	0.51
47:3C:183:PHE:CZ	47:3P:180:ALA:HA	2.45	0.51
45:3N:46:ARG:NE	45:3N:163:LEU:HD21	2.24	0.51
45:3N:46:ARG:HA	45:3N:162:PRO:HB2	1.92	0.51
47:3P:132:VAL:HA	47:3P:139:SER:HB3	1.92	0.51
57:4C:241:TYR:O	57:4C:245:VAL:HG13	2.10	0.51
5:5E:104:THR:O	6:5F:349:ARG:NE	2.43	0.51
8:5H:179:TRP:O	8:5H:183:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5I:78:ILE:C	9:5I:78:ILE:CD1	2.84	0.51
10:5J:129:ASP:N	30:5e:31:ARG:HH21	2.07	0.51
36:5k:67:LEU:O	36:5k:70:PHE:HB3	2.10	0.51
43:5r:45:SER:O	43:5r:51:ASN:ND2	2.44	0.51
45:6A:27:SER:HB3	45:6A:205:HIS:HB2	1.92	0.51
45:6A:310:PHE:C	45:6A:321:GLY:H	2.19	0.51
47:6C:226:ILE:HD12	47:6C:229:ILE:HB	1.91	0.51
45:6N:191:LYS:CE	45:6N:223:TYR:CZ	2.67	0.51
46:6O:46:ARG:HG2	46:6O:379:LEU:HD13	1.92	0.51
46:6O:163:LEU:HD22	46:6O:256:ALA:HB1	1.92	0.51
49:6R:161:GLU:HA	49:6R:178:HIS:HB3	1.93	0.51
55:8A:140:GLY:O	55:8A:141:ALA:C	2.53	0.51
59:8E:33:MET:O	59:8E:37:VAL:HG13	2.10	0.51
2:1B:100:LEU:HD21	2:1B:104:TYR:CE2	2.34	0.51
8:1H:169:GLN:NE2	8:1H:240:ILE:O	2.43	0.51
8:1H:179:TRP:O	8:1H:183:MET:HG3	2.10	0.51
15:1O:252:ASP:N	15:1O:252:ASP:OD1	2.42	0.51
69:1Y:206:3PE:H241	69:1Y:206:3PE:H342	1.93	0.51
25:1Z:129:THR:O	25:1Z:133:ILE:HG23	2.10	0.51
46:3O:167:ALA:C	46:3O:240:ARG:HG2	2.36	0.51
55:4A:299:VAL:HG11	68:4N:64:LYS:HD3	1.92	0.51
7:5G:262:TRP:HB2	7:5G:390:LEU:HD11	1.93	0.51
12:5L:524:ASN:HD22	39:5n:76:PRO:HB2	1.76	0.51
12:5L:536:LEU:HB3	12:5L:537:PRO:HD3	1.92	0.51
20:5T:11:ILE:HG22	20:5T:77:VAL:HG22	1.93	0.51
31:5f:41:SER:HB3	33:5h:88:GLU:OE1	2.10	0.51
45:6A:240:GLU:N	51:6G:19:SER:O	2.44	0.51
47:6C:48:GLY:HA3	83:6C:501:HEM:C4C	2.45	0.51
47:6C:53:MET:HG3	47:6P:177:ARG:HB2	1.91	0.51
47:6C:113:TRP:HE3	83:6C:502:HEM:HMD1	1.75	0.51
48:6D:264:THR:O	48:6D:265:PRO:C	2.53	0.51
53:6J:31:PHE:HD2	54:6Y:47:TYR:HD2	1.58	0.51
45:6N:289:HIS:HB3	46:6O:83:PHE:HA	1.92	0.51
47:6P:8:HIS:O	47:6P:12:LYS:N	2.37	0.51
53:6W:31:PHE:HA	54:6X:48:ILE:HD11	1.92	0.51
55:8A:70:VAL:HG12	55:8A:246:LEU:HD22	1.92	0.51
55:8A:193:VAL:HG13	75:8A:610:CDL:H381	1.93	0.51
55:8A:440:TYR:OH	56:8B:195:GLN:HB3	2.11	0.51
57:8C:5:THR:O	60:8F:31:TYR:HA	2.10	0.51
1:1A:62:PHE:CD2	8:1H:140:ILE:HD12	2.46	0.51
1:1A:73:LEU:O	1:1A:76:PRO:HD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:47:LEU:O	4:1D:67:GLU:HA	2.11	0.51
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.92	0.51
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.93	0.51
11:1K:15:ALA:HB3	11:1K:36:MET:HG3	1.93	0.51
12:1L:272:LEU:O	12:1L:276:MET:HG3	2.11	0.51
12:1L:590:SER:O	12:1L:594:THR:HG22	2.11	0.51
13:1M:231:LEU:HA	13:1M:235:LEU:HD12	1.93	0.51
45:3A:172:GLU:CD	45:3A:172:GLU:H	2.12	0.51
47:3C:226:ILE:CD1	48:3D:311:MET:HE2	2.40	0.51
45:3N:252:HIS:HB3	45:3N:323:HIS:HE2	1.76	0.51
55:4A:406:ASN:HB3	55:4A:409:TRP:HB2	1.93	0.51
14:5N:128:LEU:CD1	75:5N:903:CDL:HA61	2.38	0.51
46:6B:203:ARG:HD2	46:6B:230:LEU:HA	1.92	0.51
47:6C:3:ASN:HB3	47:6C:6:LYS:HG3	1.92	0.51
47:6C:107:TYR:HE1	47:6C:308:HIS:HB2	1.75	0.51
47:6C:127:ALA:O	47:6C:128:PHE:C	2.53	0.51
47:6C:241:ILE:O	47:6C:245:PHE:N	2.43	0.51
47:6C:358:TYR:O	47:6C:361:ILE:HB	2.11	0.51
45:6N:76:GLU:CD	46:6O:289:SER:HG	2.18	0.51
45:6N:174:VAL:HA	45:6N:177:LEU:HD12	1.92	0.51
45:6N:185:TYR:O	45:6N:186:VAL:C	2.52	0.51
46:6O:111:CYS:HB3	46:6O:116:ILE:HG12	1.93	0.51
53:6W:30:LEU:HA	54:6X:34:TRP:CD1	2.45	0.51
55:8A:379:TYR:O	55:8A:383:MET:HB3	2.11	0.51
57:8C:79:LEU:HB3	57:8C:233:PHE:CE2	2.46	0.51
1:1A:75:LEU:O	1:1A:76:PRO:C	2.52	0.51
9:1I:95:GLU:OE1	42:1q:133:LYS:NZ	2.42	0.51
15:1O:96:LEU:O	15:1O:100:LEU:HG	2.10	0.51
33:1h:70:PRO:HG3	41:1p:60:TYR:OH	2.10	0.51
45:3A:242:ARG:O	51:3G:16:ILE:HA	2.11	0.51
45:3A:244:ARG:O	51:3G:13:ARG:HA	2.11	0.51
47:3C:12:LYS:HA	47:3C:15:ASN:HD22	1.76	0.51
47:3C:25:SER:HB2	48:3D:316:TRP:CZ3	2.46	0.51
47:3C:214:ASP:HA	47:3C:217:LYS:HG2	1.93	0.51
48:3D:165:ASP:OD1	48:3D:165:ASP:N	2.40	0.51
48:3D:249:MET:HG3	84:3D:501:HEC:C4C	2.40	0.51
45:3N:257:VAL:HG22	45:3N:320:LEU:HB2	1.92	0.51
89:4B:303:PSC:H072	59:4E:5:HIS:CE1	2.45	0.51
57:4C:34:TRP:CD1	57:4C:40:MET:HG2	2.46	0.51
82:4C:303:PGV:H282	68:4N:45:TRP:HH2	1.75	0.51
1:5A:51:PHE:O	1:5A:52:SER:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:148:THR:HB	7:5G:150:MET:HE3	1.92	0.51
7:5G:252:PRO:HG3	7:5G:263:ILE:HG12	1.93	0.51
14:5N:71:MET:O	14:5N:75:ILE:HG12	2.10	0.51
15:5O:97:GLN:HG2	15:5O:135:LEU:HD12	1.93	0.51
15:5O:255:THR:HA	15:5O:258:ARG:HD3	1.93	0.51
32:5g:45:HIS:NE2	32:5g:58:MET:HE2	2.26	0.51
49:6E:241:SER:H	49:6E:252:GLY:HA3	1.76	0.51
45:6N:67:THR:HG23	45:6N:75:LEU:HD11	1.92	0.51
45:6N:92:ARG:O	45:6N:93:GLU:HG3	2.10	0.51
45:6N:159:GLN:NE2	45:6N:241:ILE:CG1	2.69	0.51
46:6O:45:SER:HB3	46:6O:116:ILE:HG13	1.93	0.51
46:6O:399:LEU:HA	46:6O:402:ILE:HD12	1.93	0.51
55:8A:182:PRO:O	55:8A:183:LEU:C	2.54	0.51
55:8A:248:LEU:HB2	55:8A:249:PRO:HD3	1.92	0.51
57:8C:130:PRO:HB2	57:8C:253:TYR:HE1	1.76	0.51
58:8D:78:TRP:O	58:8D:82:VAL:HG23	2.11	0.51
2:1B:104:TYR:O	2:1B:106:GLN:N	2.42	0.51
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.40	0.51
13:1M:44:GLN:HB2	32:1g:83:TYR:CE1	2.45	0.51
20:1T:70:LEU:HB3	20:1T:76:ILE:HG13	1.93	0.51
29:1d:36:PHE:HZ	69:1d:201:3PE:H3C1	1.76	0.51
47:3C:26:ASN:OD1	47:3C:26:ASN:N	2.43	0.51
49:3E:241:SER:H	49:3E:252:GLY:HA3	1.76	0.51
45:3N:140:GLU:OE2	49:3V:51:CYS:N	2.43	0.51
45:3N:162:PRO:CD	45:3N:163:LEU:H	2.01	0.51
45:3N:445:ARG:H	45:3N:445:ARG:NE	2.01	0.51
46:3O:245:ARG:HH21	46:3O:430:LEU:HB3	1.75	0.51
47:3P:278:TYR:CZ	47:3P:282:ARG:HD3	2.46	0.51
48:3Q:180:SER:HB2	52:3U:77:LEU:HD11	1.93	0.51
49:3R:197:ASP:HB3	49:3R:248:ARG:NH1	2.26	0.51
55:4A:305:PHE:O	55:4A:309:THR:HG22	2.11	0.51
4:5D:62:LEU:HB2	4:5D:425:PHE:CZ	2.45	0.51
13:5M:105:PHE:O	13:5M:109:THR:OG1	2.27	0.51
24:5Y:10:ASP:OD1	24:5Y:11:ILE:HD12	2.10	0.51
69:5Y:206:3PE:H241	69:5Y:206:3PE:H342	1.93	0.51
25:5Z:140:PHE:HB2	26:5a:45:TRP:CD1	2.46	0.51
33:5h:70:PRO:HG3	41:5p:60:TYR:OH	2.10	0.51
45:6A:343:MET:HB3	45:6A:443:TRP:CD2	2.46	0.51
48:6D:114:ILE:HG23	48:6D:278:PHE:HD1	1.75	0.51
48:6D:135:ALA:CB	48:6D:178:TYR:HA	2.41	0.51
45:6N:27:SER:O	45:6N:205:HIS:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:155:ALA:HA	45:6N:164:ALA:HB1	1.92	0.51
89:8A:611:PSC:H072	59:8E:5:HIS:CE1	2.45	0.51
56:8B:42:ILE:HG22	82:8B:301:PGV:H031	1.93	0.51
57:8C:86:PHE:HZ	82:8C:305:PGV:H301	1.76	0.51
65:8K:27:ALA:C	65:8K:31:TYR:CD2	2.88	0.51
6:1F:157:TYR:OH	6:1F:174:ASP:OD1	2.22	0.50
7:1G:148:THR:HB	7:1G:150:MET:HE3	1.92	0.50
12:1L:484:LEU:HD12	82:4J:101:PGV:C01	2.35	0.50
13:1M:71:TRP:CD2	71:1M:502:PC1:H2C2	2.46	0.50
13:1M:104:LEU:HG	13:1M:108:MET:HE2	1.91	0.50
13:1M:173:SER:HB2	33:1h:101:ALA:HB2	1.93	0.50
16:1P:260:HIS:O	16:1P:264:ARG:HG3	2.11	0.50
26:1a:1:MET:N	26:1a:1:MET:SD	2.83	0.50
26:1a:2:TRP:HZ2	75:1q:201:CDL:H522	1.76	0.50
48:3D:323:LYS:O	51:3G:17:THR:HA	2.10	0.50
52:3H:46:ARG:HG2	52:3H:90:ARG:HD2	1.93	0.50
45:3N:37:VAL:C	45:3N:99:ILE:H	2.19	0.50
45:3N:46:ARG:HE	45:3N:163:LEU:HD22	1.73	0.50
45:3N:62:LEU:HA	45:3N:65:LYS:HG3	1.93	0.50
45:3N:237:THR:HA	51:3T:22:GLU:OE2	2.11	0.50
45:3N:331:ILE:HD12	45:3N:430:GLN:HB3	1.93	0.50
49:3R:217:CYS:HB2	49:3R:224:PRO:HD3	1.92	0.50
55:4A:313:ALA:HB3	56:4B:73:LEU:HD11	1.94	0.50
57:4C:79:LEU:HB3	57:4C:233:PHE:CE2	2.46	0.50
2:5B:57:VAL:HA	2:5B:60:MET:SD	2.51	0.50
2:5B:104:TYR:O	2:5B:111:ARG:NH1	2.44	0.50
71:5B:202:PC1:H242	16:5P:275:PHE:CE1	2.46	0.50
6:5F:274:VAL:HG21	6:5F:278:GLU:OE2	2.11	0.50
7:5G:323:VAL:H	7:5G:498:SER:HB3	1.75	0.50
11:5K:15:ALA:HB3	11:5K:36:MET:HG3	1.93	0.50
12:5L:272:LEU:O	12:5L:276:MET:HG3	2.11	0.50
12:5L:554:ASP:OD2	13:5M:288:TYR:OH	2.16	0.50
13:5M:130:LEU:HD22	13:5M:150:LEU:HD13	1.91	0.50
13:5M:243:MET:SD	13:5M:302:MET:HE3	2.52	0.50
23:5X:37:LYS:HB3	23:5X:38:PRO:HD3	1.92	0.50
26:5a:14:ALA:O	26:5a:18:ILE:HG13	2.12	0.50
46:6B:254:HIS:HB3	46:6B:327:ILE:HD13	1.93	0.50
47:6C:27:ILE:HB	47:6C:31:TRP:CD2	2.47	0.50
47:6C:68:HIS:O	47:6C:72:ASP:HB2	2.11	0.50
47:6C:345:HIS:O	47:6C:347:PHE:N	2.42	0.50
45:6N:17:SER:OG	45:6N:209:LEU:HD21	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6O:342:ASP:HA	46:6O:345:LYS:HE2	1.93	0.50
55:8A:311:ILE:O	55:8A:312:ILE:C	2.52	0.50
57:8C:58:TRP:HB3	82:8C:305:PGV:H32	1.94	0.50
8:1H:312:ALA:HA	27:1b:41:ALA:HB2	1.92	0.50
10:1J:64:MET:HE3	11:1K:34:GLU:CD	2.36	0.50
38:1m:107:ASP:HA	38:1m:110:LYS:CE	2.40	0.50
47:3C:241:ILE:HG12	48:3D:298:LEU:HD21	1.94	0.50
47:3C:254:ASP:O	47:3C:255:ASN:C	2.55	0.50
47:3C:349:ILE:O	47:3C:353:LEU:HG	2.11	0.50
45:3N:32:GLN:OE1	46:3O:373:GLU:HA	2.11	0.50
45:3N:297:VAL:HG11	45:3N:337:PHE:CD2	2.46	0.50
55:4A:417:MET:O	55:4A:421:VAL:HG22	2.11	0.50
57:4C:58:TRP:HB3	82:4C:305:PGV:H32	1.93	0.50
82:4L:101:PGV:H52	82:4L:101:PGV:H92	1.92	0.50
6:5F:368:GLY:HA3	6:5F:399:ILE:HD11	1.93	0.50
8:5H:170:GLU:OE1	23:5X:97:ARG:NH2	2.43	0.50
10:5J:107:ALA:HB1	11:5K:3:LEU:HD11	1.92	0.50
10:5J:167:VAL:HG13	14:5N:42:PRO:HG3	1.94	0.50
12:5L:590:SER:O	12:5L:594:THR:HG22	2.11	0.50
71:5M:502:PC1:H2D2	71:5M:502:PC1:H292	1.92	0.50
15:5O:211:LEU:O	15:5O:215:SER:OG	2.25	0.50
16:5P:130:ILE:HG21	16:5P:214:ILE:HG23	1.92	0.50
23:5X:105:LYS:HA	23:5X:108:GLU:HG2	1.94	0.50
29:5d:120:ARG:HD2	38:5m:115:ILE:HD13	1.92	0.50
45:6A:15:GLN:HB3	45:6A:205:HIS:CB	2.40	0.50
45:6A:276:ILE:HD11	45:6A:354:VAL:HA	1.94	0.50
48:6D:215:VAL:O	48:6D:216:PHE:C	2.54	0.50
48:6D:249:MET:HA	84:6D:501:HEC:C1D	2.41	0.50
45:6N:87:ASN:ND2	45:6N:100:LYS:HG3	2.25	0.50
45:6N:258:GLU:HG2	49:6R:104:LYS:HE2	1.92	0.50
46:6O:413:ALA:HA	46:6O:416:LYS:HB3	1.92	0.50
57:8C:146:TRP:CZ2	61:8G:17:ARG:HG3	2.46	0.50
1:1A:93:PHE:HE2	10:1J:154:VAL:HG12	1.76	0.50
2:1B:37:VAL:O	2:1B:41:ARG:HB2	2.11	0.50
2:1B:78:ALA:O	2:1B:79:SER:C	2.53	0.50
4:1D:116:GLN:NE2	4:1D:276:ASP:OD2	2.36	0.50
8:1H:273:ILE:HG23	8:1H:277:TYR:CD2	2.47	0.50
12:1L:566:THR:O	12:1L:570:GLN:HG2	2.12	0.50
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.44	0.50
47:3C:151:SER:O	47:3C:153:ILE:N	2.44	0.50
47:3C:270:PRO:HD2	47:3C:275:LEU:HD23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:346:PRO:HD2	51:3G:68:PHE:CE1	2.46	0.50
46:3O:111:CYS:HB3	46:3O:119:LEU:HD22	1.94	0.50
49:3R:195:LEU:HD13	49:3R:248:ARG:HE	1.75	0.50
57:4C:197:PHE:O	57:4C:201:THR:OG1	2.23	0.50
9:5I:144:HIS:CE1	16:5P:65:LEU:HD21	2.47	0.50
10:5J:74:MET:HG3	10:5J:75:ALA:H	1.77	0.50
13:5M:6:ILE:HD12	31:5f:23:GLY:HA2	1.94	0.50
14:5N:243:LEU:HD23	69:5N:902:3PE:H262	1.92	0.50
15:5O:210:PHE:O	15:5O:214:MET:HG2	2.11	0.50
26:5a:2:TRP:HZ2	75:5q:201:CDL:H522	1.76	0.50
38:5m:23:ASP:OD1	45:6N:229:PRO:HA	2.11	0.50
45:6A:49:ASN:HD21	45:6A:51:LYS:HB3	1.74	0.50
45:6A:64:PHE:HE2	46:6B:286:LYS:HB3	1.76	0.50
45:6A:146:ARG:HH21	45:6A:147:ASP:HA	1.75	0.50
47:6C:215:MET:N	47:6C:215:MET:SD	2.84	0.50
47:6C:310:SER:HA	47:6C:374:ASN:HD21	1.74	0.50
48:6D:145:THR:O	48:6D:146:GLU:C	2.53	0.50
45:6N:58:PHE:CE1	45:6N:134:ILE:HG21	2.44	0.50
45:6N:165:GLN:HA	49:6R:84:ARG:NH2	2.27	0.50
45:6N:176:LYS:O	45:6N:177:LEU:C	2.55	0.50
57:8C:210:ILE:HG12	82:8C:305:PGV:H141	1.92	0.50
10:1J:77:GLU:O	10:1J:78:MET:SD	2.70	0.50
13:1M:104:LEU:HD21	75:1X:201:CDL:H271	1.93	0.50
13:1M:408:LEU:O	13:1M:412:ILE:HG13	2.11	0.50
15:1O:210:PHE:O	15:1O:214:MET:HG2	2.11	0.50
25:1Z:140:PHE:HB2	26:1a:45:TRP:CD1	2.46	0.50
46:3B:120:MET:HE3	46:3B:219:VAL:CG2	2.28	0.50
47:3C:377:LEU:CB	50:3F:32:TYR:HE2	2.21	0.50
45:3N:68:LYS:N	45:3N:119:ASN:HB3	2.27	0.50
46:3O:50:PHE:HB3	46:3O:387:LEU:HD21	1.94	0.50
46:3O:132:PHE:HB2	46:3O:192:HIS:NE2	2.26	0.50
55:4A:74:MET:HE3	55:4A:389:ILE:HG13	1.93	0.50
55:4A:328:HIS:NE2	63:4I:17:LEU:HD22	2.26	0.50
82:4A:602:PGV:H181	57:4C:31:LEU:HD12	1.93	0.50
58:4D:78:TRP:O	58:4D:82:VAL:HG23	2.11	0.50
4:5D:47:LEU:O	4:5D:67:GLU:HA	2.11	0.50
13:5M:71:TRP:CD2	71:5M:502:PC1:H2C2	2.46	0.50
13:5M:231:LEU:HA	13:5M:235:LEU:HD12	1.93	0.50
42:5q:2:GLU:O	42:5q:6:VAL:HG23	2.12	0.50
47:6C:68:HIS:O	47:6C:73:VAL:HG23	2.11	0.50
48:6D:112:THR:HG23	48:6D:116:ARG:HH12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:6H:50:GLU:HG2	52:6H:86:PHE:HZ	1.76	0.50
48:6Q:43:MET:HE2	48:6Q:113:LEU:HB2	1.94	0.50
55:8A:52:GLN:O	55:8A:55:ASN:HB2	2.12	0.50
55:8A:299:VAL:CG1	68:8N:64:LYS:HD3	2.41	0.50
55:8A:504:THR:O	55:8A:505:PHE:C	2.54	0.50
8:1H:65:THR:HA	16:1P:324:TYR:HB2	1.93	0.50
33:1h:123:TYR:H	81:1h:201:AME:C	2.24	0.50
48:3D:102:HIS:O	48:3D:291:LYS:NZ	2.44	0.50
45:3N:28:GLU:HA	45:3N:205:HIS:NE2	2.26	0.50
45:3N:108:LYS:HA	45:3N:111:GLU:HB2	1.94	0.50
46:3O:70:ARG:HA	46:3O:98:VAL:HG11	1.92	0.50
46:3O:314:ALA:O	46:3O:321:LEU:HB2	2.11	0.50
55:4A:86:MET:HE3	55:4A:185:VAL:HG23	1.93	0.50
58:4D:116:VAL:O	58:4D:120:THR:OG1	2.26	0.50
4:5D:112:MET:HG3	4:5D:181:TYR:CZ	2.47	0.50
10:5J:77:GLU:O	10:5J:78:MET:SD	2.70	0.50
10:5J:130:THR:HG21	25:5Z:124:LEU:HD22	1.93	0.50
12:5L:144:TRP:CD1	12:5L:223:LYS:HE2	2.47	0.50
14:5N:243:LEU:HD22	14:5N:330:ILE:HG21	1.93	0.50
20:5T:35:HIS:NE2	20:5T:71:MET:HG2	2.26	0.50
34:5i:52:ASP:HB3	34:5i:57:LYS:HE3	1.93	0.50
45:6A:25:VAL:HA	45:6A:197:LEU:HB3	1.94	0.50
46:6B:424:MET:HB2	46:6B:436:VAL:HB	1.91	0.50
47:6C:72:ASP:O	47:6C:73:VAL:C	2.55	0.50
47:6C:107:TYR:CE1	47:6C:308:HIS:HB2	2.46	0.50
48:6D:179:PHE:HE2	48:6D:278:PHE:HZ	1.59	0.50
50:6F:119:TRP:HH2	46:6O:91:ALA:HB2	1.75	0.50
48:6Q:33:TYR:HA	48:6Q:37:CYS:SG	2.50	0.50
55:8A:278:MET:HA	82:8A:603:PGV:H272	1.93	0.50
55:8A:426:PHE:HB3	55:8A:427:PRO:HD3	1.93	0.50
66:8L:15:VAL:HG12	66:8L:21:LEU:HD13	1.94	0.50
2:1B:77:ARG:HH11	2:1B:83:SER:H	1.59	0.50
7:1G:470:VAL:CG1	7:1G:490:MET:HE1	2.42	0.50
12:1L:561:ILE:HD12	71:1m:201:PC1:H291	1.94	0.50
13:1M:243:MET:SD	13:1M:302:MET:HE3	2.51	0.50
15:1O:97:GLN:HG2	15:1O:135:LEU:HD12	1.93	0.50
18:1R:10:LYS:O	18:1R:33:LYS:NZ	2.41	0.50
47:3C:72:ASP:OD1	48:3D:138:HIS:NE2	2.43	0.50
47:3C:218:ILE:HG21	48:3D:319:LEU:CD1	2.41	0.50
47:3C:248:ASP:C	47:3C:251:GLY:H	2.18	0.50
47:3C:280:ILE:HG21	47:3C:294:LEU:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:40:ASN:OD1	46:3O:40:ASN:N	2.45	0.50
46:3O:382:VAL:HG13	46:3O:392:TYR:HB2	1.93	0.50
55:4A:207:THR:O	55:4A:211:THR:HG23	2.11	0.50
7:5G:316:ALA:HB3	7:5G:519:PRO:HG3	1.94	0.50
10:5J:86:ASN:HB2	10:5J:89:VAL:HG23	1.94	0.50
45:6A:105:ASP:O	45:6A:106:LEU:C	2.55	0.50
45:6A:373:THR:O	45:6A:374:PRO:C	2.55	0.50
47:6C:78:VAL:HG11	49:6E:135:GLN:OE1	2.12	0.50
47:6C:254:ASP:HB3	47:6C:265:PRO:HB2	1.92	0.50
47:6C:315:MET:N	47:6C:315:MET:SD	2.84	0.50
47:6C:324:LEU:O	47:6C:325:PHE:C	2.55	0.50
47:6C:377:LEU:CB	50:6F:32:TYR:HE2	2.25	0.50
48:6D:129:HIS:HB3	48:6D:200:ASP:HA	1.93	0.50
49:6E:174:LEU:HD13	49:6E:214:ILE:HD13	1.94	0.50
45:6N:148:VAL:C	45:6N:152:TYR:HD2	2.18	0.50
45:6N:310:PHE:HE2	45:6N:323:HIS:HB2	1.76	0.50
46:6O:245:ARG:HD2	46:6O:435:PHE:CE2	2.46	0.50
48:6Q:180:SER:HB2	52:6U:77:LEU:HD11	1.93	0.50
57:8C:221:ARG:HB3	57:8C:226:HIS:HB2	1.94	0.50
6:1F:274:VAL:HG21	6:1F:278:GLU:OE2	2.12	0.50
10:1J:33:LEU:HD11	11:1K:34:GLU:HB3	1.93	0.50
12:1L:144:TRP:CD1	12:1L:223:LYS:HE2	2.47	0.50
69:1L:701:3PE:H221	37:1l:87:ASN:O	2.12	0.50
13:1M:163:ALA:HA	69:1M:501:3PE:H241	1.94	0.50
25:1Z:104:TRP:HH2	30:1e:74:ARG:HG3	1.77	0.50
34:1i:52:ASP:HB3	34:1i:57:LYS:HE3	1.93	0.50
36:1k:23:ILE:HD12	36:1k:29:GLU:HA	1.94	0.50
46:3B:201:SER:HB2	46:3B:228:GLY:HA2	1.92	0.50
47:3C:43:LEU:HD11	47:3C:82:LEU:HD11	1.94	0.50
47:3C:233:LEU:O	47:3C:234:PHE:C	2.54	0.50
45:3N:161:THR:HG21	45:3N:235:ARG:N	2.26	0.50
57:4C:146:TRP:CZ2	61:4G:17:ARG:HG3	2.46	0.50
57:4C:171:VAL:HG22	82:4C:304:PGV:H162	1.93	0.50
5:5E:151:ALA:HB3	5:5E:163:ASP:HA	1.93	0.50
7:5G:648:LEU:HD21	19:5S:44:LYS:HG2	1.94	0.50
12:5L:561:ILE:HD12	71:5m:201:PC1:H291	1.94	0.50
15:5O:65:ASP:OD1	15:5O:65:ASP:N	2.37	0.50
23:5X:74:LYS:NZ	26:5a:66:LEU:O	2.45	0.50
45:6A:72:GLY:O	45:6A:73:SER:C	2.55	0.50
45:6A:366:VAL:HG21	46:6B:112:LEU:HD22	1.93	0.50
46:6B:47:ILE:HB	46:6B:109:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:6C:84:ALA:HA	83:6C:501:HEM:HBA1	1.92	0.50
48:6D:97:SER:O	52:6H:95:ALA:HB1	2.11	0.50
48:6D:108:SER:HA	48:6D:287:HIS:CE1	2.47	0.50
48:6D:254:TYR:H	48:6D:257:VAL:HB	1.76	0.50
45:6N:99:ILE:HD12	45:6N:113:LEU:CG	2.40	0.50
45:6N:105:ASP:O	45:6N:106:LEU:C	2.54	0.50
45:6N:158:PHE:HA	45:6N:237:THR:H	1.77	0.50
47:6P:132:VAL:HA	47:6P:139:SER:HB3	1.93	0.50
49:6R:197:ASP:HB3	49:6R:248:ARG:NH1	2.26	0.50
54:6Y:42:LEU:HD13	54:6Y:48:ILE:HG21	1.94	0.50
55:8A:120:ALA:HA	66:8L:43:GLN:HE22	1.75	0.50
75:8D:201:CDL:H582	75:8D:201:CDL:H381	1.94	0.50
59:8E:19:PHE:O	59:8E:57:ARG:NH2	2.41	0.50
65:8K:27:ALA:C	65:8K:31:TYR:HD2	2.12	0.50
2:1B:57:VAL:HA	2:1B:60:MET:SD	2.51	0.50
6:1F:98:ASP:HA	6:1F:139:ARG:HB3	1.93	0.50
6:1F:368:GLY:HA3	6:1F:399:ILE:HD11	1.93	0.50
7:1G:424:ASP:OD2	7:1G:660:PRO:HB3	2.12	0.50
9:1I:78:ILE:C	9:1I:78:ILE:CD1	2.84	0.50
9:1I:169:ILE:O	9:1I:173:TYR:HB3	2.12	0.50
23:1X:74:LYS:NZ	26:1a:66:LEU:O	2.45	0.50
29:1d:15:PRO:HG2	29:1d:81:TYR:CZ	2.46	0.50
34:1i:102:ARG:HG2	40:1o:49:GLN:HG3	1.94	0.50
47:3C:77:TRP:CE3	48:3D:286:GLU:HG3	2.47	0.50
47:3C:135:TRP:O	47:3C:259:ALA:HB2	2.12	0.50
47:3C:227:LYS:HD2	48:3D:312:LYS:HE2	1.94	0.50
47:3C:361:ILE:HG22	47:3C:366:MET:HG3	1.94	0.50
45:3N:38:GLY:CA	45:3N:98:TYR:HA	2.41	0.50
45:3N:62:LEU:CD2	45:3N:65:LYS:NZ	2.74	0.50
45:3N:92:ARG:CG	45:3N:167:VAL:CG2	2.89	0.50
45:3N:162:PRO:HD3	45:3N:234:CYS:SG	2.52	0.50
45:3N:272:VAL:O	45:3N:276:ILE:HG13	2.12	0.50
46:3O:46:ARG:HB2	46:3O:110:GLU:HG2	1.92	0.50
75:4C:308:CDL:H541	75:4C:308:CDL:H162	1.94	0.50
63:4I:49:ASP:OD1	63:4I:49:ASP:N	2.44	0.50
4:5D:100:LEU:HD22	4:5D:195:ARG:HD3	1.93	0.50
8:5H:273:ILE:HG23	8:5H:277:TYR:CD2	2.47	0.50
15:5O:50:HIS:HA	15:5O:123:VAL:HG23	1.94	0.50
45:6A:21:ASN:HA	45:6A:222:THR:H	1.76	0.50
47:6C:149:LEU:O	47:6C:150:LEU:C	2.55	0.50
47:6C:234:PHE:O	47:6C:237:LEU:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:54:GLY:O	45:6N:55:ALA:C	2.55	0.50
45:6N:418:GLN:O	45:6N:419:CYS:C	2.55	0.50
55:8A:237:PHE:O	55:8A:241:PRO:HG2	2.12	0.50
82:8A:603:PGV:H22	75:8A:610:CDL:H461	1.93	0.50
68:8N:52:GLU:HG2	68:8N:54:TRP:CZ2	2.47	0.50
1:1A:18:VAL:HG23	8:1H:222:MET:HE1	1.94	0.50
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.77	0.50
20:1T:35:HIS:NE2	20:1T:71:MET:HG2	2.26	0.50
21:1V:57:MET:HE2	21:1V:70:GLN:HG3	1.94	0.50
46:3B:207:ILE:HD13	46:3B:383:GLY:HA2	1.94	0.50
46:3B:249:GLY:HA3	46:3O:181:TYR:CE2	2.47	0.50
47:3C:27:ILE:HG12	47:3C:224:TYR:OH	2.11	0.50
49:3E:263:TYR:HB3	49:3E:273:VAL:HG13	1.94	0.50
45:3N:60:GLU:O	45:3N:61:HIS:C	2.55	0.50
45:3N:70:ARG:CD	45:3N:75:LEU:CD2	2.66	0.50
45:3N:140:GLU:HG2	49:3V:50:LEU:HG	1.94	0.50
45:3N:244:ARG:HE	45:3N:429:GLU:HB2	1.77	0.50
82:4A:601:PGV:H282	82:4L:101:PGV:H42	1.93	0.50
4:5D:183:ARG:NH1	4:5D:210:ASP:OD2	2.29	0.50
6:5F:98:ASP:HA	6:5F:139:ARG:HB3	1.93	0.50
7:5G:522:LEU:HD22	7:5G:537:LEU:HD11	1.93	0.50
8:5H:85:MET:HE3	8:5H:233:MET:HE2	1.93	0.50
10:5J:64:MET:HE3	11:5K:34:GLU:CD	2.36	0.50
13:5M:104:LEU:HD21	75:5X:201:CDL:H271	1.93	0.50
13:5M:163:ALA:HA	69:5M:501:3PE:H241	1.94	0.50
29:5d:36:PHE:HZ	69:5d:201:3PE:H3C1	1.76	0.50
46:6B:24:LEU:HD23	46:6B:38:LEU:HB2	1.92	0.50
48:6D:256:GLU:HG3	52:6H:38:LEU:HD22	1.93	0.50
45:6N:25:VAL:HB	45:6N:209:LEU:HD22	1.93	0.50
45:6N:127:ILE:CD1	45:6N:179:ARG:CD	2.51	0.50
45:6N:247:ALA:O	45:6N:248:LEU:C	2.55	0.50
47:6P:315:MET:HE1	47:6P:325:PHE:HB2	1.94	0.50
55:8A:310:MET:HG3	56:8B:73:LEU:HB3	1.94	0.50
4:1D:100:LEU:HD22	4:1D:195:ARG:HD3	1.93	0.49
7:1G:139:ASP:OD1	7:1G:148:THR:O	2.30	0.49
10:1J:74:MET:HG3	10:1J:75:ALA:H	1.77	0.49
12:1L:562:LEU:HB2	12:1L:563:PRO:HD3	1.94	0.49
15:1O:255:THR:HA	15:1O:258:ARG:HD3	1.93	0.49
33:1h:50:ALA:HB2	41:1p:60:TYR:CE2	2.47	0.49
45:3A:70:ARG:HD3	45:3A:78:GLU:OE1	2.12	0.49
45:3A:131:ARG:HD3	45:3A:175:ARG:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3B:76:THR:HG23	46:3B:81:SER:HA	1.93	0.49
49:3E:150:SER:HB2	47:3P:168:PHE:HE1	1.77	0.49
45:3N:436:ARG:HH12	47:3P:19:ILE:HG22	1.76	0.49
48:3Q:173:ASP:OD1	48:3Q:173:ASP:N	2.37	0.49
58:4D:17:VAL:HG22	67:4M:2:TYR:CE1	2.47	0.49
3:5C:121:VAL:HG21	3:5C:146:PRO:HD3	1.94	0.49
8:5H:296:LEU:HD13	71:5I:201:PC1:H351	1.94	0.49
12:5L:331:MET:HE1	12:5L:468:ILE:HD12	1.94	0.49
34:5i:102:ARG:HG2	40:5o:49:GLN:HG3	1.94	0.49
45:6A:192:ALA:HA	45:6A:195:MET:HB2	1.94	0.49
46:6B:102:ARG:HH21	46:6B:164:HIS:HB2	1.77	0.49
46:6B:399:LEU:HA	46:6B:402:ILE:HG13	1.94	0.49
47:6C:72:ASP:CA	49:6E:144:ALA:HB3	2.42	0.49
48:6D:223:CYS:SG	48:6D:224:GLU:N	2.84	0.49
46:6O:77:THR:O	46:6O:78:LYS:C	2.54	0.49
46:6O:274:VAL:HG21	46:6O:405:VAL:HG11	1.94	0.49
46:6O:385:GLN:HA	46:6O:389:ALA:HB3	1.92	0.49
47:6P:278:TYR:CZ	47:6P:282:ARG:HD3	2.46	0.49
48:6Q:59:GLU:HG2	48:6Q:60:GLU:N	2.27	0.49
55:8A:11:ASN:O	55:8A:12:HIS:C	2.54	0.49
55:8A:376:HIS:O	55:8A:377:PHE:C	2.54	0.49
55:8A:442:ASP:CB	56:8B:135:LEU:HD21	2.42	0.49
61:8G:17:ARG:HH22	61:8G:18:PHE:HE1	1.55	0.49
61:8G:50:TYR:HA	62:8H:80:THR:HG23	1.94	0.49
10:1J:167:VAL:HG13	14:1N:42:PRO:HG3	1.94	0.49
12:1L:484:LEU:CD1	82:4J:101:PGV:H011	2.36	0.49
20:1T:11:ILE:HG22	20:1T:77:VAL:HG22	1.93	0.49
26:1a:14:ALA:O	26:1a:18:ILE:HG13	2.12	0.49
35:1j:19:ARG:NE	65:8K:12:LYS:HD2	2.27	0.49
45:3A:110:VAL:HG11	45:3A:211:LEU:HB3	1.94	0.49
47:3C:373:GLU:HB3	50:3F:32:TYR:OH	2.12	0.49
48:3D:226:PRO:HG3	52:3H:80:THR:HA	1.93	0.49
45:3N:32:GLN:OE1	46:3O:373:GLU:HG3	2.12	0.49
45:3N:55:ALA:HB1	45:3N:185:TYR:CG	2.48	0.49
45:3N:140:GLU:CG	49:3V:50:LEU:HG	2.42	0.49
46:3O:48:GLY:HA2	46:3O:108:THR:HA	1.93	0.49
48:3Q:43:MET:HE2	48:3Q:113:LEU:HB2	1.94	0.49
55:4A:131:PRO:HD2	56:4B:159:VAL:HB	1.93	0.49
61:4G:17:ARG:HH22	61:4G:18:PHE:HE1	1.56	0.49
61:4G:56:ARG:NH2	61:4G:66:ASN:O	2.30	0.49
66:4L:15:VAL:HG12	66:4L:21:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:169:GLN:NE2	8:5H:240:ILE:O	2.43	0.49
13:5M:430:PHE:HB2	13:5M:433:GLU:HG3	1.94	0.49
15:5O:33:SER:N	76:5O:401:GTP:O3G	2.43	0.49
20:5U:36:PHE:HB3	20:5U:42:LEU:HD12	1.94	0.49
33:5h:50:ALA:HB2	41:5p:60:TYR:CE2	2.47	0.49
36:5k:76:ALA:O	36:5k:79:VAL:HB	2.12	0.49
38:5m:102:TYR:O	38:5m:106:THR:OG1	2.27	0.49
48:6D:93:LEU:H	48:6D:245:GLN:NE2	2.10	0.49
48:6D:139:LEU:HD22	48:6D:142:VAL:HG12	1.95	0.49
49:6E:177:ARG:HD3	49:6E:211:VAL:CG1	2.42	0.49
45:6N:94:HIS:C	45:6N:95:THR:HG23	2.38	0.49
45:6N:378:ASP:O	45:6N:379:ILE:C	2.55	0.49
45:6N:412:SER:HA	45:6N:416:TYR:H	1.77	0.49
46:6O:77:THR:HA	46:6O:131:GLU:H	1.77	0.49
46:6O:155:PRO:O	46:6O:156:GLN:C	2.55	0.49
46:6O:316:TYR:O	46:6O:317:SER:C	2.54	0.49
55:8A:433:LEU:O	55:8A:434:SER:C	2.55	0.49
82:8A:604:PGV:H342	82:8C:303:PGV:H12	1.94	0.49
56:8B:49:LYS:HE3	82:8B:301:PGV:H282	1.93	0.49
57:8C:34:TRP:CD1	57:8C:40:MET:HG2	2.46	0.49
5:1E:27:ASN:HD21	5:1E:57:GLN:HB2	1.78	0.49
6:1F:342:ASP:CG	6:1F:429:ARG:HH12	2.21	0.49
7:1G:605:GLU:HG2	22:1W:119:LEU:HD22	1.94	0.49
13:1M:91:ARG:HE	69:1N:902:3PE:H321	1.78	0.49
37:1l:136:ASN:ND2	37:1l:153:VAL:H	2.11	0.49
45:3A:358:LYS:O	45:3A:362:ARG:HG3	2.12	0.49
47:3C:46:LEU:C	49:3E:136:PHE:HE2	2.21	0.49
47:3C:343:VAL:HG12	47:3C:348:ILE:HD11	1.95	0.49
45:3N:65:LYS:HB3	45:3N:126:GLN:OE1	2.13	0.49
45:3N:444:LEU:HB2	45:3N:445:ARG:HH21	1.77	0.49
47:3P:33:PHE:HA	47:3P:36:LEU:HB2	1.95	0.49
49:3R:248:ARG:NH2	49:3R:249:ILE:O	2.46	0.49
6:5F:301:GLY:H	6:5F:333:ALA:HB3	1.77	0.49
7:5G:424:ASP:OD2	7:5G:660:PRO:HB3	2.11	0.49
13:5M:52:PHE:O	33:5h:89:LYS:NZ	2.42	0.49
16:5P:30:LEU:HA	16:5P:207:ILE:HD11	1.94	0.49
18:5R:10:LYS:O	18:5R:33:LYS:NZ	2.41	0.49
29:5d:53:VAL:HG13	69:5d:201:3PE:H111	1.95	0.49
31:5f:5:GLN:O	31:5f:9:ASP:HB2	2.12	0.49
45:6A:291:SER:O	45:6A:292:SER:C	2.55	0.49
47:6C:281:LEU:HD12	47:6C:294:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:6C:377:LEU:HB2	50:6F:32:TYR:HE2	1.77	0.49
48:6D:157:GLU:HB2	48:6D:170:MET:HB3	1.94	0.49
45:6N:162:PRO:HA	45:6N:165:GLN:CD	2.36	0.49
46:6O:26:PHE:HE1	46:6O:382:VAL:HG13	1.76	0.49
46:6O:56:ARG:HB3	46:6O:174:ASN:HD22	1.77	0.49
54:6Y:33:VAL:O	54:6Y:34:TRP:C	2.54	0.49
55:8A:208:MET:SD	57:8C:100:ALA:HB2	2.53	0.49
55:8A:473:TRP:N	66:8L:25:MET:HE1	2.27	0.49
82:8A:601:PGV:H183	57:8C:25:LEU:HD22	1.93	0.49
64:8J:48:TYR:HE2	82:8J:101:PGV:H032	1.76	0.49
1:1A:105:GLU:HG3	1:1A:111:LEU:H	1.76	0.49
4:1D:357:GLN:O	43:1r:59:ARG:NH1	2.45	0.49
7:1G:262:TRP:HB2	7:1G:390:LEU:HD11	1.93	0.49
7:1G:316:ALA:HB3	7:1G:519:PRO:HG3	1.93	0.49
10:1J:130:THR:HG21	25:1Z:124:LEU:HD22	1.93	0.49
16:1P:90:VAL:HG23	16:1P:128:LYS:HB2	1.94	0.49
20:1T:19:LEU:HD13	20:1T:30:LEU:HD11	1.95	0.49
42:1q:2:GLU:O	42:1q:6:VAL:HG23	2.12	0.49
47:3C:100:ARG:HH12	83:3C:502:HEM:CGA	2.24	0.49
47:3C:116:GLY:HA3	83:3C:502:HEM:C4C	2.47	0.49
49:3E:174:LEU:HD13	49:3E:214:ILE:HD13	1.94	0.49
45:3N:66:GLY:HA2	45:3N:72:GLY:HA2	1.94	0.49
45:3N:344:ARG:CG	45:3N:348:SER:HB2	2.42	0.49
47:3P:131:TYR:O	47:3P:139:SER:OG	2.27	0.49
47:3P:315:MET:HE1	47:3P:325:PHE:HB2	1.94	0.49
57:4C:88:ILE:HG12	75:4C:308:CDL:H652	1.95	0.49
68:4N:52:GLU:HG2	68:4N:54:TRP:CZ2	2.47	0.49
6:5F:342:ASP:CG	6:5F:429:ARG:HH12	2.21	0.49
8:5H:14:LEU:HD21	8:5H:83:LEU:HD21	1.95	0.49
12:5L:584:ILE:HG13	14:5N:58:LYS:HE3	1.94	0.49
37:5l:136:ASN:HA	37:5l:153:VAL:HB	1.94	0.49
43:5r:7:ILE:O	43:5r:11:ARG:HG2	2.13	0.49
47:6C:22:PRO:HB3	51:6G:6:PHE:CE2	2.46	0.49
47:6C:361:ILE:HA	47:6C:365:LEU:HD12	1.94	0.49
48:6D:203:TYR:O	48:6D:204:ILE:C	2.55	0.49
49:6E:150:SER:HB2	47:6P:168:PHE:HE1	1.77	0.49
46:6O:412:ASN:HA	46:6O:415:LYS:HD2	1.94	0.49
49:6R:219:HIS:CD2	49:6R:239:HIS:HE1	2.25	0.49
55:8A:425:PHE:O	55:8A:426:PHE:C	2.55	0.49
2:1B:85:VAL:CG1	2:1B:112:TYR:HB2	2.41	0.49
2:1B:86:MET:HE1	2:1B:88:VAL:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:144:HIS:CE1	16:1P:65:LEU:HD21	2.47	0.49
12:1L:584:ILE:HG13	14:1N:58:LYS:HE3	1.94	0.49
27:1b:17:VAL:O	27:1b:21:SER:OG	2.31	0.49
45:3A:27:SER:HA	45:3A:199:ALA:O	2.12	0.49
46:3B:120:MET:CE	46:3B:219:VAL:HG21	2.30	0.49
47:3C:54:HIS:HB3	47:3C:68:HIS:HE1	1.77	0.49
47:3C:58:ASP:O	47:3C:62:ALA:N	2.36	0.49
45:3N:155:ALA:HA	45:3N:164:ALA:CB	2.41	0.49
46:3O:95:LYS:HA	49:3V:70:LEU:CD2	2.43	0.49
55:4A:8:TYR:CZ	57:4C:15:PRO:HB3	2.47	0.49
59:4E:47:ILE:HG13	59:4E:48:ILE:N	2.26	0.49
1:5A:55:PHE:HB2	10:5J:74:MET:CE	2.41	0.49
6:5F:254:LYS:NZ	6:5F:255:LEU:O	2.45	0.49
7:5G:470:VAL:HG12	7:5G:490:MET:HE1	1.94	0.49
20:5U:48:VAL:O	20:5U:52:MET:HG3	2.12	0.49
21:5V:69:GLU:OE2	21:5V:69:GLU:N	2.46	0.49
29:5d:4:GLY:HA3	33:5h:124:GLN:O	2.13	0.49
46:6B:385:GLN:O	46:6B:390:GLY:N	2.45	0.49
48:6D:120:VAL:O	48:6D:124:VAL:N	2.41	0.49
48:6D:239:PRO:HA	48:6D:245:GLN:HA	1.93	0.49
49:6E:223:VAL:O	49:6E:223:VAL:HG13	2.12	0.49
45:6N:254:ALA:HB2	45:6N:323:HIS:HD2	1.77	0.49
46:6O:147:ASP:O	46:6O:148:LYS:C	2.56	0.49
55:8A:105:LEU:O	55:8A:106:PRO:C	2.56	0.49
55:8A:324:LEU:O	55:8A:327:LEU:HB2	2.12	0.49
55:8A:423:MET:HE2	55:8A:453:ILE:HG23	1.94	0.49
59:8E:47:ILE:HG13	59:8E:48:ILE:N	2.27	0.49
71:1B:202:PC1:H242	16:1P:275:PHE:CE1	2.46	0.49
4:1D:405:MET:HE2	4:1D:417:ILE:HG23	1.95	0.49
7:1G:226:GLU:OE1	17:1Q:36:ARG:NH2	2.30	0.49
7:1G:244:THR:HB	17:1Q:73:SER:HB2	1.95	0.49
7:1G:315:VAL:O	7:1G:340:SER:OG	2.18	0.49
10:1J:86:ASN:HB2	10:1J:89:VAL:HG23	1.94	0.49
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD13	1.92	0.49
43:1r:72:GLN:N	43:1r:72:GLN:OE1	2.45	0.49
45:3A:32:GLN:HE21	45:3A:201:GLY:HA2	1.76	0.49
45:3A:280:TYR:HA	45:3A:284:TYR:CE2	2.48	0.49
47:3C:346:PRO:O	47:3C:349:ILE:N	2.45	0.49
49:3E:177:ARG:HD3	49:3E:211:VAL:CG1	2.42	0.49
46:3O:165:ALA:O	46:3O:240:ARG:HD3	2.12	0.49
46:3O:241:GLY:HA2	46:3O:423:SER:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:82:LEU:O	55:4A:86:MET:HG3	2.12	0.49
7:5G:470:VAL:CG1	7:5G:490:MET:HE1	2.42	0.49
9:5I:169:ILE:O	9:5I:173:TYR:HB3	2.12	0.49
12:5L:566:THR:O	12:5L:570:GLN:HG2	2.12	0.49
14:5N:312:LYS:HG2	14:5N:315:TRP:CZ3	2.47	0.49
15:5O:304:TYR:HE1	69:5d:201:3PE:H112	1.78	0.49
16:5P:260:HIS:O	16:5P:264:ARG:HG3	2.11	0.49
45:6A:431:LEU:HD12	45:6A:432:PRO:HD2	1.94	0.49
46:6B:143:GLN:O	46:6B:144:LEU:C	2.55	0.49
46:6B:316:TYR:O	46:6B:317:SER:C	2.56	0.49
47:6C:34:GLY:HA2	47:6C:37:LEU:HD12	1.95	0.49
48:6D:323:LYS:N	51:6G:18:TYR:O	2.43	0.49
49:6E:185:ASP:OD1	49:6E:186:GLN:N	2.44	0.49
45:6N:14:THR:CG2	45:6N:389:ARG:HH22	2.26	0.49
45:6N:64:PHE:HD2	46:6O:287:ARG:NH2	2.07	0.49
45:6N:270:LEU:HD11	45:6N:320:LEU:HD22	1.95	0.49
45:6N:317:THR:OG1	45:6N:318:GLY:N	2.46	0.49
46:6O:332:SER:O	46:6O:333:ALA:C	2.55	0.49
55:8A:129:TYR:HB3	56:8B:160:LEU:CD2	2.43	0.49
55:8A:282:PHE:HA	82:8A:603:PGV:H332	1.94	0.49
55:8A:290:HIS:HA	55:8A:293:PHE:CE2	2.48	0.49
82:8A:603:PGV:H41	68:8N:1:MET:HE3	1.95	0.49
56:8B:91:ASN:O	56:8B:93:PRO:HD3	2.12	0.49
1:1A:92:LEU:HD13	27:1b:29:ILE:HA	1.95	0.49
2:1B:61:HIS:HE1	4:1D:171:PHE:CZ	2.28	0.49
2:1B:96:MET:HG2	4:1D:82:LEU:CD2	2.05	0.49
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.93	0.49
8:1H:2:PHE:O	8:1H:6:ILE:HG13	2.13	0.49
20:1T:46:ASP:OD1	22:1W:64:ARG:NH2	2.36	0.49
20:1U:48:VAL:O	20:1U:52:MET:HG3	2.12	0.49
31:1f:5:GLN:O	31:1f:9:ASP:HB2	2.12	0.49
46:3B:109:VAL:HB	46:3B:119:LEU:HD12	1.95	0.49
47:3C:50:PHE:CG	49:3E:136:PHE:HD2	2.31	0.49
47:3C:129:MET:O	47:3C:133:LEU:N	2.44	0.49
47:3C:184:ILE:O	47:3C:185:LEU:C	2.55	0.49
48:3D:261:ASP:OD1	48:3D:262:ASP:N	2.45	0.49
49:3E:197:ASP:N	49:3E:197:ASP:OD1	2.46	0.49
51:3G:26:ARG:O	51:3G:27:ALA:C	2.56	0.49
45:3N:59:VAL:HG11	45:3N:190:TYR:HE2	1.75	0.49
45:3N:133:VAL:HG12	45:3N:137:GLU:HG3	1.94	0.49
48:3Q:224:ARG:HD3	51:3T:26:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:201:ASP:O	49:3R:205:VAL:HG12	2.13	0.49
55:4A:423:MET:CE	55:4A:456:MET:HB2	2.43	0.49
82:4C:302:PGV:H51	61:4G:69:LEU:HD21	1.95	0.49
2:5B:102:LYS:O	2:5B:106:GLN:HG3	2.12	0.49
7:5G:244:THR:HB	17:5Q:73:SER:HB2	1.95	0.49
8:5H:65:THR:HA	16:5P:324:TYR:HB2	1.93	0.49
10:5J:33:LEU:HD11	11:5K:34:GLU:HB3	1.93	0.49
12:5L:573:MET:SD	12:5L:576:MET:HE3	2.53	0.49
13:5M:91:ARG:HE	69:5N:902:3PE:H321	1.78	0.49
37:5l:3:HIS:ND1	38:5m:60:GLU:OE1	2.45	0.49
45:6A:355:VAL:HA	45:6A:358:LYS:HD3	1.93	0.49
46:6B:33:LEU:HD21	46:6B:224:LEU:HD13	1.94	0.49
46:6B:400:GLN:HE21	46:6B:401:GLN:HG3	1.78	0.49
47:6C:71:ARG:HG2	48:6D:133:TYR:HB3	1.95	0.49
48:6D:217:SER:O	48:6D:221:GLY:N	2.46	0.49
51:6G:38:ASN:O	51:6G:42:ARG:HG3	2.12	0.49
45:6N:37:VAL:CG1	45:6N:38:GLY:N	2.46	0.49
46:6O:28:ARG:HA	46:6O:34:VAL:HA	1.94	0.49
55:8A:135:ASN:ND2	61:8G:58:LYS:HB2	2.27	0.49
55:8A:244:TYR:O	55:8A:245:ILE:C	2.55	0.49
55:8A:310:MET:O	55:8A:311:ILE:C	2.55	0.49
56:8B:83:ILE:HA	56:8B:86:MET:HG2	1.95	0.49
57:8C:25:LEU:O	57:8C:29:SER:OG	2.28	0.49
90:8C:306:PEK:H302	61:8G:26:PRO:HG3	1.95	0.49
62:8H:43:MET:SD	62:8H:46:LYS:HE3	2.53	0.49
2:1B:102:LYS:O	2:1B:106:GLN:HG3	2.12	0.49
6:1F:363:THR:HG21	7:1G:97:LEU:HG	1.95	0.49
12:1L:36:VAL:HG21	12:1L:118:PHE:HB3	1.94	0.49
13:1M:52:PHE:O	33:1h:89:LYS:NZ	2.41	0.49
21:1V:22:ARG:HH11	21:1V:25:ILE:HD11	1.78	0.49
37:1l:115:MET:HA	37:1l:118:VAL:HG22	1.95	0.49
43:1r:7:ILE:O	43:1r:11:ARG:HG2	2.12	0.49
47:3C:15:ASN:HA	47:3C:19:ILE:HB	1.95	0.49
45:3N:18:GLN:HG2	45:3N:23:LEU:C	2.38	0.49
45:3N:29:GLN:NE2	45:3N:204:GLU:HG3	2.24	0.49
49:3R:167:PHE:HB3	49:3R:169:TRP:CE2	2.48	0.49
55:4A:477:ALA:HB1	66:4L:18:LYS:HG2	1.95	0.49
57:4C:221:ARG:HB3	57:4C:226:HIS:HB2	1.93	0.49
2:5B:144:ILE:HG13	2:5B:163:LEU:HB2	1.95	0.49
4:5D:343:GLU:O	4:5D:347:HIS:ND1	2.40	0.49
12:5L:161:ARG:HA	39:5n:91:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5L:583:LEU:HB2	12:5L:586:LEU:HG	1.94	0.49
69:5L:701:3PE:H221	37:5l:87:ASN:O	2.12	0.49
20:5T:70:LEU:HB3	20:5T:76:ILE:HG13	1.93	0.49
21:5V:57:MET:HE2	21:5V:70:GLN:HG3	1.94	0.49
37:5l:134:PRO:CG	40:5o:38:MET:HE2	2.40	0.49
43:5r:72:GLN:OE1	43:5r:72:GLN:N	2.45	0.49
45:6A:196:VAL:HG11	45:6A:380:GLY:HA2	1.95	0.49
47:6C:78:VAL:O	47:6C:79:ILE:C	2.56	0.49
47:6C:179:PHE:O	47:6C:183:PHE:N	2.37	0.49
47:6C:350:ILE:CD1	51:6G:64:GLY:HA3	2.41	0.49
48:6D:109:LEU:HD23	48:6D:287:HIS:ND1	2.27	0.49
52:6H:42:LEU:HD13	52:6H:98:LEU:HD22	1.94	0.49
45:6N:44:GLY:H	45:6N:47:TYR:HB2	1.77	0.49
46:6O:257:LEU:HD21	46:6O:422:LYS:HD3	1.95	0.49
55:8A:132:LEU:O	55:8A:138:HIS:HB2	2.13	0.49
55:8A:474:GLU:O	55:8A:475:ALA:C	2.56	0.49
2:1B:91:THR:HA	2:1B:119:CYS:HB3	1.93	0.49
71:1B:202:PC1:H261	71:1B:202:PC1:H351	1.95	0.49
3:1C:121:VAL:HG21	3:1C:146:PRO:HD3	1.94	0.49
6:1F:305:PRO:HD3	6:1F:413:TRP:HB3	1.95	0.49
8:1H:14:LEU:HD21	8:1H:83:LEU:HD21	1.95	0.49
12:1L:220:ALA:HB2	12:1L:260:LEU:HD13	1.95	0.49
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.94	0.49
13:1M:71:TRP:CG	71:1M:502:PC1:H2C2	2.48	0.49
34:1i:85:LEU:HA	34:1i:89:VAL:HB	1.95	0.49
37:1l:3:HIS:ND1	38:1m:60:GLU:OE1	2.45	0.49
45:3A:281:ASP:OD1	45:3A:283:THR:OG1	2.26	0.49
47:3C:58:ASP:O	47:3C:61:THR:N	2.45	0.49
48:3D:171:ARG:NH1	48:3D:177:ASP:OD2	2.39	0.49
49:3E:223:VAL:O	49:3E:223:VAL:HG13	2.12	0.49
45:3N:52:ASN:O	45:3N:55:ALA:N	2.46	0.49
46:3O:50:PHE:O	46:3O:205:ALA:N	2.46	0.49
49:3R:199:GLN:HG3	49:3R:257:ASN:ND2	2.28	0.49
82:4A:603:PGV:H41	68:4N:1:MET:HE3	1.94	0.49
56:4B:83:ILE:HA	56:4B:86:MET:HG2	1.95	0.49
82:4C:301:PGV:H012	82:4C:301:PGV:H42	1.95	0.49
2:5B:54:CYS:HB2	70:5B:201:SF4:S4	2.53	0.49
6:5F:268:VAL:HG21	6:5F:283:HIS:CG	2.48	0.49
7:5G:364:LEU:HD12	7:5G:491:ASN:HB3	1.95	0.49
7:5G:605:GLU:HG2	22:5W:119:LEU:HD22	1.94	0.49
10:5J:72:THR:O	10:5J:76:THR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:5J:175:ASN:O	15:5O:254:ARG:NH2	2.39	0.49
24:5Y:75:ILE:HG12	51:6T:56:TYR:CE2	2.46	0.49
45:6A:158:PHE:HA	45:6A:235:ARG:C	2.38	0.49
45:6A:292:SER:O	45:6A:293:THR:C	2.54	0.49
47:6C:346:PRO:O	47:6C:350:ILE:N	2.38	0.49
45:6N:94:HIS:O	45:6N:95:THR:HG23	2.13	0.49
45:6N:140:GLU:O	45:6N:143:SER:OG	2.20	0.49
45:6N:217:SER:O	45:6N:218:SER:C	2.56	0.49
49:6R:199:GLN:HG3	49:6R:257:ASN:ND2	2.28	0.49
55:8A:143:VAL:HB	55:8A:213:ARG:HH21	1.77	0.49
55:8A:313:ALA:HB3	56:8B:73:LEU:HD11	1.95	0.49
60:8F:16:LEU:O	60:8F:20:VAL:HG13	2.13	0.49
7:1G:427:LYS:NZ	7:1G:427:LYS:HB2	2.28	0.49
69:1M:503:3PE:H2F1	71:1Y:201:PC1:H281	1.95	0.49
45:3A:356:ARG:HG3	46:3B:91:ALA:HA	1.95	0.49
47:3C:315:MET:O	47:3C:316:MET:C	2.56	0.49
48:3D:235:LEU:HD13	48:3D:246:ALA:HB1	1.94	0.49
46:3O:128:ALA:HB3	46:3O:223:PHE:CE1	2.46	0.49
48:3Q:59:GLU:HG2	48:3Q:60:GLU:N	2.27	0.49
55:4A:229:ILE:HG21	82:4A:604:PGV:H062	1.94	0.49
55:4A:271:MET:HG3	68:4N:12:HIS:CE1	2.48	0.49
60:4F:16:LEU:O	60:4F:20:VAL:HG13	2.13	0.49
7:5G:427:LYS:HB2	7:5G:427:LYS:NZ	2.28	0.49
33:5h:123:TYR:H	81:5h:201:AME:C	2.25	0.49
45:6A:283:THR:HB	49:6I:73:PRO:HA	1.93	0.49
47:6C:163:TRP:HH2	49:6R:137:VAL:HG13	1.78	0.49
48:6D:98:TYR:HB2	52:6H:99:PHE:CG	2.48	0.49
53:6J:11:TYR:CD1	53:6J:15:PHE:HB3	2.48	0.49
53:6J:20:THR:HA	54:6Y:23:MET:SD	2.53	0.49
45:6N:41:ILE:HG12	45:6N:195:MET:CE	2.43	0.49
45:6N:264:ASN:HB3	45:6N:267:ASN:HB2	1.94	0.49
45:6N:439:SER:HA	45:6N:442:PHE:CE1	2.47	0.49
47:6P:131:TYR:O	47:6P:139:SER:OG	2.27	0.49
54:6Y:50:GLY:O	54:6Y:51:LYS:C	2.56	0.49
55:8A:114:ALA:O	55:8A:115:SER:C	2.56	0.49
55:8A:135:ASN:HB3	55:8A:213:ARG:HB3	1.95	0.49
55:8A:279:SER:HB3	68:8N:22:ILE:CG1	2.40	0.49
82:8A:603:PGV:H31	75:8A:610:CDL:H442	1.95	0.49
68:8N:81:ASP:N	68:8N:81:ASP:OD1	2.46	0.49
2:1B:124:GLY:HA2	9:1I:115:LYS:HG2	1.95	0.48
4:1D:112:MET:HG3	4:1D:181:TYR:CZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:151:ILE:HD11	4:1D:218:PHE:CZ	2.48	0.48
7:1G:648:LEU:HD21	19:1S:44:LYS:HG2	1.94	0.48
8:1H:296:LEU:HD13	71:1I:201:PC1:H351	1.94	0.48
12:1L:161:ARG:HA	39:1n:91:GLU:HG3	1.94	0.48
16:1P:199:GLU:OE2	16:1P:200:THR:OG1	2.31	0.48
20:1U:36:PHE:HB3	20:1U:42:LEU:HD12	1.94	0.48
21:1V:69:GLU:OE2	21:1V:69:GLU:N	2.46	0.48
29:1d:4:GLY:HA3	33:1h:124:GLN:O	2.13	0.48
47:3C:183:PHE:CE2	47:3P:180:ALA:HA	2.48	0.48
47:3C:269:LYS:HB2	47:3C:275:LEU:HD21	1.95	0.48
49:3E:185:ASP:OD1	49:3E:186:GLN:N	2.44	0.48
45:3N:192:ALA:N	45:3N:193:PRO:HD3	2.27	0.48
45:3N:216:PHE:HB3	45:3N:219:LEU:CD1	2.42	0.48
45:3N:223:TYR:HB3	45:3N:227:ALA:O	2.12	0.48
45:3N:344:ARG:O	45:3N:345:LEU:C	2.56	0.48
64:4J:33:ARG:CZ	82:4J:101:PGV:H183	2.43	0.48
68:4N:81:ASP:OD1	68:4N:81:ASP:N	2.46	0.48
2:5B:69:MET:HE3	2:5B:74:VAL:HG12	1.95	0.48
4:5D:151:ILE:HD11	4:5D:218:PHE:CZ	2.48	0.48
7:5G:284:ILE:HG23	7:5G:294:THR:HG21	1.95	0.48
10:5J:138:GLU:HG3	30:5e:28:ILE:HG21	1.95	0.48
13:5M:452:LYS:HG3	32:5g:83:TYR:HE2	1.77	0.48
16:5P:199:GLU:OE2	16:5P:200:THR:OG1	2.31	0.48
80:5T:101:EHZ:O3	80:5T:101:EHZ:N2	2.46	0.48
25:5Z:104:TRP:HH2	30:5e:74:ARG:HG3	1.77	0.48
36:5k:23:ILE:HD12	36:5k:29:GLU:HA	1.94	0.48
40:5o:28:TYR:OH	40:5o:110:ARG:NH2	2.45	0.48
45:6A:91:THR:HG23	45:6A:94:HIS:HB2	1.93	0.48
48:6D:305:LEU:O	48:6D:306:PRO:C	2.56	0.48
48:6D:317:SER:HB2	51:6G:22:PRO:HA	1.95	0.48
50:6F:61:ARG:NH2	50:6F:112:GLU:OE1	2.43	0.48
49:6R:179:ARG:HE	49:6R:184:ILE:HG12	1.78	0.48
49:6R:248:ARG:NH2	49:6R:249:ILE:O	2.46	0.48
55:8A:27:GLY:HA2	55:8A:69:MET:HG3	1.94	0.48
55:8A:360:ASN:O	55:8A:361:SER:C	2.56	0.48
55:8A:386:VAL:CG1	55:8A:387:PHE:N	2.76	0.48
1:1A:54:LYS:HG2	1:1A:114:ALA:HB3	1.95	0.48
2:1B:54:CYS:HB2	70:1B:201:SF4:S4	2.53	0.48
5:1E:109:MET:HE1	6:1F:346:ALA:HA	1.94	0.48
6:1F:268:VAL:HG21	6:1F:283:HIS:CG	2.48	0.48
8:1H:10:ILE:HG23	8:1H:83:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:321:GLN:HB3	12:1L:324:LEU:HB2	1.94	0.48
13:1M:452:LYS:HG3	32:1g:83:TYR:HE2	1.77	0.48
15:1O:240:TYR:OH	21:1V:22:ARG:NH2	2.42	0.48
29:1d:11:LEU:HD21	30:1e:3:PHE:HB3	1.95	0.48
34:1i:23:LYS:O	34:1i:26:GLU:HG2	2.13	0.48
46:3B:34:VAL:HG11	46:3B:386:ALA:HB1	1.94	0.48
47:3C:236:MET:HB2	48:3D:301:MET:HE1	1.95	0.48
48:3D:316:TRP:O	48:3D:320:LYS:HG2	2.13	0.48
45:3N:70:ARG:HB2	45:3N:75:LEU:CD2	2.42	0.48
46:3O:27:THR:N	46:3O:35:ILE:O	2.46	0.48
55:4A:51:ASP:CG	56:4B:205:SER:HG	2.20	0.48
55:4A:68:PHE:HE2	55:4A:112:LEU:HD22	1.76	0.48
4:5D:165:THR:HG23	8:5H:32:GLN:HG3	1.94	0.48
8:5H:55:LEU:HD13	8:5H:221:ALA:HB2	1.94	0.48
13:5M:220:HIS:O	13:5M:228:SER:OG	2.31	0.48
20:5T:19:LEU:HD13	20:5T:30:LEU:HD11	1.95	0.48
46:6B:59:ASP:O	46:6B:60:SER:C	2.55	0.48
46:6B:124:LEU:HD12	46:6B:128:ALA:HB2	1.95	0.48
46:6B:166:ALA:HB2	46:6B:244:ILE:HG12	1.95	0.48
47:6C:25:SER:O	47:6C:26:ASN:C	2.56	0.48
47:6C:346:PRO:O	47:6C:349:ILE:N	2.46	0.48
48:6D:187:GLU:O	48:6D:188:ALA:C	2.56	0.48
49:6E:152:ILE:HG23	49:6E:154:ILE:HG23	1.95	0.48
45:6N:92:ARG:NH1	45:6N:314:TYR:OH	2.47	0.48
45:6N:340:GLY:O	45:6N:341:GLN:C	2.56	0.48
46:6O:57:TYR:O	46:6O:58:GLU:C	2.54	0.48
48:6Q:224:ARG:HD3	51:6T:26:PHE:CE2	2.48	0.48
55:8A:507:GLU:HG3	57:8C:5:THR:HG21	1.95	0.48
89:8A:611:PSC:H21	89:8A:611:PSC:H02	1.56	0.48
64:8J:4:ARG:HH12	64:8J:8:LYS:NZ	2.04	0.48
65:8K:9:PHE:HB3	82:8K:101:PGV:O14	2.13	0.48
2:1B:101:ARG:HG2	2:1B:140:VAL:HG13	1.96	0.48
4:1D:63:ARG:HB3	4:1D:79:HIS:HB2	1.95	0.48
4:1D:112:MET:HA	4:1D:115:GLU:HG2	1.96	0.48
9:1I:135:PRO:HG3	9:1I:164:GLU:CD	2.39	0.48
10:1J:72:THR:O	10:1J:76:THR:HA	2.13	0.48
19:1S:82:SER:O	19:1S:86:VAL:HG23	2.14	0.48
38:1m:24:ILE:N	38:1m:24:ILE:HD12	2.28	0.48
47:3C:304:MET:HB2	47:3C:305:PRO:HD3	1.94	0.48
47:3C:372:ILE:O	47:3C:376:LEU:HG	2.14	0.48
45:3N:46:ARG:CZ	45:3N:163:LEU:CD2	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:191:LYS:HD2	45:3N:223:TYR:OH	2.10	0.48
55:4A:54:TYR:O	55:4A:58:VAL:HG23	2.12	0.48
55:4A:224:GLY:O	57:4C:192:VAL:HG22	2.13	0.48
55:4A:481:GLU:OE1	66:4L:7:PRO:HG2	2.13	0.48
56:4B:91:ASN:O	56:4B:93:PRO:HD3	2.12	0.48
57:4C:191:GLY:O	57:4C:195:SER:OG	2.24	0.48
90:4C:306:PEK:H302	61:4G:26:PRO:HG3	1.95	0.48
2:5B:47:PRO:HD2	2:5B:75:VAL:O	2.12	0.48
8:5H:10:ILE:HG23	8:5H:83:LEU:HD22	1.95	0.48
12:5L:562:LEU:HB2	12:5L:563:PRO:HD3	1.94	0.48
15:5O:23:LYS:HA	15:5O:167:HIS:ND1	2.28	0.48
22:5W:65:GLU:OE1	22:5W:66:MET:CE	2.61	0.48
34:5i:41:PRO:HA	34:5i:44:GLN:HB2	1.95	0.48
37:5l:97:SER:O	37:5l:101:MET:HG3	2.13	0.48
38:5m:24:ILE:HD12	38:5m:24:ILE:N	2.28	0.48
40:5o:112:LYS:O	40:5o:116:GLN:HG3	2.13	0.48
45:6A:166:SER:O	45:6A:167:VAL:C	2.56	0.48
46:6B:239:TYR:HE2	46:6B:421:ARG:HB3	1.78	0.48
48:6D:114:ILE:CD1	48:6D:281:TRP:HB3	2.43	0.48
49:6E:263:TYR:HB3	49:6E:273:VAL:HG13	1.94	0.48
46:6O:200:THR:O	46:6O:201:SER:C	2.55	0.48
54:6Y:45:VAL:O	54:6Y:46:PRO:C	2.56	0.48
55:8A:258:VAL:O	55:8A:259:THR:C	2.56	0.48
55:8A:319:LYS:HE3	55:8A:319:LYS:HB3	1.37	0.48
55:8A:321:PHE:HB3	56:8B:65:TRP:CE3	2.48	0.48
55:8A:398:PRO:O	55:8A:399:LEU:C	2.56	0.48
82:8A:603:PGV:H302	82:8A:603:PGV:H331	1.49	0.48
56:8B:105:TYR:N	56:8B:207:MET:HE3	2.28	0.48
62:8H:28:ASN:O	62:8H:32:ASN:ND2	2.47	0.48
8:1H:55:LEU:HD13	8:1H:221:ALA:HB2	1.94	0.48
8:1H:87:VAL:HG22	8:1H:88:PRO:HD3	1.96	0.48
10:1J:106:TYR:O	10:1J:110:GLU:HB2	2.13	0.48
80:1T:101:EHZ:N2	80:1T:101:EHZ:O3	2.46	0.48
37:1l:97:SER:O	37:1l:101:MET:HG3	2.13	0.48
47:3C:225:THR:O	47:3C:229:ILE:HG13	2.13	0.48
47:3C:237:LEU:HA	48:3D:301:MET:HG3	1.95	0.48
45:3N:61:HIS:CG	45:3N:134:ILE:HD11	2.48	0.48
45:3N:337:PHE:CE1	47:3P:2:THR:HA	2.47	0.48
55:4A:243:VAL:HA	85:4A:606:HEA:HAC	1.95	0.48
55:4A:297:MET:HG2	82:4A:604:PGV:H05	1.95	0.48
4:5D:357:GLN:O	43:5r:59:ARG:NH1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5F:363:THR:HG21	7:5G:97:LEU:HG	1.95	0.48
7:5G:139:ASP:OD1	7:5G:148:THR:O	2.30	0.48
8:5H:2:PHE:O	8:5H:6:ILE:HG13	2.13	0.48
21:5V:22:ARG:HH11	21:5V:25:ILE:HD11	1.78	0.48
26:5a:1:MET:SD	26:5a:1:MET:N	2.83	0.48
34:5i:85:LEU:HA	34:5i:89:VAL:HB	1.95	0.48
45:6A:192:ALA:HB2	45:6A:219:LEU:HB3	1.95	0.48
47:6C:269:LYS:HE3	47:6C:275:LEU:HD11	1.95	0.48
47:6C:357:LEU:O	47:6C:358:TYR:C	2.56	0.48
45:6N:18:GLN:HA	45:6N:24:ARG:N	2.29	0.48
49:6R:167:PHE:HB3	49:6R:169:TRP:CE2	2.48	0.48
55:8A:94:PHE:HA	82:8A:602:PGV:H041	1.95	0.48
55:8A:240:HIS:O	55:8A:241:PRO:C	2.56	0.48
55:8A:378:HIS:CD2	55:8A:382:SER:HB2	2.48	0.48
75:8A:610:CDL:H541	75:8A:610:CDL:H162	1.94	0.48
75:8A:610:CDL:H712	75:8A:610:CDL:HB61	1.63	0.48
90:8C:306:PEK:H181	82:8G:101:PGV:H162	1.95	0.48
58:8D:17:VAL:HG22	67:8M:2:TYR:CE1	2.48	0.48
6:1F:254:LYS:NZ	6:1F:255:LEU:O	2.45	0.48
7:1G:284:ILE:HG23	7:1G:294:THR:HG21	1.95	0.48
13:1M:19:LYS:HD3	31:1f:9:ASP:OD2	2.14	0.48
16:1P:30:LEU:HA	16:1P:207:ILE:HD11	1.94	0.48
23:1X:105:LYS:HA	23:1X:108:GLU:HG2	1.94	0.48
46:3B:74:SER:HB2	49:3I:70:LEU:HD12	1.95	0.48
46:3B:107:TYR:HB3	46:3B:123:LEU:HD11	1.95	0.48
47:3C:56:THR:HG21	47:3P:172:LYS:NZ	2.28	0.48
47:3C:200:LEU:HD13	83:3C:502:HEM:HAD2	1.94	0.48
47:3C:229:ILE:C	48:3D:308:VAL:HG11	2.39	0.48
47:3C:303:LEU:O	47:3C:304:MET:C	2.57	0.48
49:3E:152:ILE:HG23	49:3E:154:ILE:HG23	1.95	0.48
50:3F:119:TRP:CZ2	46:3O:88:GLY:HA2	2.48	0.48
45:3N:46:ARG:HH22	45:3N:314:TYR:CB	2.25	0.48
45:3N:68:LYS:N	45:3N:119:ASN:O	2.46	0.48
45:3N:356:ARG:HA	46:3O:91:ALA:O	2.12	0.48
46:3O:35:ILE:HG21	46:3O:217:LYS:HG2	1.96	0.48
6:5F:305:PRO:HD3	6:5F:413:TRP:HB3	1.95	0.48
13:5M:118:PHE:O	13:5M:122:PHE:HB3	2.14	0.48
16:5P:90:VAL:HG23	16:5P:128:LYS:HB2	1.94	0.48
41:5p:95:TYR:HB3	41:5p:96:LYS:HZ3	1.79	0.48
45:6A:25:VAL:HG11	45:6A:209:LEU:HA	1.93	0.48
45:6A:345:LEU:HD23	45:6A:349:ALA:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:6C:43:LEU:O	47:6C:44:GLN:C	2.54	0.48
47:6C:70:CYS:HA	47:6C:77:TRP:HB3	1.94	0.48
47:6C:233:LEU:HD12	48:6D:301:MET:HE2	1.95	0.48
47:6C:322:GLN:O	47:6C:323:CYS:C	2.55	0.48
48:6D:317:SER:HA	48:6D:320:LYS:HB2	1.95	0.48
45:6N:32:GLN:HB3	46:6O:373:GLU:CD	2.38	0.48
45:6N:41:ILE:HG22	45:6N:95:THR:OG1	2.13	0.48
45:6N:87:ASN:HD21	45:6N:100:LYS:CD	2.22	0.48
46:6O:259:ALA:HB3	46:6O:417:PHE:CD1	2.49	0.48
46:6O:305:GLN:O	46:6O:306:PRO:C	2.56	0.48
47:6P:129:MET:HE1	47:6P:181:PHE:HB3	1.96	0.48
55:8A:167:THR:O	55:8A:168:ILE:C	2.57	0.48
55:8A:231:TYR:O	55:8A:232:GLN:C	2.55	0.48
55:8A:381:LEU:HA	85:8A:606:HEA:CBC	2.44	0.48
75:8A:610:CDL:H652	57:8C:88:ILE:HG12	1.95	0.48
1:1A:47:ALA:O	1:1A:48:ARG:C	2.57	0.48
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.28	0.48
10:1J:105:TYR:CE1	10:1J:109:LYS:HG3	2.48	0.48
12:1L:13:ILE:HG21	34:1i:81:ILE:HD11	1.94	0.48
12:1L:40:VAL:HG11	12:1L:97:THR:HG23	1.96	0.48
15:1O:304:TYR:HE1	69:1d:201:3PE:H112	1.78	0.48
71:1P:401:PC1:H251	71:1P:401:PC1:H222	1.50	0.48
20:1T:52:MET:CE	22:1W:40:TYR:CD1	2.97	0.48
45:3N:79:VAL:HG22	45:3N:112:LEU:CD1	2.31	0.48
46:3O:24:LEU:HD23	46:3O:26:PHE:HB2	1.95	0.48
47:3P:246:SER:HB2	47:3P:249:LEU:HB2	1.95	0.48
55:4A:127:THR:HB	55:4A:129:TYR:CE1	2.48	0.48
1:5A:72:LEU:HA	10:5J:147:TYR:OH	2.14	0.48
4:5D:258:VAL:HG12	4:5D:296:ARG:HG2	1.96	0.48
8:5H:292:SER:OG	71:5I:201:PC1:O32	2.29	0.48
12:5L:56:HIS:CE1	41:5p:27:ASN:HD21	2.32	0.48
12:5L:321:GLN:HB3	12:5L:324:LEU:HB2	1.94	0.48
15:5O:136:GLU:OE2	15:5O:140:ARG:NE	2.47	0.48
20:5T:52:MET:CE	22:5W:40:TYR:CD1	2.97	0.48
45:6A:106:LEU:O	45:6A:107:PRO:C	2.55	0.48
47:6C:182:HIS:NE2	83:6C:501:HEM:ND	2.61	0.48
47:6C:360:LEU:O	47:6C:361:ILE:C	2.56	0.48
48:6D:121:TYR:HD1	48:6D:125:CYS:HB3	1.79	0.48
48:6D:292:ARG:CZ	48:6D:292:ARG:HB2	2.40	0.48
45:6N:15:GLN:HG3	45:6N:205:HIS:NE2	2.27	0.48
45:6N:369:LEU:HD21	45:6N:378:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6O:25:GLU:HB2	46:6O:213:HIS:CE1	2.49	0.48
46:6O:56:ARG:HH12	46:6O:235:ALA:H	1.61	0.48
48:6Q:225:HIS:CE1	51:6T:20:PRO:HB2	2.48	0.48
55:8A:62:ALA:O	55:8A:63:PHE:C	2.55	0.48
55:8A:222:PRO:HG2	56:8B:176:PRO:HB2	1.95	0.48
55:8A:341:ALA:O	55:8A:342:LEU:C	2.55	0.48
82:8A:604:PGV:H012	82:8C:303:PGV:H202	1.96	0.48
57:8C:14:SER:HG	57:8C:16:TRP:CD1	2.32	0.48
6:1F:12:PHE:CE1	6:1F:247:ARG:HG3	2.49	0.48
7:1G:685:ALA:O	7:1G:689:LYS:HG3	2.14	0.48
12:1L:331:MET:HE1	12:1L:468:ILE:HD12	1.95	0.48
13:1M:7:PRO:HB3	31:1f:16:VAL:HG13	1.95	0.48
14:1N:312:LYS:HG2	14:1N:315:TRP:CZ3	2.47	0.48
17:1Q:10:LEU:HD13	22:1W:16:SER:HB3	1.96	0.48
29:1d:53:VAL:HG13	69:1d:201:3PE:H111	1.95	0.48
40:1o:28:TYR:OH	40:1o:110:ARG:NH2	2.45	0.48
47:3C:8:HIS:O	47:3C:9:PRO:C	2.57	0.48
47:3C:20:ASP:O	47:3C:21:LEU:C	2.56	0.48
47:3C:140:PHE:CZ	47:3C:261:PRO:HB3	2.49	0.48
47:3C:244:LEU:HD13	48:3D:293:MET:C	2.38	0.48
48:3D:227:THR:HG22	52:3H:69:VAL:HB	1.95	0.48
50:3F:119:TRP:HZ3	46:3O:91:ALA:CB	2.17	0.48
45:3N:46:ARG:NH2	45:3N:314:TYR:CD2	2.82	0.48
45:3N:257:VAL:HG12	45:3N:420:PRO:HB3	1.95	0.48
45:3N:259:GLY:N	45:3N:318:GLY:O	2.43	0.48
46:3O:124:LEU:HB3	46:3O:223:PHE:CG	2.49	0.48
55:4A:448:THR:HG21	65:4K:39:GLU:HG2	1.94	0.48
71:5A:202:PC1:H151	10:5J:149:TYR:CE2	2.48	0.48
2:5B:34:ASP:HB3	2:5B:174:ARG:HH21	1.79	0.48
10:5J:105:TYR:CE1	10:5J:109:LYS:HG3	2.47	0.48
12:5L:13:ILE:HG21	34:5i:81:ILE:HD11	1.94	0.48
12:5L:386:LEU:HD13	35:5j:36:ILE:HD11	1.96	0.48
13:5M:19:LYS:HD3	31:5f:9:ASP:OD2	2.14	0.48
29:5d:17:GLU:HG3	29:5d:81:TYR:HE1	1.79	0.48
35:5j:33:TRP:CD1	36:5k:70:PHE:HA	2.49	0.48
39:5n:55:ASP:H	39:5n:58:LYS:CE	2.27	0.48
46:6B:40:ASN:H	46:6B:210:GLY:HA2	1.78	0.48
46:6B:121:GLU:O	46:6B:122:PHE:C	2.56	0.48
47:6C:137:GLN:N	47:6C:257:THR:O	2.47	0.48
47:6C:277:ALA:HB1	47:6C:294:LEU:HG	1.96	0.48
49:6E:197:ASP:N	49:6E:197:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:411:CYS:O	45:6N:415:PHE:N	2.46	0.48
46:6O:28:ARG:HD2	46:6O:34:VAL:HG23	1.95	0.48
46:6O:29:LEU:HB2	46:6O:33:LEU:HB3	1.94	0.48
46:6O:75:LEU:HD22	46:6O:136:GLU:HB3	1.96	0.48
46:6O:170:ASN:O	46:6O:171:ALA:C	2.57	0.48
46:6O:309:VAL:HB	46:6O:326:THR:HB	1.96	0.48
49:6R:201:ASP:O	49:6R:205:VAL:HG12	2.13	0.48
55:8A:100:MET:HB2	57:8C:57:TRP:HH2	1.78	0.48
55:8A:288:TRP:CH2	82:8A:604:PGV:H21	2.49	0.48
82:8C:304:PGV:H331	82:8C:304:PGV:H131	1.96	0.48
60:8F:95:GLN:HG3	60:8F:96:LEU:H	1.78	0.48
67:8M:16:ALA:O	67:8M:20:SER:OG	2.28	0.48
2:1B:118:SER:HA	2:1B:121:ASN:HB2	1.95	0.48
7:1G:364:LEU:HD12	7:1G:491:ASN:HB3	1.95	0.48
12:1L:583:LEU:HB2	12:1L:586:LEU:HG	1.94	0.48
13:1M:269:MET:HE3	13:1M:399:ASN:HB2	1.96	0.48
15:1O:50:HIS:HA	15:1O:123:VAL:HG23	1.94	0.48
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.47	0.48
46:3B:154:ASN:ND2	46:3B:156:GLN:H	2.12	0.48
46:3B:249:GLY:HA3	46:3O:181:TYR:CD2	2.49	0.48
47:3C:3:ASN:HD21	47:3C:5:ARG:HE	1.61	0.48
49:3E:93:ARG:HG2	51:3G:26:ARG:CA	2.44	0.48
46:3O:417:PHE:CE2	46:3O:422:LYS:HE3	2.48	0.48
48:3Q:225:HIS:CE1	51:3T:20:PRO:HB2	2.48	0.48
55:4A:114:ALA:O	55:4A:118:VAL:HG13	2.14	0.48
58:4D:141:ASP:O	58:4D:143:ASN:N	2.47	0.48
62:4H:43:MET:SD	62:4H:46:LYS:HE3	2.53	0.48
4:5D:405:MET:HE2	4:5D:417:ILE:HG23	1.95	0.48
7:5G:685:ALA:O	7:5G:689:LYS:HG3	2.14	0.48
12:5L:36:VAL:HG21	12:5L:118:PHE:HB3	1.95	0.48
12:5L:193:SER:HB2	12:5L:206:ASN:HD21	1.78	0.48
13:5M:269:MET:HE3	13:5M:399:ASN:HB2	1.96	0.48
17:5Q:25:VAL:HB	17:5Q:30:ILE:CD1	2.43	0.48
19:5S:82:SER:O	19:5S:86:VAL:HG23	2.14	0.48
24:5Y:71:LEU:HD21	51:6T:57:LEU:HD11	1.94	0.48
29:5d:61:GLN:O	29:5d:65:VAL:HG13	2.14	0.48
37:5l:136:ASN:ND2	37:5l:153:VAL:H	2.11	0.48
47:6C:56:THR:HB	47:6P:172:LYS:HE2	1.96	0.48
47:6C:279:ALA:O	47:6C:280:ILE:C	2.55	0.48
48:6D:183:TYR:O	48:6D:184:PRO:C	2.57	0.48
45:6N:33:PRO:CD	45:6N:34:THR:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:124:ASP:O	45:6N:125:SER:C	2.56	0.48
45:6N:191:LYS:C	45:6N:193:PRO:HD2	2.38	0.48
45:6N:335:MET:HG2	45:6N:432:PRO:HG3	1.95	0.48
46:6O:56:ARG:HD2	46:6O:171:ALA:HB1	1.96	0.48
46:6O:394:GLN:O	46:6O:395:PRO:C	2.56	0.48
55:8A:168:ILE:HG22	55:8A:169:ILE:HD13	1.95	0.48
64:8J:52:TRP:CE2	82:8J:101:PGV:H042	2.48	0.48
4:1D:171:PHE:HA	4:1D:174:ARG:HB2	1.96	0.48
7:1G:194:GLU:OE1	7:1G:194:GLU:N	2.37	0.48
8:1H:135:ALA:HB2	8:1H:201:THR:HB	1.96	0.48
8:1H:292:SER:OG	71:1I:201:PC1:O32	2.29	0.48
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.49	0.48
12:1L:193:SER:HB2	12:1L:206:ASN:HD21	1.78	0.48
15:1O:77:CYS:HB2	15:1O:96:LEU:HB2	1.96	0.48
17:1Q:93:VAL:CG1	17:1Q:97:GLU:OE1	2.62	0.48
22:1W:65:GLU:OE1	22:1W:66:MET:CE	2.61	0.48
47:3C:27:ILE:HB	47:3C:31:TRP:CD2	2.48	0.48
47:3C:111:GLU:O	47:3C:115:ILE:HG12	2.14	0.48
47:3C:230:LEU:N	48:3D:308:VAL:HG11	2.28	0.48
47:3C:257:THR:O	47:3C:258:PRO:C	2.57	0.48
49:3E:186:GLN:O	49:3E:190:VAL:HG23	2.14	0.48
45:3N:33:PRO:CD	45:3N:34:THR:H	2.24	0.48
45:3N:66:GLY:HA2	45:3N:72:GLY:CA	2.43	0.48
45:3N:87:ASN:HD21	45:3N:100:LYS:NZ	2.11	0.48
45:3N:92:ARG:CG	45:3N:167:VAL:HG22	2.43	0.48
45:3N:170:PRO:CD	45:3N:170:PRO:O	2.62	0.48
46:3O:332:SER:O	46:3O:333:ALA:C	2.57	0.48
48:3Q:21:LEU:HD21	48:3Q:191:ARG:HG2	1.96	0.48
61:4G:50:TYR:HA	62:4H:80:THR:HG23	1.94	0.48
5:5E:39:PRO:HB3	44:5s:66:PRO:HG2	1.95	0.48
13:5M:71:TRP:CG	71:5M:502:PC1:H2C2	2.48	0.48
69:5M:503:3PE:H2F1	71:5Y:201:PC1:H281	1.95	0.48
29:5d:64:TYR:CE2	75:5d:202:CDL:H312	2.49	0.48
33:5h:84:GLU:O	33:5h:88:GLU:HG2	2.14	0.48
34:5i:23:LYS:O	34:5i:26:GLU:HG2	2.13	0.48
37:5l:115:MET:HA	37:5l:118:VAL:HG22	1.95	0.48
46:6B:124:LEU:O	46:6B:125:ASN:C	2.56	0.48
47:6C:304:MET:HA	47:6C:307:LEU:HB2	1.96	0.48
48:6D:158:VAL:O	48:6D:171:ARG:N	2.47	0.48
48:6D:216:PHE:CZ	48:6D:273:LYS:HB2	2.49	0.48
53:6J:59:LYS:HB2	53:6J:59:LYS:HE2	1.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:153:LEU:O	45:6N:154:HIS:C	2.57	0.48
45:6N:304:CYS:SG	45:6N:307:PHE:HB3	2.54	0.48
45:6N:316:GLU:HG2	45:6N:317:THR:HG22	1.95	0.48
55:8A:40:GLU:HG3	55:8A:441:SER:HA	1.95	0.48
55:8A:361:SER:HB3	56:8B:84:LEU:HD13	1.95	0.48
64:8J:45:TYR:CE1	82:8J:101:PGV:H02	2.48	0.48
4:1D:404:LYS:HE2	4:1D:404:LYS:HB3	1.57	0.48
5:1E:51:LEU:HD13	5:1E:69:VAL:HG21	1.96	0.48
13:1M:430:PHE:HB2	13:1M:433:GLU:HG3	1.94	0.48
15:1O:23:LYS:HA	15:1O:167:HIS:ND1	2.29	0.48
15:1O:136:GLU:OE2	15:1O:140:ARG:NE	2.47	0.48
22:1W:27:GLU:O	22:1W:31:ARG:HG3	2.14	0.48
24:1Y:75:ILE:HG12	51:3T:56:TYR:CE2	2.46	0.48
47:3C:37:LEU:HD13	83:3C:502:HEM:C3B	2.49	0.48
47:3C:77:TRP:CH2	48:3D:290:ARG:HA	2.49	0.48
47:3C:345:HIS:HB3	47:3C:348:ILE:HB	1.96	0.48
48:3D:103:ARG:HA	48:3D:103:ARG:CZ	2.43	0.48
48:3D:228:GLY:HA3	52:3H:78:ASP:HA	1.96	0.48
46:3O:124:LEU:HD22	46:3O:223:PHE:HB3	1.96	0.48
46:3O:156:GLN:CD	46:3O:156:GLN:H	2.22	0.48
46:3O:192:HIS:O	46:3O:196:GLN:NE2	2.47	0.48
59:4E:19:PHE:O	59:4E:57:ARG:NH2	2.41	0.48
5:5E:27:ASN:HD21	5:5E:57:GLN:HB2	1.78	0.48
5:5E:51:LEU:HD13	5:5E:69:VAL:HG21	1.96	0.48
7:5G:366:THR:CB	7:5G:450:MET:HE3	2.44	0.48
8:5H:149:ILE:HG12	8:5H:181:LEU:HD22	1.96	0.48
9:5I:135:PRO:HG3	9:5I:164:GLU:CD	2.39	0.48
12:5L:147:VAL:HG13	12:5L:252:MET:HG3	1.96	0.48
15:5O:308:TYR:CE1	29:5d:51:ARG:HD3	2.49	0.48
20:5T:64:ASP:CG	22:5W:37:ARG:HH12	2.22	0.48
29:5d:11:LEU:HD21	30:5e:3:PHE:HB3	1.95	0.48
46:6B:327:ILE:CG2	49:6I:55:LEU:HD11	2.44	0.48
47:6C:75:TYR:CE2	49:6E:135:GLN:HG2	2.46	0.48
48:6D:210:GLY:O	48:6D:211:GLY:C	2.56	0.48
49:6E:186:GLN:O	49:6E:190:VAL:HG23	2.14	0.48
52:6H:47:GLU:O	52:6H:51:GLN:HG2	2.13	0.48
45:6N:4:TYR:OH	46:6O:112:LEU:CG	2.61	0.48
45:6N:117:VAL:C	45:6N:120:CYS:SG	2.95	0.48
45:6N:148:VAL:CG1	45:6N:152:TYR:OH	2.62	0.48
49:6R:155:LYS:HE2	49:6R:271:VAL:HG23	1.96	0.48
55:8A:18:LEU:HB3	55:8A:102:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:70:VAL:O	55:8A:71:MET:C	2.56	0.48
4:1D:76:CYS:O	4:1D:403:ASP:OD1	2.32	0.47
7:1G:276:ARG:NH1	7:1G:680:ALA:O	2.46	0.47
7:1G:470:VAL:HG12	7:1G:490:MET:HE1	1.94	0.47
10:1J:10:SER:O	10:1J:14:VAL:HG23	2.14	0.47
12:1L:56:HIS:CE1	41:1p:27:ASN:HD21	2.32	0.47
12:1L:203:MET:HG2	41:1p:113:GLN:HB2	1.96	0.47
15:1O:304:TYR:O	29:1d:50:ARG:HB3	2.14	0.47
29:1d:17:GLU:HG3	29:1d:81:TYR:HE1	1.79	0.47
47:3C:70:CYS:O	47:3C:77:TRP:HB3	2.13	0.47
47:3C:72:ASP:O	47:3C:73:VAL:C	2.57	0.47
47:3C:107:TYR:HB3	47:3C:113:TRP:CD2	2.49	0.47
45:3N:85:HIS:HB2	45:3N:100:LYS:HB2	1.95	0.47
45:3N:188:GLN:O	45:3N:191:LYS:HG3	2.14	0.47
45:3N:397:SER:O	45:3N:400:ALA:HB3	2.14	0.47
46:3O:123:LEU:O	46:3O:127:THR:HG23	2.13	0.47
47:3P:8:HIS:O	47:3P:12:LYS:N	2.37	0.47
55:4A:197:LEU:HD12	82:4A:603:PGV:H301	1.96	0.47
4:5D:63:ARG:HB3	4:5D:79:HIS:HB2	1.95	0.47
71:5H:401:PC1:H151	25:5Z:140:PHE:CZ	2.49	0.47
20:5T:51:ILE:HG21	20:5T:67:ALA:HB1	1.96	0.47
41:5p:166:ARG:HA	41:5p:170:LYS:NZ	2.28	0.47
45:6A:59:VAL:O	45:6A:63:ALA:N	2.40	0.47
45:6A:364:ALA:O	45:6A:365:LEU:C	2.56	0.47
45:6N:346:CYS:HA	45:6N:411:CYS:HB2	1.96	0.47
46:6O:26:PHE:HZ	46:6O:386:ALA:HB2	1.78	0.47
46:6O:247:GLN:NE2	46:6O:429:ASN:HA	2.29	0.47
46:6O:347:ILE:HA	46:6O:351:ASN:HB2	1.95	0.47
55:8A:164:PHE:O	55:8A:165:ILE:C	2.57	0.47
55:8A:513:LEU:N	60:8F:36:PRO:O	2.38	0.47
82:8G:101:PGV:H02	82:8G:101:PGV:H21	1.61	0.47
4:1D:258:VAL:HG12	4:1D:296:ARG:HG2	1.96	0.47
71:1H:401:PC1:H151	25:1Z:140:PHE:CZ	2.49	0.47
12:1L:521:LYS:HB3	12:1L:525:MET:CE	2.44	0.47
15:1O:176:VAL:O	15:1O:180:GLN:HG2	2.14	0.47
24:1Y:71:LEU:HD21	51:3T:57:LEU:HD11	1.94	0.47
37:1l:136:ASN:HA	37:1l:153:VAL:HB	1.94	0.47
39:1n:55:ASP:H	39:1n:58:LYS:CE	2.27	0.47
47:3C:5:ARG:HD2	47:3C:19:ILE:HG21	1.94	0.47
47:3C:153:ILE:HD12	47:3C:156:ILE:CG2	2.44	0.47
45:3N:60:GLU:CD	45:3N:90:SER:CB	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:106:LEU:O	45:3N:107:PRO:C	2.57	0.47
46:3O:113:ARG:O	46:3O:116:ILE:HB	2.15	0.47
46:3O:126:VAL:O	46:3O:127:THR:C	2.56	0.47
49:3R:219:HIS:CD2	49:3R:239:HIS:HE1	2.25	0.47
55:4A:71:MET:HB2	55:4A:72:PRO:HD3	1.97	0.47
57:4C:204:HIS:CE1	57:4C:249:TRP:HB2	2.49	0.47
62:4H:28:ASN:O	62:4H:32:ASN:ND2	2.47	0.47
66:4L:21:LEU:HA	66:4L:24:MET:HG2	1.96	0.47
2:5B:46:TRP:HB3	2:5B:77:ARG:HG2	1.96	0.47
6:5F:12:PHE:CE1	6:5F:247:ARG:HG3	2.49	0.47
10:5J:106:TYR:O	10:5J:110:GLU:HB2	2.13	0.47
12:5L:3:PRO:HG2	12:5L:53:MET:HE1	1.96	0.47
14:5N:256:PRO:HG2	69:5N:902:3PE:H2G2	1.96	0.47
33:5h:14:SER:OG	39:5n:110:GLU:OE1	2.30	0.47
36:5k:24:GLU:HA	36:5k:29:GLU:OE1	2.14	0.47
48:6D:102:HIS:C	48:6D:107:SER:HB3	2.39	0.47
45:6N:49:ASN:N	45:6N:52:ASN:HB2	2.25	0.47
45:6N:69:ASN:CG	45:6N:119:ASN:HD22	2.22	0.47
45:6N:115:ASP:O	45:6N:119:ASN:N	2.47	0.47
45:6N:307:PHE:HB2	45:6N:324:PHE:HB3	1.96	0.47
46:6O:181:TYR:CE2	46:6O:182:ARG:HD3	2.49	0.47
47:6P:33:PHE:HA	47:6P:36:LEU:HB2	1.94	0.47
55:8A:110:LEU:HA	55:8A:113:LEU:HD12	1.96	0.47
55:8A:193:VAL:HG11	82:8A:603:PGV:H252	1.97	0.47
55:8A:256:HIS:O	55:8A:257:ILE:C	2.58	0.47
55:8A:277:MET:HE2	55:8A:277:MET:HB2	1.77	0.47
75:8A:610:CDL:H371	75:8A:610:CDL:H251	1.96	0.47
58:8D:141:ASP:O	58:8D:143:ASN:N	2.47	0.47
2:1B:94:ASN:C	2:1B:97:ALA:HB2	2.39	0.47
9:1I:7:MET:HE2	9:1I:7:MET:HA	1.96	0.47
12:1L:544:MET:HE3	13:1M:271:MET:HE1	1.95	0.47
13:1M:449:LEU:HB3	71:1M:502:PC1:H32	1.97	0.47
29:1d:46:ASN:ND2	29:1d:51:ARG:HH11	2.12	0.47
45:3A:362:ARG:HE	45:3A:396:GLU:CD	2.23	0.47
49:3E:178:HIS:HA	49:3E:210:TRP:CD1	2.49	0.47
45:3N:32:GLN:NE2	46:3O:373:GLU:HA	2.30	0.47
45:3N:144:SER:O	45:3N:145:MET:C	2.57	0.47
49:3R:155:LYS:HE2	49:3R:271:VAL:HG23	1.96	0.47
57:4C:128:GLU:HG3	57:4C:129:VAL:H	1.79	0.47
71:5B:202:PC1:H351	71:5B:202:PC1:H261	1.95	0.47
4:5D:64:LEU:HD11	4:5D:418:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5E:109:MET:HE1	6:5F:346:ALA:HA	1.94	0.47
5:5E:174:ASP:OD1	5:5E:175:GLU:N	2.47	0.47
7:5G:256:GLU:O	7:5G:394:ARG:NH2	2.47	0.47
9:5I:7:MET:HA	9:5I:7:MET:HE2	1.96	0.47
10:5J:10:SER:O	10:5J:14:VAL:HG23	2.14	0.47
12:5L:488:MET:SD	12:5L:492:ILE:HD11	2.54	0.47
15:5O:176:VAL:O	15:5O:180:GLN:HG2	2.14	0.47
40:5o:16:PRO:HB3	40:5o:104:GLU:HG2	1.96	0.47
40:5o:46:ASN:HA	40:5o:55:ARG:HH22	1.79	0.47
45:6A:3:THR:O	45:6A:5:ALA:N	2.47	0.47
47:6C:85:ASN:HB2	47:6C:243:VAL:HG23	1.96	0.47
47:6C:137:GLN:CA	47:6C:259:ALA:HA	2.27	0.47
46:6O:203:ARG:HD3	46:6O:230:LEU:HD12	1.95	0.47
47:6P:126:THR:HG21	83:6P:501:HEM:HBB2	1.95	0.47
55:8A:33:LEU:HD23	55:8A:57:ILE:HG23	1.96	0.47
55:8A:199:LEU:HD12	55:8A:200:PRO:HD3	1.95	0.47
55:8A:220:PHE:HE1	55:8A:230:LEU:HG	1.79	0.47
55:8A:300:ASP:HB3	68:8N:65:PHE:CE2	2.49	0.47
2:1B:46:TRP:O	2:1B:84:ASP:N	2.48	0.47
12:1L:544:MET:HE2	12:1L:549:ALA:HB2	1.97	0.47
15:1O:308:TYR:CE1	29:1d:51:ARG:HD3	2.49	0.47
20:1T:48:VAL:HG13	22:1W:37:ARG:HE	1.79	0.47
20:1T:64:ASP:CG	22:1W:37:ARG:HH12	2.22	0.47
33:1h:84:GLU:O	33:1h:88:GLU:HG2	2.14	0.47
38:1m:13:LEU:HD21	38:1m:18:ASP:HA	1.96	0.47
38:1m:53:PRO:HB3	39:1n:128:ARG:HD3	1.97	0.47
47:3C:233:LEU:HB3	48:3D:301:MET:SD	2.55	0.47
45:3N:41:ILE:CD1	45:3N:195:MET:CE	2.88	0.47
45:3N:319:LEU:O	45:3N:321:GLY:N	2.47	0.47
46:3O:80:ALA:HB1	46:3O:84:LYS:HD3	1.97	0.47
46:3O:169:ARG:HD2	46:3O:238:LYS:CB	2.45	0.47
55:4A:110:LEU:HD22	82:4A:601:PGV:H181	1.96	0.47
55:4A:244:TYR:O	55:4A:245:ILE:C	2.57	0.47
57:4C:179:SER:OG	82:4G:101:PGV:H101	2.13	0.47
75:4C:308:CDL:H512	75:4C:308:CDL:HB4	1.45	0.47
1:5A:55:PHE:CB	10:5J:74:MET:CE	2.93	0.47
2:5B:150:PRO:HD3	4:5D:190:HIS:CD2	2.49	0.47
8:5H:87:VAL:HG22	8:5H:88:PRO:HD3	1.96	0.47
8:5H:196:ALA:CB	8:5H:197:PRO:HD3	2.43	0.47
10:5J:17:PHE:HA	10:5J:20:PHE:CE2	2.49	0.47
12:5L:103:PHE:HB2	12:5L:341:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5L:271:LYS:HA	12:5L:271:LYS:HD3	1.62	0.47
12:5L:488:MET:O	12:5L:492:ILE:HG13	2.14	0.47
33:5h:120:GLY:O	33:5h:124:GLN:NE2	2.47	0.47
35:5j:41:TRP:CZ2	36:5k:81:VAL:HG13	2.49	0.47
39:5n:117:TYR:HA	39:5n:120:LYS:HZ1	1.78	0.47
47:6C:346:PRO:HB2	47:6C:350:ILE:HG13	1.95	0.47
45:6N:204:GLU:O	45:6N:205:HIS:C	2.57	0.47
45:6N:333:ASP:N	45:6N:333:ASP:OD2	2.48	0.47
46:6O:50:PHE:CD1	46:6O:207:ILE:HG13	2.48	0.47
47:6P:24:PRO:HB2	47:6P:27:ILE:HG23	1.97	0.47
55:8A:318:VAL:HG13	56:8B:65:TRP:HE1	1.79	0.47
55:8A:374:VAL:HA	55:8A:377:PHE:CG	2.50	0.47
82:8A:601:PGV:H011	82:8A:601:PGV:H201	1.45	0.47
56:8B:100:MET:CE	56:8B:155:SER:HB3	2.44	0.47
57:8C:191:GLY:O	57:8C:195:SER:OG	2.24	0.47
5:1E:200:THR:HG21	6:1F:283:HIS:HA	1.97	0.47
7:1G:537:LEU:HD12	7:1G:543:ILE:HD11	1.96	0.47
71:1I:201:PC1:H3G1	25:1Z:40:ILE:HD12	1.97	0.47
10:1J:138:GLU:HG3	30:1e:28:ILE:HG21	1.95	0.47
12:1L:103:PHE:HB2	12:1L:341:MET:HE3	1.96	0.47
12:1L:144:TRP:CE2	12:1L:223:LYS:HG3	2.49	0.47
69:1L:701:3PE:H321	69:1L:701:3PE:H32	1.32	0.47
29:1d:64:TYR:CE2	75:1d:202:CDL:H312	2.49	0.47
31:1f:1:MET:SD	31:1f:2:ASN:HB2	2.54	0.47
33:1h:120:GLY:O	33:1h:124:GLN:NE2	2.47	0.47
75:1i:201:CDL:H511	75:1i:201:CDL:HB4	1.33	0.47
40:1o:46:ASN:HA	40:1o:55:ARG:HH22	1.79	0.47
40:1o:112:LYS:O	40:1o:116:GLN:HG3	2.13	0.47
82:1p:201:PGV:H171	82:1p:201:PGV:H141	1.72	0.47
45:3N:58:PHE:CE1	45:3N:134:ILE:HD13	2.50	0.47
45:3N:260:PRO:O	45:3N:313:CYS:SG	2.71	0.47
45:3N:281:ASP:HB3	45:3N:284:TYR:CD1	2.50	0.47
45:3N:397:SER:O	45:3N:401:GLU:HG2	2.13	0.47
46:3O:263:ALA:HB1	46:3O:318:ASP:HA	1.96	0.47
47:3P:126:THR:HG21	83:3P:501:HEM:HBB2	1.95	0.47
47:3P:129:MET:HE1	47:3P:181:PHE:HB3	1.96	0.47
47:3P:186:PRO:HA	47:3P:189:ILE:HD12	1.97	0.47
55:4A:34:SER:HB3	55:4A:61:HIS:NE2	2.29	0.47
55:4A:251:PHE:HB3	55:4A:319:LYS:HE2	1.97	0.47
55:4A:270:TYR:O	55:4A:274:VAL:HG13	2.14	0.47
56:4B:109:GLU:HA	56:4B:116:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:4E:67:ILE:HA	59:4E:70:VAL:HG12	1.97	0.47
62:4H:4:ILE:HD11	62:4H:55:TRP:HB2	1.97	0.47
4:5D:112:MET:HA	4:5D:115:GLU:HG2	1.96	0.47
7:5G:9:ILE:HB	7:5G:75:LYS:HG2	1.96	0.47
7:5G:285:ARG:NH2	7:5G:555:PRO:O	2.48	0.47
7:5G:514:ILE:HG23	7:5G:519:PRO:HD3	1.97	0.47
7:5G:601:ARG:NH2	7:5G:614:ASP:OD2	2.47	0.47
13:5M:12:LEU:HB2	13:5M:13:PRO:HD3	1.97	0.47
17:5Q:60:ASP:OD1	17:5Q:60:ASP:N	2.48	0.47
20:5T:24:LYS:HD3	20:5T:24:LYS:HA	1.66	0.47
28:5c:38:ASP:OD2	29:5d:77:LYS:NZ	2.33	0.47
29:5d:53:VAL:H	69:5d:201:3PE:H111	1.79	0.47
47:6C:12:LYS:O	47:6C:13:ILE:C	2.58	0.47
47:6C:252:ASP:HB3	47:6C:255:ASN:HB3	1.96	0.47
48:6D:104:GLY:CA	48:6D:107:SER:HB2	2.45	0.47
48:6D:110:ASP:HA	53:6J:51:LYS:HB3	1.96	0.47
48:6D:118:PHE:HD2	48:6D:144:TYR:HE2	1.61	0.47
48:6D:213:ASP:O	48:6D:214:TYR:C	2.56	0.47
48:6D:321:SER:HB2	49:6E:88:PHE:HE1	1.77	0.47
49:6E:271:VAL:HG23	49:6E:274:GLY:H	1.79	0.47
50:6F:116:ARG:HG2	46:6O:83:PHE:CE2	2.49	0.47
45:6N:161:THR:HB	45:6N:162:PRO:HD3	1.97	0.47
45:6N:364:ALA:O	45:6N:365:LEU:C	2.57	0.47
49:6R:219:HIS:CG	49:6R:239:HIS:CE1	3.03	0.47
55:8A:276:ALA:O	55:8A:279:SER:HB2	2.15	0.47
55:8A:332:ILE:HG13	56:8B:46:LEU:HA	1.97	0.47
5:1E:174:ASP:OD1	5:1E:175:GLU:N	2.47	0.47
6:1F:261:HIS:CD2	6:1F:338:ASP:H	2.33	0.47
71:1J:201:PC1:H252	71:1J:201:PC1:H222	1.45	0.47
12:1L:488:MET:SD	12:1L:492:ILE:HD11	2.54	0.47
12:1L:573:MET:SD	12:1L:576:MET:HE3	2.53	0.47
13:1M:131:ILE:HD12	14:1N:302:LEU:HD21	1.97	0.47
36:1k:24:GLU:HA	36:1k:29:GLU:OE1	2.14	0.47
37:1l:55:GLN:NE2	37:1l:69:LEU:O	2.33	0.47
45:3A:146:ARG:HG3	45:3A:323:HIS:CE1	2.49	0.47
46:3B:49:LEU:HD23	46:3B:127:THR:HG21	1.97	0.47
46:3B:181:TYR:CZ	46:3B:182:ARG:HG2	2.50	0.47
47:3C:376:LEU:HB2	50:3F:32:TYR:CG	2.49	0.47
49:3E:271:VAL:HG23	49:3E:274:GLY:H	1.79	0.47
51:3G:74:LYS:HD2	51:3G:75:ASN:H	1.79	0.47
45:3N:158:PHE:HB3	45:3N:161:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:158:PHE:HZ	45:3N:314:TYR:HE2	1.62	0.47
45:3N:430:GLN:O	45:3N:431:LEU:C	2.57	0.47
46:3O:77:THR:HB	46:3O:129:ALA:O	2.14	0.47
52:3U:50:THR:OG1	52:3U:51:GLU:N	2.48	0.47
60:4F:95:GLN:HG3	60:4F:96:LEU:H	1.78	0.47
64:4J:38:LEU:HA	82:4J:101:PGV:H281	1.96	0.47
2:5B:30:VAL:HG13	2:5B:173:LEU:HB3	1.96	0.47
4:5D:76:CYS:O	4:5D:403:ASP:OD1	2.32	0.47
7:5G:191:PHE:CE2	7:5G:199:ILE:HD12	2.50	0.47
8:5H:85:MET:CE	8:5H:233:MET:HE2	2.44	0.47
12:5L:203:MET:HG2	41:5p:113:GLN:HB2	1.96	0.47
13:5M:243:MET:HA	13:5M:246:ILE:HG22	1.96	0.47
14:5N:109:SER:C	14:5N:111:PHE:N	2.73	0.47
14:5N:213:LEU:HD21	75:5N:903:CDL:H191	1.96	0.47
15:5O:304:TYR:O	29:5d:50:ARG:HB3	2.14	0.47
22:5W:35:LEU:HD21	22:5W:86:GLY:HA3	1.97	0.47
31:5f:1:MET:SD	31:5f:2:ASN:HB2	2.54	0.47
45:6A:142:ASP:HA	49:6E:80:HIS:HD1	1.78	0.47
45:6A:235:ARG:HG2	45:6A:237:THR:HG23	1.95	0.47
46:6B:314:ALA:HB3	46:6B:321:LEU:CB	2.43	0.47
47:6C:67:THR:HB	47:6C:71:ARG:HD3	1.97	0.47
47:6C:166:GLY:HA3	47:6C:173:ALA:HB1	1.96	0.47
47:6C:174:THR:O	47:6C:175:LEU:C	2.57	0.47
47:6C:279:ALA:HB2	47:6C:339:GLY:N	2.30	0.47
47:6C:376:LEU:HB2	50:6F:32:TYR:CG	2.50	0.47
49:6E:205:VAL:HG22	49:6E:211:VAL:HG23	1.97	0.47
52:6H:65:CYS:HA	52:6H:68:ARG:HE	1.80	0.47
45:6N:86:LEU:CD2	45:6N:99:ILE:HD11	2.43	0.47
45:6N:110:VAL:HG13	45:6N:216:PHE:HE2	1.77	0.47
45:6N:156:THR:HG22	45:6N:241:ILE:HG13	1.95	0.47
45:6N:159:GLN:HG2	49:6R:85:VAL:HG21	1.97	0.47
46:6O:63:LEU:HB3	46:6O:182:ARG:HG3	1.96	0.47
55:8A:209:LEU:O	55:8A:212:ASP:HB2	2.15	0.47
55:8A:217:THR:HB	57:8C:195:SER:HB3	1.97	0.47
55:8A:316:THR:HG21	85:8A:606:HEA:H14	1.95	0.47
55:8A:386:VAL:HG12	55:8A:387:PHE:N	2.29	0.47
82:8A:602:PGV:H301	82:8C:305:PGV:H312	1.96	0.47
61:8G:36:TRP:CZ3	82:8G:101:PGV:H032	2.50	0.47
82:8G:101:PGV:H42	82:8G:101:PGV:H72	1.45	0.47
3:1C:104:ARG:NH2	4:1D:373:GLU:OE2	2.43	0.47
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:39:PRO:HB3	44:1s:66:PRO:HG2	1.95	0.47
6:1F:25:LEU:HD21	6:1F:267:THR:HG22	1.96	0.47
7:1G:9:ILE:HB	7:1G:75:LYS:HG2	1.96	0.47
7:1G:255:HIS:CE1	7:1G:257:ASP:HB2	2.50	0.47
7:1G:285:ARG:NH2	7:1G:555:PRO:O	2.48	0.47
12:1L:63:ILE:HG23	34:1i:96:VAL:HG22	1.96	0.47
12:1L:121:LEU:HD22	12:1L:246:LEU:HD23	1.97	0.47
13:1M:220:HIS:O	13:1M:228:SER:OG	2.31	0.47
13:1M:243:MET:HA	13:1M:246:ILE:HG22	1.95	0.47
17:1Q:25:VAL:HB	17:1Q:30:ILE:CD1	2.43	0.47
23:1X:17:VAL:HG23	23:1X:63:ASN:HD22	1.80	0.47
29:1d:61:GLN:O	29:1d:65:VAL:HG13	2.14	0.47
37:1l:136:ASN:HD22	37:1l:153:VAL:H	1.63	0.47
46:3B:24:LEU:HD23	46:3B:38:LEU:HB2	1.97	0.47
47:3C:321:SER:HA	47:3C:324:LEU:HD12	1.97	0.47
47:3C:337:TRP:CG	51:3G:61:TYR:CE2	3.03	0.47
48:3D:121:TYR:CD1	48:3D:125:CYS:HB2	2.49	0.47
49:3E:254:ALA:HB2	72:3E:301:FES:S1	2.55	0.47
45:3N:30:SER:OG	45:3N:201:GLY:C	2.57	0.47
45:3N:76:GLU:OE2	46:3O:289:SER:CB	2.63	0.47
45:3N:310:PHE:CD2	45:3N:321:GLY:HA3	2.49	0.47
45:3N:311:ASN:CA	45:3N:320:LEU:HA	2.39	0.47
45:3N:369:LEU:O	45:3N:375:VAL:HG23	2.13	0.47
46:3O:98:VAL:HA	46:3O:107:TYR:HA	1.97	0.47
46:3O:129:ALA:N	46:3O:130:PRO:HD3	2.29	0.47
46:3O:384:SER:O	46:3O:388:VAL:HG23	2.15	0.47
49:3R:179:ARG:HE	49:3R:184:ILE:HG12	1.78	0.47
82:4A:601:PGV:H302	82:4L:101:PGV:H42	1.97	0.47
82:4A:603:PGV:H31	75:4C:308:CDL:H442	1.97	0.47
58:4D:89:ILE:HG22	65:4K:29:TRP:NE1	2.30	0.47
60:4F:20:VAL:HG12	60:4F:31:TYR:CD2	2.50	0.47
4:5D:233:ARG:NH2	9:5I:23:GLN:O	2.48	0.47
6:5F:261:HIS:CD2	6:5F:338:ASP:H	2.33	0.47
8:5H:70:MET:HA	8:5H:73:ILE:HB	1.96	0.47
9:5I:150:ASN:OD1	42:5q:129:THR:HG23	2.15	0.47
12:5L:144:TRP:CZ2	12:5L:223:LYS:HG3	2.50	0.47
12:5L:144:TRP:CE2	12:5L:223:LYS:HG3	2.49	0.47
12:5L:159:HIS:HB2	13:5M:416:ARG:HB3	1.97	0.47
12:5L:220:ALA:HB2	12:5L:260:LEU:HD13	1.95	0.47
13:5M:7:PRO:HB3	31:5f:16:VAL:HG13	1.95	0.47
13:5M:131:ILE:HD12	14:5N:302:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5M:449:LEU:HB3	71:5M:502:PC1:H32	1.97	0.47
15:5O:22:SER:O	15:5O:22:SER:OG	2.31	0.47
15:5O:77:CYS:HB2	15:5O:96:LEU:HB2	1.96	0.47
17:5Q:93:VAL:CG1	17:5Q:97:GLU:OE1	2.61	0.47
21:5V:4:LEU:HD23	21:5V:4:LEU:H	1.80	0.47
22:5W:27:GLU:O	22:5W:31:ARG:HG3	2.14	0.47
23:5X:102:GLN:HA	23:5X:105:LYS:HE3	1.96	0.47
30:5e:53:LYS:HE2	30:5e:53:LYS:HB3	1.71	0.47
36:5k:52:TYR:OH	39:5n:33:ARG:HB2	2.15	0.47
45:6A:281:ASP:HB3	49:6I:39:GLU:OE2	2.15	0.47
45:6A:438:ARG:HD2	45:6A:438:ARG:HA	1.53	0.47
47:6C:41:LEU:O	47:6C:42:ILE:C	2.58	0.47
47:6C:50:PHE:CG	49:6E:136:PHE:HD2	2.32	0.47
47:6C:258:PRO:O	47:6C:260:ASN:N	2.47	0.47
47:6C:274:PHE:O	47:6C:275:LEU:C	2.58	0.47
48:6D:150:LYS:O	48:6D:151:ALA:C	2.56	0.47
45:6N:162:PRO:HA	45:6N:165:GLN:OE1	2.14	0.47
45:6N:394:GLU:HG2	45:6N:398:ARG:HE	1.79	0.47
46:6O:56:ARG:H	46:6O:56:ARG:HG3	1.17	0.47
46:6O:81:SER:O	46:6O:84:LYS:HB3	2.15	0.47
47:6P:246:SER:HB2	47:6P:249:LEU:HB2	1.95	0.47
55:8A:100:MET:HE1	57:8C:21:ALA:HA	1.96	0.47
55:8A:381:LEU:HB3	55:8A:382:SER:H	1.58	0.47
55:8A:462:LEU:HD13	66:8L:33:PHE:CZ	2.49	0.47
55:8A:510:TYR:CE1	60:8F:47:ASN:HB3	2.48	0.47
82:8A:603:PGV:H11	82:8A:603:PGV:H61	1.96	0.47
82:8K:101:PGV:H342	82:8K:101:PGV:H311	1.77	0.47
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.15	0.47
9:1I:95:GLU:HB2	9:1I:108:ARG:HB3	1.97	0.47
12:1L:147:VAL:HG13	12:1L:252:MET:HG3	1.96	0.47
12:1L:338:MET:HE1	12:1L:372:ALA:O	2.14	0.47
13:1M:118:PHE:O	13:1M:122:PHE:HB3	2.14	0.47
13:1M:126:LEU:HD21	13:1M:153:THR:HG21	1.97	0.47
14:1N:213:LEU:HD21	75:1N:903:CDL:H191	1.96	0.47
82:1p:201:PGV:H301	82:1p:201:PGV:H271	1.62	0.47
44:1s:71:GLN:OE1	44:1s:71:GLN:HA	2.15	0.47
45:3N:62:LEU:CD2	45:3N:65:LYS:HD3	2.36	0.47
45:3N:130:GLU:O	45:3N:131:ARG:C	2.56	0.47
45:3N:369:LEU:HD12	45:3N:392:LEU:HD11	1.97	0.47
46:3O:128:ALA:O	46:3O:129:ALA:C	2.57	0.47
46:3O:313:ASN:HA	46:3O:322:PHE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:382:VAL:HG22	46:3O:392:TYR:CD1	2.50	0.47
55:4A:261:TYR:O	55:4A:338:MET:HE2	2.14	0.47
3:5C:11:ILE:HD11	43:5r:56:ARG:HA	1.97	0.47
4:5D:94:LYS:HG3	4:5D:102:TYR:HE2	1.80	0.47
11:5K:73:LEU:HD21	14:5N:41:ILE:HG13	1.97	0.47
12:5L:267:MET:HE3	12:5L:267:MET:HB2	1.86	0.47
17:5Q:10:LEU:HD13	22:5W:16:SER:HB3	1.96	0.47
45:6A:77:LYS:HD3	45:6A:77:LYS:HA	1.52	0.47
45:6A:438:ARG:HA	45:6A:441:MET:HG2	1.96	0.47
46:6B:295:LEU:HB2	46:6B:309:VAL:HG11	1.97	0.47
48:6D:142:VAL:HG11	48:6D:281:TRP:CZ2	2.50	0.47
48:6D:159:GLN:CA	48:6D:170:MET:HA	2.44	0.47
49:6E:178:HIS:HA	49:6E:210:TRP:CD1	2.49	0.47
49:6E:254:ALA:HB2	72:6E:301:FES:S1	2.55	0.47
52:6H:65:CYS:SG	52:6H:78:ASP:O	2.72	0.47
53:6J:30:LEU:HD13	54:6Y:34:TRP:CD1	2.48	0.47
45:6N:50:GLU:O	45:6N:51:LYS:C	2.58	0.47
45:6N:64:PHE:CZ	45:6N:88:ALA:HB3	2.30	0.47
45:6N:303:LEU:HD11	45:6N:333:ASP:HB2	1.97	0.47
45:6N:445:ARG:O	45:6N:446:PHE:C	2.57	0.47
52:6U:50:THR:OG1	52:6U:51:GLU:N	2.48	0.47
55:8A:510:TYR:CE2	60:8F:49:VAL:HA	2.49	0.47
57:8C:204:HIS:CE1	57:8C:249:TRP:HB2	2.49	0.47
66:8L:21:LEU:HA	66:8L:24:MET:HG2	1.96	0.47
2:1B:97:ALA:C	2:1B:99:ALA:N	2.63	0.47
2:1B:150:PRO:HD3	4:1D:190:HIS:CD2	2.49	0.47
10:1J:69:GLY:HA2	10:1J:72:THR:HG22	1.97	0.47
12:1L:3:PRO:HG2	12:1L:53:MET:HE1	1.96	0.47
13:1M:105:PHE:CE2	69:1N:902:3PE:H3I1	2.50	0.47
15:1O:48:LEU:HD12	15:1O:123:VAL:HG13	1.97	0.47
22:1W:35:LEU:HD21	22:1W:86:GLY:HA3	1.97	0.47
30:1e:36:GLU:HG3	30:1e:62:PHE:CE2	2.50	0.47
34:1i:41:PRO:HA	34:1i:44:GLN:HB2	1.96	0.47
38:1m:43:LYS:HE2	38:1m:43:LYS:HB2	1.56	0.47
46:3B:247:GLN:NE2	46:3O:60:SER:OG	2.48	0.47
47:3C:357:LEU:O	47:3C:361:ILE:HG13	2.15	0.47
45:3N:64:PHE:CG	46:3O:285:VAL:HG11	2.50	0.47
45:3N:140:GLU:CG	49:3V:50:LEU:H	2.26	0.47
45:3N:204:GLU:HB2	45:3N:207:GLN:HG3	1.97	0.47
46:3O:89:ILE:HG21	46:3O:119:LEU:HD13	1.96	0.47
48:3Q:33:TYR:CD1	48:3Q:37:CYS:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:154:ILE:HD11	49:3R:270:LEU:HA	1.97	0.47
49:3R:183:GLU:O	49:3R:187:GLU:HG2	2.15	0.47
55:4A:217:THR:HB	57:4C:195:SER:HB3	1.96	0.47
56:4B:165:VAL:HG21	56:4B:211:LEU:HD11	1.97	0.47
64:4J:40:LEU:HA	64:4J:43:THR:HG22	1.97	0.47
6:5F:25:LEU:HD21	6:5F:267:THR:HG22	1.96	0.47
8:5H:317:GLN:OE1	10:5J:141:MET:CE	2.63	0.47
12:5L:338:MET:HE1	12:5L:372:ALA:O	2.14	0.47
12:5L:544:MET:HE3	13:5M:271:MET:HE1	1.95	0.47
17:5Q:69:LEU:HD11	42:5q:126:PRO:HG2	1.97	0.47
37:5l:97:SER:HB3	38:5m:6:LYS:HE3	1.96	0.47
38:5m:13:LEU:HD21	38:5m:18:ASP:HA	1.96	0.47
45:6A:161:THR:HG22	49:6E:99:SER:O	2.15	0.47
47:6C:54:HIS:HE1	49:6E:139:SER:HB2	1.78	0.47
47:6C:59:THR:O	47:6C:60:THR:C	2.56	0.47
47:6C:318:ARG:O	47:6C:322:GLN:NE2	2.48	0.47
45:6N:80:GLU:HB3	46:6O:292:THR:CG2	2.44	0.47
45:6N:119:ASN:O	45:6N:120:CYS:C	2.58	0.47
46:6O:262:ALA:N	46:6O:320:GLY:HA3	2.29	0.47
46:6O:283:PRO:HB3	49:6V:57:GLY:HA3	1.96	0.47
49:6R:230:ASP:OD1	49:6R:231:PHE:N	2.47	0.47
55:8A:77:GLY:O	55:8A:78:PHE:C	2.58	0.47
55:8A:311:ILE:O	55:8A:314:ILE:N	2.44	0.47
55:8A:507:GLU:HG2	60:8F:56:ARG:CZ	2.44	0.47
57:8C:128:GLU:HG3	57:8C:129:VAL:H	1.79	0.47
2:1B:104:TYR:O	2:1B:105:ASP:HB2	2.15	0.47
6:1F:111:ILE:HD13	6:1F:138:ILE:HD12	1.97	0.47
6:1F:287:VAL:HG11	6:1F:294:LEU:HD13	1.97	0.47
12:1L:386:LEU:HD13	35:1j:36:ILE:HD11	1.96	0.47
46:3B:25:GLU:HG2	46:3B:213:HIS:CG	2.49	0.47
45:3N:62:LEU:CA	45:3N:65:LYS:HD2	2.38	0.47
45:3N:353:GLU:C	45:3N:357:GLY:H	2.22	0.47
46:3O:214:PRO:O	46:3O:218:GLN:HG2	2.15	0.47
46:3O:316:TYR:H	46:3O:319:SER:C	2.21	0.47
49:3R:230:ASP:OD1	49:3R:231:PHE:N	2.47	0.47
54:3Y:48:ILE:HG22	54:3Y:51:LYS:HD3	1.96	0.47
89:4B:303:PSC:H02	89:4B:303:PSC:H21	1.56	0.47
75:4C:308:CDL:H251	75:4C:308:CDL:H371	1.96	0.47
7:5G:20:VAL:HG12	7:5G:32:LYS:HE2	1.97	0.47
9:5I:162:GLU:HA	9:5I:165:ILE:HG12	1.97	0.47
10:5J:69:GLY:HA2	10:5J:72:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:5J:201:3PE:H3B2	11:5K:14:ILE:HA	1.97	0.47
12:5L:346:ILE:HD11	12:5L:431:PHE:CZ	2.50	0.47
20:5T:10:ALA:O	20:5T:14:ARG:HG2	2.15	0.47
47:6C:4:ILE:H	47:6C:4:ILE:HG13	1.45	0.47
47:6C:137:GLN:HB2	47:6C:257:THR:OG1	2.14	0.47
45:6N:262:TRP:CD2	45:6N:385:THR:HB	2.50	0.47
45:6N:332:ASP:HB3	47:6P:6:LYS:HE2	1.97	0.47
46:6O:35:ILE:HG22	46:6O:213:HIS:HD2	1.79	0.47
46:6O:72:ALA:O	46:6O:73:SER:C	2.58	0.47
46:6O:118:ILE:H	46:6O:118:ILE:HG13	1.33	0.47
46:6O:172:LEU:H	46:6O:237:ALA:HB2	1.80	0.47
47:6P:186:PRO:HA	47:6P:189:ILE:HD12	1.97	0.47
49:6R:183:GLU:O	49:6R:187:GLU:HG2	2.15	0.47
53:6W:54:LYS:HB3	53:6W:54:LYS:HE3	1.78	0.47
54:6Y:5:PHE:HA	54:6Y:10:TYR:CZ	2.50	0.47
55:8A:55:ASN:O	55:8A:56:VAL:C	2.57	0.47
55:8A:320:VAL:HA	55:8A:323:TRP:CE3	2.50	0.47
55:8A:480:ARG:H	55:8A:480:ARG:HG3	1.44	0.47
55:8A:501:PRO:O	55:8A:502:TYR:C	2.57	0.47
56:8B:109:GLU:HA	56:8B:116:LEU:O	2.15	0.47
4:1D:64:LEU:HD11	4:1D:418:ILE:HD11	1.97	0.46
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.97	0.46
8:1H:85:MET:CE	8:1H:233:MET:HE2	2.44	0.46
10:1J:129:ASP:CB	30:1e:31:ARG:HH21	2.28	0.46
11:1K:73:LEU:HD21	14:1N:41:ILE:HG13	1.97	0.46
12:1L:159:HIS:HB2	13:1M:416:ARG:HB3	1.97	0.46
12:1L:601:LEU:HD12	12:1L:602:PHE:HD1	1.80	0.46
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.15	0.46
69:1Y:206:3PE:H321	69:1Y:206:3PE:H31	1.37	0.46
29:1d:53:VAL:H	69:1d:201:3PE:H111	1.79	0.46
29:1d:90:MET:HE3	29:1d:91:PHE:CE1	2.50	0.46
38:1m:22:TYR:CD2	39:1n:64:ARG:NE	2.83	0.46
45:3A:429:GLU:OE2	51:3G:9:LEU:N	2.48	0.46
46:3B:109:VAL:HG22	46:3B:123:LEU:HD22	1.97	0.46
49:3E:220:LEU:HA	47:3P:263:ASN:OD1	2.15	0.46
45:3N:35:CYS:HB2	45:3N:102:LEU:O	2.15	0.46
45:3N:280:TYR:HB3	45:3N:307:PHE:HD2	1.79	0.46
46:3O:199:PHE:HB3	46:3O:204:MET:HE3	1.96	0.46
46:3O:272:PHE:HZ	46:3O:416:LYS:HD3	1.80	0.46
54:3X:37:ASP:OD1	54:3X:51:LYS:NZ	2.32	0.46
55:4A:374:VAL:HA	55:4A:377:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:171:PHE:HA	4:5D:174:ARG:HB2	1.97	0.46
6:5F:111:ILE:HD13	6:5F:138:ILE:HD12	1.97	0.46
7:5G:255:HIS:CE1	7:5G:257:ASP:HB2	2.50	0.46
12:5L:521:LYS:HB3	12:5L:525:MET:CE	2.45	0.46
24:5Y:55:THR:O	24:5Y:59:THR:OG1	2.23	0.46
24:5Y:65:ILE:HD11	24:5Y:100:LEU:HB2	1.98	0.46
45:6A:70:ARG:O	45:6A:71:PRO:C	2.57	0.46
45:6A:418:GLN:H	45:6A:441:MET:HG3	1.78	0.46
46:6B:120:MET:HG2	46:6B:219:VAL:HG21	1.96	0.46
46:6B:295:LEU:O	46:6B:296:TYR:C	2.57	0.46
47:6C:77:TRP:HE1	48:6D:289:HIS:HE1	1.63	0.46
47:6C:221:HIS:HB3	47:6C:222:PRO:HD3	1.96	0.46
47:6C:326:TRP:CD1	51:6G:50:VAL:HG22	2.50	0.46
47:6C:378:LYS:HB3	50:6F:45:ARG:HH21	1.80	0.46
52:6H:97:LYS:C	52:6H:97:LYS:CD	2.88	0.46
46:6O:250:ASP:O	46:6O:252:LEU:N	2.48	0.46
55:8A:199:LEU:O	55:8A:200:PRO:C	2.56	0.46
56:8B:165:VAL:HG21	56:8B:211:LEU:HD11	1.97	0.46
58:8D:89:ILE:HG22	65:8K:29:TRP:NE1	2.30	0.46
67:8M:39:HIS:HA	67:8M:42:ARG:HG2	1.97	0.46
5:1E:187:ARG:HD3	5:1E:187:ARG:HA	1.59	0.46
7:1G:191:PHE:CE2	7:1G:199:ILE:HD12	2.50	0.46
7:1G:514:ILE:HG23	7:1G:519:PRO:HD3	1.97	0.46
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.80	0.46
71:1J:201:PC1:H153	71:1J:201:PC1:H111	1.67	0.46
12:1L:488:MET:O	12:1L:492:ILE:HG13	2.15	0.46
13:1M:343:ILE:O	13:1M:346:ARG:NH1	2.45	0.46
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.34	0.46
20:1T:10:ALA:O	20:1T:14:ARG:HG2	2.15	0.46
20:1T:51:ILE:HG21	20:1T:67:ALA:HB1	1.96	0.46
21:1V:4:LEU:HD23	21:1V:4:LEU:H	1.80	0.46
35:1j:37:LEU:HB3	36:1k:77:PHE:CG	2.49	0.46
46:3B:46:ARG:HD3	46:3B:379:LEU:HD22	1.97	0.46
47:3C:108:MET:HB2	47:3C:313:ARG:NH2	2.30	0.46
47:3C:270:PRO:HG3	47:3C:278:TYR:HB2	1.97	0.46
47:3C:315:MET:HG2	47:3C:321:SER:HB3	1.97	0.46
45:3N:69:ASN:HD22	45:3N:119:ASN:ND2	2.04	0.46
45:3N:396:GLU:O	45:3N:400:ALA:N	2.32	0.46
45:3N:442:PHE:CB	45:3N:446:PHE:C	2.86	0.46
46:3O:132:PHE:O	46:3O:188:PRO:HB3	2.15	0.46
46:3O:261:SER:H	46:3O:320:GLY:C	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:275:TRP:HE3	82:4A:603:PGV:H12	1.80	0.46
55:4A:305:PHE:CZ	82:4A:604:PGV:H21	2.50	0.46
56:4B:118:PHE:CD1	56:4B:226:MET:HE1	2.51	0.46
5:5E:187:ARG:HD3	5:5E:187:ARG:HA	1.59	0.46
7:5G:228:ILE:HG13	7:5G:581:GLN:HB3	1.97	0.46
11:5K:1:FME:SD	14:5N:79:LEU:HD21	2.55	0.46
14:5N:250:SER:O	14:5N:259:GLY:HA3	2.15	0.46
20:5U:36:PHE:HD1	20:5U:40:LEU:HD12	1.80	0.46
23:5X:171:MET:HG3	75:5X:201:CDL:HA4	1.97	0.46
29:5d:46:ASN:ND2	29:5d:51:ARG:HH11	2.12	0.46
71:5m:201:PC1:H11	71:5m:201:PC1:H222	1.97	0.46
45:6A:41:ILE:O	45:6A:95:THR:N	2.48	0.46
48:6D:208:ARG:HD3	48:6D:208:ARG:HA	1.67	0.46
49:6E:155:LYS:NZ	49:6E:176:VAL:HG11	2.18	0.46
49:6E:199:GLN:O	49:6E:248:ARG:HD3	2.15	0.46
45:6N:19:LEU:HD22	45:6N:213:GLN:HG2	1.98	0.46
45:6N:65:LYS:CE	45:6N:130:GLU:CD	2.87	0.46
46:6O:89:ILE:HG12	46:6O:119:LEU:HG	1.97	0.46
46:6O:140:LEU:O	46:6O:141:GLN:C	2.58	0.46
46:6O:232:LEU:HD22	46:6O:232:LEU:HA	1.77	0.46
48:6Q:195:GLU:OE2	48:6Q:201:ARG:NE	2.46	0.46
49:6R:187:GLU:CD	49:6R:244:ASP:HB2	2.40	0.46
55:8A:334:TRP:HA	55:8A:334:TRP:CE3	2.50	0.46
57:8C:117:PRO:HG2	57:8C:123:PRO:HG3	1.98	0.46
82:8C:303:PGV:H262	82:8C:303:PGV:H231	1.57	0.46
1:1A:33:LYS:NZ	2:1B:109:GLU:HG2	2.30	0.46
1:1A:64:LEU:HD13	10:1J:165:VAL:HG22	1.96	0.46
5:1E:14:GLU:O	5:1E:19:THR:OG1	2.25	0.46
7:1G:366:THR:CB	7:1G:450:MET:HE3	2.44	0.46
8:1H:317:GLN:OE1	10:1J:141:MET:CE	2.63	0.46
69:1J:202:3PE:H2C2	12:1L:592:LEU:HD21	1.97	0.46
14:1N:109:SER:C	14:1N:111:PHE:N	2.73	0.46
16:1P:133:SER:O	16:1P:168:PRO:HD2	2.15	0.46
23:1X:102:GLN:HA	23:1X:105:LYS:HE3	1.96	0.46
36:1k:52:TYR:OH	39:1n:33:ARG:HB2	2.15	0.46
45:3N:64:PHE:CG	46:3O:285:VAL:CG1	2.98	0.46
45:3N:118:GLN:NE2	45:3N:219:LEU:CG	2.77	0.46
45:3N:289:HIS:CE1	46:3O:82:SER:HB3	2.51	0.46
55:4A:487:LEU:O	55:4A:491:ASN:ND2	2.48	0.46
56:4B:98:LYS:HE3	56:4B:109:GLU:HB2	1.96	0.46
67:4M:16:ALA:O	67:4M:20:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5E:200:THR:HG21	6:5F:283:HIS:HA	1.97	0.46
8:5H:88:PRO:HG2	8:5H:105:MET:HE2	1.97	0.46
11:5K:34:GLU:OE1	11:5K:37:MET:HG2	2.15	0.46
12:5L:63:ILE:HG23	34:5i:96:VAL:HG22	1.96	0.46
12:5L:544:MET:HE2	12:5L:549:ALA:HB2	1.96	0.46
20:5U:8:LEU:N	20:5U:88:GLU:OE2	2.43	0.46
30:5e:36:GLU:HG3	30:5e:62:PHE:CE2	2.50	0.46
45:6A:31:SER:O	45:6A:32:GLN:C	2.58	0.46
45:6A:35:CYS:O	45:6A:36:THR:C	2.58	0.46
45:6A:271:GLN:HB3	45:6A:361:LEU:HD13	1.96	0.46
46:6B:394:GLN:O	46:6B:395:PRO:C	2.58	0.46
47:6C:36:LEU:HD21	47:6C:231:GLY:HA3	1.98	0.46
47:6C:220:PHE:O	47:6C:221:HIS:C	2.57	0.46
48:6D:150:LYS:HB2	48:6D:150:LYS:HE3	1.59	0.46
48:6D:325:ALA:HB2	51:6G:18:TYR:HE2	1.80	0.46
45:6N:25:VAL:HG22	45:6N:197:LEU:HD12	1.97	0.46
45:6N:270:LEU:HG	45:6N:414:TYR:CD2	2.50	0.46
46:6O:46:ARG:HA	46:6O:110:GLU:HA	1.97	0.46
55:8A:211:THR:O	55:8A:212:ASP:C	2.57	0.46
55:8A:217:THR:HB	57:8C:195:SER:CB	2.45	0.46
55:8A:373:VAL:O	55:8A:377:PHE:N	2.39	0.46
56:8B:98:LYS:HE3	56:8B:109:GLU:HB2	1.96	0.46
75:8D:201:CDL:H241	75:8D:201:CDL:H812	1.98	0.46
61:8G:39:SER:HB2	82:8G:101:PGV:H031	1.96	0.46
82:8K:101:PGV:H231	82:8K:101:PGV:H261	1.53	0.46
66:8L:17:ASN:HB3	66:8L:20:ARG:HB3	1.97	0.46
1:1A:7:LEU:HD13	71:1H:401:PC1:H362	1.97	0.46
3:1C:11:ILE:HD11	43:1r:56:ARG:HA	1.97	0.46
8:1H:70:MET:HA	8:1H:73:ILE:HB	1.96	0.46
8:1H:88:PRO:HG2	8:1H:105:MET:HE2	1.97	0.46
9:1I:162:GLU:HA	9:1I:165:ILE:HG12	1.97	0.46
69:1J:202:3PE:H3B2	11:1K:14:ILE:HA	1.97	0.46
12:1L:144:TRP:CZ2	12:1L:223:LYS:HG3	2.50	0.46
14:1N:256:PRO:HG2	69:1N:902:3PE:H2G2	1.96	0.46
15:1O:13:ARG:HG3	15:1O:16:ARG:HH21	1.81	0.46
16:1P:144:ARG:HG2	16:1P:147:ARG:HH12	1.81	0.46
17:1Q:60:ASP:OD1	17:1Q:60:ASP:N	2.48	0.46
37:1l:127:PRO:HD3	40:1o:3:HIS:CE1	2.51	0.46
40:1o:16:PRO:HB3	40:1o:104:GLU:HG2	1.96	0.46
40:1o:24:PHE:HZ	40:1o:111:LYS:HD2	1.81	0.46
49:3E:205:VAL:HG22	49:3E:211:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:62:LEU:HD11	45:3N:127:ILE:HG12	1.97	0.46
49:3R:187:GLU:CD	49:3R:244:ASP:HB2	2.41	0.46
52:3U:47:ARG:HG2	52:3U:47:ARG:HH11	1.81	0.46
2:5B:50:PHE:CD2	2:5B:86:MET:HE2	2.51	0.46
7:5G:11:VAL:HG11	7:5G:73:VAL:HB	1.98	0.46
12:5L:571:MET:HE2	12:5L:571:MET:HB3	1.78	0.46
24:5Y:103:ARG:HD2	24:5Y:103:ARG:HA	1.79	0.46
29:5d:90:MET:HE3	29:5d:91:PHE:CE1	2.51	0.46
37:5l:74:GLY:HA3	38:5m:42:LEU:HD22	1.97	0.46
38:5m:43:LYS:HE2	38:5m:43:LYS:HB2	1.56	0.46
44:5s:71:GLN:OE1	44:5s:71:GLN:HA	2.15	0.46
46:6B:250:ASP:O	46:6B:251:SER:C	2.57	0.46
47:6C:36:LEU:HD22	47:6C:235:MET:HB2	1.97	0.46
47:6C:124:MET:HE2	47:6C:124:MET:HB2	1.69	0.46
48:6D:296:LYS:O	48:6D:298:LEU:N	2.49	0.46
45:6N:67:THR:H	45:6N:75:LEU:CD1	2.23	0.46
55:8A:186:TRP:HH2	82:8A:603:PGV:H012	1.80	0.46
60:8F:20:VAL:HG12	60:8F:31:TYR:CD2	2.50	0.46
62:8H:39:CYS:O	62:8H:43:MET:HG2	2.16	0.46
64:8J:4:ARG:HG3	64:8J:4:ARG:HH11	1.80	0.46
1:1A:63:LEU:HD22	10:1J:67:VAL:HG11	1.95	0.46
69:1A:201:3PE:H3A1	69:1A:201:3PE:H3D2	1.40	0.46
7:1G:11:VAL:HG11	7:1G:73:VAL:HB	1.98	0.46
7:1G:20:VAL:HG12	7:1G:32:LYS:HE2	1.97	0.46
14:1N:320:THR:HG21	15:1O:265:ASN:HA	1.98	0.46
35:1j:54:PRO:HG3	40:1o:95:VAL:HG22	1.98	0.46
37:1l:97:SER:HB3	38:1m:6:LYS:HE3	1.96	0.46
82:1p:201:PGV:H62	82:1p:201:PGV:H32	1.49	0.46
47:3C:89:MET:HB2	47:3C:239:LEU:HD13	1.98	0.46
45:3N:259:GLY:HA3	45:3N:318:GLY:CA	2.45	0.46
46:3O:325:TYR:HE2	46:3O:327:ILE:HD11	1.79	0.46
47:3P:311:LYS:HB3	47:3P:311:LYS:HE2	1.81	0.46
55:4A:32:ALA:HB3	66:4L:36:PRO:HG2	1.98	0.46
75:4C:308:CDL:H712	75:4C:308:CDL:HB61	1.63	0.46
82:4L:101:PGV:O02	82:4L:101:PGV:H62	2.16	0.46
3:5C:96:LEU:HB2	3:5C:105:ILE:HG22	1.98	0.46
6:5F:355:LYS:HG3	6:5F:370:ASP:HA	1.98	0.46
12:5L:69:MET:HE3	13:5M:455:LEU:HD11	1.97	0.46
17:5Q:37:ILE:HG12	17:5Q:92:ALA:HB1	1.98	0.46
23:5X:17:VAL:HG23	23:5X:63:ASN:HD22	1.80	0.46
23:5X:50:LYS:HE3	23:5X:141:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:5Y:73:SER:OG	24:5Y:92:GLY:HA3	2.15	0.46
46:6B:150:VAL:O	46:6B:151:ALA:C	2.58	0.46
46:6B:177:TYR:O	46:6B:178:CYS:C	2.58	0.46
47:6C:179:PHE:HE1	83:6C:501:HEM:HHD	1.80	0.46
47:6C:199:PHE:O	47:6C:202:GLU:HB2	2.16	0.46
48:6D:251:PRO:HB2	48:6D:254:TYR:HE1	1.79	0.46
49:6I:70:LEU:O	49:6I:71:ASN:OD1	2.33	0.46
45:6N:127:ILE:O	45:6N:131:ARG:N	2.38	0.46
45:6N:186:VAL:O	45:6N:190:TYR:N	2.49	0.46
48:6Q:21:LEU:HD21	48:6Q:191:ARG:HG2	1.96	0.46
55:8A:74:MET:O	55:8A:75:ILE:C	2.59	0.46
55:8A:367:LEU:O	55:8A:368:HIS:C	2.59	0.46
82:8A:602:PGV:H241	82:8C:305:PGV:H242	1.97	0.46
57:8C:99:TRP:HB2	82:8C:303:PGV:H92	1.97	0.46
82:8C:304:PGV:H32	82:8C:304:PGV:H61	1.56	0.46
1:1A:58:VAL:HG11	1:1A:113:TRP:CZ2	2.51	0.46
2:1B:62:MET:HE3	2:1B:69:MET:HB3	1.96	0.46
2:1B:68:ASP:HB3	2:1B:71:ARG:CB	2.36	0.46
7:1G:539:LYS:HD2	7:1G:539:LYS:HA	1.57	0.46
9:1I:150:ASN:OD1	42:1q:129:THR:HG23	2.15	0.46
12:1L:346:ILE:HD11	12:1L:431:PHE:CZ	2.50	0.46
12:1L:440:LEU:HD23	12:1L:440:LEU:HA	1.79	0.46
17:1Q:59:PHE:HE1	17:1Q:82:LEU:HD12	1.81	0.46
20:1U:52:MET:HE1	39:1n:23:LEU:HB3	1.98	0.46
24:1Y:73:SER:OG	24:1Y:92:GLY:HA3	2.15	0.46
24:1Y:103:ARG:HA	24:1Y:103:ARG:HD2	1.78	0.46
29:1d:108:THR:HB	41:1p:74:THR:O	2.16	0.46
33:1h:14:SER:OG	39:1n:110:GLU:OE1	2.29	0.46
37:1l:74:GLY:HA3	38:1m:42:LEU:HD22	1.97	0.46
45:3A:396:GLU:HA	45:3A:396:GLU:OE2	2.16	0.46
46:3B:314:ALA:HA	49:3I:63:PRO:HG3	1.97	0.46
47:3C:26:ASN:HA	50:3F:82:MET:CA	2.39	0.46
47:3C:302:ILE:O	47:3C:305:PRO:HD2	2.15	0.46
49:3E:111:LYS:HA	51:3G:23:PHE:CD1	2.50	0.46
49:3E:173:PRO:O	49:3E:215:GLY:N	2.41	0.46
45:3N:61:HIS:O	45:3N:65:LYS:HE3	2.14	0.46
45:3N:430:GLN:HA	51:3T:4:PHE:HB3	1.97	0.46
55:4A:2:PHE:HZ	82:4L:101:PGV:H21	1.80	0.46
56:4B:191:LEU:HD23	58:4D:126:MET:HG2	1.98	0.46
57:4C:54:MET:HB3	57:4C:58:TRP:CZ3	2.51	0.46
68:4N:44:CYS:HB2	68:4N:53:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:76:CYS:N	4:5D:403:ASP:OD1	2.47	0.46
7:5G:537:LEU:HD12	7:5G:543:ILE:HD11	1.96	0.46
12:5L:40:VAL:HG11	12:5L:97:THR:HG23	1.96	0.46
13:5M:425:ASN:CG	38:5m:57:GLY:HA2	2.41	0.46
16:5P:81:ILE:O	16:5P:85:VAL:HB	2.16	0.46
31:5f:31:ASP:O	31:5f:35:THR:HG23	2.16	0.46
32:5g:109:GLU:O	41:5p:141:ARG:NH1	2.35	0.46
34:5i:87:TYR:CE1	41:5p:48:ARG:HG2	2.50	0.46
37:5l:127:PRO:HD3	40:5o:3:HIS:CE1	2.51	0.46
38:5m:22:TYR:CD2	39:5n:64:ARG:NE	2.83	0.46
38:5m:53:PRO:HB3	39:5n:128:ARG:HD3	1.97	0.46
41:5p:27:ASN:HB3	41:5p:30:THR:HG23	1.97	0.46
45:6A:255:ILE:HG22	45:6A:322:ALA:HB3	1.97	0.46
46:6B:266:SER:O	46:6B:267:ALA:C	2.59	0.46
46:6B:365:LYS:HG2	46:6B:399:LEU:HD22	1.98	0.46
47:6C:55:TYR:HB2	47:6C:69:ILE:HD11	1.96	0.46
48:6D:98:TYR:HD2	52:6H:98:LEU:HB3	1.80	0.46
48:6D:206:ARG:O	48:6D:207:ALA:C	2.58	0.46
53:6J:11:TYR:HA	53:6J:15:PHE:CB	2.45	0.46
53:6J:41:ASP:O	53:6J:42:ALA:C	2.59	0.46
45:6N:158:PHE:C	45:6N:164:ALA:HB2	2.40	0.46
45:6N:245:ASP:O	45:6N:246:ASP:C	2.58	0.46
45:6N:280:TYR:HB3	45:6N:307:PHE:CE2	2.51	0.46
45:6N:323:HIS:CE1	45:6N:325:VAL:HG22	2.48	0.46
55:8A:84:PRO:O	55:8A:88:GLY:N	2.48	0.46
55:8A:333:LYS:C	55:8A:335:SER:H	2.23	0.46
55:8A:419:VAL:O	55:8A:420:GLY:C	2.59	0.46
56:8B:186:SER:OG	56:8B:188:ARG:O	2.34	0.46
56:8B:191:LEU:HD23	58:8D:126:MET:HG2	1.98	0.46
57:8C:103:HIS:CE1	82:8C:303:PGV:H032	2.51	0.46
82:8C:303:PGV:H212	68:8N:36:LEU:HB3	1.98	0.46
82:8G:101:PGV:H232	82:8G:101:PGV:H202	1.36	0.46
1:1A:72:LEU:HD12	1:1A:75:LEU:HD11	1.97	0.46
13:1M:263:MET:HG3	38:1m:101:TYR:HB2	1.98	0.46
15:1O:165:PRO:HB3	15:1O:217:LYS:HD2	1.98	0.46
16:1P:192:PRO:HB3	16:1P:256:TYR:CZ	2.51	0.46
23:1X:50:LYS:HE3	23:1X:141:TYR:CZ	2.51	0.46
34:1i:87:TYR:CE1	41:1p:48:ARG:HG2	2.50	0.46
41:1p:27:ASN:HB3	41:1p:30:THR:HG23	1.98	0.46
47:3C:11:MET:N	47:3C:11:MET:SD	2.88	0.46
47:3C:64:SER:HA	48:3D:133:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3D:120:VAL:HG22	48:3D:258:LEU:HD21	1.97	0.46
46:3O:202:ALA:HB3	46:3O:229:GLY:O	2.16	0.46
46:3O:213:HIS:HB3	46:3O:214:PRO:HD3	1.97	0.46
47:3P:197:LEU:HD21	83:3P:502:HEM:HMA3	1.98	0.46
47:3P:267:HIS:CD2	47:3P:269:LYS:HG2	2.50	0.46
53:3W:5:THR:O	53:3W:9:ARG:HG2	2.16	0.46
55:4A:470:PHE:CG	67:4M:19:LEU:HD13	2.50	0.46
60:4F:40:SER:OG	60:4F:45:ASP:HB3	2.16	0.46
6:5F:108:ARG:HB2	6:5F:142:PHE:CE2	2.51	0.46
71:5I:201:PC1:H3G1	25:5Z:40:ILE:HD12	1.97	0.46
69:5J:201:3PE:H2C2	12:5L:592:LEU:HD21	1.97	0.46
15:5O:290:ASP:O	15:5O:294:GLN:HG2	2.16	0.46
16:5P:136:ASN:ND2	16:5P:289:MET:HE3	2.31	0.46
16:5P:192:PRO:HB3	16:5P:256:TYR:CZ	2.51	0.46
24:5Y:52:VAL:HG22	69:5Y:205:3PE:H262	1.98	0.46
27:5b:63:PRO:HD3	27:5b:63:PRO:HB3	1.83	0.46
35:5j:54:PRO:HG3	40:5o:95:VAL:HG22	1.98	0.46
45:6A:301:ARG:O	45:6A:302:LYS:C	2.58	0.46
46:6B:72:ALA:O	46:6B:73:SER:C	2.59	0.46
46:6B:323:GLY:HA2	46:6B:417:PHE:CE1	2.51	0.46
47:6C:327:MET:O	47:6C:328:LEU:C	2.59	0.46
47:6C:330:ALA:HB1	51:6G:57:PHE:CG	2.51	0.46
48:6D:158:VAL:N	48:6D:171:ARG:O	2.47	0.46
48:6D:318:VAL:CG2	51:6G:22:PRO:HD3	2.44	0.46
49:6E:220:LEU:HA	47:6P:263:ASN:OD1	2.15	0.46
45:6N:46:ARG:HG3	45:6N:163:LEU:HD23	1.47	0.46
46:6O:37:SER:HB3	46:6O:213:HIS:CG	2.51	0.46
46:6O:169:ARG:N	46:6O:238:LYS:O	2.43	0.46
46:6O:385:GLN:HG3	46:6O:392:TYR:HA	1.98	0.46
46:6O:397:THR:O	46:6O:398:VAL:C	2.58	0.46
46:6O:407:ASP:O	46:6O:408:ALA:C	2.58	0.46
49:6R:121:THR:O	49:6R:125:VAL:HG23	2.16	0.46
55:8A:230:LEU:HD13	57:8C:103:HIS:CB	2.45	0.46
55:8A:279:SER:CA	68:8N:22:ILE:HG12	2.45	0.46
82:8C:304:PGV:H321	82:8C:304:PGV:H291	1.46	0.46
60:8F:40:SER:OG	60:8F:45:ASP:HB3	2.16	0.46
1:1A:51:PHE:O	1:1A:52:SER:C	2.58	0.46
8:1H:149:ILE:HG12	8:1H:181:LEU:HD22	1.96	0.46
9:1I:52:PHE:CZ	42:1q:30:ALA:HA	2.51	0.46
11:1K:22:TYR:O	12:1L:585:LYS:HD2	2.16	0.46
11:1K:34:GLU:OE1	11:1K:37:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:602:PHE:CE2	69:1Y:204:3PE:H382	2.51	0.46
17:1Q:47:SER:O	17:1Q:47:SER:OG	2.32	0.46
17:1Q:69:LEU:HD11	42:1q:126:PRO:HG2	1.97	0.46
38:1m:24:ILE:HG21	38:1m:29:ARG:CZ	2.46	0.46
39:1n:45:ALA:O	39:1n:49:GLU:HG3	2.16	0.46
45:3N:34:THR:HA	45:3N:102:LEU:CA	2.23	0.46
45:3N:88:ALA:HB2	45:3N:97:TYR:CD1	2.51	0.46
45:3N:146:ARG:HB3	45:3N:150:PHE:HE2	1.79	0.46
46:3O:165:ALA:HA	46:3O:173:ALA:CB	2.45	0.46
47:3P:24:PRO:HB2	47:3P:27:ILE:HG23	1.97	0.46
48:3Q:165:TYR:CZ	48:3Q:168:VAL:HG23	2.51	0.46
49:3R:121:THR:O	49:3R:125:VAL:HG23	2.16	0.46
49:3R:207:LYS:HE3	49:3R:210:TRP:HZ3	1.80	0.46
49:3R:211:VAL:HG22	49:3R:213:LEU:HD11	1.98	0.46
49:3R:219:HIS:NE2	49:3R:239:HIS:HE1	2.11	0.46
55:4A:8:TYR:O	57:4C:13:PRO:HB3	2.15	0.46
55:4A:449:ALA:O	55:4A:453:ILE:HG12	2.15	0.46
57:4C:25:LEU:O	57:4C:29:SER:OG	2.28	0.46
58:4D:68:PHE:HA	58:4D:71:MET:HE2	1.98	0.46
4:5D:141:PHE:O	4:5D:145:THR:OG1	2.28	0.46
5:5E:87:TYR:HB3	6:5F:181:ALA:O	2.15	0.46
6:5F:20:ARG:NH2	6:5F:269:GLU:O	2.49	0.46
7:5G:135:ARG:HD3	7:5G:137:VAL:HG13	1.98	0.46
8:5H:135:ALA:HB2	8:5H:201:THR:HB	1.96	0.46
12:5L:601:LEU:HD12	12:5L:602:PHE:HD1	1.80	0.46
13:5M:14:MET:SD	13:5M:26:ASN:HB3	2.56	0.46
13:5M:401:MET:HE2	13:5M:401:MET:HB3	1.83	0.46
25:5Z:104:TRP:CH2	30:5e:74:ARG:HG3	2.50	0.46
38:5m:24:ILE:HG21	38:5m:29:ARG:CZ	2.46	0.46
40:5o:24:PHE:HZ	40:5o:111:LYS:HD2	1.81	0.46
45:6A:104:LYS:H	45:6A:104:LYS:HG3	1.51	0.46
45:6A:348:SER:HA	54:6Y:16:ASN:ND2	2.31	0.46
46:6B:150:VAL:HG11	49:6I:40:SER:HB3	1.98	0.46
46:6B:331:ALA:O	46:6B:332:SER:C	2.58	0.46
47:6C:316:MET:HB3	47:6C:317:PHE:H	1.61	0.46
48:6D:211:GLY:HA2	48:6D:214:TYR:HD2	1.81	0.46
53:6J:14:LEU:O	53:6J:15:PHE:C	2.59	0.46
45:6N:27:SER:CB	45:6N:208:LEU:HD12	2.28	0.46
46:6O:311:ALA:HA	46:6O:324:ILE:HG22	1.98	0.46
46:6O:384:SER:C	46:6O:386:ALA:H	2.24	0.46
49:6R:154:ILE:HD11	49:6R:270:LEU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:6U:47:ARG:HG2	52:6U:47:ARG:HH11	1.81	0.46
85:8A:605:HEA:HBD2	85:8A:605:HEA:HHA	1.97	0.46
56:8B:118:PHE:CD1	56:8B:226:MET:HE1	2.51	0.46
56:8B:143:VAL:HG12	56:8B:219:PHE:HD1	1.80	0.46
1:1A:25:PRO:HB2	8:1H:60:PRO:HD3	1.98	0.46
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.97	0.46
7:1G:601:ARG:NH2	7:1G:614:ASP:OD2	2.47	0.46
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.16	0.46
11:1K:1:FME:SD	14:1N:79:LEU:HD21	2.55	0.46
13:1M:14:MET:SD	13:1M:26:ASN:HB3	2.56	0.46
13:1M:207:MET:O	13:1M:294:MET:HG3	2.16	0.46
13:1M:216:LEU:HD22	13:1M:220:HIS:CE1	2.51	0.46
14:1N:183:SER:O	14:1N:187:MET:HG2	2.16	0.46
24:1Y:107:TYR:HB2	69:1Y:206:3PE:O13	2.16	0.46
45:3A:158:PHE:HB3	45:3A:161:THR:OG1	2.16	0.46
46:3B:260:GLU:O	46:3B:416:LYS:NZ	2.49	0.46
46:3B:438:GLU:OE2	46:3O:169:ARG:HD3	2.16	0.46
47:3C:3:ASN:O	47:3C:7:SER:N	2.49	0.46
47:3C:15:ASN:HA	47:3C:19:ILE:HD12	1.97	0.46
47:3C:270:PRO:HG2	47:3C:275:LEU:HA	1.97	0.46
45:3N:17:SER:CB	45:3N:209:LEU:HD13	2.44	0.46
45:3N:252:HIS:HB3	45:3N:323:HIS:NE2	2.31	0.46
46:3O:316:TYR:HB2	46:3O:319:SER:CB	2.46	0.46
85:4A:605:HEA:HHA	85:4A:605:HEA:HBD2	1.97	0.46
1:5A:48:ARG:HH11	10:5J:76:THR:HG21	1.80	0.46
9:5I:52:PHE:CZ	42:5q:30:ALA:HA	2.51	0.46
12:5L:273:VAL:O	12:5L:277:THR:HG22	2.15	0.46
12:5L:600:THR:CG2	12:5L:601:LEU:H	2.18	0.46
13:5M:105:PHE:CE2	69:5N:902:3PE:H3I1	2.50	0.46
37:5l:53:ARG:HD2	37:5l:57:GLU:OE1	2.16	0.46
39:5n:97:LYS:HG2	39:5n:173:PRO:HB2	1.97	0.46
45:6A:221:GLY:O	45:6A:222:THR:C	2.58	0.46
45:6A:301:ARG:HH21	45:6A:303:LEU:HD21	1.80	0.46
45:6A:376:CYS:HA	45:6A:379:ILE:HD12	1.97	0.46
46:6B:22:GLN:HB2	46:6B:23:ASP:H	1.53	0.46
46:6B:247:GLN:HA	46:6B:428:GLY:O	2.16	0.46
47:6C:123:VAL:HG21	83:6C:502:HEM:HBB1	1.97	0.46
47:6C:183:PHE:O	47:6C:186:PRO:HD2	2.16	0.46
47:6C:233:LEU:O	47:6C:236:MET:N	2.49	0.46
45:6N:18:GLN:HE21	45:6N:24:ARG:CG	2.28	0.46
45:6N:159:GLN:HB3	49:6R:85:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:359:ASN:HB2	46:6O:92:VAL:HG12	1.97	0.46
46:6O:338:LYS:HE3	46:6O:338:LYS:HB3	1.65	0.46
55:8A:169:ILE:HG13	75:8A:610:CDL:H321	1.97	0.46
55:8A:218:THR:HG21	57:8C:191:GLY:HA2	1.98	0.46
55:8A:301:THR:HG23	68:8N:32:TYR:HE2	1.81	0.46
55:8A:321:PHE:CD2	56:8B:65:TRP:HB2	2.51	0.46
57:8C:54:MET:HB3	57:8C:58:TRP:CZ3	2.50	0.46
6:1F:108:ARG:HB2	6:1F:142:PHE:CE2	2.51	0.46
8:1H:216:ALA:O	8:1H:217:ALA:C	2.59	0.46
12:1L:273:VAL:O	12:1L:277:THR:HG22	2.15	0.46
12:1L:383:MET:HB3	12:1L:386:LEU:HD22	1.98	0.46
13:1M:310:MET:HG2	13:1M:455:LEU:O	2.16	0.46
20:1T:51:ILE:HD12	20:1T:70:LEU:HD12	1.98	0.46
25:1Z:104:TRP:CH2	30:1e:74:ARG:HG3	2.50	0.46
31:1f:42:LEU:HD23	31:1f:45:LYS:HZ1	1.80	0.46
36:1k:84:GLU:O	36:1k:88:GLU:HG2	2.16	0.46
37:1l:53:ARG:HD2	37:1l:57:GLU:OE1	2.16	0.46
46:3B:95:LYS:HE2	49:3I:72:VAL:HB	1.98	0.46
46:3B:168:TYR:HH	46:3B:319:SER:HG	1.60	0.46
47:3C:74:ASN:ND2	49:3E:138:SER:HB3	2.30	0.46
45:3N:92:ARG:HE	45:3N:167:VAL:N	2.14	0.46
45:3N:304:CYS:HA	45:3N:326:CYS:CB	2.45	0.46
45:3N:311:ASN:HB2	45:3N:320:LEU:HD22	1.97	0.46
45:3N:344:ARG:HA	45:3N:348:SER:HB2	1.98	0.46
46:3O:27:THR:HB	46:3O:213:HIS:HE1	1.81	0.46
46:3O:99:THR:N	46:3O:106:ALA:O	2.47	0.46
55:4A:383:MET:HE2	55:4A:421:VAL:HB	1.97	0.46
55:4A:483:SER:HB3	67:4M:4:LYS:HG3	1.98	0.46
55:4A:496:HIS:HE1	55:4A:505:PHE:CE1	2.33	0.46
62:4H:39:CYS:O	62:4H:43:MET:HG2	2.16	0.46
64:4J:4:ARG:HH11	64:4J:4:ARG:HG3	1.80	0.46
3:5C:104:ARG:NH2	4:5D:373:GLU:OE2	2.43	0.46
6:5F:287:VAL:HG11	6:5F:294:LEU:HD13	1.98	0.46
8:5H:179:TRP:HE1	25:5Z:43:LEU:HG	1.81	0.46
9:5I:95:GLU:HB2	9:5I:108:ARG:HB3	1.97	0.46
12:5L:505:ASN:O	12:5L:508:THR:OG1	2.21	0.46
14:5N:88:LYS:HE2	14:5N:90:PHE:CD2	2.51	0.46
15:5O:165:PRO:HB3	15:5O:217:LYS:HD2	1.97	0.46
16:5P:133:SER:O	16:5P:168:PRO:HD2	2.16	0.46
71:5P:401:PC1:H321	71:5P:401:PC1:H31	1.67	0.46
20:5T:51:ILE:HD12	20:5T:70:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:5h:46:PHE:O	41:5p:58:ASN:ND2	2.32	0.46
40:5o:51:MET:HE2	40:5o:53:GLN:NE2	2.31	0.46
43:5r:42:VAL:HB	43:5r:46:HIS:CG	2.51	0.46
45:6A:149:VAL:HG23	45:6A:423:ALA:HB1	1.97	0.46
45:6A:231:PHE:CE1	45:6A:316:GLU:HB3	2.51	0.46
45:6A:261:GLY:O	45:6A:262:TRP:C	2.58	0.46
46:6B:352:LEU:HD12	46:6B:352:LEU:HA	1.80	0.46
47:6C:303:LEU:O	47:6C:304:MET:C	2.58	0.46
48:6D:137:ARG:H	48:6D:137:ARG:HG3	1.61	0.46
48:6D:169:PHE:O	48:6D:171:ARG:HG3	2.16	0.46
51:6G:69:GLU:HA	51:6G:72:LYS:HE2	1.98	0.46
53:6J:17:ARG:O	53:6J:18:THR:C	2.59	0.46
45:6N:14:THR:CG2	45:6N:389:ARG:HH21	2.23	0.46
45:6N:67:THR:CG2	45:6N:116:ILE:HA	2.46	0.46
45:6N:171:SER:OG	49:6R:82:ASP:OD2	2.33	0.46
46:6O:321:LEU:HD23	46:6O:321:LEU:HA	1.74	0.46
53:6W:5:THR:O	53:6W:9:ARG:HG2	2.16	0.46
55:8A:51:ASP:O	55:8A:54:TYR:N	2.49	0.46
55:8A:69:MET:O	55:8A:72:PRO:HD2	2.16	0.46
55:8A:333:LYS:HD3	55:8A:333:LYS:HA	1.60	0.46
55:8A:475:ALA:HA	55:8A:480:ARG:HH21	1.80	0.46
56:8B:104:TRP:CG	56:8B:203:ASN:HB2	2.50	0.46
57:8C:161:GLN:O	57:8C:165:ILE:HG13	2.16	0.46
82:8K:101:PGV:H252	82:8K:101:PGV:H281	1.49	0.46
68:8N:44:CYS:HB2	68:8N:53:PRO:HG3	1.98	0.46
2:1B:61:HIS:NE2	4:1D:174:ARG:NH2	2.61	0.45
8:1H:90:PRO:HG2	8:1H:240:ILE:HD13	1.98	0.45
10:1J:78:MET:HE2	10:1J:79:TYR:H	1.67	0.45
11:1K:10:MET:CE	11:1K:14:ILE:HD11	2.46	0.45
11:1K:26:LEU:HB3	11:1K:78:LEU:HD12	1.97	0.45
13:1M:74:PRO:O	13:1M:78:MET:HG3	2.16	0.45
14:1N:88:LYS:HE2	14:1N:90:PHE:CD2	2.51	0.45
14:1N:222:SER:HA	14:1N:237:MET:HE3	1.97	0.45
16:1P:274:PRO:HG2	16:1P:275:PHE:CZ	2.51	0.45
18:1R:38:ASN:HB3	18:1R:43:LEU:HD11	1.98	0.45
19:1S:36:ILE:HD13	19:1S:54:ILE:HD13	1.98	0.45
20:1U:36:PHE:HD1	20:1U:40:LEU:HD12	1.80	0.45
23:1X:90:TYR:HA	26:1a:34:LYS:HG2	1.98	0.45
26:1a:27:HIS:CE1	26:1a:36:LYS:HD3	2.52	0.45
37:1l:138:LEU:HD22	37:1l:142:ARG:NH2	2.31	0.45
71:1m:201:PC1:H222	71:1m:201:PC1:H11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:436:ARG:HH12	47:3C:20:ASP:HA	1.81	0.45
46:3B:39:GLU:OE1	46:3B:113:ARG:NH2	2.35	0.45
47:3C:237:LEU:HB2	48:3D:301:MET:SD	2.56	0.45
48:3D:115:ARG:O	48:3D:119:GLN:HG3	2.16	0.45
49:3E:199:GLN:O	49:3E:248:ARG:HD3	2.15	0.45
50:3F:107:LYS:HD3	50:3F:108:GLU:N	2.32	0.45
51:3G:51:ALA:O	51:3G:52:PRO:C	2.59	0.45
49:3I:70:LEU:O	49:3I:71:ASN:OD1	2.33	0.45
45:3N:161:THR:HB	45:3N:234:CYS:HB3	1.97	0.45
45:3N:363:ASN:O	45:3N:364:ALA:C	2.59	0.45
47:3P:121:PHE:HA	47:3P:124:MET:HE3	1.98	0.45
49:3R:219:HIS:CG	49:3R:239:HIS:CE1	3.03	0.45
55:4A:377:PHE:HA	55:4A:380:VAL:HG22	1.98	0.45
57:4C:43:LEU:HD11	82:4C:302:PGV:H292	1.98	0.45
57:4C:161:GLN:O	57:4C:165:ILE:HG13	2.16	0.45
5:5E:153:MET:HE2	5:5E:153:MET:HB2	1.90	0.45
6:5F:361:GLN:HE22	17:5Q:133:LYS:NZ	2.14	0.45
6:5F:364:PRO:HB2	6:5F:403:THR:HG22	1.97	0.45
7:5G:383:ASN:ND2	7:5G:413:VAL:HG21	2.31	0.45
9:5I:70:TYR:CE2	9:5I:76:ARG:HA	2.51	0.45
10:5J:129:ASP:CB	30:5e:31:ARG:HH21	2.28	0.45
11:5K:10:MET:CE	11:5K:14:ILE:HD11	2.46	0.45
12:5L:383:MET:HB3	12:5L:386:LEU:HD22	1.98	0.45
14:5N:222:SER:HA	14:5N:237:MET:HE3	1.97	0.45
15:5O:45:LYS:HB2	15:5O:235:VAL:HG11	1.99	0.45
15:5O:83:TYR:OH	76:5O:401:GTP:O3'	2.24	0.45
29:5d:108:THR:HB	41:5p:74:THR:O	2.16	0.45
69:5d:201:3PE:H2C2	69:5d:201:3PE:H2G2	1.98	0.45
32:5g:63:PHE:O	32:5g:67:SER:HB2	2.16	0.45
37:5l:138:LEU:HD22	37:5l:142:ARG:NH2	2.31	0.45
47:6C:85:ASN:HB2	47:6C:243:VAL:CG2	2.46	0.45
47:6C:196:HIS:NE2	83:6C:502:HEM:ND	2.63	0.45
48:6D:204:ILE:O	48:6D:205:VAL:C	2.57	0.45
45:6N:340:GLY:O	45:6N:344:ARG:N	2.46	0.45
46:6O:133:ARG:HD3	46:6O:135:TRP:CZ2	2.50	0.45
46:6O:246:ASP:HB3	46:6O:427:SER:HA	1.98	0.45
47:6P:197:LEU:HD21	83:6P:502:HEM:HMA3	1.98	0.45
49:6R:214:ILE:HD13	49:6R:214:ILE:HA	1.87	0.45
55:8A:146:THR:O	55:8A:147:ILE:C	2.59	0.45
55:8A:488:THR:O	55:8A:489:SER:C	2.58	0.45
58:8D:68:PHE:HA	58:8D:71:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:8H:4:ILE:HD11	62:8H:55:TRP:HB2	1.97	0.45
64:8J:40:LEU:HA	64:8J:43:THR:HG22	1.97	0.45
4:1D:269:LEU:HD11	4:1D:373:GLU:HG3	1.99	0.45
5:1E:115:SER:O	5:1E:118:GLU:HG3	2.16	0.45
7:1G:41:CYS:O	7:1G:161:ARG:NH2	2.46	0.45
7:1G:135:ARG:HD3	7:1G:137:VAL:HG13	1.98	0.45
12:1L:241:THR:HG21	12:1L:344:GLY:HA3	1.98	0.45
12:1L:571:MET:HE2	12:1L:571:MET:HB3	1.78	0.45
13:1M:46:GLY:HA2	32:1g:84:ARG:HG2	1.98	0.45
15:1O:45:LYS:HB2	15:1O:235:VAL:HG11	1.99	0.45
17:1Q:37:ILE:HG12	17:1Q:92:ALA:HB1	1.98	0.45
20:1U:8:LEU:N	20:1U:88:GLU:OE2	2.43	0.45
20:1U:37:MET:N	20:1U:37:MET:SD	2.90	0.45
24:1Y:65:ILE:HD11	24:1Y:100:LEU:HB2	1.97	0.45
39:1n:53:GLU:OE1	39:1n:58:LYS:HG3	2.16	0.45
47:3C:137:GLN:CB	47:3C:257:THR:HB	2.44	0.45
47:3C:244:LEU:HB3	48:3D:290:ARG:O	2.16	0.45
48:3D:159:GLN:HE21	48:3D:168:MET:HG3	1.80	0.45
50:3F:61:ARG:NH2	50:3F:112:GLU:OE1	2.43	0.45
45:3N:243:HIS:HB3	45:3N:425:LEU:HD13	1.97	0.45
45:3N:391:PRO:HD2	45:3N:394:GLU:HB2	1.97	0.45
46:3O:250:ASP:O	46:3O:251:SER:C	2.59	0.45
46:3O:295:LEU:HD23	46:3O:343:GLN:HG2	1.97	0.45
55:4A:423:MET:HE1	82:4K:101:PGV:H11	1.98	0.45
6:5F:68:ARG:HD2	6:5F:254:LYS:HE2	1.98	0.45
12:5L:2:ASN:OD1	12:5L:2:ASN:N	2.49	0.45
12:5L:121:LEU:HD22	12:5L:246:LEU:HD23	1.97	0.45
13:5M:207:MET:O	13:5M:294:MET:HG3	2.16	0.45
13:5M:263:MET:HG3	38:5m:101:TYR:HB2	1.98	0.45
37:5l:68:ASP:N	37:5l:68:ASP:OD1	2.47	0.45
45:6A:243:HIS:CG	51:6G:16:ILE:HG12	2.50	0.45
46:6B:29:LEU:HD12	46:6B:33:LEU:HD23	1.98	0.45
46:6B:246:ASP:C	46:6B:430:LEU:HD21	2.42	0.45
46:6B:435:PHE:HE2	46:6O:240:ARG:HB2	1.81	0.45
47:6C:172:LYS:HB2	47:6C:172:LYS:HE3	1.60	0.45
47:6C:331:ASP:O	47:6C:332:LEU:C	2.59	0.45
48:6D:181:LYS:HB2	48:6D:181:LYS:HE3	1.68	0.45
48:6D:293:MET:HE2	48:6D:293:MET:HB2	1.63	0.45
45:6N:18:GLN:HB3	45:6N:22:GLY:HA2	1.98	0.45
46:6O:53:ALA:HA	46:6O:57:TYR:HE2	1.81	0.45
46:6O:124:LEU:HB3	46:6O:223:PHE:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6O:182:ARG:HA	46:6O:182:ARG:HD2	1.51	0.45
47:6P:116:GLY:C	83:6P:502:HEM:HBC2	2.41	0.45
47:6P:121:PHE:HA	47:6P:124:MET:HE3	1.98	0.45
48:6Q:173:ASP:OD1	48:6Q:173:ASP:N	2.37	0.45
48:6Q:238:ARG:HD2	51:6T:14:ILE:HD12	1.98	0.45
49:6R:256:LEU:HG	49:6R:257:ASN:O	2.16	0.45
54:6Y:8:PRO:O	54:6Y:11:ARG:HG2	2.17	0.45
55:8A:324:LEU:HD13	56:8B:41:ILE:HG21	1.97	0.45
55:8A:334:TRP:HE1	75:8D:201:CDL:H261	1.81	0.45
82:8B:301:PGV:H72	82:8B:301:PGV:H41	1.58	0.45
6:1F:361:GLN:HE22	17:1Q:133:LYS:NZ	2.14	0.45
7:1G:228:ILE:HG13	7:1G:581:GLN:HB3	1.97	0.45
9:1I:70:TYR:CE2	9:1I:76:ARG:HA	2.52	0.45
9:1I:70:TYR:C	9:1I:72:SER:H	2.24	0.45
12:1L:69:MET:HE3	13:1M:455:LEU:HD11	1.97	0.45
15:1O:290:ASP:O	15:1O:294:GLN:HG2	2.16	0.45
31:1f:2:ASN:O	31:1f:6:ILE:HG13	2.17	0.45
35:1j:56:PRO:HA	35:1j:59:TRP:CE3	2.52	0.45
35:1j:68:PRO:O	40:1o:110:ARG:NH1	2.50	0.45
47:3C:51:LEU:HD21	47:3C:80:ARG:HA	1.98	0.45
47:3C:78:VAL:HG11	49:3E:135:GLN:OE1	2.15	0.45
47:3C:349:ILE:HD12	47:3C:349:ILE:HA	1.83	0.45
45:3N:25:VAL:CG1	45:3N:209:LEU:HD23	2.46	0.45
45:3N:49:ASN:H	45:3N:52:ASN:HB2	1.81	0.45
45:3N:355:VAL:HG22	45:3N:358:LYS:HD3	1.97	0.45
45:3N:443:TRP:O	45:3N:444:LEU:C	2.60	0.45
46:3O:56:ARG:HB2	46:3O:171:ALA:HB1	1.98	0.45
46:3O:77:THR:HA	46:3O:131:GLU:H	1.81	0.45
48:3Q:28:ARG:HE	48:3Q:185:ASP:CG	2.25	0.45
57:4C:99:TRP:HB2	82:4C:303:PGV:H92	1.98	0.45
57:4C:117:PRO:HG2	57:4C:123:PRO:HG3	1.98	0.45
4:5D:299:CYS:O	4:5D:303:GLU:HG3	2.17	0.45
5:5E:115:SER:O	5:5E:118:GLU:HG3	2.16	0.45
6:5F:92:TYR:CE1	6:5F:133:ALA:HB3	2.51	0.45
11:5K:22:TYR:O	12:5L:585:LYS:HD2	2.16	0.45
12:5L:201:ILE:HA	12:5L:206:ASN:HD22	1.82	0.45
12:5L:249:SER:OG	12:5L:336:LYS:HG3	2.16	0.45
12:5L:489:THR:O	12:5L:493:VAL:HG23	2.17	0.45
13:5M:432:ARG:HG3	32:5g:47:TYR:CE1	2.51	0.45
20:5T:48:VAL:HG13	22:5W:37:ARG:HE	1.79	0.45
21:5V:23:LEU:HD21	21:5V:79:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:5j:33:TRP:CD1	36:5k:69:GLY:C	2.94	0.45
39:5n:53:GLU:OE1	39:5n:58:LYS:HG3	2.16	0.45
45:6A:247:ALA:O	45:6A:248:LEU:C	2.58	0.45
45:6A:313:CYS:HA	45:6A:318:GLY:CA	2.44	0.45
45:6A:324:PHE:O	45:6A:325:VAL:C	2.59	0.45
46:6B:240:ARG:HH22	46:6O:245:ARG:HG3	1.80	0.45
47:6C:269:LYS:HB2	47:6C:269:LYS:HE3	1.64	0.45
48:6D:220:THR:HB	52:6H:40:ASP:OD2	2.17	0.45
49:6E:187:GLU:O	49:6E:190:VAL:HB	2.15	0.45
45:6N:8:LEU:HD22	45:6N:392:LEU:HB3	1.99	0.45
45:6N:43:ALA:H	45:6N:94:HIS:CA	2.29	0.45
45:6N:51:LYS:O	45:6N:177:LEU:HD23	2.16	0.45
45:6N:337:PHE:HE1	47:6P:2:THR:HA	1.81	0.45
45:6N:396:GLU:HA	45:6N:399:ILE:HD12	1.99	0.45
48:6Q:33:TYR:CD1	48:6Q:37:CYS:HB2	2.50	0.45
49:6R:191:GLU:O	49:6R:194:GLN:HG2	2.16	0.45
49:6R:207:LYS:HE3	49:6R:210:TRP:HZ3	1.80	0.45
55:8A:135:ASN:O	55:8A:136:LEU:C	2.58	0.45
55:8A:264:LYS:HA	55:8A:264:LYS:HD3	1.39	0.45
82:8C:301:PGV:H232	82:8C:301:PGV:H262	1.76	0.45
59:8E:67:ILE:HA	59:8E:70:VAL:HG12	1.97	0.45
2:1B:50:PHE:CD2	2:1B:86:MET:HE3	2.52	0.45
2:1B:171:LYS:O	2:1B:175:ILE:HG12	2.16	0.45
4:1D:94:LYS:HG3	4:1D:102:TYR:HE2	1.80	0.45
7:1G:43:HIS:HD2	7:1G:45:ARG:H	1.63	0.45
9:1I:161:TRP:CE3	42:1q:84:PRO:HB3	2.52	0.45
12:1L:201:ILE:HA	12:1L:206:ASN:HD22	1.82	0.45
15:1O:14:THR:HA	15:1O:17:LYS:HE2	1.98	0.45
20:1T:7:THR:HG23	20:1T:10:ALA:H	1.82	0.45
40:1o:17:ASP:OD1	40:1o:17:ASP:N	2.43	0.45
47:3C:85:ASN:ND2	47:3C:243:VAL:HA	2.32	0.45
47:3C:345:HIS:CB	47:3C:348:ILE:HB	2.46	0.45
45:3N:25:VAL:HG22	45:3N:197:LEU:CG	2.39	0.45
45:3N:46:ARG:NE	45:3N:163:LEU:HD22	2.23	0.45
45:3N:57:TYR:OH	45:3N:168:GLU:N	2.29	0.45
45:3N:182:LEU:HA	45:3N:185:TYR:CD2	2.50	0.45
46:3O:81:SER:O	46:3O:84:LYS:HB3	2.17	0.45
56:4B:64:ILE:HG21	89:4B:303:PSC:H281	1.98	0.45
57:4C:67:PHE:HA	64:4J:9:GLN:HG2	1.98	0.45
58:4D:45:LYS:H	58:4D:45:LYS:HG2	1.59	0.45
6:5F:61:LYS:HG2	6:5F:76:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:5H:215:TYR:HD1	8:5H:219:PRO:HB2	1.81	0.45
8:5H:310:MET:O	27:5b:37:TYR:HB2	2.16	0.45
9:5I:135:PRO:HD3	9:5I:165:ILE:HG22	1.98	0.45
10:5J:129:ASP:HB3	30:5e:31:ARG:NE	2.28	0.45
11:5K:26:LEU:HB3	11:5K:78:LEU:HD12	1.97	0.45
14:5N:183:SER:O	14:5N:187:MET:HG2	2.16	0.45
69:5N:902:3PE:H2C1	69:5d:201:3PE:H3D1	1.99	0.45
16:5P:270:PHE:CD2	16:5P:278:TRP:HB2	2.52	0.45
17:5Q:59:PHE:HE1	17:5Q:82:LEU:HD12	1.81	0.45
27:5b:17:VAL:O	27:5b:21:SER:OG	2.31	0.45
34:5i:108:THR:O	41:5p:18:ALA:N	2.43	0.45
37:5l:136:ASN:HD22	37:5l:153:VAL:H	1.63	0.45
45:6A:252:HIS:HA	45:6A:325:VAL:HG22	1.99	0.45
46:6B:67:HIS:HA	46:6B:70:ARG:CZ	2.46	0.45
46:6B:148:LYS:HB3	46:6B:177:TYR:HB3	1.99	0.45
46:6B:293:SER:HB3	46:6B:296:TYR:HB2	1.98	0.45
46:6B:434:PRO:HB2	46:6B:438:GLU:HB2	1.98	0.45
47:6C:10:LEU:O	47:6C:11:MET:C	2.59	0.45
47:6C:337:TRP:HZ2	47:6C:347:PHE:CE1	2.34	0.45
48:6D:137:ARG:O	48:6D:140:VAL:HB	2.15	0.45
48:6D:190:ARG:O	48:6D:195:GLY:N	2.50	0.45
48:6D:260:PHE:HD1	48:6D:260:PHE:HA	1.51	0.45
48:6D:273:LYS:HB3	48:6D:273:LYS:HE3	1.32	0.45
50:6F:40:LYS:HA	50:6F:92:TRP:CD1	2.51	0.45
45:6N:19:LEU:CD2	45:6N:25:VAL:HG21	2.46	0.45
45:6N:156:THR:HG22	45:6N:241:ILE:CD1	2.46	0.45
55:8A:52:GLN:O	55:8A:56:VAL:HG23	2.17	0.45
55:8A:64:VAL:O	55:8A:66:ILE:N	2.49	0.45
55:8A:245:ILE:O	55:8A:246:LEU:C	2.58	0.45
55:8A:286:ILE:HD11	55:8A:308:ALA:HB1	1.98	0.45
82:8A:603:PGV:H202	75:8A:610:CDL:H312	1.98	0.45
82:8C:304:PGV:H02	82:8C:304:PGV:H22	1.63	0.45
69:1A:201:3PE:H3A1	69:1A:201:3PE:H371	1.58	0.45
2:1B:71:ARG:HH21	8:1H:37:PRO:HD3	1.80	0.45
4:1D:119:SER:HA	4:1D:196:PRO:HG3	1.99	0.45
12:1L:44:PHE:HB2	12:1L:94:LEU:HB3	1.99	0.45
12:1L:296:ASN:H	39:1n:77:GLN:NE2	2.15	0.45
13:1M:432:ARG:HG3	32:1g:47:TYR:CE1	2.52	0.45
15:1O:173:ASP:OD1	15:1O:207:LYS:NZ	2.46	0.45
16:1P:200:THR:OG1	16:1P:288:HIS:O	2.27	0.45
20:1T:66:ASP:HA	20:1T:69:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:52:VAL:HG22	69:1Y:205:3PE:H262	1.98	0.45
32:1g:63:PHE:O	32:1g:67:SER:HB2	2.16	0.45
33:1h:77:ARG:NH1	71:1h:202:PC1:H112	2.32	0.45
47:3C:240:LEU:HB2	48:3D:297:MET:CG	2.45	0.45
47:3C:345:HIS:HA	47:3C:347:PHE:N	2.32	0.45
52:3H:46:ARG:O	52:3H:50:GLU:HG3	2.17	0.45
52:3H:61:ARG:HH22	52:3H:85:ASP:HB2	1.82	0.45
52:3H:98:LEU:O	52:3H:102:LEU:HG	2.17	0.45
53:3J:53:TRP:O	53:3J:54:LYS:HB3	2.16	0.45
45:3N:25:VAL:HG11	45:3N:209:LEU:HD23	1.98	0.45
45:3N:320:LEU:HG	45:3N:415:PHE:HZ	1.80	0.45
46:3O:219:VAL:O	46:3O:222:ARG:HB3	2.17	0.45
55:4A:243:VAL:HB	85:4A:606:HEA:C4C	2.45	0.45
55:4A:299:VAL:HB	56:4B:88:ASP:OD2	2.17	0.45
58:4D:66:GLU:HB3	58:4D:70:GLU:HB2	1.99	0.45
2:5B:171:LYS:O	2:5B:175:ILE:HG12	2.16	0.45
4:5D:62:LEU:HD22	4:5D:425:PHE:HZ	1.82	0.45
7:5G:306:MET:HG2	7:5G:542:PHE:CG	2.51	0.45
7:5G:366:THR:O	7:5G:367:THR:OG1	2.31	0.45
8:5H:190:LEU:HD21	8:5H:196:ALA:HB3	1.99	0.45
12:5L:44:PHE:HB2	12:5L:94:LEU:HB3	1.99	0.45
13:5M:36:LEU:HB2	32:5g:69:VAL:HG22	1.99	0.45
14:5N:222:SER:HA	14:5N:237:MET:CE	2.47	0.45
15:5O:13:ARG:HG3	15:5O:16:ARG:HH21	1.81	0.45
15:5O:48:LEU:HD12	15:5O:123:VAL:HG13	1.97	0.45
29:5d:14:LEU:HD13	29:5d:14:LEU:HA	1.87	0.45
35:5j:68:PRO:O	40:5o:110:ARG:NH1	2.50	0.45
39:5n:138:GLN:O	39:5n:142:GLU:HG3	2.17	0.45
45:6A:260:PRO:HD3	45:6A:270:LEU:HD12	1.99	0.45
45:6A:342:TRP:O	45:6A:343:MET:C	2.59	0.45
46:6B:52:LYS:HE3	46:6B:387:LEU:HD22	1.98	0.45
46:6B:63:LEU:HD22	46:6B:63:LEU:HA	1.66	0.45
46:6B:411:ILE:H	46:6B:411:ILE:HG13	1.59	0.45
47:6C:315:MET:HB2	47:6C:316:MET:H	1.61	0.45
47:6C:329:VAL:HB	51:6G:54:PHE:HE1	1.82	0.45
53:6J:43:ILE:H	53:6J:43:ILE:HG13	1.46	0.45
45:6N:15:GLN:CG	45:6N:205:HIS:ND1	2.78	0.45
45:6N:46:ARG:HH12	45:6N:316:GLU:H	1.63	0.45
45:6N:347:THR:HB	54:6X:17:TRP:HH2	1.79	0.45
46:6O:39:GLU:C	46:6O:41:TYR:H	2.24	0.45
46:6O:80:ALA:HB2	46:6O:125:ASN:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6Q:165:TYR:CZ	48:6Q:168:VAL:HG23	2.51	0.45
55:8A:62:ALA:HB2	85:8A:605:HEA:HBD1	1.99	0.45
55:8A:88:GLY:HA2	55:8A:505:PHE:CZ	2.52	0.45
55:8A:178:GLN:C	55:8A:180:GLN:H	2.25	0.45
55:8A:410:ALA:O	55:8A:411:LYS:C	2.59	0.45
55:8A:509:THR:HG21	60:8F:71:TRP:HZ3	1.82	0.45
82:8A:602:PGV:H251	82:8C:305:PGV:H271	1.97	0.45
56:8B:62:GLU:O	56:8B:66:THR:OG1	2.31	0.45
82:8C:303:PGV:H32	82:8C:303:PGV:H62	1.66	0.45
82:8L:101:PGV:O02	82:8L:101:PGV:H62	2.16	0.45
1:1A:39:CYS:HB3	4:1D:53:PRO:HD2	1.98	0.45
2:1B:100:LEU:HG	2:1B:104:TYR:CZ	2.41	0.45
3:1C:182:ARG:HD2	22:1W:101:THR:HG22	1.99	0.45
6:1F:92:TYR:CE1	6:1F:133:ALA:HB3	2.51	0.45
7:1G:225:THR:HG23	7:1G:240:VAL:HB	1.99	0.45
8:1H:91:MET:HE3	8:1H:91:MET:HB2	1.82	0.45
12:1L:484:LEU:HD22	12:1L:484:LEU:C	2.41	0.45
12:1L:489:THR:O	12:1L:493:VAL:HG23	2.17	0.45
12:1L:544:MET:CE	13:1M:271:MET:HE1	2.47	0.45
15:1O:24:VAL:HB	15:1O:166:PRO:HA	1.99	0.45
24:1Y:12:PRO:HG2	24:1Y:15:THR:OG1	2.16	0.45
31:1f:31:ASP:O	31:1f:35:THR:HG23	2.16	0.45
34:1i:60:ILE:HD12	34:1i:60:ILE:HA	1.83	0.45
34:1i:108:THR:O	41:1p:18:ALA:N	2.43	0.45
45:3A:240:GLU:CD	45:3A:434:TYR:HB2	2.41	0.45
47:3C:233:LEU:HD23	48:3D:308:VAL:HG21	1.97	0.45
48:3D:253:ILE:HD11	84:3D:501:HEC:HBB2	1.97	0.45
50:3F:107:LYS:NZ	50:3F:108:GLU:OE2	2.49	0.45
53:3J:52:LEU:HD12	53:3J:55:HIS:CE1	2.52	0.45
45:3N:7:ALA:HA	45:3N:10:SER:OG	2.17	0.45
45:3N:80:GLU:O	45:3N:83:GLY:N	2.40	0.45
46:3O:128:ALA:HA	46:3O:227:ARG:HH22	1.81	0.45
46:3O:369:LEU:HA	46:3O:372:VAL:HG22	1.97	0.45
49:3R:155:LYS:HB2	49:3R:271:VAL:HG23	1.99	0.45
55:4A:430:PHE:HB3	56:4B:7:LEU:HA	1.98	0.45
55:4A:440:TYR:OH	56:4B:195:GLN:HB3	2.16	0.45
56:4B:100:MET:CE	56:4B:155:SER:HB3	2.43	0.45
66:4L:17:ASN:HB3	66:4L:20:ARG:HB3	1.98	0.45
2:5B:86:MET:CE	2:5B:103:VAL:HG23	2.47	0.45
3:5C:53:HIS:NE2	21:5V:104:GLU:HB3	2.32	0.45
6:5F:191:ALA:HB2	6:5F:203:PRO:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5G:539:LYS:HD2	7:5G:539:LYS:HA	1.56	0.45
8:5H:90:PRO:HG2	8:5H:240:ILE:HD13	1.98	0.45
10:5J:18:VAL:HG22	11:5K:14:ILE:HD13	1.99	0.45
12:5L:296:ASN:H	39:5n:77:GLN:NE2	2.15	0.45
13:5M:126:LEU:HD21	13:5M:153:THR:HG21	1.97	0.45
20:5T:38:LYS:HB2	20:5T:38:LYS:HE2	1.81	0.45
32:5g:37:LEU:HD22	32:5g:40:LYS:NZ	2.22	0.45
33:5h:77:ARG:NH1	71:5h:202:PC1:H112	2.31	0.45
41:5p:84:MET:HE2	41:5p:84:MET:HB3	1.91	0.45
41:5p:166:ARG:CG	41:5p:170:LYS:HZ1	2.30	0.45
47:6C:46:LEU:C	49:6E:136:PHE:CE2	2.93	0.45
47:6C:182:HIS:HE1	83:6C:501:HEM:NB	2.15	0.45
48:6D:129:HIS:CD2	48:6D:198:PRO:HB2	2.52	0.45
53:6J:41:ASP:O	53:6J:45:GLU:N	2.45	0.45
45:6N:61:HIS:HD2	45:6N:134:ILE:HD11	1.77	0.45
45:6N:216:PHE:CD1	45:6N:219:LEU:CD1	2.96	0.45
45:6N:296:SER:HB2	47:6P:1:MET:CE	2.47	0.45
45:6N:359:ASN:ND2	46:6O:91:ALA:O	2.50	0.45
46:6O:72:ALA:HA	46:6O:75:LEU:HG	1.99	0.45
46:6O:251:SER:O	46:6O:253:VAL:N	2.49	0.45
49:6R:211:VAL:HG22	49:6R:213:LEU:HD11	1.98	0.45
55:8A:66:ILE:O	55:8A:67:PHE:C	2.60	0.45
55:8A:83:VAL:O	55:8A:87:ILE:N	2.44	0.45
55:8A:131:PRO:HD2	56:8B:159:VAL:HA	1.99	0.45
55:8A:236:TRP:CD1	55:8A:292:MET:HG2	2.51	0.45
55:8A:314:ILE:O	55:8A:315:PRO:C	2.58	0.45
55:8A:435:GLY:O	55:8A:436:MET:C	2.58	0.45
55:8A:507:GLU:O	55:8A:508:PRO:C	2.58	0.45
82:8C:302:PGV:H183	82:8C:305:PGV:H172	1.99	0.45
2:1B:118:SER:O	2:1B:122:GLY:N	2.49	0.45
2:1B:122:GLY:HA2	2:1B:135:GLY:N	2.32	0.45
4:1D:76:CYS:N	4:1D:403:ASP:OD1	2.47	0.45
4:1D:292:ASP:OD1	4:1D:292:ASP:N	2.49	0.45
8:1H:96:ILE:HG23	25:1Z:144:THR:HB	1.99	0.45
10:1J:19:GLY:HA2	10:1J:93:PHE:HD2	1.81	0.45
13:1M:12:LEU:HB2	13:1M:13:PRO:HD3	1.97	0.45
69:1N:902:3PE:H2C1	69:1d:201:3PE:H3D1	1.98	0.45
29:1d:10:PRO:HG3	30:1e:7:LYS:HE2	1.99	0.45
30:1e:64:GLU:O	30:1e:68:ARG:HA	2.16	0.45
39:1n:138:GLN:O	39:1n:142:GLU:HG3	2.17	0.45
40:1o:51:MET:HE2	40:1o:53:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:42:VAL:HB	43:1r:46:HIS:CG	2.51	0.45
49:3E:187:GLU:O	49:3E:190:VAL:HB	2.15	0.45
52:3H:67:GLN:O	52:3H:71:SER:N	2.43	0.45
45:3N:29:GLN:NE2	45:3N:204:GLU:N	2.52	0.45
45:3N:438:ARG:NH1	45:3N:442:PHE:HE2	2.15	0.45
48:3Q:238:ARG:HD2	51:3T:14:ILE:HD12	1.98	0.45
55:4A:21:LEU:HD13	82:4L:101:PGV:H71	1.98	0.45
55:4A:298:ASP:O	55:4A:302:ARG:HG3	2.16	0.45
2:5B:101:ARG:HA	2:5B:101:ARG:HD2	1.85	0.45
6:5F:157:TYR:OH	6:5F:174:ASP:OD1	2.22	0.45
7:5G:43:HIS:HD2	7:5G:45:ARG:H	1.63	0.45
9:5I:161:TRP:CE3	42:5q:84:PRO:HB3	2.52	0.45
13:5M:216:LEU:HD22	13:5M:220:HIS:CE1	2.51	0.45
13:5M:343:ILE:O	13:5M:346:ARG:NH1	2.45	0.45
42:5q:6:VAL:HG12	75:5q:201:CDL:HA61	1.99	0.45
45:6A:191:LYS:HB3	45:6A:191:LYS:HE3	1.65	0.45
47:6C:12:LYS:HE3	47:6C:12:LYS:HB3	1.58	0.45
47:6C:52:ALA:O	47:6C:53:MET:C	2.59	0.45
47:6C:238:ILE:H	47:6C:238:ILE:HG12	1.50	0.45
47:6C:342:PRO:HG2	51:6G:68:PHE:CE2	2.52	0.45
48:6D:205:VAL:HG11	48:6D:280:ARG:HA	1.97	0.45
48:6D:215:VAL:HA	48:6D:218:LEU:HD23	1.98	0.45
45:6N:41:ILE:O	45:6N:41:ILE:CG2	2.60	0.45
45:6N:53:ASN:HA	45:6N:167:VAL:HG13	1.98	0.45
45:6N:54:GLY:HA2	45:6N:168:GLU:O	2.16	0.45
45:6N:148:VAL:HG11	45:6N:152:TYR:OH	2.15	0.45
45:6N:164:ALA:O	45:6N:165:GLN:C	2.59	0.45
45:6N:438:ARG:O	45:6N:439:SER:C	2.59	0.45
55:8A:271:MET:HB3	68:8N:15:LEU:HD11	1.98	0.45
57:8C:67:PHE:HA	64:8J:9:GLN:HG2	1.98	0.45
82:8L:101:PGV:C12	82:8L:101:PGV:H292	2.47	0.45
69:1A:201:3PE:H2E1	69:1A:201:3PE:H2B2	1.55	0.45
2:1B:71:ARG:H	2:1B:71:ARG:HG2	1.37	0.45
2:1B:116:MET:HG3	2:1B:156:LEU:HD13	1.99	0.45
3:1C:96:LEU:HB2	3:1C:105:ILE:HG22	1.98	0.45
6:1F:68:ARG:HD2	6:1F:254:LYS:HE2	1.98	0.45
6:1F:429:ARG:HE	6:1F:429:ARG:HB2	1.55	0.45
7:1G:344:CYS:HB3	7:1G:510:GLY:O	2.17	0.45
11:1K:43:MET:HE3	11:1K:47:ILE:HD11	1.99	0.45
13:1M:105:PHE:HE2	69:1N:902:3PE:H3I1	1.81	0.45
13:1M:269:MET:HG3	13:1M:399:ASN:CG	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:136:ASN:ND2	16:1P:289:MET:HE3	2.31	0.45
25:1Z:6:VAL:HG11	43:1r:41:PRO:HB3	1.99	0.45
35:1j:42:HIS:CE1	36:1k:84:GLU:HG3	2.52	0.45
41:1p:95:TYR:HB3	41:1p:96:LYS:HZ2	1.81	0.45
44:1s:75:HIS:ND1	44:1s:75:HIS:N	2.64	0.45
46:3B:286:LYS:HG2	46:3B:287:ARG:HG3	1.98	0.45
47:3C:357:LEU:HA	47:3C:360:LEU:HB3	1.99	0.45
49:3E:151:LYS:NZ	49:3E:152:ILE:CD1	2.80	0.45
45:3N:25:VAL:HB	45:3N:209:LEU:HD23	1.99	0.45
45:3N:41:ILE:CG1	45:3N:195:MET:CE	2.95	0.45
45:3N:139:GLN:O	45:3N:142:ASP:HB2	2.16	0.45
45:3N:155:ALA:O	45:3N:159:GLN:HG3	2.16	0.45
45:3N:311:ASN:HA	45:3N:320:LEU:CA	2.41	0.45
55:4A:299:VAL:CG1	68:4N:64:LYS:HD3	2.47	0.45
61:4G:33:LEU:O	61:4G:37:LEU:HG	2.17	0.45
3:5C:182:ARG:HD2	22:5W:101:THR:HG22	1.99	0.45
11:5K:43:MET:HE3	11:5K:47:ILE:HD11	1.99	0.45
13:5M:7:PRO:HB2	13:5M:34:ILE:HG12	1.99	0.45
15:5O:50:HIS:HE2	15:5O:125:GLU:CD	2.25	0.45
15:5O:318:TRP:CD1	15:5O:318:TRP:H	2.33	0.45
31:5f:2:ASN:O	31:5f:6:ILE:HG13	2.17	0.45
46:6B:160:LEU:HD13	46:6B:164:HIS:CE1	2.52	0.45
46:6B:221:GLU:O	46:6B:222:ARG:C	2.59	0.45
47:6C:47:THR:O	47:6C:48:GLY:C	2.60	0.45
47:6C:50:PHE:O	47:6C:53:MET:HB2	2.16	0.45
47:6C:287:LYS:HE2	47:6C:287:LYS:HB3	1.50	0.45
47:6C:315:MET:O	47:6C:316:MET:C	2.59	0.45
48:6D:151:ALA:O	48:6D:155:GLU:N	2.49	0.45
49:6E:181:LYS:HA	49:6E:184:ILE:HB	1.99	0.45
50:6F:107:LYS:HD3	50:6F:108:GLU:N	2.32	0.45
45:6N:16:VAL:HG22	45:6N:26:ALA:HB2	1.99	0.45
45:6N:19:LEU:HD12	45:6N:23:LEU:HB2	1.99	0.45
45:6N:141:ASN:OD1	49:6V:47:ARG:NH2	2.50	0.45
45:6N:429:GLU:HB3	51:6T:5:GLY:CA	2.46	0.45
46:6O:309:VAL:HA	46:6O:326:THR:HA	1.99	0.45
49:6R:222:CYS:HB3	49:6R:238:CYS:HB3	1.50	0.45
55:8A:100:MET:HE1	57:8C:21:ALA:CA	2.47	0.45
55:8A:261:TYR:HB3	55:8A:333:LYS:HB2	1.99	0.45
55:8A:373:VAL:O	55:8A:377:PHE:HB3	2.17	0.45
55:8A:446:ALA:HB2	56:8B:4:PRO:HA	1.97	0.45
55:8A:511:ILE:O	60:8F:36:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:8A:610:CDL:HB4	75:8A:610:CDL:H512	1.45	0.45
57:8C:178:ALA:HB1	82:8C:304:PGV:H41	1.97	0.45
59:8E:27:TRP:CZ2	60:8F:81:ARG:HB2	2.52	0.45
1:1A:41:PHE:HE2	4:1D:53:PRO:HG2	1.81	0.45
5:1E:163:ASP:CG	5:1E:188:SER:HG	2.23	0.45
8:1H:190:LEU:HD21	8:1H:196:ALA:HB3	1.98	0.45
9:1I:135:PRO:HD3	9:1I:165:ILE:HG22	1.98	0.45
10:1J:18:VAL:HG22	11:1K:14:ILE:HD13	1.99	0.45
12:1L:249:SER:OG	12:1L:336:LYS:HG3	2.16	0.45
12:1L:338:MET:HE2	12:1L:338:MET:HB3	1.78	0.45
13:1M:329:LEU:O	13:1M:332:THR:OG1	2.34	0.45
23:1X:171:MET:HG3	75:1X:201:CDL:HA4	1.97	0.45
29:1d:14:LEU:HD13	29:1d:14:LEU:HA	1.87	0.45
39:1n:97:LYS:HG2	39:1n:173:PRO:HB2	1.97	0.45
40:1o:121:MET:HE3	40:1o:121:MET:HB3	1.90	0.45
45:3A:140:GLU:OE2	49:3I:50:LEU:N	2.41	0.45
45:3N:61:HIS:O	45:3N:130:GLU:OE2	2.34	0.45
45:3N:90:SER:HA	45:3N:95:THR:HG22	1.98	0.45
45:3N:124:ASP:O	45:3N:125:SER:C	2.60	0.45
45:3N:138:LEU:HD11	45:3N:174:VAL:HG21	1.99	0.45
45:3N:289:HIS:HB3	46:3O:83:PHE:HA	1.99	0.45
47:3P:116:GLY:C	83:3P:502:HEM:HBC2	2.41	0.45
49:3R:256:LEU:HG	49:3R:257:ASN:O	2.16	0.45
55:4A:217:THR:HG22	57:4C:188:ILE:HG12	1.99	0.45
82:4A:602:PGV:H61	57:4C:54:MET:HG2	1.99	0.45
56:4B:143:VAL:HG12	56:4B:219:PHE:HD1	1.80	0.45
7:5G:225:THR:HG23	7:5G:240:VAL:HB	1.99	0.45
13:5M:74:PRO:O	13:5M:78:MET:HG3	2.16	0.45
13:5M:310:MET:HG2	13:5M:455:LEU:O	2.16	0.45
15:5O:207:LYS:HA	15:5O:211:LEU:HD12	1.98	0.45
17:5Q:16:LYS:HA	17:5Q:16:LYS:HD2	1.76	0.45
20:5T:66:ASP:HA	20:5T:69:LYS:HE3	1.98	0.45
21:5V:37:ILE:HB	21:5V:44:ARG:HG3	1.99	0.45
23:5X:46:ARG:HA	23:5X:46:ARG:HD2	1.73	0.45
23:5X:90:TYR:HA	26:5a:34:LYS:HG2	1.98	0.45
24:5Y:12:PRO:HG2	24:5Y:15:THR:OG1	2.16	0.45
25:5Z:6:VAL:HG11	43:5r:41:PRO:HB3	1.99	0.45
45:6A:147:ASP:O	45:6A:148:VAL:C	2.60	0.45
45:6A:310:PHE:CD1	45:6A:321:GLY:HA3	2.51	0.45
47:6C:24:PRO:HA	47:6C:217:LYS:CA	2.39	0.45
47:6C:72:ASP:HA	49:6E:144:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:6C:75:TYR:HA	47:6C:77:TRP:CD1	2.52	0.45
47:6C:151:SER:O	47:6C:152:ALA:C	2.60	0.45
48:6D:250:ALA:O	48:6D:251:PRO:C	2.59	0.45
48:6D:307:LEU:O	48:6D:308:VAL:C	2.60	0.45
48:6D:317:SER:O	48:6D:320:LYS:N	2.50	0.45
49:6E:169:TRP:CE2	49:6E:273:VAL:HG12	2.52	0.45
45:6N:108:LYS:O	45:6N:109:ALA:C	2.59	0.45
45:6N:115:ASP:O	45:6N:116:ILE:C	2.60	0.45
45:6N:151:ASP:O	45:6N:154:HIS:HB2	2.17	0.45
45:6N:194:ARG:NH2	45:6N:223:TYR:HE2	2.15	0.45
45:6N:237:THR:HG21	49:6R:92:ARG:HH22	1.81	0.45
46:6O:169:ARG:CG	46:6O:238:LYS:HB3	2.44	0.45
55:8A:63:PHE:CZ	55:8A:126:TRP:HA	2.51	0.45
55:8A:230:LEU:O	55:8A:233:HIS:HB2	2.17	0.45
55:8A:314:ILE:HB	55:8A:315:PRO:HD3	1.99	0.45
89:8A:611:PSC:H281	56:8B:64:ILE:HG21	1.98	0.45
64:8J:31:LEU:O	64:8J:35:THR:HG22	2.17	0.45
1:1A:4:MET:HE2	1:1A:4:MET:HB2	1.74	0.45
3:1C:53:HIS:NE2	21:1V:104:GLU:HB3	2.32	0.45
3:1C:203:TRP:HE1	7:1G:115:ASP:CG	2.23	0.45
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.99	0.45
4:1D:260:LEU:HD22	4:1D:265:ILE:HD12	1.99	0.45
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.99	0.45
7:1G:256:GLU:O	7:1G:394:ARG:NH2	2.47	0.45
7:1G:346:GLU:HG2	7:1G:531:CYS:SG	2.57	0.45
7:1G:383:ASN:ND2	7:1G:413:VAL:HG21	2.31	0.45
13:1M:77:LEU:O	13:1M:81:GLN:HG2	2.17	0.45
13:1M:425:ASN:CG	38:1m:57:GLY:HA2	2.41	0.45
16:1P:81:ILE:O	16:1P:85:VAL:HB	2.16	0.45
16:1P:270:PHE:CD2	16:1P:278:TRP:HB2	2.52	0.45
20:1U:55:GLU:OE1	20:1U:62:ILE:N	2.46	0.45
32:1g:37:LEU:HD22	32:1g:40:LYS:NZ	2.22	0.45
39:1n:54:LYS:HE3	45:3N:20:ASP:O	2.17	0.45
41:1p:166:ARG:HA	41:1p:170:LYS:NZ	2.28	0.45
46:3B:56:ARG:HD2	46:3B:103:GLU:HG2	1.98	0.45
46:3B:73:SER:O	46:3B:74:SER:HB3	2.17	0.45
47:3C:301:LEU:HD23	47:3C:304:MET:HE2	1.99	0.45
48:3D:227:THR:HB	52:3H:79:CYS:SG	2.58	0.45
45:3N:60:GLU:O	45:3N:63:ALA:N	2.38	0.45
45:3N:64:PHE:CZ	45:3N:86:LEU:HB2	2.43	0.45
45:3N:117:VAL:HG11	45:3N:195:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:246:ASP:O	46:3O:427:SER:HA	2.17	0.45
49:3R:179:ARG:HB2	49:3R:183:GLU:HB2	1.99	0.45
51:3T:71:ARG:HA	51:3T:71:ARG:HD2	1.81	0.45
82:4A:601:PGV:H011	82:4A:601:PGV:H201	1.54	0.45
58:4D:52:SER:HB2	58:4D:55:GLU:HG3	1.99	0.45
64:4J:4:ARG:O	64:4J:8:LYS:HE2	2.17	0.45
64:4J:31:LEU:O	64:4J:35:THR:HG22	2.17	0.45
8:5H:156:MET:SD	25:5Z:50:MET:HG2	2.57	0.45
9:5I:31:VAL:HG13	71:5I:204:PC1:H371	1.99	0.45
9:5I:70:TYR:C	9:5I:72:SER:H	2.25	0.45
10:5J:19:GLY:HA2	10:5J:93:PHE:HD2	1.81	0.45
16:5P:144:ARG:HG2	16:5P:147:ARG:HH12	1.81	0.45
16:5P:274:PRO:HG2	16:5P:275:PHE:CZ	2.51	0.45
19:5S:36:ILE:HD13	19:5S:54:ILE:HD13	1.98	0.45
20:5U:37:MET:N	20:5U:37:MET:SD	2.89	0.45
35:5j:56:PRO:HA	35:5j:59:TRP:CE3	2.52	0.45
40:5o:102:GLU:OE1	40:5o:102:GLU:HA	2.17	0.45
45:6A:36:THR:HA	45:6A:101:ALA:H	1.82	0.45
45:6A:283:THR:HB	49:6I:74:ALA:H	1.81	0.45
46:6B:56:ARG:HA	46:6B:171:ALA:CA	2.47	0.45
46:6B:77:THR:HG21	46:6B:126:VAL:HG13	1.99	0.45
46:6B:113:ARG:NH2	46:6B:210:GLY:HA3	2.22	0.45
47:6C:152:ALA:O	47:6C:153:ILE:C	2.60	0.45
47:6C:374:ASN:O	47:6C:375:ASN:C	2.59	0.45
48:6D:160:ASP:H	48:6D:169:PHE:N	2.16	0.45
48:6D:204:ILE:HD13	48:6D:204:ILE:HA	1.69	0.45
45:6N:91:THR:OG1	45:6N:94:HIS:HB2	2.17	0.45
45:6N:199:ALA:HB1	45:6N:208:LEU:HD13	1.99	0.45
45:6N:329:MET:HA	45:6N:430:GLN:NE2	2.29	0.45
45:6N:355:VAL:HA	45:6N:358:LYS:HD3	1.99	0.45
46:6O:369:LEU:O	46:6O:370:MET:C	2.60	0.45
46:6O:381:GLU:O	46:6O:385:GLN:HG2	2.16	0.45
55:8A:3:VAL:HG22	55:8A:7:LEU:HD22	1.99	0.45
55:8A:359:ALA:O	55:8A:361:SER:N	2.50	0.45
58:8D:83:GLY:HA3	65:8K:17:ILE:HG22	1.99	0.45
66:8L:28:TYR:CD2	82:8L:101:PGV:H302	2.52	0.45
2:1B:87:ILE:O	2:1B:89:ALA:N	2.50	0.44
6:1F:355:LYS:HG3	6:1F:370:ASP:HA	1.98	0.44
7:1G:60:GLU:OE1	7:1G:78:ASN:ND2	2.46	0.44
13:1M:36:LEU:HB2	32:1g:69:VAL:HG22	1.99	0.44
19:1S:30:GLN:HG2	19:1S:33:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:24:LYS:HD3	20:1T:24:LYS:HA	1.66	0.44
37:1l:124:SER:O	37:1l:124:SER:OG	2.31	0.44
47:3C:22:PRO:HA	51:3G:6:PHE:HZ	1.82	0.44
47:3C:128:PHE:CE1	47:3C:146:ILE:HD12	2.52	0.44
45:3N:64:PHE:CE1	45:3N:86:LEU:HD12	2.23	0.44
45:3N:72:GLY:O	45:3N:75:LEU:HB2	2.16	0.44
45:3N:213:GLN:O	45:3N:217:SER:HB3	2.16	0.44
46:3O:35:ILE:HD13	46:3O:206:LEU:HB3	1.99	0.44
46:3O:381:GLU:O	46:3O:385:GLN:HG3	2.17	0.44
55:4A:208:MET:HE2	57:4C:97:PHE:CD1	2.52	0.44
4:5D:371:LYS:HE3	4:5D:422:ASP:CG	2.42	0.44
12:5L:602:PHE:CE2	69:5Y:204:3PE:H382	2.51	0.44
23:5X:149:PRO:HA	30:5e:46:ILE:HG22	1.98	0.44
26:5a:27:HIS:CE1	26:5a:36:LYS:HD3	2.52	0.44
33:5h:40:ILE:HG13	71:5h:202:PC1:H2D2	1.99	0.44
36:5k:29:GLU:O	36:5k:33:GLU:HG3	2.18	0.44
45:6A:161:THR:HG21	45:6A:235:ARG:N	2.32	0.44
47:6C:62:ALA:O	47:6C:66:VAL:N	2.46	0.44
47:6C:224:TYR:CD1	47:6C:227:LYS:HD3	2.52	0.44
47:6C:240:LEU:HB3	47:6C:244:LEU:HD12	1.99	0.44
47:6C:288:LEU:O	47:6C:292:LEU:HG	2.17	0.44
47:6C:342:PRO:HG2	51:6G:68:PHE:HE2	1.83	0.44
48:6D:232:ARG:NE	48:6D:233:GLU:HG2	2.32	0.44
48:6D:327:ARG:HD3	51:6G:16:ILE:HD12	1.98	0.44
49:6E:151:LYS:NZ	49:6E:152:ILE:CD1	2.80	0.44
45:6N:91:THR:OG1	45:6N:94:HIS:N	2.50	0.44
45:6N:170:PRO:O	45:6N:171:SER:C	2.60	0.44
45:6N:223:TYR:O	45:6N:224:VAL:C	2.60	0.44
45:6N:408:ARG:HH21	45:6N:409:GLU:HB2	1.82	0.44
46:6O:52:LYS:HA	46:6O:104:SER:HA	1.99	0.44
55:8A:417:MET:O	55:8A:418:PHE:C	2.60	0.44
82:8A:602:PGV:H261	82:8A:602:PGV:H232	1.44	0.44
57:8C:167:ILE:O	57:8C:171:VAL:HG23	2.18	0.44
61:8G:33:LEU:O	61:8G:37:LEU:HG	2.16	0.44
12:1L:473:PRO:HG2	12:1L:475:MET:HE3	1.99	0.44
69:1M:503:3PE:H242	38:1m:101:TYR:CZ	2.52	0.44
14:1N:107:GLY:HA2	14:1N:111:PHE:O	2.18	0.44
14:1N:222:SER:HA	14:1N:237:MET:CE	2.47	0.44
21:1V:22:ARG:NH2	21:1V:84:GLU:OE2	2.51	0.44
21:1V:23:LEU:HD21	21:1V:79:VAL:HG12	1.99	0.44
23:1X:149:PRO:HA	30:1e:46:ILE:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:4:LEU:HG	31:1f:5:GLN:N	2.32	0.44
36:1k:29:GLU:O	36:1k:33:GLU:HG3	2.17	0.44
45:3A:388:ARG:HH22	45:3A:394:GLU:CD	2.24	0.44
47:3C:67:THR:HG23	48:3D:203:TYR:CE2	2.53	0.44
47:3C:237:LEU:O	47:3C:241:ILE:HG13	2.16	0.44
47:3C:328:LEU:O	47:3C:332:LEU:HG	2.18	0.44
52:3H:100:ASN:N	52:3H:100:ASN:OD1	2.49	0.44
49:3R:130:LYS:NZ	54:3X:34:TRP:O	2.35	0.44
49:3R:167:PHE:HB2	49:3R:174:LEU:HB3	1.99	0.44
56:4B:186:SER:OG	56:4B:188:ARG:O	2.34	0.44
57:4C:167:ILE:O	57:4C:171:VAL:HG23	2.17	0.44
57:4C:219:LEU:HD21	82:4C:301:PGV:H231	1.98	0.44
75:4C:308:CDL:H152	75:4C:308:CDL:H211	1.99	0.44
62:4H:39:CYS:HG	62:4H:53:CYS:HG	1.55	0.44
3:5C:175:ARG:NH2	3:5C:177:ASP:OD2	2.50	0.44
7:5G:276:ARG:NH1	7:5G:680:ALA:O	2.46	0.44
9:5I:49:ASN:O	9:5I:53:GLU:N	2.43	0.44
10:5J:23:LYS:HE2	11:5K:23:ARG:HG3	1.99	0.44
10:5J:92:ALA:HB2	69:5J:201:3PE:H252	1.99	0.44
12:5L:544:MET:CE	13:5M:271:MET:HE1	2.47	0.44
13:5M:105:PHE:HE2	69:5N:902:3PE:H3I1	1.81	0.44
13:5M:188:ASN:HA	13:5M:253:LEU:HD21	1.99	0.44
16:5P:21:ALA:HA	16:5P:90:VAL:O	2.17	0.44
20:5T:7:THR:HG23	20:5T:10:ALA:H	1.82	0.44
20:5U:73:PRO:O	20:5U:77:VAL:HG12	2.16	0.44
24:5Y:107:TYR:HB2	69:5Y:206:3PE:O13	2.16	0.44
45:6A:347:THR:O	54:6Y:16:ASN:HB3	2.17	0.44
46:6B:38:LEU:HG	46:6B:40:ASN:HD22	1.81	0.44
47:6C:93:CYS:O	47:6C:94:LEU:C	2.60	0.44
48:6D:165:ASP:HB3	48:6Q:103:ALA:CB	2.47	0.44
48:6D:275:VAL:O	48:6D:279:LEU:HG	2.17	0.44
52:6H:48:GLN:OE1	52:6H:97:LYS:NZ	2.49	0.44
45:6N:99:ILE:CD1	45:6N:113:LEU:HD23	2.42	0.44
45:6N:156:THR:HG22	45:6N:241:ILE:HD12	1.98	0.44
46:6O:50:PHE:HZ	46:6O:380:ASP:HA	1.83	0.44
46:6O:279:LEU:HB3	46:6O:295:LEU:HD11	1.98	0.44
46:6O:307:PHE:N	49:6V:55:LEU:HD23	2.32	0.44
47:6P:92:ILE:HG13	47:6P:272:TRP:CH2	2.52	0.44
55:8A:390:MET:O	55:8A:391:GLY:C	2.60	0.44
82:8G:101:PGV:H91	82:8G:101:PGV:H282	1.99	0.44
4:1D:299:CYS:O	4:1D:303:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:188:ASN:HA	13:1M:253:LEU:HD21	1.99	0.44
14:1N:157:MET:O	14:1N:161:SER:OG	2.32	0.44
16:1P:325:ARG:HA	16:1P:325:ARG:HD2	1.80	0.44
25:1Z:31:SER:O	25:1Z:35:MET:HG3	2.17	0.44
26:1a:34:LYS:HE2	26:1a:34:LYS:HB2	1.80	0.44
69:1d:201:3PE:H2C2	69:1d:201:3PE:H2G2	1.98	0.44
41:1p:131:PHE:O	41:1p:135:SER:OG	2.24	0.44
46:3B:276:GLN:HG2	46:3B:281:ALA:HB2	1.99	0.44
46:3B:385:GLN:OE1	46:3B:393:VAL:HG22	2.16	0.44
47:3C:138:MET:CB	47:3C:254:ASP:HB2	2.47	0.44
47:3C:373:GLU:O	47:3C:374:ASN:C	2.60	0.44
48:3D:303:LEU:HD13	48:3D:307:LEU:HD12	1.99	0.44
49:3E:241:SER:HA	49:3E:252:GLY:HA3	1.99	0.44
53:3J:38:GLN:OE1	54:3Y:47:TYR:OH	2.28	0.44
45:3N:401:GLU:O	45:3N:402:VAL:C	2.61	0.44
48:3Q:195:GLU:OE2	48:3Q:201:ARG:NE	2.45	0.44
48:3Q:233:ARG:HG3	50:3S:71:ARG:HH22	1.82	0.44
55:4A:361:SER:HG	56:4B:84:LEU:HD13	1.82	0.44
56:4B:62:GLU:O	56:4B:66:THR:OG1	2.31	0.44
67:4M:39:HIS:HA	67:4M:42:ARG:HG2	1.97	0.44
3:5C:203:TRP:HE1	7:5G:115:ASP:CG	2.23	0.44
4:5D:404:LYS:HE2	4:5D:404:LYS:HB3	1.57	0.44
6:5F:256:PHE:CD1	6:5F:332:ALA:HB1	2.53	0.44
7:5G:252:PRO:HB3	7:5G:263:ILE:HG23	1.99	0.44
13:5M:46:GLY:HA2	32:5g:84:ARG:HG2	1.99	0.44
13:5M:71:TRP:O	13:5M:74:PRO:HD2	2.17	0.44
14:5N:313:MET:HE3	14:5N:313:MET:HB2	1.84	0.44
15:5O:14:THR:HA	15:5O:17:LYS:HE2	1.99	0.44
19:5S:18:ILE:HD11	19:5S:52:ILE:HG12	2.00	0.44
20:5U:52:MET:HE1	39:5n:23:LEU:HB3	1.98	0.44
21:5V:22:ARG:NH2	21:5V:84:GLU:OE2	2.50	0.44
22:5W:81:LEU:HA	22:5W:84:ILE:HD12	2.00	0.44
40:5o:50:LEU:HD11	40:5o:63:ILE:HG13	1.99	0.44
41:5p:168:ALA:O	41:5p:171:GLU:HG3	2.17	0.44
45:6A:113:LEU:HA	45:6A:116:ILE:HD12	1.99	0.44
45:6A:260:PRO:HG2	45:6A:267:ASN:HA	1.99	0.44
46:6B:321:LEU:HD23	46:6B:321:LEU:HA	1.76	0.44
46:6B:385:GLN:O	46:6B:386:ALA:C	2.61	0.44
47:6C:329:VAL:HB	51:6G:54:PHE:CE1	2.52	0.44
48:6D:162:PRO:HB2	48:6Q:99:GLU:HG2	2.00	0.44
48:6D:327:ARG:HE	48:6D:327:ARG:HB3	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:6E:248:ARG:HA	49:6E:257:ASN:HB3	1.99	0.44
45:6N:4:TYR:C	45:6N:8:LEU:H	2.26	0.44
45:6N:33:PRO:CD	45:6N:34:THR:H	2.30	0.44
45:6N:61:HIS:N	46:6O:287:ARG:HH22	2.15	0.44
45:6N:156:THR:O	45:6N:157:ALA:C	2.59	0.44
45:6N:170:PRO:CD	45:6N:170:PRO:O	2.65	0.44
46:6O:36:ALA:HB3	46:6O:207:ILE:HA	2.00	0.44
46:6O:257:LEU:HD11	46:6O:422:LYS:HB2	2.00	0.44
55:8A:46:THR:O	55:8A:47:LEU:C	2.60	0.44
55:8A:296:GLY:CA	62:8H:23:GLN:HB3	2.47	0.44
55:8A:484:ALA:HB3	67:8M:2:TYR:CD1	2.53	0.44
75:8D:201:CDL:H151	75:8D:201:CDL:H122	1.74	0.44
2:1B:80:PRO:HD3	4:1D:54:GLN:HE22	1.83	0.44
2:1B:98:PRO:O	2:1B:101:ARG:N	2.49	0.44
4:1D:371:LYS:HE3	4:1D:422:ASP:CG	2.42	0.44
7:1G:306:MET:HG2	7:1G:542:PHE:CG	2.52	0.44
7:1G:648:LEU:HD13	19:1S:41:VAL:HG13	1.99	0.44
20:1U:73:PRO:O	20:1U:77:VAL:HG12	2.17	0.44
26:1a:6:LEU:HB2	75:1q:201:CDL:H191	2.00	0.44
28:1c:17:VAL:O	28:1c:21:LEU:HD22	2.18	0.44
34:1i:55:PRO:HG2	82:8B:301:PGV:H142	1.99	0.44
37:1l:98:TRP:HB3	38:1m:6:LYS:HZ2	1.82	0.44
40:1o:30:PHE:CG	40:1o:33:ARG:HD3	2.52	0.44
47:3C:119:LEU:HD22	83:3C:502:HEM:HBB2	1.99	0.44
47:3C:256:TYR:O	47:3C:257:THR:C	2.58	0.44
45:3N:27:SER:OG	45:3N:205:HIS:CE1	2.67	0.44
45:3N:33:PRO:CD	45:3N:34:THR:N	2.71	0.44
47:3P:92:ILE:HG13	47:3P:272:TRP:CH2	2.52	0.44
55:4A:300:ASP:OD2	68:4N:35:ARG:NH1	2.46	0.44
82:4L:101:PGV:C12	82:4L:101:PGV:H292	2.47	0.44
13:5M:1:FME:SD	13:5M:41:LEU:HD11	2.58	0.44
13:5M:95:TYR:CE2	13:5M:132:ILE:HD12	2.53	0.44
13:5M:190:TRP:CD1	24:5Y:126:MET:HG2	2.53	0.44
69:5d:201:3PE:H32	69:5d:201:3PE:H322	1.37	0.44
37:5l:26:LYS:NZ	37:5l:46:ASP:OD2	2.41	0.44
44:5s:75:HIS:ND1	44:5s:75:HIS:N	2.64	0.44
45:6A:174:VAL:HA	45:6A:177:LEU:HD12	1.99	0.44
46:6B:21:PRO:O	46:6B:22:GLN:C	2.59	0.44
46:6B:307:PHE:N	49:6I:52:ARG:HG3	2.27	0.44
47:6C:378:LYS:HE3	47:6C:378:LYS:HB2	1.54	0.44
53:6J:54:LYS:HB2	53:6J:54:LYS:HE2	1.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:149:VAL:HG22	45:6N:425:LEU:HG	1.99	0.44
45:6N:203:VAL:O	45:6N:204:GLU:C	2.60	0.44
48:6Q:28:ARG:HE	48:6Q:185:ASP:CG	2.25	0.44
49:6R:167:PHE:HB2	49:6R:174:LEU:HB3	1.99	0.44
55:8A:58:VAL:O	55:8A:59:THR:C	2.60	0.44
55:8A:131:PRO:CG	56:8B:176:PRO:HG2	2.41	0.44
82:8C:302:PGV:H292	82:8C:302:PGV:H262	1.39	0.44
1:1A:6:THR:O	1:1A:7:LEU:C	2.60	0.44
69:1A:201:3PE:H322	69:1A:201:3PE:H32	1.75	0.44
4:1D:165:THR:OG1	8:1H:275:ALA:O	2.35	0.44
8:1H:179:TRP:CD2	8:1H:180:PRO:HD3	2.52	0.44
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.53	0.44
10:1J:107:ALA:O	10:1J:111:GLU:HG3	2.17	0.44
12:1L:296:ASN:H	39:1n:77:GLN:HE22	1.66	0.44
13:1M:43:ASN:HB2	32:1g:80:LEU:HD22	2.00	0.44
15:1O:195:THR:HG23	15:1O:198:TYR:H	1.83	0.44
25:1Z:110:VAL:CG2	30:1e:70:LYS:HB2	2.48	0.44
33:1h:111:ARG:HD3	81:1h:201:AME:HT23	1.98	0.44
37:1l:27:TYR:O	37:1l:76:PRO:HG3	2.18	0.44
47:3C:55:TYR:CD1	83:3C:501:HEM:HAD1	2.53	0.44
47:3C:218:ILE:HB	47:3C:219:PRO:HD2	2.00	0.44
49:3E:169:TRP:CE2	49:3E:273:VAL:HG12	2.52	0.44
50:3F:40:LYS:HA	50:3F:92:TRP:CD1	2.51	0.44
45:3N:35:CYS:SG	45:3N:203:VAL:CG2	2.94	0.44
45:3N:256:ALA:O	45:3N:420:PRO:HB2	2.17	0.44
46:3O:329:GLN:O	46:3O:330:ALA:C	2.60	0.44
47:3P:226:ILE:HD12	47:3P:226:ILE:HA	1.88	0.44
48:3Q:126:TYR:OH	84:3Q:501:HEC:O2A	2.19	0.44
49:3R:191:GLU:O	49:3R:194:GLN:HG2	2.16	0.44
56:4B:129:LYS:HB2	56:4B:132:GLU:HG3	1.99	0.44
57:4C:134:THR:HB	57:4C:249:TRP:HE1	1.83	0.44
3:5C:38:GLN:HG2	21:5V:102:LEU:HD21	2.00	0.44
7:5G:198:ASN:O	7:5G:202:ILE:HG23	2.18	0.44
8:5H:179:TRP:CD2	8:5H:180:PRO:HD3	2.52	0.44
9:5I:95:GLU:HG3	9:5I:108:ARG:HD2	1.99	0.44
12:5L:296:ASN:H	39:5n:77:GLN:HE22	1.66	0.44
12:5L:473:PRO:HG2	12:5L:475:MET:HE3	1.99	0.44
13:5M:77:LEU:O	13:5M:81:GLN:HG2	2.18	0.44
15:5O:315:LYS:HA	15:5O:315:LYS:HD2	1.85	0.44
16:5P:136:ASN:HD22	16:5P:289:MET:HE3	1.83	0.44
25:5Z:110:VAL:CG2	30:5e:70:LYS:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:5e:64:GLU:O	30:5e:68:ARG:HA	2.16	0.44
47:6C:322:GLN:HB3	51:6G:50:VAL:HG22	2.00	0.44
48:6D:222:TYR:CE2	48:6D:252:PRO:HD3	2.52	0.44
48:6D:233:GLU:O	48:6D:234:GLY:C	2.61	0.44
45:6N:185:TYR:O	45:6N:189:HIS:N	2.41	0.44
46:6O:65:THR:O	46:6O:66:SER:C	2.61	0.44
46:6O:202:ALA:H	46:6O:229:GLY:H	1.65	0.44
46:6O:243:GLU:HA	46:6O:424:MET:O	2.17	0.44
49:6R:179:ARG:HB2	49:6R:183:GLU:HB2	1.99	0.44
54:6Y:7:GLY:H	54:6Y:10:TYR:HB2	1.83	0.44
54:6Y:42:LEU:HD22	54:6Y:42:LEU:HA	1.80	0.44
55:8A:145:LEU:HD23	55:8A:145:LEU:HA	1.87	0.44
55:8A:157:SER:O	55:8A:158:ILE:C	2.60	0.44
55:8A:218:THR:O	55:8A:219:PHE:C	2.60	0.44
55:8A:229:ILE:HG22	57:8C:103:HIS:CE1	2.51	0.44
55:8A:346:PHE:HZ	75:8B:302:CDL:H411	1.82	0.44
55:8A:386:VAL:HG13	55:8A:390:MET:SD	2.58	0.44
55:8A:504:THR:HB	55:8A:505:PHE:CD2	2.53	0.44
2:1B:113:VAL:HB	2:1B:142:VAL:HA	1.99	0.44
3:1C:38:GLN:HG2	21:1V:102:LEU:HD21	2.00	0.44
5:1E:181:ILE:H	5:1E:181:ILE:HG13	1.50	0.44
9:1I:31:VAL:HG13	71:1I:204:PC1:H371	1.99	0.44
9:1I:95:GLU:HG3	9:1I:108:ARG:HD2	1.99	0.44
13:1M:7:PRO:HB2	13:1M:34:ILE:HG12	1.99	0.44
13:1M:190:TRP:CD1	24:1Y:126:MET:HG2	2.53	0.44
15:1O:207:LYS:HA	15:1O:211:LEU:HD12	1.98	0.44
19:1S:90:LEU:HA	19:1S:90:LEU:HD23	1.77	0.44
21:1V:37:ILE:HB	21:1V:44:ARG:HG3	1.99	0.44
22:1W:81:LEU:HA	22:1W:84:ILE:HD12	2.00	0.44
24:1Y:78:GLN:HE21	51:3T:64:GLN:HE22	1.66	0.44
28:1c:38:ASP:OD2	29:1d:77:LYS:NZ	2.33	0.44
38:1m:2:PHE:HB3	39:1n:72:TYR:CG	2.53	0.44
46:3B:36:ALA:O	46:3B:207:ILE:HA	2.17	0.44
47:3C:154:PRO:C	47:3C:156:ILE:N	2.75	0.44
47:3C:252:ASP:O	47:3C:255:ASN:HB2	2.17	0.44
45:3N:127:ILE:O	45:3N:131:ARG:HG3	2.18	0.44
45:3N:158:PHE:CZ	45:3N:314:TYR:CE2	3.03	0.44
45:3N:181:ASP:CB	45:3N:185:TYR:HE2	2.21	0.44
45:3N:395:TRP:O	45:3N:399:ILE:HG13	2.18	0.44
45:3N:433:ASP:HB2	47:3P:219:PRO:HG3	1.98	0.44
55:4A:194:LEU:HD23	55:4A:285:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:4J:7:GLU:HG3	64:4J:8:LYS:N	2.33	0.44
66:4L:28:TYR:CD2	82:4L:101:PGV:H302	2.52	0.44
12:5L:248:HIS:HA	12:5L:253:VAL:HG13	1.99	0.44
13:5M:43:ASN:HB2	32:5g:80:LEU:HD22	2.00	0.44
13:5M:269:MET:HG3	13:5M:399:ASN:CG	2.42	0.44
14:5N:320:THR:HG21	15:5O:265:ASN:HA	1.98	0.44
27:5b:66:PRO:HB3	27:5b:73:GLN:HB2	1.99	0.44
31:5f:4:LEU:HG	31:5f:5:GLN:N	2.33	0.44
37:5l:27:TYR:O	37:5l:76:PRO:HG3	2.18	0.44
39:5n:45:ALA:O	39:5n:49:GLU:HG3	2.16	0.44
42:5q:22:GLY:O	42:5q:26:VAL:HG22	2.18	0.44
45:6A:144:SER:HB2	49:6I:47:ARG:HD2	2.00	0.44
45:6A:153:LEU:O	45:6A:154:HIS:C	2.60	0.44
45:6A:319:LEU:O	45:6A:321:GLY:N	2.51	0.44
47:6C:79:ILE:H	47:6C:79:ILE:HG12	1.34	0.44
47:6C:213:SER:HB3	47:6C:216:ASP:HB2	2.00	0.44
47:6C:334:THR:CB	51:6G:57:PHE:HE1	2.30	0.44
48:6D:210:GLY:C	48:6D:214:TYR:HB3	2.43	0.44
45:6N:37:VAL:HG21	45:6N:106:LEU:CD2	2.48	0.44
45:6N:62:LEU:HD11	45:6N:182:LEU:HD13	2.00	0.44
46:6O:111:CYS:SG	46:6O:112:LEU:N	2.89	0.44
55:8A:72:PRO:O	55:8A:74:MET:N	2.50	0.44
55:8A:165:ILE:O	55:8A:166:THR:C	2.60	0.44
63:8I:49:ASP:OD1	63:8I:49:ASP:N	2.44	0.44
1:1A:54:LYS:H	1:1A:54:LYS:HG3	1.56	0.44
1:1A:95:LEU:HD13	8:1H:302:MET:HG3	1.99	0.44
4:1D:110:SER:HA	4:1D:145:THR:HG22	2.00	0.44
6:1F:20:ARG:NH2	6:1F:269:GLU:O	2.49	0.44
6:1F:229:ALA:O	6:1F:232:PRO:HD2	2.18	0.44
6:1F:261:HIS:CD2	6:1F:337:MET:HA	2.51	0.44
8:1H:156:MET:SD	25:1Z:50:MET:HG2	2.57	0.44
10:1J:125:TRP:CZ2	25:1Z:133:ILE:HD12	2.53	0.44
13:1M:95:TYR:CE2	13:1M:132:ILE:HD12	2.53	0.44
15:1O:22:SER:O	15:1O:22:SER:OG	2.31	0.44
16:1P:44:GLN:HE21	18:1R:23:TYR:HE2	1.66	0.44
71:1P:401:PC1:H321	71:1P:401:PC1:H31	1.44	0.44
40:1o:102:GLU:OE1	40:1o:102:GLU:HA	2.17	0.44
42:1q:22:GLY:O	42:1q:26:VAL:HG22	2.18	0.44
47:3C:106:SER:HA	47:3C:313:ARG:HH21	1.83	0.44
47:3C:240:LEU:HD12	48:3D:297:MET:HG3	2.00	0.44
50:3F:61:ARG:HB3	46:3O:135:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:36:THR:HG21	45:3N:372:THR:O	2.18	0.44
45:3N:61:HIS:CE1	45:3N:134:ILE:CG1	2.90	0.44
45:3N:270:LEU:O	45:3N:271:GLN:C	2.60	0.44
45:3N:310:PHE:H	45:3N:321:GLY:C	2.21	0.44
45:3N:320:LEU:HG	45:3N:415:PHE:CZ	2.53	0.44
46:3O:135:TRP:NE1	46:3O:136:GLU:HG3	2.33	0.44
47:3P:141:TRP:CD1	47:3P:265:PRO:HD3	2.53	0.44
49:3R:150:SER:HB2	49:3R:170:ARG:HD3	1.99	0.44
49:3R:222:CYS:HB3	49:3R:238:CYS:HB3	1.50	0.44
75:4C:308:CDL:HB61	75:4C:308:CDL:H542	2.00	0.44
1:5A:1:FME:O1	1:5A:2:ASN:N	2.50	0.44
2:5B:50:PHE:CE1	2:5B:96:MET:HE2	2.53	0.44
4:5D:209:ASP:O	4:5D:213:GLU:HG2	2.17	0.44
4:5D:260:LEU:HD22	4:5D:265:ILE:HD12	1.99	0.44
8:5H:54:LYS:HB3	8:5H:54:LYS:HE3	1.80	0.44
10:5J:113:VAL:HG22	10:5J:119:PHE:HB2	2.00	0.44
12:5L:241:THR:HG21	12:5L:344:GLY:HA3	1.98	0.44
12:5L:529:TYR:HB3	12:5L:530:PRO:HD3	1.99	0.44
69:5M:503:3PE:H2B1	69:5M:503:3PE:H282	1.83	0.44
19:5S:30:GLN:HG2	19:5S:33:ARG:NH1	2.32	0.44
24:5Y:124:VAL:HG22	69:5Y:203:3PE:H232	2.00	0.44
38:5m:2:PHE:HB3	39:5n:72:TYR:CG	2.53	0.44
38:5m:122:GLN:O	41:5p:139:GLN:NE2	2.44	0.44
39:5n:174:ARG:NH2	39:5n:177:PRO:O	2.51	0.44
45:6A:33:PRO:O	45:6A:34:THR:C	2.60	0.44
45:6A:73:SER:O	45:6A:74:ALA:C	2.60	0.44
45:6A:92:ARG:CZ	45:6A:166:SER:HA	2.48	0.44
47:6C:26:ASN:HB2	47:6C:207:ASN:HB2	2.00	0.44
47:6C:377:LEU:HD22	47:6C:378:LYS:HE2	1.99	0.44
49:6E:173:PRO:O	49:6E:215:GLY:N	2.41	0.44
53:6J:11:TYR:HA	53:6J:15:PHE:HB3	2.00	0.44
53:6J:30:LEU:HD13	53:6J:30:LEU:HA	1.74	0.44
45:6N:136:GLN:CD	49:6V:50:LEU:O	2.61	0.44
45:6N:158:PHE:CZ	45:6N:317:THR:HG21	2.53	0.44
46:6O:266:SER:O	46:6O:267:ALA:C	2.60	0.44
46:6O:299:VAL:O	46:6O:300:ALA:C	2.61	0.44
46:6O:385:GLN:HB2	46:6O:392:TYR:HA	2.00	0.44
55:8A:92:MET:HE1	55:8A:164:PHE:HA	1.99	0.44
56:8B:44:LEU:HD11	63:8I:20:HIS:CG	2.53	0.44
56:8B:65:TRP:CD1	56:8B:65:TRP:C	2.96	0.44
56:8B:118:PHE:CD2	56:8B:140:ASN:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:8C:26:LEU:HD21	64:8J:42:GLY:C	2.42	0.44
82:8C:304:PGV:H271	82:8C:304:PGV:H242	1.59	0.44
90:8C:306:PEK:O14	90:8C:306:PEK:N	2.38	0.44
2:1B:127:HIS:CG	9:1I:115:LYS:HD3	2.53	0.44
3:1C:83:VAL:HG12	3:1C:85:THR:HG22	2.00	0.44
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.17	0.44
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.58	0.44
7:1G:154:ILE:O	7:1G:156:CYS:N	2.51	0.44
10:1J:118:LYS:HZ1	11:1K:1:FME:HCN	1.83	0.44
12:1L:201:ILE:O	12:1L:206:ASN:HB2	2.18	0.44
13:1M:1:FME:SD	13:1M:41:LEU:HD11	2.58	0.44
16:1P:21:ALA:HA	16:1P:90:VAL:O	2.17	0.44
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.43	0.44
41:1p:168:ALA:O	41:1p:171:GLU:HG3	2.17	0.44
47:3C:264:THR:O	49:3R:220:LEU:HD13	2.18	0.44
53:3J:9:ARG:NH1	53:3J:9:ARG:HG2	2.33	0.44
45:3N:46:ARG:NH1	45:3N:93:GLU:OE2	2.50	0.44
46:3O:45:SER:CB	46:3O:113:ARG:HB2	2.48	0.44
46:3O:143:GLN:HE21	46:3O:147:ASP:HB2	1.81	0.44
49:3R:184:ILE:HG21	49:3R:208:PRO:HB3	2.00	0.44
82:4C:303:PGV:H52	82:4C:303:PGV:H281	1.99	0.44
58:4D:83:GLY:HA3	65:4K:17:ILE:HG22	1.99	0.44
12:5L:54:PHE:CZ	12:5L:84:TYR:HB2	2.53	0.44
12:5L:201:ILE:O	12:5L:206:ASN:HB2	2.18	0.44
12:5L:225:ALA:HB1	12:5L:230:HIS:HA	2.00	0.44
15:5O:195:THR:HG23	15:5O:198:TYR:H	1.82	0.44
15:5O:207:LYS:HE2	15:5O:207:LYS:HB2	1.87	0.44
18:5R:38:ASN:HB3	18:5R:43:LEU:HD11	1.98	0.44
33:5h:111:ARG:HD3	81:5h:201:AME:HT23	1.99	0.44
45:6A:46:ARG:HD2	45:6A:93:GLU:HB3	1.99	0.44
45:6A:246:ASP:O	45:6A:247:ALA:C	2.60	0.44
47:6C:350:ILE:O	47:6C:351:GLY:C	2.61	0.44
49:6E:151:LYS:NZ	49:6E:152:ILE:HD12	2.33	0.44
46:6O:83:PHE:CZ	46:6O:87:ARG:HG2	2.53	0.44
46:6O:85:ILE:HG23	46:6O:122:PHE:HB3	2.00	0.44
46:6O:87:ARG:HD3	46:6O:87:ARG:HA	1.46	0.44
46:6O:236:LYS:HA	46:6O:236:LYS:HD2	1.62	0.44
49:6R:155:LYS:HB2	49:6R:271:VAL:HG23	1.99	0.44
49:6R:211:VAL:HG11	49:6R:245:ALA:O	2.18	0.44
55:8A:16:GLY:O	55:8A:19:TYR:HB2	2.17	0.44
55:8A:162:ILE:O	55:8A:163:ASN:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:169:ILE:HG22	57:8C:81:TYR:CE2	2.53	0.44
55:8A:316:THR:HG21	85:8A:606:HEA:C14	2.48	0.44
82:8C:303:PGV:H291	82:8C:303:PGV:H321	1.39	0.44
64:8J:4:ARG:O	64:8J:8:LYS:HE2	2.17	0.44
3:1C:74:SER:HB3	3:1C:97:LEU:HB3	2.00	0.44
4:1D:62:LEU:HD22	4:1D:425:PHE:HZ	1.82	0.44
11:1K:37:MET:CE	11:1K:67:ALA:HB3	2.46	0.44
12:1L:22:SER:HA	12:1L:27:TYR:HB2	2.00	0.44
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	1.99	0.44
15:1O:65:ASP:OD1	15:1O:65:ASP:N	2.37	0.44
23:1X:152:GLU:H	23:1X:152:GLU:CD	2.11	0.44
75:1X:201:CDL:H422	29:1d:36:PHE:CE2	2.53	0.44
38:1m:117:GLU:O	38:1m:119:LYS:HG2	2.18	0.44
40:1o:50:LEU:HD11	40:1o:63:ILE:HG13	1.99	0.44
45:3A:40:TRP:CZ2	45:3A:377:GLU:HA	2.53	0.44
46:3B:312:PHE:HA	49:3I:61:GLY:HA2	1.99	0.44
47:3C:240:LEU:HB3	47:3C:244:LEU:HD12	2.00	0.44
49:3E:93:ARG:HG2	51:3G:25:GLN:C	2.43	0.44
49:3E:197:ASP:OD2	49:3E:257:ASN:CG	2.61	0.44
45:3N:34:THR:HG22	45:3N:102:LEU:HD21	1.87	0.44
45:3N:41:ILE:CG1	45:3N:195:MET:HE1	2.47	0.44
45:3N:60:GLU:C	46:3O:287:ARG:NH2	2.75	0.44
45:3N:311:ASN:CB	45:3N:320:LEU:HA	2.48	0.44
50:3S:28:LYS:HA	50:3S:80:TRP:CD1	2.53	0.44
55:4A:309:THR:HG23	55:4A:359:ALA:HB1	2.00	0.44
56:4B:65:TRP:CD1	56:4B:65:TRP:C	2.96	0.44
4:5D:119:SER:HA	4:5D:196:PRO:HG3	1.99	0.44
4:5D:269:LEU:HD11	4:5D:373:GLU:HG3	1.99	0.44
7:5G:346:GLU:HG2	7:5G:531:CYS:SG	2.57	0.44
7:5G:575:ASN:HD21	7:5G:577:GLU:CD	2.26	0.44
10:5J:7:PHE:HE2	10:5J:108:LEU:HD11	1.83	0.44
10:5J:115:ILE:O	10:5J:117:PHE:N	2.48	0.44
12:5L:263:PHE:HD1	12:5L:266:LEU:HD22	1.83	0.44
12:5L:440:LEU:HD23	12:5L:440:LEU:HA	1.79	0.44
13:5M:16:TRP:NE1	13:5M:97:THR:OG1	2.51	0.44
20:5U:14:ARG:O	20:5U:18:VAL:HG23	2.18	0.44
23:5X:123:GLU:HA	23:5X:126:LYS:HD3	2.00	0.44
45:6A:149:VAL:HA	45:6A:152:TYR:HB2	1.99	0.44
47:6C:1:MET:HE2	47:6C:1:MET:HB2	1.74	0.44
47:6C:253:PRO:O	47:6C:254:ASP:C	2.61	0.44
47:6C:341:GLN:HB3	47:6C:347:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:6E:168:LYS:HD2	49:6E:168:LYS:HA	1.85	0.44
49:6E:223:VAL:HG21	48:6Q:106:ASN:O	2.18	0.44
50:6F:119:TRP:CH2	46:6O:91:ALA:HB2	2.52	0.44
52:6H:54:LYS:CG	52:6H:89:ALA:CB	2.96	0.44
53:6J:22:ALA:HA	53:6J:25:ILE:HD12	1.99	0.44
45:6N:43:ALA:H	45:6N:94:HIS:HA	1.83	0.44
45:6N:343:MET:HE3	45:6N:441:MET:HA	2.00	0.44
47:6P:5:ARG:HA	47:6P:11:MET:HE2	2.00	0.44
49:6R:184:ILE:HG21	49:6R:208:PRO:HB3	2.00	0.44
55:8A:34:SER:HA	55:8A:37:ILE:HD12	2.00	0.44
55:8A:94:PHE:CE2	57:8C:82:GLY:HA3	2.52	0.44
55:8A:310:MET:N	55:8A:310:MET:SD	2.91	0.44
56:8B:122:MET:HG3	56:8B:208:PRO:HG2	2.00	0.44
57:8C:42:LEU:HD13	64:8J:45:TYR:CD2	2.52	0.44
82:8C:302:PGV:H272	90:8C:307:PEK:H261	2.00	0.44
58:8D:17:VAL:CG1	58:8D:19:ARG:HG3	2.48	0.44
6:1F:256:PHE:CD1	6:1F:332:ALA:HB1	2.53	0.43
7:1G:114:CYS:HB3	7:1G:117:GLN:HB2	2.00	0.43
10:1J:92:ALA:HB2	69:1J:202:3PE:H252	1.99	0.43
12:1L:263:PHE:HD1	12:1L:266:LEU:HD22	1.83	0.43
12:1L:557:TRP:O	12:1L:561:ILE:HG12	2.18	0.43
13:1M:216:LEU:HB3	13:1M:217:PRO:HD3	2.00	0.43
15:1O:211:LEU:O	15:1O:215:SER:OG	2.25	0.43
17:1Q:34:LYS:HE2	17:1Q:34:LYS:HB2	1.87	0.43
23:1X:97:ARG:HD2	25:1Z:60:LEU:HD13	2.00	0.43
39:1n:55:ASP:HB3	39:1n:58:LYS:CE	2.27	0.43
40:1o:23:THR:OG1	40:1o:104:GLU:OE2	2.36	0.43
47:3C:244:LEU:HD22	48:3D:293:MET:HB2	2.00	0.43
49:3E:181:LYS:HA	49:3E:184:ILE:HB	1.99	0.43
52:3H:44:THR:HA	52:3H:47:GLU:HG2	1.99	0.43
45:3N:69:ASN:HB2	45:3N:115:ASP:OD2	2.17	0.43
58:4D:137:LYS:H	58:4D:137:LYS:HG2	1.59	0.43
60:4F:16:LEU:HD12	60:4F:16:LEU:HA	1.81	0.43
63:4I:57:MET:O	63:4I:61:GLU:HG2	2.18	0.43
4:5D:110:SER:HA	4:5D:145:THR:HG22	2.00	0.43
7:5G:237:ASN:N	7:5G:237:ASN:HD22	2.16	0.43
7:5G:344:CYS:HB3	7:5G:510:GLY:O	2.17	0.43
10:5J:107:ALA:O	10:5J:111:GLU:HG3	2.17	0.43
12:5L:264:TYR:CD2	12:5L:265:PRO:HD3	2.53	0.43
12:5L:285:THR:HA	12:5L:308:SER:HA	1.99	0.43
75:5X:201:CDL:H422	29:5d:36:PHE:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:5l:98:TRP:HB3	38:5m:6:LYS:HZ2	1.83	0.43
45:6A:66:GLY:HA3	45:6A:72:GLY:N	2.32	0.43
45:6A:328:ASN:HA	45:6A:331:ILE:HD11	1.99	0.43
46:6B:112:LEU:O	46:6B:114:ASP:N	2.50	0.43
47:6C:371:ILE:O	47:6C:372:ILE:C	2.61	0.43
49:6E:127:TYR:HB2	53:6J:32:PHE:CE2	2.53	0.43
50:6F:107:LYS:NZ	50:6F:108:GLU:OE2	2.49	0.43
45:6N:54:GLY:C	45:6N:58:PHE:HD2	2.26	0.43
49:6R:219:HIS:NE2	49:6R:239:HIS:HE1	2.12	0.43
54:6X:23:MET:O	54:6X:27:VAL:HG23	2.18	0.43
54:6X:45:VAL:O	54:6X:49:ASN:ND2	2.51	0.43
55:8A:317:GLY:O	55:8A:318:VAL:C	2.61	0.43
58:8D:52:SER:HB2	58:8D:55:GLU:HG3	1.99	0.43
58:8D:66:GLU:HB3	58:8D:70:GLU:HB2	1.99	0.43
75:8D:201:CDL:H392	75:8D:201:CDL:H362	1.52	0.43
64:8J:7:GLU:HG3	64:8J:8:LYS:N	2.33	0.43
1:1A:111:LEU:HA	1:1A:111:LEU:HD23	1.77	0.43
6:1F:61:LYS:HG2	6:1F:76:GLY:HA3	1.98	0.43
6:1F:92:TYR:O	6:1F:220:THR:HA	2.19	0.43
6:1F:99:GLU:O	6:1F:139:ARG:NH1	2.51	0.43
7:1G:198:ASN:O	7:1G:202:ILE:HG23	2.18	0.43
10:1J:152:TRP:H	71:1J:201:PC1:H241	1.82	0.43
13:1M:95:TYR:HD2	13:1M:136:TRP:CD2	2.37	0.43
27:1b:66:PRO:HB3	27:1b:73:GLN:HB2	1.99	0.43
28:1c:40:LEU:HD23	28:1c:40:LEU:HA	1.87	0.43
32:1g:111:ASN:OD1	41:1p:161:ARG:NH1	2.51	0.43
33:1h:40:ILE:HG13	71:1h:202:PC1:H2D2	1.99	0.43
39:1n:174:ARG:NH2	39:1n:177:PRO:O	2.51	0.43
41:1p:166:ARG:C	41:1p:170:LYS:HD3	2.43	0.43
45:3A:156:THR:HA	49:3E:85:VAL:HG21	2.00	0.43
47:3C:139:SER:OG	47:3C:255:ASN:ND2	2.49	0.43
47:3C:155:TYR:HA	47:3C:159:ASP:CG	2.44	0.43
49:3E:219:HIS:C	49:3E:221:GLY:H	2.25	0.43
45:3N:79:VAL:HG21	45:3N:86:LEU:HD11	1.99	0.43
45:3N:118:GLN:CG	45:3N:219:LEU:HD23	2.48	0.43
46:3O:68:LEU:HD23	46:3O:191:LEU:HD21	1.99	0.43
49:3R:241:SER:HB3	49:3R:249:ILE:HG23	1.99	0.43
55:4A:193:VAL:HG21	82:4A:603:PGV:H231	1.99	0.43
58:4D:80:THR:HG22	65:4K:14:GLY:HA2	2.00	0.43
59:4E:27:TRP:CZ2	60:4F:81:ARG:HB2	2.52	0.43
65:4K:42:LEU:HD22	82:4K:101:PGV:H202	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:106:LEU:O	4:5D:427:GLU:N	2.51	0.43
7:5G:108:CYS:SG	7:5G:206:GLY:HA3	2.58	0.43
8:5H:96:ILE:HG23	25:5Z:144:THR:HB	1.99	0.43
10:5J:19:GLY:HA2	10:5J:93:PHE:CD2	2.53	0.43
10:5J:117:PHE:HB2	10:5J:119:PHE:CZ	2.53	0.43
12:5L:63:ILE:O	12:5L:79:SER:HA	2.18	0.43
20:5T:35:HIS:CE1	20:5T:37:MET:HB2	2.54	0.43
29:5d:10:PRO:HG3	30:5e:7:LYS:HE2	1.99	0.43
34:5i:125:GLN:O	34:5i:125:GLN:HG3	2.18	0.43
41:5p:166:ARG:HG2	41:5p:170:LYS:NZ	2.32	0.43
45:6A:244:ARG:HA	45:6A:244:ARG:HD2	1.40	0.43
45:6A:343:MET:O	45:6A:347:THR:HG23	2.18	0.43
47:6C:50:PHE:HA	47:6C:53:MET:SD	2.58	0.43
47:6C:373:GLU:O	47:6C:374:ASN:C	2.61	0.43
48:6D:185:ASN:O	48:6D:186:PRO:C	2.60	0.43
49:6E:219:HIS:C	49:6E:221:GLY:H	2.25	0.43
51:6G:41:ARG:HA	51:6G:44:ARG:HH21	1.82	0.43
45:6N:168:GLU:HB2	49:6R:81:THR:CG2	2.45	0.43
55:8A:141:ALA:O	55:8A:144:ASP:N	2.51	0.43
55:8A:407:GLN:H	55:8A:407:GLN:HG3	1.50	0.43
56:8B:102:HIS:NE2	56:8B:107:SER:OG	2.44	0.43
58:8D:80:THR:HG22	65:8K:14:GLY:HA2	1.99	0.43
62:8H:39:CYS:CB	62:8H:53:CYS:CB	2.95	0.43
4:1D:106:LEU:O	4:1D:427:GLU:N	2.51	0.43
8:1H:42:PRO:HG3	42:1q:28:PHE:CE1	2.54	0.43
8:1H:126:LYS:HA	8:1H:126:LYS:HD3	1.77	0.43
9:1I:143:THR:OG1	9:1I:146:GLU:HG3	2.19	0.43
12:1L:23:ASN:HD22	75:1L:702:CDL:H321	1.83	0.43
12:1L:54:PHE:CZ	12:1L:84:TYR:HB2	2.53	0.43
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.53	0.43
12:1L:264:TYR:O	12:1L:268:GLU:HG3	2.18	0.43
12:1L:407:TRP:CE2	12:1L:411:MET:HE3	2.54	0.43
18:1R:12:THR:HG22	18:1R:35:VAL:HG22	2.01	0.43
20:1U:21:LEU:HD22	36:1k:46:ARG:HB3	2.00	0.43
23:1X:19:VAL:O	26:1a:50:ARG:NH1	2.50	0.43
29:1d:49:ARG:HD3	29:1d:51:ARG:NH2	2.33	0.43
42:1q:6:VAL:HG12	75:1q:201:CDL:HA61	1.99	0.43
47:3C:34:GLY:O	47:3C:37:LEU:HB2	2.18	0.43
47:3C:67:THR:HG22	47:3C:71:ARG:HD2	2.00	0.43
47:3C:77:TRP:CG	48:3D:286:GLU:HB2	2.53	0.43
48:3D:325:ALA:O	51:3G:15:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:37:VAL:HG12	45:3N:113:LEU:HD11	2.00	0.43
45:3N:40:TRP:HA	45:3N:96:ALA:HB2	2.01	0.43
45:3N:46:ARG:NH1	45:3N:93:GLU:HG2	2.34	0.43
45:3N:74:ALA:O	45:3N:75:LEU:C	2.60	0.43
45:3N:92:ARG:CD	45:3N:165:GLN:O	2.63	0.43
45:3N:110:VAL:O	45:3N:111:GLU:C	2.62	0.43
45:3N:317:THR:OG1	45:3N:318:GLY:N	2.38	0.43
46:3O:275:LEU:HG	46:3O:322:PHE:CZ	2.53	0.43
54:3X:45:VAL:O	54:3X:49:ASN:ND2	2.51	0.43
4:5D:128:ILE:HD13	4:5D:330:VAL:HG11	1.99	0.43
10:5J:125:TRP:CZ2	25:5Z:133:ILE:HD12	2.53	0.43
12:5L:511:LEU:HD23	12:5L:511:LEU:HA	1.83	0.43
13:5M:329:LEU:O	13:5M:332:THR:OG1	2.34	0.43
14:5N:107:GLY:HA2	14:5N:111:PHE:O	2.18	0.43
34:5i:74:VAL:C	34:5i:77:PRO:HD2	2.43	0.43
37:5l:99:ASN:HB2	38:5m:6:LYS:HE2	2.00	0.43
40:5o:30:PHE:CG	40:5o:33:ARG:HD3	2.52	0.43
45:6A:43:ALA:HA	45:6A:47:TYR:CG	2.54	0.43
46:6B:145:ARG:O	46:6B:146:ILE:C	2.61	0.43
47:6C:66:VAL:HG21	47:6C:134:PRO:HA	2.00	0.43
47:6C:377:LEU:HD11	50:6F:38:PHE:HE2	1.83	0.43
48:6D:130:SER:H	48:6D:200:ASP:HA	1.83	0.43
48:6D:179:PHE:HE2	48:6D:278:PHE:CZ	2.36	0.43
48:6D:255:ASN:CG	52:6H:38:LEU:HB3	2.43	0.43
48:6D:310:ALA:O	48:6D:314:HIS:N	2.47	0.43
45:6N:78:GLU:O	45:6N:79:VAL:C	2.61	0.43
45:6N:373:THR:HB	45:6N:374:PRO:HD3	2.01	0.43
47:6P:141:TRP:CD1	47:6P:265:PRO:HD3	2.53	0.43
55:8A:51:ASP:HB2	56:8B:201:GLY:O	2.18	0.43
55:8A:508:PRO:HD3	57:8C:6:HIS:HB3	2.01	0.43
82:8A:603:PGV:H222	82:8A:603:PGV:H42	1.99	0.43
56:8B:134:ARG:HB2	58:8D:110:THR:HG21	2.00	0.43
59:8E:27:TRP:CH2	59:8E:31:LYS:HD3	2.53	0.43
3:1C:51:PHE:CE2	3:1C:108:LYS:HE2	2.54	0.43
7:1G:394:ARG:HD3	7:1G:394:ARG:HA	1.90	0.43
8:1H:89:LEU:HA	8:1H:89:LEU:HD23	1.83	0.43
12:1L:285:THR:HA	12:1L:308:SER:HA	1.99	0.43
13:1M:116:ILE:HD13	13:1M:116:ILE:HA	1.84	0.43
15:1O:50:HIS:HE2	15:1O:125:GLU:CD	2.25	0.43
15:1O:319:LEU:HD12	15:1O:319:LEU:HA	1.83	0.43
17:1Q:16:LYS:HA	17:1Q:16:LYS:HD2	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:166:ARG:HG2	41:1p:170:LYS:NZ	2.32	0.43
46:3B:340:ALA:O	46:3B:344:VAL:HG23	2.18	0.43
47:3C:233:LEU:O	47:3C:237:LEU:N	2.45	0.43
47:3C:329:VAL:O	47:3C:333:ILE:HG13	2.19	0.43
48:3D:226:PRO:O	48:3D:227:THR:C	2.61	0.43
49:3E:151:LYS:NZ	49:3E:152:ILE:HD12	2.33	0.43
51:3G:29:PRO:HB2	51:3G:30:HIS:CE1	2.54	0.43
45:3N:127:ILE:HD12	45:3N:179:ARG:CD	2.46	0.43
45:3N:134:ILE:HG22	45:3N:174:VAL:HG11	2.00	0.43
46:3O:329:GLN:H	46:3O:329:GLN:HG2	1.53	0.43
50:3S:12:TRP:CD1	50:3S:14:GLU:HB2	2.53	0.43
55:4A:411:LYS:O	55:4A:415:VAL:HG23	2.18	0.43
57:4C:58:TRP:CZ3	82:4C:305:PGV:H71	2.54	0.43
58:4D:121:LYS:HG3	65:4K:53:TRP:HD1	1.84	0.43
59:4E:27:TRP:CH2	59:4E:31:LYS:HD3	2.53	0.43
3:5C:83:VAL:HG12	3:5C:85:THR:HG22	2.00	0.43
4:5D:18:VAL:HG13	4:5D:20:TYR:H	1.83	0.43
7:5G:154:ILE:O	7:5G:156:CYS:N	2.51	0.43
8:5H:107:ALA:HA	10:5J:58:LEU:HD13	2.00	0.43
9:5I:175:TYR:CZ	43:5r:38:PRO:HG3	2.53	0.43
11:5K:37:MET:CE	11:5K:67:ALA:HB3	2.46	0.43
12:5L:407:TRP:CE2	12:5L:411:MET:HE3	2.54	0.43
15:5O:223:TYR:OH	15:5O:237:ASP:OD2	2.30	0.43
25:5Z:31:SER:O	25:5Z:35:MET:HG3	2.17	0.43
34:5i:75:LEU:HD22	34:5i:79:TRP:CE2	2.53	0.43
45:6A:317:THR:OG1	45:6A:318:GLY:N	2.50	0.43
46:6B:258:VAL:HG21	46:6B:321:LEU:HD13	2.00	0.43
46:6B:372:VAL:O	46:6B:373:GLU:C	2.61	0.43
46:6B:430:LEU:H	46:6B:430:LEU:HG	1.61	0.43
48:6D:159:GLN:N	48:6D:170:MET:HA	2.33	0.43
48:6D:323:LYS:HZ3	49:6E:86:PRO:HB2	1.83	0.43
53:6J:7:THR:HA	53:6J:10:LEU:HB2	2.00	0.43
45:6N:19:LEU:CD2	45:6N:213:GLN:HG2	2.49	0.43
45:6N:52:ASN:CA	45:6N:185:TYR:OH	2.66	0.43
45:6N:290:MET:O	45:6N:291:SER:C	2.60	0.43
45:6N:411:CYS:O	45:6N:412:SER:C	2.61	0.43
46:6O:173:ALA:O	46:6O:174:ASN:C	2.61	0.43
46:6O:376:GLU:OE1	46:6O:379:LEU:HD22	2.18	0.43
46:6O:409:ASP:OD1	46:6O:409:ASP:N	2.50	0.43
51:6T:71:ARG:HA	51:6T:71:ARG:HD2	1.81	0.43
55:8A:20:LEU:O	55:8A:21:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:294:THR:O	55:8A:295:VAL:C	2.60	0.43
55:8A:339:LEU:O	55:8A:340:TRP:C	2.60	0.43
55:8A:484:ALA:O	67:8M:1:ILE:HA	2.19	0.43
82:8A:601:PGV:H301	82:8A:601:PGV:H331	1.66	0.43
56:8B:59:GLN:OE1	68:8N:14:SER:OG	2.33	0.43
57:8C:250:LEU:O	57:8C:254:VAL:HG23	2.18	0.43
82:8G:101:PGV:H012	82:8G:101:PGV:H202	1.25	0.43
66:8L:26:THR:HG23	67:8M:25:SER:HB2	2.00	0.43
1:1A:54:LYS:HB2	1:1A:54:LYS:HE3	1.62	0.43
2:1B:101:ARG:CB	2:1B:104:TYR:HD2	2.30	0.43
4:1D:165:THR:HG22	4:1D:169:TRP:CE2	2.54	0.43
5:1E:7:PHE:HB3	7:1G:175:THR:HB	2.00	0.43
6:1F:274:VAL:CG2	6:1F:278:GLU:OE2	2.67	0.43
10:1J:7:PHE:HE2	10:1J:108:LEU:HD11	1.83	0.43
11:1K:34:GLU:O	11:1K:37:MET:HG3	2.18	0.43
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	2.01	0.43
13:1M:135:ARG:HD3	69:1N:902:3PE:H362	2.00	0.43
29:1d:47:ALA:HB2	69:1d:201:3PE:H331	2.01	0.43
45:3A:155:ALA:HA	45:3A:164:ALA:HB1	2.00	0.43
47:3C:188:ILE:O	47:3C:192:LEU:HG	2.18	0.43
47:3C:240:LEU:C	48:3D:297:MET:HE2	2.43	0.43
47:3C:256:TYR:HB3	48:3D:203:TYR:HB3	2.00	0.43
47:3C:320:LEU:HB2	47:3C:369:THR:HG23	2.01	0.43
52:3H:83:LEU:O	52:3H:87:LEU:HG	2.18	0.43
53:3J:30:LEU:HA	54:3Y:34:TRP:CD1	2.54	0.43
45:3N:36:THR:HG23	45:3N:372:THR:CB	2.15	0.43
45:3N:358:LYS:HE3	45:3N:362:ARG:HH22	1.83	0.43
45:3N:436:ARG:HD3	47:3P:222:PRO:HD3	2.00	0.43
46:3O:369:LEU:HD21	46:3O:399:LEU:HD11	2.00	0.43
46:3O:385:GLN:HE22	46:3O:392:TYR:HD1	1.66	0.43
50:3S:75:LEU:O	50:3S:80:TRP:NE1	2.48	0.43
54:3X:23:MET:O	54:3X:27:VAL:HG23	2.18	0.43
56:4B:118:PHE:CD2	56:4B:140:ASN:HB3	2.53	0.43
57:4C:42:LEU:HD13	64:4J:45:TYR:CD2	2.52	0.43
57:4C:178:ALA:HB1	82:4C:304:PGV:H02	2.01	0.43
59:4E:21:LYS:HB3	59:4E:21:LYS:HE3	1.79	0.43
1:5A:49:LEU:H	8:5H:126:LYS:HZ2	1.66	0.43
3:5C:39:GLN:HB3	3:5C:51:PHE:CD1	2.53	0.43
4:5D:155:THR:HB	4:5D:167:PHE:HA	1.99	0.43
4:5D:317:LYS:HA	4:5D:317:LYS:HD3	1.71	0.43
6:5F:274:VAL:CG2	6:5F:278:GLU:OE2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:5I:114:THR:HG21	9:5I:144:HIS:CE1	2.53	0.43
9:5I:143:THR:OG1	9:5I:146:GLU:HG3	2.19	0.43
69:5M:503:3PE:H242	38:5m:101:TYR:CZ	2.52	0.43
16:5P:335:LYS:H	16:5P:335:LYS:HG2	1.61	0.43
21:5V:76:ILE:HD12	21:5V:76:ILE:HA	1.92	0.43
23:5X:19:VAL:O	26:5a:50:ARG:NH1	2.50	0.43
23:5X:124:LEU:HD21	25:5Z:70:ALA:HB2	2.01	0.43
24:5Y:78:GLN:HE21	51:6T:64:GLN:HE22	1.66	0.43
28:5c:17:VAL:O	28:5c:21:LEU:HD22	2.18	0.43
33:5h:41:THR:OG1	75:5i:201:CDL:H711	2.18	0.43
45:6A:100:LYS:HA	45:6A:100:LYS:HD2	1.65	0.43
45:6A:354:VAL:HG21	45:6A:404:ALA:HA	2.00	0.43
45:6A:411:CYS:O	45:6A:412:SER:C	2.61	0.43
46:6B:39:GLU:HG3	46:6B:41:TYR:CE1	2.54	0.43
47:6C:37:LEU:HD13	83:6C:502:HEM:C2B	2.54	0.43
47:6C:162:GLU:O	47:6C:166:GLY:N	2.51	0.43
47:6C:377:LEU:HB3	47:6C:379:TRP:NE1	2.33	0.43
48:6D:104:GLY:HA3	48:6D:107:SER:HB2	1.99	0.43
45:6N:40:TRP:CE2	45:6N:377:GLU:C	2.62	0.43
45:6N:57:TYR:C	45:6N:61:HIS:CD2	2.96	0.43
45:6N:108:LYS:O	45:6N:112:LEU:HG	2.18	0.43
45:6N:225:GLU:HB2	45:6N:226:ASP:H	1.67	0.43
45:6N:254:ALA:HA	45:6N:323:HIS:HA	2.00	0.43
45:6N:391:PRO:HG2	45:6N:394:GLU:HB2	2.00	0.43
46:6O:176:LEU:HD23	46:6O:176:LEU:HA	1.85	0.43
48:6Q:233:ARG:HG3	50:6S:71:ARG:HH22	1.82	0.43
55:8A:107:PRO:O	55:8A:108:SER:C	2.60	0.43
55:8A:127:THR:HA	55:8A:235:PHE:CE2	2.54	0.43
55:8A:351:GLY:O	55:8A:352:GLY:C	2.62	0.43
8:1H:105:MET:CE	8:1H:162:LEU:HD11	2.49	0.43
8:1H:107:ALA:HA	10:1J:58:LEU:HD13	2.00	0.43
9:1I:49:ASN:O	9:1I:53:GLU:N	2.43	0.43
10:1J:175:ASN:H	14:1N:48:PHE:HD2	1.66	0.43
12:1L:225:ALA:HB1	12:1L:230:HIS:HA	2.00	0.43
13:1M:71:TRP:O	13:1M:74:PRO:HD2	2.17	0.43
13:1M:101:LEU:HD13	69:1N:902:3PE:H3I3	2.00	0.43
16:1P:193:LEU:O	16:1P:257:PRO:HA	2.19	0.43
25:1Z:87:LEU:HD11	25:1Z:119:PRO:HG3	2.01	0.43
32:1g:45:HIS:CD2	32:1g:58:MET:HE2	2.54	0.43
46:3B:232:LEU:HD12	46:3B:232:LEU:HA	1.79	0.43
47:3C:140:PHE:HD2	47:3C:141:TRP:CD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:171:ASP:OD1	47:3C:172:LYS:N	2.52	0.43
47:3C:242:LEU:O	47:3C:246:SER:N	2.44	0.43
49:3E:223:VAL:HG21	48:3Q:106:ASN:O	2.18	0.43
45:3N:53:ASN:OD1	45:3N:165:GLN:CD	2.62	0.43
45:3N:158:PHE:HB3	45:3N:163:LEU:HB2	2.01	0.43
45:3N:350:THR:OG1	45:3N:353:GLU:HG2	2.18	0.43
45:3N:378:ASP:O	45:3N:379:ILE:C	2.61	0.43
46:3O:308:ASP:OD2	49:3V:58:GLN:N	2.44	0.43
54:3Y:23:MET:O	54:3Y:27:VAL:HG23	2.17	0.43
3:5C:74:SER:HB3	3:5C:97:LEU:HB3	2.00	0.43
4:5D:165:THR:HG22	4:5D:169:TRP:CE2	2.54	0.43
5:5E:167:LYS:O	5:5E:171:GLU:HG3	2.19	0.43
6:5F:229:ALA:O	6:5F:232:PRO:HD2	2.18	0.43
13:5M:101:LEU:HD13	69:5N:902:3PE:H3I3	2.00	0.43
16:5P:83:LYS:HE2	16:5P:83:LYS:HB3	1.84	0.43
25:5Z:87:LEU:HD11	25:5Z:119:PRO:HG3	2.01	0.43
38:5m:117:GLU:O	38:5m:119:LYS:HG2	2.18	0.43
41:5p:166:ARG:C	41:5p:170:LYS:HD3	2.43	0.43
45:6A:253:VAL:O	45:6A:324:PHE:N	2.52	0.43
46:6B:305:GLN:O	46:6B:306:PRO:C	2.61	0.43
47:6C:40:CYS:O	47:6C:41:LEU:C	2.60	0.43
47:6C:58:ASP:HA	47:6C:172:LYS:HE2	2.00	0.43
48:6D:93:LEU:CD1	52:6H:87:LEU:HB3	2.48	0.43
48:6D:267:THR:HG23	48:6D:270:GLN:HB3	2.01	0.43
49:6E:197:ASP:OD2	49:6E:257:ASN:CG	2.61	0.43
45:6N:314:TYR:H	45:6N:317:THR:C	2.27	0.43
46:6O:428:GLY:O	46:6O:430:LEU:N	2.52	0.43
50:6S:28:LYS:HA	50:6S:80:TRP:CD1	2.53	0.43
55:8A:160:GLY:O	55:8A:161:ALA:C	2.61	0.43
55:8A:166:THR:HG23	57:8C:81:TYR:CB	2.47	0.43
55:8A:436:MET:HE1	55:8A:451:ASN:HD21	1.83	0.43
55:8A:480:ARG:O	55:8A:481:GLU:C	2.62	0.43
57:8C:58:TRP:CZ3	82:8C:305:PGV:H71	2.54	0.43
2:1B:134:ARG:NH1	3:1C:173:GLU:HG2	2.34	0.43
7:1G:324:ASP:CB	7:1G:571:ALA:HB1	2.45	0.43
8:1H:317:GLN:OE1	10:1J:141:MET:HE1	2.19	0.43
10:1J:23:LYS:HE2	11:1K:23:ARG:HG3	1.99	0.43
13:1M:104:LEU:HG	13:1M:108:MET:CE	2.49	0.43
13:1M:257:MET:SD	69:1M:503:3PE:H352	2.59	0.43
16:1P:99:TRP:CD2	16:1P:277:PRO:HD2	2.53	0.43
20:1U:14:ARG:O	20:1U:18:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:157:LEU:HD23	23:1X:157:LEU:HA	1.84	0.43
24:1Y:30:ALA:O	24:1Y:34:ILE:HD12	2.19	0.43
45:3A:30:SER:HB2	45:3A:32:GLN:HG3	2.01	0.43
46:3B:247:GLN:HA	46:3B:428:GLY:O	2.19	0.43
47:3C:248:ASP:HA	47:3C:251:GLY:HA3	2.00	0.43
45:3N:46:ARG:HG2	45:3N:163:LEU:HD23	2.00	0.43
45:3N:64:PHE:CE1	45:3N:86:LEU:HB2	2.39	0.43
45:3N:67:THR:HB	45:3N:119:ASN:HB2	2.01	0.43
45:3N:92:ARG:HG2	45:3N:167:VAL:HG22	2.00	0.43
45:3N:145:MET:HE1	45:3N:248:LEU:HD13	2.00	0.43
45:3N:161:THR:CB	45:3N:234:CYS:HB3	2.49	0.43
45:3N:252:HIS:HB3	45:3N:323:HIS:CE1	2.54	0.43
46:3O:62:ASN:HA	46:3O:182:ARG:CZ	2.48	0.43
55:4A:320:VAL:O	55:4A:324:LEU:HG	2.18	0.43
56:4B:122:MET:HG3	56:4B:208:PRO:HG2	2.00	0.43
57:4C:26:LEU:HD21	64:4J:42:GLY:C	2.42	0.43
66:4L:26:THR:HG23	67:4M:25:SER:HB2	2.00	0.43
6:5F:115:PRO:O	6:5F:119:VAL:HG23	2.19	0.43
6:5F:261:HIS:CD2	6:5F:337:MET:HA	2.51	0.43
7:5G:648:LEU:HD13	19:5S:41:VAL:HG13	1.99	0.43
12:5L:22:SER:HA	12:5L:27:TYR:HB2	1.99	0.43
12:5L:193:SER:CB	12:5L:206:ASN:HD21	2.32	0.43
13:5M:95:TYR:HD2	13:5M:136:TRP:CD2	2.37	0.43
15:5O:24:VAL:HB	15:5O:166:PRO:HA	1.99	0.43
16:5P:99:TRP:CD2	16:5P:277:PRO:HD2	2.53	0.43
19:5S:90:LEU:HA	19:5S:90:LEU:HD23	1.77	0.43
69:5Y:203:3PE:H2	69:5Y:203:3PE:H221	1.62	0.43
26:5a:6:LEU:HB2	75:5q:201:CDL:H191	1.99	0.43
39:5n:23:LEU:HD23	39:5n:23:LEU:HA	1.88	0.43
45:6A:35:CYS:SG	45:6A:102:LEU:O	2.74	0.43
45:6A:130:GLU:O	45:6A:131:ARG:C	2.61	0.43
45:6A:362:ARG:O	45:6A:363:ASN:C	2.61	0.43
45:6A:408:ARG:HE	45:6A:408:ARG:HB2	1.70	0.43
47:6C:27:ILE:HG22	47:6C:207:ASN:HA	2.00	0.43
47:6C:69:ILE:HA	47:6C:73:VAL:HB	2.00	0.43
47:6C:242:LEU:H	47:6C:242:LEU:HG	1.54	0.43
47:6C:269:LYS:H	47:6C:269:LYS:HG3	1.53	0.43
48:6D:215:VAL:HA	48:6D:218:LEU:CD2	2.49	0.43
49:6E:234:TYR:HD2	49:6E:247:GLY:HA2	1.83	0.43
45:6N:140:GLU:HG2	49:6V:48:SER:O	2.18	0.43
45:6N:150:PHE:HE1	45:6N:310:PHE:CE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:280:TYR:HE2	45:6N:298:ALA:HB3	1.83	0.43
46:6O:63:LEU:HD23	46:6O:63:LEU:HA	1.74	0.43
46:6O:68:LEU:O	46:6O:72:ALA:N	2.51	0.43
46:6O:328:SER:O	46:6O:329:GLN:C	2.61	0.43
50:6S:12:TRP:CD1	50:6S:14:GLU:HB2	2.53	0.43
50:6S:77:LYS:HG3	50:6S:80:TRP:CE3	2.54	0.43
55:8A:167:THR:HA	55:8A:170:ASN:HB3	1.98	0.43
55:8A:191:THR:OG1	55:8A:248:LEU:HB2	2.19	0.43
82:8A:602:PGV:H031	57:8C:61:ILE:HD13	2.01	0.43
75:8A:610:CDL:HB61	75:8A:610:CDL:H542	2.00	0.43
57:8C:134:THR:HB	57:8C:249:TRP:HE1	1.83	0.43
58:8D:20:ARG:HD3	58:8D:72:ASN:HD21	1.83	0.43
82:8G:101:PGV:H21	82:8G:101:PGV:H51	1.46	0.43
1:1A:29:ALA:HB2	8:1H:59:GLU:OE2	2.18	0.43
1:1A:70:ALA:C	1:1A:72:LEU:H	2.25	0.43
2:1B:71:ARG:HD3	8:1H:36:GLY:H	1.84	0.43
2:1B:80:PRO:HD3	4:1D:54:GLN:NE2	2.33	0.43
4:1D:227:GLU:HG2	25:1Z:25:LEU:HD22	2.00	0.43
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.53	0.43
12:1L:63:ILE:O	12:1L:79:SER:HA	2.18	0.43
13:1M:401:MET:HE2	13:1M:401:MET:HB3	1.83	0.43
23:1X:123:GLU:HA	23:1X:126:LYS:HD3	2.00	0.43
24:1Y:128:GLN:HG2	69:1Y:203:3PE:O14	2.19	0.43
33:1h:41:THR:OG1	75:1i:201:CDL:H711	2.19	0.43
45:3A:8:LEU:HD22	45:3A:392:LEU:HB3	2.01	0.43
47:3C:218:ILE:HD11	47:3C:224:TYR:CE2	2.54	0.43
47:3C:237:LEU:CA	48:3D:301:MET:HE3	2.49	0.43
47:3C:238:ILE:HD13	47:3C:241:ILE:HD12	2.00	0.43
49:3E:248:ARG:HA	49:3E:257:ASN:HB3	1.99	0.43
52:3H:47:GLU:O	52:3H:50:GLU:HB2	2.18	0.43
45:3N:123:GLU:HA	45:3N:179:ARG:NH1	2.34	0.43
45:3N:141:ASN:CB	45:3N:168:GLU:OE2	2.61	0.43
45:3N:331:ILE:N	45:3N:430:GLN:OE1	2.52	0.43
45:3N:340:GLY:O	45:3N:343:MET:HB2	2.19	0.43
45:3N:416:TYR:O	45:3N:418:GLN:HG2	2.19	0.43
48:3Q:27:ARG:HH21	48:3Q:56:TYR:HA	1.84	0.43
48:3Q:43:MET:HE3	48:3Q:43:MET:HB2	1.95	0.43
54:3X:39:ARG:HE	54:3X:39:ARG:HB3	1.66	0.43
55:4A:347:LEU:HB3	55:4A:383:MET:HB3	2.01	0.43
55:4A:367:LEU:O	55:4A:370:THR:OG1	2.33	0.43
56:4B:44:LEU:HD11	63:4I:20:HIS:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4B:59:GLN:OE1	68:4N:14:SER:OG	2.33	0.43
58:4D:17:VAL:CG1	58:4D:19:ARG:HG3	2.48	0.43
58:4D:120:THR:HG23	58:4D:134:PHE:HZ	1.84	0.43
3:5C:51:PHE:CE2	3:5C:108:LYS:HE2	2.54	0.43
4:5D:95:THR:HA	4:5D:385:ARG:HG2	2.01	0.43
4:5D:165:THR:OG1	8:5H:275:ALA:O	2.35	0.43
4:5D:227:GLU:HG2	25:5Z:25:LEU:HD22	2.00	0.43
6:5F:99:GLU:O	6:5F:139:ARG:NH1	2.51	0.43
10:5J:103:MET:HE3	10:5J:103:MET:HB2	1.85	0.43
12:5L:213:LEU:HD21	12:5L:266:LEU:HB3	2.01	0.43
12:5L:557:TRP:O	12:5L:561:ILE:HG12	2.18	0.43
13:5M:135:ARG:HD3	69:5N:902:3PE:H362	2.00	0.43
13:5M:216:LEU:HB3	13:5M:217:PRO:HD3	2.00	0.43
23:5X:97:ARG:HD2	25:5Z:60:LEU:HD13	2.00	0.43
25:5Z:98:MET:HB3	25:5Z:104:TRP:CD1	2.53	0.43
32:5g:45:HIS:CD2	32:5g:58:MET:HE2	2.54	0.43
45:6A:241:ILE:HB	51:6G:18:TYR:CD1	2.51	0.43
45:6A:438:ARG:O	45:6A:441:MET:HB2	2.18	0.43
47:6C:223:TYR:O	47:6C:224:TYR:C	2.62	0.43
47:6C:324:LEU:H	47:6C:324:LEU:HG	1.23	0.43
47:6C:341:GLN:HB3	47:6C:347:PHE:HE2	1.82	0.43
48:6D:111:HIS:HA	48:6D:114:ILE:CG1	2.37	0.43
48:6D:193:ASN:HB3	84:6D:501:HEC:HMD2	2.01	0.43
48:6D:313:ARG:O	48:6D:317:SER:N	2.51	0.43
45:6N:4:TYR:CE1	46:6O:112:LEU:CD2	3.01	0.43
45:6N:27:SER:HB2	45:6N:208:LEU:CD1	2.30	0.43
45:6N:74:ALA:O	45:6N:75:LEU:C	2.61	0.43
46:6O:311:ALA:O	49:6V:61:GLY:HA2	2.19	0.43
46:6O:315:SER:HB2	46:6O:320:GLY:HA2	2.01	0.43
47:6P:377:LEU:HD23	47:6P:377:LEU:HA	1.88	0.43
48:6Q:27:ARG:HH21	48:6Q:56:TYR:HA	1.84	0.43
49:6R:241:SER:HB3	49:6R:249:ILE:HG23	1.99	0.43
55:8A:217:THR:HB	57:8C:195:SER:OG	2.19	0.43
55:8A:328:HIS:HB2	89:8A:611:PSC:H62	2.01	0.43
55:8A:339:LEU:HA	55:8A:342:LEU:HD12	2.01	0.43
75:8A:610:CDL:H152	75:8A:610:CDL:H211	1.99	0.43
75:8B:302:CDL:H811	75:8B:302:CDL:H262	2.01	0.43
1:1A:11:VAL:O	1:1A:12:THR:C	2.60	0.43
1:1A:23:TRP:O	1:1A:24:LEU:C	2.61	0.43
1:1A:109:LYS:O	1:1A:110:GLY:C	2.62	0.43
4:1D:128:ILE:HD13	4:1D:330:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:162:GLU:OE2	6:1F:108:ARG:NH1	2.47	0.43
7:1G:237:ASN:HD22	7:1G:237:ASN:N	2.16	0.43
9:1I:26:LEU:O	71:1I:204:PC1:H261	2.19	0.43
10:1J:19:GLY:HA2	10:1J:93:PHE:CD2	2.53	0.43
10:1J:139:GLU:HG3	11:1K:49:LEU:HD21	2.01	0.43
11:1K:25:HIS:HD2	11:1K:88:ASP:OD2	2.02	0.43
12:1L:248:HIS:HA	12:1L:253:VAL:HG13	1.99	0.43
12:1L:363:TYR:CD1	12:1L:370:THR:HG21	2.53	0.43
14:1N:95:MET:HE2	14:1N:149:ILE:HA	2.01	0.43
24:1Y:57:ARG:HH21	69:1Y:202:3PE:H112	1.84	0.43
45:3A:87:ASN:ND2	45:3A:98:TYR:OH	2.42	0.43
45:3A:276:ILE:HD11	45:3A:354:VAL:HA	1.99	0.43
47:3C:46:LEU:O	47:3C:50:PHE:HD1	2.02	0.43
47:3C:78:VAL:CG1	48:3D:293:MET:HE1	2.49	0.43
47:3C:91:PHE:CZ	47:3C:124:MET:HA	2.51	0.43
49:3I:70:LEU:O	49:3I:70:LEU:HD23	2.19	0.43
45:3N:37:VAL:HB	45:3N:99:ILE:O	2.19	0.43
45:3N:182:LEU:CA	45:3N:185:TYR:HD2	2.32	0.43
49:3R:93:ARG:NH2	51:3T:21:PHE:HA	2.34	0.43
50:3S:77:LYS:HG3	50:3S:80:TRP:CE3	2.54	0.43
55:4A:76:GLY:O	55:4A:80:ASN:ND2	2.39	0.43
55:4A:367:LEU:HD21	55:4A:433:LEU:HD23	2.00	0.43
62:4H:36:PHE:O	62:4H:40:GLU:HG3	2.19	0.43
66:4L:26:THR:HG23	67:4M:25:SER:CB	2.49	0.43
2:5B:134:ARG:NH1	3:5C:173:GLU:HG2	2.34	0.43
8:5H:42:PRO:HG3	42:5q:28:PHE:CE1	2.54	0.43
12:5L:142:ILE:HD11	13:5M:371:PRO:HB3	2.00	0.43
15:5O:73:LEU:HD23	15:5O:292:VAL:HG13	2.01	0.43
45:6A:143:SER:O	45:6A:144:SER:C	2.62	0.43
46:6B:119:LEU:HD13	46:6B:119:LEU:HA	1.79	0.43
48:6D:129:HIS:HB3	48:6D:200:ASP:CA	2.48	0.43
48:6D:165:ASP:HA	48:6Q:99:GLU:HB3	2.01	0.43
48:6D:198:PRO:HG3	84:6D:501:HEC:C2D	2.49	0.43
48:6D:314:HIS:HA	51:6G:27:ALA:HB2	2.01	0.43
45:6N:46:ARG:HD3	45:6N:231:PHE:HE1	1.76	0.43
45:6N:118:GLN:HE21	45:6N:219:LEU:CG	2.32	0.43
45:6N:248:LEU:HB2	45:6N:427:PRO:CD	2.48	0.43
46:6O:35:ILE:HG21	46:6O:217:LYS:HE3	2.01	0.43
47:6P:267:HIS:CD2	47:6P:269:LYS:HG2	2.50	0.43
48:6Q:47:ALA:HA	48:6Q:90:TYR:HA	2.01	0.43
50:6S:77:LYS:HA	50:6S:80:TRP:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:94:PHE:HB3	82:8A:602:PGV:P	2.59	0.43
55:8A:170:ASN:HA	57:8C:81:TYR:HE2	1.84	0.43
55:8A:268:PHE:H	55:8A:326:THR:HG23	1.84	0.43
58:8D:81:ILE:CD1	75:8D:201:CDL:H712	2.48	0.43
61:8G:28:VAL:O	61:8G:32:THR:OG1	2.28	0.43
2:1B:70:ASP:OD1	2:1B:75:VAL:HG22	2.19	0.43
3:1C:39:GLN:HB3	3:1C:51:PHE:CD1	2.53	0.43
4:1D:18:VAL:HG13	4:1D:20:TYR:H	1.83	0.43
6:1F:96:ASN:O	6:1F:225:VAL:HG23	2.19	0.43
8:1H:196:ALA:CB	8:1H:197:PRO:HD3	2.43	0.43
10:1J:117:PHE:HB2	10:1J:119:PHE:CZ	2.53	0.43
13:1M:16:TRP:NE1	13:1M:97:THR:OG1	2.51	0.43
13:1M:122:PHE:CE1	13:1M:206:LYS:HD3	2.54	0.43
13:1M:141:GLU:HB2	13:1M:222:GLU:CD	2.43	0.43
14:1N:323:MET:HE2	14:1N:323:MET:HB2	1.87	0.43
16:1P:136:ASN:HD22	16:1P:289:MET:HE3	1.83	0.43
20:1T:35:HIS:CE1	20:1T:37:MET:HB2	2.54	0.43
24:1Y:124:VAL:HG22	69:1Y:203:3PE:H232	2.00	0.43
37:1l:99:ASN:HB2	38:1m:6:LYS:HE2	2.00	0.43
47:3C:355:SER:O	47:3C:358:TYR:HB3	2.19	0.43
48:3D:93:LEU:HD22	52:3H:84:PHE:CD2	2.54	0.43
48:3D:158:VAL:HG11	48:3D:177:ASP:OD2	2.18	0.43
52:3H:98:LEU:O	52:3H:99:PHE:C	2.61	0.43
45:3N:144:SER:HB2	45:3N:147:ASP:HB2	2.00	0.43
46:3O:53:ALA:HA	46:3O:203:ARG:HH21	1.84	0.43
49:3R:211:VAL:HG11	49:3R:245:ALA:O	2.18	0.43
56:4B:11:ASP:HB2	58:4D:129:ALA:HA	2.01	0.43
75:4B:301:CDL:H811	75:4B:301:CDL:H262	2.01	0.43
82:4C:302:PGV:H302	82:4C:302:PGV:H343	2.01	0.43
82:4C:304:PGV:H02	82:4C:304:PGV:H22	1.72	0.43
7:5G:41:CYS:O	7:5G:161:ARG:NH2	2.46	0.43
7:5G:114:CYS:HB3	7:5G:117:GLN:HB2	2.00	0.43
10:5J:175:ASN:H	14:5N:48:PHE:HD2	1.66	0.43
12:5L:23:ASN:HD22	75:5L:702:CDL:H321	1.83	0.43
12:5L:69:MET:HE2	12:5L:71:LEU:HD11	2.01	0.43
69:5L:703:3PE:H332	75:5i:201:CDL:H341	2.01	0.43
13:5M:98:MET:HE1	69:5N:902:3PE:H3D2	2.01	0.43
13:5M:141:GLU:HB2	13:5M:222:GLU:CD	2.44	0.43
16:5P:268:ARG:O	16:5P:272:VAL:HG23	2.19	0.43
16:5P:270:PHE:HE2	16:5P:278:TRP:HE3	1.67	0.43
20:5U:38:LYS:HE2	20:5U:38:LYS:HB3	1.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:5g:111:ASN:OD1	41:5p:161:ARG:NH1	2.51	0.43
45:6A:69:ASN:H	45:6A:119:ASN:HB3	1.84	0.43
45:6A:90:SER:HA	45:6A:95:THR:HA	2.01	0.43
45:6A:163:LEU:HD12	45:6A:163:LEU:HA	1.68	0.43
45:6A:241:ILE:HA	51:6G:18:TYR:HA	2.01	0.43
46:6B:232:LEU:HD12	46:6B:232:LEU:HA	1.85	0.43
47:6C:138:MET:HE1	47:6C:270:PRO:HA	2.00	0.43
47:6C:181:PHE:O	47:6C:182:HIS:C	2.61	0.43
47:6C:238:ILE:O	47:6C:242:LEU:HG	2.19	0.43
48:6D:98:TYR:HB2	52:6H:99:PHE:CE1	2.54	0.43
49:6E:241:SER:HA	49:6E:252:GLY:HA3	1.99	0.43
45:6N:2:ALA:O	45:6N:3:THR:C	2.61	0.43
45:6N:37:VAL:HA	45:6N:376:CYS:SG	2.59	0.43
45:6N:156:THR:HG22	45:6N:241:ILE:CG1	2.49	0.43
45:6N:338:LEU:HD12	45:6N:338:LEU:HA	1.85	0.43
46:6O:198:HIS:HA	46:6O:203:ARG:CZ	2.49	0.43
46:6O:255:ALA:HB3	46:6O:326:THR:HG23	2.01	0.43
55:8A:75:ILE:HG12	55:8A:191:THR:HG21	2.01	0.43
55:8A:255:SER:OG	55:8A:256:HIS:N	2.52	0.43
55:8A:293:PHE:CE1	55:8A:302:ARG:HA	2.54	0.43
55:8A:462:LEU:O	55:8A:465:VAL:HB	2.19	0.43
55:8A:506:GLU:O	57:8C:6:HIS:N	2.52	0.43
82:8C:302:PGV:H142	82:8C:305:PGV:H181	2.00	0.43
82:8C:303:PGV:H52	82:8C:303:PGV:H81	1.94	0.43
66:8L:26:THR:HG23	67:8M:25:SER:CB	2.49	0.43
1:1A:74:PRO:O	1:1A:75:LEU:C	2.62	0.42
2:1B:43:SER:C	2:1B:45:LEU:H	2.27	0.42
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.26	0.42
6:1F:302:SER:HB2	6:1F:350:LEU:HD22	2.01	0.42
9:1I:14:MET:SD	27:1b:9:LYS:NZ	2.84	0.42
12:1L:104:SER:HB2	12:1L:118:PHE:CZ	2.54	0.42
14:1N:91:ASN:OD1	14:1N:93:VAL:HG13	2.19	0.42
25:1Z:98:MET:HB3	25:1Z:104:TRP:CD1	2.53	0.42
29:1d:39:TYR:CZ	69:1d:201:3PE:H2G1	2.54	0.42
41:1p:14:ARG:HE	41:1p:14:ARG:HB3	1.68	0.42
45:3A:305:GLN:OE1	49:3I:42:VAL:HG12	2.19	0.42
49:3E:241:SER:HA	49:3E:249:ILE:HG13	2.01	0.42
45:3N:19:LEU:HD11	45:3N:212:ALA:CB	2.49	0.42
45:3N:23:LEU:CD2	45:3N:219:LEU:HD12	2.39	0.42
45:3N:294:LEU:O	45:3N:297:VAL:HB	2.18	0.42
45:3N:297:VAL:HA	47:3P:1:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:304:CYS:HA	45:3N:326:CYS:HB2	2.01	0.42
46:3O:172:LEU:C	46:3O:174:ASN:N	2.77	0.42
46:3O:312:PHE:N	46:3O:323:GLY:O	2.49	0.42
55:4A:106:PRO:HB2	55:4A:107:PRO:HD3	2.01	0.42
57:4C:250:LEU:O	57:4C:254:VAL:HG23	2.19	0.42
58:4D:20:ARG:HD3	58:4D:72:ASN:HD21	1.83	0.42
60:4F:47:ASN:HB2	60:4F:89:TYR:CD2	2.54	0.42
63:4I:59:ASP:O	63:4I:63:MET:HG3	2.19	0.42
9:5I:26:LEU:O	71:5I:204:PC1:H261	2.19	0.42
12:5L:264:TYR:O	12:5L:268:GLU:HG3	2.18	0.42
13:5M:231:LEU:HA	13:5M:235:LEU:HB2	2.01	0.42
23:5X:82:THR:HA	23:5X:85:TRP:CD1	2.54	0.42
33:5h:64:TRP:CD1	33:5h:77:ARG:HG3	2.54	0.42
35:5j:37:LEU:CB	36:5k:77:PHE:HB2	2.48	0.42
40:5o:23:THR:OG1	40:5o:104:GLU:OE2	2.36	0.42
47:6C:89:MET:O	47:6C:90:PHE:C	2.62	0.42
48:6D:154:GLU:HA	48:6D:173:GLY:O	2.19	0.42
51:6G:44:ARG:HE	51:6G:44:ARG:HB2	1.66	0.42
45:6N:110:VAL:HG12	45:6N:215:HIS:CB	2.49	0.42
46:6O:53:ALA:H	46:6O:104:SER:HA	1.83	0.42
47:6P:272:TRP:HA	47:6P:275:LEU:HG	2.01	0.42
49:6R:150:SER:HB2	49:6R:170:ARG:HD3	1.99	0.42
55:8A:467:LEU:O	55:8A:468:MET:C	2.62	0.42
55:8A:483:SER:N	67:8M:2:TYR:O	2.48	0.42
82:8B:301:PGV:H91	82:8B:301:PGV:H61	1.55	0.42
57:8C:101:PHE:HA	57:8C:196:THR:HG21	2.01	0.42
75:8D:201:CDL:H771	75:8D:201:CDL:H801	1.82	0.42
61:8G:17:ARG:NH2	61:8G:18:PHE:CE1	2.84	0.42
82:8J:101:PGV:H82	82:8J:101:PGV:H291	2.01	0.42
2:1B:37:VAL:HG22	71:1B:202:PC1:H382	2.00	0.42
3:1C:175:ARG:NH2	3:1C:177:ASP:OD2	2.50	0.42
12:1L:309:GLN:HG2	12:1L:332:HIS:CD2	2.54	0.42
15:1O:45:LYS:HE2	15:1O:232:GLU:HG2	2.01	0.42
17:1Q:65:TRP:CE2	17:1Q:74:SER:HB2	2.54	0.42
35:1j:32:MET:O	35:1j:36:ILE:HG12	2.19	0.42
82:1p:201:PGV:H261	82:1p:201:PGV:H231	1.53	0.42
43:1r:105:LEU:HD13	43:1r:110:PRO:HB3	2.00	0.42
46:3B:314:ALA:CB	49:3I:63:PRO:HG3	2.50	0.42
47:3C:377:LEU:CB	50:3F:32:TYR:CE2	3.00	0.42
49:3E:234:TYR:HD2	49:3E:247:GLY:HA2	1.83	0.42
45:3N:38:GLY:O	45:3N:198:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:60:GLU:HB3	46:3O:287:ARG:HH12	1.84	0.42
45:3N:262:TRP:HB3	45:3N:386:TYR:CE1	2.54	0.42
45:3N:262:TRP:N	45:3N:313:CYS:SG	2.92	0.42
45:3N:269:PRO:O	45:3N:272:VAL:HB	2.18	0.42
47:3P:206:ASN:HB3	83:3P:502:HEM:O1D	2.20	0.42
48:3Q:37:CYS:SG	84:3Q:501:HEC:HBB3	2.59	0.42
50:3S:77:LYS:HA	50:3S:80:TRP:CD2	2.54	0.42
55:4A:27:GLY:O	55:4A:31:THR:HG22	2.19	0.42
56:4B:134:ARG:HB2	58:4D:110:THR:HG21	2.00	0.42
57:4C:156:ARG:NH1	57:4C:222:GLN:O	2.52	0.42
6:5F:288:ILE:H	6:5F:288:ILE:HG13	1.58	0.42
6:5F:302:SER:HB2	6:5F:350:LEU:HD22	2.01	0.42
11:5K:4:VAL:O	11:5K:8:ILE:HG12	2.19	0.42
12:5L:363:TYR:CD1	12:5L:370:THR:HG21	2.53	0.42
13:5M:104:LEU:HG	13:5M:108:MET:CE	2.49	0.42
13:5M:122:PHE:CE1	13:5M:206:LYS:HD3	2.54	0.42
14:5N:91:ASN:OD1	14:5N:93:VAL:HG13	2.19	0.42
15:5O:163:TYR:OH	15:5O:269:VAL:HG22	2.19	0.42
26:5a:34:LYS:HE2	26:5a:34:LYS:HB2	1.80	0.42
32:5g:58:MET:HE3	32:5g:58:MET:HB3	1.79	0.42
46:6B:42:ALA:O	46:6B:43:PRO:C	2.61	0.42
47:6C:145:VAL:O	47:6C:146:ILE:C	2.62	0.42
47:6C:345:HIS:C	47:6C:347:PHE:N	2.77	0.42
45:6N:138:LEU:HD11	45:6N:174:VAL:HG21	2.01	0.42
45:6N:428:ILE:O	45:6N:430:GLN:N	2.50	0.42
47:6P:376:LEU:O	50:6S:17:ARG:HD3	2.19	0.42
49:6R:93:ARG:NH2	51:6T:21:PHE:HA	2.34	0.42
54:6Y:15:ARG:O	54:6Y:16:ASN:C	2.63	0.42
55:8A:51:ASP:HB3	55:8A:55:ASN:OD1	2.20	0.42
55:8A:107:PRO:O	55:8A:111:LEU:HG	2.18	0.42
55:8A:115:SER:CB	55:8A:142:SER:HA	2.48	0.42
55:8A:134:GLY:O	55:8A:138:HIS:N	2.49	0.42
55:8A:417:MET:HE1	85:8A:605:HEA:H263	2.00	0.42
82:8A:604:PGV:H61	82:8A:604:PGV:H91	1.71	0.42
58:8D:48:TRP:HA	58:8D:51:LEU:HD13	2.01	0.42
58:8D:120:THR:HG23	58:8D:134:PHE:HZ	1.84	0.42
75:8D:201:CDL:H172	75:8D:201:CDL:H551	1.99	0.42
61:8G:36:TRP:HE3	82:8G:101:PGV:H251	1.84	0.42
2:1B:59:MET:HE3	2:1B:76:PHE:CE1	2.53	0.42
4:1D:379:VAL:HB	4:1D:388:ARG:HB3	2.01	0.42
12:1L:142:ILE:HD11	13:1M:371:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:514:LYS:HE3	12:1L:514:LYS:HB2	1.87	0.42
69:1Y:205:3PE:H322	69:1Y:205:3PE:H32	1.66	0.42
34:1i:75:LEU:HD22	34:1i:79:TRP:CE2	2.53	0.42
34:1i:125:GLN:O	34:1i:125:GLN:HG3	2.18	0.42
37:1l:65:ASP:OD1	38:1m:43:LYS:NZ	2.46	0.42
44:1s:31:GLU:N	44:1s:32:PRO:HD2	2.34	0.42
45:3A:68:LYS:CG	45:3A:119:ASN:HB3	2.49	0.42
46:3B:71:LEU:HD23	49:3I:68:VAL:HG11	2.01	0.42
47:3C:153:ILE:C	47:3C:158:THR:H	2.22	0.42
47:3C:320:LEU:HB2	47:3C:369:THR:CG2	2.50	0.42
45:3N:363:ASN:ND2	45:3N:363:ASN:H	2.13	0.42
45:3N:383:LEU:HD12	45:3N:383:LEU:HA	1.86	0.42
46:3O:200:THR:HB	46:3O:229:GLY:N	2.34	0.42
46:3O:245:ARG:NH2	46:3O:430:LEU:HB3	2.34	0.42
61:4G:17:ARG:NH1	61:4G:18:PHE:CE1	2.84	0.42
82:4K:101:PGV:H52	82:4K:101:PGV:H271	2.02	0.42
7:5G:399:TRP:O	17:5Q:127:ARG:HD2	2.19	0.42
10:5J:150:GLY:HA2	30:5e:16:TRP:CZ2	2.55	0.42
11:5K:34:GLU:O	11:5K:37:MET:HG3	2.18	0.42
12:5L:484:LEU:HD13	12:5L:484:LEU:C	2.45	0.42
15:5O:138:MET:HG2	15:5O:143:PHE:HD2	1.84	0.42
15:5O:304:TYR:CE1	69:5d:201:3PE:H112	2.54	0.42
20:5U:21:LEU:HD22	36:5k:46:ARG:HB3	2.00	0.42
23:5X:29:HIS:HB3	23:5X:119:PRO:HD2	2.00	0.42
69:5Y:203:3PE:H331	69:5Y:203:3PE:H231	2.01	0.42
29:5d:39:TYR:CZ	69:5d:201:3PE:H2G1	2.54	0.42
34:5i:39:VAL:HG12	34:5i:44:GLN:HG3	2.01	0.42
46:6B:213:HIS:HD1	46:6B:213:HIS:HA	1.66	0.42
47:6C:1:MET:H3	47:6C:1:MET:HG3	1.76	0.42
47:6C:91:PHE:O	47:6C:92:ILE:C	2.62	0.42
47:6C:235:MET:HE2	47:6C:236:MET:HG2	2.01	0.42
47:6C:332:LEU:HA	47:6C:335:LEU:HD12	2.01	0.42
48:6D:98:TYR:N	48:6D:98:TYR:CD1	2.87	0.42
48:6D:141:GLY:C	53:6J:53:TRP:HD1	2.27	0.42
48:6D:238:ASN:H	48:6D:246:ALA:HA	1.84	0.42
49:6E:151:LYS:HZ1	49:6E:152:ILE:CD1	2.33	0.42
52:6H:50:GLU:HG2	52:6H:86:PHE:CZ	2.53	0.42
53:6J:35:ALA:O	53:6J:36:PHE:C	2.62	0.42
45:6N:55:ALA:O	45:6N:59:VAL:N	2.39	0.42
45:6N:136:GLN:OE1	49:6V:51:CYS:HA	2.20	0.42
45:6N:280:TYR:CE2	45:6N:298:ALA:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:322:ALA:HB3	45:6N:338:LEU:HD21	2.01	0.42
45:6N:369:LEU:HD22	45:6N:369:LEU:HA	1.70	0.42
47:6P:149:LEU:HD23	47:6P:287:LYS:NZ	2.34	0.42
48:6Q:12:TRP:HB3	48:6Q:14:HIS:CE1	2.54	0.42
51:6T:74:PRO:HB2	51:6T:74:PRO:HD2	1.49	0.42
55:8A:32:ALA:O	55:8A:36:LEU:HG	2.19	0.42
55:8A:91:ASP:HB2	57:8C:10:MET:HE1	2.01	0.42
55:8A:183:LEU:HG	55:8A:274:VAL:HG12	2.00	0.42
55:8A:233:HIS:HA	55:8A:288:TRP:HE1	1.83	0.42
55:8A:360:ASN:O	55:8A:363:LEU:N	2.52	0.42
55:8A:495:LEU:HD22	55:8A:495:LEU:HA	1.82	0.42
55:8A:508:PRO:HB2	60:8F:32:ASN:HB3	2.02	0.42
63:8I:57:MET:O	63:8I:61:GLU:HG2	2.18	0.42
82:8J:101:PGV:H232	82:8J:101:PGV:H261	1.80	0.42
82:8J:101:PGV:H261	82:8J:101:PGV:H292	1.38	0.42
1:1A:80:GLN:H	1:1A:80:GLN:HG2	1.68	0.42
2:1B:39:TRP:C	2:1B:41:ARG:H	2.27	0.42
2:1B:62:MET:HE3	2:1B:69:MET:CB	2.49	0.42
2:1B:85:VAL:HB	2:1B:86:MET:H	1.58	0.42
6:1F:90:PRO:O	6:1F:218:CYS:HB3	2.20	0.42
6:1F:115:PRO:O	6:1F:119:VAL:HG23	2.19	0.42
10:1J:113:VAL:HG22	10:1J:119:PHE:HB2	2.00	0.42
11:1K:4:VAL:O	11:1K:8:ILE:HG12	2.19	0.42
13:1M:54:LEU:HD23	33:1h:93:ILE:HG23	2.01	0.42
15:1O:73:LEU:HD23	15:1O:292:VAL:HG13	2.01	0.42
16:1P:186:ARG:HD3	16:1P:251:ARG:HG3	2.02	0.42
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.54	0.42
69:1Y:203:3PE:H331	69:1Y:203:3PE:H231	2.01	0.42
28:1c:41:GLU:OE2	28:1c:45:ARG:NE	2.49	0.42
34:1i:39:VAL:HG12	34:1i:44:GLN:HG3	2.01	0.42
34:1i:101:PRO:CD	41:1p:14:ARG:HH22	2.30	0.42
35:1j:53:TYR:CZ	40:1o:98:MET:HE1	2.54	0.42
45:3A:176:LYS:HD3	45:3A:176:LYS:HA	1.58	0.42
47:3C:8:HIS:ND1	47:3C:11:MET:SD	2.93	0.42
52:3H:77:GLU:HA	52:3H:78:ASP:OD1	2.19	0.42
45:3N:146:ARG:HB3	45:3N:150:PHE:CE2	2.55	0.42
45:3N:223:TYR:CE1	45:3N:228:VAL:HG23	2.55	0.42
45:3N:319:LEU:HD22	45:3N:319:LEU:HA	1.84	0.42
45:3N:329:MET:CG	51:3T:6:HIS:CE1	3.02	0.42
46:3O:381:GLU:HG3	46:3O:385:GLN:NE2	2.33	0.42
47:3P:5:ARG:HA	47:3P:11:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3P:337:TRP:CH2	51:3T:59:TYR:HA	2.55	0.42
7:5G:255:HIS:HE1	7:5G:257:ASP:HB2	1.85	0.42
8:5H:90:PRO:HG3	8:5H:162:LEU:HB3	2.02	0.42
8:5H:104:PHE:O	8:5H:108:MET:HG2	2.19	0.42
10:5J:143:ILE:HG13	11:5K:57:ASN:HB3	2.01	0.42
13:5M:127:VAL:O	13:5M:131:ILE:HG12	2.20	0.42
14:5N:287:LEU:HB3	69:5N:901:3PE:H291	2.01	0.42
16:5P:193:LEU:O	16:5P:257:PRO:HA	2.19	0.42
17:5Q:10:LEU:HD22	22:5W:16:SER:C	2.45	0.42
24:5Y:30:ALA:O	24:5Y:34:ILE:HD12	2.19	0.42
69:5Y:205:3PE:H322	69:5Y:205:3PE:H32	1.66	0.42
35:5j:37:LEU:CD1	36:5k:77:PHE:HB3	2.39	0.42
35:5j:53:TYR:CZ	40:5o:98:MET:HE1	2.54	0.42
37:5l:50:LEU:HB2	37:5l:78:HIS:CD2	2.54	0.42
38:5m:3:PRO:HD2	39:5n:72:TYR:CE1	2.55	0.42
44:5s:31:GLU:N	44:5s:32:PRO:HD2	2.34	0.42
45:6A:47:TYR:CE2	45:6A:230:ALA:HA	2.54	0.42
48:6D:158:VAL:C	48:6D:170:MET:HA	2.45	0.42
48:6D:189:ALA:HB3	48:6D:197:LEU:HB2	2.01	0.42
48:6D:254:TYR:O	48:6D:255:ASN:C	2.61	0.42
45:6N:64:PHE:HD2	46:6O:287:ARG:HH21	1.59	0.42
45:6N:69:ASN:ND2	45:6N:115:ASP:CG	2.71	0.42
45:6N:170:PRO:O	45:6N:174:VAL:N	2.39	0.42
45:6N:171:SER:N	49:6R:82:ASP:OD1	2.50	0.42
45:6N:186:VAL:HA	45:6N:190:TYR:HD2	1.84	0.42
45:6N:283:THR:O	45:6N:284:TYR:C	2.63	0.42
46:6O:240:ARG:O	46:6O:241:GLY:C	2.61	0.42
49:6R:213:LEU:CD2	49:6R:258:LEU:HB2	2.42	0.42
55:8A:38:ARG:HD2	85:8A:605:HEA:OMA	2.18	0.42
55:8A:241:PRO:O	55:8A:242:GLU:C	2.61	0.42
55:8A:271:MET:HB3	55:8A:271:MET:HE3	1.89	0.42
55:8A:303:ALA:O	55:8A:304:TYR:C	2.62	0.42
55:8A:478:SER:O	67:8M:6:ALA:HB1	2.19	0.42
55:8A:500:PRO:HA	55:8A:501:PRO:HD3	1.88	0.42
57:8C:220:LEU:O	57:8C:224:LYS:HG3	2.19	0.42
75:8D:201:CDL:H401	75:8D:201:CDL:H331	2.01	0.42
1:1A:17:LEU:HA	1:1A:20:ILE:HD12	2.00	0.42
5:1E:167:LYS:O	5:1E:171:GLU:HG3	2.19	0.42
8:1H:81:LEU:HA	8:1H:84:THR:HG22	2.02	0.42
10:1J:150:GLY:HA2	30:1e:16:TRP:CZ2	2.55	0.42
12:1L:193:SER:CB	12:1L:206:ASN:HD21	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:289:ALA:O	12:1L:293:ILE:HG23	2.19	0.42
14:1N:274:GLU:HG2	24:1Y:139:LYS:HE2	2.01	0.42
15:1O:315:LYS:HA	15:1O:315:LYS:HD2	1.85	0.42
17:1Q:10:LEU:HD22	22:1W:16:SER:C	2.45	0.42
18:1R:31:ARG:HE	42:1q:125:VAL:HG22	1.84	0.42
19:1S:18:ILE:HD11	19:1S:52:ILE:HG12	2.00	0.42
21:1V:49:GLN:HA	21:1V:52:ASN:HD21	1.85	0.42
23:1X:29:HIS:HB3	23:1X:119:PRO:HD2	2.00	0.42
24:1Y:44:PRO:HA	24:1Y:45:PRO:HD3	1.87	0.42
45:3A:21:ASN:HA	45:3A:221:GLY:HA2	2.01	0.42
47:3C:77:TRP:CG	48:3D:286:GLU:CB	3.02	0.42
47:3C:101:GLY:HA2	47:3C:106:SER:HB2	2.01	0.42
45:3N:39:VAL:HG11	45:3N:195:MET:HE3	2.01	0.42
45:3N:111:GLU:O	45:3N:112:LEU:C	2.61	0.42
45:3N:149:VAL:HA	45:3N:152:TYR:HD2	1.84	0.42
45:3N:276:ILE:HG21	45:3N:345:LEU:HD21	2.02	0.42
46:3O:314:ALA:HB1	49:3V:63:PRO:HB3	2.02	0.42
49:3R:134:SER:O	49:3R:138:SER:OG	2.32	0.42
50:3S:59:VAL:HG11	51:3T:10:MET:HG3	2.02	0.42
2:5B:96:MET:HE3	2:5B:99:ALA:HB3	2.02	0.42
3:5C:15:ASN:HB3	3:5C:46:ASN:ND2	2.35	0.42
6:5F:96:ASN:O	6:5F:225:VAL:HG23	2.19	0.42
7:5G:543:ILE:O	7:5G:558:ASP:N	2.48	0.42
12:5L:316:THR:HG23	12:5L:325:ALA:HB2	2.02	0.42
13:5M:74:PRO:HA	13:5M:77:LEU:HD12	2.01	0.42
16:5P:44:GLN:HE21	18:5R:23:TYR:HE2	1.66	0.42
17:5Q:65:TRP:CE2	17:5Q:74:SER:HB2	2.54	0.42
22:5W:91:GLU:OE1	22:5W:91:GLU:HA	2.19	0.42
23:5X:68:ASP:O	23:5X:72:GLN:HG3	2.19	0.42
45:6A:285:GLY:N	49:6I:71:ASN:H	2.17	0.42
45:6A:419:CYS:SG	51:6G:23:PHE:HB2	2.59	0.42
46:6B:77:THR:HB	46:6B:130:PRO:HA	2.01	0.42
46:6B:89:ILE:O	46:6B:93:GLY:N	2.53	0.42
46:6B:385:GLN:HA	46:6B:389:ALA:HB3	2.02	0.42
47:6C:156:ILE:H	47:6C:156:ILE:HG13	1.32	0.42
47:6C:324:LEU:HD11	47:6C:369:THR:HG21	2.01	0.42
47:6C:328:LEU:HD12	47:6C:328:LEU:HA	1.76	0.42
48:6D:190:ARG:O	48:6D:191:ALA:C	2.62	0.42
48:6D:297:MET:HE3	48:6D:297:MET:HB3	1.79	0.42
53:6J:11:TYR:O	53:6J:12:SER:C	2.62	0.42
45:6N:111:GLU:O	45:6N:112:LEU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6O:84:LYS:O	46:6O:85:ILE:C	2.62	0.42
46:6O:168:TYR:HE2	46:6O:321:LEU:HG	1.84	0.42
48:6Q:144:ARG:HG2	48:6Q:147:LEU:HD12	2.02	0.42
49:6R:150:SER:HB3	49:6R:170:ARG:N	2.34	0.42
49:6V:71:ASN:OD1	49:6V:71:ASN:N	2.52	0.42
55:8A:78:PHE:HE2	55:8A:389:ILE:HA	1.84	0.42
55:8A:132:LEU:HA	56:8B:159:VAL:HG11	2.00	0.42
55:8A:154:GLY:O	55:8A:155:VAL:C	2.63	0.42
55:8A:300:ASP:HB3	68:8N:65:PHE:CD2	2.54	0.42
55:8A:408:ALA:O	55:8A:409:TRP:C	2.63	0.42
57:8C:175:LEU:HD13	82:8C:304:PGV:H212	2.00	0.42
62:8H:36:PHE:O	62:8H:40:GLU:HG3	2.18	0.42
2:1B:154:GLU:HG2	9:1I:50:TYR:CE2	2.55	0.42
3:1C:125:LYS:HA	3:1C:125:LYS:HD3	1.78	0.42
5:1E:140:ILE:HD12	5:1E:140:ILE:HA	1.89	0.42
8:1H:124:ASN:C	8:1H:126:LYS:H	2.27	0.42
11:1K:50:ASN:O	30:1e:31:ARG:HD2	2.19	0.42
12:1L:375:ILE:HG12	35:1j:32:MET:SD	2.60	0.42
12:1L:484:LEU:HD13	12:1L:484:LEU:C	2.44	0.42
12:1L:528:TYR:CG	37:1l:101:MET:HB3	2.54	0.42
69:1L:703:3PE:H332	75:1i:201:CDL:H341	2.00	0.42
16:1P:268:ARG:O	16:1P:272:VAL:HG23	2.19	0.42
17:1Q:59:PHE:CE2	17:1Q:79:LEU:HD13	2.55	0.42
22:1W:91:GLU:OE1	22:1W:91:GLU:HA	2.19	0.42
34:1i:6:ASP:OD2	39:1n:157:ARG:NH2	2.49	0.42
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.44	0.42
46:3B:116:ILE:HD12	46:3B:211:VAL:HG12	2.02	0.42
46:3B:200:THR:OG1	46:3B:229:GLY:O	2.26	0.42
47:3C:111:GLU:HA	47:3C:114:ASN:HD22	1.83	0.42
47:3C:141:TRP:CE2	47:3C:264:THR:HA	2.54	0.42
47:3C:206:ASN:H	83:3C:502:HEM:CGD	2.33	0.42
45:3N:310:PHE:O	45:3N:312:ILE:HG13	2.20	0.42
46:3O:263:ALA:O	46:3O:264:THR:C	2.63	0.42
48:3Q:12:TRP:HB3	48:3Q:14:HIS:CE1	2.54	0.42
49:3R:244:ASP:CG	49:3R:248:ARG:HB2	2.45	0.42
5:5E:39:PRO:HA	44:5s:65:GLN:HB3	2.01	0.42
10:5J:45:LEU:HD23	10:5J:50:SER:HA	2.02	0.42
10:5J:139:GLU:HG3	11:5K:49:LEU:HD21	2.01	0.42
12:5L:213:LEU:HB3	12:5L:273:VAL:HG11	2.01	0.42
12:5L:233:LEU:HB3	12:5L:234:PRO:HD3	2.02	0.42
13:5M:257:MET:SD	69:5M:503:3PE:H352	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5M:336:ARG:HD3	13:5M:426:ILE:HA	2.01	0.42
14:5N:49:ASN:OD1	14:5N:52:ALA:N	2.42	0.42
14:5N:97:MET:HA	14:5N:97:MET:HE3	2.01	0.42
20:5U:55:GLU:OE1	20:5U:62:ILE:N	2.46	0.42
29:5d:49:ARG:HD3	29:5d:51:ARG:NH2	2.33	0.42
29:5d:59:HIS:H	29:5d:59:HIS:CD2	2.38	0.42
75:5i:201:CDL:OA7	75:5i:201:CDL:H742	2.20	0.42
35:5j:6:HIS:CD2	35:5j:7:ILE:HG12	2.55	0.42
35:5j:67:LEU:HD12	35:5j:67:LEU:HA	1.88	0.42
45:6A:68:LYS:HG3	45:6A:69:ASN:N	2.33	0.42
45:6A:112:LEU:HD23	45:6A:112:LEU:HA	1.66	0.42
45:6A:250:LEU:HD23	45:6A:250:LEU:HA	1.84	0.42
45:6A:335:MET:HE2	45:6A:335:MET:HB2	1.69	0.42
46:6B:79:GLY:HA3	46:6B:125:ASN:HB3	2.01	0.42
46:6B:226:MET:HE3	46:6B:226:MET:HB2	1.87	0.42
46:6B:301:LYS:HE3	46:6B:301:LYS:HB3	1.54	0.42
47:6C:143:ALA:O	47:6C:144:THR:C	2.61	0.42
47:6C:158:THR:O	47:6C:159:ASP:C	2.62	0.42
47:6C:179:PHE:O	47:6C:180:ALA:C	2.63	0.42
48:6D:208:ARG:HB3	48:6D:211:GLY:HA3	2.02	0.42
53:6J:59:LYS:HD3	53:6J:60:TYR:HD2	1.84	0.42
45:6N:38:GLY:C	45:6N:98:TYR:CD1	2.97	0.42
45:6N:62:LEU:CD1	45:6N:182:LEU:CD1	2.92	0.42
46:6O:197:ASN:O	46:6O:232:LEU:HB2	2.20	0.42
46:6O:261:SER:HB3	46:6O:321:LEU:N	2.35	0.42
46:6O:430:LEU:HD22	46:6O:433:THR:HG21	2.01	0.42
47:6P:284:ILE:CD1	47:6P:285:PRO:HD2	2.50	0.42
47:6P:337:TRP:CH2	51:6T:59:TYR:HA	2.55	0.42
48:6Q:231:LYS:HD3	50:6S:70:MET:HE3	2.02	0.42
54:6Y:7:GLY:O	54:6Y:8:PRO:C	2.62	0.42
55:8A:165:ILE:HG22	57:8C:85:LEU:HD11	2.00	0.42
55:8A:203:ALA:HA	55:8A:206:ILE:HD13	2.00	0.42
56:8B:129:LYS:HB2	56:8B:132:GLU:HG3	1.99	0.42
57:8C:3:HIS:NE2	60:8F:96:LEU:HD11	2.34	0.42
58:8D:137:LYS:H	58:8D:137:LYS:HG2	1.58	0.42
4:1D:317:LYS:HA	4:1D:317:LYS:HD3	1.71	0.42
5:1E:205:PRO:HA	5:1E:206:PRO:HD3	1.93	0.42
6:1F:202:LYS:HD3	6:1F:361:GLN:HB2	2.01	0.42
7:1G:24:THR:O	7:1G:73:VAL:HG22	2.19	0.42
7:1G:399:TRP:O	17:1Q:127:ARG:HD2	2.19	0.42
8:1H:66:SER:HA	8:1H:122:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:90:PRO:HG3	8:1H:162:LEU:HB3	2.02	0.42
10:1J:14:VAL:O	10:1J:18:VAL:HG23	2.20	0.42
11:1K:87:THR:HG21	11:1K:89:TYR:CD2	2.55	0.42
12:1L:69:MET:HE2	12:1L:71:LEU:HD11	2.01	0.42
13:1M:8:THR:O	13:1M:11:LEU:HB2	2.20	0.42
13:1M:74:PRO:HA	13:1M:77:LEU:HD12	2.01	0.42
14:1N:287:LEU:HB3	69:1N:901:3PE:H291	2.01	0.42
33:1h:64:TRP:CD1	33:1h:77:ARG:HG3	2.54	0.42
36:1k:48:GLU:OE1	39:1n:33:ARG:NE	2.42	0.42
40:1o:112:LYS:HE2	40:1o:112:LYS:HB3	1.80	0.42
45:3A:398:ARG:O	45:3A:401:GLU:HG2	2.19	0.42
46:3B:120:MET:O	46:3B:124:LEU:HD23	2.19	0.42
46:3B:163:LEU:HD11	46:3B:258:VAL:HG22	2.01	0.42
46:3B:213:HIS:CD2	46:3B:217:LYS:HE3	2.54	0.42
46:3B:349:GLN:OE1	46:3B:349:GLN:HA	2.19	0.42
47:3C:59:THR:CG2	47:3C:172:LYS:HB2	2.47	0.42
47:3C:85:ASN:HB2	47:3C:243:VAL:CG2	2.50	0.42
47:3C:315:MET:SD	47:3C:325:PHE:HB2	2.59	0.42
45:3N:33:PRO:HD2	45:3N:34:THR:HG23	2.01	0.42
45:3N:255:ILE:HG13	45:3N:422:VAL:HG22	2.02	0.42
45:3N:262:TRP:NE1	45:3N:315:ALA:HA	2.35	0.42
45:3N:336:PHE:HD2	45:3N:337:PHE:CD1	2.37	0.42
46:3O:342:ASP:O	46:3O:346:THR:HG23	2.20	0.42
46:3O:420:GLY:O	46:3O:421:ARG:C	2.63	0.42
55:4A:328:HIS:ND1	89:4B:303:PSC:O02	2.52	0.42
85:4A:605:HEA:H202	85:4A:605:HEA:H171	1.76	0.42
57:4C:35:PHE:O	61:4G:58:LYS:NZ	2.43	0.42
2:5B:63:ALA:HB2	2:5B:69:MET:SD	2.59	0.42
5:5E:162:GLU:OE2	6:5F:108:ARG:NH1	2.47	0.42
7:5G:60:GLU:OE1	7:5G:78:ASN:ND2	2.46	0.42
7:5G:616:LEU:HA	7:5G:619:VAL:HG12	2.02	0.42
10:5J:26:PRO:HG3	10:5J:77:GLU:HG3	2.01	0.42
14:5N:95:MET:HE2	14:5N:149:ILE:HA	2.01	0.42
15:5O:193:LYS:H	15:5O:193:LYS:HG2	1.73	0.42
16:5P:186:ARG:HD3	16:5P:251:ARG:HG3	2.01	0.42
18:5R:12:THR:HG22	18:5R:35:VAL:HG22	2.01	0.42
19:5S:75:ASN:OD1	19:5S:75:ASN:N	2.53	0.42
23:5X:21:SER:OG	26:5a:51:ASP:OD2	2.35	0.42
24:5Y:22:TYR:O	24:5Y:25:THR:HG22	2.20	0.42
39:5n:123:GLN:O	39:5n:126:ARG:HG2	2.19	0.42
43:5r:105:LEU:HD13	43:5r:110:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6A:333:ASP:O	45:6A:334:MET:C	2.62	0.42
47:6C:125:ALA:O	47:6C:126:THR:C	2.63	0.42
47:6C:236:MET:HA	47:6C:239:LEU:HD23	2.01	0.42
47:6C:260:ASN:C	47:6C:262:LEU:H	2.28	0.42
47:6C:347:PHE:HA	47:6C:350:ILE:HD12	2.02	0.42
48:6D:289:HIS:O	48:6D:290:ARG:C	2.63	0.42
49:6I:70:LEU:O	49:6I:70:LEU:HD23	2.19	0.42
45:6N:19:LEU:CG	45:6N:23:LEU:HB2	2.50	0.42
45:6N:136:GLN:OE1	49:6V:51:CYS:CA	2.66	0.42
45:6N:415:PHE:O	45:6N:416:TYR:C	2.61	0.42
46:6O:90:GLU:O	46:6O:91:ALA:C	2.62	0.42
46:6O:258:VAL:HB	46:6O:321:LEU:HD22	2.02	0.42
46:6O:391:SER:O	46:6O:392:TYR:C	2.63	0.42
48:6Q:37:CYS:SG	84:6Q:501:HEC:HBB3	2.59	0.42
55:8A:254:ILE:O	55:8A:255:SER:C	2.62	0.42
56:8B:5:PHE:HE2	65:8K:42:LEU:HD23	1.83	0.42
56:8B:11:ASP:HB2	58:8D:129:ALA:HA	2.01	0.42
57:8C:58:TRP:HD1	57:8C:61:ILE:HD12	1.85	0.42
60:8F:47:ASN:HB2	60:8F:89:TYR:CD2	2.54	0.42
64:8J:37:THR:HG23	82:8J:101:PGV:H142	2.00	0.42
82:8J:101:PGV:H232	82:8J:101:PGV:H292	2.02	0.42
2:1B:76:PHE:HD1	2:1B:76:PHE:HA	1.74	0.42
6:1F:45:THR:O	6:1F:49:LEU:HG	2.20	0.42
7:1G:199:ILE:CG2	7:1G:208:LEU:HD13	2.50	0.42
7:1G:375:ASP:HB2	7:1G:448:LYS:H	1.85	0.42
7:1G:616:LEU:HA	7:1G:619:VAL:HG12	2.01	0.42
8:1H:124:ASN:HB3	8:1H:125:SER:H	1.58	0.42
10:1J:65:LEU:O	10:1J:66:VAL:HG23	2.20	0.42
11:1K:41:PHE:CE2	11:1K:64:LEU:HD13	2.55	0.42
12:1L:383:MET:HE2	35:1j:36:ILE:HD12	2.02	0.42
13:1M:2:LEU:HD23	13:1M:2:LEU:HA	1.91	0.42
13:1M:346:ARG:O	13:1M:419:TYR:HA	2.19	0.42
14:1N:284:MET:HB3	69:1N:901:3PE:H2F2	2.02	0.42
71:1P:401:PC1:H272	71:1P:401:PC1:H242	1.38	0.42
20:1T:42:LEU:HB3	20:1T:46:ASP:HB2	2.02	0.42
23:1X:46:ARG:HD2	23:1X:46:ARG:HA	1.73	0.42
24:1Y:80:ARG:CA	24:1Y:81:GLU:OE2	2.68	0.42
46:3B:308:ASP:OD2	49:3I:56:SER:CA	2.67	0.42
47:3C:138:MET:HB2	47:3C:255:ASN:N	2.35	0.42
47:3C:153:ILE:HD12	47:3C:156:ILE:HG21	2.02	0.42
47:3C:224:TYR:O	47:3C:225:THR:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:113:LEU:O	45:3N:114:ALA:C	2.61	0.42
45:3N:262:TRP:HB3	45:3N:386:TYR:CZ	2.55	0.42
45:3N:369:LEU:HD23	45:3N:369:LEU:HA	1.86	0.42
46:3O:200:THR:OG1	46:3O:203:ARG:HD3	2.19	0.42
47:3P:10:LEU:O	47:3P:13:ILE:HG12	2.19	0.42
47:3P:32:ASN:ND2	47:3P:228:ASP:HA	2.35	0.42
49:3R:150:SER:HB3	49:3R:170:ARG:N	2.34	0.42
49:3R:182:LYS:HB2	49:3R:182:LYS:HE2	1.89	0.42
54:3X:9:ARG:NH1	54:3X:13:LEU:HD11	2.35	0.42
55:4A:106:PRO:HB2	82:4A:601:PGV:H162	2.00	0.42
55:4A:334:TRP:CH2	56:4B:46:LEU:HB3	2.55	0.42
55:4A:398:PRO:O	55:4A:498:CYS:HB3	2.20	0.42
57:4C:220:LEU:O	57:4C:224:LYS:HG3	2.19	0.42
2:5B:91:THR:HA	2:5B:119:CYS:HB3	2.01	0.42
4:5D:379:VAL:HB	4:5D:388:ARG:HB3	2.01	0.42
6:5F:45:THR:O	6:5F:49:LEU:HG	2.20	0.42
6:5F:92:TYR:O	6:5F:220:THR:HA	2.19	0.42
7:5G:199:ILE:CG2	7:5G:208:LEU:HD13	2.50	0.42
8:5H:81:LEU:HA	8:5H:84:THR:HG22	2.01	0.42
8:5H:317:GLN:OE1	10:5J:141:MET:HE1	2.19	0.42
10:5J:65:LEU:O	10:5J:66:VAL:HG23	2.20	0.42
11:5K:25:HIS:HD2	11:5K:88:ASP:OD2	2.02	0.42
12:5L:104:SER:HB2	12:5L:118:PHE:CZ	2.54	0.42
69:5M:501:3PE:H341	14:5N:277:ILE:HG12	2.02	0.42
16:5P:135:LEU:HA	16:5P:167:LYS:HB3	2.01	0.42
23:5X:10:GLU:HA	23:5X:13:LYS:HE3	2.02	0.42
28:5c:21:LEU:O	28:5c:25:VAL:HG23	2.20	0.42
34:5i:76:ILE:H	34:5i:76:ILE:HG12	1.70	0.42
42:5q:42:ASP:C	42:5q:42:ASP:OD1	2.63	0.42
45:6A:407:VAL:O	45:6A:408:ARG:C	2.62	0.42
46:6B:137:VAL:HG21	46:6B:188:PRO:HB3	2.01	0.42
46:6B:245:ARG:HE	46:6B:245:ARG:HB3	1.73	0.42
46:6B:280:GLY:HA3	46:6B:293:SER:HB2	2.02	0.42
47:6C:24:PRO:CA	47:6C:217:LYS:HA	2.40	0.42
47:6C:101:GLY:HA2	47:6C:106:SER:CB	2.48	0.42
47:6C:355:SER:O	47:6C:358:TYR:HB3	2.20	0.42
49:6E:241:SER:HA	49:6E:249:ILE:HG13	2.01	0.42
50:6F:119:TRP:HH2	46:6O:91:ALA:CB	2.33	0.42
53:6J:55:HIS:O	53:6J:58:HIS:ND1	2.49	0.42
45:6N:19:LEU:HD12	45:6N:23:LEU:CB	2.50	0.42
45:6N:40:TRP:NE1	45:6N:377:GLU:C	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:378:ASP:HA	45:6N:381:ARG:NE	2.33	0.42
46:6O:37:SER:HB3	46:6O:213:HIS:CD2	2.55	0.42
46:6O:68:LEU:HD21	46:6O:137:VAL:HG13	2.01	0.42
46:6O:90:GLU:C	46:6O:93:GLY:H	2.28	0.42
46:6O:166:ALA:HA	46:6O:240:ARG:HD3	2.02	0.42
46:6O:365:LYS:HD2	46:6O:403:ASP:OD1	2.19	0.42
55:8A:320:VAL:O	55:8A:324:LEU:HG	2.20	0.42
55:8A:334:TRP:HZ3	56:8B:46:LEU:HD13	1.80	0.42
55:8A:443:TYR:HE1	55:8A:448:THR:HA	1.85	0.42
5:1E:39:PRO:HA	44:1s:65:GLN:HB3	2.01	0.42
7:1G:39:ARG:HB2	72:1G:803:FES:S2	2.60	0.42
10:1J:115:ILE:O	10:1J:117:PHE:N	2.48	0.42
13:1M:16:TRP:HA	13:1M:93:LYS:HD3	2.02	0.42
13:1M:98:MET:HE1	69:1N:902:3PE:H3D2	2.01	0.42
15:1O:163:TYR:OH	15:1O:269:VAL:HG22	2.20	0.42
20:1T:63:PRO:HD2	20:1T:66:ASP:OD1	2.20	0.42
23:1X:10:GLU:HA	23:1X:13:LYS:HE3	2.02	0.42
23:1X:68:ASP:O	23:1X:72:GLN:HG3	2.19	0.42
32:1g:108:MET:HE2	41:1p:98:ASP:HB3	2.01	0.42
39:1n:91:GLU:HB2	39:1n:94:GLU:HG3	2.02	0.42
45:3A:154:HIS:NE2	45:3A:314:TYR:OH	2.39	0.42
47:3C:71:ARG:NH1	48:3D:133:TYR:HB2	2.35	0.42
47:3C:211:ILE:O	47:3C:212:SER:C	2.62	0.42
47:3C:244:LEU:CA	48:3D:290:ARG:HG2	2.33	0.42
45:3N:36:THR:OG1	45:3N:200:ALA:CB	2.54	0.42
45:3N:223:TYR:CD1	45:3N:228:VAL:HG23	2.55	0.42
45:3N:262:TRP:HE1	45:3N:315:ALA:HA	1.85	0.42
45:3N:294:LEU:HD13	45:3N:337:PHE:HB2	2.01	0.42
45:3N:351:GLU:CA	45:3N:354:VAL:HB	2.41	0.42
45:3N:392:LEU:HA	45:3N:395:TRP:HD1	1.83	0.42
45:3N:438:ARG:HD3	45:3N:438:ARG:HA	1.76	0.42
46:3O:195:VAL:HG13	46:3O:199:PHE:HB2	2.00	0.42
46:3O:343:GLN:O	46:3O:346:THR:OG1	2.38	0.42
49:3R:191:GLU:HG3	49:3R:194:GLN:H	1.85	0.42
49:3R:213:LEU:CD2	49:3R:258:LEU:HB2	2.42	0.42
55:4A:420:GLY:O	55:4A:424:THR:OG1	2.35	0.42
56:4B:5:PHE:HE2	65:4K:42:LEU:HD23	1.83	0.42
89:4B:303:PSC:H252	89:4B:303:PSC:H302	2.02	0.42
57:4C:22:LEU:O	57:4C:26:LEU:HG	2.20	0.42
6:5F:90:PRO:O	6:5F:218:CYS:HB3	2.19	0.42
10:5J:119:PHE:CD1	11:5K:6:MET:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5L:207:GLU:HG2	12:5L:269:THR:HG23	2.02	0.42
12:5L:289:ALA:O	12:5L:293:ILE:HG23	2.19	0.42
12:5L:528:TYR:CG	37:5l:101:MET:HB3	2.54	0.42
13:5M:88:THR:O	13:5M:92:LYS:HG3	2.20	0.42
13:5M:346:ARG:O	13:5M:419:TYR:HA	2.19	0.42
15:5O:45:LYS:HE2	15:5O:232:GLU:HG2	2.01	0.42
24:5Y:80:ARG:CA	24:5Y:81:GLU:OE2	2.68	0.42
24:5Y:128:GLN:HG2	69:5Y:203:3PE:O14	2.19	0.42
32:5g:95:ARG:HH22	41:5p:64:HIS:CD2	2.38	0.42
35:5j:32:MET:O	35:5j:36:ILE:HG12	2.19	0.42
35:5j:37:LEU:HB3	36:5k:77:PHE:CB	2.50	0.42
41:5p:136:LYS:HD2	41:5p:136:LYS:O	2.20	0.42
46:6B:96:LEU:HB3	49:6I:70:LEU:HD22	2.01	0.42
47:6C:91:PHE:HB3	47:6C:95:PHE:CZ	2.54	0.42
47:6C:160:LEU:HA	47:6C:160:LEU:HD12	1.91	0.42
48:6D:114:ILE:HG12	48:6D:277:THR:C	2.45	0.42
50:6F:61:ARG:HB3	46:6O:135:TRP:CD2	2.54	0.42
51:6G:36:ILE:HB	51:6G:37:PRO:HD3	2.01	0.42
45:6N:61:HIS:HA	46:6O:287:ARG:NH2	2.35	0.42
45:6N:134:ILE:HG22	45:6N:138:LEU:HG	2.02	0.42
45:6N:171:SER:HG	49:6R:82:ASP:CG	2.28	0.42
45:6N:289:HIS:O	45:6N:290:MET:C	2.63	0.42
45:6N:349:ALA:HB3	54:6X:16:ASN:ND2	2.30	0.42
46:6O:28:ARG:HE	46:6O:32:GLY:C	2.28	0.42
46:6O:69:LEU:HD13	46:6O:69:LEU:HA	1.89	0.42
46:6O:315:SER:CB	46:6O:320:GLY:HA2	2.50	0.42
50:6S:59:VAL:HG11	51:6T:10:MET:HG3	2.02	0.42
54:6Y:32:LEU:HD12	54:6Y:32:LEU:HA	1.79	0.42
55:8A:34:SER:HB3	55:8A:61:HIS:CE1	2.55	0.42
55:8A:53:ILE:O	55:8A:54:TYR:C	2.62	0.42
55:8A:118:VAL:O	55:8A:120:ALA:N	2.52	0.42
55:8A:190:ILE:O	55:8A:193:VAL:HB	2.19	0.42
55:8A:513:LEU:HA	60:8F:35:ALA:HB3	2.02	0.42
82:8A:601:PGV:H272	82:8A:601:PGV:H242	1.61	0.42
82:8A:602:PGV:H02	82:8C:305:PGV:H211	2.02	0.42
58:8D:121:LYS:HG3	65:8K:53:TRP:HD1	1.84	0.42
63:8I:59:ASP:O	63:8I:63:MET:HG3	2.19	0.42
2:1B:179:ARG:O	16:1P:103:ASN:ND2	2.53	0.42
7:1G:183:VAL:HG21	70:1G:802:SF4:S1	2.60	0.42
8:1H:104:PHE:O	8:1H:108:MET:HG2	2.19	0.42
14:1N:30:TRP:CG	14:1N:71:MET:HE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:135:LEU:HA	16:1P:167:LYS:HB3	2.01	0.42
16:1P:196:LEU:HD12	16:1P:196:LEU:HA	1.94	0.42
20:1T:19:LEU:HD23	20:1T:19:LEU:HA	1.88	0.42
37:1l:158:ILE:HA	40:1o:33:ARG:HH21	1.84	0.42
41:1p:84:MET:HE2	41:1p:84:MET:HB3	1.91	0.42
43:1r:105:LEU:HD23	43:1r:105:LEU:HA	1.84	0.42
45:3A:30:SER:HB2	45:3A:32:GLN:HE21	1.85	0.42
45:3A:429:GLU:OE1	51:3G:9:LEU:HB2	2.20	0.42
46:3B:74:SER:O	46:3B:74:SER:OG	2.28	0.42
47:3C:138:MET:CG	47:3C:254:ASP:HB2	2.50	0.42
49:3E:223:VAL:O	49:3E:223:VAL:CG1	2.68	0.42
45:3N:16:VAL:HG22	45:3N:26:ALA:CB	2.49	0.42
45:3N:52:ASN:HA	45:3N:185:TYR:CZ	2.55	0.42
45:3N:58:PHE:CE1	45:3N:174:VAL:HG13	2.53	0.42
45:3N:80:GLU:CD	46:3O:292:THR:OG1	2.63	0.42
45:3N:144:SER:OG	45:3N:148:VAL:HG23	2.20	0.42
45:3N:292:SER:HB3	45:3N:295:ALA:HB2	2.01	0.42
47:3P:284:ILE:CD1	47:3P:285:PRO:HD2	2.50	0.42
55:4A:64:VAL:HA	55:4A:68:PHE:HD2	1.85	0.42
57:4C:58:TRP:HD1	57:4C:61:ILE:HD12	1.85	0.42
58:4D:20:ARG:HD2	59:4E:73:ASP:OD2	2.20	0.42
65:4K:12:LYS:HB2	65:4K:12:LYS:HE3	1.35	0.42
2:5B:71:ARG:NH2	9:5I:49:ASN:OD1	2.53	0.42
4:5D:371:LYS:HE2	4:5D:424:VAL:CG2	2.44	0.42
6:5F:256:PHE:CE2	6:5F:270:GLU:HB3	2.55	0.42
8:5H:126:LYS:HD3	8:5H:126:LYS:HA	1.77	0.42
10:5J:135:PHE:CD2	25:5Z:68:ARG:HD3	2.55	0.42
12:5L:309:GLN:HG2	12:5L:332:HIS:CD2	2.54	0.42
13:5M:16:TRP:HA	13:5M:93:LYS:HD3	2.02	0.42
19:5S:39:ARG:HD2	19:5S:87:THR:OG1	2.20	0.42
24:5Y:48:PHE:O	24:5Y:52:VAL:HG23	2.20	0.42
27:5b:77:LEU:O	27:5b:81:LYS:HG3	2.20	0.42
32:5g:108:MET:HE2	41:5p:98:ASP:HB3	2.01	0.42
43:5r:15:SER:OG	43:5r:19:LEU:HD23	2.20	0.42
45:6A:64:PHE:CE2	46:6B:286:LYS:HB3	2.53	0.42
45:6A:153:LEU:HA	45:6A:156:THR:HG22	2.01	0.42
45:6A:208:LEU:HA	45:6A:211:LEU:HD12	2.01	0.42
45:6A:304:CYS:SG	45:6A:307:PHE:HB3	2.60	0.42
45:6A:359:ASN:HA	45:6A:362:ARG:HD2	2.02	0.42
46:6B:56:ARG:HG3	46:6B:57:TYR:CD2	2.55	0.42
46:6B:238:LYS:HB2	46:6B:238:LYS:HE2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:6C:302:ILE:H	47:6C:302:ILE:HG13	1.47	0.42
47:6C:328:LEU:HD13	47:6C:361:ILE:HG21	2.02	0.42
49:6E:155:LYS:HE2	49:6E:159:ILE:HD11	2.02	0.42
49:6E:234:TYR:HB2	49:6E:243:TYR:HB3	2.02	0.42
50:6F:99:LYS:HD3	50:6F:99:LYS:HA	1.77	0.42
45:6N:58:PHE:CD2	45:6N:177:LEU:HD13	2.55	0.42
45:6N:89:TYR:HB2	45:6N:96:ALA:HB3	2.02	0.42
45:6N:130:GLU:O	45:6N:131:ARG:C	2.62	0.42
45:6N:191:LYS:O	45:6N:195:MET:HG2	2.19	0.42
45:6N:270:LEU:HD13	45:6N:311:ASN:HD21	1.85	0.42
45:6N:288:THR:HA	45:6N:296:SER:HB3	2.02	0.42
45:6N:349:ALA:HB1	45:6N:404:ALA:HB1	2.02	0.42
49:6R:130:LYS:HD3	54:6X:34:TRP:CZ2	2.55	0.42
49:6R:177:ARG:HD2	49:6R:234:TYR:OH	2.20	0.42
55:8A:2:PHE:O	55:8A:3:VAL:C	2.63	0.42
55:8A:62:ALA:HB3	55:8A:126:TRP:HB3	2.00	0.42
55:8A:182:PRO:HB3	55:8A:256:HIS:CE1	2.49	0.42
55:8A:187:SER:HB3	55:8A:277:MET:HE3	2.02	0.42
55:8A:253:MET:HE2	55:8A:253:MET:HB2	1.71	0.42
55:8A:445:ASP:HB3	65:8K:41:ASN:ND2	2.35	0.42
82:8A:604:PGV:O14	68:8N:40:ASN:ND2	2.52	0.42
1:1A:104:TYR:O	1:1A:108:GLN:HG2	2.20	0.41
2:1B:69:MET:HG3	2:1B:74:VAL:O	2.19	0.41
3:1C:15:ASN:HB3	3:1C:46:ASN:ND2	2.35	0.41
5:1E:136:LEU:HD23	5:1E:136:LEU:HA	1.93	0.41
6:1F:256:PHE:CE2	6:1F:270:GLU:HB3	2.55	0.41
10:1J:119:PHE:CD1	11:1K:6:MET:HB2	2.55	0.41
10:1J:135:PHE:CD2	25:1Z:68:ARG:HD3	2.55	0.41
10:1J:143:ILE:HG13	11:1K:57:ASN:HB3	2.01	0.41
12:1L:178:GLY:HA2	12:1L:218:LEU:HG	2.02	0.41
13:1M:150:LEU:HG	13:1M:154:LEU:HD12	2.02	0.41
13:1M:153:THR:OG1	13:1M:206:LYS:NZ	2.48	0.41
13:1M:452:LYS:HG3	32:1g:83:TYR:CE2	2.55	0.41
14:1N:245:MET:HE2	69:1N:902:3PE:H371	2.01	0.41
17:1Q:125:ASN:O	44:1s:70:ARG:NE	2.52	0.41
19:1S:39:ARG:HD2	19:1S:87:THR:OG1	2.20	0.41
21:1V:76:ILE:HD12	21:1V:76:ILE:HA	1.92	0.41
32:1g:58:MET:HE3	32:1g:58:MET:HB3	1.79	0.41
37:1l:40:ASP:N	37:1l:40:ASP:OD1	2.53	0.41
42:1q:53:LYS:HB2	42:1q:53:LYS:HE2	1.88	0.41
43:1r:15:SER:OG	43:1r:19:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:163:LEU:HB2	45:3A:234:CYS:SG	2.60	0.41
46:3B:22:GLN:OE1	46:3B:39:GLU:HB3	2.20	0.41
46:3B:46:ARG:HG3	46:3B:110:GLU:HG3	2.01	0.41
47:3C:107:TYR:HE1	47:3C:308:HIS:HB2	1.85	0.41
47:3C:186:PRO:HG2	83:3C:501:HEM:HMC3	2.02	0.41
48:3D:238:ASN:O	48:3D:245:GLN:HA	2.20	0.41
52:3H:74:GLN:NE2	52:3H:76:GLU:OE2	2.52	0.41
45:3N:57:TYR:CE2	45:3N:167:VAL:HG13	2.40	0.41
45:3N:153:LEU:O	45:3N:154:HIS:C	2.63	0.41
45:3N:298:ALA:O	45:3N:302:LYS:HA	2.20	0.41
45:3N:383:LEU:O	45:3N:387:GLY:HA2	2.19	0.41
46:3O:54:GLY:HA3	46:3O:103:GLU:C	2.45	0.41
47:3P:272:TRP:HA	47:3P:275:LEU:HG	2.01	0.41
47:3P:376:LEU:O	50:3S:17:ARG:HD3	2.19	0.41
48:3Q:231:LYS:HA	48:3Q:231:LYS:HD3	1.90	0.41
49:3R:130:LYS:HD3	54:3X:34:TRP:CZ2	2.55	0.41
55:4A:225:GLY:HA3	57:4C:112:LEU:HD21	2.02	0.41
55:4A:491:ASN:HB3	55:4A:494:TRP:HD1	1.83	0.41
57:4C:178:ALA:CB	82:4C:304:PGV:H22	2.50	0.41
3:5C:32:ILE:HG21	3:5C:63:PHE:CE1	2.55	0.41
5:5E:7:PHE:HB3	7:5G:175:THR:HB	2.00	0.41
7:5G:24:THR:O	7:5G:73:VAL:HG22	2.19	0.41
7:5G:110:GLN:HE22	17:5Q:45:MET:HE3	1.85	0.41
8:5H:98:MET:HE1	8:5H:104:PHE:CD2	2.55	0.41
8:5H:316:PRO:HG3	25:5Z:57:ARG:HB3	2.02	0.41
10:5J:3:MET:HE1	25:5Z:133:ILE:HD11	2.01	0.41
13:5M:72:LEU:HD21	13:5M:230:VAL:HA	2.01	0.41
13:5M:116:ILE:HA	13:5M:116:ILE:HD13	1.84	0.41
13:5M:150:LEU:HG	13:5M:154:LEU:HD12	2.02	0.41
14:5N:274:GLU:HG2	24:5Y:139:LYS:HE2	2.02	0.41
37:5l:114:PHE:O	37:5l:118:VAL:HG13	2.20	0.41
45:6A:19:LEU:HB2	45:6A:23:LEU:HB3	2.02	0.41
45:6A:44:GLY:H	45:6A:47:TYR:HB2	1.85	0.41
45:6A:178:SER:H	45:6A:181:ASP:CG	2.29	0.41
45:6A:417:ASP:HB3	49:6E:111:LYS:HD2	2.01	0.41
45:6A:418:GLN:O	45:6A:420:PRO:HD3	2.19	0.41
46:6B:313:ASN:N	49:6I:61:GLY:O	2.53	0.41
46:6B:422:LYS:HA	46:6B:422:LYS:HD3	1.40	0.41
47:6C:3:ASN:O	47:6C:6:LYS:N	2.53	0.41
47:6C:86:GLY:HA2	47:6C:239:LEU:CD1	2.50	0.41
48:6D:160:ASP:HB3	48:6D:167:GLU:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:6D:311:MET:O	48:6D:312:LYS:C	2.61	0.41
45:6N:4:TYR:CZ	46:6O:112:LEU:CG	3.02	0.41
45:6N:244:ARG:N	51:6T:13:VAL:O	2.51	0.41
45:6N:350:THR:OG1	45:6N:351:GLU:N	2.50	0.41
45:6N:444:LEU:HA	45:6N:444:LEU:HD13	1.76	0.41
47:6P:10:LEU:O	47:6P:13:ILE:HG12	2.19	0.41
55:8A:103:TRP:O	55:8A:106:PRO:HD2	2.20	0.41
55:8A:273:MET:HB3	55:8A:319:LYS:HZ1	1.84	0.41
55:8A:383:MET:O	55:8A:384:GLY:C	2.63	0.41
55:8A:431:LEU:HD22	55:8A:447:TYR:HD1	1.85	0.41
55:8A:468:MET:HE2	55:8A:468:MET:HB2	1.58	0.41
1:1A:74:PRO:HD2	10:1J:147:TYR:OH	2.20	0.41
4:1D:413:ASP:OD1	8:1H:281:ARG:NH1	2.53	0.41
5:1E:34:ILE:HD12	5:1E:49:PRO:HB2	2.02	0.41
5:1E:153:MET:HE2	5:1E:153:MET:HB2	1.91	0.41
6:1F:48:ILE:HD11	6:1F:236:ARG:HG3	2.02	0.41
8:1H:119:SER:HB2	8:1H:215:TYR:CE2	2.55	0.41
10:1J:3:MET:HE1	25:1Z:133:ILE:HD11	2.01	0.41
10:1J:26:PRO:HG3	10:1J:77:GLU:HG3	2.01	0.41
12:1L:271:LYS:HD3	12:1L:271:LYS:HA	1.62	0.41
12:1L:558:LEU:HD21	69:1Y:206:3PE:H2H2	2.01	0.41
13:1M:72:LEU:HD21	13:1M:230:VAL:HA	2.01	0.41
13:1M:127:VAL:O	13:1M:131:ILE:HG12	2.20	0.41
18:1R:27:ARG:HE	18:1R:27:ARG:HB3	1.68	0.41
24:1Y:22:TYR:O	24:1Y:25:THR:HG22	2.20	0.41
37:1l:50:LEU:HB2	37:1l:78:HIS:CD2	2.54	0.41
40:1o:24:PHE:CZ	40:1o:111:LYS:HD2	2.55	0.41
45:3A:145:MET:HE3	45:3A:425:LEU:HG	2.02	0.41
47:3C:153:ILE:O	47:3C:158:THR:N	2.32	0.41
47:3C:337:TRP:CD1	51:3G:61:TYR:CZ	3.09	0.41
49:3E:222:CYS:SG	72:3E:301:FES:S2	3.18	0.41
50:3F:99:LYS:HA	50:3F:99:LYS:HD3	1.76	0.41
51:3G:43:THR:O	51:3G:47:ILE:HB	2.20	0.41
46:3O:25:GLU:HB2	46:3O:37:SER:O	2.20	0.41
46:3O:133:ARG:O	46:3O:137:VAL:HG23	2.19	0.41
46:3O:256:ALA:CB	46:3O:325:TYR:HA	2.49	0.41
47:3P:119:LEU:HD22	83:3P:502:HEM:HBB2	2.03	0.41
47:3P:150:LEU:HD23	47:3P:150:LEU:HA	1.89	0.41
48:3Q:47:ALA:HA	48:3Q:90:TYR:HA	2.01	0.41
55:4A:144:ASP:OD2	57:4C:36:HIS:NE2	2.48	0.41
55:4A:510:TYR:HB3	60:4F:58:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4C:3:HIS:NE2	60:4F:96:LEU:HD11	2.34	0.41
59:4E:37:VAL:HG11	59:4E:70:VAL:HG21	2.02	0.41
62:4H:18:SER:O	68:4N:57:LEU:HD13	2.20	0.41
64:4J:4:ARG:HH12	64:4J:8:LYS:NZ	2.04	0.41
2:5B:154:GLU:HG2	9:5I:50:TYR:CE2	2.55	0.41
3:5C:16:ASP:O	3:5C:20:LYS:HG2	2.20	0.41
4:5D:413:ASP:OD1	8:5H:281:ARG:NH1	2.53	0.41
7:5G:39:ARG:HB2	72:5G:803:FES:S2	2.60	0.41
7:5G:237:ASN:HB3	7:5G:253:ARG:HB3	2.02	0.41
7:5G:391:PHE:O	7:5G:395:ILE:HG13	2.20	0.41
9:5I:30:LEU:HD13	71:5I:201:PC1:H261	2.02	0.41
11:5K:50:ASN:O	30:5e:31:ARG:HD2	2.19	0.41
12:5L:178:GLY:HA2	12:5L:218:LEU:HG	2.02	0.41
12:5L:383:MET:HE2	35:5j:36:ILE:HD12	2.02	0.41
12:5L:558:LEU:HD21	69:5Y:206:3PE:H2H2	2.02	0.41
13:5M:357:THR:O	13:5M:361:MET:HG3	2.20	0.41
13:5M:458:LEU:HA	13:5M:458:LEU:HD23	1.81	0.41
16:5P:319:ARG:NH1	22:5W:51:GLN:HG2	2.35	0.41
21:5V:37:ILE:O	21:5V:44:ARG:HD2	2.21	0.41
23:5X:39:ASN:HB3	25:5Z:73:PRO:HG2	2.02	0.41
24:5Y:116:TYR:HB3	71:5m:201:PC1:H3E1	2.02	0.41
69:5Y:206:3PE:H31	69:5Y:206:3PE:H321	1.37	0.41
45:6A:186:VAL:O	45:6A:190:TYR:N	2.53	0.41
45:6A:204:GLU:CD	45:6A:206:ARG:HB3	2.45	0.41
45:6A:294:LEU:HD22	45:6A:341:GLN:HG3	2.01	0.41
45:6A:303:LEU:HD22	45:6A:330:SER:HB3	2.02	0.41
45:6A:326:CYS:SG	45:6A:327:ASP:N	2.93	0.41
45:6A:378:ASP:HB3	45:6A:389:ARG:HH21	1.85	0.41
46:6B:321:LEU:O	46:6B:322:PHE:C	2.63	0.41
46:6B:435:PHE:HB2	46:6B:438:GLU:CD	2.45	0.41
47:6C:129:MET:HE2	47:6C:129:MET:HB2	1.83	0.41
47:6C:200:LEU:HD13	83:6C:502:HEM:HAD2	2.02	0.41
47:6C:281:LEU:O	47:6C:282:ARG:C	2.63	0.41
47:6C:345:HIS:O	51:6G:68:PHE:HB2	2.20	0.41
45:6N:16:VAL:CG1	45:6N:17:SER:N	2.69	0.41
45:6N:40:TRP:CE2	45:6N:98:TYR:CZ	3.01	0.41
45:6N:43:ALA:HA	45:6N:47:TYR:CD2	2.55	0.41
45:6N:48:GLU:O	45:6N:49:ASN:CG	2.62	0.41
45:6N:127:ILE:HB	45:6N:179:ARG:HE	1.81	0.41
46:6O:246:ASP:H	46:6O:430:LEU:HD12	1.85	0.41
47:6P:32:ASN:ND2	47:6P:228:ASP:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:6Y:52:PHE:HD1	54:6Y:52:PHE:HA	1.63	0.41
55:8A:135:ASN:OD1	55:8A:135:ASN:N	2.53	0.41
55:8A:283:LEU:HD21	68:8N:22:ILE:HG13	2.02	0.41
55:8A:334:TRP:CZ2	82:8B:301:PGV:H242	2.47	0.41
55:8A:363:LEU:HD13	56:8B:20:LEU:HD22	2.02	0.41
82:8A:602:PGV:H031	57:8C:61:ILE:CD1	2.49	0.41
82:8B:301:PGV:H12	82:8B:301:PGV:H152	1.93	0.41
1:1A:60:ILE:HD12	1:1A:60:ILE:HA	1.86	0.41
4:1D:218:PHE:HB3	4:1D:308:LEU:HD21	2.03	0.41
5:1E:202:LEU:H	5:1E:202:LEU:HD12	1.85	0.41
6:1F:272:MET:HG3	6:1F:273:SER:H	1.84	0.41
9:1I:31:VAL:HG13	71:1I:204:PC1:H392	2.02	0.41
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	2.03	0.41
12:1L:37:LYS:HB3	12:1L:37:LYS:HE2	1.88	0.41
12:1L:90:ILE:HG12	12:1L:129:MET:SD	2.60	0.41
12:1L:600:THR:O	12:1L:602:PHE:N	2.53	0.41
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	2.01	0.41
13:1M:329:LEU:HB3	13:1M:359:TRP:CE2	2.55	0.41
14:1N:44:LEU:HD22	14:1N:122:ILE:HD12	2.02	0.41
15:1O:138:MET:HG2	15:1O:143:PHE:HD2	1.84	0.41
16:1P:270:PHE:HE2	16:1P:278:TRP:HE3	1.67	0.41
23:1X:21:SER:OG	26:1a:51:ASP:OD2	2.34	0.41
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.54	0.41
30:1e:53:LYS:HE2	30:1e:53:LYS:HB3	1.71	0.41
34:1i:9:LEU:O	34:1i:13:GLN:HG3	2.21	0.41
42:1q:42:ASP:C	42:1q:42:ASP:OD1	2.63	0.41
45:3A:124:ASP:OD1	45:3A:179:ARG:HD2	2.19	0.41
47:3C:39:ILE:HB	47:3C:235:MET:HE1	2.00	0.41
47:3C:133:LEU:N	47:3C:134:PRO:HD2	2.35	0.41
47:3C:240:LEU:O	47:3C:244:LEU:N	2.53	0.41
47:3C:328:LEU:HD22	47:3C:366:MET:HE1	2.02	0.41
48:3D:208:ARG:HD3	48:3D:208:ARG:HA	1.84	0.41
49:3E:234:TYR:HB2	49:3E:243:TYR:HB3	2.02	0.41
50:3F:64:GLU:OE1	51:3G:13:ARG:NH1	2.52	0.41
51:3G:26:ARG:O	51:3G:29:PRO:HD3	2.20	0.41
51:3G:34:LYS:C	51:3G:37:PRO:HD2	2.44	0.41
45:3N:246:ASP:OD1	45:3N:427:PRO:HA	2.20	0.41
45:3N:291:SER:HA	46:3O:87:ARG:NH2	2.35	0.41
45:3N:396:GLU:O	45:3N:397:SER:C	2.62	0.41
45:3N:422:VAL:HG21	45:3N:437:ILE:HD13	2.00	0.41
46:3O:140:LEU:O	46:3O:141:GLN:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3P:337:TRP:O	47:3P:341:GLN:HG2	2.20	0.41
51:3T:67:GLU:OE1	51:3T:70:LYS:NZ	2.50	0.41
55:4A:168:ILE:HG12	55:4A:185:VAL:HG13	2.02	0.41
55:4A:289:ALA:HB3	55:4A:305:PHE:CE2	2.56	0.41
57:4C:247:VAL:CG2	75:4C:308:CDL:H842	2.49	0.41
58:4D:48:TRP:HA	58:4D:51:LEU:HD13	2.01	0.41
59:4E:61:PHE:O	59:4E:65:VAL:HG23	2.20	0.41
2:5B:178:ARG:NH2	16:5P:50:ARG:O	2.50	0.41
2:5B:179:ARG:O	16:5P:103:ASN:ND2	2.53	0.41
3:5C:10:THR:HG22	4:5D:325:VAL:HG23	2.02	0.41
5:5E:43:LYS:HD2	5:5E:43:LYS:HA	1.86	0.41
6:5F:48:ILE:HD11	6:5F:236:ARG:HG3	2.02	0.41
6:5F:309:LYS:HA	6:5F:312:CYS:SG	2.61	0.41
7:5G:150:MET:HA	7:5G:150:MET:CE	2.45	0.41
7:5G:241:SER:HB2	7:5G:249:ARG:HG3	2.01	0.41
8:5H:105:MET:CE	8:5H:162:LEU:HD11	2.49	0.41
12:5L:367:PRO:HG3	35:5j:22:LEU:HD23	2.02	0.41
13:5M:73:LEU:HB3	13:5M:74:PRO:HD3	2.02	0.41
13:5M:452:LYS:HG3	32:5g:83:TYR:CE2	2.55	0.41
16:5P:98:GLU:OE1	16:5P:286:ARG:NH2	2.53	0.41
18:5R:31:ARG:HE	42:5q:125:VAL:HG22	1.84	0.41
20:5T:63:PRO:HD2	20:5T:66:ASP:OD1	2.20	0.41
39:5n:91:GLU:HB2	39:5n:94:GLU:HG3	2.02	0.41
45:6A:157:ALA:HB1	45:6A:236:PHE:HD2	1.85	0.41
45:6A:252:HIS:HA	45:6A:325:VAL:HG13	2.02	0.41
46:6B:84:LYS:HD2	50:6S:107:TRP:HZ3	1.85	0.41
47:6C:5:ARG:NH1	47:6C:15:ASN:OD1	2.52	0.41
48:6D:109:LEU:HD13	48:6D:280:ARG:HB2	2.02	0.41
48:6D:160:ASP:HB3	48:6D:168:MET:HA	2.03	0.41
48:6D:242:PHE:O	48:6D:244:GLY:N	2.53	0.41
48:6D:311:MET:HE3	48:6D:311:MET:HB2	1.64	0.41
49:6E:235:TYR:HD1	49:6E:242:HIS:HA	1.86	0.41
45:6N:17:SER:HG	45:6N:209:LEU:HD21	1.86	0.41
45:6N:49:ASN:O	45:6N:50:GLU:C	2.62	0.41
45:6N:185:TYR:O	45:6N:189:HIS:CD2	2.73	0.41
45:6N:209:LEU:O	45:6N:213:GLN:HG3	2.21	0.41
45:6N:281:ASP:HB3	45:6N:284:TYR:CE1	2.55	0.41
45:6N:314:TYR:N	45:6N:317:THR:O	2.45	0.41
46:6O:165:ALA:C	46:6O:167:ALA:H	2.27	0.41
46:6O:385:GLN:HG2	46:6O:385:GLN:H	1.53	0.41
47:6P:206:ASN:HB3	83:6P:502:HEM:O1D	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:6R:244:ASP:CG	49:6R:248:ARG:HB2	2.45	0.41
50:6S:75:LEU:O	50:6S:80:TRP:NE1	2.48	0.41
54:6X:9:ARG:NH1	54:6X:13:LEU:HD11	2.35	0.41
55:8A:15:ILE:HA	55:8A:18:LEU:HD12	2.01	0.41
55:8A:94:PHE:HB2	55:8A:163:ASN:HD21	1.85	0.41
55:8A:130:PRO:HD3	55:8A:209:LEU:HD21	2.02	0.41
55:8A:254:ILE:HG13	55:8A:344:PHE:CD1	2.55	0.41
55:8A:278:MET:H	55:8A:278:MET:HG2	1.51	0.41
55:8A:279:SER:HB3	68:8N:22:ILE:CD1	2.50	0.41
55:8A:343:GLY:O	55:8A:344:PHE:C	2.63	0.41
55:8A:376:HIS:O	55:8A:380:VAL:HG22	2.20	0.41
82:8A:601:PGV:H32	82:8A:601:PGV:H211	2.02	0.41
82:8A:603:PGV:H282	82:8A:603:PGV:H251	1.87	0.41
75:8A:610:CDL:H152	75:8A:610:CDL:H111	2.03	0.41
1:1A:6:THR:OG1	1:1A:7:LEU:N	2.53	0.41
1:1A:84:LEU:O	1:1A:85:LYS:C	2.63	0.41
4:1D:232:ASN:O	4:1D:236:ARG:HG3	2.21	0.41
5:1E:50:VAL:HG12	5:1E:69:VAL:HG22	2.01	0.41
7:1G:21:GLU:CD	7:1G:21:GLU:N	2.77	0.41
7:1G:575:ASN:HD21	7:1G:577:GLU:CD	2.26	0.41
8:1H:102:VAL:HG21	8:1H:154:LEU:HD11	2.02	0.41
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	2.02	0.41
12:1L:551:SER:HA	12:1L:555:LEU:HD12	2.02	0.41
13:1M:336:ARG:HD3	13:1M:426:ILE:HA	2.01	0.41
14:1N:133:TRP:HE3	75:1N:903:CDL:H201	1.84	0.41
16:1P:98:GLU:OE1	16:1P:286:ARG:NH2	2.53	0.41
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	2.01	0.41
29:1d:46:ASN:HD22	29:1d:51:ARG:HD2	1.85	0.41
29:1d:46:ASN:CB	29:1d:53:VAL:HA	2.51	0.41
34:1i:65:ARG:HE	34:1i:65:ARG:HB2	1.57	0.41
75:1i:201:CDL:H742	75:1i:201:CDL:OA7	2.20	0.41
43:1r:39:LYS:HA	43:1r:39:LYS:HD2	1.81	0.41
47:3C:73:VAL:HG22	49:3E:143:SER:HB3	2.00	0.41
47:3C:120:LEU:O	47:3C:124:MET:HG3	2.20	0.41
47:3C:377:LEU:HD13	47:3C:379:TRP:NE1	2.35	0.41
48:3D:254:TYR:CZ	48:3D:257:VAL:HG23	2.56	0.41
45:3N:70:ARG:CB	45:3N:75:LEU:CD2	2.98	0.41
45:3N:433:ASP:HB2	47:3P:219:PRO:CG	2.50	0.41
46:3O:112:LEU:O	46:3O:115:ASP:N	2.53	0.41
46:3O:252:LEU:HB3	46:3O:327:ILE:HG22	2.02	0.41
49:3R:187:GLU:OE1	49:3R:244:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:3T:34:ILE:HB	51:3T:35:PRO:HD3	2.02	0.41
49:3V:71:ASN:OD1	49:3V:71:ASN:N	2.52	0.41
53:3W:54:LYS:HA	53:3W:57:LYS:HD3	2.02	0.41
56:4B:217:LYS:HB2	56:4B:217:LYS:HE3	1.84	0.41
90:4C:306:PEK:H101	61:4G:25:LEU:HD11	2.01	0.41
59:4E:27:TRP:CZ3	59:4E:31:LYS:HD3	2.56	0.41
60:4F:16:LEU:HD11	60:4F:31:TYR:CE1	2.55	0.41
65:4K:9:PHE:O	65:4K:10:HIS:C	2.64	0.41
65:4K:13:TYR:O	65:4K:14:GLY:C	2.63	0.41
4:5D:168:PHE:CD2	8:5H:34:ARG:HD3	2.56	0.41
5:5E:50:VAL:HG12	5:5E:69:VAL:HG22	2.01	0.41
6:5F:202:LYS:HD3	6:5F:361:GLN:HB2	2.01	0.41
7:5G:283:MET:HE1	42:5q:139:PRO:HG3	2.02	0.41
7:5G:640:ASN:CG	7:5G:641:TYR:H	2.27	0.41
10:5J:94:VAL:O	10:5J:98:MET:HG2	2.21	0.41
13:5M:54:LEU:HD23	33:5h:93:ILE:HG23	2.01	0.41
13:5M:329:LEU:HB3	13:5M:359:TRP:CE2	2.56	0.41
14:5N:133:TRP:HE3	75:5N:903:CDL:H201	1.84	0.41
20:5T:42:LEU:HB3	20:5T:46:ASP:HB2	2.02	0.41
20:5U:6:LEU:HD23	20:5U:6:LEU:HA	1.89	0.41
21:5V:94:LEU:HD12	21:5V:94:LEU:HA	1.90	0.41
23:5X:168:PHE:CE1	75:5X:201:CDL:H142	2.55	0.41
31:5f:25:TYR:CZ	31:5f:29:ARG:HD2	2.56	0.41
32:5g:108:MET:HB3	41:5p:137:ALA:CB	2.51	0.41
37:5l:40:ASP:N	37:5l:40:ASP:OD1	2.53	0.41
40:5o:24:PHE:CZ	40:5o:111:LYS:HD2	2.55	0.41
45:6A:259:GLY:H	45:6A:318:GLY:C	2.29	0.41
45:6A:281:ASP:HB2	45:6A:306:SER:HA	2.03	0.41
46:6B:76:THR:HA	46:6B:82:SER:H	1.85	0.41
46:6B:313:ASN:CA	46:6B:322:PHE:HA	2.40	0.41
47:6C:68:HIS:O	47:6C:73:VAL:N	2.41	0.41
47:6C:364:VAL:O	47:6C:365:LEU:C	2.62	0.41
47:6C:377:LEU:HD21	50:6F:38:PHE:CE2	2.55	0.41
48:6D:128:CYS:HB2	48:6D:129:HIS:HD2	1.86	0.41
48:6D:139:LEU:HD22	48:6D:139:LEU:HA	1.76	0.41
48:6D:177:ASP:OD1	48:6D:177:ASP:N	2.53	0.41
48:6D:319:LEU:O	48:6D:320:LYS:C	2.63	0.41
45:6N:27:SER:HA	45:6N:199:ALA:HB3	2.01	0.41
45:6N:46:ARG:CD	45:6N:93:GLU:OE2	2.68	0.41
45:6N:58:PHE:CE2	45:6N:177:LEU:CD1	3.03	0.41
45:6N:67:THR:OG1	45:6N:75:LEU:HD21	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:86:LEU:HD21	45:6N:99:ILE:HD11	1.97	0.41
45:6N:136:GLN:O	49:6V:50:LEU:HD12	2.20	0.41
45:6N:192:ALA:N	45:6N:193:PRO:CD	2.81	0.41
45:6N:208:LEU:O	45:6N:209:LEU:C	2.63	0.41
45:6N:246:ASP:CB	51:6T:9:ARG:HG3	2.46	0.41
46:6O:75:LEU:HD13	46:6O:136:GLU:HB3	2.00	0.41
46:6O:97:SER:HB3	46:6O:108:THR:HB	2.03	0.41
46:6O:158:GLN:O	46:6O:159:VAL:C	2.63	0.41
46:6O:169:ARG:HG2	46:6O:239:TYR:C	2.46	0.41
47:6P:92:ILE:HG13	47:6P:272:TRP:HH2	1.85	0.41
47:6P:237:LEU:HB2	48:6Q:212:MET:SD	2.61	0.41
49:6R:134:SER:O	49:6R:138:SER:OG	2.32	0.41
49:6R:243:TYR:HA	49:6R:248:ARG:O	2.21	0.41
55:8A:272:GLY:N	68:8N:15:LEU:HD21	2.35	0.41
89:8A:611:PSC:H302	89:8A:611:PSC:H252	2.02	0.41
59:8E:27:TRP:CZ3	59:8E:31:LYS:HD3	2.56	0.41
62:8H:18:SER:O	68:8N:57:LEU:HD13	2.20	0.41
63:8I:64:ARG:HD2	63:8I:72:ALA:HB1	2.01	0.41
1:1A:110:GLY:HA3	10:1J:169:MET:HE1	2.02	0.41
2:1B:60:MET:O	2:1B:61:HIS:CA	2.51	0.41
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	2.02	0.41
6:1F:320:ASP:O	6:1F:324:GLN:HG3	2.21	0.41
7:1G:283:MET:HE1	42:1q:139:PRO:HG3	2.02	0.41
10:1J:129:ASP:HB3	30:1e:31:ARG:NE	2.28	0.41
13:1M:88:THR:O	13:1M:92:LYS:HG3	2.20	0.41
14:1N:1:FME:HCN	15:1O:258:ARG:NH1	2.33	0.41
16:1P:69:ILE:HD12	18:1R:26:VAL:HG13	2.01	0.41
16:1P:224:LYS:H	16:1P:224:LYS:HG2	1.68	0.41
75:1X:201:CDL:H273	75:1X:201:CDL:H612	2.02	0.41
25:1Z:56:GLU:HG2	25:1Z:59:ARG:HH21	1.84	0.41
26:1a:64:LYS:HD3	26:1a:64:LYS:HA	1.86	0.41
35:1j:19:ARG:HH21	65:8K:12:LYS:HD2	1.82	0.41
37:1l:114:PHE:O	37:1l:118:VAL:HG13	2.20	0.41
37:1l:134:PRO:HG3	40:1o:38:MET:CE	2.46	0.41
39:1n:123:GLN:O	39:1n:126:ARG:HG2	2.19	0.41
46:3B:213:HIS:O	46:3B:217:LYS:HG3	2.20	0.41
45:3N:158:PHE:CG	45:3N:163:LEU:CB	3.03	0.41
45:3N:298:ALA:HA	45:3N:303:LEU:H	1.85	0.41
45:3N:392:LEU:HD23	45:3N:392:LEU:HA	1.95	0.41
45:3N:429:GLU:OE2	51:3T:5:GLY:N	2.53	0.41
46:3O:172:LEU:O	46:3O:173:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:238:LYS:HA	46:3O:238:LYS:HD2	1.75	0.41
48:3Q:120:ARG:HD3	48:3Q:120:ARG:HA	1.90	0.41
49:3R:214:ILE:HD13	49:3R:214:ILE:HA	1.87	0.41
55:4A:440:TYR:CZ	56:4B:205:SER:HA	2.55	0.41
56:4B:104:TRP:CD2	56:4B:203:ASN:HB2	2.55	0.41
56:4B:191:LEU:HD22	63:4I:68:ILE:HD12	2.02	0.41
75:4C:308:CDL:H741	75:4C:308:CDL:H552	2.03	0.41
58:4D:33:LEU:HD12	58:4D:37:GLN:HB3	2.02	0.41
5:5E:201:SER:HB2	6:5F:26:TYR:CE2	2.52	0.41
6:5F:215:VAL:H	6:5F:220:THR:HG21	1.85	0.41
12:5L:151:SER:HB2	12:5L:252:MET:SD	2.60	0.41
12:5L:403:TYR:CD2	37:5l:125:TYR:HB3	2.55	0.41
13:5M:84:LEU:HD22	13:5M:87:GLU:HG3	2.03	0.41
14:5N:14:MET:HG2	14:5N:14:MET:H	1.66	0.41
14:5N:284:MET:HB3	69:5N:901:3PE:H2F2	2.02	0.41
16:5P:195:SER:HB2	16:5P:199:GLU:OE1	2.20	0.41
19:5S:19:ARG:HB2	19:5S:65:TRP:HB2	2.03	0.41
25:5Z:56:GLU:HG2	25:5Z:59:ARG:HH21	1.84	0.41
25:5Z:91:LEU:HA	25:5Z:94:GLU:HG2	2.02	0.41
29:5d:46:ASN:HD22	29:5d:51:ARG:HD2	1.85	0.41
41:5p:50:PHE:HA	41:5p:53:GLN:HG3	2.03	0.41
45:6A:52:ASN:HA	45:6A:177:LEU:HD21	2.02	0.41
45:6A:332:ASP:HA	45:6A:432:PRO:HG3	2.02	0.41
45:6A:443:TRP:CB	45:6A:446:PHE:HB2	2.44	0.41
46:6B:261:SER:H	46:6B:320:GLY:C	2.27	0.41
46:6B:407:ASP:O	46:6B:408:ALA:C	2.64	0.41
47:6C:61:THR:HG21	47:6P:58:ASP:OD2	2.19	0.41
47:6C:130:GLY:O	47:6C:133:LEU:HB2	2.20	0.41
47:6C:327:MET:CG	51:6G:53:PRO:HB3	2.51	0.41
48:6D:321:SER:OG	48:6D:322:ARG:N	2.54	0.41
45:6N:204:GLU:HB2	45:6N:207:GLN:CD	2.45	0.41
45:6N:255:ILE:HB	45:6N:422:VAL:HG13	2.03	0.41
45:6N:268:VAL:HB	45:6N:269:PRO:HD3	2.02	0.41
46:6O:366:ALA:O	46:6O:367:GLY:C	2.62	0.41
49:6R:187:GLU:OE1	49:6R:244:ASP:HB2	2.21	0.41
51:6T:34:ILE:HB	51:6T:35:PRO:HD3	2.02	0.41
55:8A:52:GLN:HE22	55:8A:123:GLY:N	2.17	0.41
55:8A:67:PHE:HA	55:8A:71:MET:SD	2.60	0.41
55:8A:129:TYR:HA	55:8A:130:PRO:HD2	1.90	0.41
55:8A:132:LEU:HA	55:8A:132:LEU:HD12	1.88	0.41
55:8A:253:MET:O	55:8A:254:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:311:ILE:H	55:8A:311:ILE:HG12	1.55	0.41
55:8A:479:LYS:CB	67:8M:7:ARG:HB2	2.49	0.41
90:8C:306:PEK:H101	61:8G:25:LEU:HD11	2.01	0.41
1:1A:102:LEU:O	1:1A:103:ALA:C	2.64	0.41
2:1B:68:ASP:CG	8:1H:34:ARG:HB3	2.44	0.41
2:1B:71:ARG:HH11	8:1H:34:ARG:NH1	2.18	0.41
2:1B:104:TYR:C	2:1B:106:GLN:H	2.24	0.41
3:1C:16:ASP:O	3:1C:20:LYS:HG2	2.20	0.41
4:1D:95:THR:HA	4:1D:385:ARG:HG2	2.01	0.41
6:1F:384:ALA:O	6:1F:430:MET:HG2	2.20	0.41
73:1F:501:FMN:HM81	73:1F:501:FMN:HM73	1.90	0.41
7:1G:241:SER:HB2	7:1G:249:ARG:HG3	2.01	0.41
12:1L:213:LEU:HD21	12:1L:266:LEU:HB3	2.01	0.41
13:1M:197:LEU:O	13:1M:201:MET:HG2	2.21	0.41
14:1N:128:LEU:HD23	14:1N:129:LEU:N	2.36	0.41
14:1N:153:LEU:CD1	14:1N:157:MET:HE2	2.51	0.41
28:1c:38:ASP:CG	29:1d:19:ARG:HH12	2.29	0.41
29:1d:59:HIS:H	29:1d:59:HIS:CD2	2.38	0.41
35:1j:37:LEU:HB3	36:1k:77:PHE:CD1	2.56	0.41
45:3A:433:ASP:O	45:3A:437:ILE:HG13	2.21	0.41
47:3C:256:TYR:CD1	48:3D:206:ARG:HD3	2.56	0.41
47:3C:350:ILE:HD11	51:3G:63:TRP:HZ3	1.85	0.41
48:3D:194:ASN:O	48:3D:194:ASN:CG	2.64	0.41
48:3D:307:LEU:HB3	49:3E:121:THR:OG1	2.21	0.41
45:3N:262:TRP:CD1	45:3N:315:ALA:HA	2.55	0.41
47:3P:72:ASP:CG	48:3Q:49:ARG:HH22	2.28	0.41
47:3P:315:MET:HG3	47:3P:318:ARG:NH2	2.36	0.41
48:3Q:208:MET:HE3	48:3Q:208:MET:HB3	1.90	0.41
54:3Y:42:LEU:HD23	54:3Y:42:LEU:HA	1.88	0.41
55:4A:151:HIS:CD2	90:4C:307:PEK:H361	2.55	0.41
61:4G:35:SER:HB2	82:4G:101:PGV:H252	2.01	0.41
63:4I:64:ARG:HD2	63:4I:72:ALA:HB1	2.01	0.41
3:5C:34:PRO:HD2	21:5V:98:PRO:O	2.21	0.41
5:5E:136:LEU:HD23	5:5E:136:LEU:HA	1.93	0.41
7:5G:183:VAL:HG21	70:5G:802:SF4:S1	2.60	0.41
7:5G:640:ASN:OD1	7:5G:641:TYR:N	2.47	0.41
8:5H:124:ASN:C	8:5H:126:LYS:H	2.27	0.41
8:5H:204:GLU:HA	8:5H:208:VAL:O	2.21	0.41
8:5H:294:LEU:O	8:5H:298:LEU:HG	2.21	0.41
10:5J:122:LEU:HD13	30:5e:76:SER:HA	2.02	0.41
12:5L:524:ASN:ND2	39:5n:76:PRO:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:5L:551:SER:HA	12:5L:555:LEU:HD12	2.02	0.41
12:5L:600:THR:O	12:5L:602:PHE:N	2.53	0.41
14:5N:332:LEU:HD21	75:5d:202:CDL:H431	2.03	0.41
15:5O:35:LYS:HE2	15:5O:126:ARG:CZ	2.51	0.41
22:5W:119:LEU:HA	22:5W:119:LEU:HD12	1.81	0.41
75:5X:201:CDL:H273	75:5X:201:CDL:H612	2.02	0.41
24:5Y:57:ARG:HH21	69:5Y:202:3PE:H112	1.84	0.41
28:5c:38:ASP:CG	29:5d:19:ARG:HH12	2.29	0.41
29:5d:47:ALA:HB2	69:5d:201:3PE:H331	2.01	0.41
35:5j:33:TRP:CZ2	36:5k:67:LEU:HG	2.55	0.41
37:5l:158:ILE:HA	40:5o:33:ARG:HH21	1.84	0.41
45:6A:385:THR:OG1	45:6A:386:TYR:N	2.53	0.41
46:6B:71:LEU:HA	49:6I:68:VAL:HG21	2.03	0.41
47:6C:207:ASN:O	47:6C:208:PRO:C	2.64	0.41
48:6D:304:LEU:HA	48:6D:304:LEU:HD23	1.72	0.41
48:6D:323:LYS:HB3	49:6E:86:PRO:HG2	2.02	0.41
45:6N:34:THR:HG21	46:6O:370:MET:HG2	2.02	0.41
45:6N:46:ARG:HD2	45:6N:93:GLU:OE2	2.19	0.41
45:6N:204:GLU:HB2	45:6N:207:GLN:HB2	2.03	0.41
45:6N:401:GLU:O	45:6N:402:VAL:C	2.63	0.41
45:6N:425:LEU:HA	45:6N:425:LEU:HD13	1.77	0.41
49:6R:191:GLU:HG3	49:6R:194:GLN:H	1.85	0.41
51:6T:19:SER:O	51:6T:23:GLN:HG2	2.21	0.41
55:8A:292:MET:HE2	55:8A:292:MET:HB2	1.84	0.41
56:8B:191:LEU:HD22	63:8I:68:ILE:HD12	2.02	0.41
58:8D:20:ARG:HD2	59:8E:73:ASP:OD2	2.20	0.41
59:8E:61:PHE:O	59:8E:65:VAL:HG23	2.20	0.41
3:1C:178:ASP:O	3:1C:181:LYS:HD2	2.20	0.41
4:1D:169:TRP:CH2	9:1I:36:MET:HG3	2.56	0.41
12:1L:316:THR:HG23	12:1L:325:ALA:HB2	2.02	0.41
13:1M:318:ALA:HB1	13:1M:374:ASN:CG	2.46	0.41
14:1N:87:THR:HG22	33:1h:126:PRO:HG2	2.02	0.41
15:1O:183:ILE:O	15:1O:186:LYS:HG2	2.21	0.41
15:1O:304:TYR:CE1	69:1d:201:3PE:H112	2.54	0.41
23:1X:168:PHE:CE1	75:1X:201:CDL:H142	2.55	0.41
27:1b:77:LEU:O	27:1b:81:LYS:HG3	2.20	0.41
38:1m:3:PRO:HD2	39:1n:72:TYR:CE1	2.55	0.41
39:1n:21:ARG:HG2	39:1n:70:PHE:CZ	2.56	0.41
42:1q:84:PRO:HA	42:1q:87:HIS:HB3	2.03	0.41
50:3F:47:ASP:OD1	50:3F:101:TYR:OH	2.37	0.41
45:3N:130:GLU:O	45:3N:133:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:328:ASN:ND2	51:3T:5:GLY:O	2.52	0.41
45:3N:358:LYS:HG2	45:3N:402:VAL:CB	2.50	0.41
46:3O:74:SER:O	46:3O:75:LEU:C	2.63	0.41
46:3O:89:ILE:HG13	46:3O:89:ILE:H	1.58	0.41
47:3P:117:VAL:N	83:3P:502:HEM:HBC2	2.36	0.41
49:3R:177:ARG:HD2	49:3R:234:TYR:OH	2.20	0.41
51:3T:19:SER:O	51:3T:23:GLN:HG2	2.21	0.41
57:4C:34:TRP:CH2	82:4C:302:PGV:H251	2.56	0.41
3:5C:178:ASP:O	3:5C:181:LYS:HD2	2.20	0.41
4:5D:253:TYR:CE1	4:5D:404:LYS:HD3	2.56	0.41
6:5F:320:ASP:O	6:5F:324:GLN:HG3	2.21	0.41
10:5J:41:CYS:O	10:5J:45:LEU:HG	2.21	0.41
11:5K:41:PHE:CE2	11:5K:64:LEU:HD13	2.55	0.41
12:5L:90:ILE:HG12	12:5L:129:MET:SD	2.60	0.41
12:5L:145:GLU:HG2	13:5M:370:PRO:HD2	2.03	0.41
12:5L:375:ILE:HG12	35:5j:32:MET:SD	2.60	0.41
12:5L:573:MET:HA	12:5L:576:MET:HE3	2.03	0.41
17:5Q:59:PHE:CE2	17:5Q:79:LEU:HD13	2.55	0.41
21:5V:49:GLN:HA	21:5V:52:ASN:HD21	1.85	0.41
35:5j:37:LEU:HB2	36:5k:77:PHE:HB2	2.02	0.41
37:5l:40:ASP:OD2	38:5m:84:LYS:NZ	2.54	0.41
45:6A:181:ASP:N	45:6A:181:ASP:OD1	2.52	0.41
45:6A:433:ASP:OD2	45:6A:435:ASN:HB2	2.21	0.41
46:6B:160:LEU:HD23	46:6B:160:LEU:HA	1.75	0.41
47:6C:96:ILE:H	47:6C:96:ILE:HG12	1.64	0.41
47:6C:164:ILE:O	47:6C:165:TRP:C	2.64	0.41
47:6C:298:ILE:H	47:6C:298:ILE:HG13	1.42	0.41
48:6D:131:MET:HE2	48:6D:201:LEU:HD12	2.02	0.41
48:6D:164:GLU:O	48:6Q:103:ALA:HB2	2.21	0.41
48:6D:254:TYR:O	48:6D:268:MET:HB3	2.21	0.41
50:6F:116:ARG:HG2	46:6O:83:PHE:CZ	2.55	0.41
45:6N:211:LEU:CA	45:6N:215:HIS:HD2	2.33	0.41
45:6N:224:VAL:HB	45:6N:225:GLU:H	1.56	0.41
45:6N:394:GLU:O	45:6N:395:TRP:C	2.63	0.41
45:6N:445:ARG:H	45:6N:445:ARG:NE	2.16	0.41
46:6O:42:ALA:O	46:6O:44:ALA:N	2.54	0.41
46:6O:250:ASP:O	46:6O:251:SER:C	2.63	0.41
48:6Q:132:THR:HG22	48:6Q:179:MET:HE3	2.03	0.41
49:6R:199:GLN:HG3	49:6R:257:ASN:HD21	1.85	0.41
49:6R:219:HIS:CE1	49:6R:239:HIS:CE1	3.09	0.41
49:6R:248:ARG:HH22	49:6R:249:ILE:HB	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8A:32:ALA:HA	55:8A:35:LEU:HD12	2.02	0.41
55:8A:200:PRO:HB2	57:8C:92:LEU:CB	2.44	0.41
55:8A:265:LYS:HD2	55:8A:265:LYS:HA	1.30	0.41
55:8A:356:ILE:H	55:8A:356:ILE:HG12	1.74	0.41
55:8A:357:VAL:O	55:8A:360:ASN:ND2	2.54	0.41
55:8A:412:ILE:O	55:8A:413:HIS:C	2.63	0.41
1:1A:13:LEU:HA	1:1A:16:LEU:HD12	2.03	0.41
2:1B:125:TYR:HD1	2:1B:125:TYR:HA	1.63	0.41
2:1B:171:LYS:HD3	2:1B:174:ARG:CZ	2.51	0.41
3:1C:10:THR:HG22	4:1D:325:VAL:HG23	2.02	0.41
6:1F:215:VAL:H	6:1F:220:THR:HG21	1.85	0.41
6:1F:423:ARG:N	6:1F:424:PRO:HD2	2.36	0.41
7:1G:359:ARG:HG3	7:1G:362:TYR:OH	2.21	0.41
7:1G:391:PHE:O	7:1G:395:ILE:HG13	2.20	0.41
12:1L:151:SER:HB2	12:1L:252:MET:SD	2.60	0.41
12:1L:367:PRO:HG3	35:1j:22:LEU:HD23	2.02	0.41
13:1M:357:THR:O	13:1M:361:MET:HG3	2.20	0.41
14:1N:97:MET:HA	14:1N:97:MET:HE3	2.01	0.41
14:1N:274:GLU:CD	24:1Y:139:LYS:HE2	2.46	0.41
16:1P:32:ARG:HG3	16:1P:33:TYR:CD1	2.56	0.41
16:1P:319:ARG:NH1	22:1W:51:GLN:HG2	2.35	0.41
20:1U:3:ALA:HA	20:1U:4:PRO:HD3	1.89	0.41
24:1Y:116:TYR:HB3	71:1m:201:PC1:H3E1	2.02	0.41
29:1d:94:VAL:HA	29:1d:101:PHE:CD2	2.56	0.41
45:3A:332:ASP:OD1	45:3A:432:PRO:HG3	2.20	0.41
47:3C:150:LEU:O	47:3C:151:SER:C	2.64	0.41
48:3D:269:SER:HB2	52:3H:98:LEU:HD21	2.02	0.41
51:3G:5:GLU:N	51:3G:5:GLU:OE2	2.54	0.41
46:3O:324:ILE:HD12	46:3O:340:ALA:HB1	2.02	0.41
46:3O:412:ASN:HA	46:3O:415:LYS:HE2	2.03	0.41
49:3R:248:ARG:HH22	49:3R:249:ILE:HB	1.84	0.41
54:3X:42:LEU:HD23	54:3X:42:LEU:HA	1.87	0.41
55:4A:512:ASN:ND2	60:4F:47:ASN:OD1	2.54	0.41
82:4A:602:PGV:O14	57:4C:57:TRP:NE1	2.42	0.41
56:4B:98:LYS:HE3	56:4B:98:LYS:HB2	1.79	0.41
1:5A:39:CYS:O	4:5D:53:PRO:HD2	2.21	0.41
2:5B:32:LYS:HD2	2:5B:32:LYS:HA	1.73	0.41
2:5B:47:PRO:HA	2:5B:85:VAL:O	2.21	0.41
4:5D:49:LEU:HD12	4:5D:49:LEU:HA	1.90	0.41
4:5D:78:PRO:HG3	4:5D:402:LEU:HD23	2.03	0.41
4:5D:348:HIS:HE1	9:5I:125:ALA:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5D:417:ILE:O	4:5D:420:THR:HG22	2.21	0.41
6:5F:261:HIS:NE2	6:5F:341:THR:OG1	2.54	0.41
6:5F:272:MET:HG3	6:5F:273:SER:H	1.84	0.41
7:5G:359:ARG:HG3	7:5G:362:TYR:OH	2.21	0.41
11:5K:87:THR:HG21	11:5K:89:TYR:CD2	2.55	0.41
12:5L:108:MET:HE3	12:5L:108:MET:HB3	1.93	0.41
12:5L:208:CYS:HB2	12:5L:209:PRO:HD2	2.03	0.41
13:5M:207:MET:HE3	13:5M:207:MET:HB3	1.88	0.41
14:5N:128:LEU:HD23	14:5N:129:LEU:N	2.36	0.41
16:5P:273:SER:HA	16:5P:274:PRO:HD3	1.95	0.41
17:5Q:116:LYS:HD3	17:5Q:116:LYS:HA	1.88	0.41
38:5m:22:TYR:CA	39:5n:64:ARG:NH2	2.84	0.41
39:5n:21:ARG:HG2	39:5n:70:PHE:CZ	2.55	0.41
45:6A:82:MET:HE2	45:6A:82:MET:HB3	1.68	0.41
46:6B:85:ILE:HA	46:6B:122:PHE:HE1	1.86	0.41
46:6B:303:VAL:C	49:6I:52:ARG:HH22	2.29	0.41
47:6C:132:VAL:O	47:6C:133:LEU:C	2.64	0.41
47:6C:282:ARG:CZ	47:6C:343:VAL:HG22	2.49	0.41
47:6C:377:LEU:HD21	50:6F:38:PHE:HE2	1.85	0.41
48:6D:314:HIS:CE1	49:6E:114:SER:HB3	2.56	0.41
49:6E:151:LYS:HZ1	49:6E:152:ILE:HD11	1.86	0.41
49:6E:207:LYS:O	49:6E:209:GLU:N	2.54	0.41
49:6E:266:THR:HB	49:6E:270:LEU:HG	2.03	0.41
51:6G:47:ILE:HG23	51:6G:48:LEU:HD13	2.03	0.41
53:6J:23:LEU:O	53:6J:24:THR:C	2.64	0.41
53:6J:37:ASP:O	53:6J:38:GLN:C	2.64	0.41
45:6N:136:GLN:HB3	49:6V:50:LEU:CB	2.50	0.41
45:6N:217:SER:OG	45:6N:218:SER:N	2.53	0.41
45:6N:436:ARG:HD3	47:6P:222:PRO:CD	2.34	0.41
46:6O:314:ALA:O	46:6O:315:SER:C	2.63	0.41
47:6P:72:ASP:CG	48:6Q:49:ARG:HH22	2.28	0.41
47:6P:119:LEU:HD22	83:6P:502:HEM:HBB2	2.03	0.41
47:6P:337:TRP:O	47:6P:341:GLN:HG2	2.20	0.41
49:6R:176:VAL:HG13	49:6R:212:ILE:HD11	2.03	0.41
53:6W:54:LYS:HA	53:6W:57:LYS:HD3	2.01	0.41
54:6Y:41:ILE:H	54:6Y:41:ILE:HG12	1.52	0.41
55:8A:74:MET:O	55:8A:78:PHE:N	2.54	0.41
55:8A:218:THR:HG21	55:8A:224:GLY:HA3	2.03	0.41
55:8A:218:THR:HB	55:8A:221:ASP:HB3	2.02	0.41
55:8A:349:THR:O	55:8A:350:VAL:C	2.64	0.41
82:8A:604:PGV:H182	82:8A:604:PGV:H151	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:8B:29:MET:HB3	56:8B:29:MET:HE2	1.81	0.41
56:8B:44:LEU:HD12	56:8B:44:LEU:HA	1.87	0.41
75:8B:302:CDL:H652	75:8B:302:CDL:H152	2.03	0.41
57:8C:22:LEU:O	57:8C:26:LEU:HG	2.20	0.41
60:8F:16:LEU:HD11	60:8F:31:TYR:CE1	2.55	0.41
62:8H:10:ASN:OD1	62:8H:10:ASN:N	2.54	0.41
1:1A:95:LEU:O	1:1A:96:ILE:C	2.64	0.41
2:1B:58:GLU:C	2:1B:60:MET:H	2.27	0.41
2:1B:82:GLN:HB2	2:1B:83:SER:H	1.74	0.41
3:1C:34:PRO:HD2	21:1V:98:PRO:O	2.21	0.41
3:1C:161:PRO:HA	3:1C:166:PHE:CD2	2.56	0.41
3:1C:171:TYR:CD1	17:1Q:78:PRO:HG2	2.56	0.41
4:1D:253:TYR:CE1	4:1D:404:LYS:HD3	2.56	0.41
4:1D:309:ARG:HG2	4:1D:313:GLN:HE21	1.85	0.41
5:1E:201:SER:HB2	6:1F:26:TYR:CE2	2.52	0.41
6:1F:20:ARG:HG2	6:1F:269:GLU:HG2	2.03	0.41
7:1G:110:GLN:HE22	17:1Q:45:MET:HE3	1.85	0.41
7:1G:216:THR:CG2	7:1G:248:MET:HE3	2.51	0.41
7:1G:237:ASN:HB3	7:1G:253:ARG:HB3	2.02	0.41
7:1G:255:HIS:HE1	7:1G:257:ASP:HB2	1.85	0.41
7:1G:359:ARG:O	7:1G:363:LEU:HG	2.21	0.41
8:1H:98:MET:HE1	8:1H:104:PHE:CD2	2.55	0.41
10:1J:45:LEU:HD23	10:1J:50:SER:HA	2.02	0.41
10:1J:52:LEU:O	10:1J:56:VAL:HG23	2.21	0.41
10:1J:125:TRP:HB2	25:1Z:137:THR:HG21	2.03	0.41
11:1K:10:MET:HE3	11:1K:10:MET:HB3	1.92	0.41
12:1L:208:CYS:HB2	12:1L:209:PRO:HD2	2.03	0.41
13:1M:1:FME:HE3	13:1M:111:THR:HG21	2.02	0.41
13:1M:73:LEU:HB3	13:1M:74:PRO:HD3	2.02	0.41
13:1M:128:PRO:O	13:1M:132:ILE:HG12	2.21	0.41
14:1N:106:LEU:HG	14:1N:138:PRO:HB2	2.02	0.41
14:1N:332:LEU:HD21	75:1d:202:CDL:H431	2.03	0.41
16:1P:132:ILE:HD13	16:1P:166:ILE:HB	2.03	0.41
20:1T:56:ASP:OD1	20:1T:57:GLU:N	2.54	0.41
24:1Y:48:PHE:O	24:1Y:52:VAL:HG23	2.20	0.41
24:1Y:94:CYS:HB2	24:1Y:114:CYS:C	2.46	0.41
25:1Z:40:ILE:HD13	25:1Z:40:ILE:HA	1.90	0.41
25:1Z:91:LEU:HA	25:1Z:94:GLU:HG2	2.02	0.41
28:1c:21:LEU:O	28:1c:25:VAL:HG23	2.20	0.41
29:1d:100:ASP:CG	33:1h:117:ARG:HH22	2.26	0.41
31:1f:25:TYR:CZ	31:1f:29:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:95:ARG:HH22	41:1p:64:HIS:CD2	2.38	0.41
35:1j:37:LEU:HD13	36:1k:74:PHE:HA	2.02	0.41
38:1m:48:LEU:HD23	39:1n:165:LEU:HD21	2.02	0.41
39:1n:100:GLU:H	39:1n:100:GLU:HG3	1.69	0.41
45:3A:45:SER:O	45:3A:165:GLN:NE2	2.54	0.41
45:3A:124:ASP:O	45:3A:128:GLU:HG2	2.20	0.41
45:3A:364:ALA:HB2	49:3I:33:ALA:HB1	2.03	0.41
46:3B:86:THR:HA	49:3I:70:LEU:HD11	2.02	0.41
46:3B:435:PHE:CZ	46:3O:169:ARG:HA	2.55	0.41
47:3C:23:ALA:H	47:3C:218:ILE:H	1.67	0.41
47:3C:50:PHE:HA	47:3C:53:MET:SD	2.61	0.41
47:3C:223:TYR:HB2	47:3C:224:TYR:H	1.72	0.41
49:3E:223:VAL:HG11	48:3Q:144:ARG:HH22	1.86	0.41
49:3E:235:TYR:HD1	49:3E:242:HIS:HA	1.86	0.41
52:3H:67:GLN:HE21	52:3H:68:ARG:N	2.18	0.41
53:3J:49:GLN:HA	53:3J:55:HIS:CE1	2.56	0.41
45:3N:52:ASN:CA	45:3N:185:TYR:CE1	3.03	0.41
45:3N:56:GLY:O	45:3N:57:TYR:C	2.64	0.41
45:3N:78:GLU:O	45:3N:81:SER:OG	2.23	0.41
45:3N:91:THR:OG1	45:3N:94:HIS:O	2.32	0.41
45:3N:156:THR:HG22	45:3N:241:ILE:CB	2.45	0.41
45:3N:188:GLN:O	45:3N:191:LYS:HE3	2.21	0.41
45:3N:382:SER:O	45:3N:387:GLY:N	2.54	0.41
45:3N:436:ARG:CD	47:3P:222:PRO:HD3	2.50	0.41
48:3Q:110:PRO:HA	48:3Q:111:PRO:HD3	1.93	0.41
48:3Q:144:ARG:HG2	48:3Q:147:LEU:HD12	2.01	0.41
48:3Q:230:LEU:O	48:3Q:233:ARG:HG2	2.21	0.41
49:3R:169:TRP:CD1	49:3R:174:LEU:HD22	2.56	0.41
49:3R:219:HIS:CE1	49:3R:239:HIS:CE1	3.09	0.41
55:4A:407:GLN:O	55:4A:411:LYS:HG3	2.21	0.41
56:4B:105:TYR:H	56:4B:207:MET:HE3	1.86	0.41
57:4C:27:MET:HE2	57:4C:47:LEU:HD23	2.03	0.41
57:4C:101:PHE:HA	57:4C:196:THR:HG21	2.02	0.41
57:4C:179:SER:HB3	82:4G:101:PGV:H82	2.02	0.41
58:4D:34:SER:O	58:4D:38:LYS:HG3	2.21	0.41
82:4G:101:PGV:H21	82:4G:101:PGV:H02	1.88	0.41
62:4H:10:ASN:N	62:4H:10:ASN:OD1	2.54	0.41
1:5A:42:ASP:OD1	1:5A:42:ASP:N	2.40	0.41
1:5A:68:GLU:OE1	1:5A:98:LEU:HG	2.21	0.41
1:5A:98:LEU:HD13	8:5H:298:LEU:HD22	2.02	0.41
5:5E:61:LEU:HD23	5:5E:61:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5E:100:ILE:HG13	5:5E:156:ILE:CD1	2.50	0.41
5:5E:202:LEU:HD12	5:5E:202:LEU:H	1.85	0.41
6:5F:384:ALA:O	6:5F:430:MET:HG2	2.20	0.41
6:5F:423:ARG:N	6:5F:424:PRO:HD2	2.36	0.41
7:5G:216:THR:CG2	7:5G:248:MET:HE3	2.51	0.41
8:5H:66:SER:HA	8:5H:122:ALA:O	2.20	0.41
8:5H:102:VAL:HG21	8:5H:154:LEU:HD11	2.02	0.41
8:5H:181:LEU:HG	8:5H:300:LEU:HD13	2.03	0.41
10:5J:14:VAL:O	10:5J:18:VAL:HG23	2.20	0.41
12:5L:257:VAL:HG12	12:5L:314:MET:CE	2.51	0.41
13:5M:352:LEU:HB3	13:5M:355:MET:HB2	2.03	0.41
14:5N:30:TRP:CG	14:5N:71:MET:HE2	2.55	0.41
14:5N:106:LEU:HG	14:5N:138:PRO:HB2	2.02	0.41
14:5N:153:LEU:HG	14:5N:157:MET:HE2	2.03	0.41
14:5N:167:TRP:CZ2	69:5N:901:3PE:H2I1	2.56	0.41
14:5N:245:MET:HE2	69:5N:902:3PE:H371	2.01	0.41
15:5O:76:ASN:O	15:5O:95:ARG:NE	2.32	0.41
15:5O:112:LEU:HD23	15:5O:112:LEU:HA	1.97	0.41
16:5P:278:TRP:CZ2	71:5P:401:PC1:H12	2.56	0.41
17:5Q:47:SER:O	17:5Q:47:SER:OG	2.32	0.41
17:5Q:125:ASN:O	44:5s:70:ARG:NE	2.53	0.41
24:5Y:82:LYS:O	24:5Y:88:ASN:ND2	2.54	0.41
28:5c:36:LYS:HB2	28:5c:36:LYS:HE3	1.77	0.41
33:5h:119:ASP:OD1	33:5h:119:ASP:N	2.52	0.41
34:5i:9:LEU:O	34:5i:13:GLN:HG3	2.21	0.41
75:5i:201:CDL:HB4	75:5i:201:CDL:H511	1.34	0.41
36:5k:67:LEU:CB	36:5k:70:PHE:HB3	2.47	0.41
36:5k:84:GLU:HA	36:5k:87:LEU:HD12	2.03	0.41
37:5l:65:ASP:OD1	38:5m:43:LYS:NZ	2.46	0.41
45:6A:148:VAL:HG13	49:6E:80:HIS:CD2	2.56	0.41
45:6A:335:MET:O	45:6A:336:PHE:C	2.63	0.41
45:6A:434:TYR:HA	45:6A:437:ILE:HD12	2.03	0.41
46:6B:297:GLN:O	46:6B:298:ALA:C	2.63	0.41
47:6C:72:ASP:CB	49:6E:144:ALA:HB3	2.51	0.41
47:6C:117:VAL:HG21	47:6C:302:ILE:HG12	2.03	0.41
47:6C:250:LEU:HD23	47:6C:250:LEU:HA	1.77	0.41
48:6D:181:LYS:H	48:6D:181:LYS:HG3	1.53	0.41
48:6D:238:ASN:O	48:6D:242:PHE:HB3	2.20	0.41
48:6D:327:ARG:H	48:6D:327:ARG:HG2	1.81	0.41
49:6E:222:CYS:SG	72:6E:301:FES:S2	3.18	0.41
53:6J:17:ARG:HA	53:6J:17:ARG:HD2	1.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6N:33:PRO:HG2	46:6O:369:LEU:HB3	2.03	0.41
45:6N:51:LYS:O	45:6N:177:LEU:CD2	2.69	0.41
45:6N:135:LEU:O	45:6N:136:GLN:C	2.64	0.41
45:6N:215:HIS:O	45:6N:216:PHE:C	2.64	0.41
45:6N:280:TYR:CE1	45:6N:284:TYR:HB2	2.56	0.41
45:6N:369:LEU:HD13	45:6N:375:VAL:HG22	2.02	0.41
46:6O:238:LYS:HD2	46:6O:239:TYR:H	1.84	0.41
46:6O:258:VAL:O	46:6O:423:SER:N	2.51	0.41
46:6O:295:LEU:O	46:6O:296:TYR:C	2.63	0.41
47:6P:226:ILE:HD12	47:6P:226:ILE:HA	1.88	0.41
47:6P:315:MET:HG3	47:6P:318:ARG:NH2	2.36	0.41
48:6Q:27:ARG:NH2	48:6Q:60:GLU:OE1	2.40	0.41
48:6Q:109:LEU:HD12	48:6Q:110:PRO:HD2	2.03	0.41
51:6T:45:ILE:HD12	51:6T:45:ILE:HA	1.88	0.41
54:6Y:15:ARG:HA	54:6Y:18:ILE:HD12	2.02	0.41
54:6Y:26:ALA:O	54:6Y:27:VAL:C	2.64	0.41
55:8A:11:ASN:HB3	55:8A:14:ASP:HB2	2.02	0.41
55:8A:94:PHE:O	55:8A:95:PRO:C	2.63	0.41
55:8A:94:PHE:HZ	57:8C:82:GLY:HA3	1.83	0.41
55:8A:100:MET:O	55:8A:101:SER:C	2.64	0.41
55:8A:182:PRO:HB2	55:8A:185:VAL:HB	2.02	0.41
55:8A:186:TRP:O	55:8A:189:LEU:HB3	2.21	0.41
55:8A:307:SER:O	55:8A:308:ALA:C	2.64	0.41
55:8A:390:MET:SD	85:8A:605:HEA:H273	2.61	0.41
55:8A:460:ILE:H	55:8A:460:ILE:HG12	1.60	0.41
55:8A:492:LEU:HD22	60:8F:71:TRP:CZ2	2.56	0.41
55:8A:492:LEU:O	55:8A:493:GLU:C	2.64	0.41
55:8A:500:PRO:HB2	55:8A:504:THR:HG21	2.03	0.41
56:8B:105:TYR:HE1	56:8B:119:ASP:OD1	2.04	0.41
57:8C:243:HIS:O	57:8C:247:VAL:HG13	2.21	0.41
65:8K:9:PHE:CE2	82:8K:101:PGV:H212	2.56	0.41
1:1A:12:THR:O	1:1A:16:LEU:HG	2.21	0.41
6:1F:132:ARG:CZ	44:1s:66:PRO:HD3	2.51	0.41
6:1F:309:LYS:HA	6:1F:312:CYS:SG	2.61	0.41
7:1G:147:LYS:HB3	7:1G:147:LYS:HE2	1.92	0.41
7:1G:640:ASN:CG	7:1G:641:TYR:H	2.27	0.41
8:1H:181:LEU:HG	8:1H:300:LEU:HD13	2.03	0.41
12:1L:145:GLU:HG2	13:1M:370:PRO:HD2	2.03	0.41
12:1L:403:TYR:CD2	37:1l:125:TYR:HB3	2.55	0.41
69:1M:501:3PE:H341	14:1N:277:ILE:HG12	2.02	0.41
69:1M:501:3PE:H321	24:1Y:132:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:48:GLU:O	21:1V:52:ASN:ND2	2.54	0.41
33:1h:87:TYR:O	33:1h:91:MET:HG3	2.21	0.41
35:1j:6:HIS:CD2	35:1j:7:ILE:HG12	2.55	0.41
35:1j:19:ARG:HE	65:8K:12:LYS:CG	2.32	0.41
47:3C:75:TYR:CD1	49:3E:135:GLN:HG2	2.56	0.41
49:3E:93:ARG:HG2	51:3G:26:ARG:N	2.36	0.41
45:3N:41:ILE:HG12	45:3N:195:MET:CE	2.50	0.41
45:3N:41:ILE:N	45:3N:95:THR:O	2.44	0.41
45:3N:135:LEU:HD11	45:3N:175:ARG:HG2	2.02	0.41
45:3N:143:SER:O	49:3V:47:ARG:HG3	2.21	0.41
46:3O:253:VAL:N	46:3O:328:SER:O	2.54	0.41
46:3O:310:SER:HB2	49:3V:60:ALA:O	2.21	0.41
47:3P:253:PRO:O	48:3Q:119:ALA:HA	2.21	0.41
48:3Q:138:PRO:HB2	52:3U:54:CYS:HB2	2.03	0.41
54:3Y:48:ILE:CG2	54:3Y:51:LYS:HD3	2.51	0.41
90:4C:306:PEK:O14	90:4C:306:PEK:N	2.38	0.41
1:5A:54:LYS:HB3	1:5A:113:TRP:CE3	2.56	0.41
2:5B:171:LYS:HD3	2:5B:174:ARG:CZ	2.51	0.41
4:5D:151:ILE:HG21	4:5D:174:ARG:HG3	2.03	0.41
7:5G:254:MET:HA	7:5G:260:GLU:O	2.21	0.41
7:5G:375:ASP:HB2	7:5G:448:LYS:H	1.85	0.41
13:5M:1:FME:HE3	13:5M:111:THR:HG21	2.02	0.41
13:5M:197:LEU:O	13:5M:201:MET:HG2	2.21	0.41
14:5N:44:LEU:HD22	14:5N:122:ILE:HD12	2.02	0.41
15:5O:183:ILE:O	15:5O:186:LYS:HG2	2.21	0.41
16:5P:69:ILE:HD12	18:5R:26:VAL:HG13	2.01	0.41
25:5Z:96:ILE:HA	25:5Z:99:LYS:NZ	2.36	0.41
35:5j:37:LEU:HD11	36:5k:74:PHE:HA	2.01	0.41
38:5m:22:TYR:CB	39:5n:64:ARG:NE	2.83	0.41
38:5m:47:LEU:HB3	39:5n:165:LEU:HD13	2.03	0.41
42:5q:84:PRO:HA	42:5q:87:HIS:HB3	2.03	0.41
45:6A:67:THR:HA	45:6A:120:CYS:HA	2.03	0.41
46:6B:30:PRO:C	46:6B:32:GLY:H	2.28	0.41
46:6B:352:LEU:HD23	46:6B:411:ILE:HG12	2.02	0.41
47:6C:94:LEU:O	47:6C:98:VAL:HG23	2.20	0.41
47:6C:130:GLY:O	47:6C:134:PRO:HD3	2.21	0.41
47:6C:130:GLY:HA3	83:6C:501:HEM:C1A	2.56	0.41
47:6C:138:MET:O	47:6C:141:TRP:N	2.54	0.41
47:6C:207:ASN:OD1	47:6C:210:GLY:N	2.52	0.41
47:6C:369:THR:O	47:6C:370:SER:C	2.63	0.41
48:6D:270:GLN:O	48:6D:271:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:6J:40:ALA:O	53:6J:41:ASP:C	2.65	0.41
45:6N:67:THR:HG21	45:6N:116:ILE:HA	2.02	0.41
45:6N:139:GLN:HB2	49:6V:50:LEU:CD1	2.51	0.41
45:6N:191:LYS:HB3	45:6N:193:PRO:CD	2.50	0.41
45:6N:399:ILE:H	45:6N:399:ILE:HG13	1.69	0.41
46:6O:140:LEU:HD12	46:6O:140:LEU:HA	1.86	0.41
46:6O:160:LEU:HB3	46:6O:164:HIS:CE1	2.56	0.41
55:8A:97:MET:N	82:8A:602:PGV:O13	2.54	0.41
55:8A:166:THR:OG1	57:8C:85:LEU:HD12	2.21	0.41
55:8A:169:ILE:HG13	75:8A:610:CDL:CA7	2.50	0.41
55:8A:186:TRP:CH2	82:8A:603:PGV:H012	2.56	0.41
55:8A:278:MET:HB3	82:8A:603:PGV:H241	2.02	0.41
55:8A:301:THR:O	55:8A:302:ARG:C	2.64	0.41
55:8A:347:LEU:O	55:8A:350:VAL:HB	2.21	0.41
55:8A:421:VAL:HG12	55:8A:425:PHE:HE2	1.86	0.41
57:8C:27:MET:HE2	57:8C:47:LEU:HD23	2.03	0.41
57:8C:176:LEU:HA	82:8G:101:PGV:H11	2.02	0.41
58:8D:33:LEU:HD12	58:8D:37:GLN:HB3	2.02	0.41
75:8D:201:CDL:H311	75:8D:201:CDL:H341	1.31	0.41
64:8J:55:PHE:HB2	64:8J:57:HIS:CE1	2.56	0.41
5:1E:160:TYR:O	5:1E:185:GLY:N	2.45	0.40
6:1F:206:LYS:N	6:1F:207:PRO:HD2	2.36	0.40
6:1F:261:HIS:NE2	6:1F:341:THR:OG1	2.53	0.40
7:1G:526:GLY:N	7:1G:546:GLN:O	2.51	0.40
8:1H:204:GLU:HA	8:1H:208:VAL:O	2.21	0.40
8:1H:294:LEU:O	8:1H:298:LEU:HG	2.21	0.40
10:1J:122:LEU:HD13	30:1e:76:SER:HA	2.02	0.40
21:1V:57:MET:HE2	21:1V:70:GLN:CG	2.51	0.40
23:1X:39:ASN:HB3	25:1Z:73:PRO:HG2	2.02	0.40
25:1Z:43:LEU:HD23	25:1Z:43:LEU:HA	1.89	0.40
27:1b:39:ASN:O	27:1b:43:ARG:HG3	2.20	0.40
32:1g:40:LYS:H	32:1g:40:LYS:HG3	1.73	0.40
38:1m:4:LYS:NZ	39:1n:68:GLU:OE1	2.50	0.40
41:1p:6:LYS:H	41:1p:6:LYS:HG2	1.68	0.40
41:1p:101:ILE:O	41:1p:105:ILE:HG12	2.21	0.40
41:1p:136:LYS:O	41:1p:136:LYS:HD2	2.20	0.40
45:3N:124:ASP:OD1	45:3N:127:ILE:HD12	2.21	0.40
45:3N:148:VAL:C	45:3N:152:TYR:HD2	2.30	0.40
45:3N:179:ARG:O	45:3N:183:THR:HG23	2.21	0.40
45:3N:191:LYS:O	45:3N:192:ALA:C	2.64	0.40
45:3N:316:GLU:OE1	45:3N:316:GLU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:371:GLY:C	45:3N:374:PRO:HD2	2.46	0.40
46:3O:33:LEU:HB2	46:3O:201:SER:HB3	2.02	0.40
46:3O:385:GLN:OE1	46:3O:392:TYR:HA	2.21	0.40
47:3P:92:ILE:HG13	47:3P:272:TRP:HH2	1.86	0.40
48:3Q:41:HIS:HE1	48:3Q:111:PRO:HD2	1.86	0.40
48:3Q:231:LYS:HD3	50:3S:70:MET:HE3	2.02	0.40
82:4A:601:PGV:H142	57:4C:22:LEU:HD21	2.03	0.40
57:4C:112:LEU:HB3	57:4C:118:PRO:HB3	2.03	0.40
82:4C:304:PGV:O13	82:4C:304:PGV:O05	2.30	0.40
58:4D:19:ARG:HE	58:4D:19:ARG:HB3	1.71	0.40
64:4J:55:PHE:HB2	64:4J:57:HIS:CE1	2.56	0.40
1:5A:30:TYR:OH	2:5B:111:ARG:NH2	2.40	0.40
3:5C:161:PRO:HA	3:5C:166:PHE:CD2	2.56	0.40
4:5D:169:TRP:CH2	9:5I:36:MET:HG3	2.56	0.40
4:5D:306:GLN:O	4:5D:310:ILE:HG13	2.22	0.40
5:5E:34:ILE:HD12	5:5E:49:PRO:HB2	2.02	0.40
5:5E:150:ASN:HA	5:5E:190:ARG:HH12	1.86	0.40
5:5E:216:GLY:O	5:5E:217:LEU:HD23	2.22	0.40
10:5J:127:ILE:HG21	11:5K:2:PRO:HG3	2.03	0.40
13:5M:2:LEU:HD23	13:5M:2:LEU:HA	1.91	0.40
13:5M:128:PRO:O	13:5M:132:ILE:HG12	2.21	0.40
13:5M:176:PHE:CE1	13:5M:245:ARG:HB3	2.57	0.40
13:5M:318:ALA:HB1	13:5M:374:ASN:CG	2.46	0.40
15:5O:129:TYR:CE2	15:5O:166:PRO:HD3	2.57	0.40
33:5h:87:TYR:O	33:5h:91:MET:HG3	2.21	0.40
34:5i:10:ARG:NH1	39:5n:154:PRO:O	2.53	0.40
41:5p:14:ARG:HE	41:5p:14:ARG:HB3	1.68	0.40
45:6A:196:VAL:HG23	45:6A:384:LEU:HD23	2.03	0.40
45:6A:319:LEU:O	45:6A:320:LEU:C	2.63	0.40
45:6A:425:LEU:O	45:6A:426:GLY:C	2.64	0.40
46:6B:185:LYS:HE2	46:6B:185:LYS:HB3	1.53	0.40
47:6C:36:LEU:HA	47:6C:39:ILE:HD12	2.03	0.40
47:6C:177:ARG:O	47:6C:178:PHE:C	2.63	0.40
48:6D:98:TYR:CD2	52:6H:98:LEU:HB3	2.55	0.40
51:6G:43:THR:O	51:6G:47:ILE:HB	2.21	0.40
45:6N:14:THR:HG23	45:6N:389:ARG:HH22	1.84	0.40
45:6N:140:GLU:HG2	49:6V:48:SER:C	2.46	0.40
45:6N:170:PRO:CD	45:6N:173:ASN:CB	2.78	0.40
45:6N:246:ASP:CG	51:6T:9:ARG:HA	2.46	0.40
45:6N:407:VAL:HA	45:6N:410:VAL:HG22	2.02	0.40
46:6O:176:LEU:O	46:6O:177:TYR:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:6O:300:ALA:O	46:6O:302:GLY:N	2.54	0.40
55:8A:152:LEU:O	55:8A:153:ALA:C	2.64	0.40
55:8A:204:ALA:C	55:8A:208:MET:HE3	2.45	0.40
55:8A:268:PHE:HE1	56:8B:56:MET:HB3	1.85	0.40
55:8A:508:PRO:HB2	60:8F:32:ASN:CB	2.51	0.40
75:8A:610:CDL:H842	57:8C:247:VAL:CG2	2.49	0.40
57:8C:127:LEU:HD23	57:8C:127:LEU:HA	1.90	0.40
59:8E:37:VAL:HG11	59:8E:70:VAL:HG21	2.02	0.40
68:8N:7:THR:O	68:8N:11:LYS:HG3	2.21	0.40
2:1B:58:GLU:HG3	4:1D:189:MET:SD	2.61	0.40
3:1C:32:ILE:HG21	3:1C:63:PHE:CE1	2.55	0.40
4:1D:348:HIS:HE1	9:1I:125:ALA:O	2.04	0.40
5:1E:150:ASN:HA	5:1E:190:ARG:HH12	1.86	0.40
7:1G:622:ARG:NH2	19:1S:73:GLU:OE2	2.40	0.40
9:1I:30:LEU:HD13	71:1I:201:PC1:H261	2.02	0.40
14:1N:167:TRP:CZ2	69:1N:901:3PE:H2I1	2.56	0.40
15:1O:35:LYS:HE2	15:1O:126:ARG:CZ	2.51	0.40
15:1O:223:TYR:OH	15:1O:237:ASP:OD2	2.30	0.40
19:1S:19:ARG:HB2	19:1S:65:TRP:HB2	2.03	0.40
28:1c:35:HIS:CG	29:1d:26:LEU:HD21	2.56	0.40
29:1d:64:TYR:CZ	75:1d:202:CDL:H312	2.56	0.40
31:1f:8:ARG:HA	31:1f:8:ARG:HD2	1.79	0.40
32:1g:81:PRO:HG3	33:1h:76:ALA:HB2	2.04	0.40
39:1n:54:LYS:HZ2	45:3N:20:ASP:HA	1.86	0.40
43:1r:31:SER:HB2	43:1r:35:GLN:NE2	2.37	0.40
46:3B:181:TYR:CE2	46:3O:249:GLY:HA3	2.56	0.40
46:3B:216:LEU:HD23	46:3B:216:LEU:HA	1.92	0.40
47:3C:50:PHE:CD1	49:3E:136:PHE:CD2	3.09	0.40
47:3C:315:MET:HA	47:3C:318:ARG:HB2	2.04	0.40
47:3C:316:MET:O	47:3C:322:GLN:NE2	2.55	0.40
49:3E:180:THR:O	49:3E:184:ILE:HG13	2.21	0.40
49:3R:167:PHE:O	49:3R:173:PRO:HA	2.22	0.40
49:3R:176:VAL:HG13	49:3R:212:ILE:HD11	2.03	0.40
56:4B:102:HIS:CD2	56:4B:107:SER:HG	2.37	0.40
1:5A:94:LEU:HD23	1:5A:94:LEU:HA	1.93	0.40
2:5B:42:ARG:O	2:5B:164:GLN:NE2	2.54	0.40
5:5E:163:ASP:CG	5:5E:188:SER:HG	2.23	0.40
13:5M:8:THR:O	13:5M:11:LEU:HB2	2.20	0.40
13:5M:343:ILE:HD11	38:5m:64:LEU:HD11	2.03	0.40
14:5N:231:SER:O	14:5N:234:TRP:HD1	2.05	0.40
15:5O:82:PHE:CE1	15:5O:138:MET:HE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5P:209:ASP:OD1	16:5P:209:ASP:N	2.53	0.40
21:5V:57:MET:HE2	21:5V:70:GLN:CG	2.51	0.40
22:5W:65:GLU:OE1	22:5W:66:MET:HE1	2.21	0.40
28:5c:35:HIS:CG	29:5d:26:LEU:HD21	2.57	0.40
75:5i:201:CDL:HB61	75:5i:201:CDL:H712	1.51	0.40
35:5j:69:ASP:HB3	40:5o:117:ARG:HH12	1.86	0.40
46:6B:295:LEU:H	46:6B:295:LEU:HG	1.73	0.40
47:6C:53:MET:HG2	49:6E:140:MET:HG2	2.03	0.40
48:6D:159:GLN:HA	48:6D:170:MET:CA	2.49	0.40
48:6D:260:PHE:O	48:6D:263:GLY:N	2.54	0.40
45:6N:86:LEU:HD21	45:6N:99:ILE:HD13	1.99	0.40
46:6O:197:ASN:O	46:6O:232:LEU:N	2.54	0.40
46:6O:218:GLN:O	46:6O:221:GLU:HG2	2.21	0.40
47:6P:296:ALA:O	47:6P:300:ILE:HB	2.22	0.40
48:6Q:230:LEU:O	48:6Q:233:ARG:HG2	2.21	0.40
49:6R:159:ILE:HA	49:6R:160:PRO:HD3	1.93	0.40
49:6V:53:GLU:H	49:6V:53:GLU:HG2	1.73	0.40
55:8A:66:ILE:HB	55:8A:67:PHE:H	1.69	0.40
55:8A:100:MET:HB2	57:8C:57:TRP:CH2	2.56	0.40
55:8A:249:PRO:O	55:8A:250:GLY:C	2.64	0.40
55:8A:431:LEU:CD2	55:8A:447:TYR:HA	2.50	0.40
55:8A:480:ARG:HA	67:8M:6:ALA:HA	2.03	0.40
55:8A:486:GLU:C	55:8A:488:THR:H	2.29	0.40
82:8A:602:PGV:H181	57:8C:31:LEU:HD12	2.03	0.40
82:8A:603:PGV:H201	75:8A:610:CDL:H442	2.02	0.40
58:8D:34:SER:O	58:8D:38:LYS:HG3	2.21	0.40
61:8G:69:LEU:HD12	61:8G:69:LEU:HA	1.91	0.40
2:1B:47:PRO:HD2	2:1B:75:VAL:O	2.22	0.40
2:1B:101:ARG:C	2:1B:103:VAL:H	2.23	0.40
4:1D:151:ILE:HG21	4:1D:174:ARG:HG3	2.03	0.40
5:1E:216:GLY:O	5:1E:217:LEU:HD23	2.22	0.40
6:1F:97:ALA:HB3	6:1F:138:ILE:HA	2.03	0.40
7:1G:159:CYS:HA	7:1G:202:ILE:HD11	2.04	0.40
7:1G:543:ILE:O	7:1G:558:ASP:N	2.48	0.40
8:1H:316:PRO:HG3	25:1Z:57:ARG:HB3	2.02	0.40
10:1J:41:CYS:O	10:1J:45:LEU:HG	2.21	0.40
12:1L:7:LEU:HD22	12:1L:46:LEU:HD11	2.02	0.40
12:1L:108:MET:HE3	12:1L:108:MET:HB3	1.93	0.40
13:1M:19:LYS:HB3	13:1M:19:LYS:HE3	1.89	0.40
13:1M:343:ILE:HD11	38:1m:64:LEU:HD11	2.03	0.40
15:1O:82:PHE:CE1	15:1O:138:MET:HE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:195:SER:HB2	16:1P:199:GLU:OE1	2.20	0.40
16:1P:265:TRP:CD1	16:1P:268:ARG:HH21	2.39	0.40
17:1Q:77:ASP:HA	17:1Q:78:PRO:HD3	1.92	0.40
19:1S:64:LEU:O	19:1S:75:ASN:HA	2.22	0.40
20:1T:79:TYR:O	20:1T:83:LYS:HG2	2.22	0.40
20:1U:63:PRO:HB3	37:1l:61:TRP:CD2	2.56	0.40
20:1U:83:LYS:HE3	20:1U:83:LYS:HB3	1.82	0.40
25:1Z:96:ILE:HA	25:1Z:99:LYS:NZ	2.36	0.40
26:1a:21:MET:HE3	26:1a:21:MET:HB3	1.85	0.40
31:1f:38:ARG:HG3	31:1f:56:TRP:CE2	2.56	0.40
46:3B:308:ASP:OD2	49:3I:57:GLY:N	2.54	0.40
48:3D:297:MET:HE3	48:3D:297:MET:HB3	1.86	0.40
49:3E:155:LYS:HE2	49:3E:159:ILE:HD11	2.02	0.40
52:3H:99:PHE:HA	52:3H:102:LEU:HD12	2.02	0.40
45:3N:36:THR:CG2	45:3N:372:THR:C	2.90	0.40
45:3N:60:GLU:C	46:3O:287:ARG:HH22	2.29	0.40
45:3N:67:THR:HA	45:3N:121:SER:H	1.83	0.40
45:3N:179:ARG:O	45:3N:180:ALA:C	2.64	0.40
45:3N:339:GLN:O	45:3N:343:MET:N	2.39	0.40
45:3N:419:CYS:HB3	45:3N:438:ARG:CD	2.51	0.40
46:3O:152:PHE:O	46:3O:153:GLN:C	2.65	0.40
48:3Q:109:LEU:HD12	48:3Q:110:PRO:HD2	2.03	0.40
57:4C:31:LEU:HD23	57:4C:31:LEU:HA	1.93	0.40
1:5A:84:LEU:HD23	1:5A:84:LEU:HA	1.85	0.40
3:5C:171:TYR:CD1	17:5Q:78:PRO:HG2	2.56	0.40
5:5E:205:PRO:HA	5:5E:206:PRO:HD3	1.93	0.40
6:5F:132:ARG:CZ	44:5s:66:PRO:HD3	2.51	0.40
7:5G:391:PHE:CE2	7:5G:395:ILE:HD11	2.57	0.40
69:5M:501:3PE:H321	24:5Y:132:TRP:CZ3	2.56	0.40
14:5N:87:THR:HG22	33:5h:126:PRO:HG2	2.02	0.40
14:5N:153:LEU:CD1	14:5N:157:MET:HE2	2.51	0.40
16:5P:65:LEU:HB3	17:5Q:69:LEU:HD22	2.03	0.40
16:5P:265:TRP:CD1	16:5P:268:ARG:HH21	2.39	0.40
20:5T:79:TYR:O	20:5T:83:LYS:HG2	2.22	0.40
75:5X:201:CDL:H252	75:5X:201:CDL:H441	2.04	0.40
25:5Z:105:LYS:HB3	25:5Z:105:LYS:HE3	1.91	0.40
26:5a:4:GLU:O	26:5a:7:PRO:HD2	2.21	0.40
29:5d:46:ASN:CB	29:5d:53:VAL:HA	2.51	0.40
37:5l:81:LEU:O	37:5l:85:ILE:HG23	2.22	0.40
38:5m:48:LEU:HD23	39:5n:165:LEU:HD21	2.02	0.40
40:5o:121:MET:HE3	40:5o:121:MET:HB3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:6A:204:GLU:O	45:6A:205:HIS:C	2.63	0.40
45:6A:214:LYS:HZ3	45:6A:214:LYS:HG3	1.78	0.40
47:6C:185:LEU:HA	47:6C:188:ILE:HD12	2.02	0.40
48:6D:226:PRO:HG3	52:6H:83:LEU:HD22	2.03	0.40
48:6D:235:LEU:HD23	48:6D:235:LEU:HA	1.91	0.40
49:6E:182:LYS:HD2	49:6E:182:LYS:HA	1.79	0.40
49:6E:206:LYS:HD2	49:6E:265:PHE:HD1	1.85	0.40
49:6E:219:HIS:HB3	72:6E:301:FES:S1	2.60	0.40
45:6N:15:GLN:CB	45:6N:205:HIS:CG	3.02	0.40
45:6N:382:SER:HA	45:6N:386:TYR:CD2	2.56	0.40
46:6O:22:GLN:HE21	46:6O:22:GLN:HB2	1.55	0.40
46:6O:297:GLN:O	46:6O:298:ALA:C	2.64	0.40
47:6P:5:ARG:HA	47:6P:11:MET:CE	2.52	0.40
47:6P:185:LEU:HD23	47:6P:185:LEU:HA	1.85	0.40
48:6Q:41:HIS:HE1	48:6Q:111:PRO:HD2	1.86	0.40
49:6R:214:ILE:HG22	49:6R:216:VAL:HG12	2.03	0.40
55:8A:247:ILE:HD11	55:8A:344:PHE:HE2	1.86	0.40
55:8A:306:THR:OG1	55:8A:361:SER:HB2	2.21	0.40
55:8A:356:ILE:O	55:8A:359:ALA:HB3	2.20	0.40
55:8A:438:ARG:HD2	55:8A:439:ARG:HG3	2.02	0.40
55:8A:440:TYR:HE1	56:8B:204:HIS:CE1	2.40	0.40
55:8A:508:PRO:C	60:8F:56:ARG:HH21	2.22	0.40
55:8A:508:PRO:HG2	60:8F:32:ASN:HB2	2.04	0.40
57:8C:112:LEU:HB3	57:8C:118:PRO:HB3	2.03	0.40
1:1A:72:LEU:HD13	1:1A:72:LEU:HA	1.92	0.40
2:1B:114:VAL:HG22	2:1B:163:LEU:HD22	2.04	0.40
4:1D:417:ILE:O	4:1D:420:THR:HG22	2.21	0.40
7:1G:622:ARG:HH22	19:1S:73:GLU:CD	2.27	0.40
12:1L:249:SER:HB2	12:1L:340:PHE:CD2	2.56	0.40
12:1L:573:MET:HA	12:1L:576:MET:HE3	2.03	0.40
13:1M:281:ASP:OD1	13:1M:340:ARG:HB3	2.22	0.40
13:1M:299:VAL:HG11	13:1M:396:MET:HE1	2.04	0.40
13:1M:458:LEU:HD23	13:1M:458:LEU:HA	1.81	0.40
22:1W:65:GLU:OE1	22:1W:66:MET:HE1	2.21	0.40
23:1X:171:MET:HE2	23:1X:171:MET:HB3	1.83	0.40
43:1r:31:SER:HB2	43:1r:35:GLN:HE22	1.87	0.40
47:3C:103:TYR:HB2	47:3C:325:PHE:CE1	2.55	0.40
47:3C:124:MET:HE1	47:3C:298:ILE:HD13	2.03	0.40
47:3C:240:LEU:O	47:3C:241:ILE:C	2.65	0.40
48:3D:162:PRO:HD3	48:3D:168:MET:HE1	2.03	0.40
49:3E:199:GLN:OE1	49:3E:204:ARG:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:206:LYS:HD2	49:3E:265:PHE:HD1	1.85	0.40
49:3E:207:LYS:O	49:3E:209:GLU:N	2.54	0.40
49:3E:213:LEU:CD1	49:3E:247:GLY:HA3	2.52	0.40
47:3P:237:LEU:HB2	48:3Q:212:MET:SD	2.60	0.40
48:3Q:87:LEU:HD23	48:3Q:87:LEU:HA	1.91	0.40
48:3Q:160:MET:HG2	48:3Q:161:ALA:O	2.21	0.40
48:3Q:167:GLU:HG2	52:3U:13:LEU:HD22	2.03	0.40
49:3R:163:LYS:HB2	49:3R:163:LYS:HE2	1.88	0.40
49:3R:170:ARG:C	49:3R:172:LYS:H	2.30	0.40
55:4A:49:GLY:HA3	55:4A:53:ILE:HG21	2.04	0.40
89:4B:303:PSC:H012	89:4B:303:PSC:P	2.61	0.40
75:4C:308:CDL:H152	75:4C:308:CDL:H111	2.03	0.40
1:5A:63:LEU:HB2	10:5J:67:VAL:HG21	2.04	0.40
4:5D:55:HIS:CD2	4:5D:57:ALA:HB3	2.56	0.40
4:5D:232:ASN:O	4:5D:236:ARG:HG3	2.21	0.40
6:5F:262:VAL:CG1	6:5F:284:ALA:HB1	2.52	0.40
7:5G:148:THR:HA	7:5G:207:ALA:O	2.22	0.40
8:5H:187:ILE:HG13	71:5I:201:PC1:H251	2.03	0.40
12:5L:484:LEU:HD22	12:5L:484:LEU:C	2.41	0.40
13:5M:84:LEU:HD23	13:5M:84:LEU:HA	1.92	0.40
13:5M:299:VAL:HG11	13:5M:396:MET:HE1	2.04	0.40
16:5P:325:ARG:HA	16:5P:325:ARG:HD2	1.80	0.40
20:5T:56:ASP:OD1	20:5T:57:GLU:N	2.54	0.40
27:5b:39:ASN:O	27:5b:43:ARG:HG3	2.20	0.40
29:5d:64:TYR:CZ	75:5d:202:CDL:H312	2.56	0.40
42:5q:49:TYR:HB2	42:5q:61:TRP:CE2	2.56	0.40
44:5s:71:GLN:HB2	44:5s:75:HIS:HD2	1.87	0.40
45:6A:365:LEU:H	45:6A:365:LEU:HG	1.73	0.40
45:6A:394:GLU:O	45:6A:395:TRP:C	2.64	0.40
46:6B:153:GLN:HB2	49:6I:46:LYS:CE	2.52	0.40
47:6C:111:GLU:HB3	47:6C:199:PHE:CG	2.57	0.40
48:6D:251:PRO:HA	48:6D:252:PRO:HD3	1.78	0.40
48:6D:275:VAL:HA	48:6D:278:PHE:HB3	2.03	0.40
53:6J:40:ALA:HA	53:6J:43:ILE:HD12	2.04	0.40
45:6N:16:VAL:CG1	45:6N:17:SER:H	2.31	0.40
45:6N:347:THR:HB	54:6X:17:TRP:CZ2	2.56	0.40
45:6N:351:GLU:O	45:6N:352:SER:C	2.64	0.40
46:6O:133:ARG:HB3	46:6O:135:TRP:CH2	2.56	0.40
46:6O:195:VAL:HG13	46:6O:199:PHE:HB2	2.04	0.40
46:6O:298:ALA:O	46:6O:301:LYS:HB2	2.21	0.40
46:6O:411:ILE:H	46:6O:411:ILE:HG12	1.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:6P:117:VAL:N	83:6P:502:HEM:HBC2	2.36	0.40
47:6P:313:ARG:HB2	50:6S:38:TYR:CD1	2.57	0.40
48:6Q:138:PRO:HB2	52:6U:54:CYS:HB2	2.03	0.40
48:6Q:160:MET:HG2	48:6Q:161:ALA:O	2.21	0.40
49:6R:169:TRP:CD1	49:6R:174:LEU:HD22	2.56	0.40
54:6Y:40:LEU:O	54:6Y:44:TRP:NE1	2.55	0.40
55:8A:496:HIS:HE1	55:8A:505:PHE:H	1.69	0.40
57:8C:117:PRO:HA	57:8C:118:PRO:HD3	1.98	0.40
75:8D:201:CDL:H332	75:8D:201:CDL:H542	2.04	0.40
68:8N:40:ASN:HB3	68:8N:43:VAL:HG23	2.04	0.40
1:1A:38:GLU:CD	1:1A:43:PRO:HA	2.46	0.40
1:1A:71:LEU:HD11	11:1K:65:VAL:HG11	2.03	0.40
4:1D:55:HIS:CD2	4:1D:57:ALA:HB3	2.56	0.40
4:1D:371:LYS:HE2	4:1D:424:VAL:CG2	2.44	0.40
6:1F:262:VAL:CG1	6:1F:284:ALA:HB1	2.52	0.40
7:1G:148:THR:HA	7:1G:207:ALA:O	2.22	0.40
8:1H:2:PHE:CE2	8:1H:6:ILE:HD11	2.57	0.40
8:1H:289:LEU:HD23	8:1H:290:TRP:CD1	2.56	0.40
12:1L:207:GLU:HG2	12:1L:269:THR:HG23	2.02	0.40
12:1L:257:VAL:HG12	12:1L:314:MET:CE	2.51	0.40
75:1L:702:CDL:H332	33:1h:25:MET:HE3	2.04	0.40
13:1M:246:ILE:HD12	13:1M:246:ILE:HA	1.93	0.40
20:1T:52:MET:HE3	22:1W:41:ARG:NE	2.37	0.40
23:1X:13:LYS:HE3	23:1X:13:LYS:HB2	1.79	0.40
34:1i:5:PRO:O	34:1i:8:LYS:HG3	2.21	0.40
34:1i:82:HIS:HD2	41:1p:44:VAL:HG21	1.86	0.40
37:1l:40:ASP:OD2	38:1m:84:LYS:NZ	2.54	0.40
40:1o:80:LYS:HE2	40:1o:80:LYS:HB2	1.91	0.40
42:1q:49:TYR:HB2	42:1q:61:TRP:CE2	2.56	0.40
45:3A:12:PRO:O	45:3A:12:PRO:HG2	2.10	0.40
45:3A:260:PRO:HG2	45:3A:267:ASN:OD1	2.22	0.40
45:3A:429:GLU:CG	51:3G:7:GLY:H	2.32	0.40
46:3B:154:ASN:ND2	46:3B:154:ASN:C	2.71	0.40
47:3C:5:ARG:NH1	47:3C:20:ASP:OD1	2.55	0.40
47:3C:23:ALA:O	47:3C:218:ILE:N	2.53	0.40
47:3C:67:THR:HG21	48:3D:133:TYR:HB3	2.03	0.40
49:3E:219:HIS:HB3	72:3E:301:FES:S1	2.60	0.40
45:3N:108:LYS:O	45:3N:111:GLU:N	2.54	0.40
45:3N:259:GLY:H	45:3N:318:GLY:H	1.70	0.40
46:3O:79:GLY:HA3	46:3O:125:ASN:CB	2.48	0.40
46:3O:115:ASP:O	46:3O:118:ILE:HG13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3P:377:LEU:HD23	47:3P:377:LEU:HA	1.89	0.40
48:3Q:123:GLY:O	48:3Q:127:VAL:HG23	2.22	0.40
49:3R:211:VAL:HG22	49:3R:213:LEU:CD1	2.51	0.40
55:4A:232:GLN:HB2	55:4A:292:MET:HE3	2.02	0.40
55:4A:347:LEU:HD11	55:4A:418:PHE:CE1	2.56	0.40
75:4B:301:CDL:H152	75:4B:301:CDL:H652	2.03	0.40
57:4C:243:HIS:O	57:4C:247:VAL:HG13	2.21	0.40
82:4G:101:PGV:H012	82:4G:101:PGV:H202	1.69	0.40
62:4H:39:CYS:CB	62:4H:53:CYS:CB	2.95	0.40
62:4H:56:TYR:CZ	68:4N:80:PRO:HD2	2.56	0.40
63:4I:58:LYS:HE3	63:4I:62:GLU:OE2	2.21	0.40
66:4L:44:LEU:HD22	67:4M:41:LYS:HG2	2.04	0.40
4:5D:329:LYS:HE2	43:5r:53:TYR:CE2	2.56	0.40
10:5J:52:LEU:O	10:5J:56:VAL:HG23	2.21	0.40
12:5L:249:SER:HB2	12:5L:340:PHE:CD2	2.56	0.40
69:5N:901:3PE:H2C2	69:5N:901:3PE:H281	2.04	0.40
20:5T:52:MET:HE3	22:5W:41:ARG:NE	2.37	0.40
23:5X:157:LEU:HD23	23:5X:157:LEU:HA	1.84	0.40
34:5i:5:PRO:O	34:5i:8:LYS:HG3	2.21	0.40
36:5k:67:LEU:HD23	36:5k:70:PHE:CG	2.57	0.40
43:5r:31:SER:HB2	43:5r:35:GLN:NE2	2.36	0.40
45:6A:163:LEU:HB2	45:6A:234:CYS:SG	2.62	0.40
46:6B:83:PHE:CZ	50:6S:104:ARG:HA	2.56	0.40
47:6C:186:PRO:HG2	83:6C:501:HEM:CMC	2.50	0.40
49:6E:199:GLN:OE1	49:6E:204:ARG:HB3	2.22	0.40
50:6F:110:ILE:O	50:6F:114:LYS:HG2	2.22	0.40
51:6G:73:ARG:HA	51:6G:73:ARG:HD2	1.75	0.40
45:6N:106:LEU:HD13	45:6N:208:LEU:HD21	2.04	0.40
45:6N:254:ALA:HB2	45:6N:323:HIS:CD2	2.54	0.40
45:6N:396:GLU:O	45:6N:397:SER:C	2.65	0.40
46:6O:67:HIS:CE1	46:6O:144:LEU:HA	2.54	0.40
47:6P:6:LYS:O	47:6P:12:LYS:HD2	2.22	0.40
47:6P:361:ILE:HA	47:6P:365:LEU:HB2	2.04	0.40
48:6Q:167:GLU:HG2	52:6U:13:LEU:HD22	2.03	0.40
55:8A:59:THR:HG23	55:8A:125:GLY:C	2.46	0.40
55:8A:73:ILE:HD13	55:8A:73:ILE:HA	1.89	0.40
55:8A:80:ASN:O	55:8A:81:TRP:C	2.64	0.40
56:8B:171:LYS:HE3	56:8B:171:LYS:HB2	1.86	0.40
62:8H:56:TYR:CZ	68:8N:80:PRO:HD2	2.56	0.40
63:8I:58:LYS:HE3	63:8I:62:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1A	112/115 (97%)	79 (70%)	27 (24%)	6 (5%)	1 15
1	5A	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	7 35
2	1B	147/258 (57%)	115 (78%)	22 (15%)	10 (7%)	1 11
2	5B	153/258 (59%)	147 (96%)	6 (4%)	0	100 100
3	1C	207/264 (78%)	202 (98%)	5 (2%)	0	100 100
3	5C	207/264 (78%)	202 (98%)	5 (2%)	0	100 100
4	1D	427/466 (92%)	409 (96%)	18 (4%)	0	100 100
4	5D	427/466 (92%)	410 (96%)	17 (4%)	0	100 100
5	1E	212/249 (85%)	199 (94%)	13 (6%)	0	100 100
5	5E	212/249 (85%)	199 (94%)	13 (6%)	0	100 100
6	1F	430/464 (93%)	411 (96%)	17 (4%)	2 (0%)	25 64
6	5F	430/464 (93%)	411 (96%)	17 (4%)	2 (0%)	25 64
7	1G	697/727 (96%)	675 (97%)	19 (3%)	3 (0%)	30 68
7	5G	697/727 (96%)	675 (97%)	19 (3%)	3 (0%)	30 68
8	1H	316/318 (99%)	293 (93%)	21 (7%)	2 (1%)	22 60
8	5H	316/318 (99%)	295 (93%)	20 (6%)	1 (0%)	37 73
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100 100
9	5I	174/239 (73%)	167 (96%)	7 (4%)	0	100 100
10	1J	172/175 (98%)	155 (90%)	15 (9%)	2 (1%)	11 44
10	5J	172/175 (98%)	158 (92%)	12 (7%)	2 (1%)	11 44
11	1K	96/98 (98%)	93 (97%)	3 (3%)	0	100 100
11	5K	96/98 (98%)	93 (97%)	3 (3%)	0	100 100
12	1L	604/606 (100%)	568 (94%)	33 (6%)	3 (0%)	25 64
12	5L	604/606 (100%)	568 (94%)	33 (6%)	3 (0%)	25 64
13	1M	457/459 (100%)	450 (98%)	6 (1%)	1 (0%)	44 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	5M	457/459 (100%)	450 (98%)	6 (1%)	1 (0%)	44 78
14	1N	345/347 (99%)	337 (98%)	7 (2%)	1 (0%)	37 73
14	5N	345/347 (99%)	337 (98%)	7 (2%)	1 (0%)	37 73
15	1O	318/357 (89%)	308 (97%)	10 (3%)	0	100 100
15	5O	318/357 (89%)	308 (97%)	10 (3%)	0	100 100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100 100
16	5P	340/377 (90%)	324 (95%)	16 (5%)	0	100 100
17	1Q	127/175 (73%)	122 (96%)	5 (4%)	0	100 100
17	5Q	127/175 (73%)	122 (96%)	5 (4%)	0	100 100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100 100
18	5R	94/123 (76%)	89 (95%)	5 (5%)	0	100 100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100 100
19	5S	85/99 (86%)	81 (95%)	4 (5%)	0	100 100
20	1T	83/156 (53%)	83 (100%)	0	0	100 100
20	1U	84/156 (54%)	83 (99%)	1 (1%)	0	100 100
20	5T	83/156 (53%)	83 (100%)	0	0	100 100
20	5U	84/156 (54%)	83 (99%)	1 (1%)	0	100 100
21	1V	113/116 (97%)	111 (98%)	2 (2%)	0	100 100
21	5V	113/116 (97%)	111 (98%)	2 (2%)	0	100 100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100 100
22	5W	113/128 (88%)	107 (95%)	6 (5%)	0	100 100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	22 60
23	5X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	22 60
24	1Y	137/141 (97%)	136 (99%)	1 (1%)	0	100 100
24	5Y	137/141 (97%)	136 (99%)	1 (1%)	0	100 100
25	1Z	139/144 (96%)	138 (99%)	1 (1%)	0	100 100
25	5Z	139/144 (96%)	138 (99%)	1 (1%)	0	100 100
26	1a	68/70 (97%)	68 (100%)	0	0	100 100
26	5a	68/70 (97%)	68 (100%)	0	0	100 100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100 100
27	5b	81/84 (96%)	77 (95%)	4 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	1c	47/76 (62%)	47 (100%)	0	0	100	100
28	5c	47/76 (62%)	47 (100%)	0	0	100	100
29	1d	117/122 (96%)	116 (99%)	1 (1%)	0	100	100
29	5d	117/122 (96%)	116 (99%)	1 (1%)	0	100	100
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
30	5e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
31	5f	55/58 (95%)	51 (93%)	4 (7%)	0	100	100
32	1g	98/154 (64%)	88 (90%)	10 (10%)	0	100	100
32	5g	98/154 (64%)	88 (90%)	10 (10%)	0	100	100
33	1h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
33	5h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	1i	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
34	5i	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
35	5j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	77 (98%)	2 (2%)	0	100	100
36	5k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
37	5l	154/186 (83%)	149 (97%)	5 (3%)	0	100	100
38	1m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
38	5m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
39	1n	170/179 (95%)	162 (95%)	8 (5%)	0	100	100
39	5n	170/179 (95%)	162 (95%)	8 (5%)	0	100	100
40	1o	120/136 (88%)	120 (100%)	0	0	100	100
40	5o	120/136 (88%)	120 (100%)	0	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
41	5p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
42	5q	143/145 (99%)	141 (99%)	2 (1%)	0	100	100
43	1r	90/113 (80%)	87 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
43	5r	90/113 (80%)	87 (97%)	3 (3%)	0	100 100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100 100
44	5s	43/471 (9%)	41 (95%)	2 (5%)	0	100 100
45	3A	436/480 (91%)	428 (98%)	6 (1%)	2 (0%)	25 64
45	3N	443/480 (92%)	387 (87%)	44 (10%)	12 (3%)	4 25
45	6A	436/480 (91%)	297 (68%)	110 (25%)	29 (7%)	1 12
45	6N	443/480 (92%)	289 (65%)	113 (26%)	41 (9%)	0 8
46	3B	416/453 (92%)	407 (98%)	9 (2%)	0	100 100
46	3O	415/453 (92%)	366 (88%)	40 (10%)	9 (2%)	5 29
46	6B	416/453 (92%)	302 (73%)	96 (23%)	18 (4%)	2 17
46	6O	415/453 (92%)	288 (69%)	103 (25%)	24 (6%)	1 14
47	3C	377/379 (100%)	333 (88%)	35 (9%)	9 (2%)	5 27
47	3P	377/379 (100%)	370 (98%)	7 (2%)	0	100 100
47	6C	377/379 (100%)	223 (59%)	115 (30%)	39 (10%)	0 6
47	6P	377/379 (100%)	370 (98%)	7 (2%)	0	100 100
48	3D	235/326 (72%)	230 (98%)	5 (2%)	0	100 100
48	3Q	237/326 (73%)	231 (98%)	6 (2%)	0	100 100
48	6D	235/326 (72%)	156 (66%)	47 (20%)	32 (14%)	0 4
48	6Q	237/326 (73%)	231 (98%)	6 (2%)	0	100 100
49	3E	194/274 (71%)	176 (91%)	17 (9%)	1 (0%)	25 64
49	3I	45/274 (16%)	40 (89%)	5 (11%)	0	100 100
49	3R	194/274 (71%)	173 (89%)	17 (9%)	4 (2%)	5 30
49	3V	29/274 (11%)	29 (100%)	0	0	100 100
49	6E	194/274 (71%)	175 (90%)	18 (9%)	1 (0%)	25 64
49	6I	45/274 (16%)	40 (89%)	5 (11%)	0	100 100
49	6R	194/274 (71%)	173 (89%)	17 (9%)	4 (2%)	5 30
49	6V	29/274 (11%)	29 (100%)	0	0	100 100
50	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100 100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100 100
50	6F	96/111 (86%)	95 (99%)	1 (1%)	0	100 100
50	6S	96/111 (86%)	95 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	3G	70/82 (85%)	59 (84%)	10 (14%)	1 (1%)	9 41
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100 100
51	6G	70/82 (85%)	70 (100%)	0	0	100 100
51	6T	72/82 (88%)	71 (99%)	1 (1%)	0	100 100
52	3H	63/91 (69%)	59 (94%)	2 (3%)	2 (3%)	3 21
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100 100
52	6H	63/91 (69%)	58 (92%)	4 (6%)	1 (2%)	8 38
52	6U	63/91 (69%)	62 (98%)	1 (2%)	0	100 100
53	3J	54/64 (84%)	53 (98%)	0	1 (2%)	6 32
53	3W	54/64 (84%)	54 (100%)	0	0	100 100
53	6J	54/64 (84%)	36 (67%)	15 (28%)	3 (6%)	1 14
53	6W	54/64 (84%)	54 (100%)	0	0	100 100
54	3X	50/56 (89%)	49 (98%)	1 (2%)	0	100 100
54	3Y	49/56 (88%)	45 (92%)	4 (8%)	0	100 100
54	6X	50/56 (89%)	49 (98%)	1 (2%)	0	100 100
54	6Y	49/56 (88%)	32 (65%)	12 (24%)	5 (10%)	0 7
55	4A	511/514 (99%)	493 (96%)	15 (3%)	3 (1%)	22 60
55	8A	511/514 (99%)	329 (64%)	146 (29%)	36 (7%)	1 11
56	4B	225/229 (98%)	215 (96%)	9 (4%)	1 (0%)	30 68
56	8B	225/229 (98%)	215 (96%)	9 (4%)	1 (0%)	30 68
57	4C	257/261 (98%)	248 (96%)	9 (4%)	0	100 100
57	8C	257/261 (98%)	248 (96%)	9 (4%)	0	100 100
58	4D	137/169 (81%)	131 (96%)	6 (4%)	0	100 100
58	8D	137/169 (81%)	131 (96%)	6 (4%)	0	100 100
59	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100 100
59	8E	103/152 (68%)	99 (96%)	4 (4%)	0	100 100
60	4F	95/129 (74%)	92 (97%)	3 (3%)	0	100 100
60	8F	95/129 (74%)	92 (97%)	3 (3%)	0	100 100
61	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100 100
61	8G	73/97 (75%)	69 (94%)	4 (6%)	0	100 100
62	4H	80/86 (93%)	77 (96%)	3 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	8H	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
63	4I	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
63	8I	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
64	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
64	8J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
65	4K	47/80 (59%)	44 (94%)	3 (6%)	0	100	100
65	8K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
66	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
66	8L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
67	8M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	10	43
68	8N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	10	43
All	All	28141/33842 (83%)	26038 (92%)	1775 (6%)	328 (1%)	14	44

All (328) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1B	59	MET
2	1B	84	ASP
2	1B	98	PRO
2	1B	102	LYS
2	1B	114	VAL
10	1J	66	VAL
13	1M	82	SER
23	1X	28	ALA
47	3C	152	ALA
49	3E	271	VAL
45	3N	107	PRO
45	3N	200	ALA
49	3R	150	SER
55	4A	242	GLU
55	4A	243	VAL
68	4N	33	VAL
10	5J	66	VAL
13	5M	82	SER
23	5X	28	ALA

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Mol	Chain	Res	Type
46	6B	155	PRO
46	6B	157	ALA
47	6C	25	SER
47	6C	26	ASN
47	6C	73	VAL
47	6C	222	PRO
47	6C	259	ALA
47	6C	319	PRO
48	6D	199	PRO
48	6D	252	PRO
48	6D	287	HIS
49	6E	271	VAL
45	6N	3	THR
45	6N	10	SER
45	6N	16	VAL
45	6N	24	ARG
45	6N	90	SER
45	6N	167	VAL
45	6N	199	ALA
45	6N	217	SER
45	6N	428	ILE
49	6R	150	SER
55	8A	5	ARG
55	8A	83	VAL
55	8A	142	SER
55	8A	509	THR
68	8N	33	VAL
1	1A	51	PHE
1	1A	110	GLY
2	1B	83	SER
2	1B	88	VAL
2	1B	97	ALA
7	1G	155	GLN
8	1H	208	VAL
10	1J	78	MET
47	3C	59	THR
47	3C	222	PRO
47	3C	266	PRO
47	3C	319	PRO
53	3J	54	LYS
45	3N	145	MET
45	3N	177	LEU

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Mol	Chain	Res	Type
45	3N	224	VAL
46	3O	171	ALA
49	3R	228	ALA
49	3R	273	VAL
55	4A	239	GLY
7	5G	155	GLN
8	5H	208	VAL
10	5J	78	MET
45	6A	53	ASN
45	6A	72	GLY
45	6A	144	SER
45	6A	157	ALA
45	6A	202	GLY
45	6A	220	SER
45	6A	311	ASN
45	6A	320	LEU
45	6A	331	ILE
45	6A	411	CYS
45	6A	426	GLY
46	6B	76	THR
46	6B	113	ARG
46	6B	156	GLN
46	6B	231	GLY
46	6B	293	SER
46	6B	330	ALA
47	6C	59	THR
47	6C	74	ASN
47	6C	156	ILE
47	6C	223	TYR
47	6C	253	PRO
47	6C	323	CYS
47	6C	373	GLU
48	6D	170	MET
48	6D	184	PRO
48	6D	233	GLU
48	6D	236	TYR
48	6D	261	ASP
45	6N	15	GLN
45	6N	36	THR
45	6N	56	GLY
45	6N	71	PRO
45	6N	223	TYR

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Mol	Chain	Res	Type
45	6N	245	ASP
45	6N	312	ILE
46	6O	58	GLU
46	6O	172	LEU
46	6O	225	ASN
46	6O	301	LYS
46	6O	429	ASN
49	6R	228	ALA
49	6R	273	VAL
54	6Y	38	TRP
54	6Y	40	LEU
55	8A	73	ILE
55	8A	74	MET
55	8A	120	ALA
55	8A	239	GLY
55	8A	345	ILE
55	8A	360	ASN
55	8A	437	PRO
55	8A	446	ALA
1	1A	73	LEU
1	1A	112	GLU
6	1F	249	ARG
7	1G	186	TYR
7	1G	654	GLN
12	1L	208	CYS
47	3C	253	PRO
47	3C	283	SER
52	3H	98	LEU
45	3N	43	ALA
45	3N	260	PRO
45	3N	317	THR
46	3O	39	GLU
46	3O	199	PHE
49	3R	181	LYS
1	5A	52	SER
6	5F	249	ARG
7	5G	186	TYR
7	5G	654	GLN
12	5L	208	CYS
45	6A	120	CYS
45	6A	170	PRO
45	6A	291	SER

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Mol	Chain	Res	Type
45	6A	388	ARG
46	6B	24	LEU
46	6B	147	ASP
46	6B	227	ARG
46	6B	313	ASN
47	6C	9	PRO
47	6C	139	SER
47	6C	270	PRO
47	6C	315	MET
48	6D	147	GLU
48	6D	211	GLY
48	6D	265	PRO
48	6D	285	PRO
48	6D	288	ASP
48	6D	318	VAL
53	6J	17	ARG
53	6J	37	ASP
45	6N	17	SER
45	6N	30	SER
45	6N	41	ILE
45	6N	198	ALA
45	6N	219	LEU
45	6N	224	VAL
45	6N	351	GLU
46	6O	173	ALA
46	6O	251	SER
46	6O	252	LEU
46	6O	293	SER
49	6R	181	LYS
55	8A	65	MET
55	8A	119	GLU
55	8A	162	ILE
55	8A	288	TRP
55	8A	359	ALA
55	8A	381	LEU
55	8A	511	ILE
1	1A	109	LYS
1	1A	114	ALA
2	1B	78	ALA
6	1F	297	VAL
8	1H	217	ALA
12	1L	601	LEU

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Mol	Chain	Res	Type
45	3A	350	THR
47	3C	156	ILE
51	3G	27	ALA
45	3N	53	ASN
45	3N	120	CYS
45	3N	262	TRP
45	3N	320	LEU
46	3O	43	PRO
46	3O	84	LYS
6	5F	297	VAL
12	5L	601	LEU
45	6A	4	TYR
45	6A	61	HIS
45	6A	71	PRO
45	6A	143	SER
45	6A	165	GLN
45	6A	292	SER
45	6A	385	THR
47	6C	47	THR
47	6C	78	VAL
47	6C	256	TYR
47	6C	308	HIS
47	6C	316	MET
47	6C	344	GLU
48	6D	94	HIS
48	6D	146	GLU
48	6D	160	ASP
48	6D	166	GLY
48	6D	297	MET
48	6D	298	LEU
45	6N	31	SER
45	6N	50	GLU
45	6N	159	GLN
45	6N	176	LYS
45	6N	249	PRO
45	6N	342	TRP
46	6O	57	TYR
46	6O	201	SER
46	6O	224	LEU
46	6O	283	PRO
46	6O	350	GLY
46	6O	425	ALA

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Mol	Chain	Res	Type
55	8A	49	GLY
55	8A	166	THR
55	8A	174	PRO
55	8A	310	MET
55	8A	334	TRP
55	8A	382	SER
55	8A	444	PRO
55	8A	448	THR
2	1B	85	VAL
14	1N	110	PRO
47	3C	286	ASN
52	3H	80	THR
46	3O	388	VAL
56	4B	159	VAL
12	5L	205	ASN
14	5N	110	PRO
45	6A	73	SER
45	6A	148	VAL
45	6A	230	ALA
45	6A	364	ALA
46	6B	171	ALA
46	6B	306	PRO
47	6C	12	LYS
47	6C	21	LEU
47	6C	110	LEU
47	6C	111	GLU
47	6C	151	SER
47	6C	155	TYR
47	6C	327	MET
48	6D	178	TYR
48	6D	190	ARG
48	6D	243	PRO
48	6D	253	ILE
48	6D	255	ASN
48	6D	300	MET
48	6D	306	PRO
52	6H	78	ASP
53	6J	11	TYR
45	6N	33	PRO
45	6N	107	PRO
45	6N	110	VAL
45	6N	204	GLU

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Mol	Chain	Res	Type
45	6N	222	THR
45	6N	234	CYS
45	6N	286	GLY
45	6N	379	ILE
45	6N	411	CYS
46	6O	84	LYS
46	6O	114	ASP
46	6O	171	ALA
46	6O	249	GLY
55	8A	69	MET
55	8A	374	VAL
12	1L	205	ASN
45	3A	231	PHE
46	3O	89	ILE
46	3O	317	SER
1	5A	109	LYS
45	6A	264	ASN
46	6B	63	LEU
46	6B	131	GLU
47	6C	42	ILE
47	6C	324	LEU
47	6C	374	ASN
48	6D	212	GLU
48	6D	322	ARG
46	6O	78	LYS
46	6O	396	SER
54	6Y	6	LEU
54	6Y	48	ILE
54	6Y	49	ASN
55	8A	72	PRO
55	8A	164	PHE
46	3O	280	GLY
46	6B	130	PRO
47	6C	27	ILE
46	6O	130	PRO
55	8A	84	PRO
55	8A	435	GLY
56	8B	159	VAL
47	6C	14	ILE
48	6D	172	PRO
45	6N	186	VAL
55	8A	312	ILE

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Mol	Chain	Res	Type
45	6A	203	VAL
47	6C	157	GLY
47	6C	285	PRO
45	6N	12	PRO
45	6A	107	PRO
46	6B	350	GLY
47	6C	258	PRO
48	6D	204	ILE
45	6N	72	GLY
55	8A	258	VAL
47	6C	361	ILE
48	6D	99	PRO
46	6O	109	VAL
46	6O	116	ILE
55	8A	182	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1A	99/99 (100%)	64 (65%)	35 (35%)	0 1
1	5A	99/99 (100%)	90 (91%)	9 (9%)	7 24
2	1B	131/212 (62%)	112 (86%)	19 (14%)	2 12
2	5B	131/212 (62%)	123 (94%)	8 (6%)	15 37
3	1C	191/228 (84%)	187 (98%)	4 (2%)	48 66
3	5C	191/228 (84%)	187 (98%)	4 (2%)	48 66
4	1D	371/396 (94%)	362 (98%)	9 (2%)	44 62
4	5D	371/396 (94%)	362 (98%)	9 (2%)	44 62
5	1E	183/207 (88%)	176 (96%)	7 (4%)	28 49
5	5E	183/207 (88%)	176 (96%)	7 (4%)	28 49
6	1F	346/368 (94%)	335 (97%)	11 (3%)	34 53
6	5F	346/368 (94%)	335 (97%)	11 (3%)	34 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1G	588/610 (96%)	570 (97%)	18 (3%)	35	54
7	5G	588/610 (96%)	568 (97%)	20 (3%)	32	51
8	1H	274/274 (100%)	264 (96%)	10 (4%)	30	50
8	5H	274/274 (100%)	264 (96%)	10 (4%)	30	50
9	1I	151/201 (75%)	147 (97%)	4 (3%)	41	59
9	5I	151/201 (75%)	147 (97%)	4 (3%)	41	59
10	1J	140/141 (99%)	132 (94%)	8 (6%)	17	38
10	5J	140/141 (99%)	132 (94%)	8 (6%)	17	38
11	1K	84/84 (100%)	84 (100%)	0	100	100
11	5K	84/84 (100%)	83 (99%)	1 (1%)	67	79
12	1L	539/539 (100%)	526 (98%)	13 (2%)	44	62
12	5L	539/539 (100%)	527 (98%)	12 (2%)	47	65
13	1M	408/408 (100%)	397 (97%)	11 (3%)	40	58
13	5M	408/408 (100%)	397 (97%)	11 (3%)	40	58
14	1N	310/310 (100%)	305 (98%)	5 (2%)	58	74
14	5N	310/310 (100%)	305 (98%)	5 (2%)	58	74
15	1O	283/307 (92%)	268 (95%)	15 (5%)	19	40
15	5O	283/307 (92%)	269 (95%)	14 (5%)	21	42
16	1P	296/323 (92%)	289 (98%)	7 (2%)	44	62
16	5P	296/323 (92%)	289 (98%)	7 (2%)	44	62
17	1Q	117/152 (77%)	110 (94%)	7 (6%)	16	37
17	5Q	117/152 (77%)	110 (94%)	7 (6%)	16	37
18	1R	79/97 (81%)	78 (99%)	1 (1%)	65	77
18	5R	79/97 (81%)	78 (99%)	1 (1%)	65	77
19	1S	77/82 (94%)	74 (96%)	3 (4%)	27	48
19	5S	77/82 (94%)	74 (96%)	3 (4%)	27	48
20	1T	79/133 (59%)	78 (99%)	1 (1%)	65	77
20	1U	79/133 (59%)	73 (92%)	6 (8%)	11	30
20	5T	79/133 (59%)	78 (99%)	1 (1%)	65	77
20	5U	79/133 (59%)	73 (92%)	6 (8%)	11	30
21	1V	100/101 (99%)	97 (97%)	3 (3%)	36	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	5V	100/101 (99%)	97 (97%)	3 (3%)	36	55
22	1W	107/112 (96%)	105 (98%)	2 (2%)	52	69
22	5W	107/112 (96%)	105 (98%)	2 (2%)	52	69
23	1X	153/154 (99%)	148 (97%)	5 (3%)	33	52
23	5X	153/154 (99%)	147 (96%)	6 (4%)	27	48
24	1Y	101/102 (99%)	97 (96%)	4 (4%)	27	47
24	5Y	101/102 (99%)	97 (96%)	4 (4%)	27	47
25	1Z	123/124 (99%)	121 (98%)	2 (2%)	58	74
25	5Z	123/124 (99%)	121 (98%)	2 (2%)	58	74
26	1a	58/58 (100%)	57 (98%)	1 (2%)	56	72
26	5a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	64 (93%)	5 (7%)	12	32
27	5b	69/70 (99%)	64 (93%)	5 (7%)	12	32
28	1c	45/66 (68%)	42 (93%)	3 (7%)	13	34
28	5c	45/66 (68%)	42 (93%)	3 (7%)	13	34
29	1d	106/109 (97%)	101 (95%)	5 (5%)	22	44
29	5d	106/109 (97%)	101 (95%)	5 (5%)	22	44
30	1e	87/94 (93%)	84 (97%)	3 (3%)	32	51
30	5e	87/94 (93%)	84 (97%)	3 (3%)	32	51
31	1f	54/55 (98%)	53 (98%)	1 (2%)	52	69
31	5f	54/55 (98%)	53 (98%)	1 (2%)	52	69
32	1g	92/129 (71%)	91 (99%)	1 (1%)	70	80
32	5g	92/129 (71%)	91 (99%)	1 (1%)	70	80
33	1h	121/158 (77%)	117 (97%)	4 (3%)	33	52
33	5h	121/158 (77%)	117 (97%)	4 (3%)	33	52
34	1i	120/120 (100%)	118 (98%)	2 (2%)	56	72
34	5i	120/120 (100%)	118 (98%)	2 (2%)	56	72
35	1j	62/84 (74%)	61 (98%)	1 (2%)	58	74
35	5j	62/84 (74%)	60 (97%)	2 (3%)	34	53
36	1k	63/76 (83%)	62 (98%)	1 (2%)	58	74
36	5k	63/76 (83%)	59 (94%)	4 (6%)	15	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	1l	141/161 (88%)	139 (99%)	2 (1%)	62 75
37	5l	141/161 (88%)	139 (99%)	2 (1%)	62 75
38	1m	113/114 (99%)	109 (96%)	4 (4%)	31 51
38	5m	113/114 (99%)	109 (96%)	4 (4%)	31 51
39	1n	156/160 (98%)	153 (98%)	3 (2%)	52 69
39	5n	156/160 (98%)	153 (98%)	3 (2%)	52 69
40	1o	110/119 (92%)	104 (94%)	6 (6%)	18 39
40	5o	110/119 (92%)	104 (94%)	6 (6%)	18 39
41	1p	154/156 (99%)	150 (97%)	4 (3%)	41 59
41	5p	154/156 (99%)	150 (97%)	4 (3%)	41 59
42	1q	131/131 (100%)	129 (98%)	2 (2%)	60 75
42	5q	131/131 (100%)	129 (98%)	2 (2%)	60 75
43	1r	85/98 (87%)	83 (98%)	2 (2%)	44 62
43	5r	85/98 (87%)	83 (98%)	2 (2%)	44 62
44	1s	44/351 (12%)	39 (89%)	5 (11%)	4 16
44	5s	44/351 (12%)	39 (89%)	5 (11%)	4 16
45	3A	367/397 (92%)	360 (98%)	7 (2%)	52 69
45	3N	371/397 (94%)	353 (95%)	18 (5%)	21 42
45	6A	367/397 (92%)	234 (64%)	133 (36%)	0 1
45	6N	371/397 (94%)	295 (80%)	76 (20%)	1 6
46	3B	329/355 (93%)	322 (98%)	7 (2%)	48 66
46	3O	328/355 (92%)	298 (91%)	30 (9%)	7 24
46	6B	329/355 (93%)	195 (59%)	134 (41%)	0 0
46	6O	328/355 (92%)	202 (62%)	126 (38%)	0 0
47	3C	332/332 (100%)	300 (90%)	32 (10%)	7 22
47	3P	332/332 (100%)	330 (99%)	2 (1%)	84 88
47	6C	332/332 (100%)	212 (64%)	120 (36%)	0 1
47	6P	332/332 (100%)	331 (100%)	1 (0%)	91 92
48	3D	202/259 (78%)	198 (98%)	4 (2%)	50 68
48	3Q	204/259 (79%)	202 (99%)	2 (1%)	73 82
48	6D	202/259 (78%)	123 (61%)	79 (39%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	6Q	204/259 (79%)	201 (98%)	3 (2%)	60 75
49	3E	166/225 (74%)	164 (99%)	2 (1%)	67 79
49	3I	36/225 (16%)	30 (83%)	6 (17%)	2 9
49	3R	166/225 (74%)	158 (95%)	8 (5%)	21 43
49	3V	24/225 (11%)	22 (92%)	2 (8%)	9 27
49	6E	166/225 (74%)	164 (99%)	2 (1%)	67 79
49	6I	36/225 (16%)	31 (86%)	5 (14%)	3 13
49	6R	166/225 (74%)	158 (95%)	8 (5%)	21 43
49	6V	24/225 (11%)	22 (92%)	2 (8%)	9 27
50	3F	90/99 (91%)	90 (100%)	0	100 100
50	3S	90/99 (91%)	90 (100%)	0	100 100
50	6F	90/99 (91%)	90 (100%)	0	100 100
50	6S	90/99 (91%)	90 (100%)	0	100 100
51	3G	66/73 (90%)	60 (91%)	6 (9%)	7 24
51	3T	67/73 (92%)	67 (100%)	0	100 100
51	6G	66/73 (90%)	66 (100%)	0	100 100
51	6T	67/73 (92%)	67 (100%)	0	100 100
52	3H	62/85 (73%)	57 (92%)	5 (8%)	9 28
52	3U	62/85 (73%)	57 (92%)	5 (8%)	9 28
52	6H	62/85 (73%)	59 (95%)	3 (5%)	21 43
52	6U	62/85 (73%)	57 (92%)	5 (8%)	9 28
53	3J	46/52 (88%)	46 (100%)	0	100 100
53	3W	46/52 (88%)	46 (100%)	0	100 100
53	6J	46/52 (88%)	25 (54%)	21 (46%)	0 0
53	6W	46/52 (88%)	46 (100%)	0	100 100
54	3X	42/46 (91%)	42 (100%)	0	100 100
54	3Y	41/46 (89%)	40 (98%)	1 (2%)	44 62
54	6X	42/46 (91%)	42 (100%)	0	100 100
54	6Y	41/46 (89%)	23 (56%)	18 (44%)	0 0
55	4A	424/424 (100%)	417 (98%)	7 (2%)	56 72
55	8A	424/424 (100%)	296 (70%)	128 (30%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	4B	210/211 (100%)	198 (94%)	12 (6%)	17	38
56	8B	210/211 (100%)	200 (95%)	10 (5%)	21	43
57	4C	223/225 (99%)	215 (96%)	8 (4%)	30	50
57	8C	223/225 (99%)	215 (96%)	8 (4%)	30	50
58	4D	124/149 (83%)	121 (98%)	3 (2%)	44	62
58	8D	124/149 (83%)	121 (98%)	3 (2%)	44	62
59	4E	92/124 (74%)	87 (95%)	5 (5%)	18	40
59	8E	92/124 (74%)	87 (95%)	5 (5%)	18	40
60	4F	80/101 (79%)	74 (92%)	6 (8%)	11	31
60	8F	80/101 (79%)	74 (92%)	6 (8%)	11	31
61	4G	65/80 (81%)	60 (92%)	5 (8%)	10	30
61	8G	65/80 (81%)	60 (92%)	5 (8%)	10	30
62	4H	73/76 (96%)	70 (96%)	3 (4%)	26	47
62	8H	73/76 (96%)	70 (96%)	3 (4%)	26	47
63	4I	54/61 (88%)	54 (100%)	0	100	100
63	8I	54/61 (88%)	54 (100%)	0	100	100
64	4J	49/68 (72%)	47 (96%)	2 (4%)	26	47
64	8J	49/68 (72%)	47 (96%)	2 (4%)	26	47
65	4K	38/66 (58%)	35 (92%)	3 (8%)	10	29
65	8K	38/66 (58%)	36 (95%)	2 (5%)	19	40
66	4L	39/55 (71%)	38 (97%)	1 (3%)	41	59
66	8L	39/55 (71%)	38 (97%)	1 (3%)	41	59
67	4M	37/57 (65%)	36 (97%)	1 (3%)	40	58
67	8M	37/57 (65%)	36 (97%)	1 (3%)	40	58
68	4N	70/70 (100%)	67 (96%)	3 (4%)	25	46
68	8N	70/70 (100%)	67 (96%)	3 (4%)	25	46
All	All	24534/28538 (86%)	22927 (93%)	1607 (7%)	16	34

All (1607) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	5	LEU
1	1A	8	LEU

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Mol	Chain	Res	Type
1	1A	9	THR
1	1A	13	LEU
1	1A	15	SER
1	1A	17	LEU
1	1A	18	VAL
1	1A	19	LEU
1	1A	20	ILE
1	1A	27	LEU
1	1A	32	GLU
1	1A	48	ARG
1	1A	51	PHE
1	1A	52	SER
1	1A	53	MET
1	1A	54	LYS
1	1A	57	LEU
1	1A	65	PHE
1	1A	69	ILE
1	1A	71	LEU
1	1A	72	LEU
1	1A	73	LEU
1	1A	76	PRO
1	1A	79	SER
1	1A	80	GLN
1	1A	83	ASN
1	1A	86	THR
1	1A	87	MET
1	1A	88	LEU
1	1A	90	MET
1	1A	96	ILE
1	1A	97	LEU
1	1A	109	LYS
1	1A	111	LEU
1	1A	112	GLU
2	1B	32	LYS
2	1B	39	TRP
2	1B	42	ARG
2	1B	48	MET
2	1B	54	CYS
2	1B	74	VAL
2	1B	76	PHE
2	1B	82	GLN
2	1B	83	SER

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Mol	Chain	Res	Type
2	1B	85	VAL
2	1B	88	VAL
2	1B	91	THR
2	1B	111	ARG
2	1B	114	VAL
2	1B	118	SER
2	1B	125	TYR
2	1B	133	VAL
2	1B	142	VAL
2	1B	143	ASP
3	1C	32	ILE
3	1C	33	LEU
3	1C	114	LEU
3	1C	115	THR
4	1D	18	VAL
4	1D	22	THR
4	1D	36	VAL
4	1D	61	VAL
4	1D	85	ARG
4	1D	95	THR
4	1D	184	VAL
4	1D	246	THR
4	1D	281	VAL
5	1E	68	LYS
5	1E	121	GLN
5	1E	122	LYS
5	1E	132	THR
5	1E	149	VAL
5	1E	164	LEU
5	1E	181	ILE
6	1F	10	THR
6	1F	105	CYS
6	1F	148	ASN
6	1F	221	THR
6	1F	227	THR
6	1F	250	ASN
6	1F	267	THR
6	1F	277	LYS
6	1F	287	VAL
6	1F	334	VAL
6	1F	395	ILE
7	1G	33	VAL

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Mol	Chain	Res	Type
7	1G	151	THR
7	1G	153	CYS
7	1G	181	MET
7	1G	187	ILE
7	1G	190	MET
7	1G	216	THR
7	1G	227	SER
7	1G	348	VAL
7	1G	371	VAL
7	1G	376	VAL
7	1G	403	ASP
7	1G	471	SER
7	1G	475	GLN
7	1G	503	LEU
7	1G	531	CYS
7	1G	613	TYR
7	1G	651	LEU
8	1H	25	ARG
8	1H	72	ILE
8	1H	87	VAL
8	1H	102	VAL
8	1H	119	SER
8	1H	177	THR
8	1H	178	SER
8	1H	201	THR
8	1H	227	GLU
8	1H	285	LEU
9	1I	7	MET
9	1I	37	THR
9	1I	93	THR
9	1I	103	SER
10	1J	33	LEU
10	1J	50	SER
10	1J	55	MET
10	1J	84	VAL
10	1J	97	LEU
10	1J	100	GLU
10	1J	113	VAL
10	1J	163	ILE
12	1L	140	LEU
12	1L	147	VAL
12	1L	149	ILE

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Mol	Chain	Res	Type
12	1L	163	ASP
12	1L	190	LEU
12	1L	203	MET
12	1L	380	LEU
12	1L	440	LEU
12	1L	491	LEU
12	1L	517	SER
12	1L	531	SER
12	1L	543	SER
12	1L	560	THR
13	1M	83	HIS
13	1M	94	LEU
13	1M	104	LEU
13	1M	116	ILE
13	1M	253	LEU
13	1M	292	SER
13	1M	303	ILE
13	1M	305	THR
13	1M	350	THR
13	1M	365	THR
13	1M	391	ILE
14	1N	43	VAL
14	1N	93	VAL
14	1N	227	THR
14	1N	250	SER
14	1N	268	GLN
15	1O	14	THR
15	1O	15	THR
15	1O	18	LEU
15	1O	19	THR
15	1O	24	VAL
15	1O	28	ASP
15	1O	60	ASP
15	1O	87	LYS
15	1O	96	LEU
15	1O	106	LEU
15	1O	154	GLU
15	1O	209	THR
15	1O	218	CYS
15	1O	263	VAL
15	1O	282	ILE
16	1P	85	VAL

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Mol	Chain	Res	Type
16	1P	126	VAL
16	1P	143	SER
16	1P	275	PHE
16	1P	311	GLU
16	1P	318	LEU
16	1P	340	VAL
17	1Q	30	ILE
17	1Q	44	ASN
17	1Q	61	THR
17	1Q	80	SER
17	1Q	105	VAL
17	1Q	110	VAL
17	1Q	128	THR
18	1R	10	LYS
19	1S	58	SER
19	1S	87	THR
19	1S	93	VAL
20	1T	70	LEU
20	1U	19	LEU
20	1U	31	SER
20	1U	32	VAL
20	1U	64	ASP
20	1U	77	VAL
20	1U	86	VAL
21	1V	78	GLU
21	1V	94	LEU
21	1V	103	VAL
22	1W	22	SER
22	1W	27	GLU
23	1X	63	ASN
23	1X	99	CYS
23	1X	130	VAL
23	1X	136	LEU
23	1X	152	GLU
24	1Y	20	LYS
24	1Y	34	ILE
24	1Y	39	SER
24	1Y	76	SER
25	1Z	133	ILE
25	1Z	137	THR
26	1a	48	MET
27	1b	21	SER

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Mol	Chain	Res	Type
27	1b	29	ILE
27	1b	34	LEU
27	1b	54	VAL
27	1b	83	LEU
28	1c	4	ILE
28	1c	24	SER
28	1c	33	LYS
29	1d	14	LEU
29	1d	43	LEU
29	1d	53	VAL
29	1d	54	VAL
29	1d	65	VAL
30	1e	18	THR
30	1e	57	ILE
30	1e	76	SER
31	1f	4	LEU
32	1g	101	GLU
33	1h	36	VAL
33	1h	55	ILE
33	1h	103	LEU
33	1h	113	LEU
34	1i	58	ASN
34	1i	68	ILE
35	1j	67	LEU
36	1k	86	TYR
37	1l	138	LEU
37	1l	158	ILE
38	1m	8	SER
38	1m	24	ILE
38	1m	91	LEU
38	1m	106	THR
39	1n	84	SER
39	1n	136	VAL
39	1n	169	ILE
40	1o	19	LEU
40	1o	23	THR
40	1o	30	PHE
40	1o	34	LYS
40	1o	39	VAL
40	1o	52	LEU
41	1p	2	ASP
41	1p	11	GLU

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Mol	Chain	Res	Type
41	1p	35	ILE
41	1p	119	SER
42	1q	109	ILE
42	1q	118	SER
43	1r	24	GLN
43	1r	112	LEU
44	1s	37	THR
44	1s	47	SER
44	1s	59	SER
44	1s	71	GLN
44	1s	75	HIS
45	3A	11	VAL
45	3A	121	SER
45	3A	184	GLU
45	3A	186	VAL
45	3A	203	VAL
45	3A	232	THR
45	3A	308	GLN
46	3B	200	THR
46	3B	308	ASP
46	3B	315	SER
46	3B	319	SER
46	3B	338	LYS
46	3B	376	GLU
46	3B	436	VAL
47	3C	2	THR
47	3C	15	ASN
47	3C	18	PHE
47	3C	26	ASN
47	3C	27	ILE
47	3C	53	MET
47	3C	59	THR
47	3C	68	HIS
47	3C	74	ASN
47	3C	80	ARG
47	3C	122	THR
47	3C	135	TRP
47	3C	137	GLN
47	3C	138	MET
47	3C	146	ILE
47	3C	150	LEU
47	3C	153	ILE

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Mol	Chain	Res	Type
47	3C	162	GLU
47	3C	165	TRP
47	3C	207	ASN
47	3C	209	THR
47	3C	215	MET
47	3C	225	THR
47	3C	234	PHE
47	3C	248	ASP
47	3C	264	THR
47	3C	273	TYR
47	3C	300	ILE
47	3C	337	TRP
47	3C	345	HIS
47	3C	349	ILE
47	3C	377	LEU
48	3D	146	GLU
48	3D	158	VAL
48	3D	165	ASP
48	3D	232	ARG
49	3E	180	THR
49	3E	217	CYS
51	3G	10	THR
51	3G	25	GLN
51	3G	30	HIS
51	3G	61	TYR
51	3G	73	ARG
51	3G	74	LYS
52	3H	67	GLN
52	3H	75	THR
52	3H	78	ASP
52	3H	97	LYS
52	3H	100	ASN
49	3I	41	PRO
49	3I	65	VAL
49	3I	67	SER
49	3I	70	LEU
49	3I	72	VAL
49	3I	78	TYR
45	3N	244	ARG
45	3N	269	PRO
45	3N	279	HIS
45	3N	290	MET

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Mol	Chain	Res	Type
45	3N	307	PHE
45	3N	308	GLN
45	3N	313	CYS
45	3N	319	LEU
45	3N	320	LEU
45	3N	332	ASP
45	3N	347	THR
45	3N	350	THR
45	3N	355	VAL
45	3N	363	ASN
45	3N	442	PHE
45	3N	443	TRP
45	3N	445	ARG
45	3N	446	PHE
46	3O	25	GLU
46	3O	26	PHE
46	3O	37	SER
46	3O	38	LEU
46	3O	39	GLU
46	3O	46	ARG
46	3O	63	LEU
46	3O	89	ILE
46	3O	92	VAL
46	3O	99	THR
46	3O	107	TYR
46	3O	113	ARG
46	3O	116	ILE
46	3O	131	GLU
46	3O	134	ARG
46	3O	187	THR
46	3O	189	ASP
46	3O	195	VAL
46	3O	221	GLU
46	3O	248	ASN
46	3O	264	THR
46	3O	292	THR
46	3O	309	VAL
46	3O	319	SER
46	3O	324	ILE
46	3O	329	GLN
46	3O	335	ASP
46	3O	379	LEU

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Mol	Chain	Res	Type
46	3O	393	VAL
46	3O	437	ASP
47	3P	43	LEU
47	3P	345	HIS
48	3Q	3	LEU
48	3Q	114	SER
49	3R	83	ILE
49	3R	150	SER
49	3R	180	THR
49	3R	218	THR
49	3R	219	HIS
49	3R	263	TYR
49	3R	265	PHE
49	3R	271	VAL
52	3U	20	VAL
52	3U	39	LEU
52	3U	45	SER
52	3U	48	SER
52	3U	50	THR
49	3V	71	ASN
49	3V	75	SER
54	3Y	18	ILE
55	4A	212	ASP
55	4A	241	PRO
55	4A	243	VAL
55	4A	247	ILE
55	4A	298	ASP
55	4A	316	THR
55	4A	513	LEU
56	4B	16	ILE
56	4B	27	THR
56	4B	33	LEU
56	4B	54	SER
56	4B	65	TRP
56	4B	95	LEU
56	4B	103	GLN
56	4B	110	TYR
56	4B	138	VAL
56	4B	149	THR
56	4B	185	MET
56	4B	191	LEU
57	4C	29	SER

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Mol	Chain	Res	Type
57	4C	44	SER
57	4C	129	VAL
57	4C	143	SER
57	4C	183	GLU
57	4C	192	VAL
57	4C	230	ASN
57	4C	245	VAL
58	4D	17	VAL
58	4D	27	VAL
58	4D	80	THR
59	4E	17	THR
59	4E	47	ILE
59	4E	80	GLU
59	4E	95	GLU
59	4E	109	VAL
60	4F	49	VAL
60	4F	67	SER
60	4F	76	LYS
60	4F	79	THR
60	4F	84	SER
60	4F	96	LEU
61	4G	15	THR
61	4G	25	LEU
61	4G	30	LEU
61	4G	44	ARG
61	4G	75	VAL
62	4H	6	THR
62	4H	26	THR
62	4H	50	VAL
64	4J	1	LEU
64	4J	10	LYS
65	4K	8	ASP
65	4K	12	LYS
65	4K	20	SER
66	4L	14	SER
67	4M	20	SER
68	4N	6	ILE
68	4N	14	SER
68	4N	33	VAL
1	5A	5	LEU
1	5A	6	THR
1	5A	17	LEU

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Mol	Chain	Res	Type
1	5A	18	VAL
1	5A	34	THR
1	5A	60	ILE
1	5A	68	GLU
1	5A	98	LEU
1	5A	111	LEU
2	5B	30	VAL
2	5B	37	VAL
2	5B	54	CYS
2	5B	76	PHE
2	5B	85	VAL
2	5B	91	THR
2	5B	125	TYR
2	5B	133	VAL
3	5C	32	ILE
3	5C	33	LEU
3	5C	114	LEU
3	5C	115	THR
4	5D	18	VAL
4	5D	22	THR
4	5D	36	VAL
4	5D	61	VAL
4	5D	85	ARG
4	5D	95	THR
4	5D	184	VAL
4	5D	246	THR
4	5D	281	VAL
5	5E	68	LYS
5	5E	121	GLN
5	5E	122	LYS
5	5E	132	THR
5	5E	149	VAL
5	5E	164	LEU
5	5E	181	ILE
6	5F	10	THR
6	5F	105	CYS
6	5F	148	ASN
6	5F	221	THR
6	5F	227	THR
6	5F	250	ASN
6	5F	267	THR
6	5F	277	LYS

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Mol	Chain	Res	Type
6	5F	287	VAL
6	5F	334	VAL
6	5F	395	ILE
7	5G	33	VAL
7	5G	151	THR
7	5G	153	CYS
7	5G	181	MET
7	5G	187	ILE
7	5G	190	MET
7	5G	216	THR
7	5G	227	SER
7	5G	348	VAL
7	5G	371	VAL
7	5G	376	VAL
7	5G	403	ASP
7	5G	471	SER
7	5G	475	GLN
7	5G	503	LEU
7	5G	531	CYS
7	5G	539	LYS
7	5G	613	TYR
7	5G	651	LEU
7	5G	657	LEU
8	5H	70	MET
8	5H	72	ILE
8	5H	87	VAL
8	5H	102	VAL
8	5H	119	SER
8	5H	177	THR
8	5H	178	SER
8	5H	201	THR
8	5H	227	GLU
8	5H	285	LEU
9	5I	7	MET
9	5I	37	THR
9	5I	93	THR
9	5I	103	SER
10	5J	33	LEU
10	5J	50	SER
10	5J	84	VAL
10	5J	97	LEU
10	5J	100	GLU

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Mol	Chain	Res	Type
10	5J	113	VAL
10	5J	151	THR
10	5J	163	ILE
11	5K	10	MET
12	5L	140	LEU
12	5L	147	VAL
12	5L	149	ILE
12	5L	163	ASP
12	5L	190	LEU
12	5L	380	LEU
12	5L	440	LEU
12	5L	491	LEU
12	5L	517	SER
12	5L	531	SER
12	5L	543	SER
12	5L	560	THR
13	5M	83	HIS
13	5M	94	LEU
13	5M	104	LEU
13	5M	116	ILE
13	5M	253	LEU
13	5M	292	SER
13	5M	303	ILE
13	5M	305	THR
13	5M	350	THR
13	5M	365	THR
13	5M	391	ILE
14	5N	43	VAL
14	5N	93	VAL
14	5N	227	THR
14	5N	250	SER
14	5N	268	GLN
15	5O	14	THR
15	5O	15	THR
15	5O	18	LEU
15	5O	19	THR
15	5O	24	VAL
15	5O	60	ASP
15	5O	87	LYS
15	5O	96	LEU
15	5O	106	LEU
15	5O	154	GLU

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Mol	Chain	Res	Type
15	5O	209	THR
15	5O	218	CYS
15	5O	263	VAL
15	5O	282	ILE
16	5P	85	VAL
16	5P	126	VAL
16	5P	143	SER
16	5P	275	PHE
16	5P	311	GLU
16	5P	318	LEU
16	5P	340	VAL
17	5Q	30	ILE
17	5Q	44	ASN
17	5Q	61	THR
17	5Q	80	SER
17	5Q	105	VAL
17	5Q	110	VAL
17	5Q	128	THR
18	5R	10	LYS
19	5S	58	SER
19	5S	87	THR
19	5S	93	VAL
20	5T	70	LEU
20	5U	19	LEU
20	5U	31	SER
20	5U	32	VAL
20	5U	64	ASP
20	5U	77	VAL
20	5U	86	VAL
21	5V	78	GLU
21	5V	94	LEU
21	5V	103	VAL
22	5W	22	SER
22	5W	27	GLU
23	5X	63	ASN
23	5X	64	GLN
23	5X	74	LYS
23	5X	99	CYS
23	5X	130	VAL
23	5X	136	LEU
24	5Y	20	LYS
24	5Y	34	ILE

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Mol	Chain	Res	Type
24	5Y	39	SER
24	5Y	76	SER
25	5Z	133	ILE
25	5Z	137	THR
27	5b	21	SER
27	5b	29	ILE
27	5b	34	LEU
27	5b	54	VAL
27	5b	83	LEU
28	5c	4	ILE
28	5c	24	SER
28	5c	33	LYS
29	5d	14	LEU
29	5d	43	LEU
29	5d	53	VAL
29	5d	54	VAL
29	5d	65	VAL
30	5e	18	THR
30	5e	57	ILE
30	5e	76	SER
31	5f	4	LEU
32	5g	101	GLU
33	5h	36	VAL
33	5h	55	ILE
33	5h	103	LEU
33	5h	113	LEU
34	5i	58	ASN
34	5i	68	ILE
35	5j	19	ARG
35	5j	67	LEU
36	5k	71	LYS
36	5k	77	PHE
36	5k	86	TYR
36	5k	90	GLN
37	5l	138	LEU
37	5l	158	ILE
38	5m	8	SER
38	5m	68	THR
38	5m	91	LEU
38	5m	106	THR
39	5n	84	SER
39	5n	136	VAL

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Mol	Chain	Res	Type
39	5n	169	ILE
40	5o	19	LEU
40	5o	23	THR
40	5o	30	PHE
40	5o	34	LYS
40	5o	39	VAL
40	5o	52	LEU
41	5p	2	ASP
41	5p	11	GLU
41	5p	35	ILE
41	5p	119	SER
42	5q	109	ILE
42	5q	118	SER
43	5r	24	GLN
43	5r	112	LEU
44	5s	37	THR
44	5s	47	SER
44	5s	48	THR
44	5s	59	SER
44	5s	75	HIS
45	6A	8	LEU
45	6A	9	GLN
45	6A	18	GLN
45	6A	19	LEU
45	6A	20	ASP
45	6A	21	ASN
45	6A	25	VAL
45	6A	27	SER
45	6A	29	GLN
45	6A	30	SER
45	6A	32	GLN
45	6A	34	THR
45	6A	37	VAL
45	6A	39	VAL
45	6A	45	SER
45	6A	49	ASN
45	6A	50	GLU
45	6A	60	GLU
45	6A	62	LEU
45	6A	65	LYS
45	6A	68	LYS
45	6A	70	ARG

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Mol	Chain	Res	Type
45	6A	77	LYS
45	6A	82	MET
45	6A	86	LEU
45	6A	91	THR
45	6A	93	GLU
45	6A	95	THR
45	6A	103	SER
45	6A	104	LYS
45	6A	107	PRO
45	6A	108	LYS
45	6A	111	GLU
45	6A	112	LEU
45	6A	115	ASP
45	6A	118	GLN
45	6A	122	LEU
45	6A	129	LYS
45	6A	130	GLU
45	6A	133	VAL
45	6A	140	GLU
45	6A	145	MET
45	6A	147	ASP
45	6A	149	VAL
45	6A	151	ASP
45	6A	163	LEU
45	6A	166	SER
45	6A	172	GLU
45	6A	177	LEU
45	6A	179	ARG
45	6A	181	ASP
45	6A	182	LEU
45	6A	184	GLU
45	6A	188	GLN
45	6A	191	LYS
45	6A	203	VAL
45	6A	207	GLN
45	6A	208	LEU
45	6A	209	LEU
45	6A	213	GLN
45	6A	214	LYS
45	6A	231	PHE
45	6A	232	THR
45	6A	237	THR

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Mol	Chain	Res	Type
45	6A	239	SER
45	6A	240	GLU
45	6A	241	ILE
45	6A	244	ARG
45	6A	250	LEU
45	6A	253	VAL
45	6A	255	ILE
45	6A	257	VAL
45	6A	258	GLU
45	6A	266	ASP
45	6A	270	LEU
45	6A	281	ASP
45	6A	283	THR
45	6A	293	THR
45	6A	296	SER
45	6A	301	ARG
45	6A	302	LYS
45	6A	303	LEU
45	6A	305	GLN
45	6A	306	SER
45	6A	307	PHE
45	6A	308	GLN
45	6A	312	ILE
45	6A	313	CYS
45	6A	319	LEU
45	6A	320	LEU
45	6A	324	PHE
45	6A	327	ASP
45	6A	331	ILE
45	6A	333	ASP
45	6A	335	MET
45	6A	338	LEU
45	6A	339	GLN
45	6A	344	ARG
45	6A	348	SER
45	6A	351	GLU
45	6A	353	GLU
45	6A	356	ARG
45	6A	365	LEU
45	6A	368	HIS
45	6A	369	LEU
45	6A	372	THR

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Mol	Chain	Res	Type
45	6A	373	THR
45	6A	376	CYS
45	6A	381	ARG
45	6A	388	ARG
45	6A	390	ILE
45	6A	392	LEU
45	6A	396	GLU
45	6A	398	ARG
45	6A	401	GLU
45	6A	406	VAL
45	6A	408	ARG
45	6A	410	VAL
45	6A	411	CYS
45	6A	413	LYS
45	6A	415	PHE
45	6A	417	ASP
45	6A	418	GLN
45	6A	422	VAL
45	6A	425	LEU
45	6A	428	ILE
45	6A	433	ASP
45	6A	434	TYR
45	6A	438	ARG
45	6A	439	SER
45	6A	441	MET
45	6A	445	ARG
45	6A	446	PHE
46	6B	22	GLN
46	6B	24	LEU
46	6B	28	ARG
46	6B	31	ASN
46	6B	34	VAL
46	6B	35	ILE
46	6B	41	TYR
46	6B	46	ARG
46	6B	47	ILE
46	6B	51	ILE
46	6B	55	SER
46	6B	56	ARG
46	6B	58	GLU
46	6B	59	ASP
46	6B	61	ASN

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Mol	Chain	Res	Type
46	6B	63	LEU
46	6B	69	LEU
46	6B	70	ARG
46	6B	74	SER
46	6B	75	LEU
46	6B	78	LYS
46	6B	81	SER
46	6B	84	LYS
46	6B	89	ILE
46	6B	95	LYS
46	6B	97	SER
46	6B	101	THR
46	6B	102	ARG
46	6B	105	MET
46	6B	109	VAL
46	6B	111	CYS
46	6B	112	LEU
46	6B	113	ARG
46	6B	115	ASP
46	6B	116	ILE
46	6B	117	GLU
46	6B	119	LEU
46	6B	120	MET
46	6B	121	GLU
46	6B	122	PHE
46	6B	124	LEU
46	6B	131	GLU
46	6B	145	ARG
46	6B	148	LYS
46	6B	150	VAL
46	6B	155	PRO
46	6B	159	VAL
46	6B	160	LEU
46	6B	161	GLU
46	6B	169	ARG
46	6B	176	LEU
46	6B	181	TYR
46	6B	182	ARG
46	6B	185	LYS
46	6B	187	THR
46	6B	189	ASP
46	6B	196	GLN

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Mol	Chain	Res	Type
46	6B	200	THR
46	6B	201	SER
46	6B	203	ARG
46	6B	209	LEU
46	6B	213	HIS
46	6B	219	VAL
46	6B	222	ARG
46	6B	223	PHE
46	6B	224	LEU
46	6B	226	MET
46	6B	227	ARG
46	6B	232	LEU
46	6B	233	SER
46	6B	236	LYS
46	6B	238	LYS
46	6B	240	ARG
46	6B	244	ILE
46	6B	245	ARG
46	6B	252	LEU
46	6B	253	VAL
46	6B	254	HIS
46	6B	261	SER
46	6B	264	THR
46	6B	266	SER
46	6B	268	GLU
46	6B	272	PHE
46	6B	274	VAL
46	6B	278	VAL
46	6B	286	LYS
46	6B	287	ARG
46	6B	295	LEU
46	6B	301	LYS
46	6B	305	GLN
46	6B	307	PHE
46	6B	308	ASP
46	6B	309	VAL
46	6B	310	SER
46	6B	321	LEU
46	6B	324	ILE
46	6B	326	THR
46	6B	327	ILE
46	6B	329	GLN

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Mol	Chain	Res	Type
46	6B	335	ASP
46	6B	338	LYS
46	6B	344	VAL
46	6B	346	THR
46	6B	347	ILE
46	6B	356	ASP
46	6B	361	LYS
46	6B	363	LYS
46	6B	364	LEU
46	6B	369	LEU
46	6B	370	MET
46	6B	374	SER
46	6B	375	SER
46	6B	379	LEU
46	6B	381	GLU
46	6B	384	SER
46	6B	393	VAL
46	6B	394	GLN
46	6B	397	THR
46	6B	399	LEU
46	6B	400	GLN
46	6B	402	ILE
46	6B	403	ASP
46	6B	407	ASP
46	6B	409	ASP
46	6B	411	ILE
46	6B	416	LYS
46	6B	421	ARG
46	6B	422	LYS
46	6B	423	SER
46	6B	424	MET
46	6B	430	LEU
46	6B	432	HIS
46	6B	436	VAL
46	6B	437	ASP
47	6C	1	MET
47	6C	2	THR
47	6C	4	ILE
47	6C	6	LYS
47	6C	9	PRO
47	6C	11	MET
47	6C	12	LYS

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Mol	Chain	Res	Type
47	6C	15	ASN
47	6C	19	ILE
47	6C	25	SER
47	6C	26	ASN
47	6C	27	ILE
47	6C	43	LEU
47	6C	46	LEU
47	6C	53	MET
47	6C	56	THR
47	6C	57	SER
47	6C	58	ASP
47	6C	61	THR
47	6C	63	PHE
47	6C	64	SER
47	6C	65	SER
47	6C	68	HIS
47	6C	70	CYS
47	6C	72	ASP
47	6C	74	ASN
47	6C	79	ILE
47	6C	80	ARG
47	6C	83	HIS
47	6C	94	LEU
47	6C	96	ILE
47	6C	108	MET
47	6C	110	LEU
47	6C	111	GLU
47	6C	112	THR
47	6C	117	VAL
47	6C	120	LEU
47	6C	124	MET
47	6C	126	THR
47	6C	129	MET
47	6C	132	VAL
47	6C	133	LEU
47	6C	137	GLN
47	6C	156	ILE
47	6C	158	THR
47	6C	159	ASP
47	6C	160	LEU
47	6C	163	TRP
47	6C	170	VAL

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Mol	Chain	Res	Type
47	6C	171	ASP
47	6C	172	LYS
47	6C	174	THR
47	6C	175	LEU
47	6C	177	ARG
47	6C	178	PHE
47	6C	184	ILE
47	6C	186	PRO
47	6C	195	VAL
47	6C	197	LEU
47	6C	198	LEU
47	6C	203	THR
47	6C	205	SER
47	6C	209	THR
47	6C	214	ASP
47	6C	215	MET
47	6C	217	LYS
47	6C	218	ILE
47	6C	225	THR
47	6C	228	ASP
47	6C	229	ILE
47	6C	230	LEU
47	6C	233	LEU
47	6C	236	MET
47	6C	238	ILE
47	6C	242	LEU
47	6C	247	PRO
47	6C	250	LEU
47	6C	254	ASP
47	6C	256	TYR
47	6C	257	THR
47	6C	262	LEU
47	6C	263	ASN
47	6C	264	THR
47	6C	268	ILE
47	6C	269	LYS
47	6C	271	GLU
47	6C	273	TYR
47	6C	276	PHE
47	6C	281	LEU
47	6C	287	LYS
47	6C	288	LEU

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Mol	Chain	Res	Type
47	6C	292	LEU
47	6C	295	VAL
47	6C	298	ILE
47	6C	300	ILE
47	6C	302	ILE
47	6C	304	MET
47	6C	310	SER
47	6C	311	LYS
47	6C	315	MET
47	6C	316	MET
47	6C	317	PHE
47	6C	318	ARG
47	6C	320	LEU
47	6C	322	GLN
47	6C	324	LEU
47	6C	334	THR
47	6C	337	TRP
47	6C	343	VAL
47	6C	344	GLU
47	6C	352	GLN
47	6C	362	ILE
47	6C	366	MET
47	6C	368	ILE
47	6C	369	THR
47	6C	372	ILE
47	6C	374	ASN
47	6C	376	LEU
47	6C	377	LEU
47	6C	378	LYS
48	6D	98	TYR
48	6D	102	HIS
48	6D	103	ARG
48	6D	107	SER
48	6D	111	HIS
48	6D	112	THR
48	6D	115	ARG
48	6D	116	ARG
48	6D	123	GLN
48	6D	124	VAL
48	6D	128	CYS
48	6D	131	MET
48	6D	137	ARG

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Mol	Chain	Res	Type
48	6D	139	LEU
48	6D	142	VAL
48	6D	150	LYS
48	6D	152	LEU
48	6D	154	GLU
48	6D	155	GLU
48	6D	156	VAL
48	6D	157	GLU
48	6D	158	VAL
48	6D	164	GLU
48	6D	168	MET
48	6D	169	PHE
48	6D	170	MET
48	6D	171	ARG
48	6D	174	LYS
48	6D	177	ASP
48	6D	181	LYS
48	6D	184	PRO
48	6D	190	ARG
48	6D	197	LEU
48	6D	199	PRO
48	6D	204	ILE
48	6D	205	VAL
48	6D	208	ARG
48	6D	213	ASP
48	6D	216	PHE
48	6D	217	SER
48	6D	218	LEU
48	6D	219	LEU
48	6D	224	GLU
48	6D	231	LEU
48	6D	232	ARG
48	6D	235	LEU
48	6D	257	VAL
48	6D	258	LEU
48	6D	260	PHE
48	6D	262	ASP
48	6D	264	THR
48	6D	267	THR
48	6D	273	LYS
48	6D	281	TRP
48	6D	284	GLU

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Mol	Chain	Res	Type
48	6D	286	GLU
48	6D	288	ASP
48	6D	289	HIS
48	6D	291	LYS
48	6D	292	ARG
48	6D	293	MET
48	6D	295	LEU
48	6D	297	MET
48	6D	299	MET
48	6D	300	MET
48	6D	303	LEU
48	6D	304	LEU
48	6D	305	LEU
48	6D	306	PRO
48	6D	307	LEU
48	6D	311	MET
48	6D	313	ARG
48	6D	314	HIS
48	6D	315	LYS
48	6D	320	LYS
48	6D	323	LYS
48	6D	324	LEU
48	6D	327	ARG
48	6D	329	PRO
49	6E	180	THR
49	6E	217	CYS
52	6H	44	THR
52	6H	77	GLU
52	6H	78	ASP
49	6I	41	PRO
49	6I	65	VAL
49	6I	70	LEU
49	6I	72	VAL
49	6I	78	TYR
53	6J	5	THR
53	6J	6	LEU
53	6J	7	THR
53	6J	9	ARG
53	6J	11	TYR
53	6J	13	LEU
53	6J	14	LEU
53	6J	15	PHE

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Mol	Chain	Res	Type
53	6J	16	ARG
53	6J	17	ARG
53	6J	30	LEU
53	6J	36	PHE
53	6J	43	ILE
53	6J	45	GLU
53	6J	52	LEU
53	6J	54	LYS
53	6J	55	HIS
53	6J	56	ILE
53	6J	57	LYS
53	6J	58	HIS
53	6J	59	LYS
45	6N	224	VAL
45	6N	225	GLU
45	6N	226	ASP
45	6N	228	VAL
45	6N	234	CYS
45	6N	240	GLU
45	6N	241	ILE
45	6N	242	ARG
45	6N	243	HIS
45	6N	245	ASP
45	6N	250	LEU
45	6N	253	VAL
45	6N	262	TRP
45	6N	266	ASP
45	6N	270	LEU
45	6N	276	ILE
45	6N	281	ASP
45	6N	283	THR
45	6N	289	HIS
45	6N	290	MET
45	6N	291	SER
45	6N	292	SER
45	6N	294	LEU
45	6N	296	SER
45	6N	297	VAL
45	6N	301	ARG
45	6N	303	LEU
45	6N	307	PHE
45	6N	308	GLN

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Mol	Chain	Res	Type
45	6N	309	THR
45	6N	312	ILE
45	6N	313	CYS
45	6N	319	LEU
45	6N	325	VAL
45	6N	327	ASP
45	6N	329	MET
45	6N	330	SER
45	6N	331	ILE
45	6N	333	ASP
45	6N	343	MET
45	6N	345	LEU
45	6N	348	SER
45	6N	353	GLU
45	6N	354	VAL
45	6N	355	VAL
45	6N	356	ARG
45	6N	359	ASN
45	6N	360	ILE
45	6N	361	LEU
45	6N	368	HIS
45	6N	369	LEU
45	6N	370	ASP
45	6N	373	THR
45	6N	376	CYS
45	6N	381	ARG
45	6N	388	ARG
45	6N	390	ILE
45	6N	392	LEU
45	6N	405	SER
45	6N	406	VAL
45	6N	407	VAL
45	6N	408	ARG
45	6N	412	SER
45	6N	413	LYS
45	6N	415	PHE
45	6N	419	CYS
45	6N	422	VAL
45	6N	425	LEU
45	6N	428	ILE
45	6N	436	ARG
45	6N	438	ARG

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Mol	Chain	Res	Type
45	6N	439	SER
45	6N	442	PHE
45	6N	443	TRP
45	6N	444	LEU
45	6N	445	ARG
46	6O	22	GLN
46	6O	24	LEU
46	6O	27	THR
46	6O	33	LEU
46	6O	34	VAL
46	6O	37	SER
46	6O	45	SER
46	6O	49	LEU
46	6O	52	LYS
46	6O	55	SER
46	6O	56	ARG
46	6O	57	TYR
46	6O	58	GLU
46	6O	59	ASP
46	6O	61	ASN
46	6O	62	ASN
46	6O	63	LEU
46	6O	66	SER
46	6O	69	LEU
46	6O	70	ARG
46	6O	73	SER
46	6O	77	THR
46	6O	78	LYS
46	6O	81	SER
46	6O	82	SER
46	6O	84	LYS
46	6O	85	ILE
46	6O	87	ARG
46	6O	90	GLU
46	6O	92	VAL
46	6O	95	LYS
46	6O	100	SER
46	6O	101	THR
46	6O	103	GLU
46	6O	105	MET
46	6O	108	THR
46	6O	109	VAL

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Mol	Chain	Res	Type
46	6O	112	LEU
46	6O	113	ARG
46	6O	115	ASP
46	6O	116	ILE
46	6O	118	ILE
46	6O	119	LEU
46	6O	120	MET
46	6O	121	GLU
46	6O	123	LEU
46	6O	125	ASN
46	6O	131	GLU
46	6O	134	ARG
46	6O	140	LEU
46	6O	145	ARG
46	6O	147	ASP
46	6O	148	LYS
46	6O	150	VAL
46	6O	160	LEU
46	6O	162	ASN
46	6O	172	LEU
46	6O	180	ASP
46	6O	182	ARG
46	6O	185	LYS
46	6O	187	THR
46	6O	189	ASP
46	6O	193	TYR
46	6O	207	ILE
46	6O	212	SER
46	6O	213	HIS
46	6O	219	VAL
46	6O	221	GLU
46	6O	226	MET
46	6O	227	ARG
46	6O	230	LEU
46	6O	232	LEU
46	6O	236	LYS
46	6O	238	LYS
46	6O	240	ARG
46	6O	245	ARG
46	6O	253	VAL
46	6O	257	LEU
46	6O	258	VAL

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Mol	Chain	Res	Type
46	6O	261	SER
46	6O	268	GLU
46	6O	270	ASN
46	6O	273	SER
46	6O	276	GLN
46	6O	278	VAL
46	6O	284	HIS
46	6O	286	LYS
46	6O	292	THR
46	6O	301	LYS
46	6O	308	ASP
46	6O	309	VAL
46	6O	319	SER
46	6O	321	LEU
46	6O	324	ILE
46	6O	326	THR
46	6O	327	ILE
46	6O	328	SER
46	6O	329	GLN
46	6O	335	ASP
46	6O	338	LYS
46	6O	344	VAL
46	6O	347	ILE
46	6O	352	LEU
46	6O	353	SER
46	6O	363	LYS
46	6O	364	LEU
46	6O	370	MET
46	6O	373	GLU
46	6O	379	LEU
46	6O	385	GLN
46	6O	393	VAL
46	6O	394	GLN
46	6O	397	THR
46	6O	400	GLN
46	6O	403	ASP
46	6O	409	ASP
46	6O	411	ILE
46	6O	416	LYS
46	6O	421	ARG
46	6O	422	LYS
46	6O	423	SER

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Mol	Chain	Res	Type
46	6O	424	MET
46	6O	430	LEU
46	6O	432	HIS
46	6O	436	VAL
46	6O	437	ASP
47	6P	345	HIS
48	6Q	3	LEU
48	6Q	109	LEU
48	6Q	114	SER
49	6R	83	ILE
49	6R	150	SER
49	6R	180	THR
49	6R	218	THR
49	6R	219	HIS
49	6R	263	TYR
49	6R	265	PHE
49	6R	271	VAL
52	6U	20	VAL
52	6U	39	LEU
52	6U	45	SER
52	6U	48	SER
52	6U	50	THR
49	6V	71	ASN
49	6V	75	SER
54	6Y	2	LEU
54	6Y	4	ARG
54	6Y	6	LEU
54	6Y	9	ARG
54	6Y	11	ARG
54	6Y	18	ILE
54	6Y	20	THR
54	6Y	23	MET
54	6Y	32	LEU
54	6Y	33	VAL
54	6Y	38	TRP
54	6Y	39	ARG
54	6Y	41	ILE
54	6Y	42	LEU
54	6Y	44	TRP
54	6Y	49	ASN
54	6Y	51	LYS
54	6Y	52	PHE

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Mol	Chain	Res	Type
55	8A	3	VAL
55	8A	4	ASN
55	8A	5	ARG
55	8A	10	THR
55	8A	12	HIS
55	8A	13	LYS
55	8A	31	THR
55	8A	33	LEU
55	8A	35	LEU
55	8A	38	ARG
55	8A	41	LEU
55	8A	43	GLN
55	8A	47	LEU
55	8A	48	LEU
55	8A	52	GLN
55	8A	53	ILE
55	8A	58	VAL
55	8A	65	MET
55	8A	66	ILE
55	8A	73	ILE
55	8A	75	ILE
55	8A	81	TRP
55	8A	86	MET
55	8A	87	ILE
55	8A	92	MET
55	8A	96	ARG
55	8A	99	ASN
55	8A	104	LEU
55	8A	108	SER
55	8A	112	LEU
55	8A	116	SER
55	8A	117	MET
55	8A	136	LEU
55	8A	142	SER
55	8A	144	ASP
55	8A	147	ILE
55	8A	150	LEU
55	8A	152	LEU
55	8A	156	SER
55	8A	157	SER
55	8A	158	ILE
55	8A	167	THR

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Mol	Chain	Res	Type
55	8A	172	LYS
55	8A	176	MET
55	8A	178	GLN
55	8A	180	GLN
55	8A	183	LEU
55	8A	186	TRP
55	8A	191	THR
55	8A	194	LEU
55	8A	199	LEU
55	8A	202	LEU
55	8A	206	ILE
55	8A	207	THR
55	8A	209	LEU
55	8A	218	THR
55	8A	227	ASP
55	8A	234	LEU
55	8A	238	PHE
55	8A	240	HIS
55	8A	241	PRO
55	8A	242	GLU
55	8A	243	VAL
55	8A	245	ILE
55	8A	253	MET
55	8A	264	LYS
55	8A	265	LYS
55	8A	277	MET
55	8A	278	MET
55	8A	286	ILE
55	8A	287	VAL
55	8A	290	HIS
55	8A	292	MET
55	8A	293	PHE
55	8A	294	THR
55	8A	298	ASP
55	8A	299	VAL
55	8A	301	THR
55	8A	309	THR
55	8A	310	MET
55	8A	311	ILE
55	8A	316	THR
55	8A	319	LYS
55	8A	326	THR

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Mol	Chain	Res	Type
55	8A	363	LEU
55	8A	364	ASP
55	8A	366	VAL
55	8A	370	THR
55	8A	371	TYR
55	8A	377	PHE
55	8A	380	VAL
55	8A	381	LEU
55	8A	386	VAL
55	8A	390	MET
55	8A	403	TYR
55	8A	404	THR
55	8A	405	LEU
55	8A	407	GLN
55	8A	416	ILE
55	8A	417	MET
55	8A	421	VAL
55	8A	423	MET
55	8A	433	LEU
55	8A	434	SER
55	8A	438	ARG
55	8A	439	ARG
55	8A	440	TYR
55	8A	454	SER
55	8A	455	SER
55	8A	460	ILE
55	8A	462	LEU
55	8A	467	LEU
55	8A	468	MET
55	8A	469	ILE
55	8A	471	ILE
55	8A	476	PHE
55	8A	478	SER
55	8A	479	LYS
55	8A	480	ARG
55	8A	482	VAL
55	8A	483	SER
55	8A	485	VAL
55	8A	486	GLU
55	8A	487	LEU
55	8A	493	GLU
55	8A	495	LEU

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Mol	Chain	Res	Type
55	8A	496	HIS
55	8A	504	THR
56	8B	16	ILE
56	8B	27	THR
56	8B	33	LEU
56	8B	54	SER
56	8B	65	TRP
56	8B	95	LEU
56	8B	110	TYR
56	8B	138	VAL
56	8B	149	THR
56	8B	191	LEU
57	8C	29	SER
57	8C	44	SER
57	8C	129	VAL
57	8C	143	SER
57	8C	183	GLU
57	8C	192	VAL
57	8C	230	ASN
57	8C	245	VAL
58	8D	17	VAL
58	8D	27	VAL
58	8D	80	THR
59	8E	17	THR
59	8E	47	ILE
59	8E	80	GLU
59	8E	95	GLU
59	8E	109	VAL
60	8F	49	VAL
60	8F	67	SER
60	8F	76	LYS
60	8F	79	THR
60	8F	84	SER
60	8F	96	LEU
61	8G	15	THR
61	8G	25	LEU
61	8G	30	LEU
61	8G	44	ARG
61	8G	75	VAL
62	8H	6	THR
62	8H	26	THR
62	8H	50	VAL

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Mol	Chain	Res	Type
64	8J	1	LEU
64	8J	10	LYS
65	8K	20	SER
65	8K	26	VAL
66	8L	14	SER
67	8M	20	SER
68	8N	6	ILE
68	8N	14	SER
68	8N	33	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (378) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	80	GLN
1	1A	108	GLN
2	1B	162	GLN
2	1B	164	GLN
3	1C	19	HIS
3	1C	71	GLN
3	1C	160	HIS
4	1D	13	GLN
4	1D	150	HIS
4	1D	201	GLN
4	1D	348	HIS
5	1E	101	GLN
6	1F	250	ASN
6	1F	257	ASN
6	1F	356	HIS
6	1F	361	GLN
7	1G	110	GLN
7	1G	421	HIS
7	1G	646	ASN
8	1H	287	HIS
11	1K	7	ASN
11	1K	25	HIS
11	1K	52	HIS
11	1K	83	ASN
11	1K	92	ASN
11	1K	97	GLN
12	1L	30	ASN
12	1L	206	ASN
12	1L	309	GLN

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Mol	Chain	Res	Type
12	1L	447	ASN
12	1L	524	ASN
12	1L	605	HIS
13	1M	81	GLN
13	1M	144	ASN
13	1M	188	ASN
13	1M	220	HIS
13	1M	331	ASN
14	1N	120	GLN
14	1N	174	GLN
14	1N	268	GLN
15	1O	107	GLN
15	1O	141	GLN
15	1O	200	GLN
15	1O	204	ASN
15	1O	265	ASN
15	1O	288	GLN
16	1P	44	GLN
16	1P	87	HIS
16	1P	93	ASN
16	1P	103	ASN
19	1S	61	GLN
19	1S	85	GLN
20	1U	33	ASN
22	1W	58	GLN
22	1W	95	ASN
23	1X	94	GLN
26	1a	27	HIS
26	1a	46	ASN
29	1d	16	ASN
29	1d	46	ASN
29	1d	59	HIS
29	1d	61	GLN
29	1d	88	HIS
30	1e	96	HIS
31	1f	5	GLN
32	1g	57	ASN
33	1h	143	ASN
34	1i	25	GLN
34	1i	125	GLN
35	1j	6	HIS
36	1k	47	ASN

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Mol	Chain	Res	Type
36	1k	58	ASN
36	1k	91	ASN
37	1l	99	ASN
37	1l	136	ASN
39	1n	77	GLN
40	1o	49	GLN
41	1p	27	ASN
41	1p	53	GLN
42	1q	5	GLN
42	1q	112	ASN
43	1r	35	GLN
44	1s	43	HIS
44	1s	75	HIS
45	3A	32	GLN
45	3A	52	ASN
45	3A	87	ASN
45	3A	118	GLN
45	3A	159	GLN
45	3A	165	GLN
46	3B	153	GLN
46	3B	154	ASN
46	3B	247	GLN
46	3B	277	HIS
46	3B	304	HIS
46	3B	400	GLN
47	3C	3	ASN
47	3C	15	ASN
47	3C	85	ASN
47	3C	114	ASN
47	3C	206	ASN
47	3C	255	ASN
47	3C	263	ASN
47	3C	322	GLN
47	3C	341	GLN
48	3D	119	GLN
48	3D	238	ASN
48	3D	314	HIS
49	3E	219	HIS
49	3E	257	ASN
51	3G	8	HIS
51	3G	30	HIS
52	3H	67	GLN

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Mol	Chain	Res	Type
52	3H	92	HIS
52	3H	96	HIS
53	3J	55	HIS
45	3N	18	GLN
45	3N	29	GLN
45	3N	61	HIS
45	3N	69	ASN
45	3N	87	ASN
45	3N	118	GLN
45	3N	119	ASN
45	3N	154	HIS
45	3N	159	GLN
45	3N	173	ASN
45	3N	189	HIS
45	3N	215	HIS
45	3N	271	GLN
45	3N	308	GLN
45	3N	328	ASN
45	3N	363	ASN
46	3O	143	GLN
46	3O	196	GLN
46	3O	197	ASN
46	3O	248	ASN
46	3O	290	ASN
46	3O	329	GLN
46	3O	385	GLN
47	3P	85	ASN
47	3P	196	HIS
47	3P	267	HIS
47	3P	341	GLN
48	3Q	150	ASN
48	3Q	181	GLN
49	3R	219	HIS
49	3R	239	HIS
49	3R	257	ASN
50	3S	79	GLN
51	3T	6	HIS
51	3T	64	GLN
52	3U	67	HIS
49	3V	58	GLN
54	3X	16	ASN
55	4A	360	ASN

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Mol	Chain	Res	Type
55	4A	496	HIS
56	4B	52	HIS
56	4B	103	GLN
57	4C	12	ASN
57	4C	76	GLN
57	4C	122	HIS
57	4C	204	HIS
57	4C	243	HIS
59	4E	59	ASN
60	4F	94	HIS
61	4G	38	HIS
61	4G	71	HIS
61	4G	72	ASN
61	4G	84	GLN
62	4H	32	ASN
65	4K	35	GLN
68	4N	69	ASN
1	5A	26	GLN
1	5A	82	ASN
3	5C	19	HIS
3	5C	71	GLN
3	5C	160	HIS
4	5D	13	GLN
4	5D	150	HIS
4	5D	201	GLN
4	5D	348	HIS
5	5E	101	GLN
6	5F	150	GLN
6	5F	200	GLN
6	5F	250	ASN
6	5F	257	ASN
6	5F	356	HIS
6	5F	361	GLN
7	5G	110	GLN
7	5G	392	ASN
7	5G	421	HIS
7	5G	646	ASN
8	5H	287	HIS
11	5K	7	ASN
11	5K	52	HIS
11	5K	83	ASN
11	5K	92	ASN

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Mol	Chain	Res	Type
11	5K	97	GLN
12	5L	30	ASN
12	5L	206	ASN
12	5L	309	GLN
12	5L	447	ASN
12	5L	518	GLN
12	5L	524	ASN
12	5L	605	HIS
13	5M	81	GLN
13	5M	144	ASN
13	5M	188	ASN
13	5M	220	HIS
13	5M	331	ASN
14	5N	2	ASN
14	5N	120	GLN
14	5N	174	GLN
14	5N	268	GLN
15	5O	107	GLN
15	5O	114	HIS
15	5O	141	GLN
15	5O	200	GLN
15	5O	204	ASN
15	5O	265	ASN
15	5O	288	GLN
16	5P	44	GLN
16	5P	87	HIS
16	5P	93	ASN
16	5P	234	ASN
18	5R	93	GLN
19	5S	61	GLN
19	5S	85	GLN
22	5W	58	GLN
22	5W	95	ASN
23	5X	94	GLN
25	5Z	76	GLN
26	5a	27	HIS
26	5a	46	ASN
29	5d	16	ASN
29	5d	46	ASN
29	5d	59	HIS
29	5d	61	GLN
29	5d	88	HIS

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Mol	Chain	Res	Type
30	5e	96	HIS
31	5f	5	GLN
32	5g	57	ASN
33	5h	143	ASN
34	5i	25	GLN
34	5i	125	GLN
35	5j	6	HIS
35	5j	42	HIS
36	5k	47	ASN
36	5k	58	ASN
37	5l	99	ASN
37	5l	104	HIS
37	5l	136	ASN
39	5n	77	GLN
40	5o	49	GLN
41	5p	27	ASN
41	5p	53	GLN
41	5p	130	GLN
42	5q	5	GLN
42	5q	112	ASN
43	5r	35	GLN
44	5s	43	HIS
44	5s	75	HIS
45	6A	9	GLN
45	6A	15	GLN
45	6A	29	GLN
45	6A	49	ASN
45	6A	52	ASN
45	6A	53	ASN
45	6A	165	GLN
45	6A	188	GLN
45	6A	207	GLN
45	6A	267	ASN
45	6A	289	HIS
45	6A	339	GLN
46	6B	22	GLN
46	6B	40	ASN
46	6B	225	ASN
46	6B	247	GLN
46	6B	248	ASN
46	6B	349	GLN
46	6B	362	ASN

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Mol	Chain	Res	Type
46	6B	400	GLN
47	6C	3	ASN
47	6C	54	HIS
47	6C	85	ASN
47	6C	221	HIS
47	6C	263	ASN
47	6C	312	GLN
47	6C	341	GLN
47	6C	345	HIS
47	6C	352	GLN
47	6C	374	ASN
47	6C	375	ASN
48	6D	111	HIS
48	6D	129	HIS
48	6D	159	GLN
48	6D	163	ASN
48	6D	245	GLN
48	6D	270	GLN
49	6E	219	HIS
49	6E	257	ASN
52	6H	51	GLN
52	6H	67	GLN
45	6N	18	GLN
45	6N	52	ASN
45	6N	53	ASN
45	6N	61	HIS
45	6N	69	ASN
45	6N	87	ASN
45	6N	118	GLN
45	6N	159	GLN
45	6N	173	ASN
45	6N	252	HIS
45	6N	267	ASN
45	6N	271	GLN
45	6N	311	ASN
45	6N	323	HIS
45	6N	328	ASN
45	6N	341	GLN
45	6N	359	ASN
45	6N	363	ASN
45	6N	368	HIS
46	6O	22	GLN

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Mol	Chain	Res	Type
46	6O	62	ASN
46	6O	153	GLN
46	6O	158	GLN
46	6O	248	ASN
46	6O	290	ASN
46	6O	400	GLN
47	6P	85	ASN
47	6P	221	HIS
47	6P	267	HIS
47	6P	341	GLN
48	6Q	150	ASN
48	6Q	181	GLN
49	6R	219	HIS
49	6R	239	HIS
49	6R	257	ASN
50	6S	79	GLN
51	6T	6	HIS
51	6T	28	HIS
51	6T	64	GLN
52	6U	67	HIS
49	6V	58	GLN
54	6Y	16	ASN
55	8A	99	ASN
55	8A	163	ASN
55	8A	240	HIS
55	8A	406	ASN
55	8A	407	GLN
55	8A	491	ASN
55	8A	496	HIS
55	8A	512	ASN
56	8B	24	HIS
56	8B	52	HIS
56	8B	195	GLN
57	8C	12	ASN
57	8C	71	HIS
57	8C	76	GLN
57	8C	103	HIS
57	8C	122	HIS
57	8C	204	HIS
57	8C	243	HIS
59	8E	59	ASN
60	8F	94	HIS

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Mol	Chain	Res	Type
61	8G	38	HIS
61	8G	71	HIS
61	8G	72	ASN
61	8G	84	GLN
62	8H	22	ASN
62	8H	32	ASN
65	8K	35	GLN
65	8K	41	ASN
66	8L	43	GLN
68	8N	4	GLN
68	8N	8	GLN
68	8N	49	ASN
68	8N	69	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

14 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	5H	1	8	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
1	FME	1A	1	-	8,9,10	0.54	0	8,9,11	1.09	1 (12%)
56	FME	4B	1	56	8,9,10	0.54	0	8,9,11	1.02	1 (12%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
56	FME	8B	1	56	8,9,10	0.53	0	8,9,11	1.02	1 (12%)
1	FME	5A	1	1	8,9,10	0.59	0	8,9,11	1.00	1 (12%)
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
13	FME	5M	1	13	8,9,10	0.54	0	8,9,11	1.08	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	FME	5N	1	14	8,9,10	0.59	0	8,9,11	0.98	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	0.92	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	0.97	1 (12%)
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	1.07	1 (12%)
12	FME	5L	1	12	8,9,10	0.53	0	8,9,11	0.90	1 (12%)
11	FME	5K	1	11	8,9,10	0.55	0	8,9,11	0.98	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	5H	1	8	-	1/7/9/11	-
1	FME	1A	1	-	-	5/7/9/11	-
56	FME	4B	1	56	-	4/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
56	FME	8B	1	56	-	4/7/9/11	-
1	FME	5A	1	1	-	0/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
13	FME	5M	1	13	-	1/7/9/11	-
14	FME	5N	1	14	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
12	FME	5L	1	12	-	0/7/9/11	-
11	FME	5K	1	11	-	1/7/9/11	-

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1	FME	O-C-CA	-2.87	117.40	124.77
11	5K	1	FME	O-C-CA	-2.68	117.89	124.77
14	5N	1	FME	O-C-CA	-2.66	117.92	124.77
11	1K	1	FME	O-C-CA	-2.65	117.95	124.77
13	5M	1	FME	O-C-CA	-2.65	117.96	124.77
56	4B	1	FME	O-C-CA	-2.62	118.02	124.77
56	8B	1	FME	O-C-CA	-2.62	118.02	124.77
8	1H	1	FME	O-C-CA	-2.61	118.05	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	1N	1	FME	O-C-CA	-2.61	118.06	124.77
13	1M	1	FME	O-C-CA	-2.60	118.07	124.77
8	5H	1	FME	O-C-CA	-2.59	118.10	124.77
12	1L	1	FME	O-C-CA	-2.42	118.54	124.77
1	5A	1	FME	O-C-CA	-2.40	118.59	124.77
12	5L	1	FME	O-C-CA	-2.38	118.66	124.77

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	O1-CN-N-CA
1	1A	1	FME	C-CA-CB-CG
1	1A	1	FME	O-C-CA-CB
8	1H	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	C-CA-CB-CG
8	5H	1	FME	O1-CN-N-CA
56	8B	1	FME	O1-CN-N-CA
56	8B	1	FME	C-CA-CB-CG
1	1A	1	FME	N-CA-CB-CG
13	1M	1	FME	C-CA-CB-CG
13	5M	1	FME	C-CA-CB-CG
11	1K	1	FME	N-CA-CB-CG
11	5K	1	FME	N-CA-CB-CG
1	1A	1	FME	CB-CG-SD-CE
56	4B	1	FME	CB-CG-SD-CE
56	8B	1	FME	CB-CG-SD-CE
56	4B	1	FME	N-CA-CB-CG
56	8B	1	FME	N-CA-CB-CG

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	4B	1	FME	1	0
56	8B	1	FME	1	0
1	5A	1	FME	3	0
11	1K	1	FME	2	0
13	5M	1	FME	2	0
14	5N	1	FME	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1N	1	FME	3	0
13	1M	1	FME	2	0
11	5K	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 169 ligands modelled in this entry, 14 are monoatomic - leaving 155 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
82	PGV	4A	604	-	50,50,50	0.31	0	53,56,56	0.34	0
69	3PE	1J	202	-	43,43,50	0.29	0	46,48,55	0.39	0
70	SF4	1F	502	6	0,12,12	-	-	-		
72	FES	3E	301	49	0,4,4	-	-	-		
83	HEM	6C	502	47	42,50,50	1.36	6 (14%)	46,82,82	1.68	9 (19%)
91	PO4	8H	101	-	4,4,4	1.01	0	6,6,6	0.44	0
69	3PE	1L	703	-	44,44,50	0.29	0	47,49,55	0.42	0
82	PGV	8A	604	-	50,50,50	0.31	0	53,56,56	0.35	0
73	FMN	1F	501	-	33,33,33	0.61	0	48,50,50	0.66	1 (2%)
69	3PE	1M	501	-	44,44,50	0.30	0	47,49,55	0.37	0
69	3PE	1Y	205	-	26,26,50	0.35	0	29,31,55	0.43	0
71	PC1	1B	202	-	45,45,53	0.28	0	51,53,61	0.33	0
90	PEK	4C	307	-	51,51,52	0.27	0	54,56,57	0.39	0
72	FES	1G	803	7	0,4,4	-	-	-		
69	3PE	5A	201	-	46,46,50	0.28	0	49,51,55	0.36	0
82	PGV	4A	603	-	50,50,50	0.29	0	53,56,56	0.37	0
71	PC1	1J	201	-	34,34,53	0.33	0	40,42,61	0.35	0
80	EHZ	5n	201	-	31,36,37	0.18	0	36,44,47	1.14	1 (2%)
82	PGV	4C	301	-	50,50,50	0.30	0	53,56,56	0.72	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
85	HEA	4A	605	55	58,67,67	2.14	18 (31%)	63,103,103	2.51	26 (41%)
82	PGV	8K	101	-	50,50,50	0.30	0	53,56,56	0.32	0
78	NDP	1P	402	-	47,52,52	0.66	0	61,80,80	0.92	3 (4%)
71	PC1	5B	202	-	45,45,53	0.28	0	51,53,61	0.33	0
83	HEM	6C	501	47	42,50,50	1.41	7 (16%)	46,82,82	1.79	9 (19%)
83	HEM	6P	502	47	42,50,50	1.31	6 (14%)	46,82,82	1.77	11 (23%)
70	SF4	1G	802	7	0,12,12	-	-	-		
82	PGV	8C	304	-	50,50,50	0.29	0	53,56,56	0.33	0
90	PEK	4C	306	-	52,52,52	0.26	0	55,57,57	0.47	0
70	SF4	1B	201	2	0,12,12	-	-	-		
82	PGV	4C	305	-	50,50,50	0.31	0	53,56,56	0.38	0
71	PC1	5M	502	-	43,43,53	0.32	0	49,51,61	0.37	0
80	EHZ	1T	101	-	31,36,37	0.20	0	36,44,47	1.14	1 (2%)
75	CDL	8A	610	-	99,99,99	0.28	0	105,111,111	0.42	1 (0%)
91	PO4	4H	101	-	4,4,4	1.00	0	6,6,6	0.44	0
71	PC1	1Y	201	-	34,34,53	0.32	0	40,42,61	0.42	0
71	PC1	5A	202	-	34,34,53	0.33	0	40,42,61	0.39	0
69	3PE	5j	101	-	43,43,50	0.28	0	46,48,55	0.48	0
71	PC1	5I	204	-	43,43,53	0.29	0	49,51,61	0.33	0
69	3PE	5Y	202	-	39,39,50	0.29	0	42,44,55	0.39	0
71	PC1	5H	401	-	47,47,53	0.28	0	53,55,61	0.37	0
70	SF4	1I	203	9	0,12,12	-	-	-		
71	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.32	0
72	FES	3R	301	49	0,4,4	-	-	-		
81	AME	1h	201	-	9,10,11	0.52	0	9,11,13	1.08	1 (11%)
84	HEC	6Q	501	48	32,50,50	2.33	12 (37%)	30,82,82	2.29	6 (20%)
82	PGV	1p	201	-	50,50,50	0.29	0	53,56,56	0.33	0
71	PC1	1H	401	-	47,47,53	0.28	0	53,55,61	0.37	0
82	PGV	4C	304	-	50,50,50	0.30	0	53,56,56	0.61	1 (1%)
85	HEA	4A	606	55	58,67,67	2.19	17 (29%)	63,103,103	2.42	26 (41%)
69	3PE	5Y	204	-	32,32,50	0.33	0	35,37,55	0.45	0
71	PC1	5P	401	-	32,32,53	0.33	0	38,40,61	0.43	0
80	EHZ	1n	201	-	31,36,37	0.19	0	36,44,47	1.14	1 (2%)
72	FES	5E	301	5	0,4,4	-	-	-		
69	3PE	5Y	206	-	40,40,50	0.30	0	43,45,55	0.68	1 (2%)
84	HEC	3Q	501	48	32,50,50	2.33	12 (37%)	30,82,82	2.30	6 (20%)
70	SF4	5G	802	7	0,12,12	-	-	-		
75	CDL	5d	202	-	64,64,99	0.33	0	70,76,111	0.41	0
71	PC1	5m	201	-	45,45,53	0.30	0	51,53,61	1.06	3 (5%)
71	PC1	5Y	201	-	34,34,53	0.33	0	40,42,61	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.32	0
75	CDL	5L	702	-	75,75,99	0.30	0	81,87,111	0.39	0
82	PGV	4C	302	-	50,50,50	0.30	0	53,56,56	0.34	0
83	HEM	3P	501	47	42,50,50	1.28	6 (14%)	46,82,82	1.74	8 (17%)
82	PGV	8C	302	-	50,50,50	0.29	0	53,56,56	0.32	0
78	NDP	5P	402	-	47,52,52	0.66	0	61,80,80	0.92	3 (4%)
80	EHZ	5T	101	-	31,36,37	0.19	0	36,44,47	1.14	1 (2%)
69	3PE	5Y	205	-	26,26,50	0.36	0	29,31,55	0.43	0
71	PC1	1m	201	-	45,45,53	0.31	0	51,53,61	1.07	3 (5%)
75	CDL	8B	302	-	99,99,99	0.27	0	105,111,111	0.31	0
82	PGV	8C	303	-	50,50,50	0.31	0	53,56,56	0.33	0
75	CDL	4B	301	-	99,99,99	0.27	0	105,111,111	0.32	0
75	CDL	5X	201	-	85,85,99	0.28	0	91,97,111	0.39	0
69	3PE	5J	201	-	43,43,50	0.29	0	46,48,55	0.38	0
69	3PE	5d	201	-	47,47,50	0.29	0	50,52,55	0.42	0
88	CUA	4B	302	56	0,1,1	-	-	-		
71	PC1	1I	201	-	53,53,53	0.27	0	59,61,61	0.34	0
75	CDL	5q	201	-	60,60,99	0.34	0	66,72,111	0.41	0
69	3PE	1M	503	-	49,49,50	0.27	0	52,54,55	0.36	0
70	SF4	5F	502	6	0,12,12	-	-	-		
69	3PE	1j	101	-	43,43,50	0.28	0	46,48,55	0.48	0
72	FES	1E	301	5	0,4,4	-	-	-		
69	3PE	5Y	203	-	29,29,50	0.34	0	32,34,55	0.68	1 (3%)
75	CDL	1d	202	-	64,64,99	0.33	0	70,76,111	0.41	0
83	HEM	3P	502	47	42,50,50	1.30	6 (14%)	46,82,82	1.77	11 (23%)
69	3PE	1Y	206	-	40,40,50	0.30	0	43,45,55	0.68	1 (2%)
72	FES	6E	301	49	0,4,4	-	-	-		
73	FMN	5F	501	-	33,33,33	0.61	0	48,50,50	0.66	1 (2%)
70	SF4	5I	203	9	0,12,12	-	-	-		
70	SF4	5B	201	2	0,12,12	-	-	-		
82	PGV	8A	602	-	50,50,50	0.29	0	53,56,56	0.44	0
75	CDL	1i	201	-	79,79,99	0.30	0	85,91,111	0.44	0
84	HEC	3D	501	48	30,49,50	2.34	12 (40%)	28,80,82	2.25	5 (17%)
82	PGV	4L	101	-	50,50,50	0.31	0	53,56,56	0.40	0
69	3PE	5M	501	-	44,44,50	0.29	0	47,49,55	0.37	0
70	SF4	5G	801	7	0,12,12	-	-	-		
75	CDL	1L	702	-	75,75,99	0.30	0	81,87,111	0.39	0
75	CDL	5i	201	-	79,79,99	0.30	0	85,91,111	0.44	0
70	SF4	5I	202	9	0,12,12	-	-	-		
82	PGV	4C	303	-	50,50,50	0.31	0	53,56,56	0.42	0
82	PGV	8G	101	-	50,50,50	0.29	0	53,56,56	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	1Y	203	-	29,29,50	0.34	0	32,34,55	0.69	1 (3%)
69	3PE	1Y	202	-	39,39,50	0.29	0	42,44,55	0.39	0
71	PC1	1M	502	-	43,43,53	0.31	0	49,51,61	0.37	0
69	3PE	1L	704	-	30,30,50	0.34	0	33,35,55	0.68	1 (3%)
71	PC1	5I	201	-	53,53,53	0.27	0	59,61,61	0.35	0
82	PGV	8C	301	-	50,50,50	0.29	0	53,56,56	0.39	0
69	3PE	1Y	204	-	32,32,50	0.33	0	35,37,55	0.45	0
72	FES	6R	301	49	0,4,4	-	-	-		
71	PC1	1P	401	-	32,32,53	0.35	0	38,40,61	0.40	0
83	HEM	3C	501	47	42,50,50	1.33	7 (16%)	46,82,82	1.90	10 (21%)
69	3PE	5M	503	-	49,49,50	0.27	0	52,54,55	0.36	0
76	GTP	1O	401	77	29,34,34	1.01	2 (6%)	35,54,54	1.06	1 (2%)
83	HEM	6P	501	47	42,50,50	1.27	5 (11%)	46,82,82	1.74	9 (19%)
85	HEA	8A	606	55	58,67,67	2.19	18 (31%)	63,103,103	2.42	26 (41%)
69	3PE	1d	201	-	47,47,50	0.29	0	50,52,55	0.43	0
89	PSC	8A	611	-	51,51,51	0.29	0	57,59,59	0.44	0
69	3PE	1N	902	-	50,50,50	0.28	0	53,55,55	0.41	0
81	AME	5h	201	-	9,10,11	0.52	0	9,11,13	1.07	1 (11%)
75	CDL	5N	903	-	61,61,99	0.31	0	67,73,111	0.57	1 (1%)
69	3PE	5L	703	-	44,44,50	0.28	0	47,49,55	0.42	0
69	3PE	5L	704	-	30,30,50	0.34	0	33,35,55	0.69	1 (3%)
83	HEM	3C	502	47	42,50,50	1.32	5 (11%)	46,82,82	1.79	10 (21%)
82	PGV	8A	601	-	50,50,50	0.30	0	53,56,56	0.31	0
69	3PE	5N	902	-	50,50,50	0.28	0	53,55,55	0.41	0
72	FES	5G	803	7	0,4,4	-	-	-		
75	CDL	4C	308	-	99,99,99	0.28	0	105,111,111	0.42	1 (0%)
69	3PE	1L	701	-	45,45,50	0.30	0	48,50,55	0.42	0
82	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.44	1 (1%)
75	CDL	1q	201	-	60,60,99	0.34	0	66,72,111	0.41	0
82	PGV	8J	101	-	50,50,50	0.29	0	53,56,56	0.34	0
75	CDL	8D	201	-	99,99,99	0.28	0	105,111,111	0.33	0
82	PGV	4A	601	-	50,50,50	0.27	0	53,56,56	0.33	0
82	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.33	0
90	PEK	8C	306	-	52,52,52	0.26	0	55,57,57	0.47	0
82	PGV	8B	301	-	50,50,50	0.31	0	53,56,56	0.31	0
70	SF4	1G	801	7	0,12,12	-	-	-		
76	GTP	5O	401	77	29,34,34	1.02	2 (6%)	35,54,54	1.05	1 (2%)
71	PC1	1h	202	-	46,46,53	0.28	0	52,54,61	0.31	0
82	PGV	4J	101	-	50,50,50	0.32	0	53,56,56	0.38	0
82	PGV	8C	305	-	50,50,50	0.31	0	53,56,56	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
69	3PE	5L	701	-	45,45,50	0.29	0	48,50,55	0.42	0
90	PEK	8C	307	-	51,51,52	0.27	0	54,56,57	0.39	0
82	PGV	8L	101	-	50,50,50	0.31	0	53,56,56	0.40	0
70	SF4	1I	202	9	0,12,12	-	-	-		
85	HEA	8A	605	55	58,67,67	2.13	18 (31%)	63,103,103	2.52	26 (41%)
82	PGV	8A	603	-	50,50,50	0.33	0	53,56,56	0.36	0
75	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.39	0
84	HEC	6D	501	-	30,49,50	2.55	12 (40%)	28,80,82	2.04	3 (10%)
89	PSC	4B	303	-	51,51,51	0.30	0	57,59,59	0.43	0
88	CUA	8B	303	56	0,1,1	-	-	-		
82	PGV	4K	101	-	50,50,50	0.29	0	53,56,56	0.35	0
75	CDL	1N	903	-	61,61,99	0.31	0	67,73,111	0.57	1 (1%)
69	3PE	5N	901	-	48,48,50	0.32	0	51,53,55	0.39	0
69	3PE	1N	901	-	48,48,50	0.33	0	51,53,55	0.39	0
71	PC1	5h	202	-	46,46,53	0.27	0	52,54,61	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PGV	4A	604	-	-	10/55/55/55	-
69	3PE	1J	202	-	-	10/47/47/54	-
70	SF4	1F	502	6	-	-	0/6/5/5
72	FES	3E	301	49	-	-	0/1/1/1
83	HEM	6C	502	47	-	3/12/54/54	-
69	3PE	1L	703	-	-	9/48/48/54	-
82	PGV	8A	604	-	-	35/55/55/55	-
73	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
69	3PE	1M	501	-	-	7/48/48/54	-
69	3PE	1Y	205	-	-	5/30/30/54	-
71	PC1	1B	202	-	-	8/49/49/57	-
90	PEK	4C	307	-	-	6/55/55/56	-
72	FES	1G	803	7	-	-	0/1/1/1
69	3PE	5A	201	-	-	9/50/50/54	-
82	PGV	4A	603	-	-	7/55/55/55	-
71	PC1	1J	201	-	-	27/38/38/57	-
80	EHZ	5n	201	-	-	3/42/44/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PGV	4C	301	-	-	7/55/55/55	-
85	HEA	4A	605	55	-	9/32/76/76	-
82	PGV	8K	101	-	-	29/55/55/55	-
78	NDP	1P	402	-	-	3/30/77/77	0/5/5/5
71	PC1	5B	202	-	-	8/49/49/57	-
83	HEM	6C	501	47	-	6/12/54/54	-
83	HEM	6P	502	47	-	6/12/54/54	-
70	SF4	1G	802	7	-	-	0/6/5/5
82	PGV	8C	304	-	-	35/55/55/55	-
90	PEK	4C	306	-	-	10/56/56/56	-
70	SF4	1B	201	2	-	-	0/6/5/5
82	PGV	4C	305	-	-	5/55/55/55	-
71	PC1	5M	502	-	-	7/47/47/57	-
80	EHZ	1T	101	-	-	15/42/44/45	-
75	CDL	8A	610	-	-	28/110/110/110	-
71	PC1	1Y	201	-	-	8/38/38/57	-
71	PC1	5A	202	-	-	3/38/38/57	-
69	3PE	5j	101	-	-	5/47/47/54	-
71	PC1	5I	204	-	-	1/47/47/57	-
69	3PE	5Y	202	-	-	9/43/43/54	-
71	PC1	5H	401	-	-	11/51/51/57	-
70	SF4	1I	203	9	-	-	0/6/5/5
71	PC1	1I	204	-	-	1/47/47/57	-
72	FES	3R	301	49	-	-	0/1/1/1
81	AME	1h	201	-	-	2/9/10/12	-
84	HEC	6Q	501	48	-	3/10/54/54	-
82	PGV	1p	201	-	-	40/55/55/55	-
71	PC1	1H	401	-	-	11/51/51/57	-
82	PGV	4C	304	-	-	16/55/55/55	-
85	HEA	4A	606	55	-	5/32/76/76	-
69	3PE	5Y	204	-	-	3/36/36/54	-
71	PC1	5P	401	-	-	9/36/36/57	-
80	EHZ	1n	201	-	-	3/42/44/45	-
84	HEC	3Q	501	48	-	3/10/54/54	-
69	3PE	5Y	206	-	-	12/44/44/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	FES	5E	301	5	-	-	0/1/1/1
70	SF4	5G	802	7	-	-	0/6/5/5
75	CDL	5d	202	-	-	22/75/75/110	-
71	PC1	5m	201	-	-	12/49/49/57	-
71	PC1	5Y	201	-	-	8/38/38/57	-
69	3PE	1A	201	-	-	26/50/50/54	-
75	CDL	5L	702	-	-	9/86/86/110	-
82	PGV	4C	302	-	-	11/55/55/55	-
83	HEM	3P	501	47	-	6/12/54/54	-
82	PGV	8C	302	-	-	31/55/55/55	-
78	NDP	5P	402	-	-	3/30/77/77	0/5/5/5
80	EHZ	5T	101	-	-	15/42/44/45	-
69	3PE	5Y	205	-	-	5/30/30/54	-
71	PC1	1m	201	-	-	12/49/49/57	-
75	CDL	8B	302	-	-	21/110/110/110	-
82	PGV	8C	303	-	-	32/55/55/55	-
75	CDL	4B	301	-	-	21/110/110/110	-
75	CDL	5X	201	-	-	18/96/96/110	-
69	3PE	5J	201	-	-	10/47/47/54	-
69	3PE	5d	201	-	-	15/51/51/54	-
71	PC1	1I	201	-	-	10/57/57/57	-
75	CDL	5q	201	-	-	7/71/71/110	-
69	3PE	1M	503	-	-	5/53/53/54	-
70	SF4	5F	502	6	-	-	0/6/5/5
69	3PE	1j	101	-	-	5/47/47/54	-
72	FES	1E	301	5	-	-	0/1/1/1
69	3PE	5Y	203	-	-	14/33/33/54	-
75	CDL	1d	202	-	-	22/75/75/110	-
83	HEM	3P	502	47	-	6/12/54/54	-
69	3PE	1Y	206	-	-	12/44/44/54	-
72	FES	6E	301	49	-	-	0/1/1/1
73	FMN	5F	501	-	-	1/18/18/18	0/3/3/3
70	SF4	5I	203	9	-	-	0/6/5/5
70	SF4	5B	201	2	-	-	0/6/5/5
82	PGV	8A	602	-	-	30/55/55/55	-
75	CDL	1i	201	-	-	9/90/90/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
84	HEC	3D	501	48	-	3/9/53/54	-
82	PGV	4L	101	-	-	7/55/55/55	-
69	3PE	5M	501	-	-	7/48/48/54	-
70	SF4	5G	801	7	-	-	0/6/5/5
75	CDL	1L	702	-	-	9/86/86/110	-
75	CDL	5i	201	-	-	9/90/90/110	-
82	PGV	4C	303	-	-	16/55/55/55	-
82	PGV	8G	101	-	-	29/55/55/55	-
70	SF4	5I	202	9	-	-	0/6/5/5
69	3PE	1Y	203	-	-	14/33/33/54	-
69	3PE	1Y	202	-	-	9/43/43/54	-
71	PC1	1M	502	-	-	7/47/47/57	-
69	3PE	1L	704	-	-	7/34/34/54	-
71	PC1	5I	201	-	-	10/57/57/57	-
82	PGV	8C	301	-	-	34/55/55/55	-
69	3PE	1Y	204	-	-	3/36/36/54	-
72	FES	6R	301	49	-	-	0/1/1/1
71	PC1	1P	401	-	-	19/36/36/57	-
83	HEM	3C	501	47	-	5/12/54/54	-
69	3PE	5M	503	-	-	5/53/53/54	-
76	GTP	1O	401	77	-	4/18/38/38	0/3/3/3
83	HEM	6P	501	47	-	6/12/54/54	-
85	HEA	8A	606	55	-	5/32/76/76	-
69	3PE	1d	201	-	-	15/51/51/54	-
89	PSC	8A	611	-	-	13/55/55/55	-
69	3PE	1N	902	-	-	8/54/54/54	-
81	AME	5h	201	-	-	2/9/10/12	-
75	CDL	5N	903	-	-	8/71/71/110	-
69	3PE	5L	703	-	-	9/48/48/54	-
69	3PE	5L	704	-	-	7/34/34/54	-
83	HEM	3C	502	47	-	4/12/54/54	-
82	PGV	8A	601	-	-	32/55/55/55	-
69	3PE	5N	902	-	-	8/54/54/54	-
72	FES	5G	803	7	-	-	0/1/1/1
75	CDL	4C	308	-	-	27/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1L	701	-	-	5/49/49/54	-
82	PGV	4G	101	-	-	11/55/55/55	-
75	CDL	1q	201	-	-	7/71/71/110	-
82	PGV	8J	101	-	-	29/55/55/55	-
75	CDL	8D	201	-	-	66/110/110/110	-
82	PGV	4A	601	-	-	13/55/55/55	-
82	PGV	4A	602	-	-	2/55/55/55	-
90	PEK	8C	306	-	-	10/56/56/56	-
82	PGV	8B	301	-	-	40/55/55/55	-
82	PGV	8C	305	-	-	5/55/55/55	-
76	GTP	5O	401	77	-	4/18/38/38	0/3/3/3
71	PC1	1h	202	-	-	12/50/50/57	-
82	PGV	4J	101	-	-	11/55/55/55	-
90	PEK	8C	307	-	-	6/55/55/56	-
69	3PE	5L	701	-	-	5/49/49/54	-
70	SF4	1G	801	7	-	-	0/6/5/5
82	PGV	8L	101	-	-	7/55/55/55	-
85	HEA	8A	605	55	-	9/32/76/76	-
70	SF4	1I	202	9	-	-	0/6/5/5
82	PGV	8A	603	-	-	28/55/55/55	-
75	CDL	1X	201	-	-	18/96/96/110	-
84	HEC	6D	501	-	-	3/9/53/54	-
89	PSC	4B	303	-	-	13/55/55/55	-
82	PGV	4K	101	-	-	14/55/55/55	-
75	CDL	1N	903	-	-	8/71/71/110	-
69	3PE	5N	901	-	-	11/52/52/54	-
69	3PE	1N	901	-	-	11/52/52/54	-
71	PC1	5h	202	-	-	12/50/50/57	-

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	6D	501	HEC	C3C-C2C	7.19	1.48	1.40
84	6D	501	HEC	C2B-C3B	7.09	1.48	1.40
84	6Q	501	HEC	C3C-C2C	6.57	1.48	1.40
84	3Q	501	HEC	C3C-C2C	6.57	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	6Q	501	HEC	C2B-C3B	6.43	1.48	1.40
84	3Q	501	HEC	C2B-C3B	6.38	1.47	1.40
84	3D	501	HEC	C3C-C2C	6.38	1.47	1.40
84	3D	501	HEC	C2B-C3B	6.33	1.47	1.40
85	4A	606	HEA	C3B-C2B	5.48	1.47	1.34
85	8A	606	HEA	C3B-C2B	5.42	1.47	1.34
85	8A	606	HEA	CHD-C1D	5.36	1.47	1.34
85	4A	606	HEA	CHD-C1D	5.34	1.47	1.34
85	8A	606	HEA	C3A-C2A	5.27	1.47	1.40
85	8A	606	HEA	CHC-C4B	5.26	1.47	1.34
85	4A	605	HEA	C3B-C2B	5.25	1.46	1.34
85	8A	605	HEA	C3A-C2A	5.24	1.47	1.40
85	4A	606	HEA	CHC-C4B	5.23	1.47	1.34
85	8A	605	HEA	C3B-C2B	5.21	1.46	1.34
85	4A	606	HEA	C3A-C2A	5.21	1.47	1.40
85	8A	605	HEA	CHD-C1D	5.20	1.47	1.34
85	4A	605	HEA	CHD-C1D	5.19	1.47	1.34
85	4A	605	HEA	C3A-C2A	5.19	1.47	1.40
85	4A	605	HEA	CHC-C4B	5.02	1.46	1.34
85	8A	605	HEA	CHC-C4B	5.02	1.46	1.34
85	4A	606	HEA	C3C-C2C	4.96	1.47	1.40
85	4A	606	HEA	C3D-C2D	4.94	1.47	1.36
85	8A	606	HEA	C3D-C2D	4.93	1.47	1.36
85	8A	606	HEA	C3C-C2C	4.89	1.47	1.40
85	4A	606	HEA	C3A-C4A	4.89	1.48	1.41
85	8A	606	HEA	C3A-C4A	4.77	1.48	1.41
85	4A	605	HEA	C3C-C2C	4.76	1.46	1.40
85	8A	605	HEA	C3C-C2C	4.69	1.46	1.40
85	8A	605	HEA	C3A-C4A	4.68	1.48	1.41
85	4A	605	HEA	C3A-C4A	4.67	1.48	1.41
85	4A	605	HEA	C3D-C2D	4.56	1.46	1.36
85	8A	605	HEA	C3D-C2D	4.56	1.46	1.36
83	6C	501	HEM	C1B-NB	-3.91	1.33	1.40
83	6C	502	HEM	C1B-NB	-3.77	1.33	1.40
83	6C	501	HEM	C4D-ND	-3.75	1.33	1.40
83	3C	502	HEM	C1B-NB	-3.60	1.34	1.40
83	6C	502	HEM	C4D-ND	-3.60	1.34	1.40
84	6D	501	HEC	C2A-C3A	3.50	1.48	1.37
84	6D	501	HEC	C3D-C2D	3.50	1.48	1.37
83	6P	502	HEM	C1B-NB	-3.45	1.34	1.40
83	3C	501	HEM	C1B-NB	-3.39	1.34	1.40
83	3P	502	HEM	C1B-NB	-3.38	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	3C	501	HEM	C4D-ND	-3.36	1.34	1.40
83	6P	502	HEM	C4D-ND	-3.31	1.34	1.40
84	3D	501	HEC	C3D-C2D	3.31	1.47	1.37
84	3Q	501	HEC	C3D-C2D	3.31	1.47	1.37
84	6Q	501	HEC	C3D-C2D	3.29	1.47	1.37
83	3P	502	HEM	C4D-ND	-3.27	1.34	1.40
84	3D	501	HEC	C2A-C3A	3.25	1.47	1.37
84	3Q	501	HEC	C2A-C3A	3.25	1.47	1.37
83	3C	502	HEM	C4D-ND	-3.22	1.34	1.40
84	6Q	501	HEC	C2A-C3A	3.22	1.47	1.37
83	3P	501	HEM	C4D-ND	-3.19	1.34	1.40
83	6P	501	HEM	C1B-NB	-3.17	1.34	1.40
83	3P	501	HEM	C1B-NB	-3.15	1.34	1.40
83	6P	501	HEM	C4D-ND	-3.14	1.34	1.40
84	3Q	501	HEC	C3C-C4C	3.14	1.48	1.43
84	6Q	501	HEC	C3C-C4C	3.14	1.48	1.43
84	6D	501	HEC	C4B-C3B	3.09	1.48	1.43
84	3D	501	HEC	C3C-C4C	3.04	1.48	1.43
84	3Q	501	HEC	C4B-C3B	2.97	1.48	1.43
84	6Q	501	HEC	C4B-C3B	2.91	1.48	1.43
83	6C	501	HEM	C1D-ND	-2.88	1.33	1.38
84	3D	501	HEC	C4B-C3B	2.86	1.48	1.43
84	3Q	501	HEC	C2A-C1A	2.80	1.48	1.42
85	4A	606	HEA	C4B-C3B	2.80	1.49	1.44
85	8A	606	HEA	C4B-C3B	2.78	1.49	1.44
84	6D	501	HEC	C2A-C1A	2.78	1.48	1.42
85	8A	605	HEA	C1D-ND	-2.77	1.35	1.40
84	6Q	501	HEC	C2A-C1A	2.76	1.48	1.42
84	3D	501	HEC	C2A-C1A	2.75	1.48	1.42
85	4A	605	HEA	C1D-ND	-2.74	1.35	1.40
76	5O	401	GTP	C5-C6	-2.74	1.42	1.47
84	6Q	501	HEC	C3A-C4A	2.74	1.48	1.42
84	6D	501	HEC	C3A-C4A	2.72	1.48	1.42
84	3Q	501	HEC	C3A-C4A	2.71	1.48	1.42
84	6D	501	HEC	C1D-CHD	2.69	1.48	1.41
84	6D	501	HEC	C1C-CHC	2.69	1.48	1.41
84	6D	501	HEC	C3C-C4C	2.68	1.47	1.43
84	6D	501	HEC	C4D-CHA	2.66	1.48	1.41
85	8A	605	HEA	C4B-C3B	2.66	1.49	1.44
85	8A	606	HEA	C1D-ND	-2.66	1.35	1.40
76	1O	401	GTP	C5-C6	-2.65	1.42	1.47
84	3D	501	HEC	C3A-C4A	2.64	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	4A	605	HEA	C4B-NB	-2.63	1.35	1.40
85	4A	606	HEA	C1D-ND	-2.61	1.35	1.40
84	6D	501	HEC	C1B-CHB	2.61	1.48	1.41
85	8A	605	HEA	C4B-NB	-2.60	1.35	1.40
85	4A	605	HEA	C4B-C3B	2.60	1.49	1.44
84	6Q	501	HEC	C1D-CHD	2.58	1.48	1.41
84	3Q	501	HEC	C1D-CHD	2.57	1.48	1.41
85	8A	605	HEA	C2A-C1A	2.57	1.48	1.42
85	4A	605	HEA	FE-NB	2.56	2.12	1.98
85	8A	605	HEA	FE-ND	2.55	2.12	1.98
85	4A	606	HEA	FE-NB	2.54	2.12	1.98
85	4A	605	HEA	FE-ND	2.53	2.12	1.98
85	8A	606	HEA	FE-NB	2.53	2.12	1.98
85	8A	606	HEA	C2A-C1A	2.53	1.48	1.42
84	3D	501	HEC	C4D-CHA	2.52	1.48	1.41
85	8A	605	HEA	FE-NB	2.52	2.12	1.98
85	8A	606	HEA	FE-ND	2.52	2.12	1.98
85	4A	605	HEA	C2A-C1A	2.52	1.48	1.42
84	3D	501	HEC	C1D-CHD	2.51	1.48	1.41
85	4A	606	HEA	FE-ND	2.49	2.11	1.98
85	4A	606	HEA	C2A-C1A	2.49	1.48	1.42
85	8A	606	HEA	C4B-NB	-2.48	1.35	1.40
84	6Q	501	HEC	C4D-CHA	2.48	1.47	1.41
83	6C	501	HEM	C4B-NB	-2.46	1.34	1.38
84	3Q	501	HEC	C4D-CHA	2.46	1.47	1.41
85	4A	606	HEA	C4B-NB	-2.45	1.36	1.40
83	6P	501	HEM	FE-NB	2.45	2.11	1.98
85	4A	606	HEA	C1D-C2D	2.44	1.49	1.44
83	3P	501	HEM	FE-NB	2.44	2.11	1.98
83	3C	501	HEM	C1D-ND	-2.42	1.34	1.38
83	6C	501	HEM	CHB-C1B	2.42	1.40	1.34
84	6Q	501	HEC	C1C-CHC	2.40	1.47	1.41
85	4A	606	HEA	C4C-CHD	2.39	1.47	1.41
83	3P	501	HEM	CHB-C1B	2.38	1.40	1.34
84	6Q	501	HEC	C1B-CHB	2.37	1.47	1.41
85	8A	606	HEA	C1D-C2D	2.37	1.49	1.44
85	8A	606	HEA	C4C-CHD	2.36	1.47	1.41
83	3C	501	HEM	CHB-C1B	2.36	1.40	1.34
84	3D	501	HEC	C1B-CHB	2.35	1.47	1.41
83	6P	501	HEM	CHB-C1B	2.34	1.40	1.34
84	3Q	501	HEC	C1C-CHC	2.34	1.47	1.41
83	6P	502	HEM	FE-NB	2.31	2.10	1.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
84	3Q	501	HEC	C1B-CHB	2.31	1.47	1.41
83	3P	502	HEM	FE-NB	2.30	2.10	1.98
83	6C	502	HEM	C1D-ND	-2.30	1.34	1.38
84	3D	501	HEC	C1C-CHC	2.29	1.47	1.41
85	4A	605	HEA	C4C-CHD	2.29	1.47	1.41
85	4A	606	HEA	C1C-CHC	2.28	1.47	1.41
83	6P	502	HEM	CHB-C1B	2.28	1.40	1.34
85	8A	606	HEA	C1C-CHC	2.26	1.47	1.41
83	6C	501	HEM	FE-ND	-2.25	1.85	1.98
85	8A	605	HEA	C4C-CHD	2.25	1.47	1.41
83	3C	502	HEM	FE-NB	2.24	2.10	1.98
83	3C	501	HEM	FE-NB	2.23	2.10	1.98
83	3C	502	HEM	C4B-NB	-2.21	1.34	1.38
85	8A	605	HEA	C1C-CHC	2.21	1.47	1.41
83	6C	502	HEM	FE-NB	2.21	2.10	1.98
85	8A	605	HEA	C4D-C3D	2.21	1.48	1.45
83	3P	502	HEM	CHB-C1B	2.20	1.40	1.34
83	3C	502	HEM	C1D-ND	-2.20	1.34	1.38
85	4A	605	HEA	C1C-CHC	2.19	1.47	1.41
85	4A	605	HEA	C4D-C3D	2.18	1.48	1.45
83	6P	502	HEM	C1D-ND	-2.17	1.34	1.38
83	6C	502	HEM	C4B-NB	-2.16	1.34	1.38
83	6P	502	HEM	C4B-NB	-2.15	1.34	1.38
76	1O	401	GTP	C8-N7	-2.14	1.31	1.34
76	5O	401	GTP	C8-N7	-2.14	1.31	1.34
85	4A	605	HEA	C1D-C2D	2.13	1.48	1.44
85	8A	605	HEA	CHA-C4D	2.13	1.46	1.40
83	6C	502	HEM	FE-ND	-2.12	1.86	1.98
83	3P	502	HEM	C1D-ND	-2.12	1.34	1.38
83	3P	502	HEM	C4B-NB	-2.10	1.34	1.38
85	8A	605	HEA	C1D-C2D	2.10	1.48	1.44
83	3C	501	HEM	C4B-NB	-2.09	1.34	1.38
85	4A	605	HEA	CHA-C4D	2.09	1.46	1.40
83	3C	501	HEM	FE-ND	-2.08	1.86	1.98
85	8A	606	HEA	C1B-C2B	2.07	1.48	1.44
85	4A	606	HEA	C1B-C2B	2.06	1.48	1.44
85	8A	606	HEA	CHB-C1B	2.05	1.46	1.40
83	3P	501	HEM	C1D-ND	-2.04	1.34	1.38
83	6C	501	HEM	FE-NB	2.02	2.09	1.98
83	6P	501	HEM	C1D-ND	-2.01	1.34	1.38
83	3P	501	HEM	C4B-NB	-2.00	1.34	1.38

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	4A	606	HEA	C3D-C4D-ND	6.93	117.05	110.35
85	8A	606	HEA	C3D-C4D-ND	6.90	117.02	110.35
85	8A	605	HEA	C3D-C4D-ND	6.45	116.58	110.35
80	5n	201	EHZ	C10-S1-C9	6.37	120.68	101.84
80	1n	201	EHZ	C10-S1-C9	6.37	120.67	101.84
84	3Q	501	HEC	C1D-C2D-C3D	-6.36	102.57	107.00
85	4A	605	HEA	C3D-C4D-ND	6.35	116.49	110.35
84	6Q	501	HEC	C1D-C2D-C3D	-6.26	102.64	107.00
84	3D	501	HEC	C1D-C2D-C3D	-6.23	102.67	107.00
80	1T	101	EHZ	C10-S1-C9	6.02	119.63	101.84
80	5T	101	EHZ	C10-S1-C9	6.00	119.59	101.84
85	8A	605	HEA	C2B-C1B-NB	5.89	116.71	109.90
85	4A	605	HEA	C2B-C1B-NB	5.79	116.60	109.90
85	8A	606	HEA	C2B-C1B-NB	5.73	116.53	109.90
71	1m	201	PC1	O21-C21-C22	5.72	123.86	111.48
85	4A	606	HEA	C2B-C1B-NB	5.71	116.51	109.90
71	5m	201	PC1	O21-C21-C22	5.68	123.76	111.48
85	4A	606	HEA	C3B-C4B-NB	5.63	116.32	109.84
85	8A	606	HEA	C3B-C4B-NB	5.63	116.31	109.84
85	4A	605	HEA	C3B-C4B-NB	5.59	116.27	109.84
85	8A	605	HEA	C3B-C4B-NB	5.58	116.25	109.84
84	6D	501	HEC	CMC-C2C-C3C	5.56	132.36	125.82
84	6D	501	HEC	CMB-C2B-C3B	5.55	132.34	125.82
84	6Q	501	HEC	CMC-C2C-C3C	5.44	132.22	125.82
84	3D	501	HEC	CMC-C2C-C3C	5.43	132.21	125.82
84	3Q	501	HEC	CMC-C2C-C3C	5.41	132.18	125.82
85	4A	605	HEA	C2D-C1D-ND	5.39	116.03	109.84
85	8A	605	HEA	C2D-C1D-ND	5.39	116.03	109.84
85	8A	605	HEA	CBA-CAA-C2A	-5.35	103.73	112.55
85	8A	606	HEA	C2D-C1D-ND	5.32	115.95	109.84
85	4A	605	HEA	CBA-CAA-C2A	-5.31	103.80	112.55
85	4A	606	HEA	C2D-C1D-ND	5.30	115.93	109.84
84	3D	501	HEC	CMB-C2B-C3B	5.18	131.92	125.82
83	6C	501	HEM	C1B-NB-C4B	5.17	111.33	105.21
84	6Q	501	HEC	CMB-C2B-C3B	5.15	131.88	125.82
84	3Q	501	HEC	CMB-C2B-C3B	5.14	131.86	125.82
83	3C	501	HEM	CHC-C4B-NB	5.11	129.94	124.44
83	3C	501	HEM	CHD-C1D-ND	5.05	129.87	124.44
83	3C	502	HEM	CHC-C4B-NB	5.03	129.84	124.44
83	6P	501	HEM	CHC-C4B-NB	5.00	129.82	124.44
84	6D	501	HEC	C1D-C2D-C3D	-4.99	103.52	107.00
83	3P	501	HEM	CHC-C4B-NB	4.95	129.76	124.44
83	3P	502	HEM	CHC-C4B-NB	4.80	129.60	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	6P	502	HEM	CHC-C4B-NB	4.79	129.59	124.44
85	8A	606	HEA	CBA-CAA-C2A	-4.59	104.99	112.55
85	4A	606	HEA	CBA-CAA-C2A	-4.58	105.01	112.55
78	5P	402	NDP	P2B-O2B-C2B	-4.52	111.37	123.43
78	1P	402	NDP	P2B-O2B-C2B	-4.48	111.46	123.43
76	1O	401	GTP	C4'-O4'-C1'	-4.48	105.82	109.92
83	6C	501	HEM	C3B-C4B-NB	-4.46	106.27	109.47
76	5O	401	GTP	C4'-O4'-C1'	-4.43	105.87	109.92
85	4A	606	HEA	C1D-C2D-C3D	-4.39	102.36	106.98
85	8A	606	HEA	C1D-C2D-C3D	-4.32	102.44	106.98
83	3C	502	HEM	CHD-C1D-ND	4.22	128.97	124.44
83	3P	501	HEM	CHD-C1D-ND	4.22	128.97	124.44
83	6P	501	HEM	CHD-C1D-ND	4.22	128.97	124.44
83	6C	502	HEM	CHC-C4B-NB	4.16	128.91	124.44
83	3P	502	HEM	CHD-C1D-ND	4.11	128.85	124.44
83	6P	502	HEM	CHD-C1D-ND	4.07	128.82	124.44
83	6C	501	HEM	CHC-C4B-NB	4.05	128.80	124.44
85	4A	605	HEA	C1D-C2D-C3D	-3.95	102.83	106.98
85	4A	605	HEA	C3C-C4C-NC	3.90	114.25	109.21
85	8A	605	HEA	C1D-C2D-C3D	-3.88	102.90	106.98
83	3C	501	HEM	C1B-NB-C4B	3.87	109.79	105.21
85	8A	605	HEA	C3C-C4C-NC	3.81	114.13	109.21
85	8A	605	HEA	C13-C14-C15	-3.80	118.92	127.62
85	4A	606	HEA	C3C-C4C-NC	3.79	114.11	109.21
85	8A	606	HEA	C3C-C4C-NC	3.78	114.10	109.21
85	4A	605	HEA	C13-C14-C15	-3.77	119.00	127.62
83	6P	502	HEM	C1B-NB-C4B	3.65	109.52	105.21
83	3P	502	HEM	C1B-NB-C4B	3.63	109.51	105.21
83	3P	502	HEM	CHA-C4D-ND	3.61	128.84	124.37
83	6P	502	HEM	CHA-C4D-ND	3.59	128.82	124.37
83	6C	502	HEM	C1B-NB-C4B	3.58	109.44	105.21
82	4C	301	PGV	O01-C1-C2	3.56	119.19	111.48
83	6C	502	HEM	CHD-C1D-ND	3.54	128.25	124.44
85	8A	605	HEA	C13-C12-C11	-3.51	108.78	114.39
83	3C	502	HEM	CHA-C4D-ND	3.50	128.71	124.37
85	8A	606	HEA	C1B-C2B-C3B	-3.48	102.77	106.80
85	4A	605	HEA	C13-C12-C11	-3.48	108.83	114.39
85	4A	606	HEA	C1B-C2B-C3B	-3.45	102.81	106.80
85	8A	605	HEA	C1B-C2B-C3B	-3.44	102.81	106.80
83	3C	502	HEM	CHB-C1B-NB	3.44	128.63	124.37
85	4A	605	HEA	C1B-C2B-C3B	-3.43	102.82	106.80
83	3C	501	HEM	CHB-C1B-NB	3.43	128.62	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	3C	501	HEM	C3B-C4B-NB	-3.39	107.04	109.47
85	8A	605	HEA	CAD-C3D-C4D	3.38	130.60	124.70
84	3Q	501	HEC	CBD-CAD-C3D	-3.38	106.85	112.54
84	6Q	501	HEC	CBD-CAD-C3D	-3.37	106.88	112.54
83	3P	502	HEM	CHB-C1B-NB	3.36	128.54	124.37
85	4A	605	HEA	CHA-C4D-ND	-3.36	120.82	124.44
83	6P	502	HEM	CHB-C1B-NB	3.35	128.52	124.37
85	8A	605	HEA	CHA-C4D-ND	-3.35	120.84	124.44
85	4A	605	HEA	CAD-C3D-C4D	3.33	130.50	124.70
85	8A	605	HEA	C4D-C3D-C2D	-3.29	102.11	106.89
83	3C	501	HEM	CHA-C4D-ND	3.27	128.42	124.37
83	6C	502	HEM	CHA-C4D-ND	3.26	128.41	124.37
83	6C	501	HEM	CHD-C1D-ND	3.25	127.94	124.44
83	3P	501	HEM	CHA-C4D-ND	3.24	128.39	124.37
83	6P	501	HEM	CHA-C4D-ND	3.24	128.39	124.37
85	4A	606	HEA	C4B-C3B-C2B	-3.23	102.01	107.44
85	8A	605	HEA	CMC-C2C-C3C	3.22	131.11	124.68
85	4A	605	HEA	CMC-C2C-C3C	3.21	131.09	124.68
85	8A	605	HEA	C4B-C3B-C2B	-3.20	102.06	107.44
85	4A	605	HEA	C4D-C3D-C2D	-3.20	102.23	106.89
85	4A	605	HEA	C4B-C3B-C2B	-3.20	102.06	107.44
85	8A	606	HEA	C4D-C3D-C2D	-3.19	102.25	106.89
85	8A	606	HEA	C4B-C3B-C2B	-3.19	102.08	107.44
69	1Y	206	3PE	O21-C21-C22	3.17	118.34	111.48
75	5N	903	CDL	OB6-CB5-C51	3.16	116.73	111.09
69	5Y	206	3PE	O21-C21-C22	3.15	118.31	111.48
83	3C	501	HEM	CHD-C1D-C2D	-3.15	120.05	125.03
83	3P	501	HEM	C1B-NB-C4B	3.15	108.94	105.21
83	3C	502	HEM	C1B-NB-C4B	3.13	108.92	105.21
85	4A	606	HEA	C4D-C3D-C2D	-3.13	102.34	106.89
75	1N	903	CDL	OB6-CB5-C51	3.13	116.66	111.09
83	3P	501	HEM	CHB-C1B-NB	3.12	128.24	124.37
83	6P	501	HEM	CBA-CAA-C2A	-3.11	107.31	112.54
83	6P	501	HEM	C1B-NB-C4B	3.11	108.89	105.21
83	3P	501	HEM	CBA-CAA-C2A	-3.10	107.33	112.54
83	6C	502	HEM	C3B-C4B-NB	-3.08	107.25	109.47
84	3Q	501	HEC	CAA-CBA-CGA	-3.07	105.55	113.83
84	6Q	501	HEC	CAA-CBA-CGA	-3.07	105.56	113.83
85	8A	606	HEA	CMC-C2C-C3C	3.05	130.78	124.68
83	6P	501	HEM	CHB-C1B-NB	3.04	128.14	124.37
85	4A	606	HEA	CMC-C2C-C3C	3.03	130.74	124.68
81	1h	201	AME	O-C-CA	-3.01	117.03	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	5h	201	AME	O-C-CA	-3.01	117.04	124.77
85	8A	606	HEA	CHA-C4D-C3D	-2.96	120.45	124.77
83	6P	502	HEM	C3B-C4B-NB	-2.95	107.35	109.47
84	3D	501	HEC	CAA-CBA-CGA	-2.95	105.90	113.83
83	6C	501	HEM	C4D-ND-C1D	2.92	108.67	105.21
83	6C	502	HEM	C4D-ND-C1D	2.91	108.66	105.21
85	4A	606	HEA	CHA-C4D-C3D	-2.91	120.54	124.77
83	3P	502	HEM	C3B-C4B-NB	-2.89	107.39	109.47
82	4C	304	PGV	O01-C1-C2	2.86	117.67	111.48
85	8A	605	HEA	C17-C18-C19	-2.82	121.16	127.62
85	4A	605	HEA	C17-C18-C19	-2.82	121.17	127.62
85	4A	605	HEA	C27-C19-C20	2.79	120.07	115.23
78	5P	402	NDP	O4D-C1D-C2D	-2.78	100.66	106.62
78	1P	402	NDP	O4D-C1D-C2D	-2.77	100.69	106.62
85	8A	606	HEA	C27-C19-C20	2.77	120.03	115.23
85	4A	606	HEA	C27-C19-C20	2.76	120.01	115.23
85	8A	605	HEA	C27-C19-C20	2.76	120.01	115.23
69	1Y	203	3PE	O21-C21-C22	2.75	117.44	111.48
83	6C	502	HEM	CBD-CAD-C3D	-2.75	104.94	112.53
85	4A	605	HEA	C26-C15-C16	2.72	119.96	115.23
85	8A	605	HEA	C26-C15-C16	2.72	119.94	115.23
85	8A	606	HEA	C26-C15-C16	2.71	119.93	115.23
71	5m	201	PC1	O21-C21-O22	-2.71	117.37	123.70
69	5Y	203	3PE	O21-C21-C22	2.71	117.33	111.48
71	1m	201	PC1	O21-C21-O22	-2.71	117.38	123.70
85	4A	605	HEA	CMD-C2D-C1D	2.70	129.25	125.03
85	4A	606	HEA	C26-C15-C16	2.68	119.87	115.23
83	3P	501	HEM	CHD-C1D-C2D	-2.67	120.81	125.03
69	5L	704	3PE	O21-C21-C22	2.66	117.23	111.48
83	6P	501	HEM	CHD-C1D-C2D	-2.65	120.84	125.03
85	8A	605	HEA	CMD-C2D-C1D	2.64	129.16	125.03
85	4A	606	HEA	CMD-C2D-C1D	2.61	129.10	125.03
69	1L	704	3PE	O21-C21-C22	2.60	117.10	111.48
85	4A	606	HEA	C13-C14-C15	-2.58	121.71	127.62
83	6C	501	HEM	CAD-CBD-CGD	-2.58	106.82	113.67
85	8A	606	HEA	CMD-C2D-C1D	2.58	129.07	125.03
85	8A	605	HEA	C4B-NB-C1B	-2.57	102.17	105.21
85	8A	606	HEA	C13-C14-C15	-2.55	121.78	127.62
85	8A	605	HEA	CHB-C1B-NB	-2.53	121.71	124.44
83	3C	502	HEM	CHD-C1D-C2D	-2.50	121.07	125.03
85	4A	605	HEA	C4B-NB-C1B	-2.50	102.25	105.21
85	4A	605	HEA	CHB-C1B-NB	-2.45	121.80	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	3C	502	HEM	C3B-C4B-NB	-2.44	107.71	109.47
85	8A	606	HEA	C4B-NB-C1B	-2.44	102.32	105.21
85	4A	606	HEA	C17-C18-C19	-2.44	122.04	127.62
85	4A	606	HEA	C1D-ND-C4D	-2.43	102.33	105.21
71	5m	201	PC1	C2-O21-C21	2.42	123.58	117.80
85	8A	606	HEA	C1D-ND-C4D	-2.42	102.35	105.21
85	8A	606	HEA	C17-C18-C19	-2.41	122.11	127.62
85	4A	606	HEA	C4B-NB-C1B	-2.41	102.36	105.21
85	8A	606	HEA	CHB-C1B-NB	-2.39	121.86	124.44
85	4A	606	HEA	CMB-C2B-C1B	2.39	128.77	125.03
85	8A	605	HEA	C1D-ND-C4D	-2.39	102.38	105.21
85	8A	605	HEA	CMB-C2B-C1B	2.38	128.75	125.03
71	1m	201	PC1	C2-O21-C21	2.37	123.47	117.80
85	4A	605	HEA	CMB-C2B-C1B	2.37	128.73	125.03
85	4A	605	HEA	C1D-ND-C4D	-2.36	102.41	105.21
85	4A	606	HEA	CHB-C1B-NB	-2.35	121.90	124.44
83	3C	501	HEM	CAA-CBA-CGA	-2.35	107.50	113.83
85	8A	606	HEA	CMB-C2B-C1B	2.35	128.71	125.03
83	3C	501	HEM	CAD-CBD-CGD	-2.35	107.44	113.67
85	4A	606	HEA	C25-C23-C24	2.34	119.98	114.59
85	8A	606	HEA	C25-C23-C24	2.32	119.93	114.59
83	6P	502	HEM	CHD-C1D-C2D	-2.27	121.44	125.03
83	3P	502	HEM	CHD-C1D-C2D	-2.26	121.45	125.03
83	6C	501	HEM	CHA-C4D-ND	2.24	127.15	124.37
85	4A	605	HEA	CHD-C1D-C2D	-2.22	120.65	126.94
85	4A	605	HEA	C25-C23-C24	2.21	119.67	114.59
85	8A	605	HEA	C25-C23-C24	2.21	119.67	114.59
78	5P	402	NDP	C5A-C6A-N6A	2.21	123.67	120.31
78	1P	402	NDP	C5A-C6A-N6A	2.20	123.67	120.31
85	8A	605	HEA	CHD-C1D-C2D	-2.19	120.73	126.94
85	4A	606	HEA	CHB-C1B-C2B	-2.19	121.58	125.03
85	8A	605	HEA	CHB-C1B-C2B	-2.18	121.58	125.03
75	4C	308	CDL	OB6-CB5-C51	2.18	116.19	111.48
85	4A	605	HEA	CHB-C1B-C2B	-2.17	121.60	125.03
84	3D	501	HEC	CMA-C3A-C2A	2.17	129.03	124.94
83	3P	502	HEM	O2D-CGD-CBD	2.17	120.86	114.00
85	8A	606	HEA	CHB-C1B-C2B	-2.17	121.60	125.03
83	3C	502	HEM	CHB-C1B-C2B	-2.16	120.81	126.94
83	3P	502	HEM	C4D-ND-C1D	2.16	107.76	105.21
75	8A	610	CDL	OB6-CB5-C51	2.15	116.14	111.48
83	6P	502	HEM	O2D-CGD-CBD	2.15	120.80	114.00
83	6P	502	HEM	C4D-ND-C1D	2.15	107.75	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
73	5F	501	FMN	C4-N3-C2	-2.15	121.83	125.64
83	6C	502	HEM	CHB-C1B-NB	2.14	127.03	124.37
84	6Q	501	HEC	CMA-C3A-C2A	2.12	128.94	124.94
84	3Q	501	HEC	CMA-C3A-C2A	2.12	128.94	124.94
85	8A	606	HEA	CAD-CBD-CGD	-2.10	108.09	113.67
83	6P	502	HEM	CHA-C4D-C3D	-2.10	121.35	125.23
73	1F	501	FMN	C4-N3-C2	-2.09	121.94	125.64
83	6C	502	HEM	C3C-C4C-NC	-2.09	107.00	110.94
85	4A	606	HEA	CAD-CBD-CGD	-2.08	108.14	113.67
83	3P	502	HEM	CHA-C4D-C3D	-2.07	121.41	125.23
83	3C	501	HEM	C4D-ND-C1D	2.07	107.66	105.21
83	6P	502	HEM	O2A-CGA-CBA	2.07	120.55	114.00
85	4A	606	HEA	C13-C12-C11	-2.06	111.09	114.39
83	3P	502	HEM	O2A-CGA-CBA	2.05	120.47	114.00
83	3C	502	HEM	C4D-ND-C1D	2.02	107.61	105.21
85	8A	606	HEA	C21-C22-C23	-2.02	120.90	127.64
83	3P	501	HEM	CHA-C4D-C3D	-2.02	121.50	125.23
83	6C	501	HEM	C4C-CHD-C1D	-2.02	119.89	122.56
83	6P	501	HEM	CHA-C4D-C3D	-2.02	121.50	125.23
85	8A	606	HEA	C13-C12-C11	-2.02	111.17	114.39
85	4A	606	HEA	C21-C22-C23	-2.01	120.95	127.64
83	6C	501	HEM	CHB-C1B-NB	2.00	126.86	124.37
82	4G	101	PGV	O01-C1-C2	2.00	115.81	111.48
83	6P	501	HEM	C3B-C4B-NB	-2.00	108.03	109.47
83	3C	502	HEM	CHA-C4D-C3D	-2.00	121.54	125.23

There are no chirality outliers.

All (1552) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C1-O11-P-O14
69	1A	201	3PE	O13-C11-C12-N
69	1A	201	3PE	O32-C31-O31-C3
69	1A	201	3PE	C32-C31-O31-C3
69	1J	202	3PE	C1-O11-P-O13
69	1J	202	3PE	C1-O11-P-O14
69	1J	202	3PE	C11-O13-P-O12
69	1J	202	3PE	C12-C11-O13-P
69	1L	701	3PE	O32-C31-O31-C3
69	1L	701	3PE	C32-C31-O31-C3
69	1L	704	3PE	O22-C21-O21-C2
69	1L	704	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	1M	501	3PE	C1-O11-P-O14
69	1N	901	3PE	C11-O13-P-O14
69	1N	902	3PE	C2-C1-O11-P
69	1Y	202	3PE	C1-O11-P-O12
69	1Y	202	3PE	C1-O11-P-O13
69	1Y	202	3PE	C2-C1-O11-P
69	1Y	203	3PE	O22-C21-O21-C2
69	1Y	203	3PE	C22-C21-O21-C2
69	1Y	204	3PE	O21-C2-C3-O31
69	1Y	205	3PE	C11-O13-P-O14
69	1Y	205	3PE	C12-C11-O13-P
69	1Y	205	3PE	O32-C31-O31-C3
69	1Y	205	3PE	C32-C31-O31-C3
69	1Y	206	3PE	C1-O11-P-O13
69	1Y	206	3PE	O32-C31-O31-C3
69	1Y	206	3PE	C32-C31-O31-C3
69	1Y	206	3PE	O22-C21-O21-C2
69	1Y	206	3PE	C22-C21-O21-C2
69	1d	201	3PE	C11-O13-P-O14
69	1d	201	3PE	C2-C1-O11-P
69	1d	201	3PE	O32-C31-O31-C3
69	1d	201	3PE	C32-C31-O31-C3
69	1j	101	3PE	O22-C21-O21-C2
69	1j	101	3PE	C22-C21-O21-C2
69	5A	201	3PE	C1-O11-P-O14
69	5J	201	3PE	C1-O11-P-O13
69	5J	201	3PE	C1-O11-P-O14
69	5J	201	3PE	C11-O13-P-O12
69	5J	201	3PE	C12-C11-O13-P
69	5L	701	3PE	O32-C31-O31-C3
69	5L	701	3PE	C32-C31-O31-C3
69	5L	704	3PE	O22-C21-O21-C2
69	5L	704	3PE	C22-C21-O21-C2
69	5M	501	3PE	C1-O11-P-O14
69	5N	901	3PE	C11-O13-P-O14
69	5N	902	3PE	C2-C1-O11-P
69	5Y	202	3PE	C1-O11-P-O12
69	5Y	202	3PE	C1-O11-P-O13
69	5Y	202	3PE	C2-C1-O11-P
69	5Y	203	3PE	O22-C21-O21-C2
69	5Y	203	3PE	C22-C21-O21-C2
69	5Y	204	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
69	5Y	205	3PE	C11-O13-P-O14
69	5Y	205	3PE	C12-C11-O13-P
69	5Y	205	3PE	O32-C31-O31-C3
69	5Y	205	3PE	C32-C31-O31-C3
69	5Y	206	3PE	C1-O11-P-O13
69	5Y	206	3PE	O32-C31-O31-C3
69	5Y	206	3PE	C32-C31-O31-C3
69	5Y	206	3PE	O22-C21-O21-C2
69	5Y	206	3PE	C22-C21-O21-C2
69	5d	201	3PE	C11-O13-P-O14
69	5d	201	3PE	C2-C1-O11-P
69	5d	201	3PE	O32-C31-O31-C3
69	5d	201	3PE	C32-C31-O31-C3
69	5j	101	3PE	O22-C21-O21-C2
69	5j	101	3PE	C22-C21-O21-C2
71	1H	401	PC1	C11-O13-P-O11
71	1H	401	PC1	C1-O11-P-O14
71	1H	401	PC1	C1-O11-P-O13
71	1H	401	PC1	C12-C11-O13-P
71	1H	401	PC1	O13-C11-C12-N
71	1I	201	PC1	C11-O13-P-O14
71	1I	204	PC1	C1-O11-P-O14
71	1J	201	PC1	C1-O11-P-O12
71	1J	201	PC1	C1-O11-P-O14
71	1J	201	PC1	C1-O11-P-O13
71	1J	201	PC1	O13-C11-C12-N
71	1J	201	PC1	C22-C21-O21-C2
71	1P	401	PC1	O32-C31-O31-C3
71	1P	401	PC1	C32-C31-O31-C3
71	1Y	201	PC1	C1-O11-P-O14
71	1h	202	PC1	C11-O13-P-O14
71	1h	202	PC1	O32-C31-O31-C3
71	1h	202	PC1	C32-C31-O31-C3
71	1m	201	PC1	C11-O13-P-O14
71	1m	201	PC1	C12-C11-O13-P
71	1m	201	PC1	O13-C11-C12-N
71	1m	201	PC1	O22-C21-O21-C2
71	1m	201	PC1	C22-C21-O21-C2
71	5A	202	PC1	C1-O11-P-O14
71	5H	401	PC1	C11-O13-P-O11
71	5H	401	PC1	C1-O11-P-O14
71	5H	401	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
71	5H	401	PC1	C12-C11-O13-P
71	5H	401	PC1	O13-C11-C12-N
71	5I	201	PC1	C11-O13-P-O14
71	5I	204	PC1	C1-O11-P-O14
71	5P	401	PC1	O32-C31-O31-C3
71	5P	401	PC1	C32-C31-O31-C3
71	5Y	201	PC1	C1-O11-P-O14
71	5h	202	PC1	C11-O13-P-O14
71	5h	202	PC1	O32-C31-O31-C3
71	5h	202	PC1	C32-C31-O31-C3
71	5m	201	PC1	C11-O13-P-O14
71	5m	201	PC1	C12-C11-O13-P
71	5m	201	PC1	O13-C11-C12-N
71	5m	201	PC1	O22-C21-O21-C2
71	5m	201	PC1	C22-C21-O21-C2
75	1L	702	CDL	CB2-OB2-PB2-OB4
75	1L	702	CDL	CB2-OB2-PB2-OB5
75	1N	903	CDL	CA3-OA5-PA1-OA3
75	1X	201	CDL	C1-CA2-OA2-PA1
75	1X	201	CDL	CA2-OA2-PA1-OA4
75	1X	201	CDL	CA2-OA2-PA1-OA5
75	1d	202	CDL	CA2-OA2-PA1-OA4
75	1d	202	CDL	CA2-OA2-PA1-OA5
75	1d	202	CDL	CA3-OA5-PA1-OA2
75	1d	202	CDL	CA3-OA5-PA1-OA3
75	1d	202	CDL	CA3-OA5-PA1-OA4
75	1d	202	CDL	CB3-OB5-PB2-OB2
75	1d	202	CDL	CB3-OB5-PB2-OB3
75	1d	202	CDL	CB3-OB5-PB2-OB4
75	1d	202	CDL	OB5-CB3-CB4-OB6
75	1i	201	CDL	CA2-OA2-PA1-OA4
75	1i	201	CDL	CA2-OA2-PA1-OA5
75	1i	201	CDL	OB7-CB5-OB6-CB4
75	1i	201	CDL	C51-CB5-OB6-CB4
75	1i	201	CDL	OB9-CB7-OB8-CB6
75	1i	201	CDL	C71-CB7-OB8-CB6
75	4B	301	CDL	CA3-OA5-PA1-OA3
75	4B	301	CDL	OA9-CA7-OA8-CA6
75	4B	301	CDL	C31-CA7-OA8-CA6
75	4B	301	CDL	CB3-OB5-PB2-OB2
75	4B	301	CDL	CB3-OB5-PB2-OB3
75	4C	308	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
75	4C	308	CDL	OB7-CB5-OB6-CB4
75	4C	308	CDL	C51-CB5-OB6-CB4
75	4C	308	CDL	OB9-CB7-OB8-CB6
75	4C	308	CDL	C71-CB7-OB8-CB6
75	5L	702	CDL	CB2-OB2-PB2-OB4
75	5L	702	CDL	CB2-OB2-PB2-OB5
75	5N	903	CDL	CA3-OA5-PA1-OA3
75	5X	201	CDL	C1-CA2-OA2-PA1
75	5X	201	CDL	CA2-OA2-PA1-OA4
75	5X	201	CDL	CA2-OA2-PA1-OA5
75	5d	202	CDL	CA2-OA2-PA1-OA4
75	5d	202	CDL	CA2-OA2-PA1-OA5
75	5d	202	CDL	CA3-OA5-PA1-OA2
75	5d	202	CDL	CA3-OA5-PA1-OA3
75	5d	202	CDL	CA3-OA5-PA1-OA4
75	5d	202	CDL	CB3-OB5-PB2-OB2
75	5d	202	CDL	CB3-OB5-PB2-OB3
75	5d	202	CDL	CB3-OB5-PB2-OB4
75	5d	202	CDL	OB5-CB3-CB4-OB6
75	5i	201	CDL	CA2-OA2-PA1-OA4
75	5i	201	CDL	CA2-OA2-PA1-OA5
75	5i	201	CDL	OB7-CB5-OB6-CB4
75	5i	201	CDL	C51-CB5-OB6-CB4
75	5i	201	CDL	OB9-CB7-OB8-CB6
75	5i	201	CDL	C71-CB7-OB8-CB6
75	8A	610	CDL	C1-CA2-OA2-PA1
75	8A	610	CDL	OB7-CB5-OB6-CB4
75	8A	610	CDL	C51-CB5-OB6-CB4
75	8A	610	CDL	OB9-CB7-OB8-CB6
75	8A	610	CDL	C71-CB7-OB8-CB6
75	8B	302	CDL	CA3-OA5-PA1-OA3
75	8B	302	CDL	OA9-CA7-OA8-CA6
75	8B	302	CDL	C31-CA7-OA8-CA6
75	8B	302	CDL	CB3-OB5-PB2-OB2
75	8B	302	CDL	CB3-OB5-PB2-OB3
75	8D	201	CDL	CA2-OA2-PA1-OA3
75	8D	201	CDL	CA2-OA2-PA1-OA5
75	8D	201	CDL	CA3-OA5-PA1-OA2
75	8D	201	CDL	CA3-OA5-PA1-OA3
75	8D	201	CDL	CA3-OA5-PA1-OA4
75	8D	201	CDL	C11-CA5-OA6-CA4
75	8D	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
75	8D	201	CDL	C51-CB5-OB6-CB4
80	1T	101	EHZ	N2-C15-C16-C17
80	1T	101	EHZ	N2-C15-C16-O5
80	1T	101	EHZ	O4-C15-C16-C17
80	1T	101	EHZ	O4-C15-C16-O5
80	1T	101	EHZ	C15-C16-C17-C19
80	1T	101	EHZ	C15-C16-C17-C20
80	5T	101	EHZ	N2-C15-C16-C17
80	5T	101	EHZ	N2-C15-C16-O5
80	5T	101	EHZ	O4-C15-C16-C17
80	5T	101	EHZ	O4-C15-C16-O5
80	5T	101	EHZ	C15-C16-C17-C19
80	5T	101	EHZ	C15-C16-C17-C20
82	1p	201	PGV	C03-O11-P-O13
82	1p	201	PGV	C04-O12-P-O11
82	1p	201	PGV	C04-O12-P-O14
82	4A	601	PGV	C03-O11-P-O12
82	4A	601	PGV	C03-O11-P-O13
82	4A	601	PGV	C03-O11-P-O14
82	4A	601	PGV	O04-C19-O03-C01
82	4A	601	PGV	C20-C19-O03-C01
82	4A	603	PGV	C04-O12-P-O11
82	4A	603	PGV	C04-O12-P-O14
82	4A	603	PGV	C02-C03-O11-P
82	4A	604	PGV	O03-C01-C02-O01
82	4C	301	PGV	C03-O11-P-O13
82	4C	301	PGV	O02-C1-O01-C02
82	4C	301	PGV	C2-C1-O01-C02
82	4C	302	PGV	C04-O12-P-O11
82	4C	302	PGV	C04-O12-P-O14
82	4C	302	PGV	O04-C19-O03-C01
82	4C	302	PGV	C20-C19-O03-C01
82	4C	303	PGV	C03-O11-P-O12
82	4C	303	PGV	C03-O11-P-O14
82	4C	303	PGV	C02-C03-O11-P
82	4C	304	PGV	C03-O11-P-O12
82	4C	304	PGV	C03-O11-P-O14
82	4C	304	PGV	O02-C1-O01-C02
82	4C	304	PGV	C2-C1-O01-C02
82	4G	101	PGV	C04-O12-P-O11
82	4G	101	PGV	C04-O12-P-O14
82	4G	101	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
82	4G	101	PGV	C2-C1-O01-C02
82	4G	101	PGV	O04-C19-O03-C01
82	4G	101	PGV	C20-C19-O03-C01
82	4K	101	PGV	C03-O11-P-O12
82	4K	101	PGV	C03-O11-P-O14
82	4K	101	PGV	O04-C19-O03-C01
82	4K	101	PGV	C20-C19-O03-C01
82	8A	601	PGV	C03-O11-P-O12
82	8A	601	PGV	C03-O11-P-O14
82	8A	601	PGV	C04-C05-C06-O06
82	8A	602	PGV	C03-O11-P-O12
82	8A	602	PGV	C04-O12-P-O14
82	8A	603	PGV	C03-O11-P-O12
82	8A	603	PGV	C03-O11-P-O14
82	8A	603	PGV	C04-O12-P-O11
82	8A	603	PGV	C04-O12-P-O14
82	8A	604	PGV	C03-O11-P-O12
82	8A	604	PGV	C03-O11-P-O13
82	8A	604	PGV	C03-O11-P-O14
82	8A	604	PGV	C04-O12-P-O14
82	8A	604	PGV	C04-C05-C06-O06
82	8A	604	PGV	O05-C05-C06-O06
82	8B	301	PGV	C03-O11-P-O12
82	8B	301	PGV	C03-O11-P-O13
82	8B	301	PGV	C03-O11-P-O14
82	8B	301	PGV	C04-O12-P-O11
82	8B	301	PGV	C04-C05-C06-O06
82	8B	301	PGV	C11-C10-C9-C8
82	8C	301	PGV	C04-O12-P-O11
82	8C	301	PGV	C04-O12-P-O13
82	8C	301	PGV	C04-O12-P-O14
82	8C	301	PGV	C04-C05-C06-O06
82	8C	301	PGV	O05-C05-C06-O06
82	8C	301	PGV	O02-C1-O01-C02
82	8C	301	PGV	C2-C1-O01-C02
82	8C	302	PGV	C03-O11-P-O13
82	8C	302	PGV	C04-O12-P-O11
82	8C	302	PGV	C04-O12-P-O13
82	8C	302	PGV	C04-O12-P-O14
82	8C	303	PGV	C03-O11-P-O12
82	8C	303	PGV	C03-O11-P-O14
82	8C	303	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
82	8C	303	PGV	O12-C04-C05-O05
82	8C	304	PGV	C04-O12-P-O11
82	8C	304	PGV	O12-C04-C05-C06
82	8C	304	PGV	O02-C1-O01-C02
82	8C	304	PGV	C2-C1-O01-C02
82	8G	101	PGV	C04-O12-P-O13
82	8G	101	PGV	C04-C05-C06-O06
82	8G	101	PGV	O02-C1-O01-C02
82	8G	101	PGV	C2-C1-O01-C02
82	8G	101	PGV	O04-C19-O03-C01
82	8G	101	PGV	C20-C19-O03-C01
82	8J	101	PGV	C04-O12-P-O11
82	8J	101	PGV	C04-O12-P-O13
82	8J	101	PGV	C04-O12-P-O14
82	8J	101	PGV	C2-C1-O01-C02
82	8J	101	PGV	C11-C10-C9-C8
82	8K	101	PGV	C03-O11-P-O12
82	8K	101	PGV	C03-O11-P-O13
82	8K	101	PGV	C03-O11-P-O14
82	8K	101	PGV	C04-O12-P-O13
83	3C	501	HEM	C2B-C3B-CAB-CBB
83	3C	502	HEM	C2B-C3B-CAB-CBB
83	3P	501	HEM	C2B-C3B-CAB-CBB
83	3P	502	HEM	C2B-C3B-CAB-CBB
83	6C	501	HEM	C2B-C3B-CAB-CBB
83	6P	501	HEM	C2B-C3B-CAB-CBB
83	6P	502	HEM	C2B-C3B-CAB-CBB
84	6D	501	HEC	C2D-C3D-CAD-CBD
84	6D	501	HEC	C4D-C3D-CAD-CBD
85	4A	605	HEA	C3B-C11-C12-C13
85	4A	605	HEA	O11-C11-C12-C13
85	8A	605	HEA	C3B-C11-C12-C13
85	8A	605	HEA	O11-C11-C12-C13
89	4B	303	PSC	C03-O11-P-O12
89	4B	303	PSC	C03-O11-P-O13
89	4B	303	PSC	O02-C1-O01-C02
89	4B	303	PSC	C2-C1-O01-C02
89	8A	611	PSC	C03-O11-P-O12
89	8A	611	PSC	C03-O11-P-O13
89	8A	611	PSC	O02-C1-O01-C02
89	8A	611	PSC	C2-C1-O01-C02
90	4C	306	PEK	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
90	4C	306	PEK	C04-O12-P-O13
90	8C	306	PEK	C04-O12-P-O11
90	8C	306	PEK	C04-O12-P-O13
75	8D	201	CDL	OA9-CA7-OA8-CA6
82	8A	601	PGV	O04-C19-O03-C01
75	8D	201	CDL	C31-CA7-OA8-CA6
82	8A	601	PGV	C20-C19-O03-C01
75	8D	201	CDL	OB9-CB7-OB8-CB6
82	1p	201	PGV	O04-C19-O03-C01
82	8B	301	PGV	O04-C19-O03-C01
82	8C	301	PGV	O04-C19-O03-C01
82	8K	101	PGV	O04-C19-O03-C01
71	1J	201	PC1	O22-C21-O21-C2
75	8D	201	CDL	OA7-CA5-OA6-CA4
82	8J	101	PGV	O02-C1-O01-C02
75	8D	201	CDL	C71-CB7-OB8-CB6
82	8B	301	PGV	C20-C19-O03-C01
82	8C	301	PGV	C20-C19-O03-C01
80	1T	101	EHZ	C13-C12-N1-C11
80	5T	101	EHZ	C13-C12-N1-C11
82	1p	201	PGV	C20-C19-O03-C01
82	8C	302	PGV	C20-C19-O03-C01
82	8K	101	PGV	C20-C19-O03-C01
82	8G	101	PGV	C7-C8-C9-C10
82	8A	604	PGV	C10-C11-C12-C13
82	1p	201	PGV	C14-C15-C16-C17
82	8B	301	PGV	C30-C31-C32-C33
82	8C	301	PGV	C14-C15-C16-C17
69	1A	201	3PE	C3A-C3B-C3C-C3D
75	8D	201	CDL	C54-C55-C56-C57
75	8D	201	CDL	O1-C1-CB2-OB2
82	8A	601	PGV	O12-C04-C05-O05
82	8C	304	PGV	O12-C04-C05-O05
75	1N	903	CDL	OB7-CB5-OB6-CB4
75	1N	903	CDL	C51-CB5-OB6-CB4
75	5N	903	CDL	OB7-CB5-OB6-CB4
75	5N	903	CDL	C51-CB5-OB6-CB4
82	1p	201	PGV	C2-C1-O01-C02
82	8A	604	PGV	C2-C1-O01-C02
82	1p	201	PGV	C23-C24-C25-C26
82	1p	201	PGV	C3-C4-C5-C6
82	8C	302	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
82	1p	201	PGV	O02-C1-O01-C02
71	1P	401	PC1	C24-C25-C26-C27
75	8D	201	CDL	C31-C32-C33-C34
75	8D	201	CDL	C42-C43-C44-C45
82	4C	304	PGV	C02-C03-O11-P
82	4C	304	PGV	C05-C04-O12-P
82	8C	303	PGV	C3-C4-C5-C6
82	8A	604	PGV	C4-C5-C6-C7
82	8A	604	PGV	C6-C7-C8-C9
82	8C	303	PGV	C13-C14-C15-C16
82	8C	304	PGV	C29-C30-C31-C32
82	8C	303	PGV	C29-C30-C31-C32
80	1T	101	EHZ	O3-C12-N1-C11
80	5T	101	EHZ	O3-C12-N1-C11
75	8D	201	CDL	C52-C53-C54-C55
75	8D	201	CDL	C72-C73-C74-C75
82	8A	603	PGV	C10-C11-C12-C13
82	8B	301	PGV	C10-C11-C12-C13
82	8A	601	PGV	C24-C25-C26-C27
82	8C	302	PGV	C26-C27-C28-C29
71	1J	201	PC1	C22-C23-C24-C25
82	8A	604	PGV	C20-C21-C22-C23
82	8B	301	PGV	C6-C7-C8-C9
82	8C	301	PGV	C23-C24-C25-C26
82	8A	601	PGV	O12-C04-C05-C06
71	1J	201	PC1	C32-C31-O31-C3
75	8D	201	CDL	C81-C82-C83-C84
82	8J	101	PGV	C26-C27-C28-C29
82	8A	601	PGV	C7-C8-C9-C10
82	8A	603	PGV	C28-C29-C30-C31
82	8B	301	PGV	C4-C5-C6-C7
82	8G	101	PGV	C20-C21-C22-C23
82	8J	101	PGV	C4-C5-C6-C7
82	8A	602	PGV	C23-C24-C25-C26
82	8K	101	PGV	C7-C8-C9-C10
82	8K	101	PGV	C25-C26-C27-C28
82	8A	601	PGV	C22-C23-C24-C25
82	8G	101	PGV	C27-C28-C29-C30
69	1A	201	3PE	C37-C38-C39-C3A
82	8A	603	PGV	C30-C31-C32-C33
82	8A	604	PGV	C29-C30-C31-C32
82	8G	101	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
82	1p	201	PGV	C27-C28-C29-C30
69	1A	201	3PE	C29-C2A-C2B-C2C
75	8D	201	CDL	C12-C13-C14-C15
82	8K	101	PGV	C23-C24-C25-C26
82	8B	301	PGV	O03-C01-C02-O01
71	1J	201	PC1	C21-C22-C23-C24
82	1p	201	PGV	C19-C20-C21-C22
82	8G	101	PGV	C2-C3-C4-C5
75	8D	201	CDL	C36-C37-C38-C39
82	8C	304	PGV	C6-C7-C8-C9
83	6C	502	HEM	C2A-CAA-CBA-CGA
84	6D	501	HEC	C2A-CAA-CBA-CGA
82	8G	101	PGV	O05-C05-C06-O06
82	8C	302	PGV	C11-C10-C9-C8
76	1O	401	GTP	O4'-C4'-C5'-O5'
76	1O	401	GTP	C3'-C4'-C5'-O5'
76	5O	401	GTP	O4'-C4'-C5'-O5'
76	5O	401	GTP	C3'-C4'-C5'-O5'
71	1P	401	PC1	C22-C23-C24-C25
82	8C	303	PGV	C5-C6-C7-C8
82	8C	301	PGV	C19-C20-C21-C22
82	8C	303	PGV	C23-C24-C25-C26
82	8J	101	PGV	C6-C7-C8-C9
82	8J	101	PGV	C28-C29-C30-C31
82	8K	101	PGV	C3-C4-C5-C6
82	8A	604	PGV	O02-C1-O01-C02
69	1A	201	3PE	C2B-C2C-C2D-C2E
82	8C	304	PGV	C24-C25-C26-C27
71	5I	201	PC1	C31-C32-C33-C34
75	8D	201	CDL	CA7-C31-C32-C33
82	4G	101	PGV	C1-C2-C3-C4
82	8G	101	PGV	C19-C20-C21-C22
71	1J	201	PC1	O32-C31-O31-C3
69	1L	703	3PE	C2-C1-O11-P
69	5L	703	3PE	C2-C1-O11-P
82	8C	303	PGV	C05-C04-O12-P
71	1I	201	PC1	C31-C32-C33-C34
71	5P	401	PC1	C21-C22-C23-C24
75	8D	201	CDL	CA5-C11-C12-C13
82	4J	101	PGV	C19-C20-C21-C22
82	8A	601	PGV	C1-C2-C3-C4
82	8C	302	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
89	4B	303	PSC	C19-C20-C21-C22
89	8A	611	PSC	C19-C20-C21-C22
71	1H	401	PC1	C22-C23-C24-C25
71	5H	401	PC1	C22-C23-C24-C25
82	8A	602	PGV	C26-C27-C28-C29
82	8C	304	PGV	C3-C4-C5-C6
69	1A	201	3PE	C27-C28-C29-C2A
82	8A	602	PGV	O12-C04-C05-O05
82	8B	301	PGV	O12-C04-C05-O05
71	1J	201	PC1	C31-C32-C33-C34
82	4L	101	PGV	C1-C2-C3-C4
82	8A	602	PGV	C19-C20-C21-C22
82	8L	101	PGV	C1-C2-C3-C4
82	1p	201	PGV	C12-C13-C14-C15
82	8B	301	PGV	C25-C26-C27-C28
75	4C	308	CDL	C80-C81-C82-C83
75	8A	610	CDL	C80-C81-C82-C83
82	8C	303	PGV	C19-C20-C21-C22
75	8D	201	CDL	C44-C45-C46-C47
75	8D	201	CDL	CA2-C1-CB2-OB2
82	8A	602	PGV	O12-C04-C05-C06
82	8B	301	PGV	O12-C04-C05-C06
82	8C	301	PGV	C27-C28-C29-C30
82	8C	304	PGV	C11-C10-C9-C8
75	8A	610	CDL	C75-C76-C77-C78
75	4C	308	CDL	C75-C76-C77-C78
82	8C	304	PGV	C19-C20-C21-C22
82	8A	602	PGV	C4-C5-C6-C7
82	8G	101	PGV	O12-C04-C05-O05
71	1h	202	PC1	C2-C1-O11-P
71	5H	401	PC1	C2-C1-O11-P
71	5h	202	PC1	C2-C1-O11-P
82	4A	604	PGV	C05-C04-O12-P
83	3C	501	HEM	C3D-CAD-CBD-CGD
82	8A	601	PGV	C30-C31-C32-C33
82	8A	602	PGV	C04-C05-C06-O06
82	8C	303	PGV	C04-C05-C06-O06
82	8C	304	PGV	C04-C05-C06-O06
82	8J	101	PGV	C04-C05-C06-O06
82	8K	101	PGV	C04-C05-C06-O06
75	8A	610	CDL	C82-C83-C84-C85
75	4C	308	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
71	1P	401	PC1	C22-C21-O21-C2
75	5d	202	CDL	C32-C33-C34-C35
75	1d	202	CDL	C32-C33-C34-C35
75	8D	201	CDL	C78-C79-C80-C81
82	1p	201	PGV	C29-C30-C31-C32
82	8K	101	PGV	C24-C25-C26-C27
71	1P	401	PC1	C25-C26-C27-C28
82	8C	301	PGV	C2-C3-C4-C5
71	1M	502	PC1	C21-C22-C23-C24
71	5M	502	PC1	C21-C22-C23-C24
82	8C	301	PGV	C10-C11-C12-C13
82	8B	301	PGV	C3-C4-C5-C6
82	8C	302	PGV	C6-C7-C8-C9
82	4J	101	PGV	C22-C23-C24-C25
82	8B	301	PGV	C27-C28-C29-C30
82	8C	304	PGV	C22-C23-C24-C25
82	8L	101	PGV	C2-C3-C4-C5
82	8A	601	PGV	O05-C05-C06-O06
82	8A	602	PGV	O05-C05-C06-O06
82	4L	101	PGV	C2-C3-C4-C5
82	8A	604	PGV	C22-C23-C24-C25
82	8C	303	PGV	C25-C26-C27-C28
75	8D	201	CDL	CB5-C51-C52-C53
69	1L	703	3PE	C33-C34-C35-C36
69	1d	201	3PE	C32-C33-C34-C35
69	5L	703	3PE	C33-C34-C35-C36
69	5d	201	3PE	C32-C33-C34-C35
82	8A	603	PGV	C24-C25-C26-C27
69	1A	201	3PE	C25-C26-C27-C28
82	8B	301	PGV	C13-C14-C15-C16
82	8A	603	PGV	C2-C1-O01-C02
82	8C	303	PGV	C2-C1-O01-C02
69	1L	703	3PE	C39-C3A-C3B-C3C
69	5L	703	3PE	C39-C3A-C3B-C3C
71	1Y	201	PC1	C32-C33-C34-C35
75	1L	702	CDL	C37-C38-C39-C40
75	5L	702	CDL	C37-C38-C39-C40
82	1p	201	PGV	C21-C22-C23-C24
82	8B	301	PGV	C2-C3-C4-C5
82	8C	304	PGV	C5-C6-C7-C8
82	8G	101	PGV	C21-C22-C23-C24
71	5Y	201	PC1	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
82	1p	201	PGV	C24-C25-C26-C27
75	8D	201	CDL	C37-C38-C39-C40
75	8D	201	CDL	C75-C76-C77-C78
82	8C	301	PGV	C26-C27-C28-C29
82	8C	304	PGV	C26-C27-C28-C29
82	8A	601	PGV	C13-C14-C15-C16
82	8K	101	PGV	C21-C22-C23-C24
71	1P	401	PC1	O22-C21-O21-C2
75	8D	201	CDL	C62-C63-C64-C65
82	8A	601	PGV	C29-C30-C31-C32
82	8A	602	PGV	C22-C23-C24-C25
82	8C	302	PGV	C14-C15-C16-C17
82	8C	302	PGV	C29-C30-C31-C32
69	1d	201	3PE	C23-C24-C25-C26
69	5d	201	3PE	C23-C24-C25-C26
75	8D	201	CDL	C40-C41-C42-C43
82	1p	201	PGV	C2-C3-C4-C5
82	8A	604	PGV	C2-C3-C4-C5
69	1A	201	3PE	C23-C24-C25-C26
71	1I	201	PC1	C34-C35-C36-C37
71	5I	201	PC1	C34-C35-C36-C37
75	8D	201	CDL	C34-C35-C36-C37
75	8D	201	CDL	C83-C84-C85-C86
82	8A	601	PGV	C21-C22-C23-C24
82	8A	604	PGV	C14-C15-C16-C17
82	8G	101	PGV	C23-C24-C25-C26
82	8G	101	PGV	C26-C27-C28-C29
75	8D	201	CDL	C57-C58-C59-C60
82	8C	302	PGV	C28-C29-C30-C31
82	8C	303	PGV	C15-C16-C17-C18
75	8D	201	CDL	C23-C24-C25-C26
82	8C	303	PGV	C12-C13-C14-C15
82	8K	101	PGV	C11-C10-C9-C8
71	1H	401	PC1	C2-C1-O11-P
82	4C	305	PGV	C02-C03-O11-P
82	8C	305	PGV	C02-C03-O11-P
82	8C	303	PGV	C24-C25-C26-C27
82	8C	304	PGV	C27-C28-C29-C30
83	6C	501	HEM	C3D-CAD-CBD-CGD
82	8C	304	PGV	C14-C15-C16-C17
82	8J	101	PGV	C1-C2-C3-C4
82	8A	604	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
82	8G	101	PGV	C15-C16-C17-C18
82	8A	603	PGV	C14-C15-C16-C17
82	8C	301	PGV	C30-C31-C32-C33
71	1P	401	PC1	C23-C24-C25-C26
82	4C	303	PGV	C24-C25-C26-C27
82	8B	301	PGV	C29-C30-C31-C32
82	8J	101	PGV	C14-C15-C16-C17
82	8K	101	PGV	C31-C32-C33-C34
82	8B	301	PGV	C28-C29-C30-C31
82	8K	101	PGV	C2-C3-C4-C5
82	8C	303	PGV	C20-C19-O03-C01
71	5h	202	PC1	C32-C33-C34-C35
75	8D	201	CDL	C60-C61-C62-C63
71	1h	202	PC1	C32-C33-C34-C35
69	1A	201	3PE	C34-C35-C36-C37
82	8J	101	PGV	C25-C26-C27-C28
78	1P	402	NDP	O4D-C1D-N1N-C6N
78	5P	402	NDP	O4D-C1D-N1N-C6N
71	1J	201	PC1	C32-C33-C34-C35
75	8D	201	CDL	C35-C36-C37-C38
82	8A	602	PGV	C20-C21-C22-C23
82	8A	601	PGV	C4-C5-C6-C7
82	1p	201	PGV	C25-C26-C27-C28
69	1A	201	3PE	C22-C21-O21-C2
82	8A	603	PGV	O02-C1-O01-C02
82	8C	303	PGV	O02-C1-O01-C02
80	5T	101	EHZ	C21-C22-C23-C24
82	1p	201	PGV	C4-C5-C6-C7
82	8A	602	PGV	C12-C13-C14-C15
82	8B	301	PGV	C12-C13-C14-C15
80	1T	101	EHZ	C21-C22-C23-C24
82	8G	101	PGV	C5-C6-C7-C8
75	5d	202	CDL	C42-C43-C44-C45
82	8C	302	PGV	C7-C8-C9-C10
75	1X	201	CDL	C19-C20-C21-C22
75	1d	202	CDL	C42-C43-C44-C45
75	5X	201	CDL	C19-C20-C21-C22
75	8D	201	CDL	C38-C39-C40-C41
82	1p	201	PGV	C13-C14-C15-C16
82	8A	602	PGV	C14-C15-C16-C17
82	8A	603	PGV	C29-C30-C31-C32
82	8A	604	PGV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
83	6C	502	HEM	C2B-C3B-CAB-CBB
71	1J	201	PC1	C11-C12-N-C15
82	8B	301	PGV	C21-C22-C23-C24
71	1J	201	PC1	C34-C35-C36-C37
75	5L	702	CDL	C33-C34-C35-C36
71	1m	201	PC1	C22-C23-C24-C25
75	1L	702	CDL	C33-C34-C35-C36
83	3C	501	HEM	C4B-C3B-CAB-CBB
83	3C	502	HEM	C4B-C3B-CAB-CBB
83	3P	501	HEM	C4B-C3B-CAB-CBB
83	3P	502	HEM	C4B-C3B-CAB-CBB
83	6C	501	HEM	C4B-C3B-CAB-CBB
83	6P	501	HEM	C4B-C3B-CAB-CBB
83	6P	502	HEM	C4B-C3B-CAB-CBB
71	5m	201	PC1	C22-C23-C24-C25
75	8D	201	CDL	C51-C52-C53-C54
82	1p	201	PGV	C26-C27-C28-C29
82	8C	301	PGV	C6-C7-C8-C9
82	8B	301	PGV	C26-C27-C28-C29
82	8A	603	PGV	C19-C20-C21-C22
82	8A	601	PGV	C11-C10-C9-C8
82	8A	603	PGV	C11-C10-C9-C8
82	8C	301	PGV	C12-C13-C14-C15
69	1A	201	3PE	C26-C27-C28-C29
69	5N	902	3PE	C2D-C2E-C2F-C2G
69	1N	902	3PE	C2D-C2E-C2F-C2G
82	8C	302	PGV	C27-C28-C29-C30
89	8A	611	PSC	C25-C26-C27-C28
75	8D	201	CDL	C33-C34-C35-C36
82	1p	201	PGV	C28-C29-C30-C31
89	4B	303	PSC	C25-C26-C27-C28
75	8D	201	CDL	C15-C16-C17-C18
73	1F	501	FMN	C4'-C5'-O5'-P
73	5F	501	FMN	C4'-C5'-O5'-P
75	1d	202	CDL	C1-CA2-OA2-PA1
75	1i	201	CDL	C1-CB2-OB2-PB2
75	5d	202	CDL	C1-CA2-OA2-PA1
75	5i	201	CDL	C1-CB2-OB2-PB2
89	4B	303	PSC	C02-C03-O11-P
89	8A	611	PSC	C02-C03-O11-P
75	1q	201	CDL	CA5-C11-C12-C13
75	5q	201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
69	1M	503	3PE	C2B-C2C-C2D-C2E
69	5M	503	3PE	C2B-C2C-C2D-C2E
71	5B	202	PC1	C38-C39-C3A-C3B
82	8A	602	PGV	C21-C22-C23-C24
82	8A	603	PGV	C23-C24-C25-C26
71	1B	202	PC1	C38-C39-C3A-C3B
82	8G	101	PGV	C3-C4-C5-C6
83	6C	501	HEM	C2A-CAA-CBA-CGA
82	8C	303	PGV	O04-C19-O03-C01
82	8A	603	PGV	C22-C23-C24-C25
71	5A	202	PC1	C21-C22-C23-C24
82	8C	301	PGV	C5-C6-C7-C8
69	1A	201	3PE	C2D-C2E-C2F-C2G
82	8J	101	PGV	O05-C05-C06-O06
71	1M	502	PC1	C2A-C2B-C2C-C2D
71	5M	502	PC1	C2A-C2B-C2C-C2D
71	1M	502	PC1	C32-C33-C34-C35
71	5M	502	PC1	C32-C33-C34-C35
82	8G	101	PGV	C22-C23-C24-C25
82	8A	604	PGV	C7-C8-C9-C10
82	8B	301	PGV	C7-C8-C9-C10
82	8C	303	PGV	C30-C31-C32-C33
82	8C	304	PGV	C21-C22-C23-C24
82	8A	601	PGV	C28-C29-C30-C31
71	5P	401	PC1	O11-C1-C2-C3
82	8B	301	PGV	C24-C25-C26-C27
90	4C	307	PEK	C23-C24-C25-C26
90	8C	307	PEK	C23-C24-C25-C26
82	1p	201	PGV	C5-C6-C7-C8
75	1q	201	CDL	C14-C15-C16-C17
75	5q	201	CDL	C14-C15-C16-C17
82	8B	301	PGV	C23-C24-C25-C26
71	1H	401	PC1	C37-C38-C39-C3A
71	5H	401	PC1	C37-C38-C39-C3A
82	8A	602	PGV	C10-C11-C12-C13
69	1L	703	3PE	C1-C2-C3-O31
69	5L	703	3PE	C1-C2-C3-O31
71	1h	202	PC1	C1-C2-C3-O31
71	5h	202	PC1	C1-C2-C3-O31
75	1X	201	CDL	CB3-CB4-CB6-OB8
75	4B	301	CDL	CB3-CB4-CB6-OB8
75	5X	201	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
75	8B	302	CDL	CB3-CB4-CB6-OB8
82	1p	201	PGV	O03-C01-C02-C03
82	4J	101	PGV	O03-C01-C02-C03
82	8B	301	PGV	O03-C01-C02-C03
69	1N	901	3PE	C28-C29-C2A-C2B
69	5N	901	3PE	C28-C29-C2A-C2B
82	8A	604	PGV	C25-C26-C27-C28
82	8C	304	PGV	C4-C5-C6-C7
82	8G	101	PGV	C28-C29-C30-C31
82	8G	101	PGV	C12-C13-C14-C15
82	4C	302	PGV	C5-C6-C7-C8
82	4L	101	PGV	C5-C6-C7-C8
82	8C	302	PGV	C5-C6-C7-C8
82	8L	101	PGV	C5-C6-C7-C8
71	1H	401	PC1	C21-C22-C23-C24
71	5H	401	PC1	C21-C22-C23-C24
82	8A	602	PGV	C6-C7-C8-C9
71	1J	201	PC1	C11-C12-N-C13
82	1p	201	PGV	C7-C8-C9-C10
75	8A	610	CDL	C71-C72-C73-C74
82	8C	303	PGV	C02-C03-O11-P
82	8C	304	PGV	C05-C04-O12-P
69	1A	201	3PE	O22-C21-O21-C2
69	1d	201	3PE	C26-C27-C28-C29
75	4B	301	CDL	C59-C60-C61-C62
75	8B	302	CDL	C59-C60-C61-C62
69	5d	201	3PE	C26-C27-C28-C29
75	4C	308	CDL	C71-C72-C73-C74
71	1h	202	PC1	C2B-C2C-C2D-C2E
71	5h	202	PC1	C2B-C2C-C2D-C2E
82	8J	101	PGV	C2-C3-C4-C5
82	8C	304	PGV	C23-C24-C25-C26
82	8A	604	PGV	C11-C10-C9-C8
82	8C	302	PGV	C12-C13-C14-C15
82	8G	101	PGV	C11-C10-C9-C8
82	8C	303	PGV	C6-C7-C8-C9
82	8C	304	PGV	C10-C11-C12-C13
82	8G	101	PGV	C10-C11-C12-C13
82	8A	602	PGV	C30-C31-C32-C33
75	8D	201	CDL	C21-C22-C23-C24
69	1Y	203	3PE	O11-C1-C2-O21
69	5Y	203	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
75	4B	301	CDL	OA5-CA3-CA4-OA6
75	8B	302	CDL	OA5-CA3-CA4-OA6
82	8A	601	PGV	O01-C02-C03-O11
82	8J	101	PGV	C3-C4-C5-C6
71	1J	201	PC1	C23-C24-C25-C26
82	8C	304	PGV	C28-C29-C30-C31
82	8K	101	PGV	C26-C27-C28-C29
69	1A	201	3PE	C36-C37-C38-C39
75	1X	201	CDL	C58-C59-C60-C61
75	5X	201	CDL	C58-C59-C60-C61
90	8C	306	PEK	C26-C27-C28-C29
69	1Y	202	3PE	O21-C2-C3-O31
69	5Y	202	3PE	O21-C2-C3-O31
71	1J	201	PC1	O21-C2-C3-O31
71	1Y	201	PC1	O21-C2-C3-O31
71	5Y	201	PC1	O21-C2-C3-O31
75	1N	903	CDL	OA6-CA4-CA6-OA8
75	5N	903	CDL	OA6-CA4-CA6-OA8
82	4C	304	PGV	O03-C01-C02-O01
82	8C	302	PGV	C31-C32-C33-C34
71	1P	401	PC1	C11-C12-N-C15
82	8J	101	PGV	C15-C16-C17-C18
69	1Y	203	3PE	O31-C31-C32-C33
69	5Y	203	3PE	O31-C31-C32-C33
82	8A	601	PGV	C27-C28-C29-C30
90	4C	306	PEK	C26-C27-C28-C29
82	8C	304	PGV	C15-C16-C17-C18
82	8A	601	PGV	C15-C16-C17-C18
80	1T	101	EHZ	O5-C16-C17-C19
80	5T	101	EHZ	O5-C16-C17-C19
85	4A	606	HEA	C3B-C11-C12-C13
85	8A	606	HEA	C3B-C11-C12-C13
71	1m	201	PC1	C23-C24-C25-C26
82	8B	301	PGV	C14-C15-C16-C17
71	5m	201	PC1	C23-C24-C25-C26
82	8C	302	PGV	C30-C31-C32-C33
69	1A	201	3PE	C2E-C2F-C2G-C2H
82	8B	301	PGV	C31-C32-C33-C34
75	4C	308	CDL	C59-C60-C61-C62
75	8A	610	CDL	C59-C60-C61-C62
75	8A	610	CDL	C51-C52-C53-C54
82	8J	101	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
82	8C	304	PGV	O05-C05-C06-O06
82	8K	101	PGV	O05-C05-C06-O06
69	1Y	203	3PE	C2-C1-O11-P
69	5Y	203	3PE	C2-C1-O11-P
75	1d	202	CDL	CA4-CA3-OA5-PA1
75	5d	202	CDL	CA4-CA3-OA5-PA1
82	4C	302	PGV	C05-C04-O12-P
82	4K	101	PGV	C02-C03-O11-P
75	4C	308	CDL	C51-C52-C53-C54
75	8D	201	CDL	C73-C74-C75-C76
75	1N	903	CDL	C32-C31-CA7-OA8
75	5N	903	CDL	C32-C31-CA7-OA8
82	8C	302	PGV	C24-C25-C26-C27
69	1A	201	3PE	C39-C3A-C3B-C3C
69	1A	201	3PE	C2A-C2B-C2C-C2D
82	8A	604	PGV	C13-C14-C15-C16
69	1Y	202	3PE	O11-C1-C2-C3
69	5Y	202	3PE	O11-C1-C2-C3
75	8D	201	CDL	OB5-CB3-CB4-CB6
69	1A	201	3PE	C3B-C3C-C3D-C3E
75	1d	202	CDL	C12-C11-CA5-OA6
82	8C	303	PGV	C1-C2-C3-C4
82	8C	303	PGV	C28-C29-C30-C31
71	1I	201	PC1	O31-C31-C32-C33
71	5I	201	PC1	O31-C31-C32-C33
75	1q	201	CDL	C52-C51-CB5-OB6
75	5d	202	CDL	C12-C11-CA5-OA6
75	5q	201	CDL	C52-C51-CB5-OB6
82	8C	302	PGV	C10-C11-C12-C13
75	1X	201	CDL	C61-C62-C63-C64
75	8B	302	CDL	C38-C39-C40-C41
69	5N	901	3PE	C32-C33-C34-C35
75	4B	301	CDL	C38-C39-C40-C41
75	5X	201	CDL	C61-C62-C63-C64
82	4C	301	PGV	C22-C23-C24-C25
82	8K	101	PGV	C4-C5-C6-C7
71	1I	201	PC1	C1-C2-C3-O31
71	5I	201	PC1	C1-C2-C3-O31
71	5P	401	PC1	C1-C2-C3-O31
75	1N	903	CDL	CA3-CA4-CA6-OA8
75	5N	903	CDL	CA3-CA4-CA6-OA8
82	4A	604	PGV	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
82	4C	304	PGV	O03-C01-C02-C03
82	8C	302	PGV	O03-C01-C02-C03
71	1J	201	PC1	C35-C36-C37-C38
69	1N	901	3PE	C32-C33-C34-C35
71	1M	502	PC1	C23-C24-C25-C26
89	4B	303	PSC	C1-C2-C3-C4
71	5M	502	PC1	C23-C24-C25-C26
75	4C	308	CDL	C38-C39-C40-C41
75	8A	610	CDL	C38-C39-C40-C41
75	8D	201	CDL	C63-C64-C65-C66
82	8J	101	PGV	C27-C28-C29-C30
89	8A	611	PSC	C1-C2-C3-C4
69	1N	901	3PE	O11-C1-C2-O21
69	5N	901	3PE	O11-C1-C2-O21
71	1J	201	PC1	O11-C1-C2-O21
82	1p	201	PGV	O01-C02-C03-O11
82	8C	302	PGV	C22-C23-C24-C25
82	8A	604	PGV	O12-C04-C05-O05
75	4B	301	CDL	C1-CA2-OA2-PA1
75	8B	302	CDL	C1-CA2-OA2-PA1
76	1O	401	GTP	C4'-C5'-O5'-PA
76	5O	401	GTP	C4'-C5'-O5'-PA
82	4A	604	PGV	C02-C03-O11-P
82	8A	603	PGV	C02-C03-O11-P
82	8K	101	PGV	C29-C30-C31-C32
69	5J	201	3PE	C3A-C3B-C3C-C3D
69	1J	202	3PE	C3A-C3B-C3C-C3D
69	1A	201	3PE	O21-C21-C22-C23
69	1d	201	3PE	O21-C21-C22-C23
69	5A	201	3PE	O31-C31-C32-C33
69	5d	201	3PE	O21-C21-C22-C23
71	1B	202	PC1	O31-C31-C32-C33
71	5B	202	PC1	O31-C31-C32-C33
69	1d	201	3PE	O21-C2-C3-O31
69	5d	201	3PE	O21-C2-C3-O31
82	8C	301	PGV	O03-C01-C02-O01
82	8C	303	PGV	O03-C01-C02-O01
89	4B	303	PSC	O03-C01-C02-O01
89	8A	611	PSC	O03-C01-C02-O01
75	8D	201	CDL	C84-C85-C86-C87
90	4C	306	PEK	C6-C7-C8-C9
90	4C	306	PEK	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
90	4C	307	PEK	C11-C12-C13-C14
90	8C	306	PEK	C6-C7-C8-C9
90	8C	306	PEK	C9-C10-C11-C12
90	8C	307	PEK	C11-C12-C13-C14
75	8D	201	CDL	C32-C33-C34-C35
82	4K	101	PGV	C5-C6-C7-C8
82	8A	604	PGV	C21-C22-C23-C24
71	1P	401	PC1	C21-C22-C23-C24
82	8K	101	PGV	C1-C2-C3-C4
75	1X	201	CDL	C18-C19-C20-C21
75	5X	201	CDL	C18-C19-C20-C21
82	4C	305	PGV	C19-C20-C21-C22
82	8C	305	PGV	C19-C20-C21-C22
75	8D	201	CDL	C39-C40-C41-C42
82	8J	101	PGV	C29-C30-C31-C32
69	5A	201	3PE	O21-C21-C22-C23
76	1O	401	GTP	PB-O3A-PA-O5'
76	5O	401	GTP	PB-O3A-PA-O5'
82	8C	304	PGV	C31-C32-C33-C34
82	8C	304	PGV	C7-C8-C9-C10
82	8K	101	PGV	C30-C31-C32-C33
85	4A	605	HEA	C19-C20-C21-C22
85	8A	605	HEA	C19-C20-C21-C22
75	1N	903	CDL	C12-C13-C14-C15
75	8D	201	CDL	C41-C42-C43-C44
82	8A	602	PGV	C24-C25-C26-C27
75	5N	903	CDL	C12-C13-C14-C15
82	8B	301	PGV	O05-C05-C06-O06
82	8C	303	PGV	O05-C05-C06-O06
82	8B	301	PGV	C19-C20-C21-C22
82	8G	101	PGV	O12-C04-C05-C06
75	4C	308	CDL	C16-C17-C18-C19
75	8A	610	CDL	C16-C17-C18-C19
82	8C	301	PGV	C3-C4-C5-C6
82	4A	601	PGV	C11-C10-C9-C8
69	5d	201	3PE	C2C-C2D-C2E-C2F
69	1d	201	3PE	C2C-C2D-C2E-C2F
75	1X	201	CDL	C36-C37-C38-C39
82	8C	303	PGV	C26-C27-C28-C29
71	1P	401	PC1	O11-C1-C2-C3
75	4B	301	CDL	OA5-CA3-CA4-CA6
75	8B	302	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
75	1X	201	CDL	C1-CB2-OB2-PB2
75	5X	201	CDL	C1-CB2-OB2-PB2
82	8A	604	PGV	C23-C24-C25-C26
82	8A	602	PGV	C3-C4-C5-C6
71	1P	401	PC1	C33-C34-C35-C36
69	1N	901	3PE	C31-C32-C33-C34
69	5N	901	3PE	C31-C32-C33-C34
82	8G	101	PGV	C1-C2-C3-C4
69	1M	503	3PE	C26-C27-C28-C29
75	5X	201	CDL	C36-C37-C38-C39
69	5M	503	3PE	C26-C27-C28-C29
71	1J	201	PC1	C11-C12-N-C14
71	1P	401	PC1	C11-C12-N-C13
69	1Y	204	3PE	C35-C36-C37-C38
69	5Y	204	3PE	C35-C36-C37-C38
81	1h	201	AME	CB-CA-N-CT1
81	5h	201	AME	CB-CA-N-CT1
82	8A	603	PGV	C15-C16-C17-C18
69	1N	902	3PE	C1-C2-C3-O31
69	1Y	203	3PE	C1-C2-C3-O31
69	1Y	204	3PE	C1-C2-C3-O31
69	5N	902	3PE	C1-C2-C3-O31
69	5Y	203	3PE	C1-C2-C3-O31
69	5Y	204	3PE	C1-C2-C3-O31
71	1Y	201	PC1	C1-C2-C3-O31
71	5Y	201	PC1	C1-C2-C3-O31
75	1d	202	CDL	CA3-CA4-CA6-OA8
75	5d	202	CDL	CA3-CA4-CA6-OA8
82	4A	601	PGV	O03-C01-C02-C03
89	4B	303	PSC	O03-C01-C02-C03
89	8A	611	PSC	O03-C01-C02-C03
69	1L	704	3PE	C12-C11-O13-P
69	1M	503	3PE	C12-C11-O13-P
69	1N	902	3PE	C12-C11-O13-P
69	1j	101	3PE	C12-C11-O13-P
69	5L	704	3PE	C12-C11-O13-P
69	5M	503	3PE	C12-C11-O13-P
69	5N	902	3PE	C12-C11-O13-P
69	5j	101	3PE	C12-C11-O13-P
80	1T	101	EHZ	C15-C16-C17-C18
80	5T	101	EHZ	C15-C16-C17-C18
69	1N	902	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
69	1Y	203	3PE	O21-C2-C3-O31
69	5N	902	3PE	O21-C2-C3-O31
69	5Y	203	3PE	O21-C2-C3-O31
75	4B	301	CDL	OB6-CB4-CB6-OB8
75	8B	302	CDL	OB6-CB4-CB6-OB8
82	8A	603	PGV	O03-C01-C02-O01
90	4C	307	PEK	O03-C21-C22-C23
82	8A	604	PGV	C28-C29-C30-C31
69	5Y	202	3PE	C23-C24-C25-C26
69	1Y	202	3PE	C23-C24-C25-C26
69	1A	201	3PE	C31-C32-C33-C34
90	8C	307	PEK	O03-C21-C22-C23
82	4K	101	PGV	C22-C23-C24-C25
82	8C	301	PGV	C20-C21-C22-C23
82	4C	304	PGV	C19-C20-C21-C22
82	4J	101	PGV	C6-C7-C8-C9
71	1h	202	PC1	O13-C11-C12-N
71	5A	202	PC1	O13-C11-C12-N
71	5h	202	PC1	O13-C11-C12-N
75	4C	308	CDL	CB2-C1-CA2-OA2
75	8A	610	CDL	CB2-C1-CA2-OA2
82	8C	302	PGV	O12-C04-C05-C06
75	8A	610	CDL	O1-C1-CA2-OA2
82	8A	603	PGV	C20-C19-O03-C01
69	5M	503	3PE	C27-C28-C29-C2A
69	1M	503	3PE	C27-C28-C29-C2A
82	1p	201	PGV	C31-C32-C33-C34
75	8D	201	CDL	C77-C78-C79-C80
75	1d	202	CDL	OB5-CB3-CB4-CB6
75	5d	202	CDL	OB5-CB3-CB4-CB6
75	8D	201	CDL	OA5-CA3-CA4-CA6
82	1p	201	PGV	C01-C02-C03-O11
82	8A	601	PGV	C01-C02-C03-O11
82	8C	304	PGV	C20-C21-C22-C23
75	4C	308	CDL	O1-C1-CA2-OA2
82	8A	603	PGV	O04-C19-O03-C01
82	8B	301	PGV	C5-C6-C7-C8
82	4C	303	PGV	C11-C12-C13-C14
82	1p	201	PGV	C22-C23-C24-C25
69	1Y	205	3PE	C2-C1-O11-P
69	5A	201	3PE	C2-C1-O11-P
69	5Y	205	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
75	8D	201	CDL	C1-CA2-OA2-PA1
82	4C	302	PGV	C02-C03-O11-P
82	8A	601	PGV	C05-C04-O12-P
69	1Y	202	3PE	O11-C1-C2-O21
69	5Y	202	3PE	O11-C1-C2-O21
71	1P	401	PC1	O11-C1-C2-O21
71	5P	401	PC1	O11-C1-C2-O21
75	8D	201	CDL	OA5-CA3-CA4-OA6
75	8D	201	CDL	OB5-CB3-CB4-OB6
82	8A	601	PGV	C3-C4-C5-C6
75	1X	201	CDL	C31-C32-C33-C34
82	8A	601	PGV	C25-C26-C27-C28
69	1L	703	3PE	O21-C2-C3-O31
69	5L	703	3PE	O21-C2-C3-O31
71	1I	201	PC1	O21-C2-C3-O31
71	1h	202	PC1	O21-C2-C3-O31
71	5I	201	PC1	O21-C2-C3-O31
71	5h	202	PC1	O21-C2-C3-O31
75	1X	201	CDL	OB6-CB4-CB6-OB8
75	5X	201	CDL	OB6-CB4-CB6-OB8
82	1p	201	PGV	O03-C01-C02-O01
82	4J	101	PGV	O03-C01-C02-O01
82	8C	302	PGV	O03-C01-C02-O01
82	8J	101	PGV	C31-C32-C33-C34
75	5X	201	CDL	C31-C32-C33-C34
82	4A	604	PGV	C1-C2-C3-C4
75	4C	308	CDL	C81-C82-C83-C84
69	1Y	202	3PE	C1-C2-C3-O31
69	5Y	202	3PE	C1-C2-C3-O31
71	1J	201	PC1	C1-C2-C3-O31
80	1T	101	EHZ	C10-C11-N1-C12
80	1n	201	EHZ	C10-C11-N1-C12
80	5T	101	EHZ	C10-C11-N1-C12
80	5n	201	EHZ	C10-C11-N1-C12
82	8A	602	PGV	O03-C01-C02-C03
75	1X	201	CDL	C12-C11-CA5-OA6
82	4C	303	PGV	C23-C24-C25-C26
69	1N	902	3PE	C3F-C3G-C3H-C3I
69	5N	902	3PE	C3F-C3G-C3H-C3I
82	4A	602	PGV	C11-C12-C13-C14
82	4G	101	PGV	C11-C12-C13-C14
75	8A	610	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
69	5Y	206	3PE	C2D-C2E-C2F-C2G
82	8A	602	PGV	C5-C6-C7-C8
69	1Y	206	3PE	C2D-C2E-C2F-C2G
82	4A	603	PGV	C28-C29-C30-C31
71	1h	202	PC1	C2A-C2B-C2C-C2D
71	5h	202	PC1	C2A-C2B-C2C-C2D
75	8D	201	CDL	C59-C60-C61-C62
75	5X	201	CDL	C12-C11-CA5-OA6
69	5J	201	3PE	C34-C35-C36-C37
82	8A	604	PGV	C24-C25-C26-C27
69	1A	201	3PE	C1-O11-P-O13
69	1J	202	3PE	C1-O11-P-O12
69	1L	701	3PE	C11-O13-P-O14
69	1L	704	3PE	C11-O13-P-O14
69	1M	501	3PE	C1-O11-P-O13
69	1N	901	3PE	C11-O13-P-O12
69	1Y	203	3PE	C11-O13-P-O14
69	1Y	206	3PE	C1-O11-P-O14
69	1j	101	3PE	C1-O11-P-O12
69	1j	101	3PE	C1-O11-P-O13
69	5A	201	3PE	C1-O11-P-O13
69	5J	201	3PE	C1-O11-P-O12
69	5L	701	3PE	C11-O13-P-O14
69	5L	704	3PE	C11-O13-P-O14
69	5M	501	3PE	C1-O11-P-O13
69	5N	901	3PE	C11-O13-P-O12
69	5Y	203	3PE	C11-O13-P-O14
69	5Y	206	3PE	C1-O11-P-O14
69	5j	101	3PE	C1-O11-P-O12
69	5j	101	3PE	C1-O11-P-O13
71	1H	401	PC1	C11-O13-P-O14
71	1H	401	PC1	C1-O11-P-O12
71	1J	201	PC1	C11-O13-P-O14
71	5H	401	PC1	C11-O13-P-O14
71	5H	401	PC1	C1-O11-P-O12
75	1d	202	CDL	CA2-OA2-PA1-OA3
75	1d	202	CDL	CB2-OB2-PB2-OB3
75	1q	201	CDL	CA3-OA5-PA1-OA3
75	4B	301	CDL	CA2-OA2-PA1-OA3
75	4B	301	CDL	CA3-OA5-PA1-OA2
75	4B	301	CDL	CB3-OB5-PB2-OB4
75	4C	308	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
75	4C	308	CDL	CB3-OB5-PB2-OB3
75	5d	202	CDL	CA2-OA2-PA1-OA3
75	5d	202	CDL	CB2-OB2-PB2-OB3
75	5q	201	CDL	CA3-OA5-PA1-OA3
75	8A	610	CDL	CB2-OB2-PB2-OB3
75	8A	610	CDL	CB3-OB5-PB2-OB3
75	8B	302	CDL	CA2-OA2-PA1-OA3
75	8B	302	CDL	CA3-OA5-PA1-OA2
75	8B	302	CDL	CB3-OB5-PB2-OB4
75	8D	201	CDL	CA2-OA2-PA1-OA4
82	1p	201	PGV	C03-O11-P-O12
82	1p	201	PGV	C03-O11-P-O14
82	4K	101	PGV	C04-O12-P-O13
82	4L	101	PGV	C03-O11-P-O13
82	8A	602	PGV	C03-O11-P-O13
82	8A	602	PGV	C04-O12-P-O11
82	8A	602	PGV	C04-O12-P-O13
82	8A	604	PGV	C04-O12-P-O11
82	8A	604	PGV	C04-O12-P-O13
82	8B	301	PGV	C04-O12-P-O13
82	8C	304	PGV	C03-O11-P-O13
82	8C	304	PGV	C04-O12-P-O13
82	8K	101	PGV	C04-O12-P-O11
82	8K	101	PGV	C04-O12-P-O14
82	8L	101	PGV	C03-O11-P-O13
69	1J	202	3PE	C34-C35-C36-C37
71	1J	201	PC1	C2-C1-O11-P
82	1p	201	PGV	C05-C04-O12-P
82	4C	303	PGV	C05-C04-O12-P
82	4K	101	PGV	C05-C04-O12-P
82	8A	602	PGV	C02-C03-O11-P
82	8A	602	PGV	C05-C04-O12-P
82	8B	301	PGV	C05-C04-O12-P
82	8C	302	PGV	C05-C04-O12-P
69	1N	901	3PE	C2D-C2E-C2F-C2G
82	8C	301	PGV	C15-C16-C17-C18
69	5N	901	3PE	C2D-C2E-C2F-C2G
71	1J	201	PC1	C33-C34-C35-C36
82	8C	303	PGV	C03-C02-O01-C1
69	1Y	203	3PE	O11-C1-C2-C3
69	5Y	203	3PE	O11-C1-C2-C3
75	5X	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
82	4K	101	PGV	C9-C10-C11-C12
82	8C	302	PGV	C11-C12-C13-C14
69	5d	201	3PE	C3C-C3D-C3E-C3F
69	1d	201	3PE	C3C-C3D-C3E-C3F
69	5A	201	3PE	C36-C37-C38-C39
75	1X	201	CDL	C55-C56-C57-C58
82	8C	301	PGV	C4-C5-C6-C7
69	5N	901	3PE	C2B-C2C-C2D-C2E
75	8A	610	CDL	C52-C53-C54-C55
82	8A	604	PGV	O04-C19-O03-C01
75	4C	308	CDL	C52-C53-C54-C55
82	1p	201	PGV	C02-C03-O11-P
82	8C	301	PGV	C25-C26-C27-C28
71	5P	401	PC1	O21-C2-C3-O31
75	1d	202	CDL	OA6-CA4-CA6-OA8
75	5d	202	CDL	OA6-CA4-CA6-OA8
82	4A	601	PGV	O03-C01-C02-O01
69	1N	901	3PE	C2B-C2C-C2D-C2E
82	8A	604	PGV	C20-C19-O03-C01
71	1P	401	PC1	C11-C12-N-C14
75	5i	201	CDL	CB7-C71-C72-C73
85	4A	605	HEA	C4D-C3D-CAD-CBD
85	8A	605	HEA	C4D-C3D-CAD-CBD
82	8C	303	PGV	C11-C10-C9-C8
80	1T	101	EHZ	O5-C16-C17-C18
80	5T	101	EHZ	O5-C16-C17-C18
69	5M	501	3PE	C23-C24-C25-C26
75	1i	201	CDL	CB7-C71-C72-C73
82	4C	303	PGV	O03-C19-C20-C21
75	4C	308	CDL	C11-C12-C13-C14
80	1n	201	EHZ	C7-C8-C9-O2
80	5n	201	EHZ	C7-C8-C9-O2
69	1M	501	3PE	C23-C24-C25-C26
75	8A	610	CDL	C11-C12-C13-C14
82	8J	101	PGV	C10-C11-C12-C13
75	1X	201	CDL	CA7-C31-C32-C33
82	8A	603	PGV	C12-C13-C14-C15
75	1L	702	CDL	C11-C12-C13-C14
75	5L	702	CDL	C11-C12-C13-C14
82	4C	303	PGV	C21-C22-C23-C24
75	5X	201	CDL	CA7-C31-C32-C33
71	1P	401	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
75	4C	308	CDL	CA2-C1-CB2-OB2
75	8A	610	CDL	CA2-C1-CB2-OB2
82	8A	604	PGV	C05-C04-O12-P
90	4C	306	PEK	C02-C03-O11-P
90	8C	306	PEK	C02-C03-O11-P
75	5X	201	CDL	C35-C36-C37-C38
69	1L	704	3PE	C23-C24-C25-C26
83	6C	501	HEM	CAD-CBD-CGD-O2D
75	8D	201	CDL	C11-C12-C13-C14
69	5L	704	3PE	C23-C24-C25-C26
75	1X	201	CDL	C35-C36-C37-C38
69	1M	501	3PE	C21-C22-C23-C24
69	1L	703	3PE	C28-C29-C2A-C2B
69	5L	703	3PE	C28-C29-C2A-C2B
82	4K	101	PGV	C13-C14-C15-C16
69	1Y	203	3PE	O32-C31-C32-C33
69	5Y	203	3PE	O32-C31-C32-C33
82	4C	302	PGV	C11-C12-C13-C14
82	4C	304	PGV	C9-C10-C11-C12
82	8K	101	PGV	C9-C10-C11-C12
83	6C	502	HEM	C4B-C3B-CAB-CBB
75	8A	610	CDL	C72-C73-C74-C75
75	4C	308	CDL	C72-C73-C74-C75
75	8D	201	CDL	C22-C23-C24-C25
71	1B	202	PC1	C23-C24-C25-C26
71	5B	202	PC1	C23-C24-C25-C26
82	8C	304	PGV	C30-C31-C32-C33
82	8K	101	PGV	O12-C04-C05-O05
82	4C	303	PGV	C3-C4-C5-C6
69	1N	902	3PE	C24-C25-C26-C27
82	4A	604	PGV	C2-C3-C4-C5
89	8A	611	PSC	C7-C8-C9-C10
90	4C	306	PEK	C3-C4-C5-C6
90	8C	306	PEK	C3-C4-C5-C6
82	4C	303	PGV	O03-C01-C02-O01
69	5N	902	3PE	C24-C25-C26-C27
69	5A	201	3PE	C28-C29-C2A-C2B
75	4B	301	CDL	C61-C62-C63-C64
89	4B	303	PSC	C7-C8-C9-C10
75	8B	302	CDL	C61-C62-C63-C64
80	5T	101	EHZ	C1-C2-C3-C4
69	1Y	206	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
69	5Y	206	3PE	C2-C1-O11-P
75	1d	202	CDL	CB4-CB3-OB5-PB2
75	5d	202	CDL	CB4-CB3-OB5-PB2
80	1T	101	EHZ	C1-C2-C3-C4
69	5M	501	3PE	C21-C22-C23-C24
75	1X	201	CDL	C12-C13-C14-C15
69	1d	201	3PE	O22-C21-C22-C23
69	5d	201	3PE	O22-C21-C22-C23
83	3P	502	HEM	CAA-CBA-CGA-O1A
83	3P	502	HEM	CAA-CBA-CGA-O2A
83	6C	501	HEM	CAD-CBD-CGD-O1D
83	6P	502	HEM	CAA-CBA-CGA-O1A
83	6P	502	HEM	CAA-CBA-CGA-O2A
85	4A	605	HEA	CAD-CBD-CGD-O1D
85	8A	605	HEA	CAD-CBD-CGD-O1D
75	5X	201	CDL	C12-C13-C14-C15
82	4J	101	PGV	C11-C12-C13-C14
82	8C	302	PGV	C25-C26-C27-C28
82	4C	305	PGV	C14-C15-C16-C17
71	5h	202	PC1	C22-C23-C24-C25
82	4C	304	PGV	C20-C21-C22-C23
82	8C	305	PGV	C14-C15-C16-C17
82	1p	201	PGV	C01-C02-O01-C1
82	1p	201	PGV	C03-C02-O01-C1
71	1h	202	PC1	C22-C23-C24-C25
82	8C	301	PGV	C22-C23-C24-C25
75	1i	201	CDL	C34-C35-C36-C37
71	5I	201	PC1	C2B-C2C-C2D-C2E
75	5i	201	CDL	C34-C35-C36-C37
71	1I	201	PC1	C2B-C2C-C2D-C2E
69	5L	703	3PE	C25-C26-C27-C28
82	4J	101	PGV	C2-C3-C4-C5
69	1L	703	3PE	C25-C26-C27-C28
69	5A	201	3PE	O32-C31-C32-C33
82	4C	303	PGV	C02-C01-O03-C19
71	5B	202	PC1	O32-C31-C32-C33
82	8J	101	PGV	C23-C24-C25-C26
69	1M	501	3PE	C2-C1-O11-P
69	5M	501	3PE	C2-C1-O11-P
75	1L	702	CDL	CA4-CA3-OA5-PA1
75	5L	702	CDL	CA4-CA3-OA5-PA1
82	8A	601	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
81	1h	201	AME	C-CA-N-CT1
81	5h	201	AME	C-CA-N-CT1
83	3C	502	HEM	CAA-CBA-CGA-O2A
85	4A	605	HEA	CAD-CBD-CGD-O2D
85	4A	606	HEA	CAD-CBD-CGD-O1D
85	8A	605	HEA	CAD-CBD-CGD-O2D
85	8A	606	HEA	CAD-CBD-CGD-O1D
71	1J	201	PC1	O11-C1-C2-C3
75	1d	202	CDL	OA5-CA3-CA4-CA6
75	5d	202	CDL	OA5-CA3-CA4-CA6
71	1B	202	PC1	O32-C31-C32-C33
75	8D	201	CDL	C24-C25-C26-C27
82	8A	603	PGV	C20-C21-C22-C23
83	3C	501	HEM	CAA-CBA-CGA-O1A
90	4C	306	PEK	C14-C15-C16-C17
90	8C	306	PEK	C14-C15-C16-C17
82	8C	304	PGV	O03-C01-C02-O01
83	3P	501	HEM	CAA-CBA-CGA-O2A
83	3P	501	HEM	CAD-CBD-CGD-O1D
83	6P	501	HEM	CAA-CBA-CGA-O2A
83	6P	501	HEM	CAD-CBD-CGD-O1D
78	1P	402	NDP	C2N-C3N-C7N-N7N
78	5P	402	NDP	C2N-C3N-C7N-N7N
82	8G	101	PGV	C25-C26-C27-C28
83	3P	501	HEM	CAA-CBA-CGA-O1A
83	6P	501	HEM	CAA-CBA-CGA-O1A
82	4L	101	PGV	C24-C25-C26-C27
82	8L	101	PGV	C24-C25-C26-C27
82	8C	305	PGV	C5-C6-C7-C8
82	8A	601	PGV	O02-C1-O01-C02
75	4B	301	CDL	C11-C12-C13-C14
75	8B	302	CDL	C11-C12-C13-C14
82	4C	305	PGV	C5-C6-C7-C8
82	4A	602	PGV	C22-C23-C24-C25
82	4K	101	PGV	C3-C4-C5-C6
82	4A	603	PGV	C11-C12-C13-C14
82	4J	101	PGV	C5-C6-C7-C8
75	4C	308	CDL	C18-C19-C20-C21
82	4C	304	PGV	C4-C5-C6-C7
75	8A	610	CDL	C18-C19-C20-C21
75	8D	201	CDL	C53-C54-C55-C56
85	4A	606	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
85	8A	606	HEA	CAD-CBD-CGD-O2D
82	4A	604	PGV	C5-C6-C7-C8
82	8C	301	PGV	C24-C25-C26-C27
69	1A	201	3PE	C22-C23-C24-C25
83	3C	502	HEM	CAA-CBA-CGA-O1A
85	4A	606	HEA	C26-C15-C16-C17
85	8A	606	HEA	C26-C15-C16-C17
83	3P	501	HEM	CAD-CBD-CGD-O2D
71	1Y	201	PC1	C2-C1-O11-P
71	5Y	201	PC1	C2-C1-O11-P
82	8C	304	PGV	C02-C03-O11-P
69	1L	701	3PE	C28-C29-C2A-C2B
69	5L	701	3PE	C28-C29-C2A-C2B
82	4A	603	PGV	C14-C15-C16-C17
83	6P	501	HEM	CAD-CBD-CGD-O2D
75	1q	201	CDL	C52-C51-CB5-OB7
75	5q	201	CDL	C52-C51-CB5-OB7
75	4C	308	CDL	C37-C38-C39-C40
82	8A	604	PGV	C1-C2-C3-C4
85	4A	605	HEA	C2D-C3D-CAD-CBD
85	8A	605	HEA	C2D-C3D-CAD-CBD
75	8A	610	CDL	C37-C38-C39-C40
82	8C	303	PGV	O03-C01-C02-C03
82	8C	301	PGV	C7-C8-C9-C10
75	8D	201	CDL	C74-C75-C76-C77
75	5X	201	CDL	C63-C64-C65-C66
69	1Y	203	3PE	C23-C24-C25-C26
82	4C	304	PGV	C6-C7-C8-C9
69	5Y	203	3PE	C23-C24-C25-C26
82	8A	602	PGV	C15-C16-C17-C18
75	1X	201	CDL	C63-C64-C65-C66
69	5d	201	3PE	C36-C37-C38-C39
80	5T	101	EHZ	C1-C21-C22-C23
82	1p	201	PGV	C9-C10-C11-C12
82	4C	303	PGV	C9-C10-C11-C12
82	8A	604	PGV	O03-C19-C20-C21
75	8D	201	CDL	C80-C81-C82-C83
69	1d	201	3PE	C36-C37-C38-C39
82	4C	302	PGV	C14-C15-C16-C17
82	8C	303	PGV	C2-C3-C4-C5
71	1I	201	PC1	C38-C39-C3A-C3B
71	5I	201	PC1	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
80	1T	101	EHZ	C1-C21-C22-C23
69	1N	901	3PE	O11-C1-C2-C3
69	5N	901	3PE	O11-C1-C2-C3
82	8K	101	PGV	C01-C02-C03-O11
82	8C	302	PGV	O01-C1-C2-C3
69	1J	202	3PE	C23-C24-C25-C26
69	5J	201	3PE	C23-C24-C25-C26
69	1J	202	3PE	C28-C29-C2A-C2B
83	3C	501	HEM	CAA-CBA-CGA-O2A
84	3Q	501	HEC	CAA-CBA-CGA-O2A
84	6Q	501	HEC	CAA-CBA-CGA-O2A
69	5J	201	3PE	C28-C29-C2A-C2B
71	1B	202	PC1	C35-C36-C37-C38
71	5B	202	PC1	C33-C34-C35-C36
82	4C	302	PGV	C1-C2-C3-C4
71	5B	202	PC1	C35-C36-C37-C38
75	8A	610	CDL	C36-C37-C38-C39
82	8A	601	PGV	C12-C13-C14-C15
75	4C	308	CDL	C36-C37-C38-C39
71	1B	202	PC1	C33-C34-C35-C36
69	1A	201	3PE	O22-C21-C22-C23
75	1N	903	CDL	C32-C31-CA7-OA9
82	4A	601	PGV	C9-C10-C11-C12
82	8C	304	PGV	C11-C12-C13-C14
75	4B	301	CDL	C60-C61-C62-C63
75	5N	903	CDL	C32-C31-CA7-OA9
82	1p	201	PGV	C04-C05-C06-O06
82	8A	603	PGV	C04-C05-C06-O06
69	5Y	206	3PE	C2A-C2B-C2C-C2D
82	4C	305	PGV	C11-C12-C13-C14
82	4K	101	PGV	C11-C12-C13-C14
82	8C	305	PGV	C11-C12-C13-C14
75	8B	302	CDL	C60-C61-C62-C63
69	1L	701	3PE	C25-C26-C27-C28
69	1Y	206	3PE	C2A-C2B-C2C-C2D
84	3Q	501	HEC	CAA-CBA-CGA-O1A
69	5Y	203	3PE	C21-C22-C23-C24
69	1M	501	3PE	C36-C37-C38-C39
69	5M	501	3PE	C36-C37-C38-C39
84	6Q	501	HEC	CAA-CBA-CGA-O1A
82	8J	101	PGV	C05-C04-O12-P
75	8B	302	CDL	CB5-C51-C52-C53

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Mol	Chain	Res	Type	Atoms
82	8J	101	PGV	C24-C25-C26-C27
82	4C	301	PGV	C20-C19-O03-C01
69	1d	201	3PE	C1-C2-C3-O31
69	5d	201	3PE	C1-C2-C3-O31
82	8A	603	PGV	O03-C01-C02-C03
82	8C	301	PGV	O03-C01-C02-C03
69	1Y	203	3PE	C21-C22-C23-C24
75	4B	301	CDL	CB5-C51-C52-C53
69	5L	701	3PE	C25-C26-C27-C28
89	8A	611	PSC	C3-C4-C5-C6
85	4A	605	HEA	C26-C15-C16-C17
85	8A	605	HEA	C26-C15-C16-C17
82	8J	101	PGV	C20-C21-C22-C23
90	4C	306	PEK	C05-C04-O12-P
90	8C	306	PEK	C05-C04-O12-P
69	5L	703	3PE	C29-C2A-C2B-C2C
89	8A	611	PSC	C27-C28-C29-C30
71	5B	202	PC1	C37-C38-C39-C3A
69	1L	703	3PE	C29-C2A-C2B-C2C
82	4A	601	PGV	C7-C8-C9-C10
84	3D	501	HEC	CAA-CBA-CGA-O2A
89	4B	303	PSC	C3-C4-C5-C6
71	1P	401	PC1	O21-C2-C3-O31
89	4B	303	PSC	C27-C28-C29-C30
82	1p	201	PGV	O12-C04-C05-O05
82	8A	604	PGV	C11-C12-C13-C14
71	1B	202	PC1	C37-C38-C39-C3A
82	8C	301	PGV	C01-C02-C03-O11
71	1m	201	PC1	C24-C25-C26-C27
82	4G	101	PGV	C21-C22-C23-C24
75	1d	202	CDL	C12-C11-CA5-OA7
75	5d	202	CDL	C12-C11-CA5-OA7
82	8A	603	PGV	C25-C26-C27-C28
71	5m	201	PC1	C24-C25-C26-C27
82	4K	101	PGV	C2-C3-C4-C5
71	5P	401	PC1	C22-C23-C24-C25
82	4J	101	PGV	C9-C10-C11-C12
82	8A	602	PGV	C11-C12-C13-C14
82	8G	101	PGV	C02-C03-O11-P
83	3P	502	HEM	CAD-CBD-CGD-O1D
71	1Y	201	PC1	C2-C3-O31-C31
71	5Y	201	PC1	C2-C3-O31-C31

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Mol	Chain	Res	Type	Atoms
71	1J	201	PC1	O31-C31-C32-C33
71	1I	201	PC1	C32-C33-C34-C35
83	6P	502	HEM	CAD-CBD-CGD-O1D
82	8C	302	PGV	O02-C1-O01-C02
82	4L	101	PGV	C9-C10-C11-C12
82	8C	301	PGV	C11-C12-C13-C14
82	8L	101	PGV	C9-C10-C11-C12
82	8A	601	PGV	C2-C1-O01-C02
71	1I	201	PC1	O32-C31-C32-C33
71	5I	201	PC1	O32-C31-C32-C33
71	5I	201	PC1	C32-C33-C34-C35
75	1L	702	CDL	C72-C71-CB7-OB8
82	8B	301	PGV	O03-C19-C20-C21
75	4C	308	CDL	C22-C23-C24-C25
82	4C	301	PGV	C24-C25-C26-C27
82	8C	301	PGV	O01-C02-C03-O11
75	8A	610	CDL	C22-C23-C24-C25
75	8D	201	CDL	C61-C62-C63-C64
82	4C	304	PGV	C24-C25-C26-C27
82	8A	603	PGV	C4-C5-C6-C7
82	4A	603	PGV	C6-C7-C8-C9
75	5L	702	CDL	C72-C71-CB7-OB8
69	1L	703	3PE	C34-C35-C36-C37
90	4C	306	PEK	C21-C22-C23-C24
69	5Y	202	3PE	C2D-C2E-C2F-C2G
82	4G	101	PGV	C7-C8-C9-C10
90	8C	306	PEK	C21-C22-C23-C24
69	5L	704	3PE	O21-C21-C22-C23
71	1m	201	PC1	O21-C21-C22-C23
71	5m	201	PC1	O21-C21-C22-C23
82	8B	301	PGV	O01-C1-C2-C3
71	1P	401	PC1	C1-C2-C3-O31
69	5L	703	3PE	C34-C35-C36-C37
71	1m	201	PC1	C39-C3A-C3B-C3C
69	1L	704	3PE	O21-C21-C22-C23
69	1Y	203	3PE	O21-C21-C22-C23
69	5Y	203	3PE	O21-C21-C22-C23
82	8A	601	PGV	O03-C19-C20-C21
71	5m	201	PC1	C39-C3A-C3B-C3C
69	1Y	202	3PE	C2D-C2E-C2F-C2G
69	5Y	206	3PE	C26-C27-C28-C29
84	3D	501	HEC	C3D-CAD-CBD-CGD

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Mol	Chain	Res	Type	Atoms
69	1Y	206	3PE	C26-C27-C28-C29
90	4C	307	PEK	O04-C21-C22-C23
90	8C	307	PEK	O04-C21-C22-C23
69	1M	501	3PE	C3A-C3B-C3C-C3D
69	1N	901	3PE	O31-C31-C32-C33
69	5N	901	3PE	O31-C31-C32-C33
71	5P	401	PC1	O21-C21-C22-C23
82	4A	601	PGV	O03-C19-C20-C21
82	4C	303	PGV	C29-C30-C31-C32
69	1M	503	3PE	C3A-C3B-C3C-C3D
82	4C	304	PGV	O03-C19-C20-C21
82	1p	201	PGV	O12-C04-C05-C06
90	4C	307	PEK	C22-C23-C24-C25
90	8C	307	PEK	C22-C23-C24-C25
69	5M	503	3PE	C3A-C3B-C3C-C3D
83	6P	502	HEM	CAD-CBD-CGD-O2D
69	1N	902	3PE	C3-C2-O21-C21
69	5N	902	3PE	C3-C2-O21-C21
82	4C	303	PGV	C01-C02-O01-C1
69	5M	501	3PE	C3A-C3B-C3C-C3D
83	3P	502	HEM	CAD-CBD-CGD-O2D
82	4L	101	PGV	C21-C22-C23-C24
69	5A	201	3PE	O22-C21-C22-C23
84	3D	501	HEC	CAA-CBA-CGA-O1A
75	4B	301	CDL	C12-C11-CA5-OA6
80	1n	201	EHZ	C11-C10-S1-C9
80	5n	201	EHZ	C11-C10-S1-C9
75	1L	702	CDL	C72-C71-CB7-OB9
75	5L	702	CDL	C72-C71-CB7-OB9
82	8L	101	PGV	C21-C22-C23-C24
75	8B	302	CDL	C12-C11-CA5-OA6
75	8D	201	CDL	C12-C11-CA5-OA6
82	4A	604	PGV	C26-C27-C28-C29
69	1L	704	3PE	O22-C21-C22-C23
75	4B	301	CDL	C56-C57-C58-C59
75	8B	302	CDL	C56-C57-C58-C59
82	4C	303	PGV	O01-C02-C03-O11
82	4J	101	PGV	C26-C27-C28-C29
82	8C	304	PGV	C2-C3-C4-C5
71	5m	201	PC1	C37-C38-C39-C3A
75	5q	201	CDL	C53-C54-C55-C56
69	5L	704	3PE	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
71	1J	201	PC1	O32-C31-C32-C33
75	1q	201	CDL	C53-C54-C55-C56
71	1m	201	PC1	C37-C38-C39-C3A
82	8A	603	PGV	C3-C4-C5-C6
82	8B	301	PGV	O04-C19-C20-C21
90	4C	307	PEK	C3-C4-C5-C6
82	4C	304	PGV	O04-C19-C20-C21
82	8K	101	PGV	C5-C6-C7-C8
69	5Y	206	3PE	C23-C24-C25-C26
71	5M	502	PC1	O21-C21-C22-C23
84	3Q	501	HEC	CAD-CBD-CGD-O2D
84	6Q	501	HEC	CAD-CBD-CGD-O2D
82	8B	301	PGV	O02-C1-C2-C3
75	1L	702	CDL	C36-C37-C38-C39
75	5L	702	CDL	C36-C37-C38-C39
71	1Y	201	PC1	O22-C21-C22-C23
71	5Y	201	PC1	O22-C21-C22-C23
82	4A	601	PGV	O04-C19-C20-C21
82	8A	601	PGV	O04-C19-C20-C21
71	1M	502	PC1	O21-C21-C22-C23
82	8K	101	PGV	O01-C1-C2-C3
69	1Y	206	3PE	C23-C24-C25-C26
82	8J	101	PGV	O03-C01-C02-C03
90	8C	307	PEK	C3-C4-C5-C6
69	5Y	203	3PE	O22-C21-C22-C23
71	1M	502	PC1	O22-C21-C22-C23
71	1m	201	PC1	O22-C21-C22-C23
71	5m	201	PC1	O22-C21-C22-C23
71	1Y	201	PC1	O21-C21-C22-C23
71	5Y	201	PC1	O21-C21-C22-C23
85	4A	605	HEA	CAA-CBA-CGA-O2A
69	1Y	203	3PE	O22-C21-C22-C23
71	5M	502	PC1	O22-C21-C22-C23
82	4A	604	PGV	C20-C21-C22-C23
82	8C	301	PGV	C31-C32-C33-C34
69	1N	901	3PE	O32-C31-C32-C33
69	5N	901	3PE	O32-C31-C32-C33
82	4J	101	PGV	C28-C29-C30-C31
71	1h	202	PC1	O31-C31-C32-C33
71	5h	202	PC1	O31-C31-C32-C33
82	4G	101	PGV	O03-C19-C20-C21
69	1J	202	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
71	5M	502	PC1	C2D-C2E-C2F-C2G
71	1M	502	PC1	C2D-C2E-C2F-C2G
85	8A	605	HEA	CAA-CBA-CGA-O2A
71	1B	202	PC1	C3D-C3E-C3F-C3G
75	8D	201	CDL	C12-C11-CA5-OA7
71	5B	202	PC1	C3D-C3E-C3F-C3G
69	1Y	206	3PE	O31-C31-C32-C33
69	5Y	206	3PE	O31-C31-C32-C33
69	5d	201	3PE	O31-C31-C32-C33
82	8A	602	PGV	O03-C19-C20-C21
82	4C	302	PGV	C2-C3-C4-C5
82	4A	601	PGV	C15-C16-C17-C18
82	8C	302	PGV	C2-C1-O01-C02
78	1P	402	NDP	PN-O3-PA-O2A
78	5P	402	NDP	PN-O3-PA-O2A
75	8A	610	CDL	C20-C21-C22-C23
69	1d	201	3PE	O31-C31-C32-C33
71	1P	401	PC1	O21-C21-C22-C23
75	1q	201	CDL	C12-C11-CA5-OA6
75	5q	201	CDL	C12-C11-CA5-OA6
82	4C	301	PGV	O03-C19-C20-C21
82	8J	101	PGV	O03-C19-C20-C21
69	5J	201	3PE	C37-C38-C39-C3A
85	4A	606	HEA	CAA-CBA-CGA-O2A
85	8A	606	HEA	CAA-CBA-CGA-O2A
75	4C	308	CDL	C43-C44-C45-C46
75	8A	610	CDL	C43-C44-C45-C46
82	4A	604	PGV	C24-C25-C26-C27

There are no ring outliers.

144 monomers are involved in 752 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	4A	604	PGV	7	0
69	1J	202	3PE	5	0
70	1F	502	SF4	2	0
72	3E	301	FES	4	0
83	6C	502	HEM	6	0
69	1L	703	3PE	4	0
82	8A	604	PGV	7	0
73	1F	501	FMN	2	0
69	1M	501	3PE	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	1Y	205	3PE	4	0
71	1B	202	PC1	3	0
90	4C	307	PEK	4	0
72	1G	803	FES	1	0
69	5A	201	3PE	2	0
82	4A	603	PGV	10	0
71	1J	201	PC1	4	0
80	5n	201	EHZ	1	0
82	4C	301	PGV	4	0
85	4A	605	HEA	5	0
82	8K	101	PGV	9	0
78	1P	402	NDP	1	0
71	5B	202	PC1	2	0
83	6C	501	HEM	10	0
83	6P	502	HEM	5	0
70	1G	802	SF4	1	0
82	8C	304	PGV	10	0
90	4C	306	PEK	3	0
70	1B	201	SF4	5	0
82	4C	305	PGV	7	0
71	5M	502	PC1	8	0
80	1T	101	EHZ	1	0
75	8A	610	CDL	28	0
71	1Y	201	PC1	3	0
71	5A	202	PC1	1	0
71	5I	204	PC1	4	0
69	5Y	202	3PE	1	0
71	5H	401	PC1	5	0
71	1I	204	PC1	5	0
72	3R	301	FES	1	0
81	1h	201	AME	3	0
84	6Q	501	HEC	2	0
82	1p	201	PGV	4	0
71	1H	401	PC1	7	0
82	4C	304	PGV	6	0
85	4A	606	HEA	3	0
69	5Y	204	3PE	2	0
71	5P	401	PC1	2	0
80	1n	201	EHZ	1	0
72	5E	301	FES	1	0
69	5Y	206	3PE	5	0
84	3Q	501	HEC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	5G	802	SF4	1	0
75	5d	202	CDL	7	0
71	5m	201	PC1	5	0
71	5Y	201	PC1	3	0
69	1A	201	3PE	4	0
75	5L	702	CDL	2	0
82	4C	302	PGV	9	0
83	3P	501	HEM	1	0
82	8C	302	PGV	6	0
78	5P	402	NDP	1	0
80	5T	101	EHZ	1	0
69	5Y	205	3PE	4	0
71	1m	201	PC1	5	0
75	8B	302	CDL	7	0
82	8C	303	PGV	11	0
75	4B	301	CDL	6	0
75	5X	201	CDL	13	0
69	5J	201	3PE	5	0
69	5d	201	3PE	12	0
88	4B	302	CUA	3	0
71	1I	201	PC1	6	0
75	5q	201	CDL	5	0
69	1M	503	3PE	7	0
70	5F	502	SF4	2	0
72	1E	301	FES	1	0
69	5Y	203	3PE	5	0
75	1d	202	CDL	7	0
83	3P	502	HEM	5	0
69	1Y	206	3PE	5	0
72	6E	301	FES	4	0
73	5F	501	FMN	1	0
70	5B	201	SF4	2	0
82	8A	602	PGV	13	0
75	1i	201	CDL	8	0
84	3D	501	HEC	2	0
82	4L	101	PGV	12	0
69	5M	501	3PE	5	0
75	1L	702	CDL	3	0
75	5i	201	CDL	9	0
82	4C	303	PGV	8	0
82	8G	101	PGV	12	0
69	1Y	203	3PE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	1Y	202	3PE	1	0
71	1M	502	PC1	8	0
69	1L	704	3PE	1	0
71	5I	201	PC1	7	0
82	8C	301	PGV	2	0
69	1Y	204	3PE	2	0
72	6R	301	FES	1	0
71	1P	401	PC1	5	0
83	3C	501	HEM	5	0
69	5M	503	3PE	8	0
76	1O	401	GTP	4	0
83	6P	501	HEM	1	0
85	8A	606	HEA	6	0
69	1d	201	3PE	11	0
89	8A	611	PSC	7	0
69	1N	902	3PE	15	0
81	5h	201	AME	3	0
75	5N	903	CDL	4	0
69	5L	703	3PE	4	0
69	5L	704	3PE	1	0
83	3C	502	HEM	6	0
82	8A	601	PGV	7	0
69	5N	902	3PE	15	0
72	5G	803	FES	1	0
75	4C	308	CDL	18	0
69	1L	701	3PE	3	0
82	4G	101	PGV	8	0
75	1q	201	CDL	5	0
82	8J	101	PGV	11	0
75	8D	201	CDL	19	0
82	4A	601	PGV	10	0
82	4A	602	PGV	3	0
90	8C	306	PEK	4	0
82	8B	301	PGV	10	0
76	5O	401	GTP	5	0
71	1h	202	PC1	3	0
82	4J	101	PGV	11	0
82	8C	305	PGV	12	0
69	5L	701	3PE	2	0
90	8C	307	PEK	5	0
82	8L	101	PGV	7	0
85	8A	605	HEA	10	0

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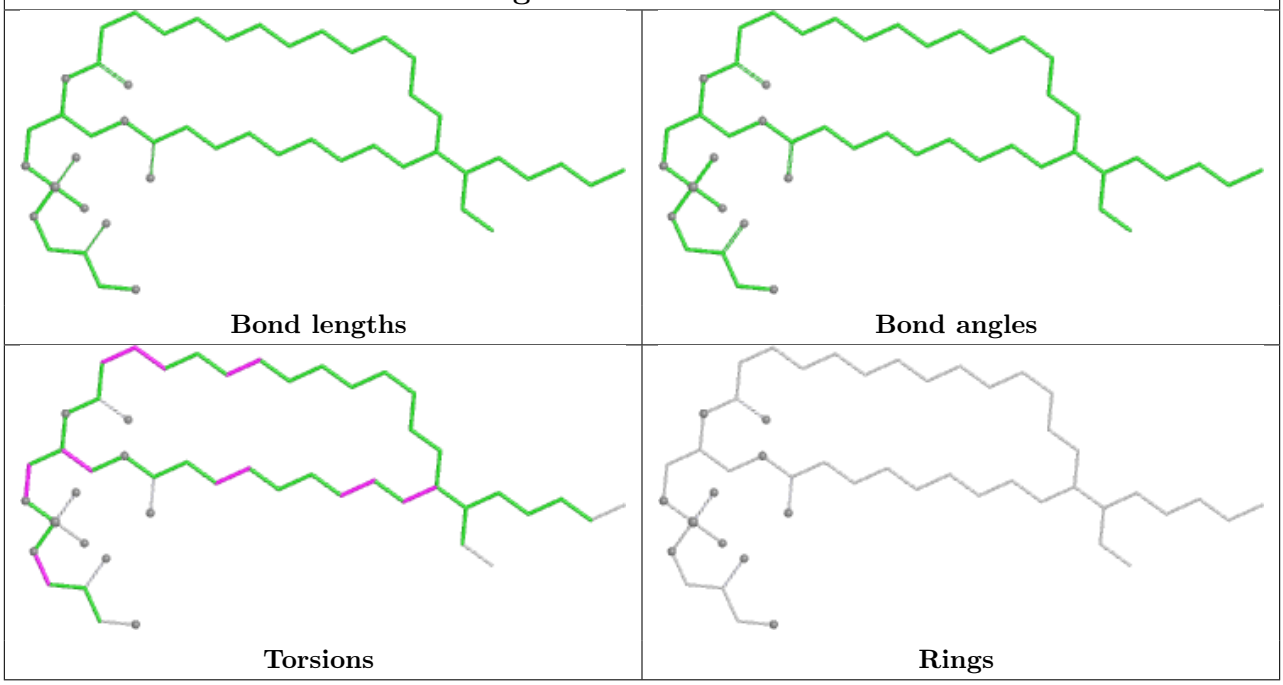
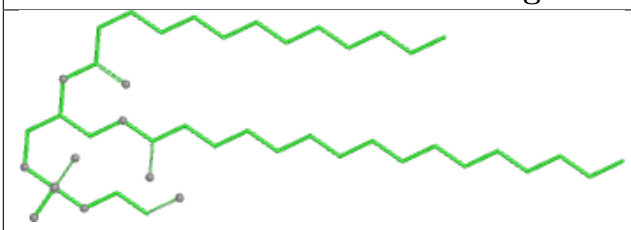
Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	8A	603	PGV	19	0
75	1X	201	CDL	12	0
84	6D	501	HEC	5	0
89	4B	303	PSC	7	0
82	4K	101	PGV	7	0
75	1N	903	CDL	4	0
69	5N	901	3PE	5	0
69	1N	901	3PE	4	0
71	5h	202	PC1	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

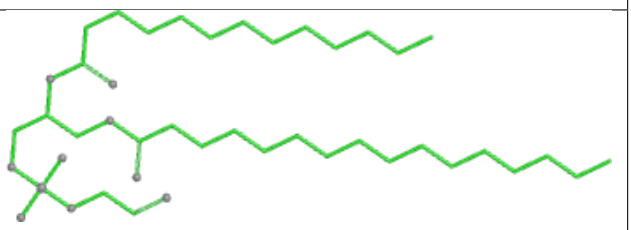
Ligand PGV 4A 604



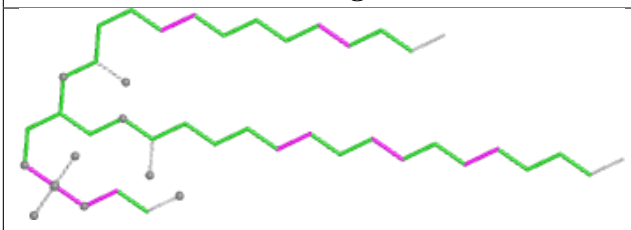
Ligand 3PE 1J 202



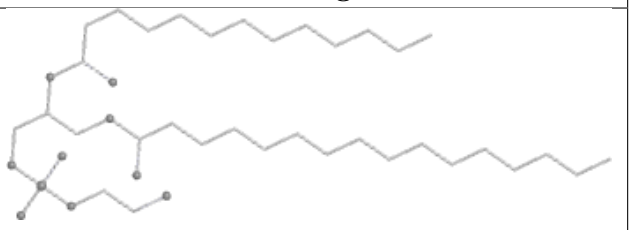
Bond lengths



Bond angles

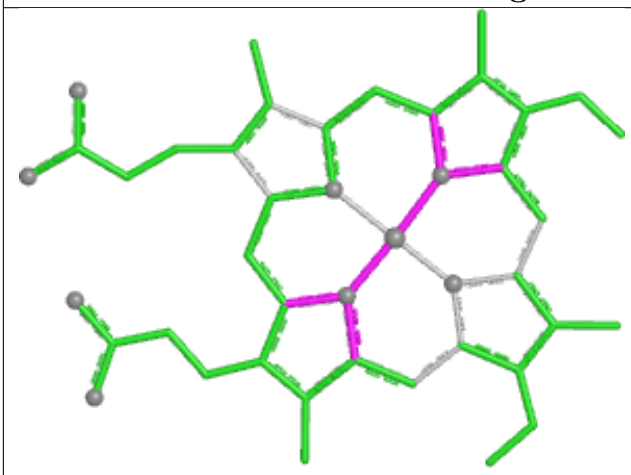


Torsions

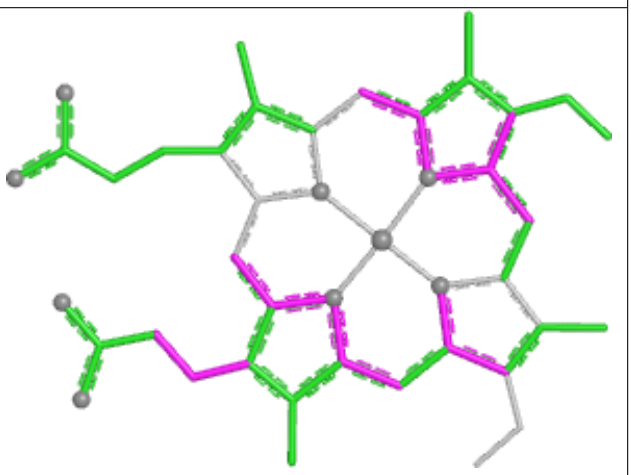


Rings

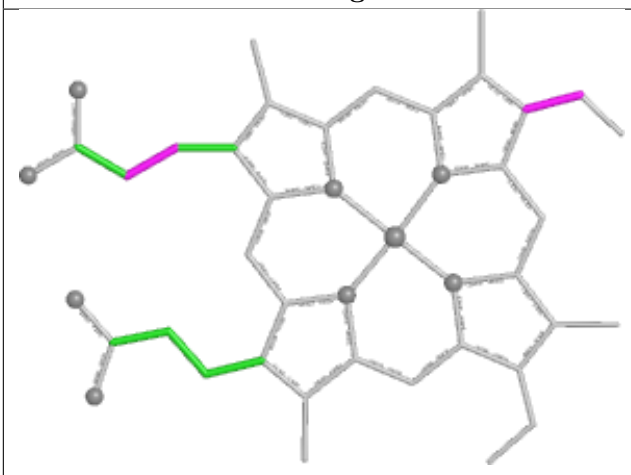
Ligand HEM 6C 502



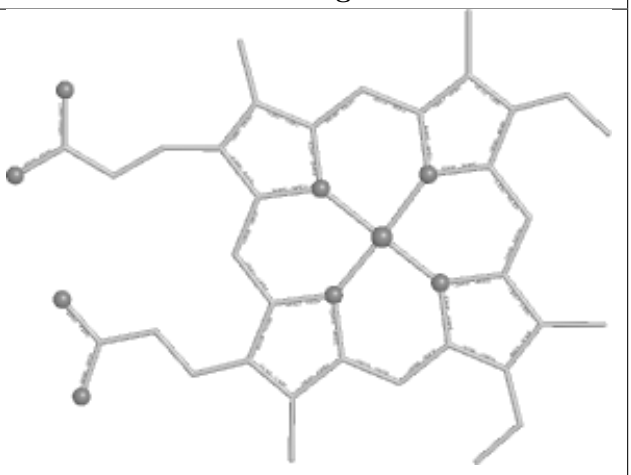
Bond lengths



Bond angles

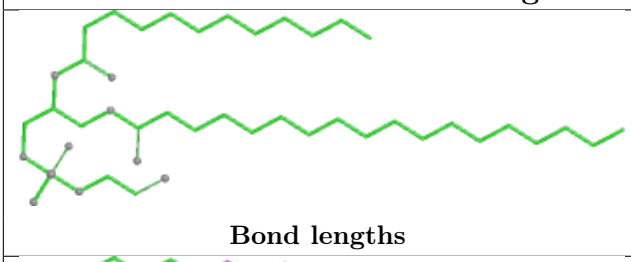


Torsions

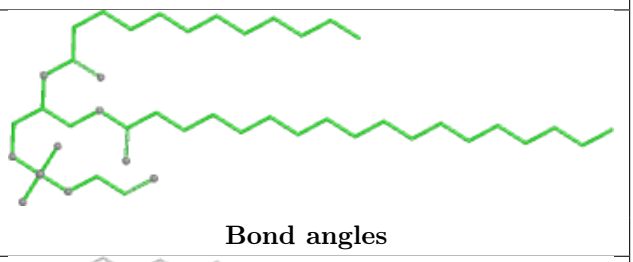


Rings

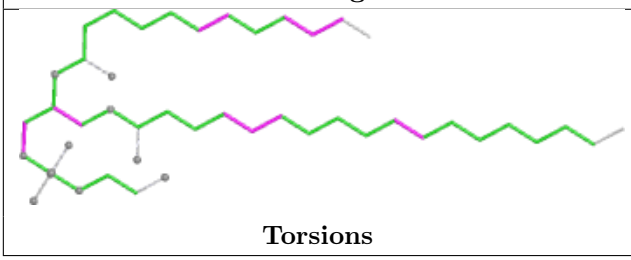
Ligand 3PE 1L 703



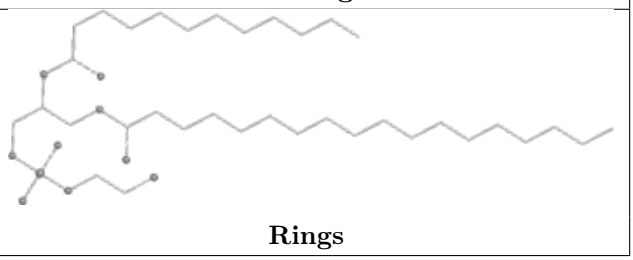
Bond lengths



Bond angles



Torsions

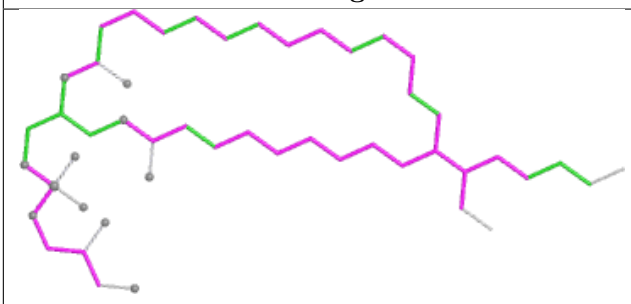


Rings

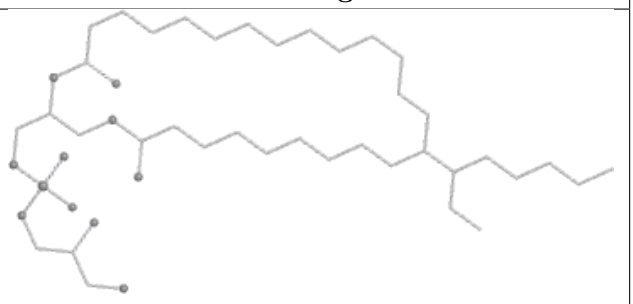
Ligand PGV 8A 604

Bond lengths

Bond angles

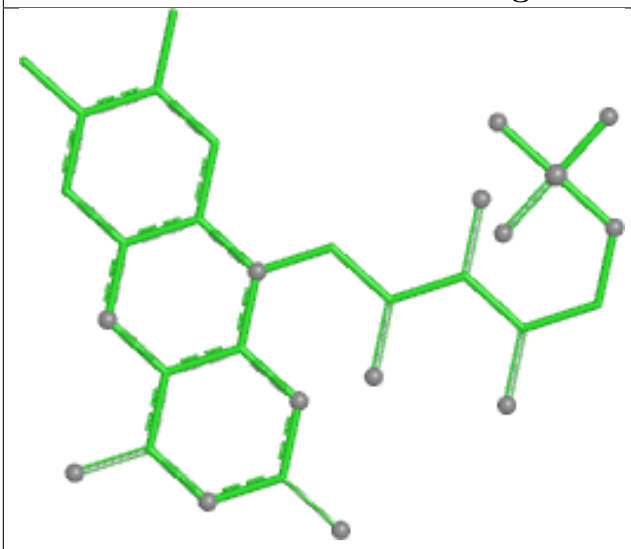


Torsions



Rings

Ligand FMN 1F 501



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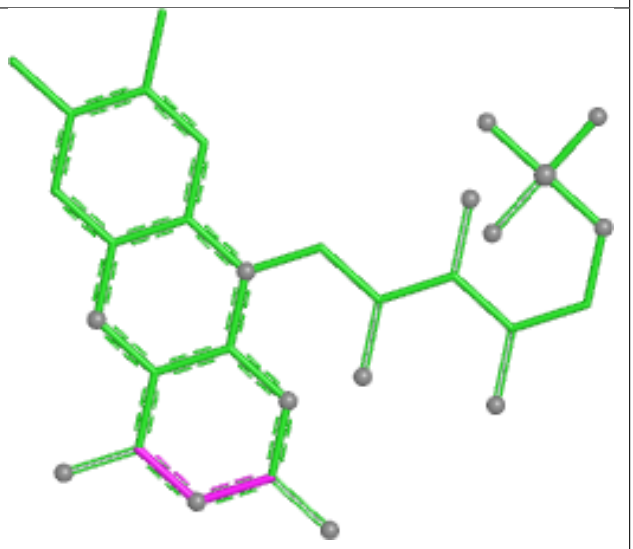
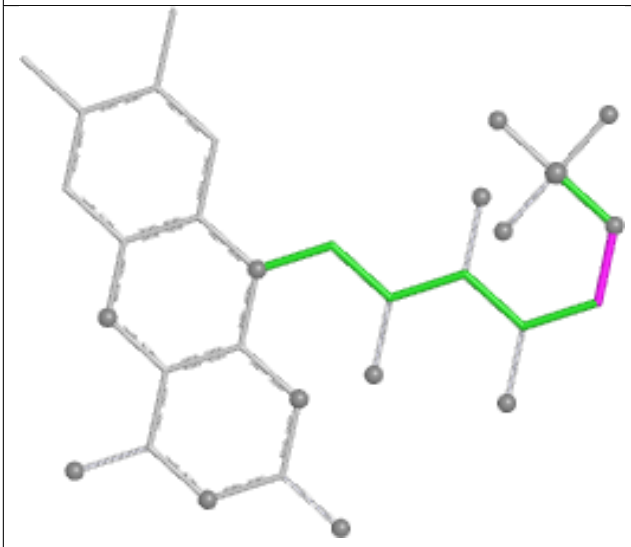


Bond angles



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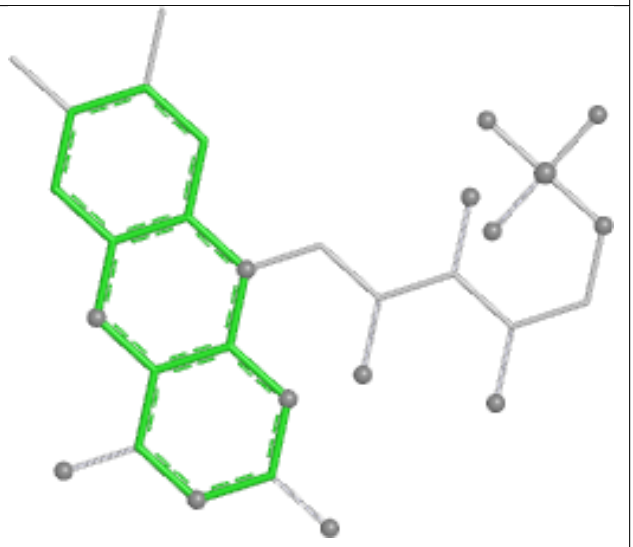
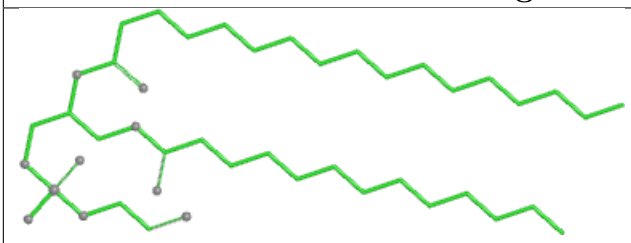


Rings

Ligand 3PE 1M 501



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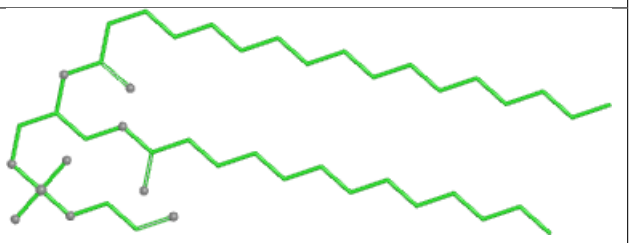

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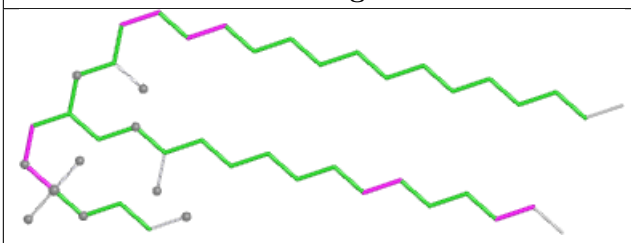

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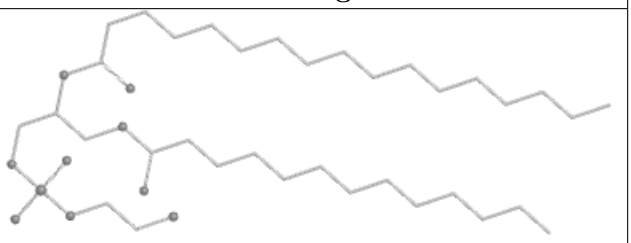
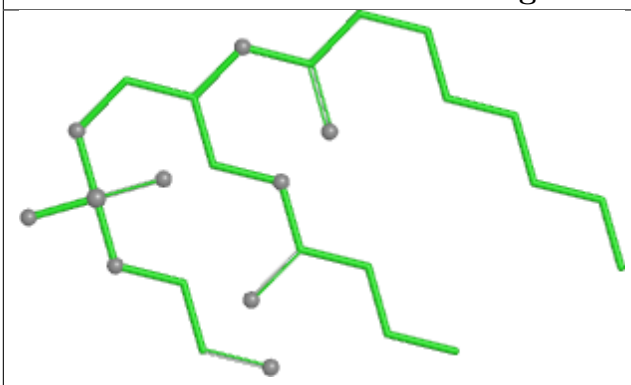


Rings

Ligand 3PE 1Y 205



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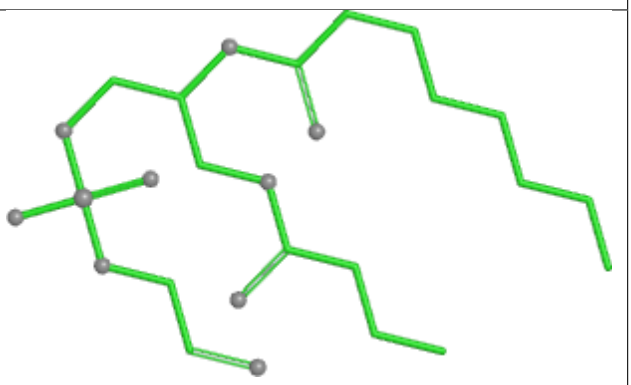
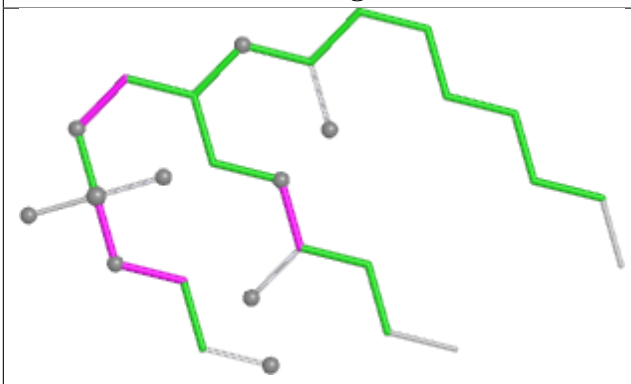


Bond angles



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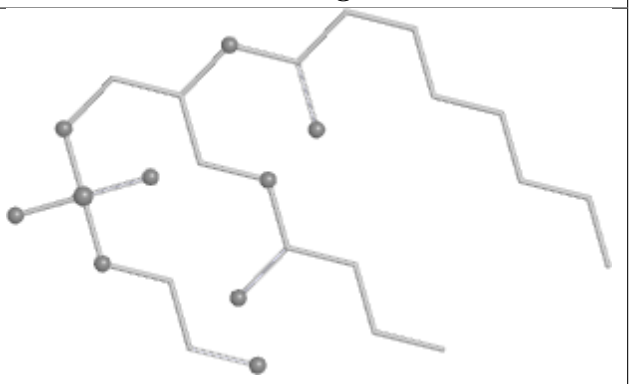
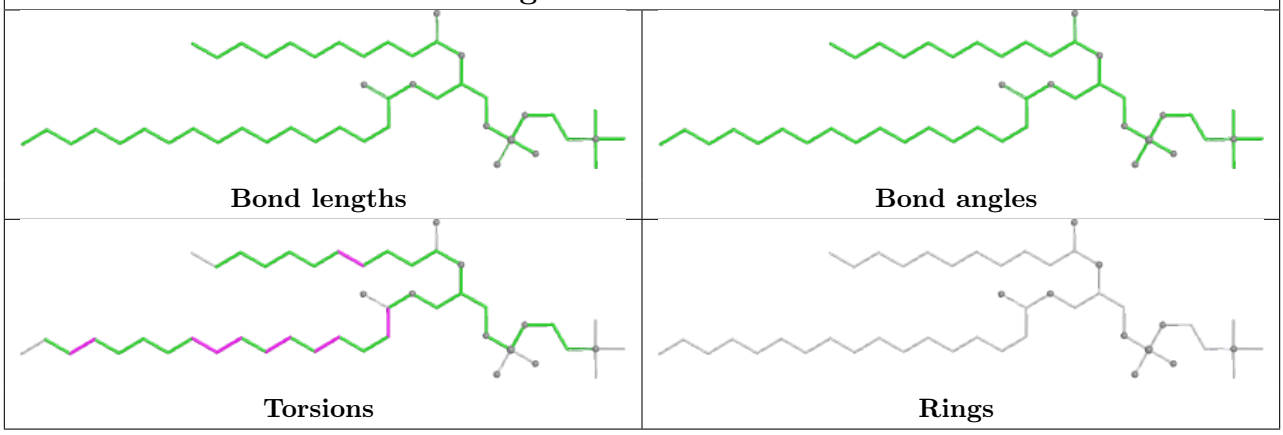
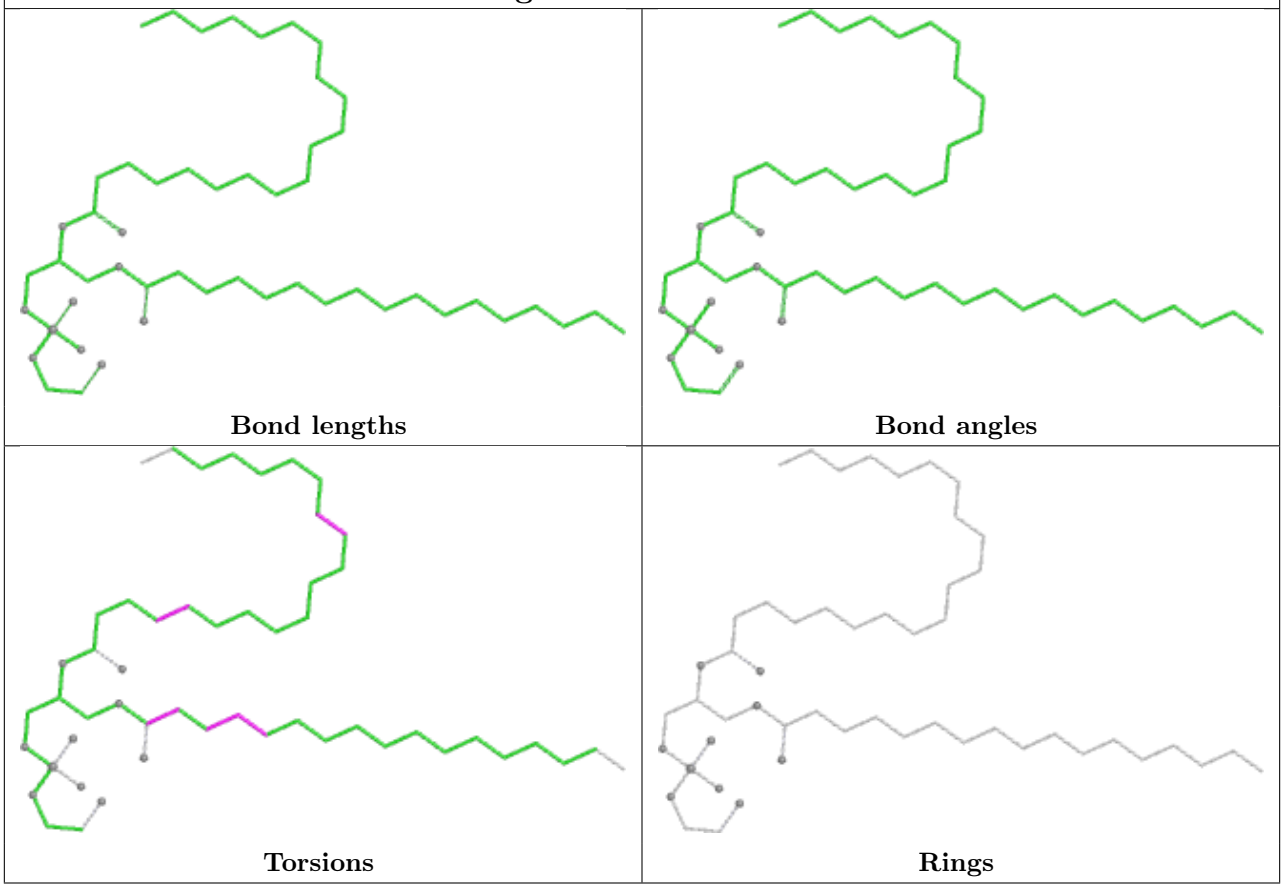


Rings

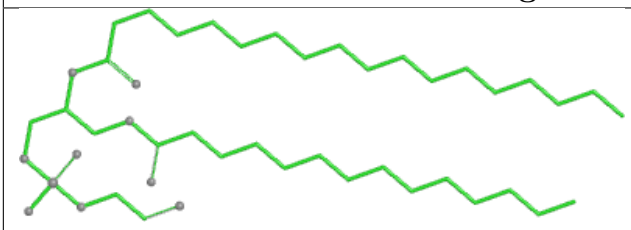
Ligand PC1 1B 202



Ligand PEK 4C 307



Ligand 3PE 5A 201



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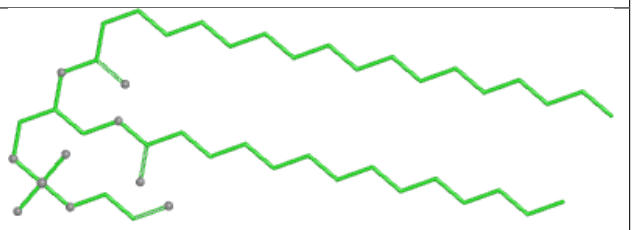
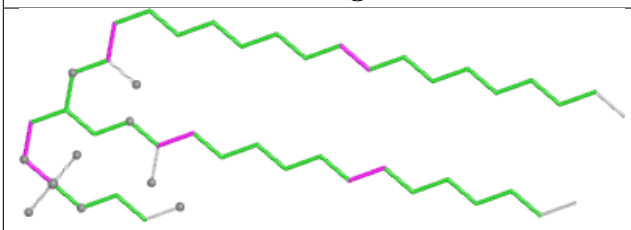


Bond angles



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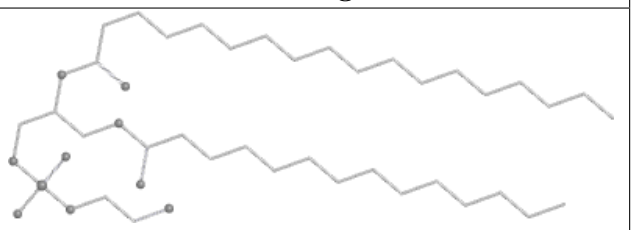
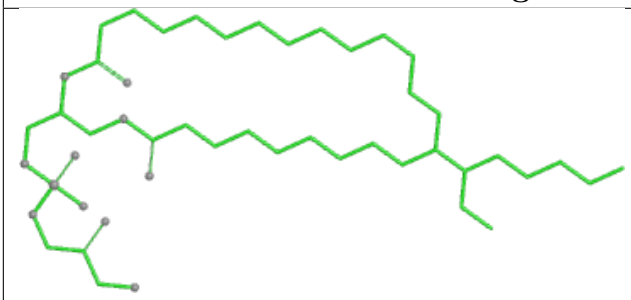


Rings

Ligand PGV 4A 603



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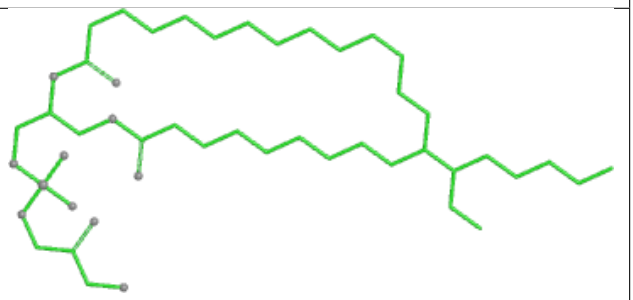
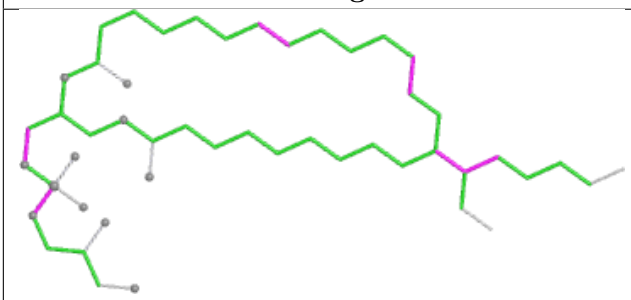


Bond angles



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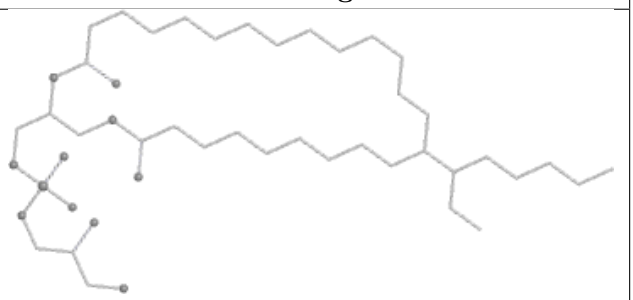
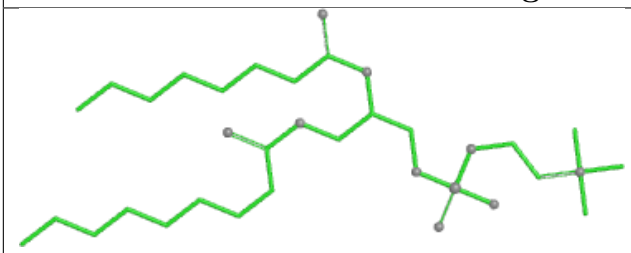


Rings

Ligand PC1 1J 201



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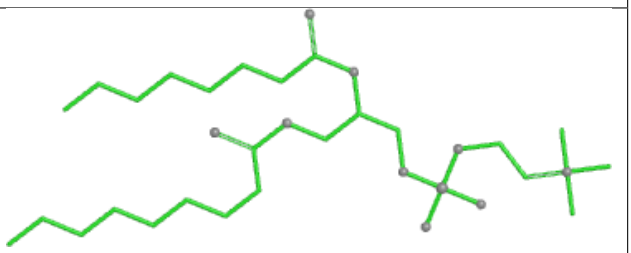
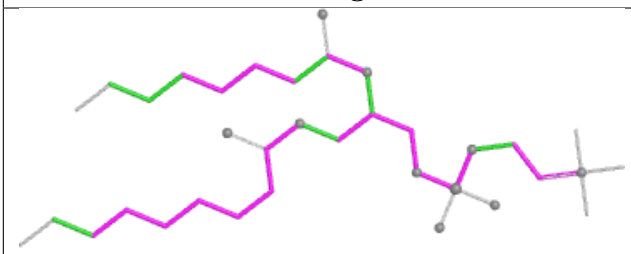


Bond angles



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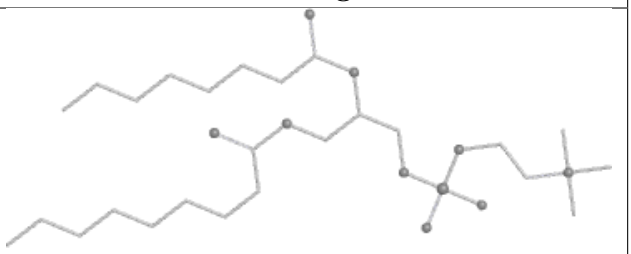
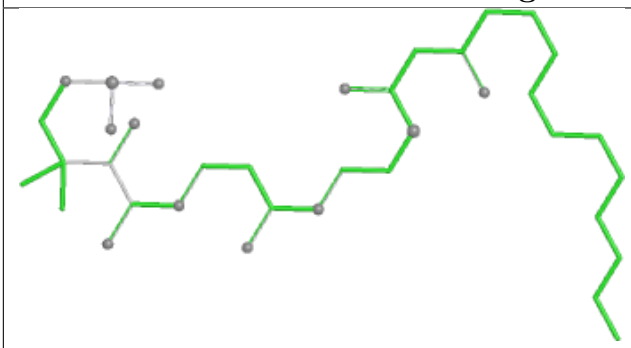


Rings

Ligand EHZ 5n 201



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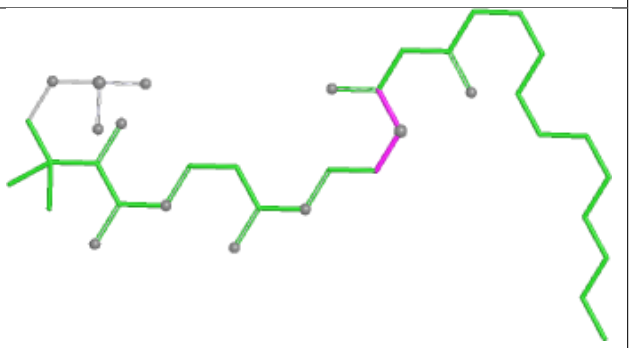
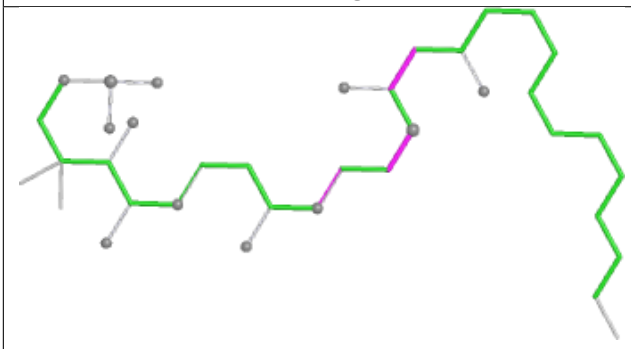


Bond angles



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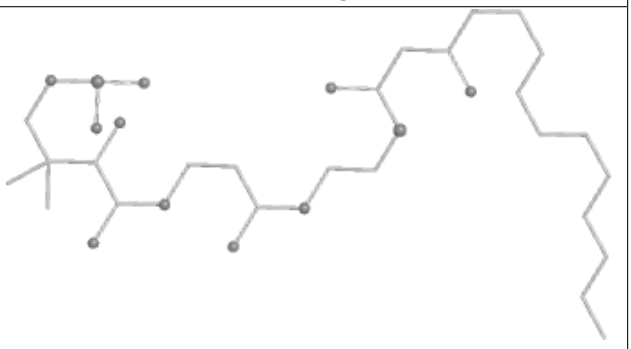
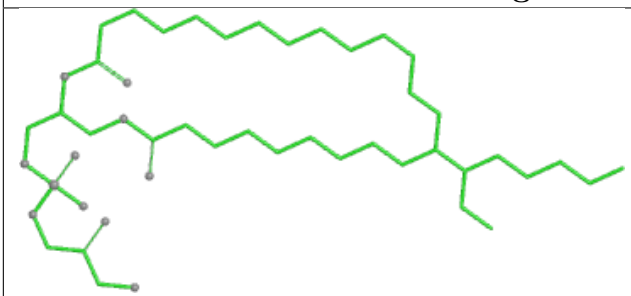


Rings

Ligand PGV 4C 301



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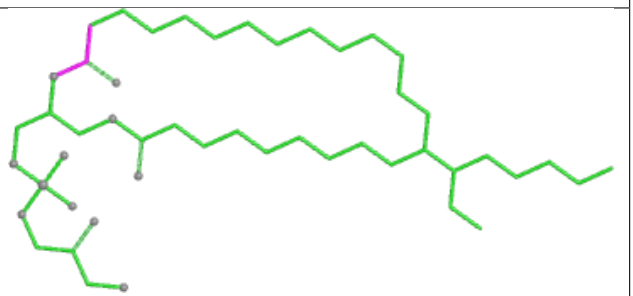
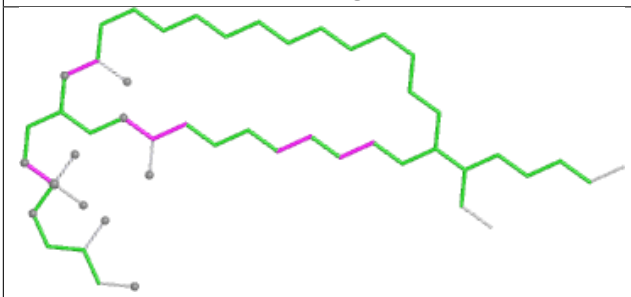


Bond angles



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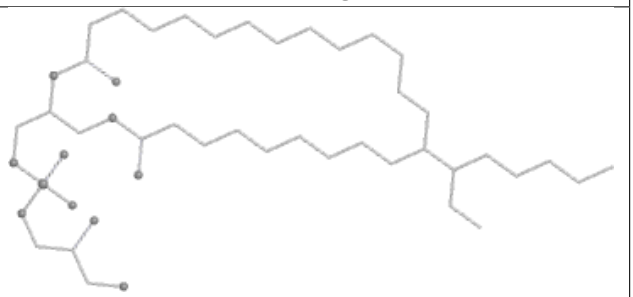
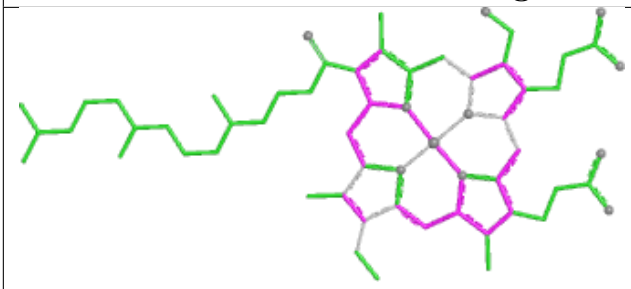


Rings

Ligand HEA 4A 605



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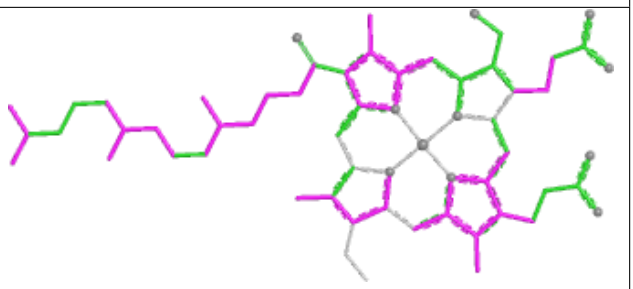
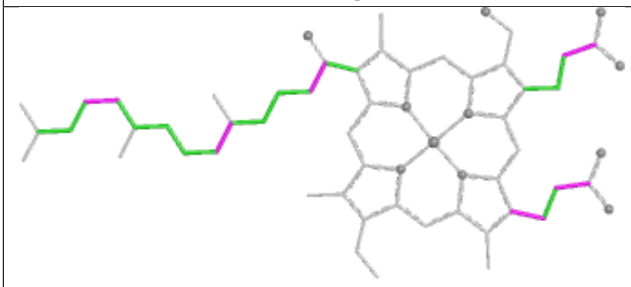


Bond angles



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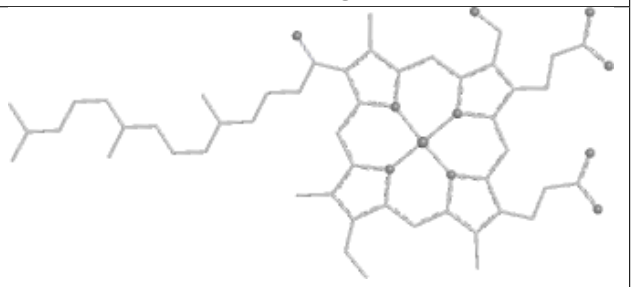
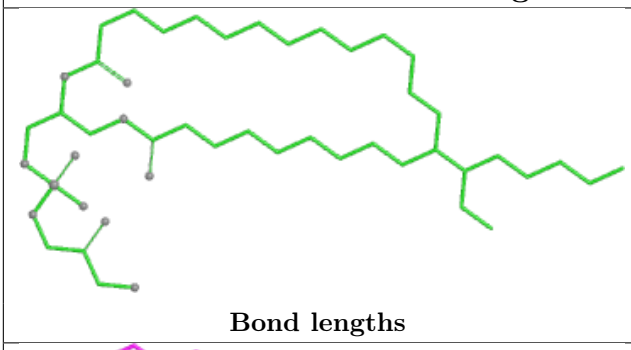


Rings

Ligand PGV 8K 101



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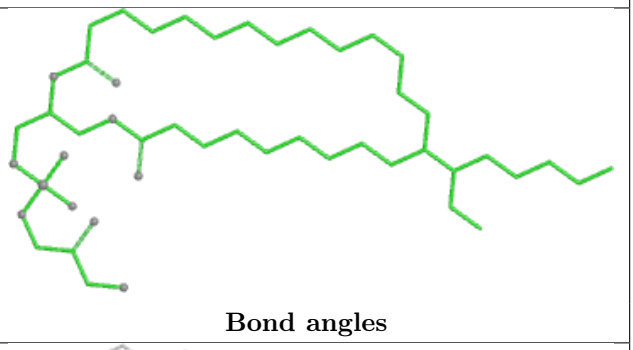
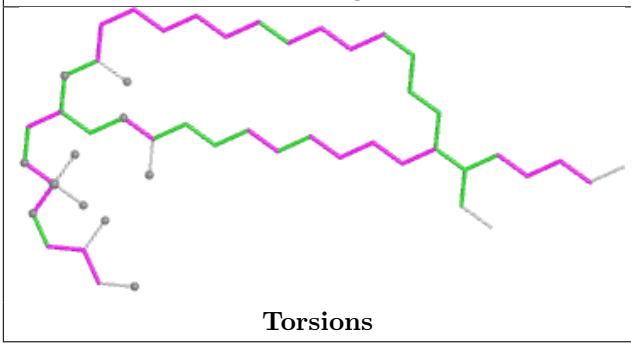


Bond angles



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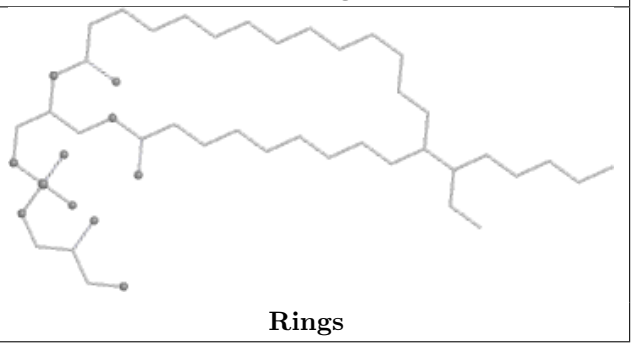
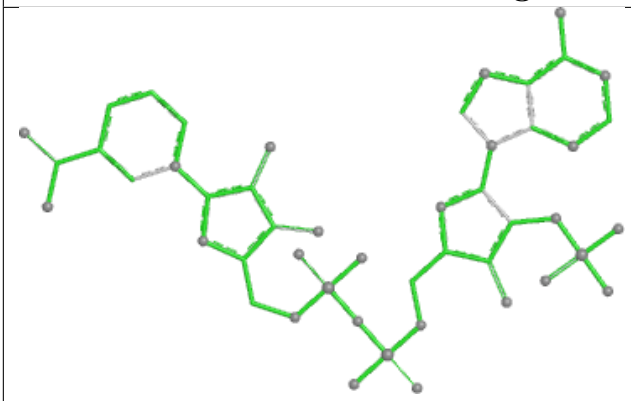


Rings

Ligand NDP 1P 402



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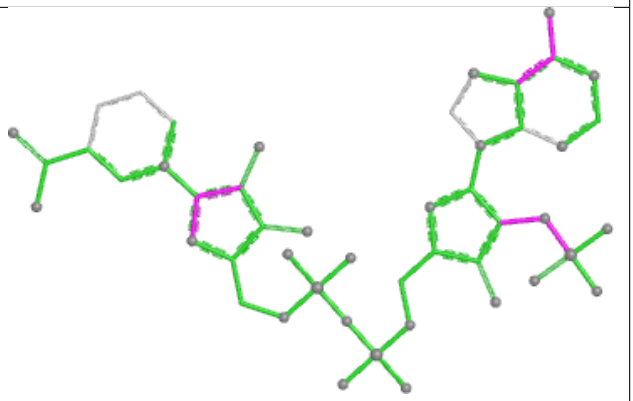
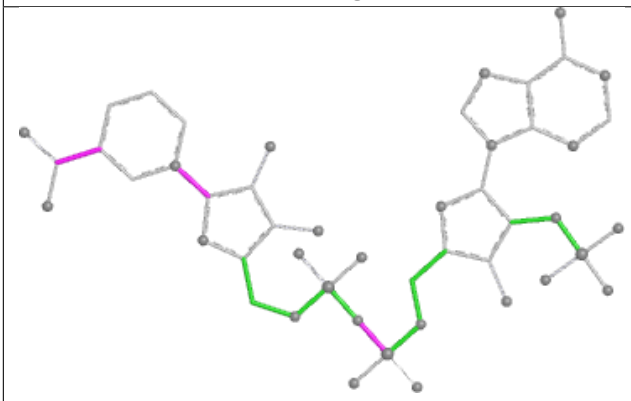
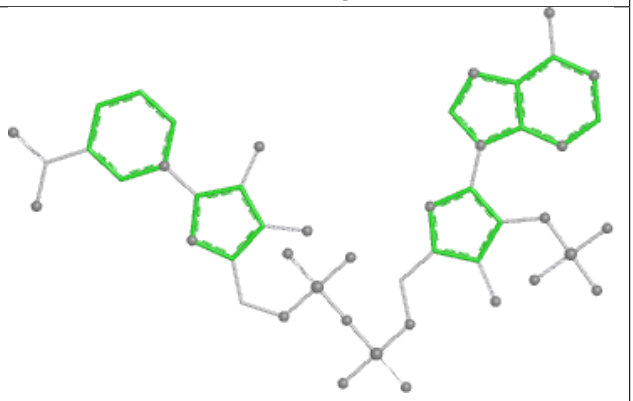


Bond angles

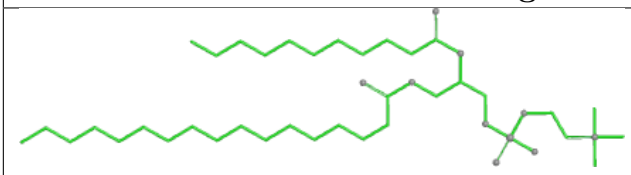


Torsions



Rings

Ligand PC1 5B 202



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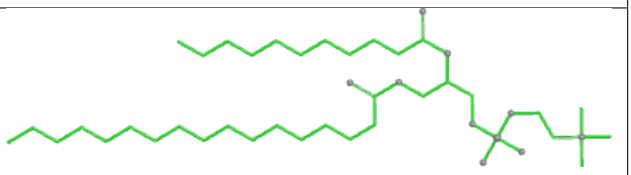
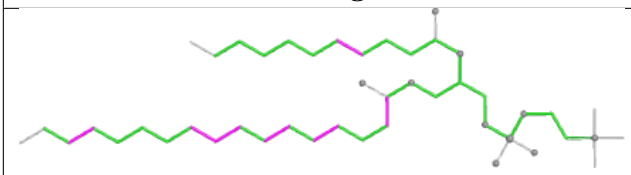


Bond angles



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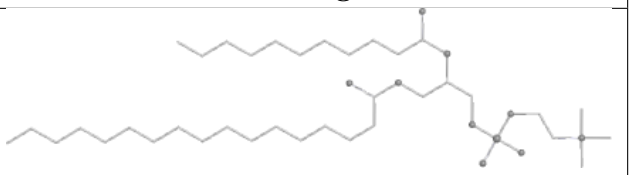
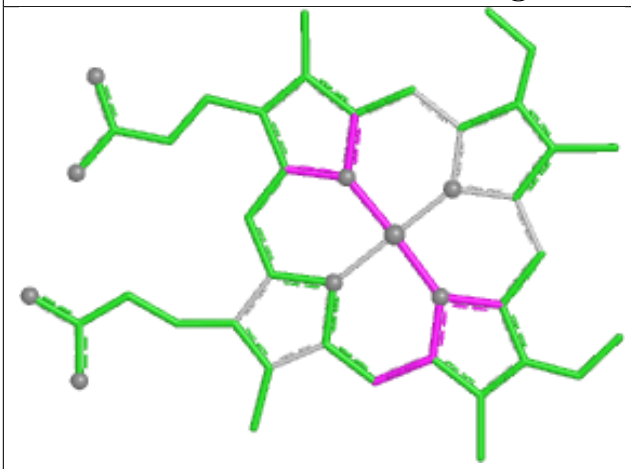
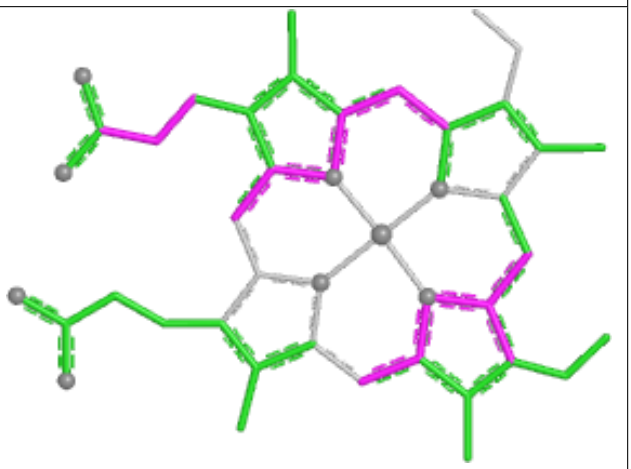


Rings

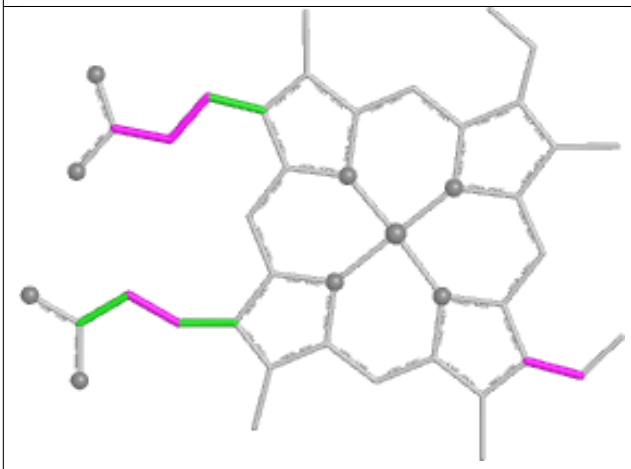
Ligand HEM 6C 501



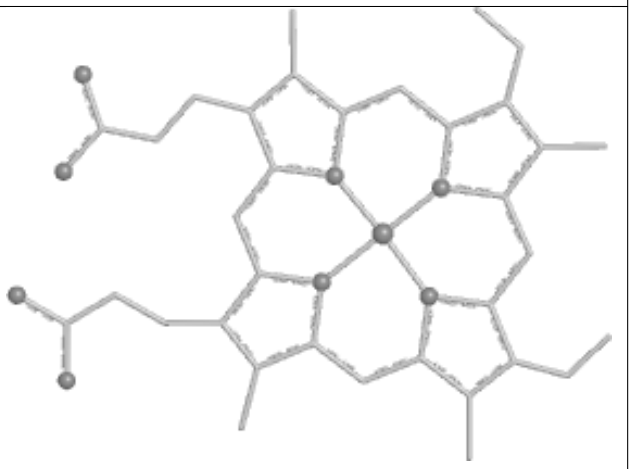
Bond lengths



Bond angles

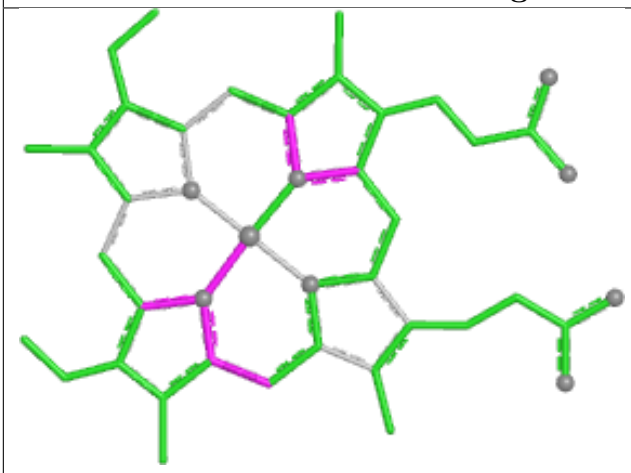


Torsions



Rings

Ligand HEM 6P 502



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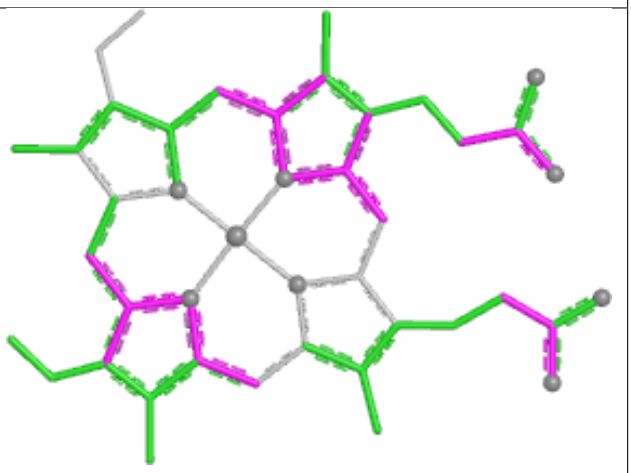
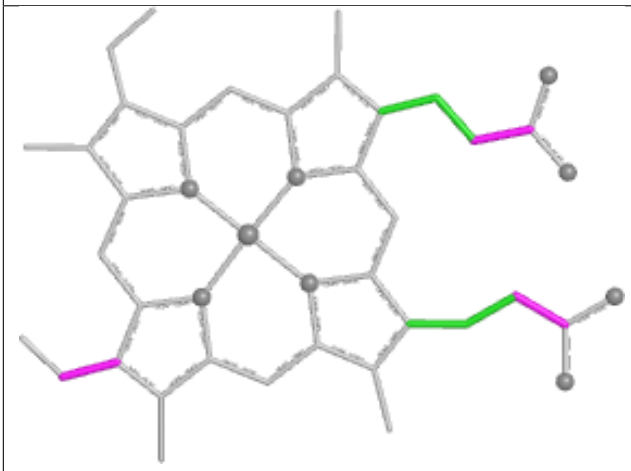


Bond angles



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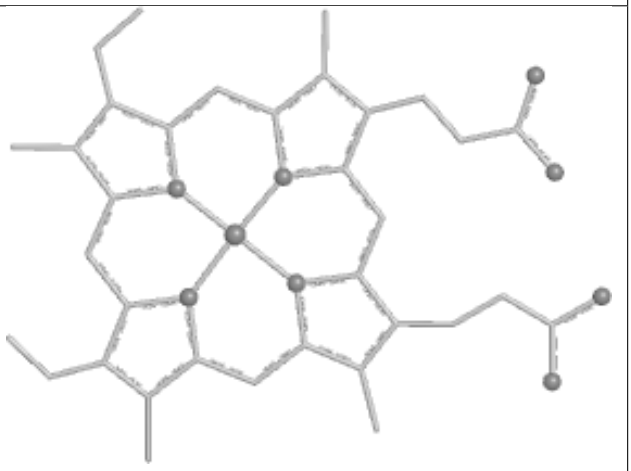
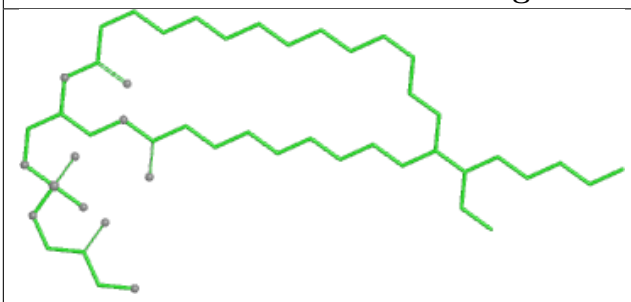


Rings

Ligand PGV 8C 304



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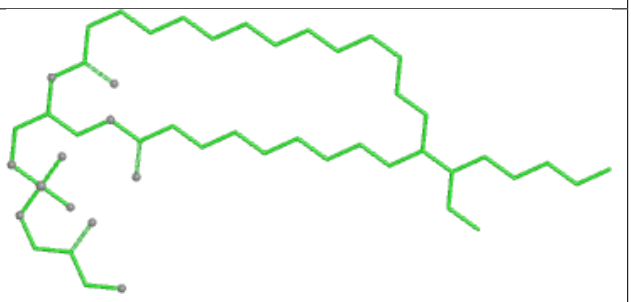

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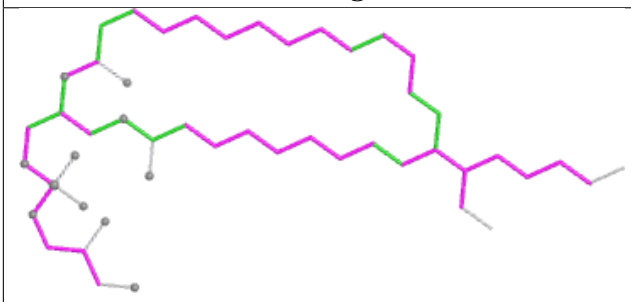

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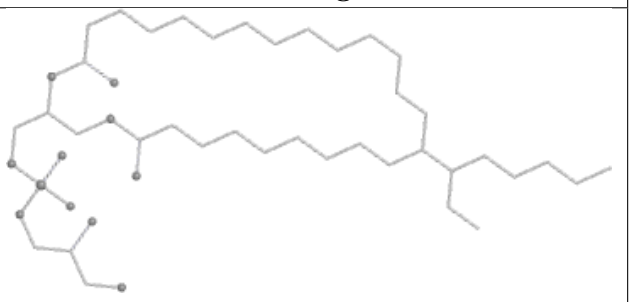
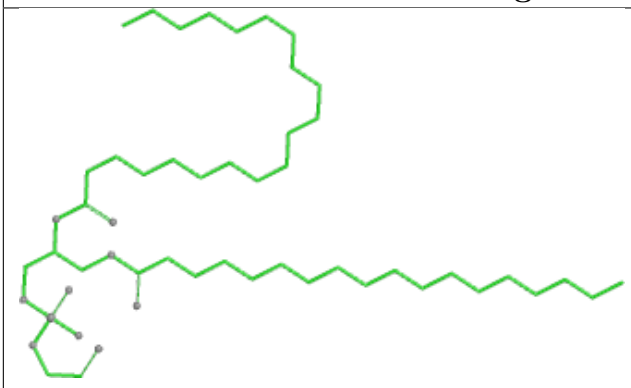


Rings

Ligand PEK 4C 306



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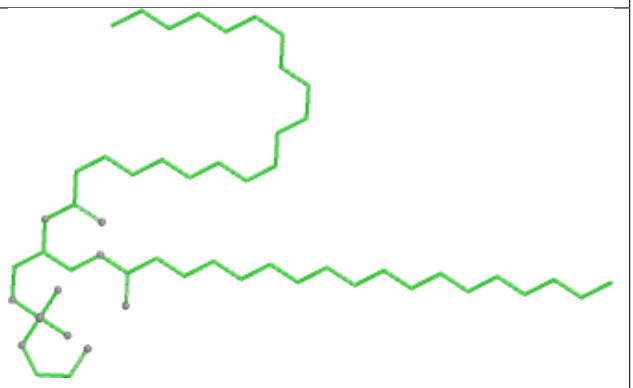

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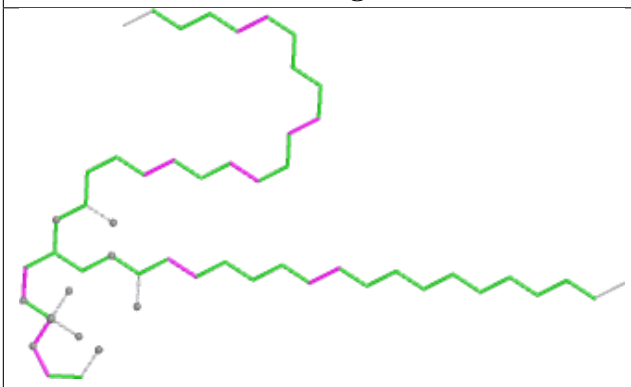

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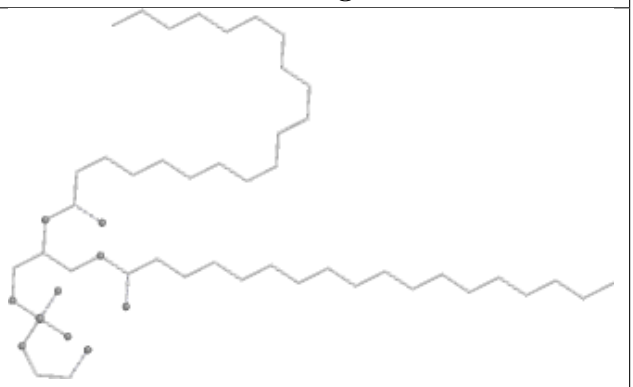
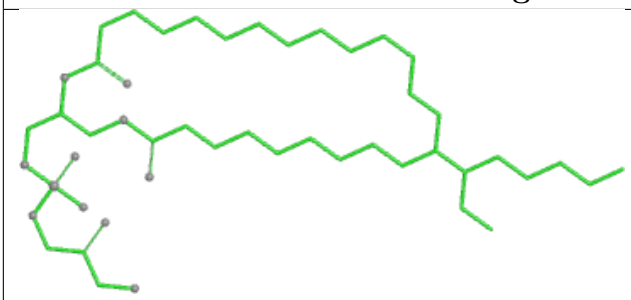


Rings

Ligand PGV 4C 305



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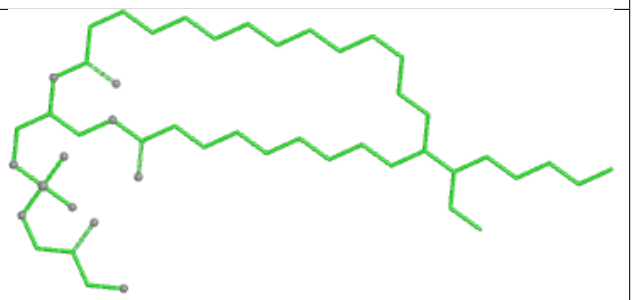

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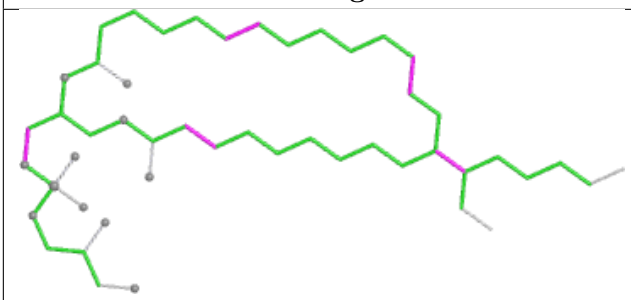

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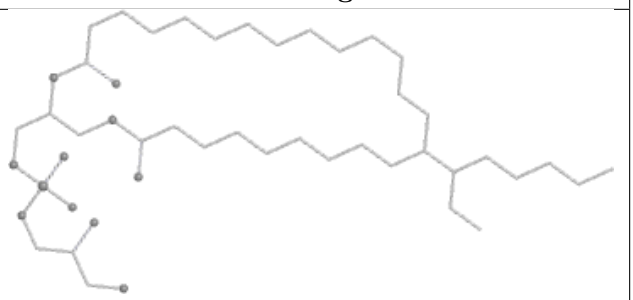
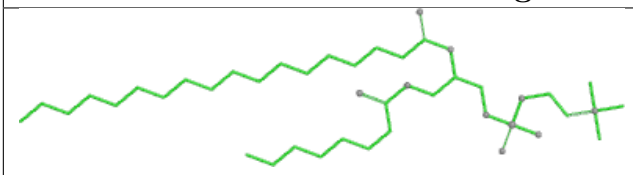


Rings

Ligand PC1 5M 502



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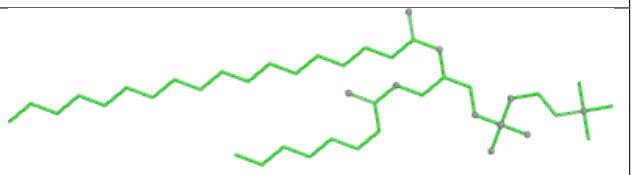

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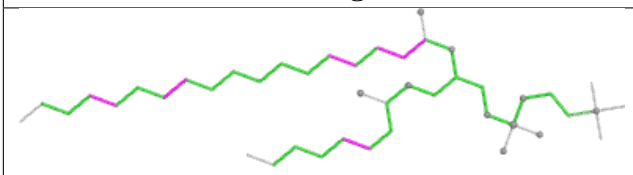

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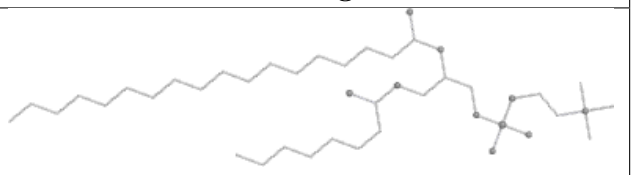
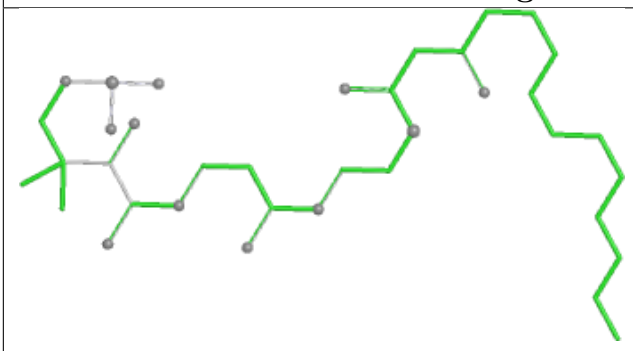


Rings

Ligand EHZ 1T 101



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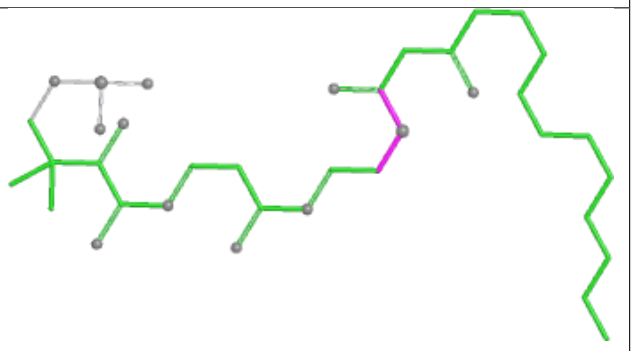

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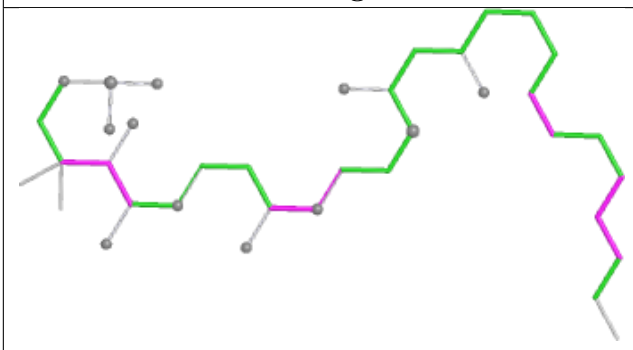

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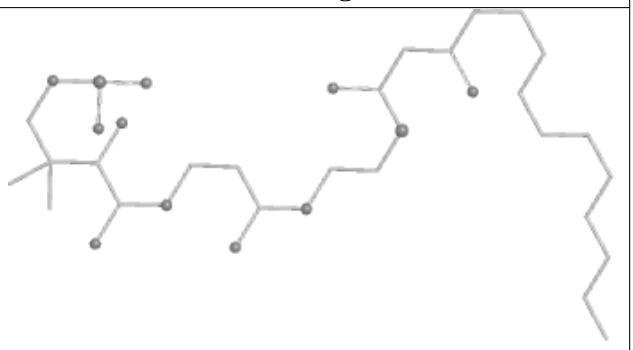
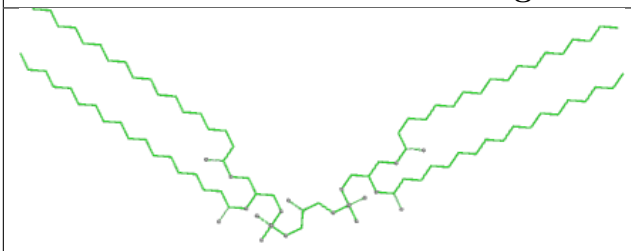


Rings

Ligand CDL 8A 610



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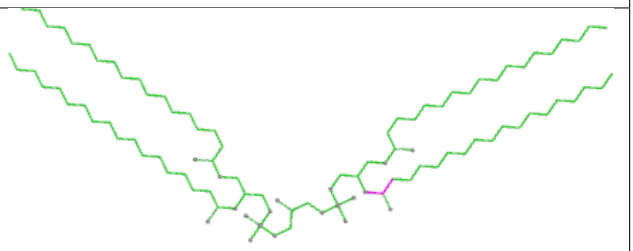
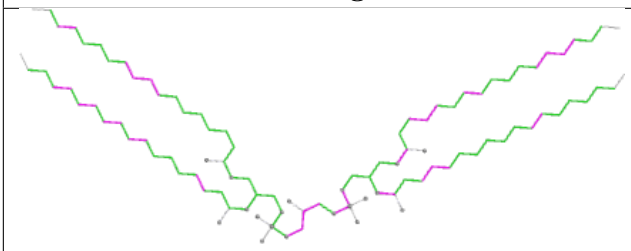


Bond angles



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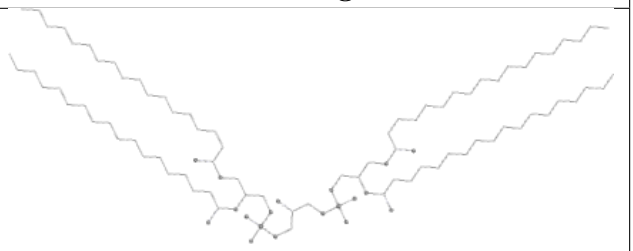
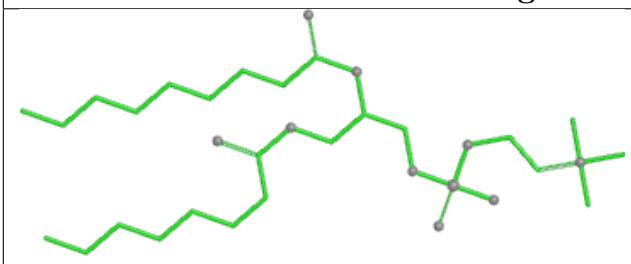


Rings

Ligand PC1 1Y 201



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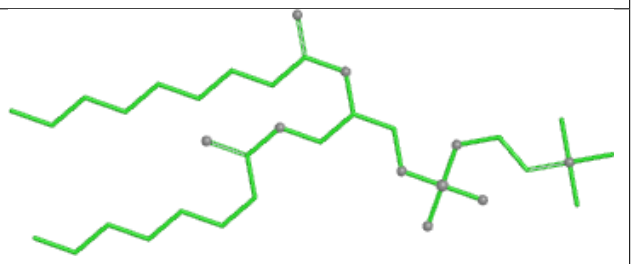

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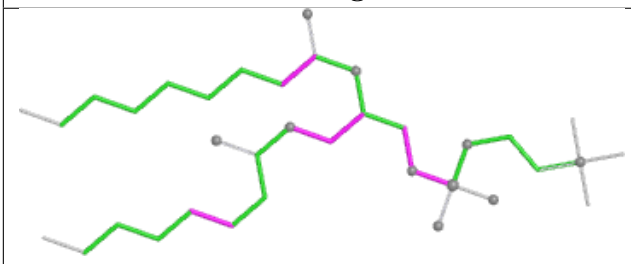

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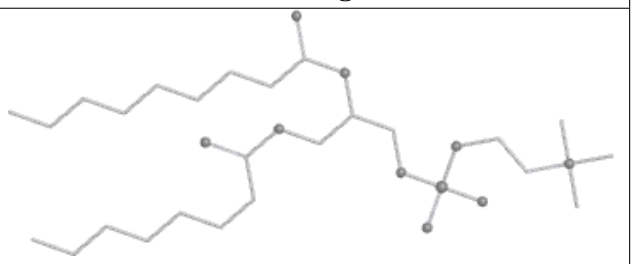
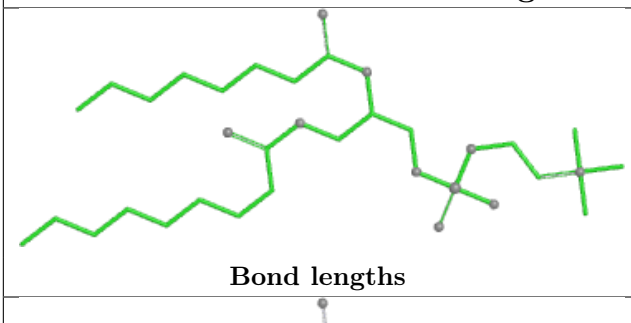


Rings

Ligand PC1 5A 202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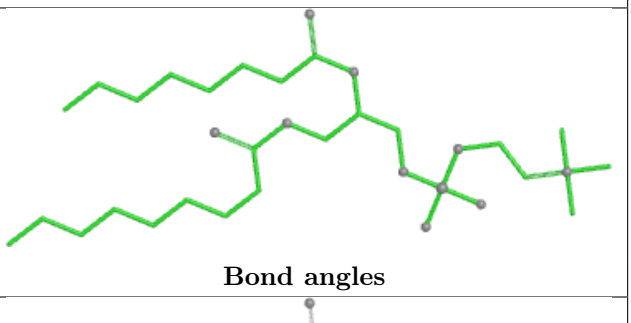
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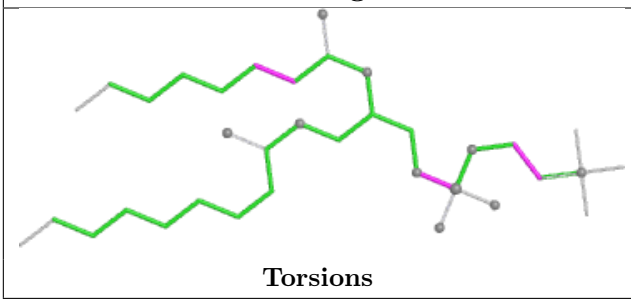
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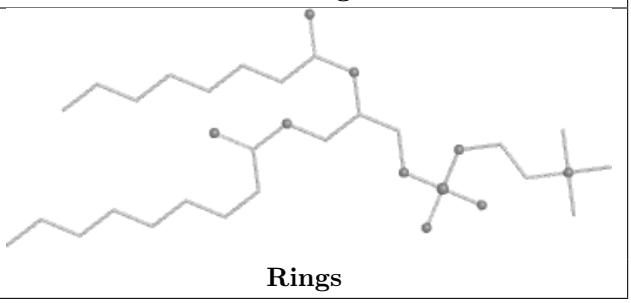
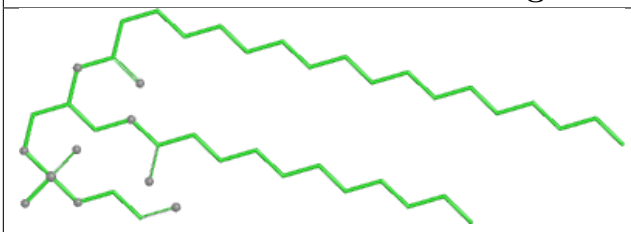

Rings

Ligand 3PE 5j 101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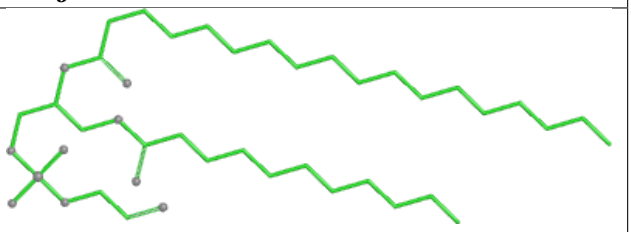
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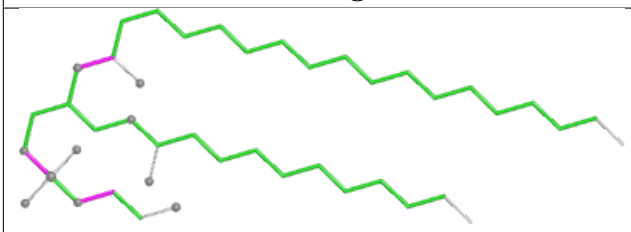
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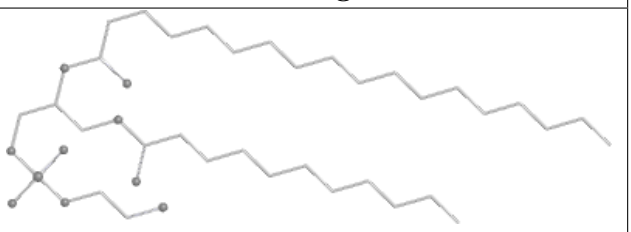
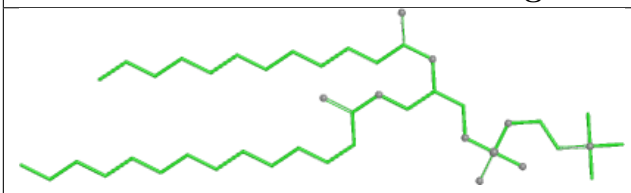

Rings

Ligand PC1 5I 204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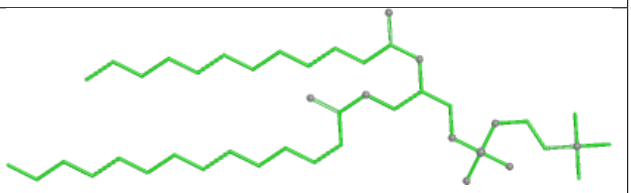
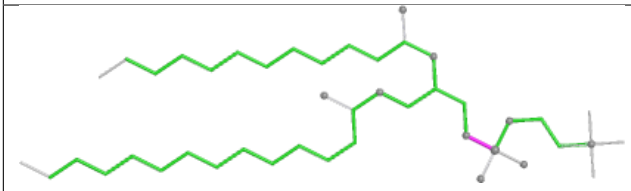

Bond angles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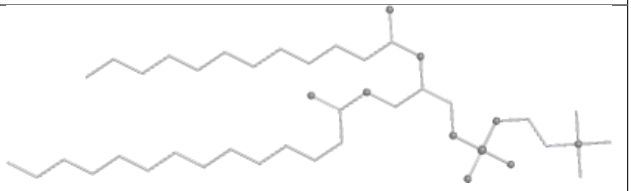
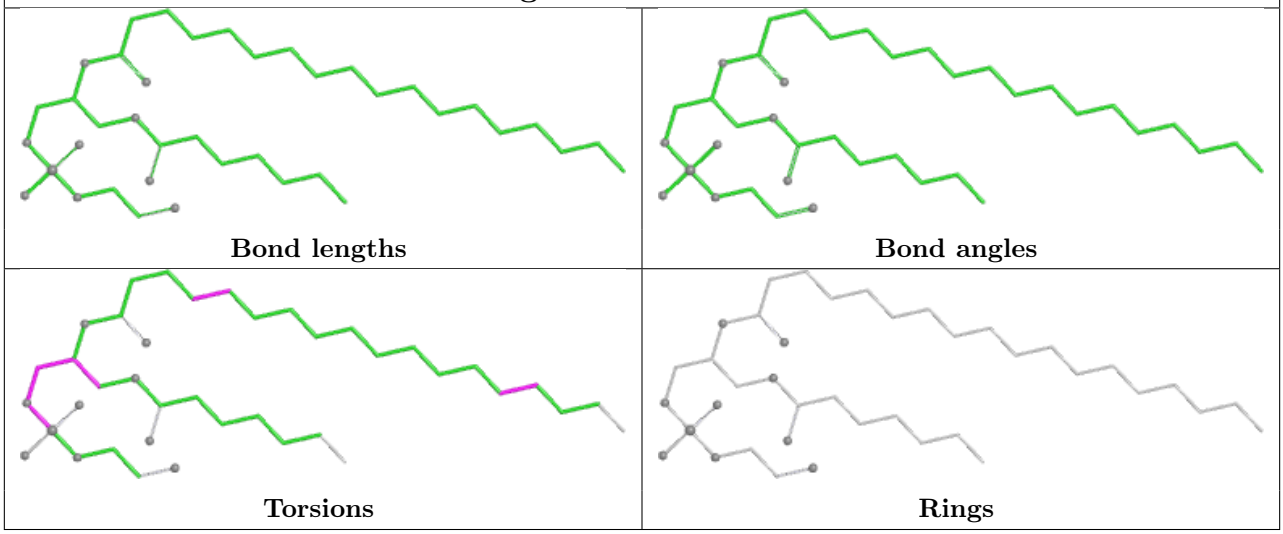
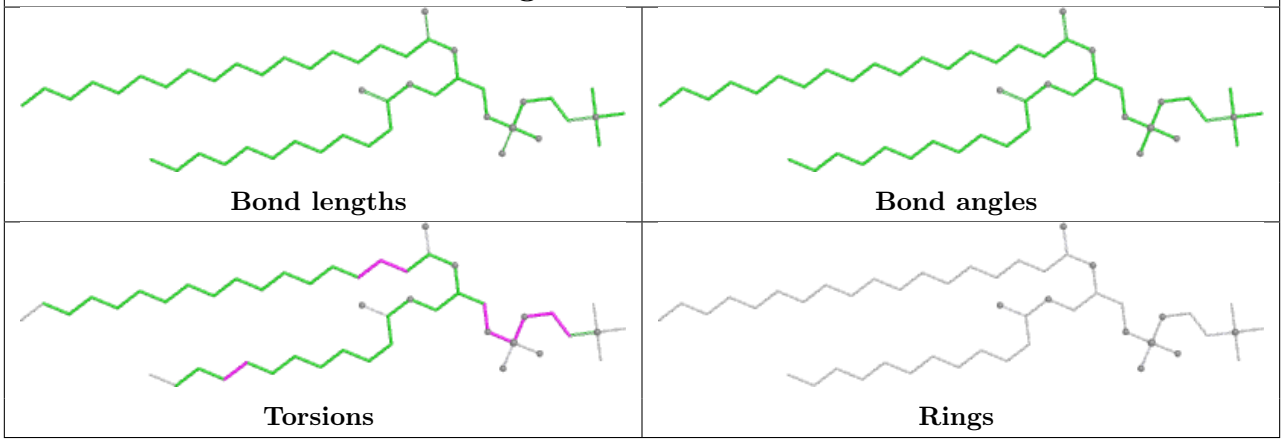

Rings

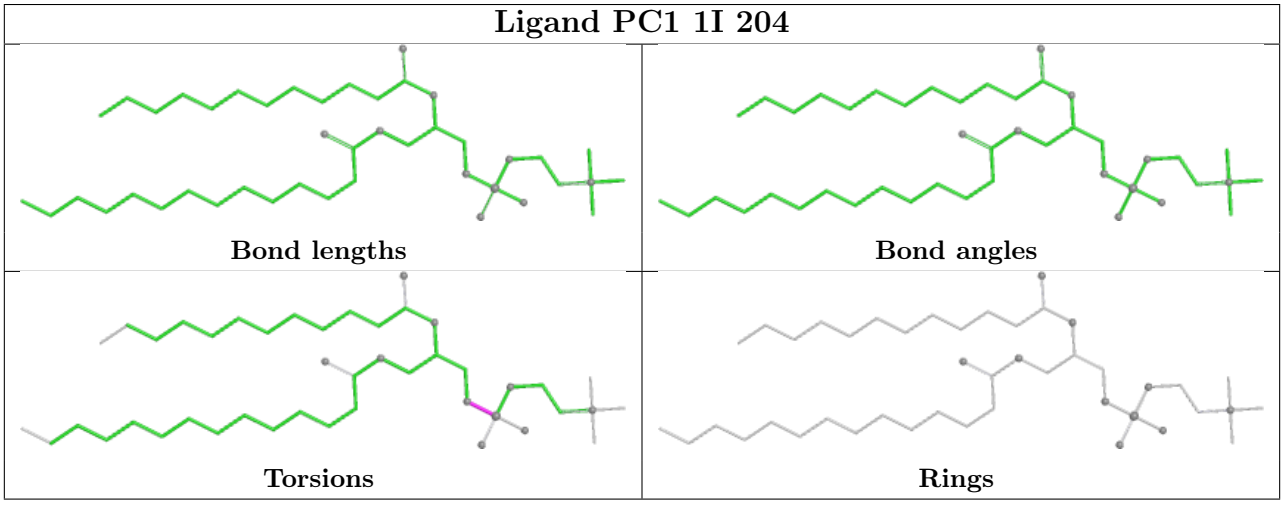
Ligand 3PE 5Y 202



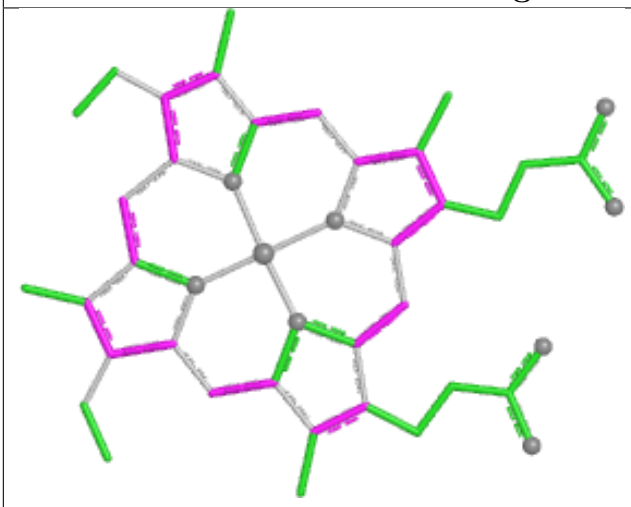
Ligand PC1 5H 401



Ligand PC1 1I 204



Ligand HEC 6Q 501



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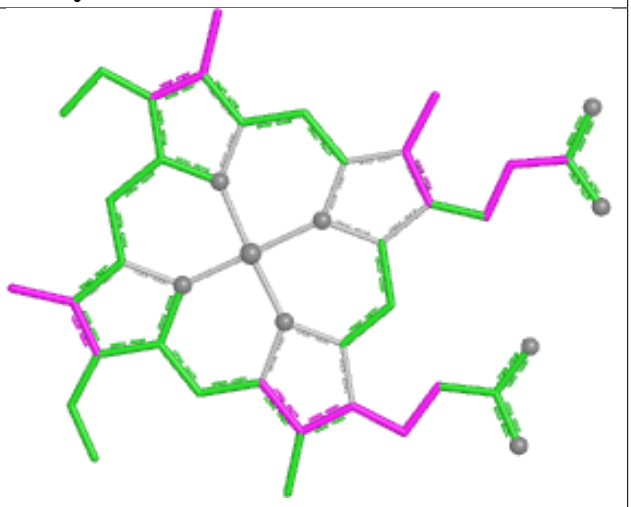
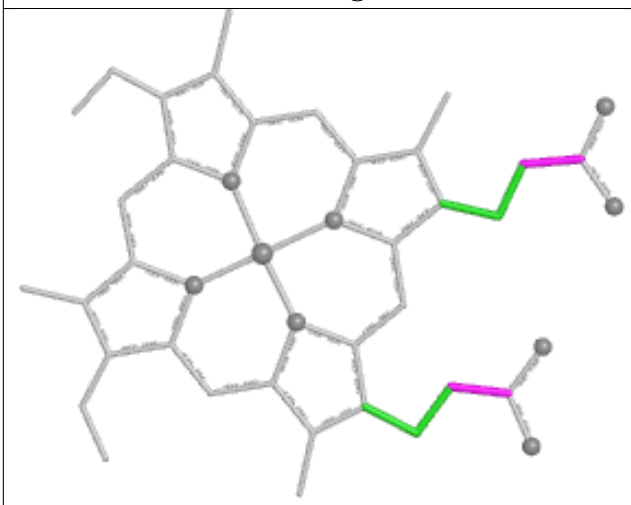
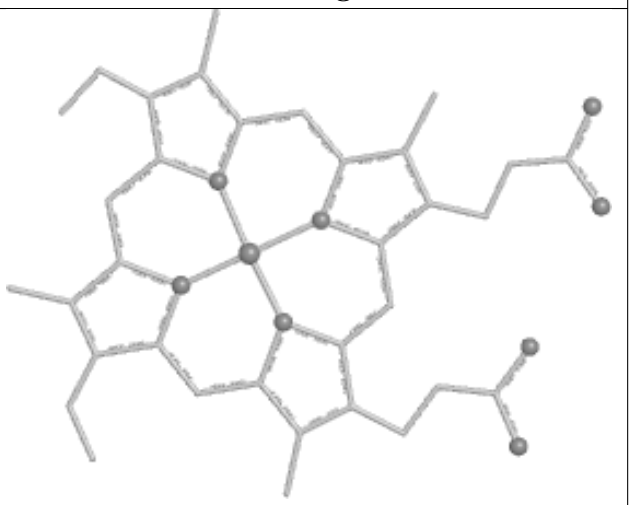


Bond angles

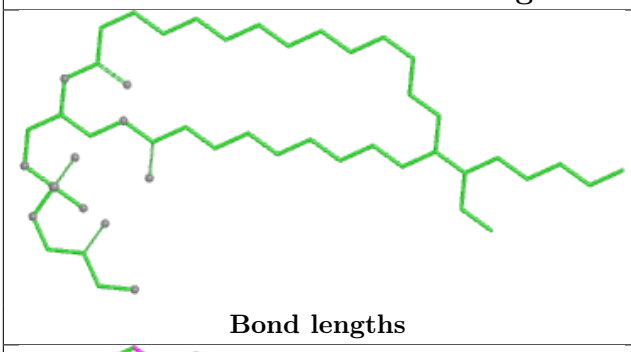


Torsions

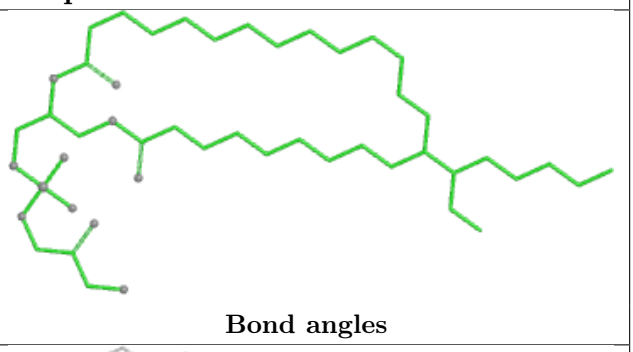


Rings

Ligand PGV 1p 201



Bond lengths



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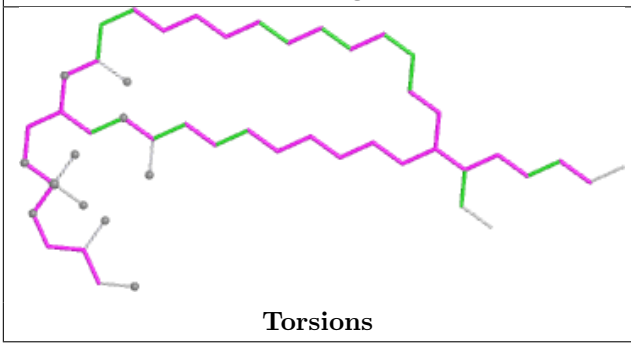
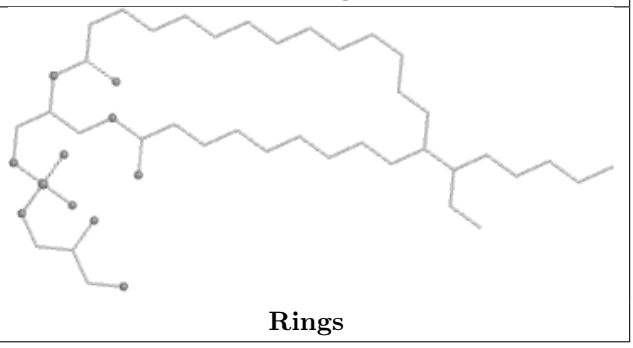
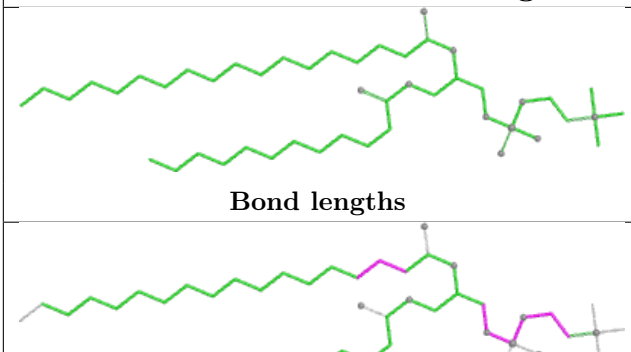


Torsions



Rings

Ligand PC1 1H 401



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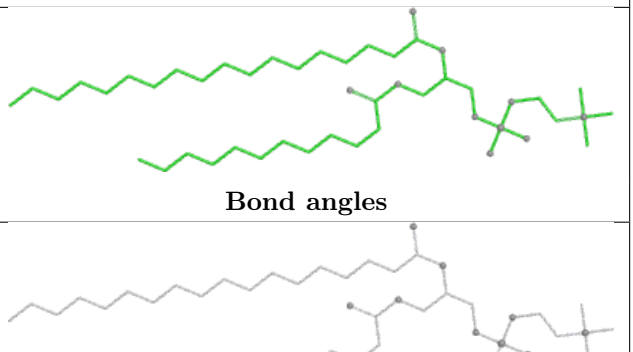

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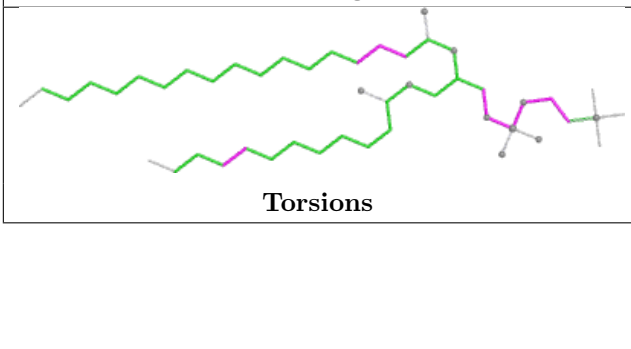

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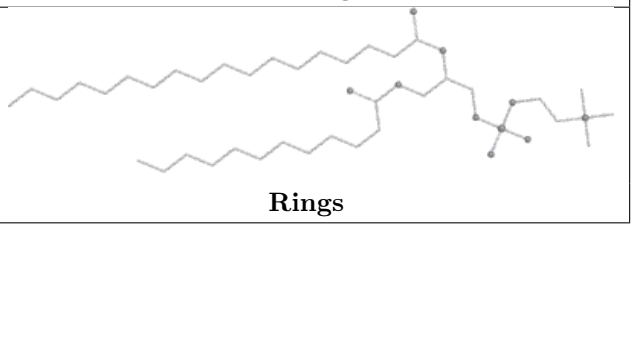
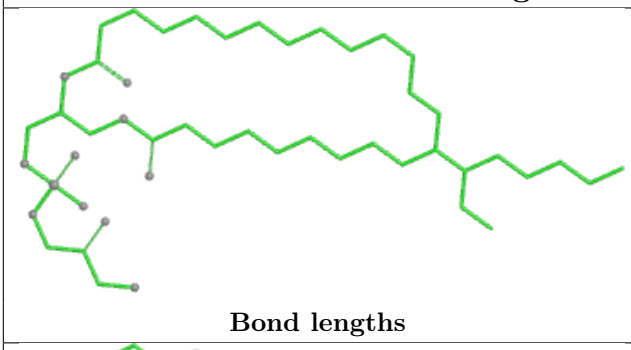


Rings

Ligand PGV 4C 304



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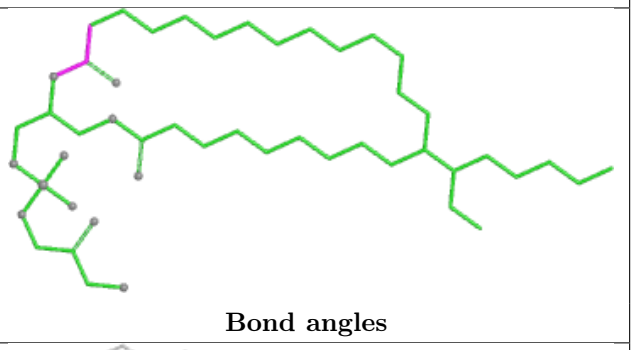

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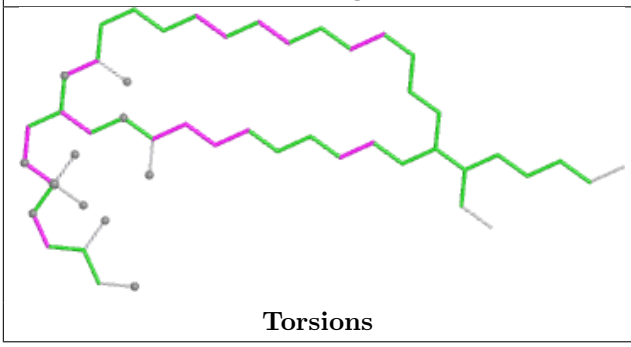

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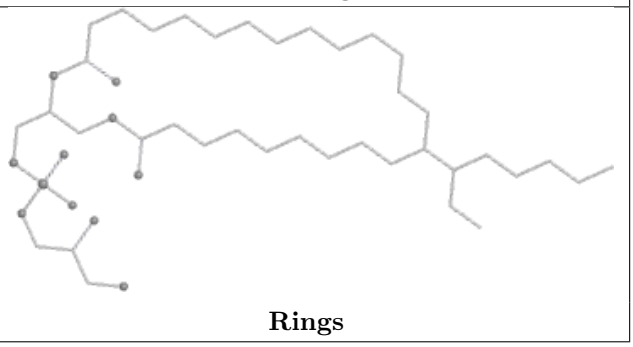
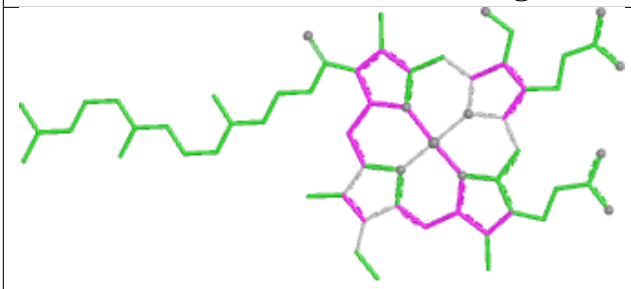


Rings

Ligand HEA 4A 606



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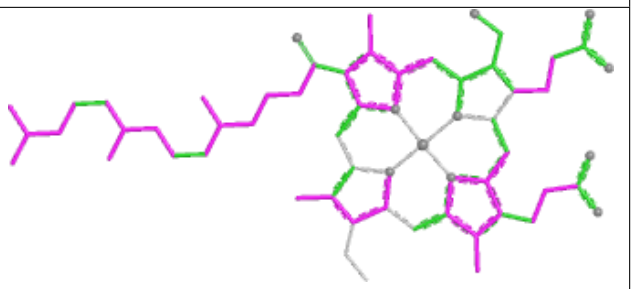

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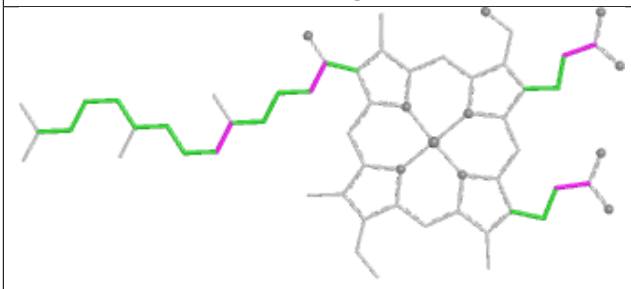

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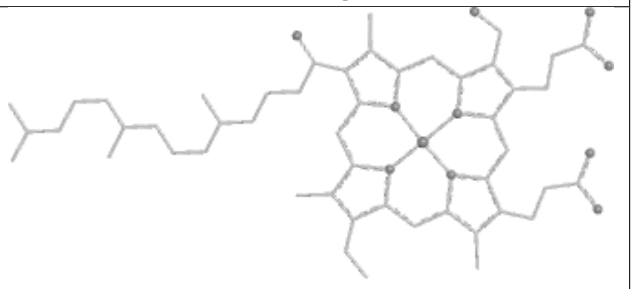
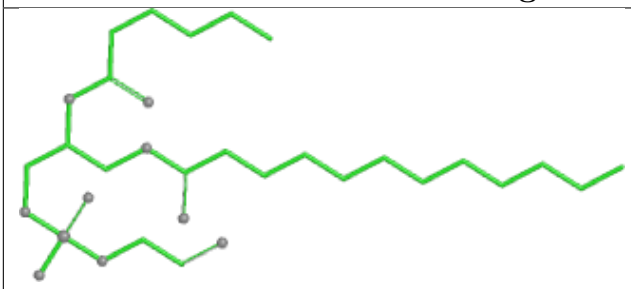


Rings

Ligand 3PE 5Y 204



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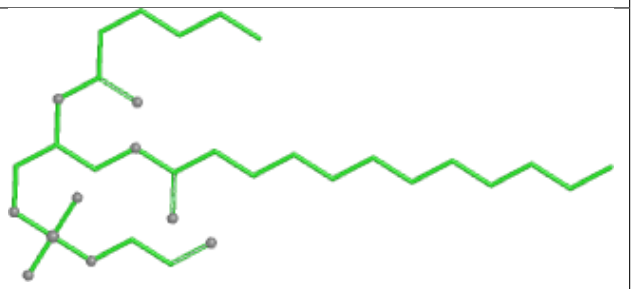

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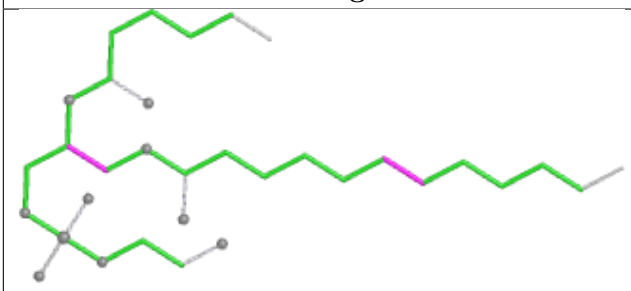

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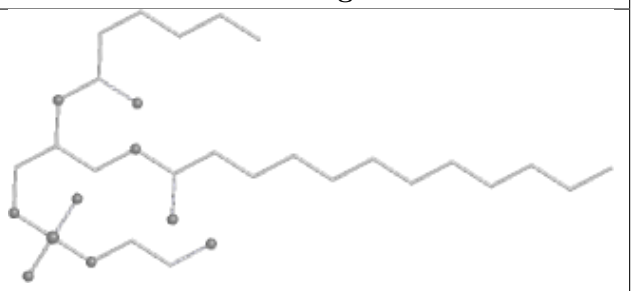
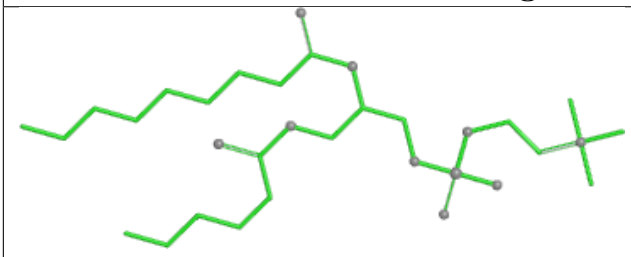


Rings

Ligand PC1 5P 401



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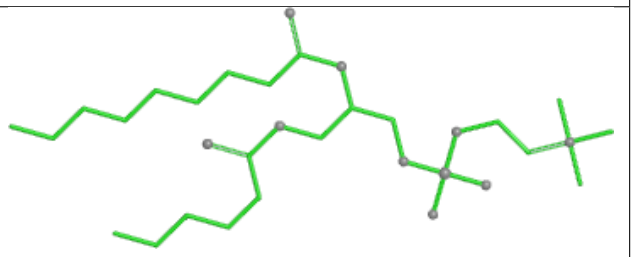

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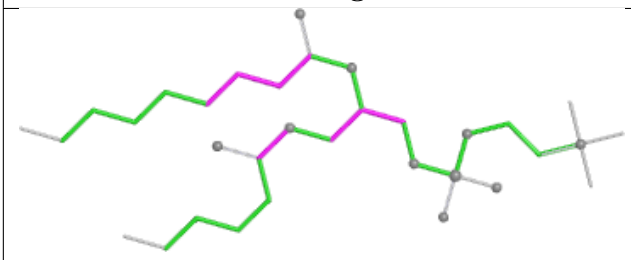

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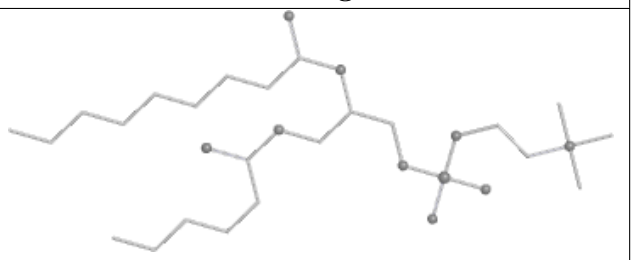
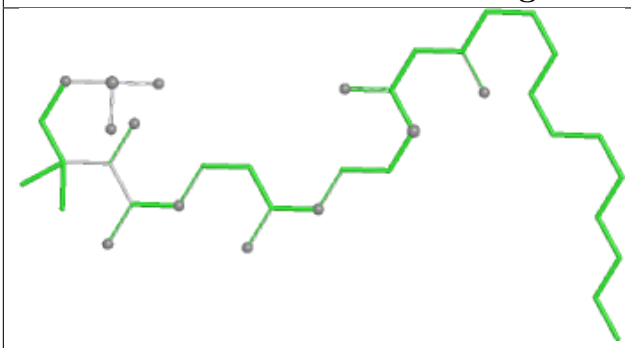


Rings

Ligand EHZ 1n 201



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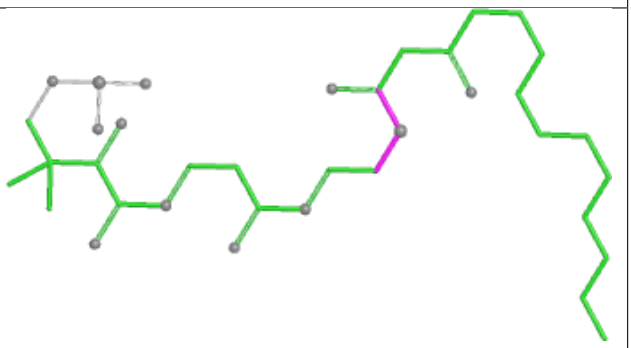
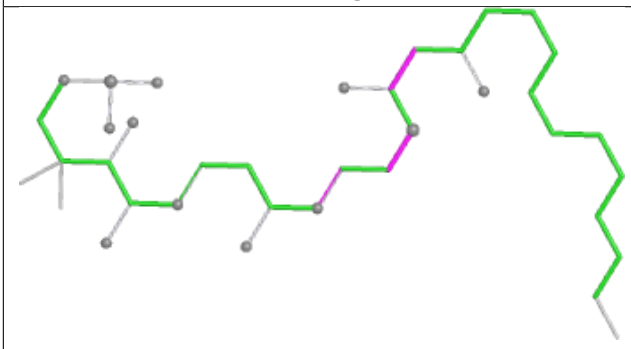


Bond angles



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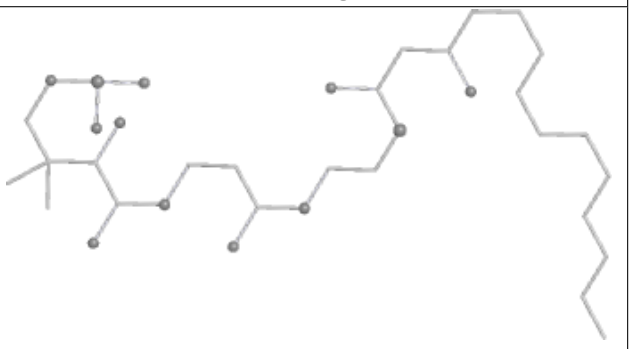
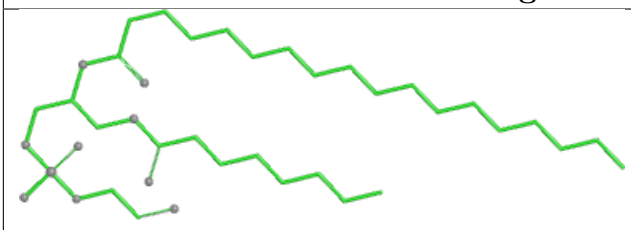


Rings

Ligand 3PE 5Y 206



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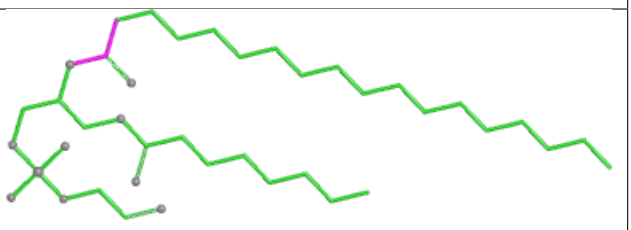

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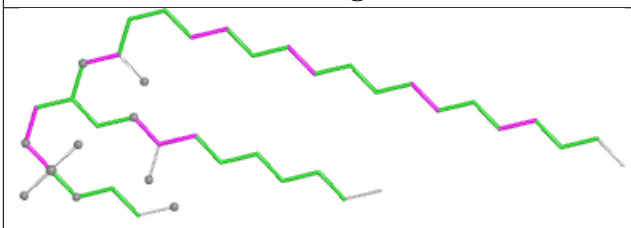

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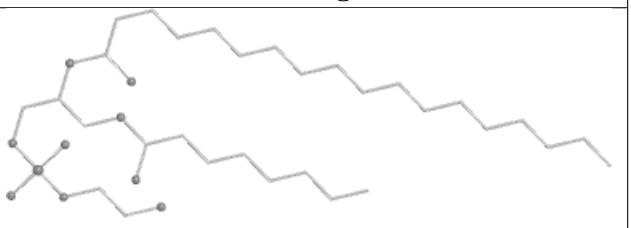
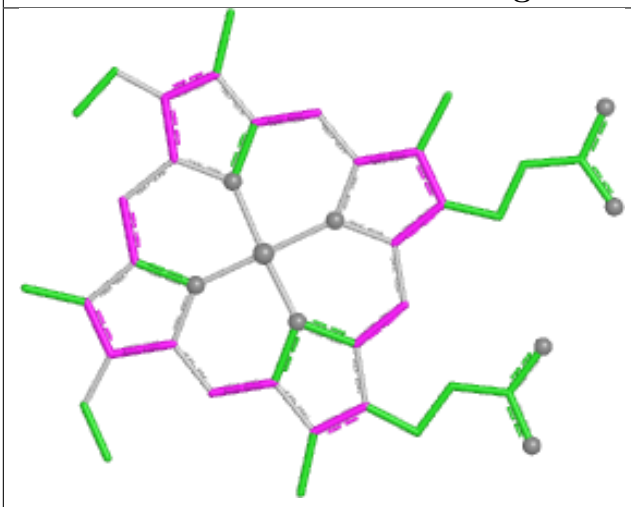


Rings

Ligand HEC 3Q 501



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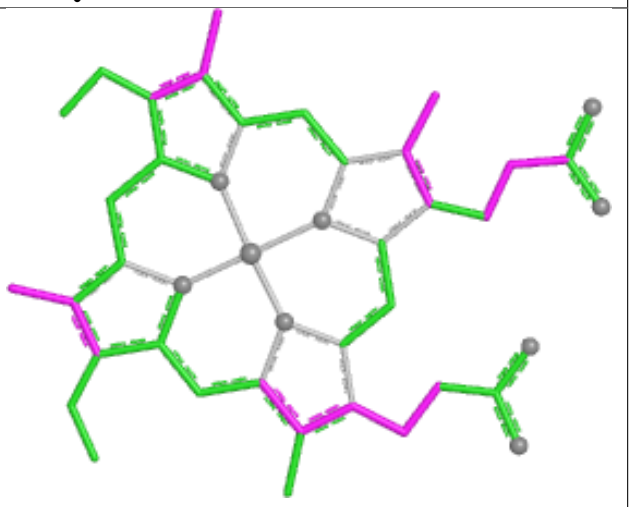

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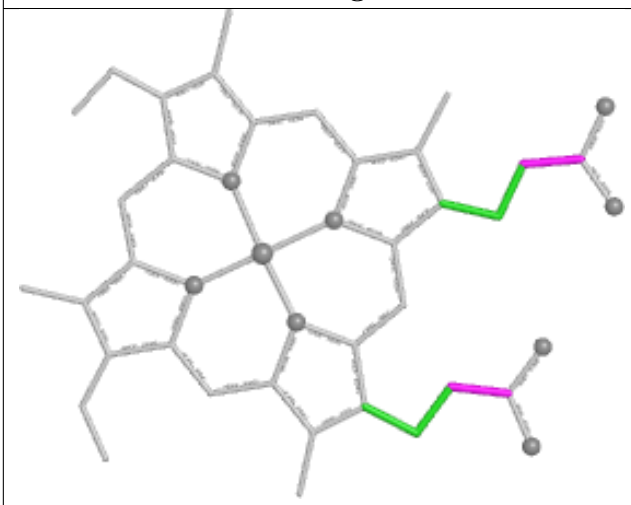

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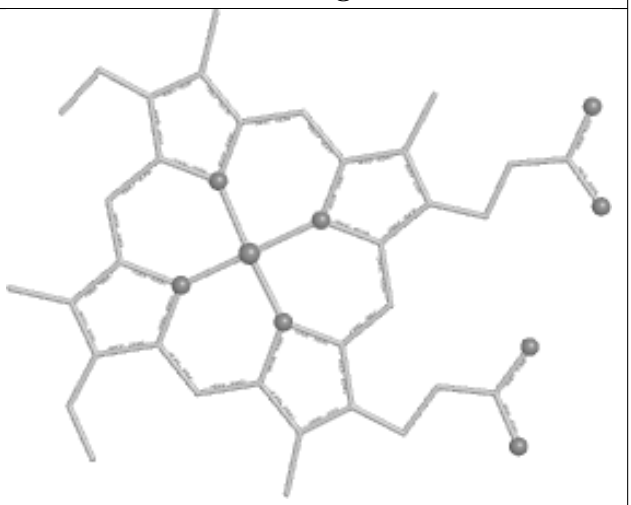
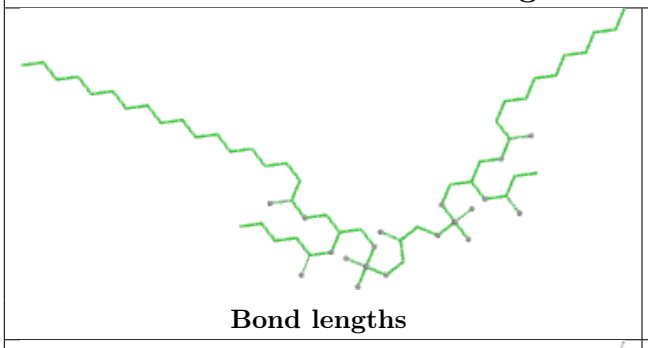


Rings

Ligand CDL 5d 202



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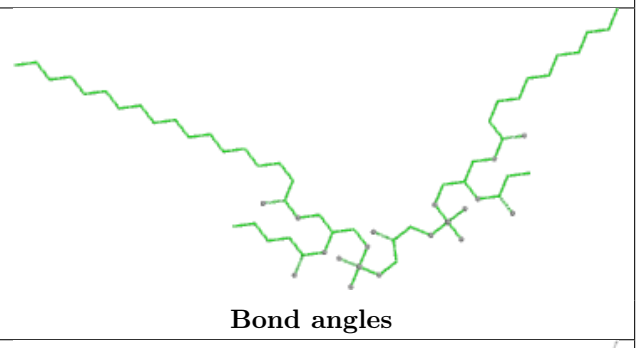

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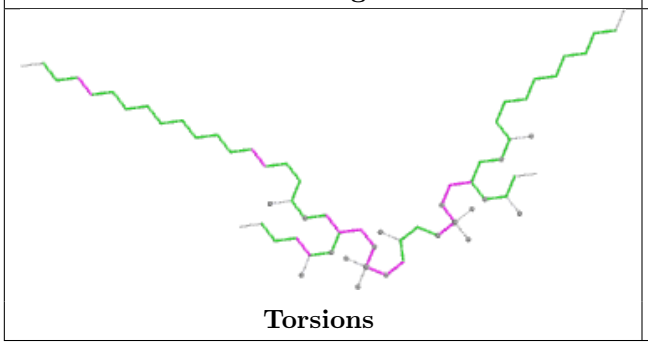

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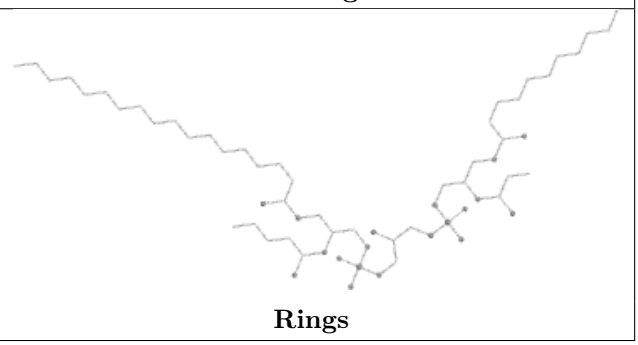
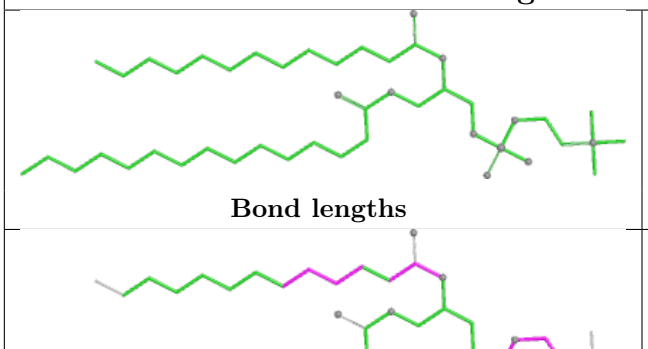


Rings

Ligand PC1 5m 201



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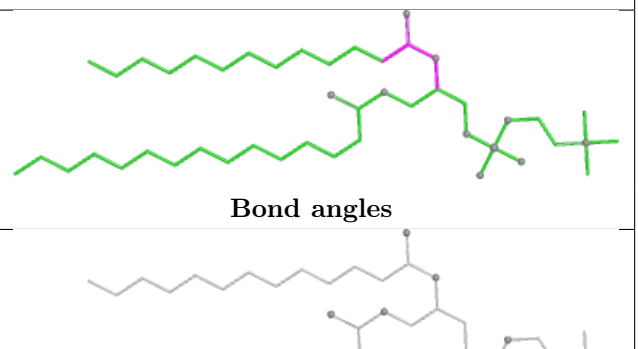
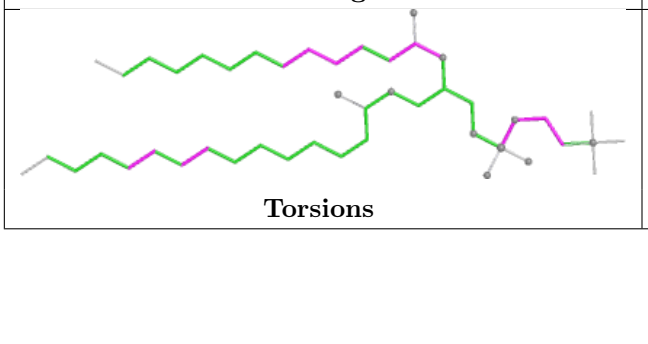


Bond angles



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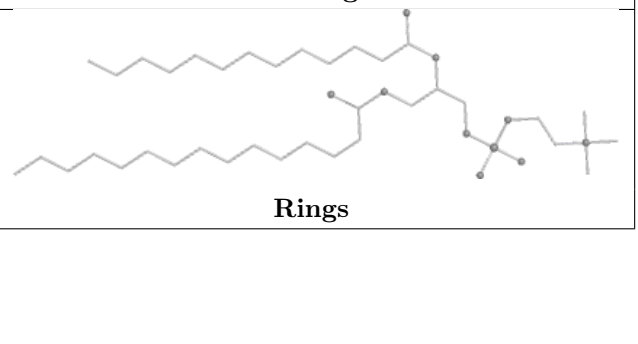
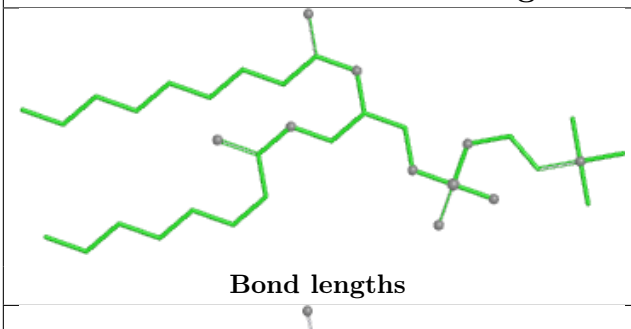


Rings

Ligand PC1 5Y 201



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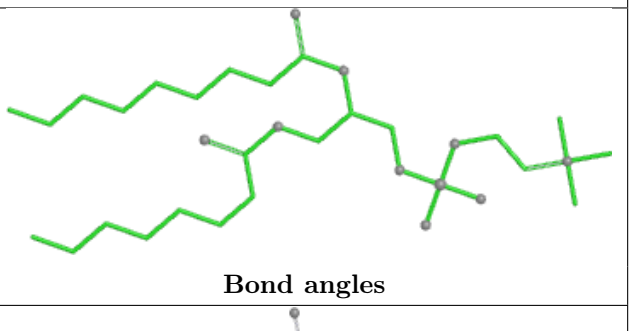
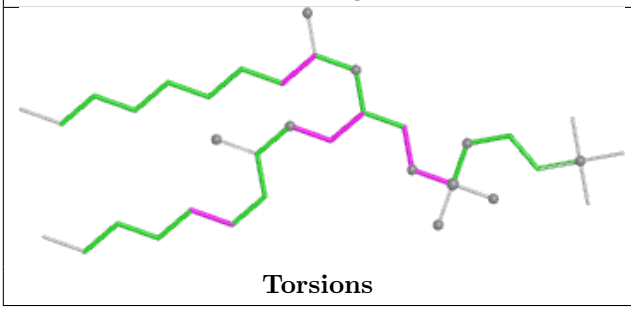
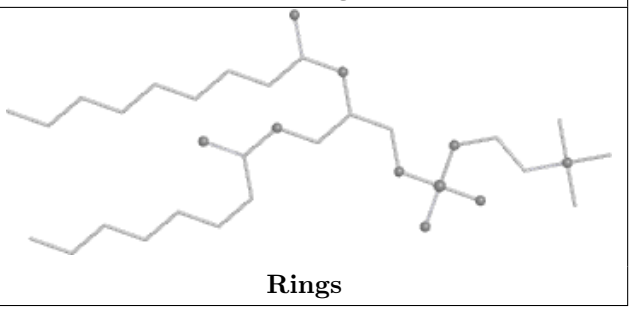


Bond angles

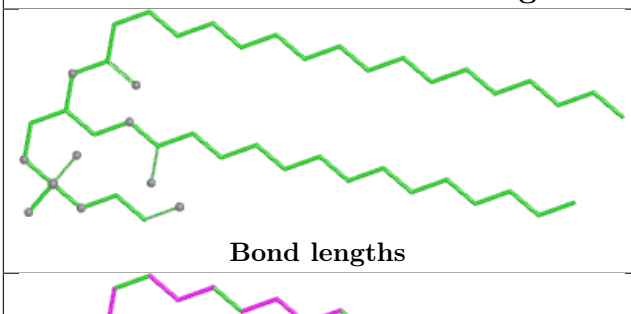


Torsions



Rings

Ligand 3PE 1A 201



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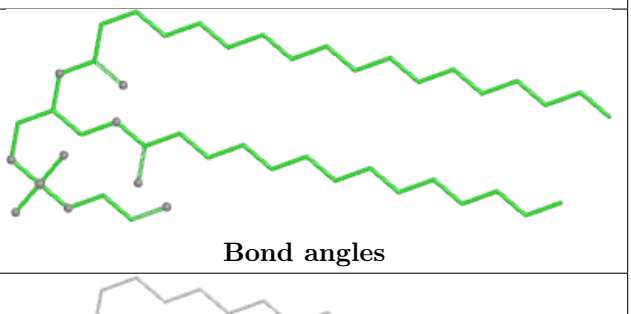
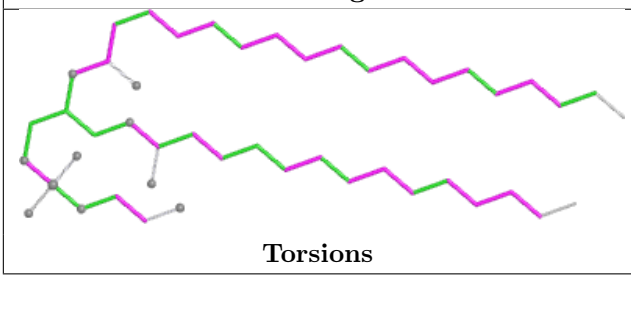


Bond angles



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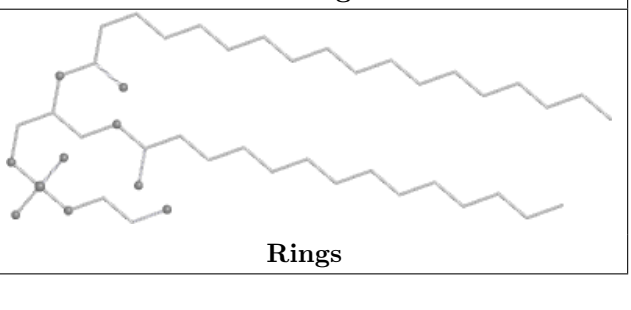
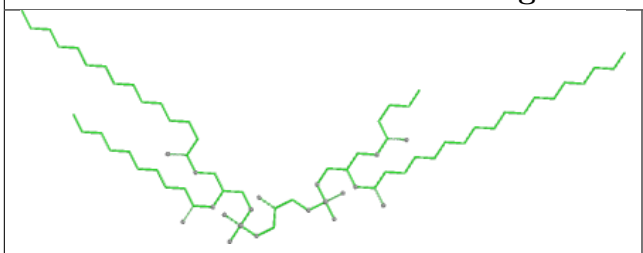


Rings

Ligand CDL 5L 702



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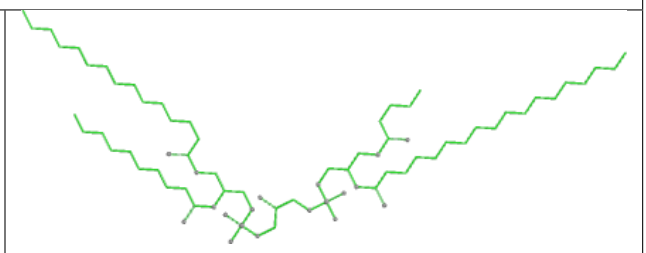
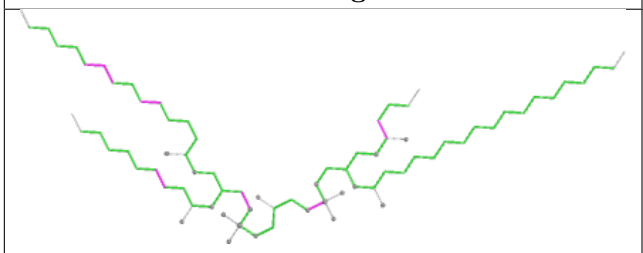
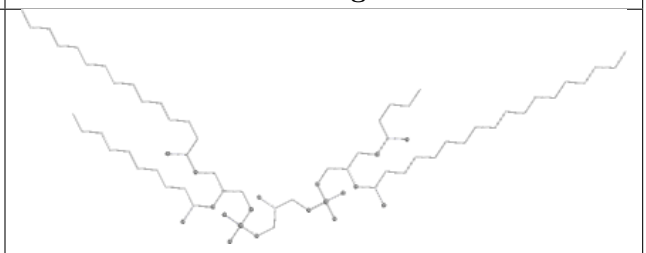


Bond angles

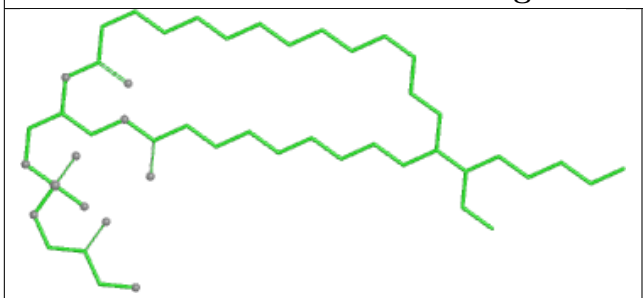


Torsions

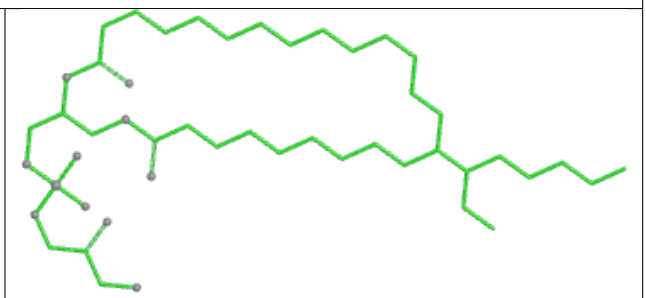


Rings

Ligand PGV 4C 302

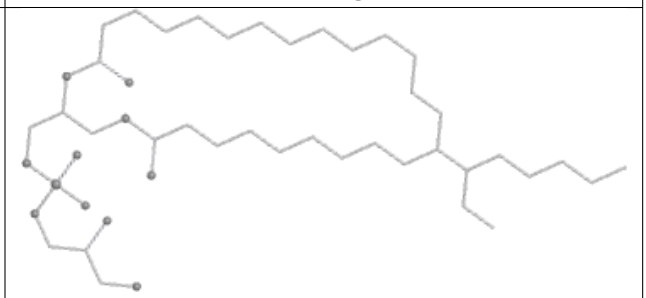


Bond lengths



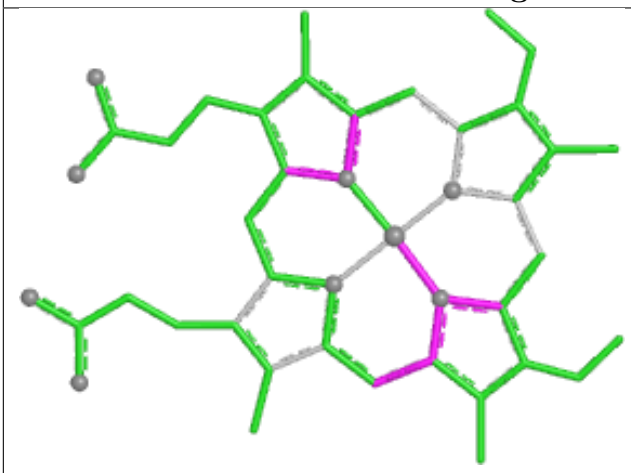
Bond angles

Torsions



Rings

Ligand HEM 3P 501



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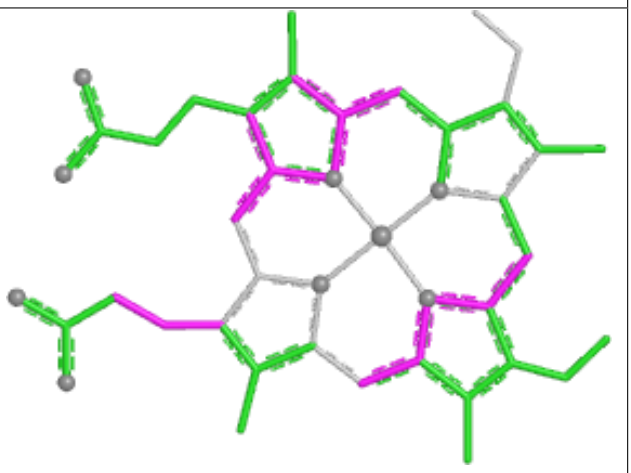
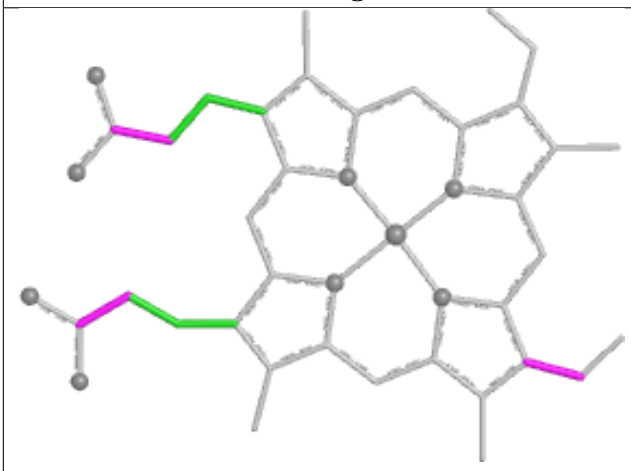


Bond angles



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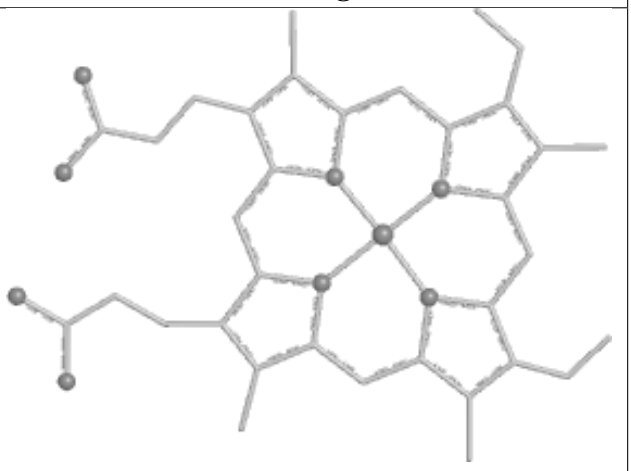
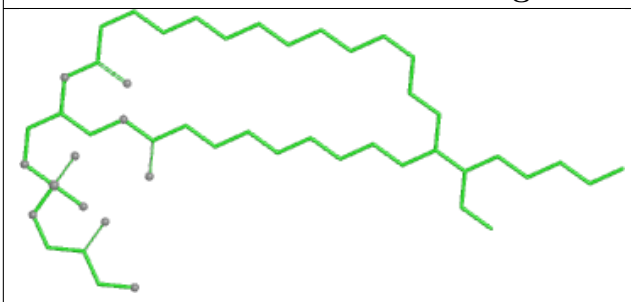


Rings

Ligand PGV 8C 302



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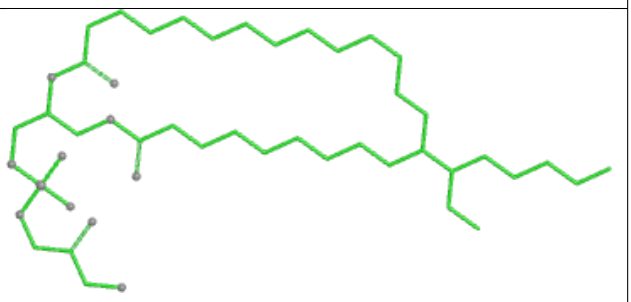
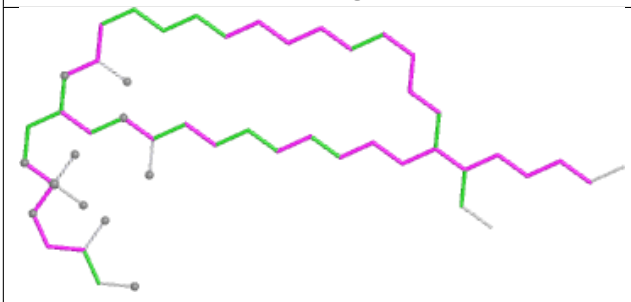


Bond angles



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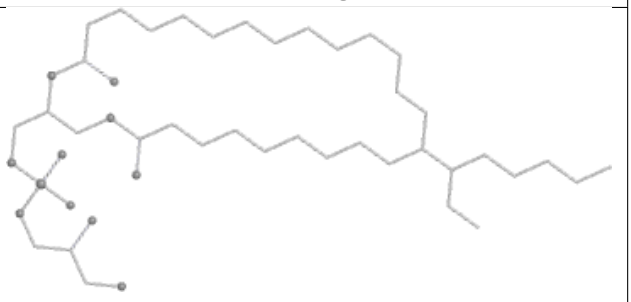
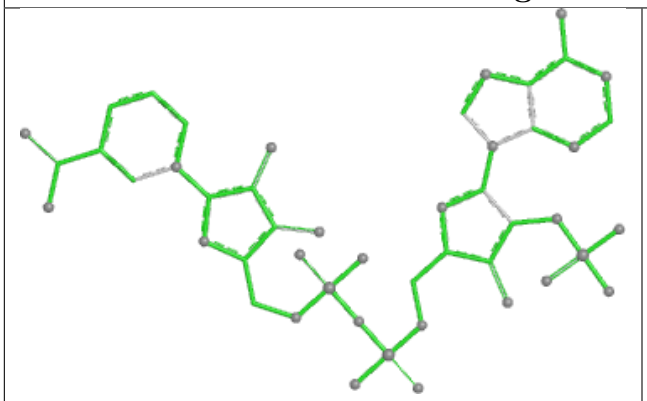


Rings

Ligand NDP 5P 402



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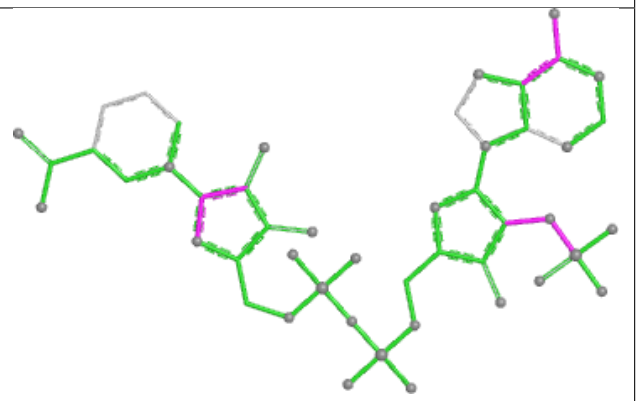
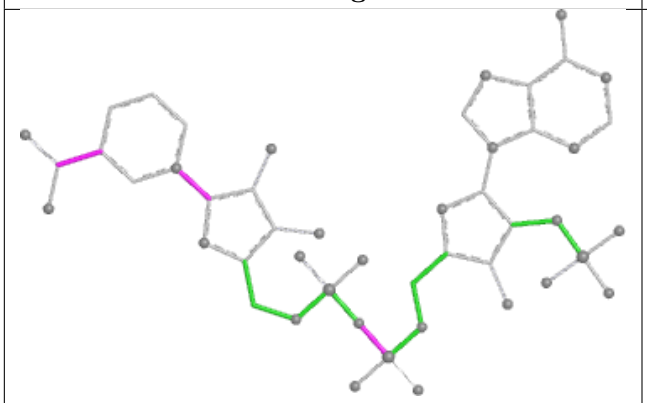


Bond angles



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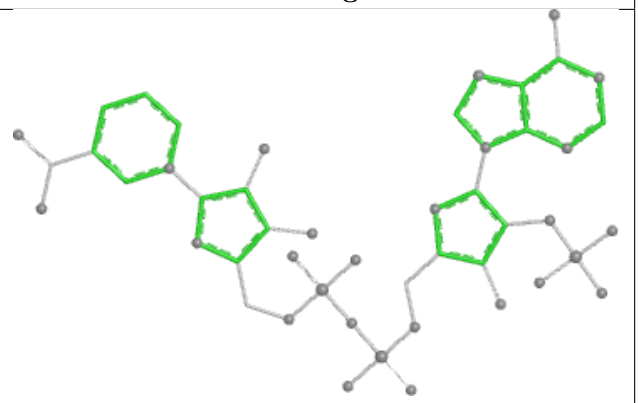
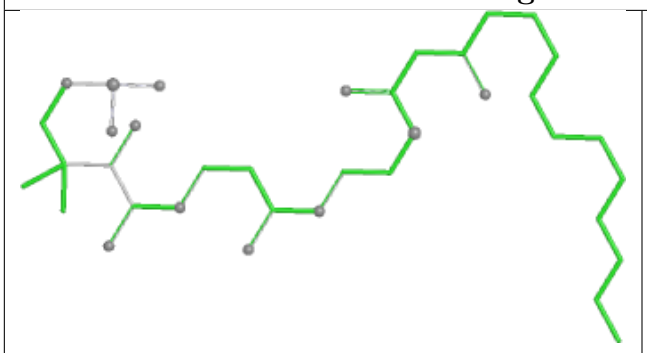


Rings

Ligand EHZ 5T 101



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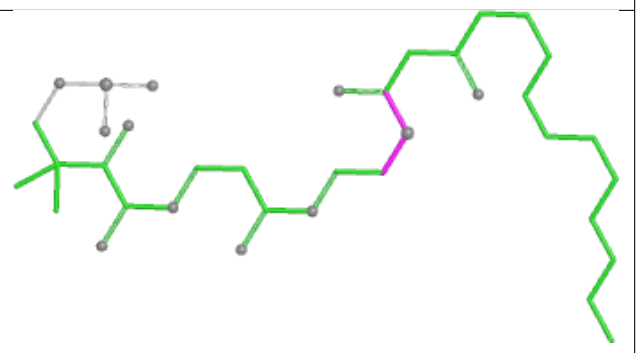

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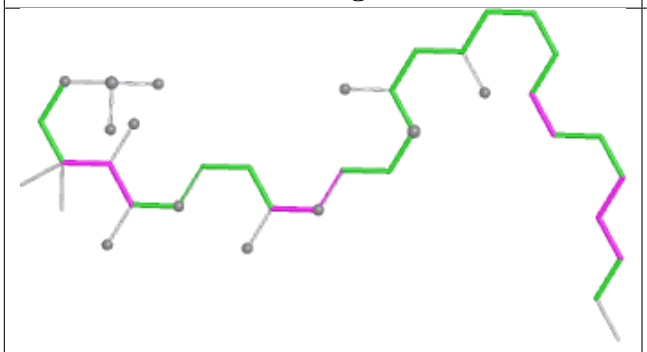

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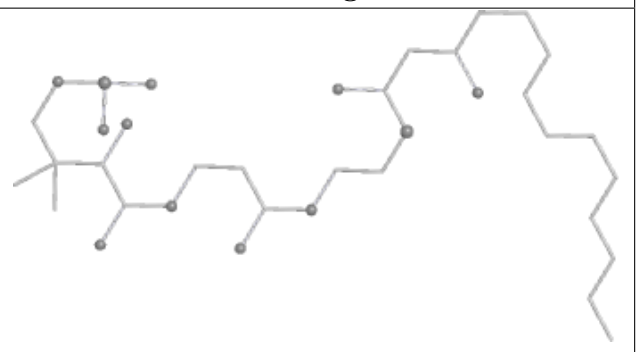
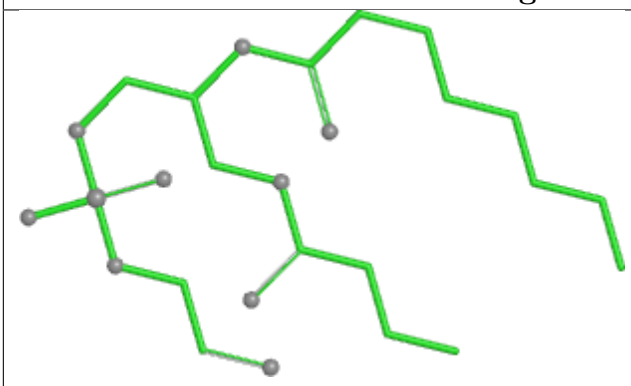


Rings

Ligand 3PE 5Y 205



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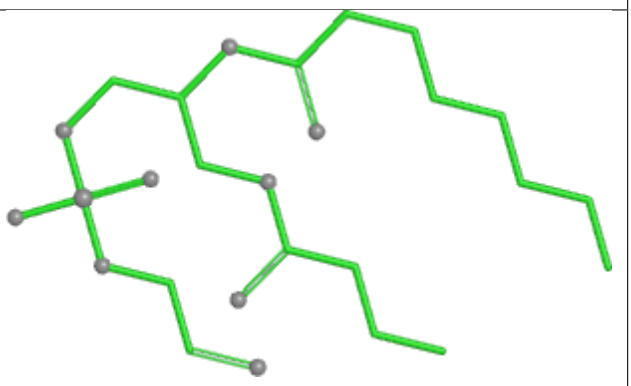
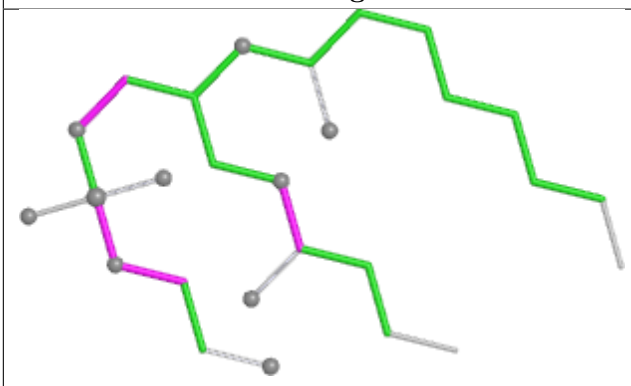
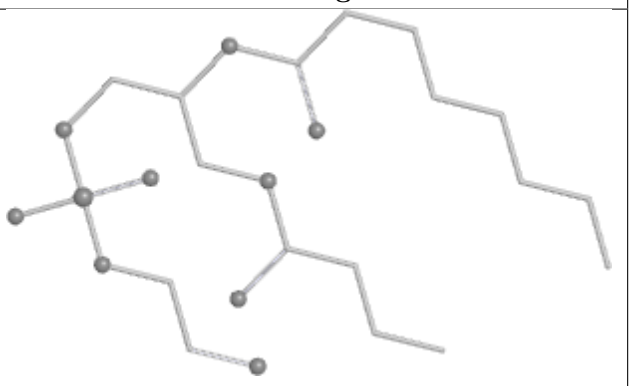


Bond angles

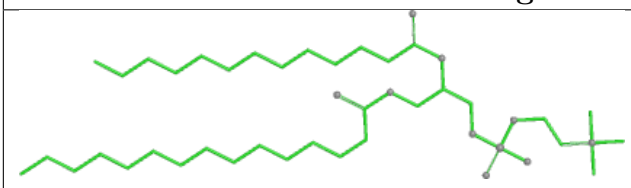


Torsions



Rings

Ligand PC1 1m 201



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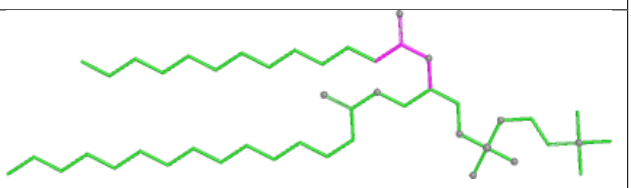

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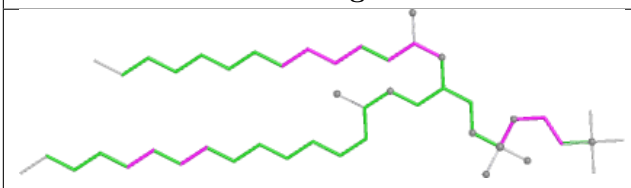

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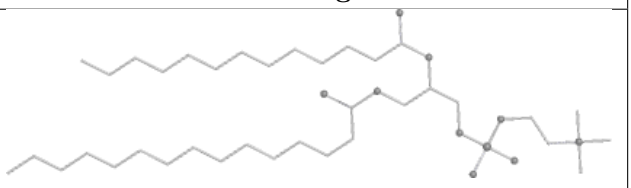
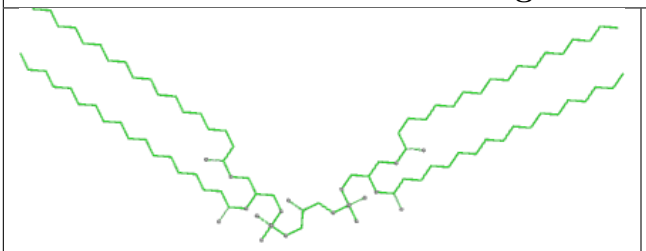


Rings

Ligand CDL 8B 302



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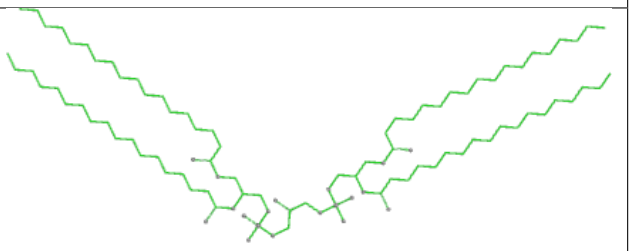
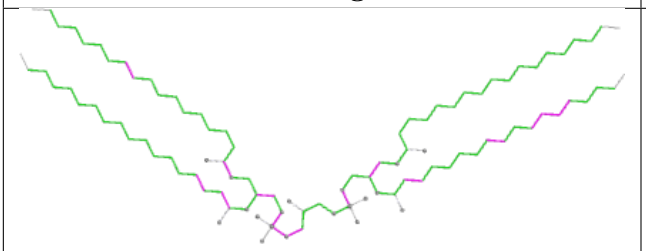


Bond angles



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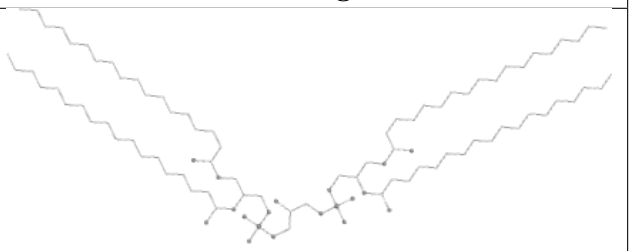
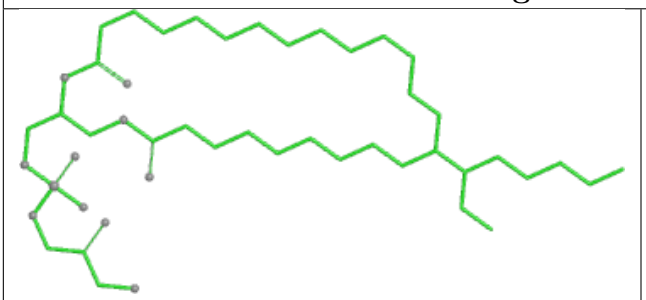


Rings

Ligand PGV 8C 303



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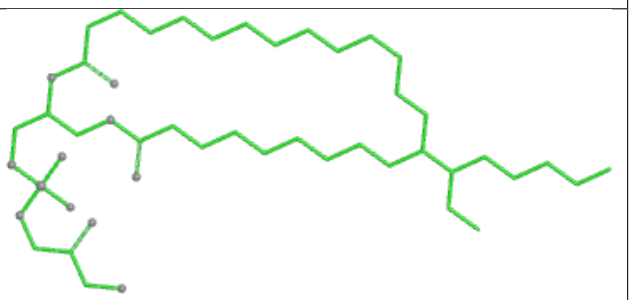
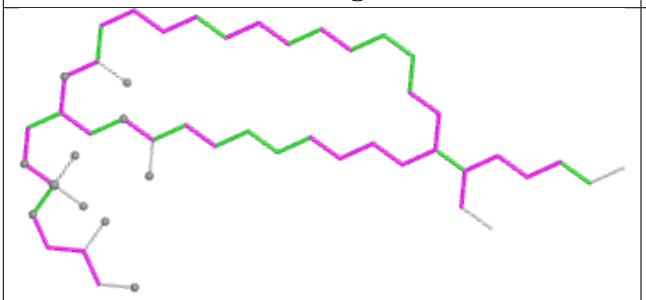


Bond angles



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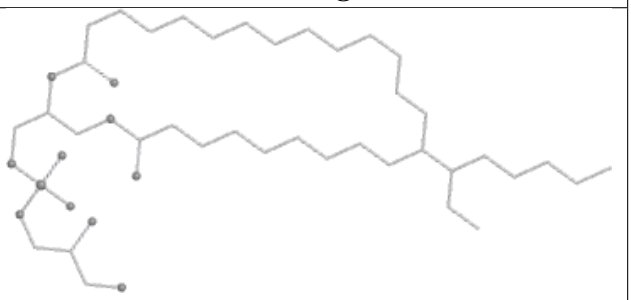
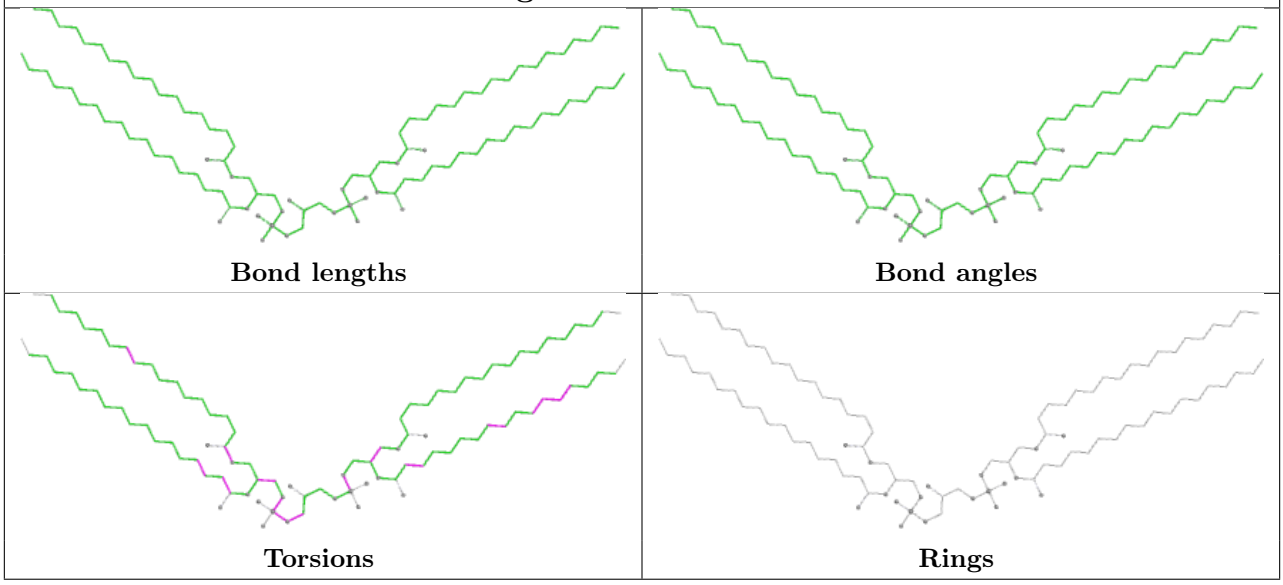
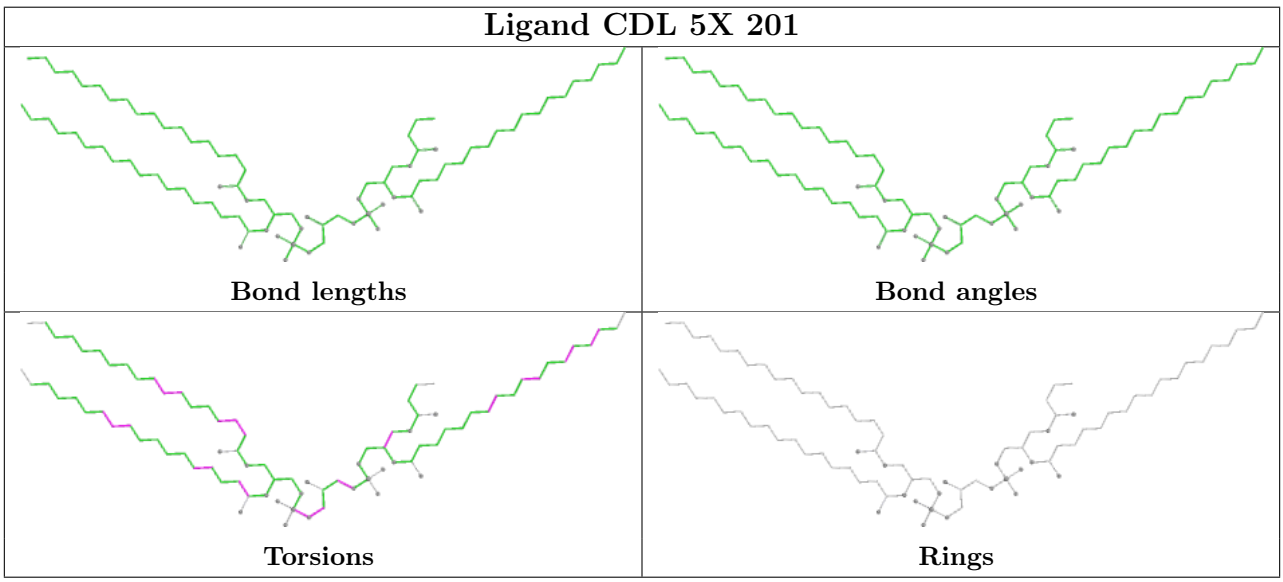


Rings

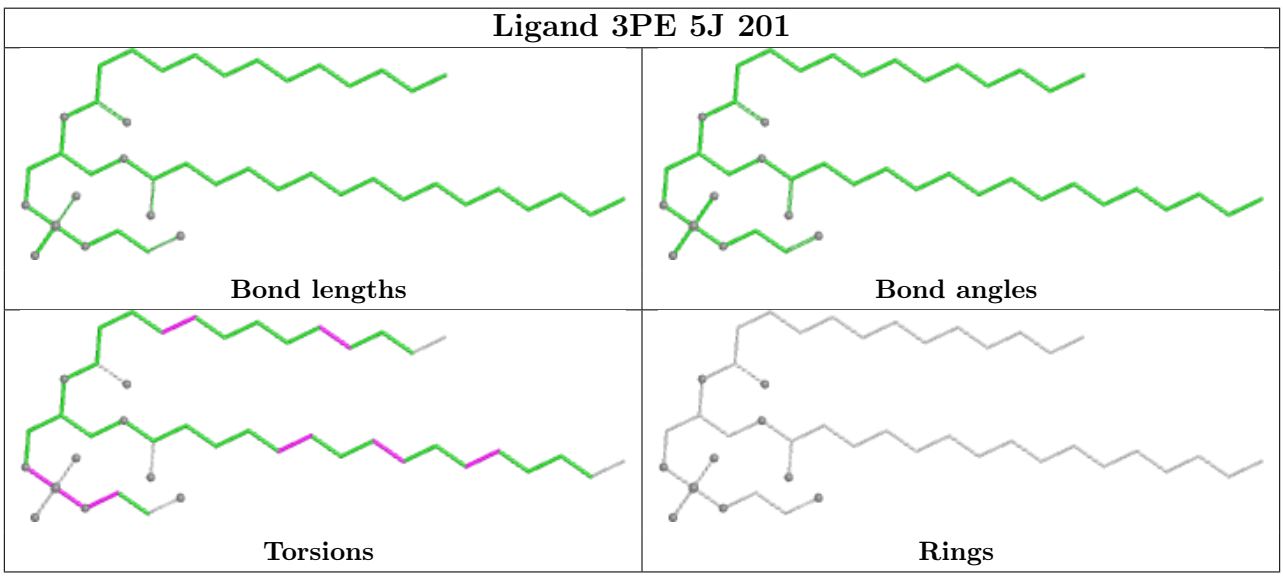
Ligand CDL 4B 301



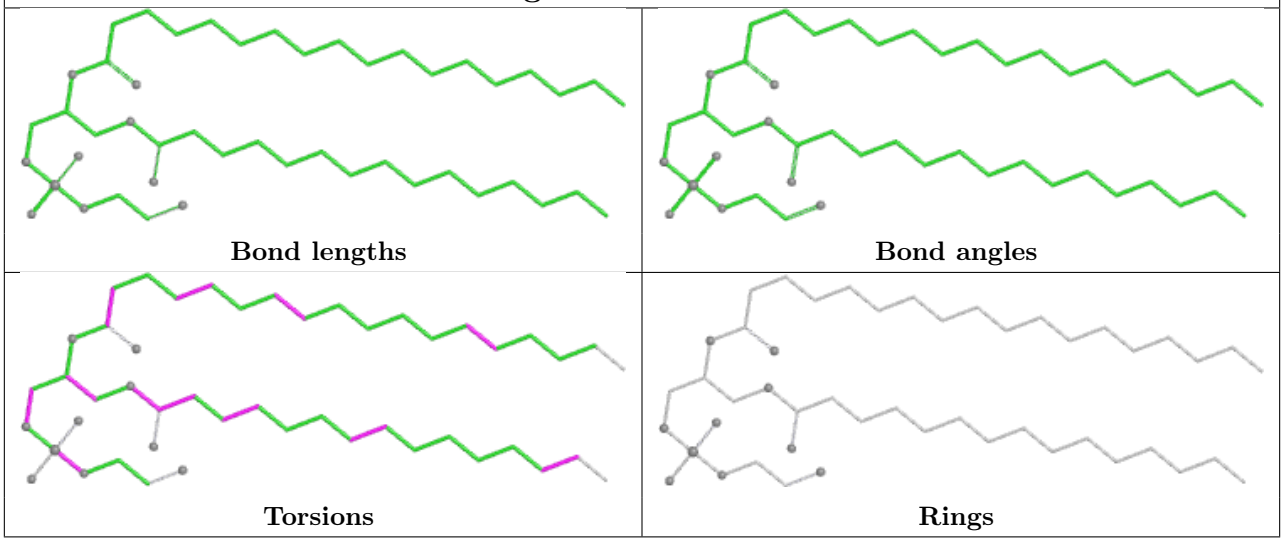
Ligand CDL 5X 201



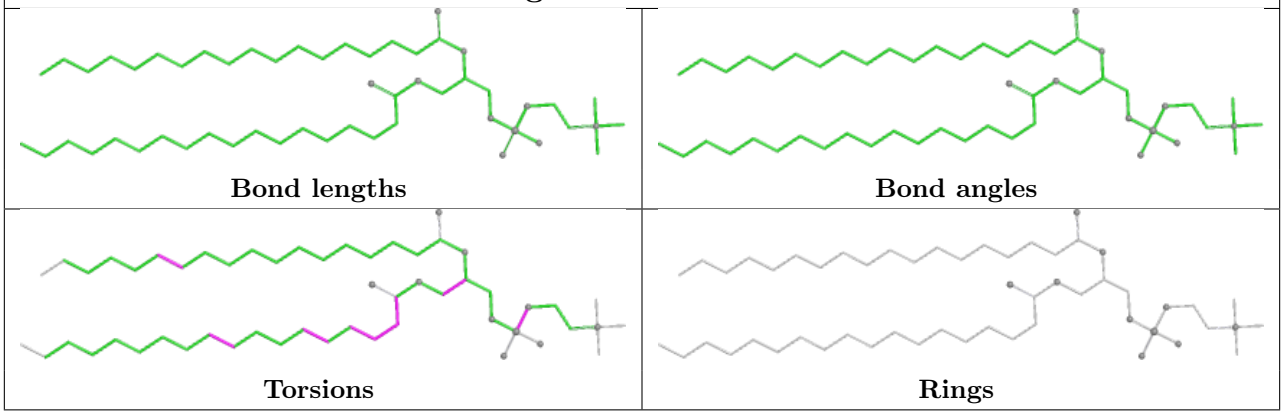
Ligand 3PE 5J 201



Ligand 3PE 5d 201



Ligand PC1 1I 201



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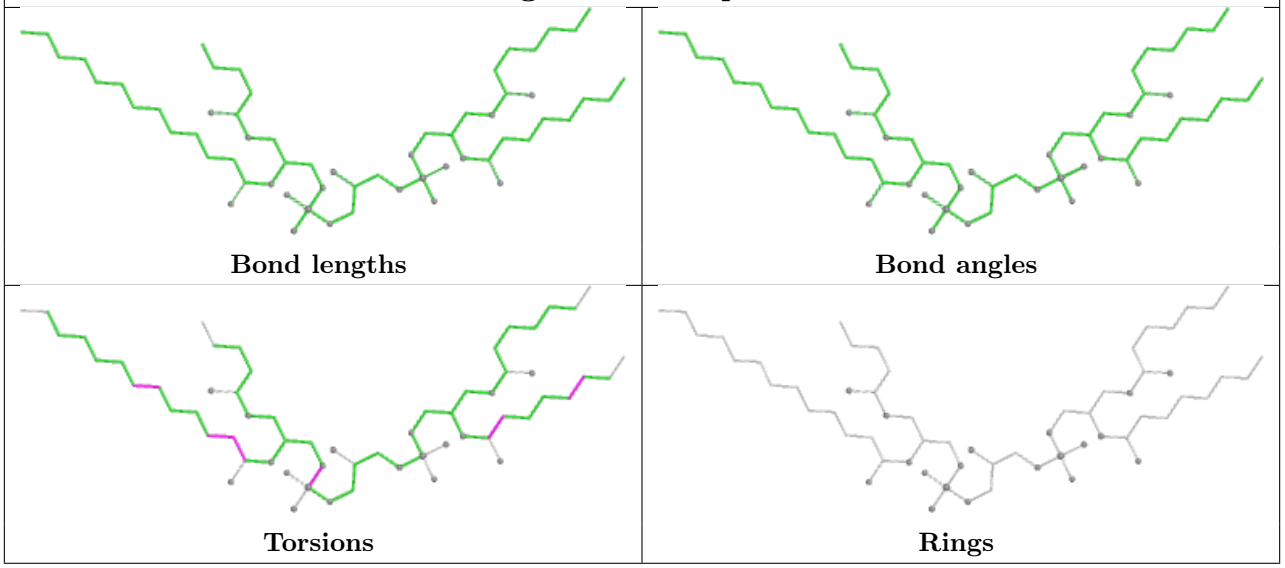
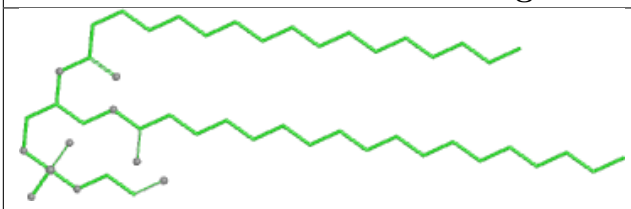
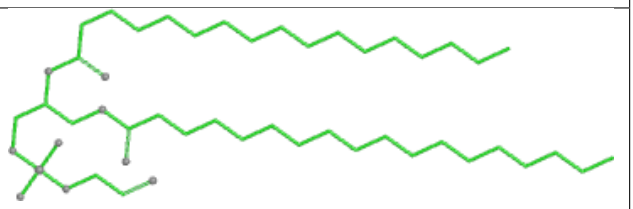
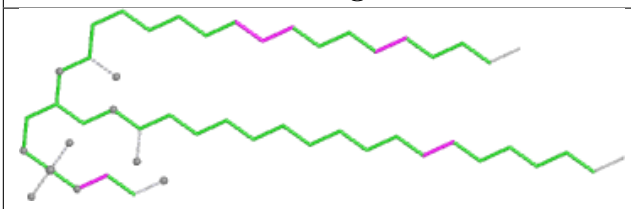
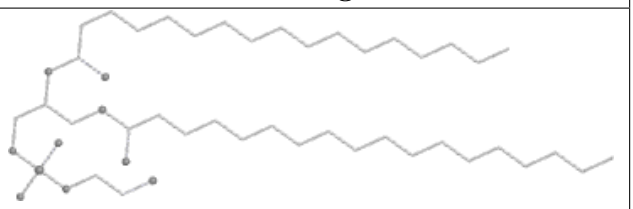
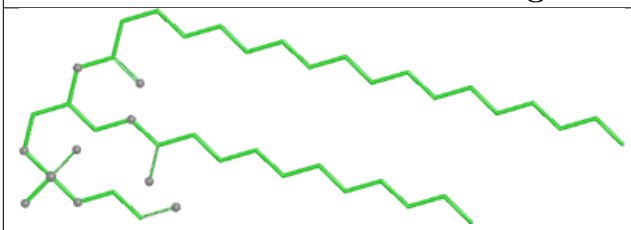
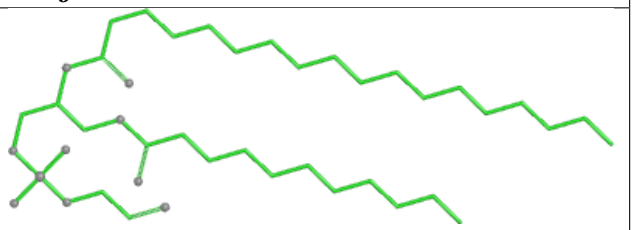
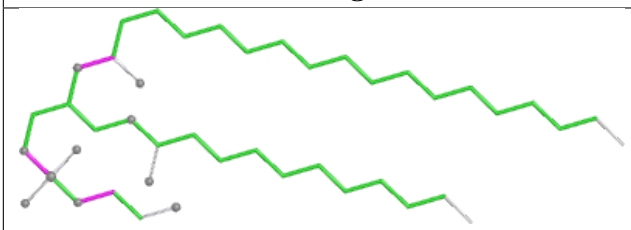
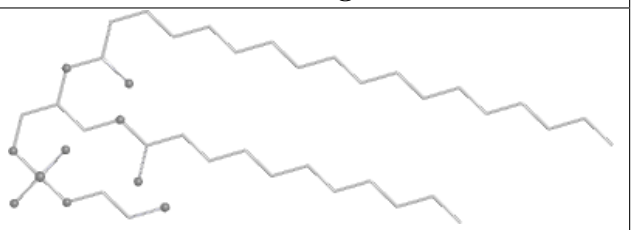
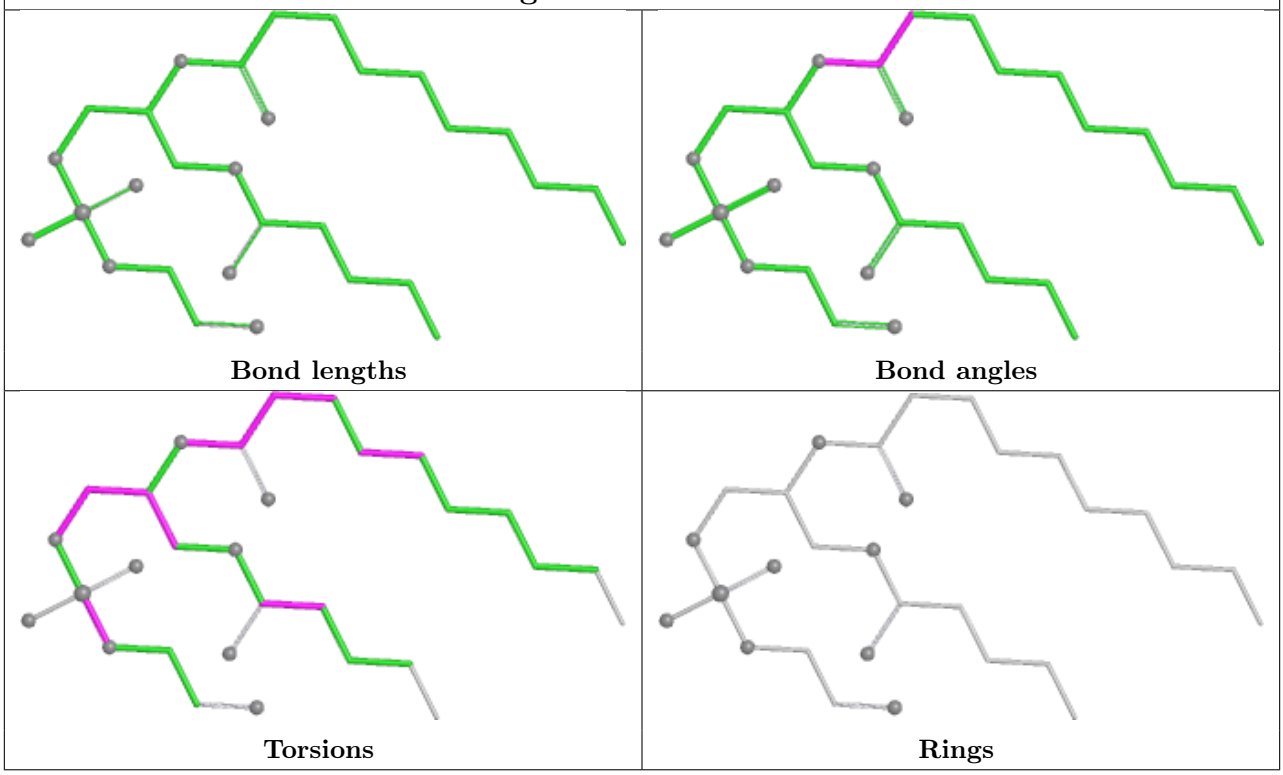


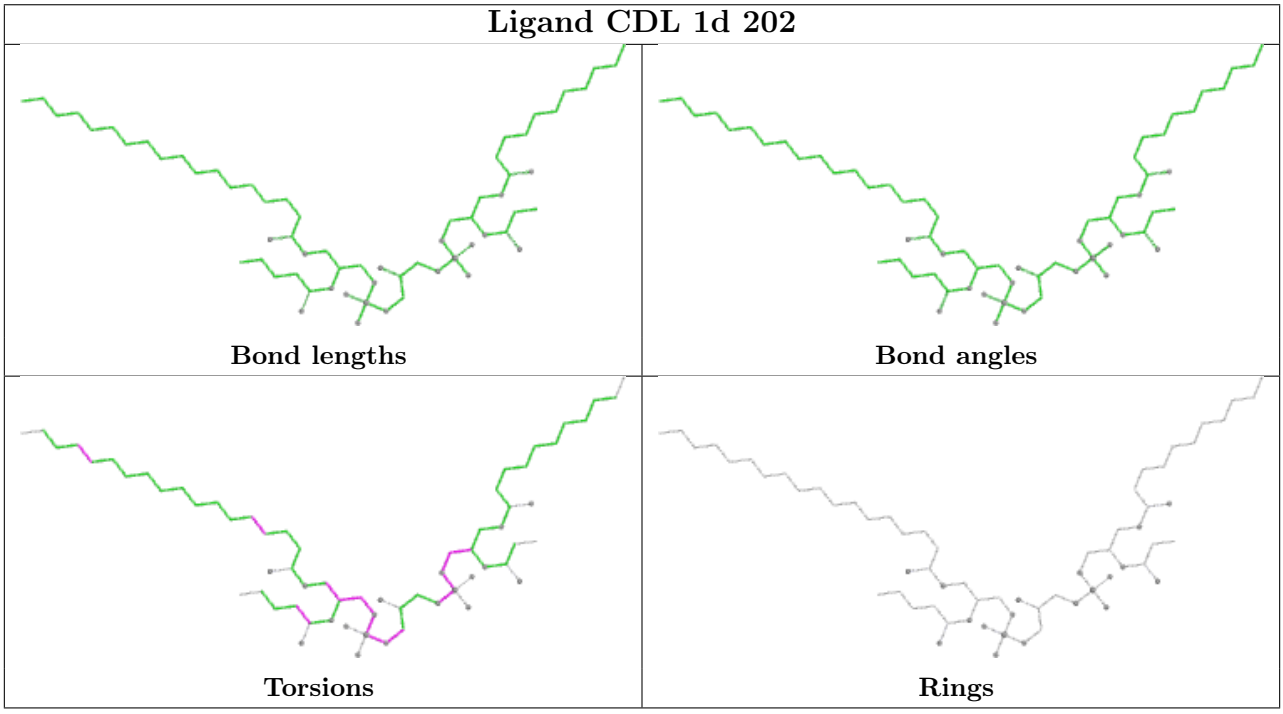
Ligand 3PE 1M 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE 1j 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

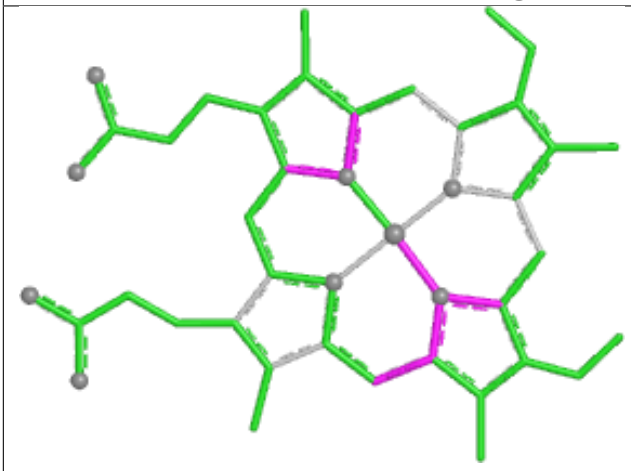
Ligand 3PE 5Y 203



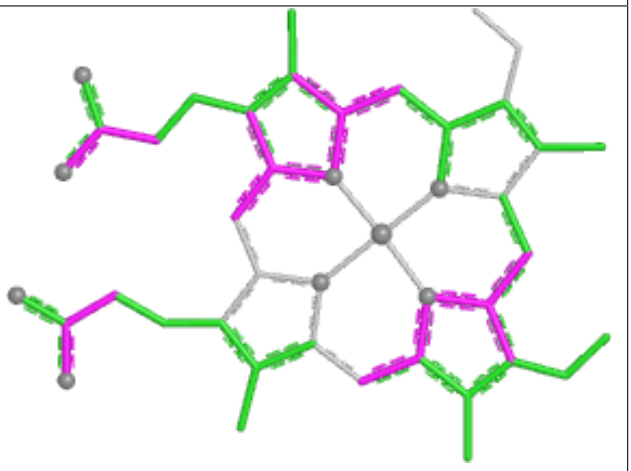
Ligand CDL 1d 202



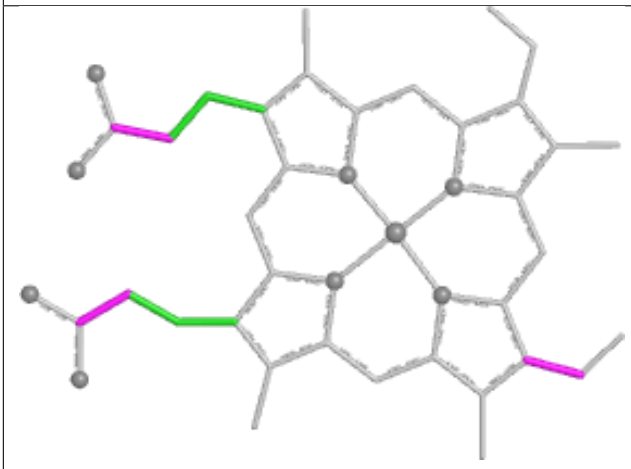
Ligand HEM 3P 502



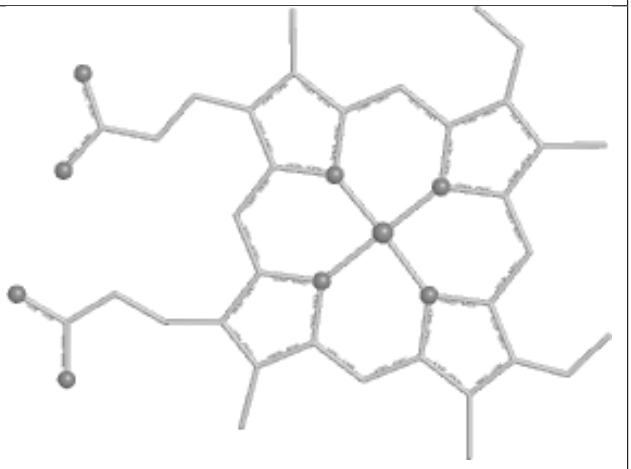
Bond lengths



Bond angles

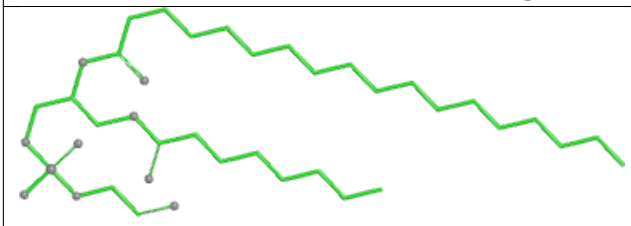


Torsions

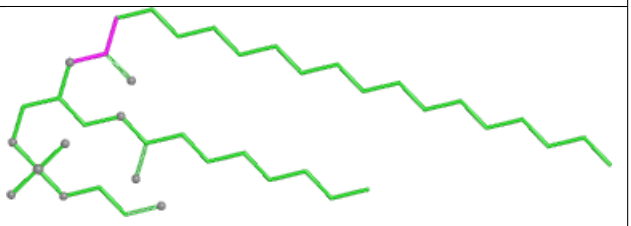


Rings

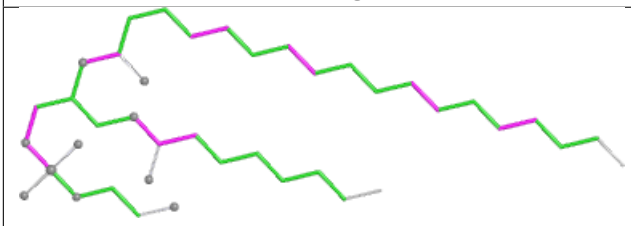
Ligand 3PE 1Y 206



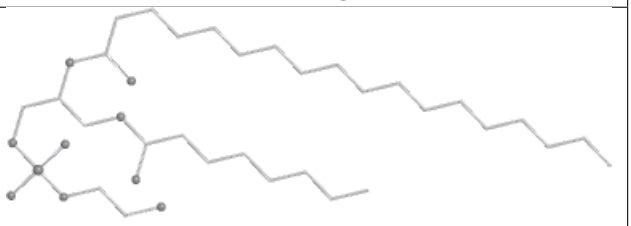
Bond lengths



Bond angles

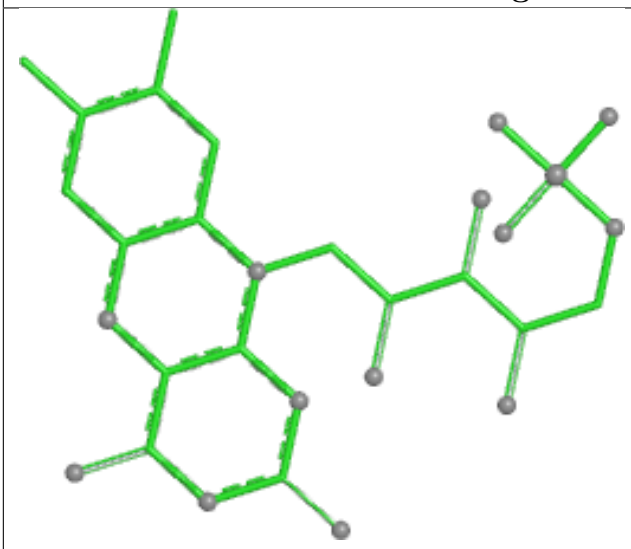


Torsions

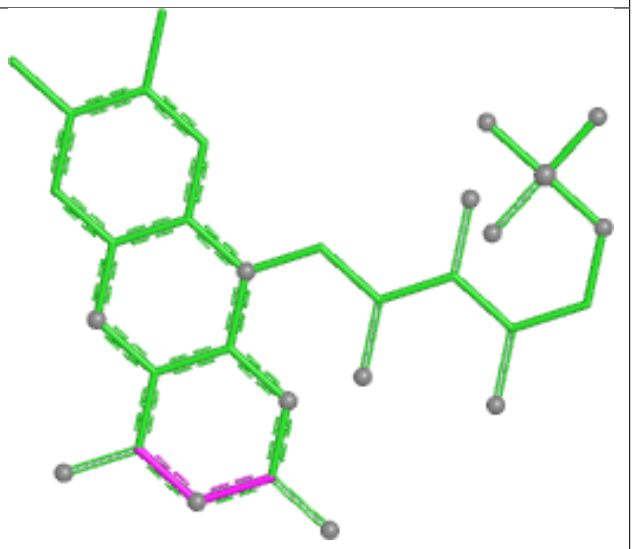


Rings

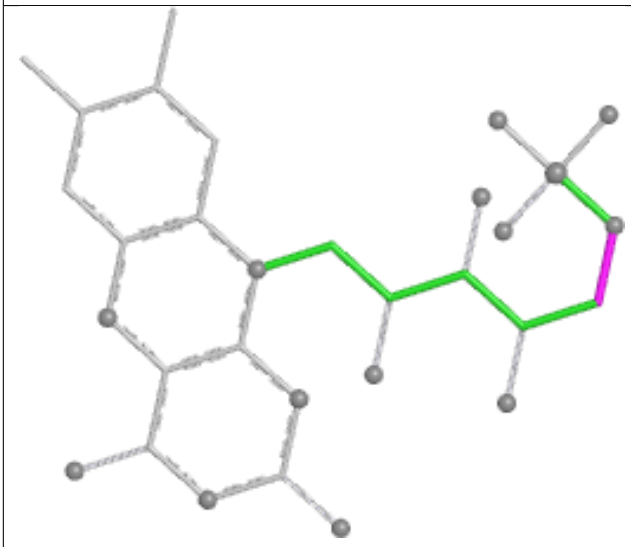
Ligand FMN 5F 501



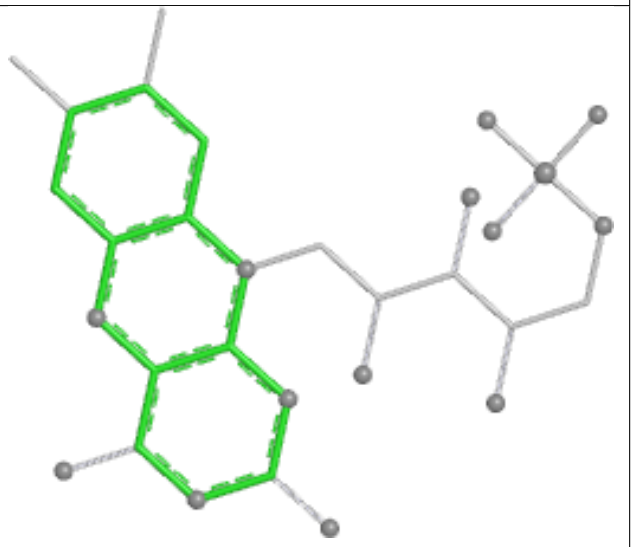
Bond lengths



Bond angles

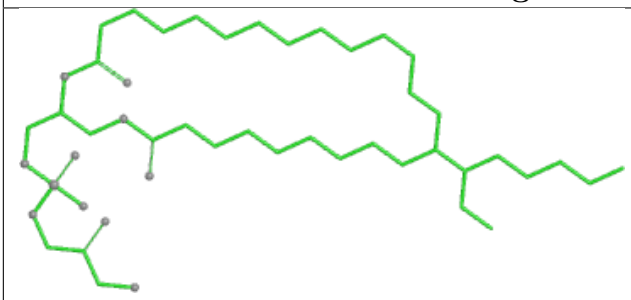


Torsions

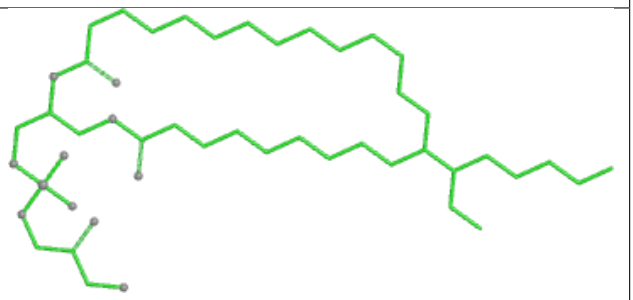


Rings

Ligand PGV 8A 602

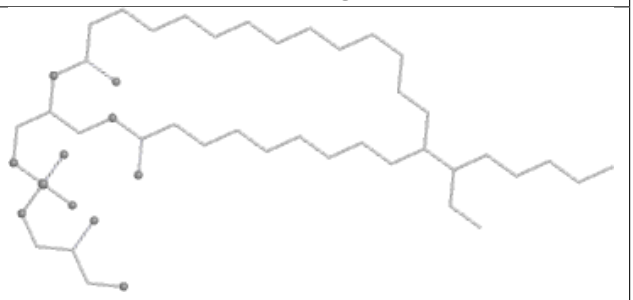


Bond lengths



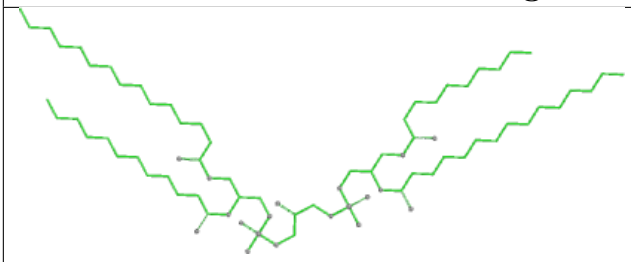
Bond angles

Torsions

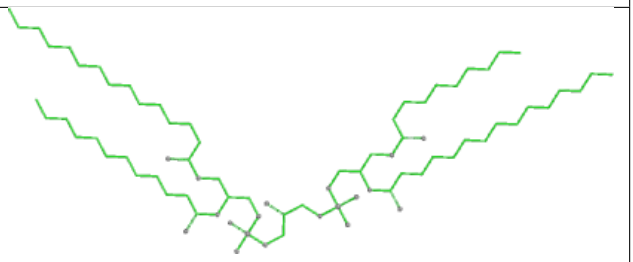


Rings

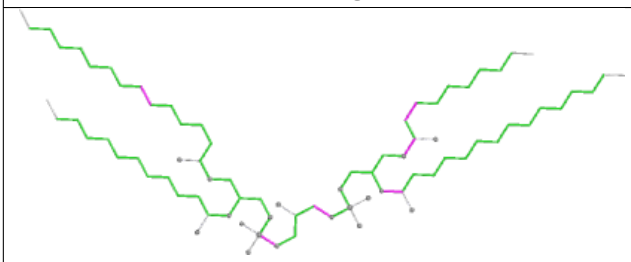
Ligand CDL 1i 201



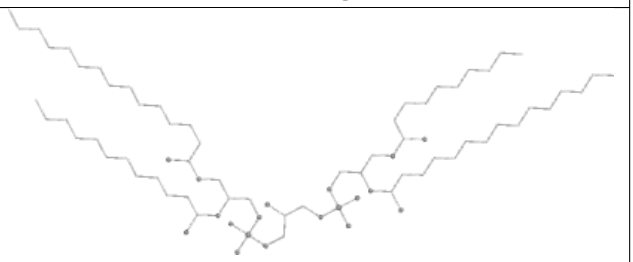
Bond lengths



Bond angles

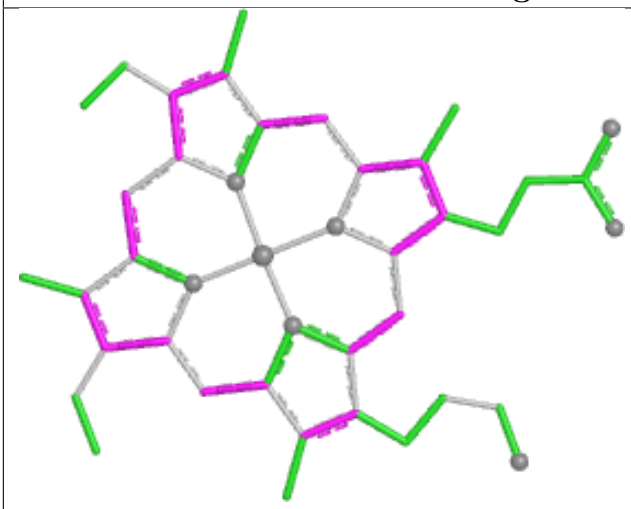


Torsions

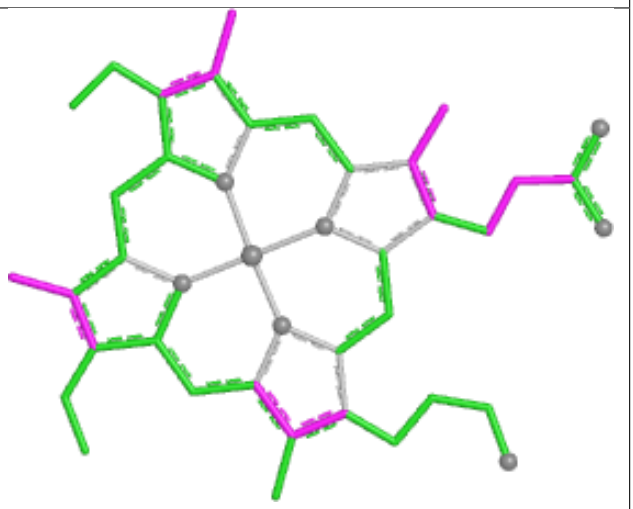


Rings

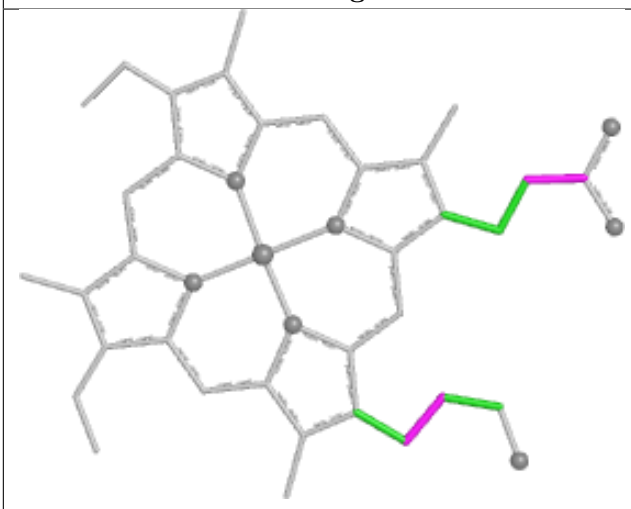
Ligand HEC 3D 501



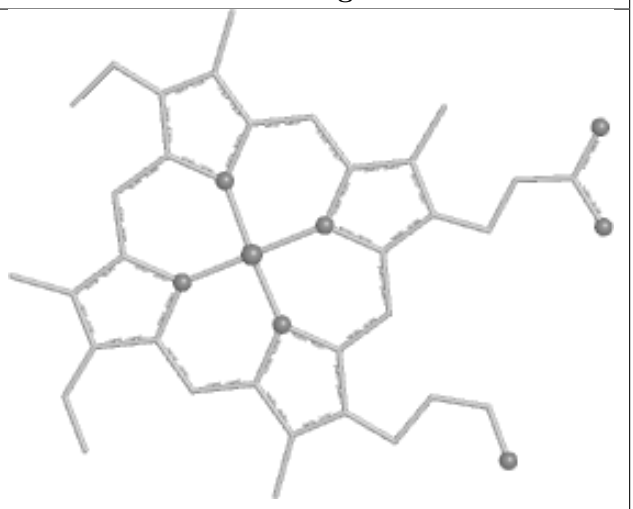
Bond lengths



Bond angles

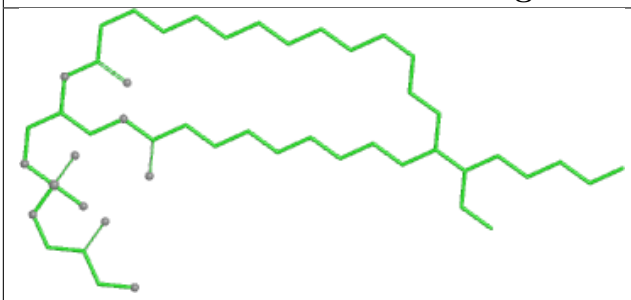


Torsions



Rings

Ligand PGV 4L 101



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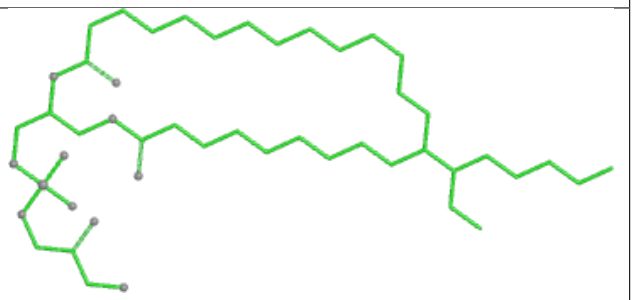
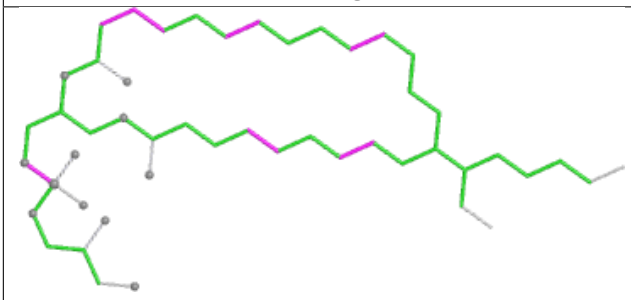


Bond angles



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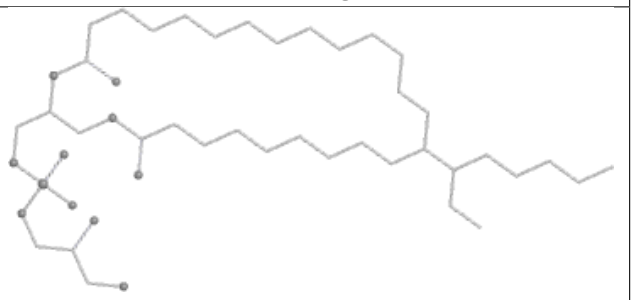
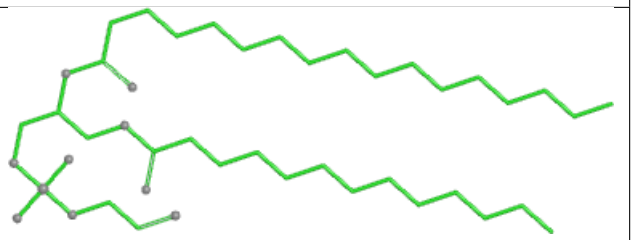


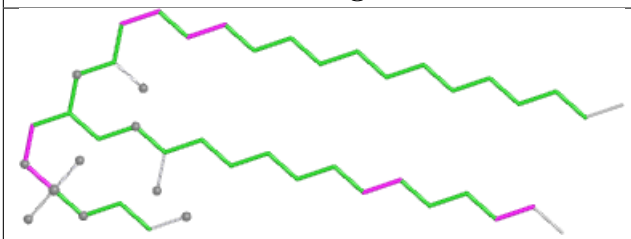
Rings

Ligand 3PE 5M 501

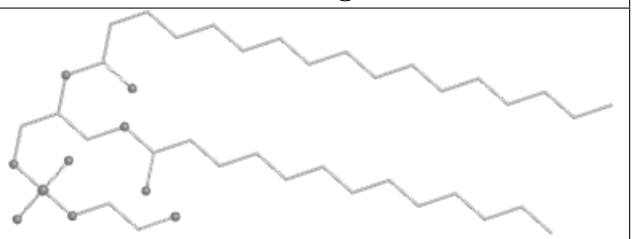
Bond lengths



Bond angles

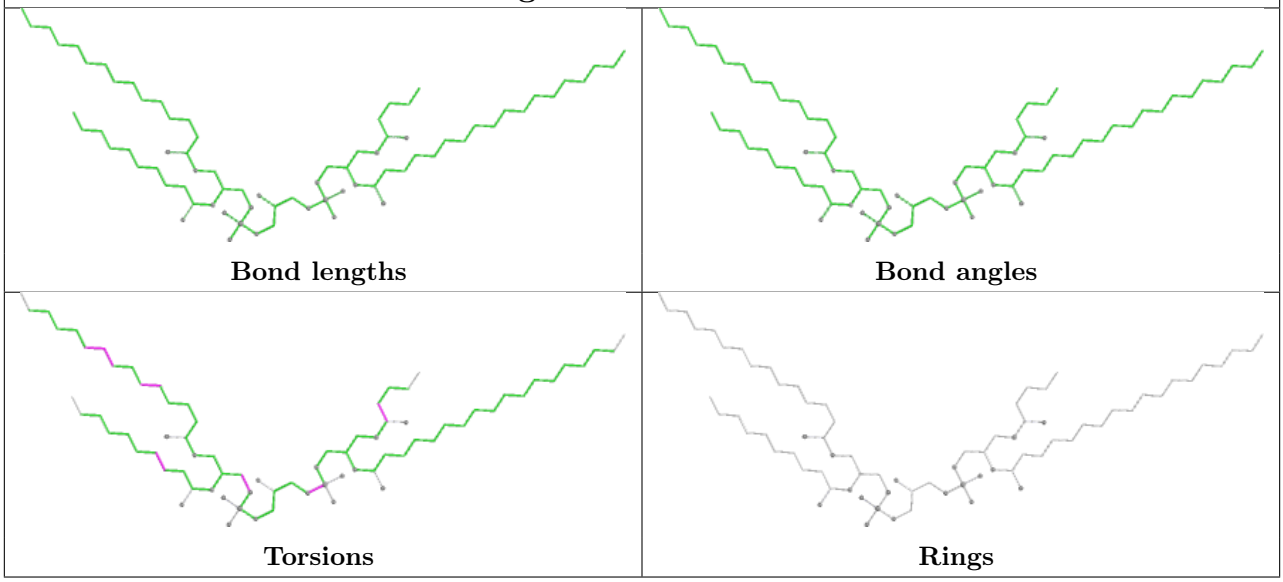


Torsions

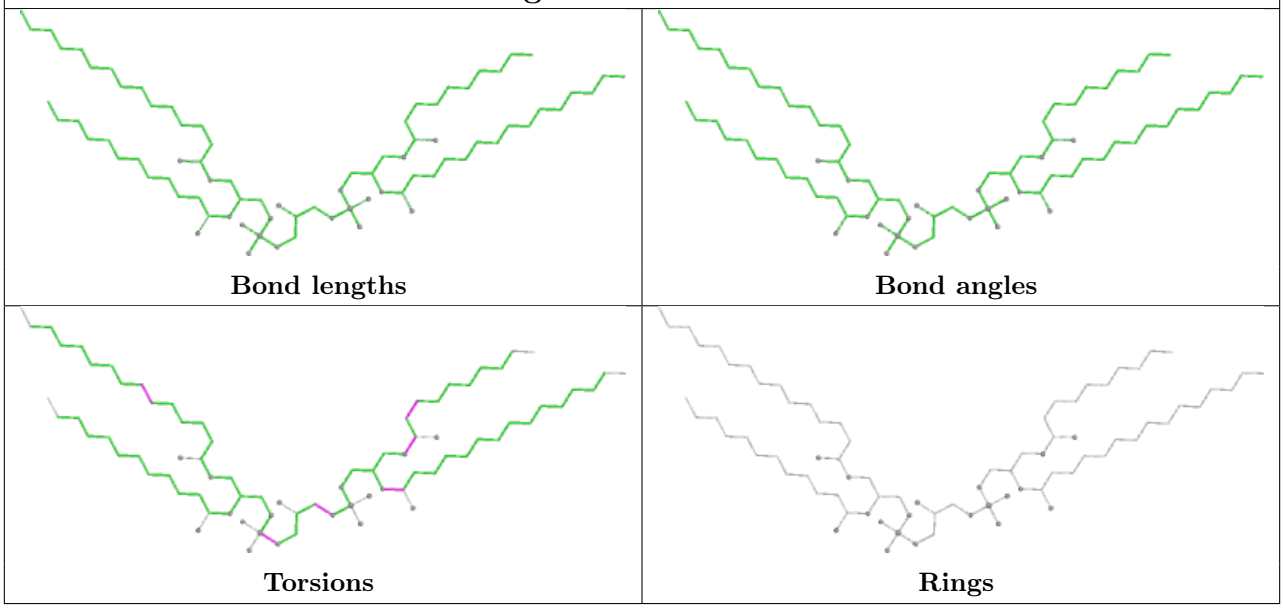


Rings

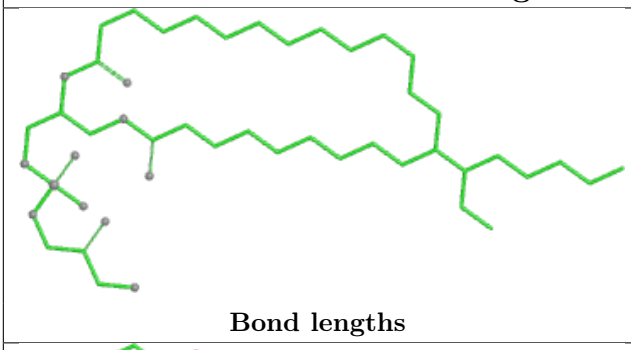
Ligand CDL 1L 702



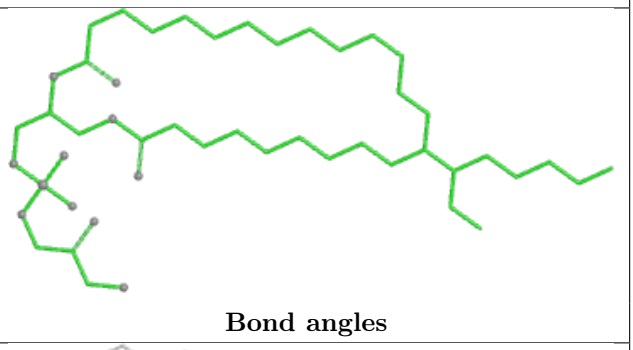
Ligand CDL 5i 201



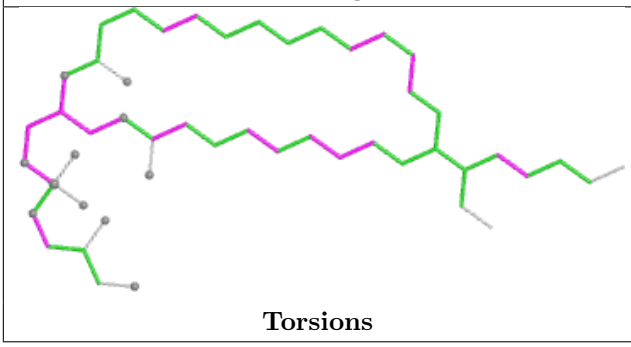
Ligand PGV 4C 303



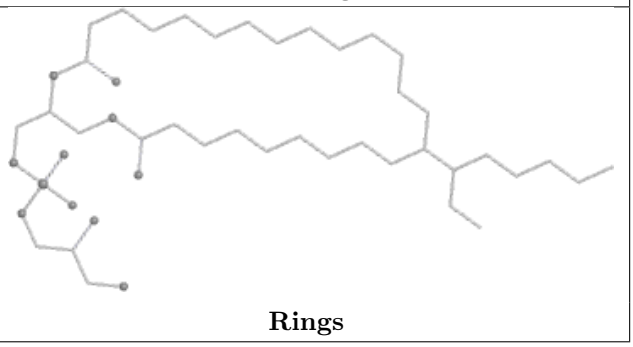
Bond lengths



Bond angles

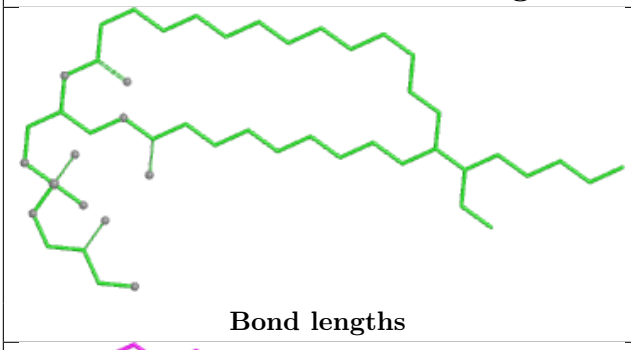


Torsions



Rings

Ligand PGV 8G 101



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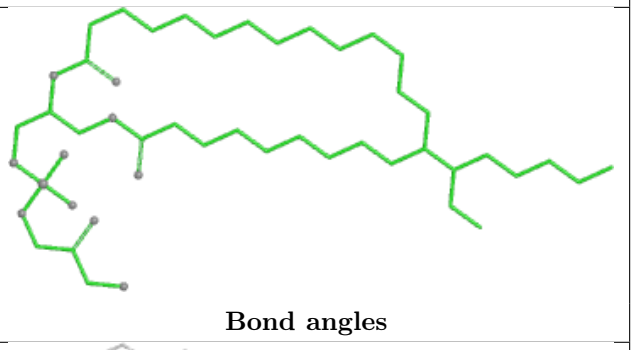
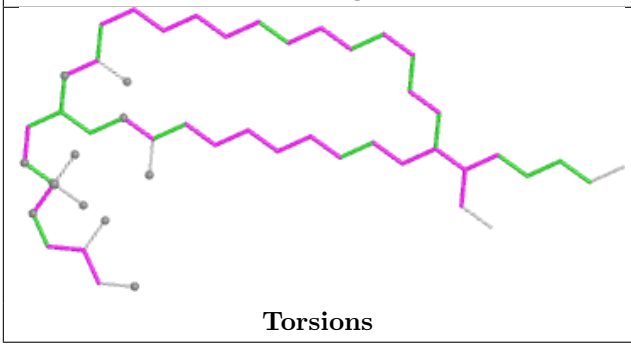


Bond angles



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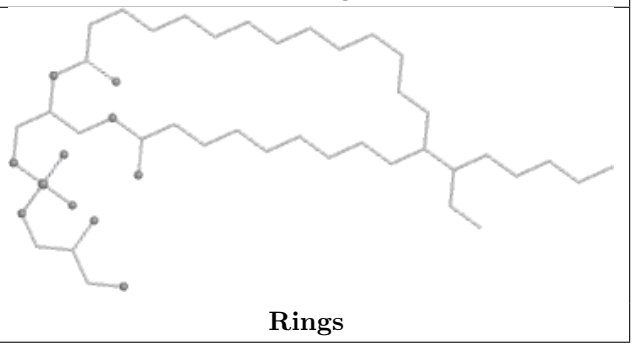
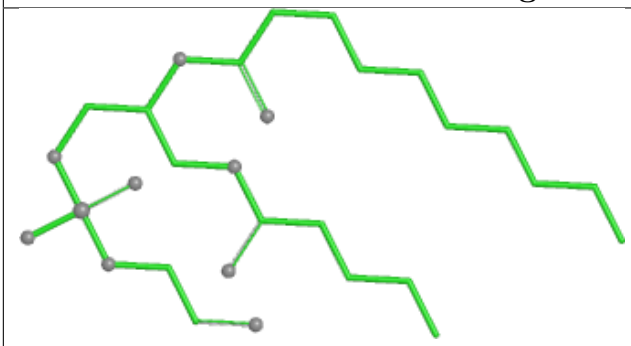


Rings

Ligand 3PE 1Y 203



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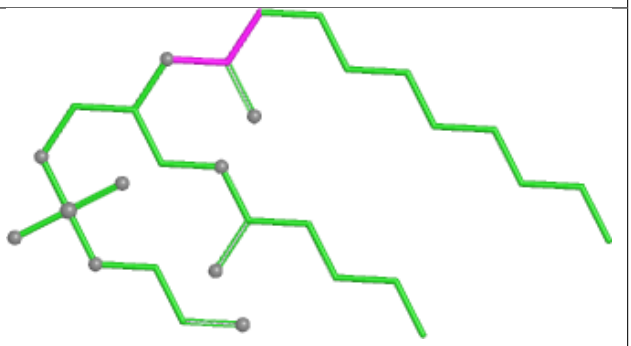
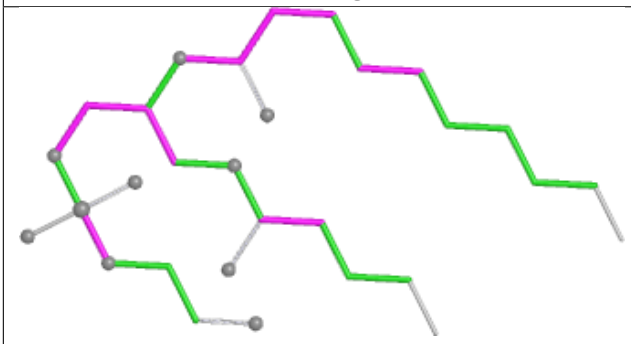


Bond angles



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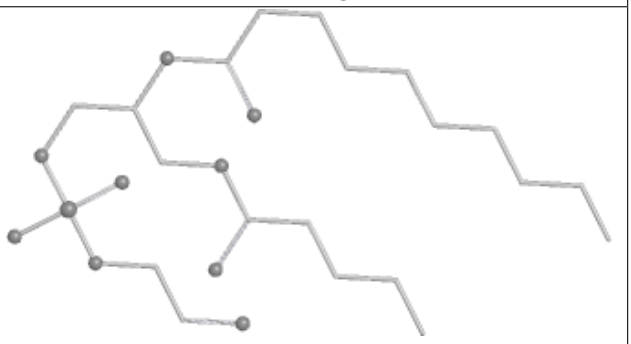
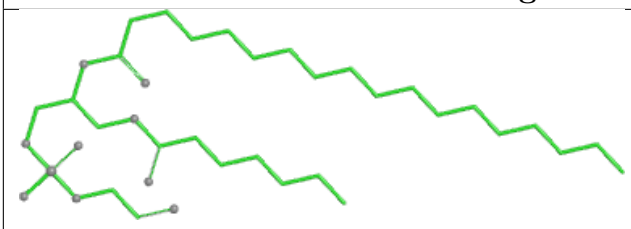


Rings

Ligand 3PE 1Y 202



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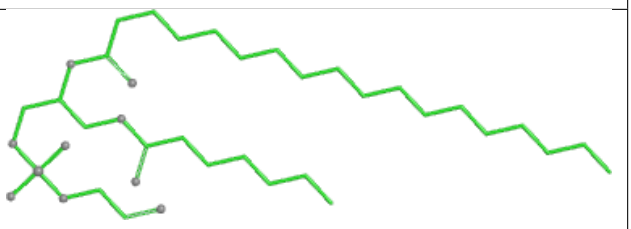
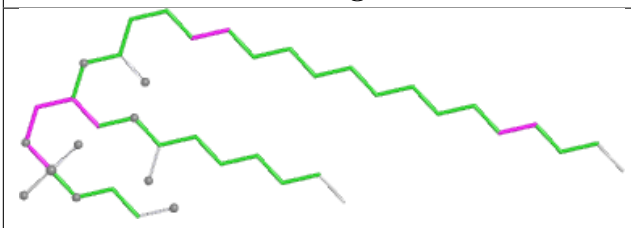
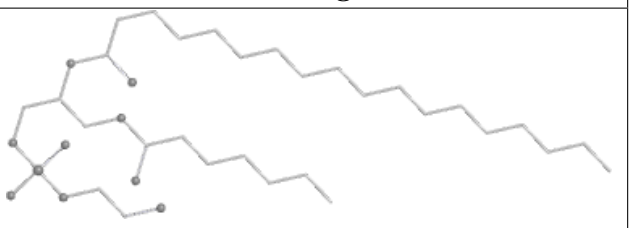


Bond angles

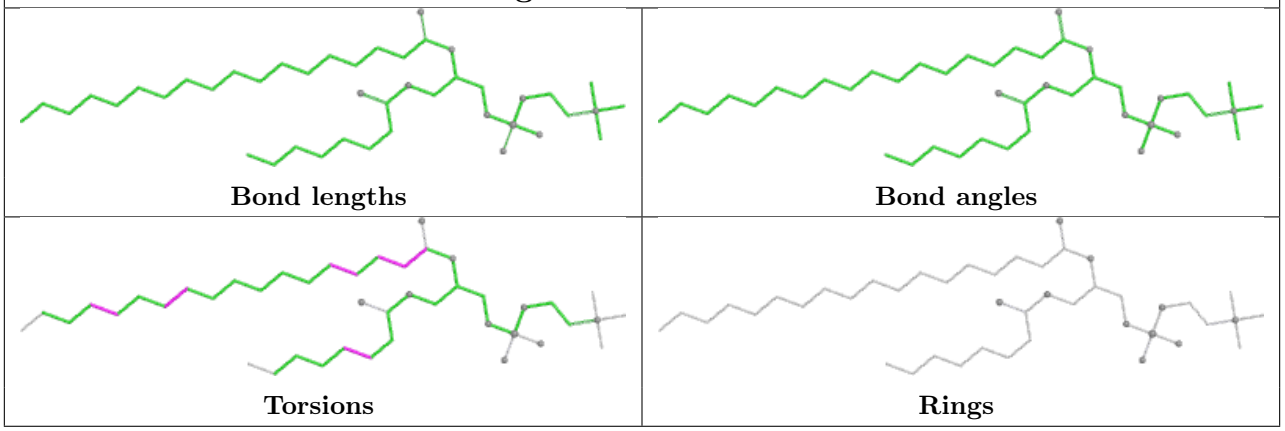


Torsions

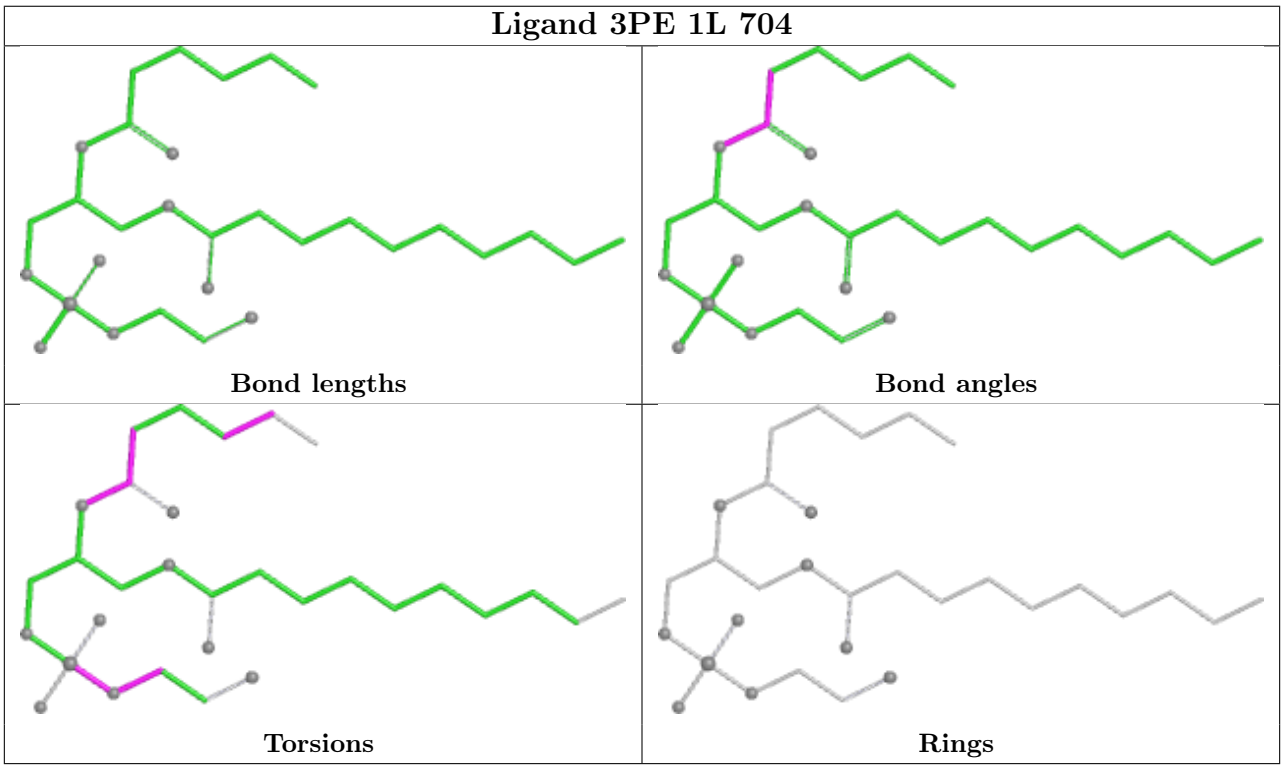


Rings

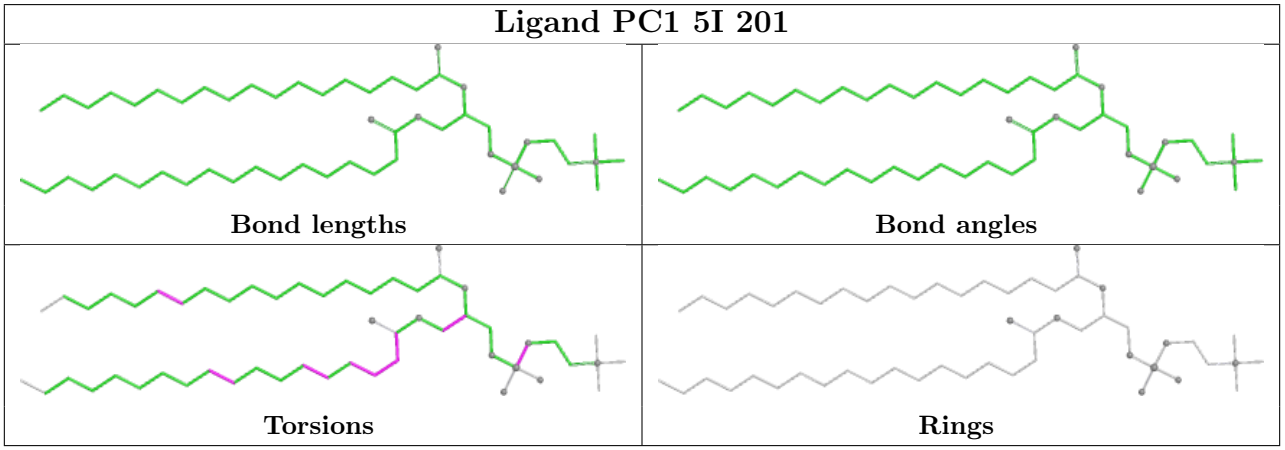
Ligand PC1 1M 502



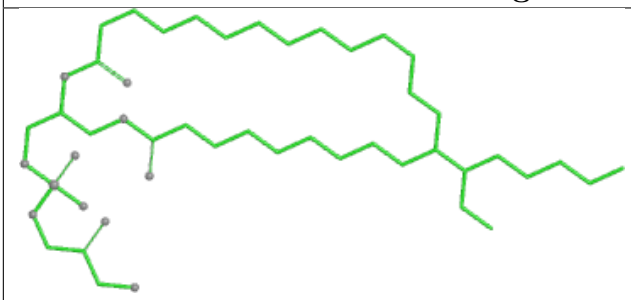
Ligand 3PE 1L 704



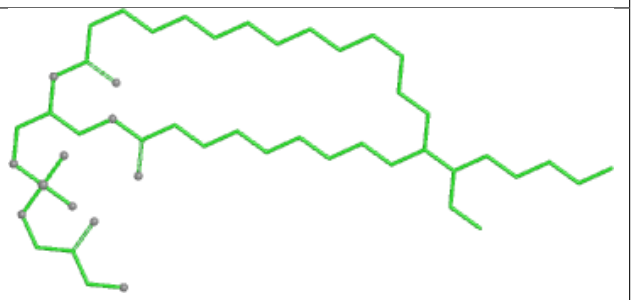
Ligand PC1 5I 201



Ligand PGV 8C 301

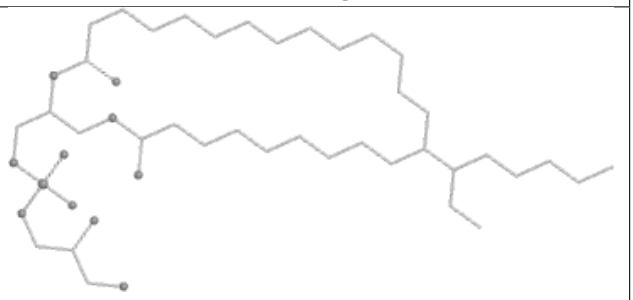


Bond lengths



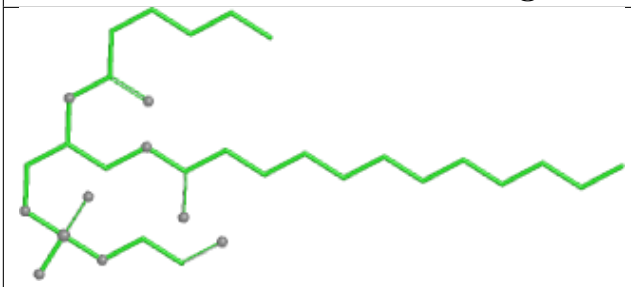
Bond angles

Torsions



Rings

Ligand 3PE 1Y 204



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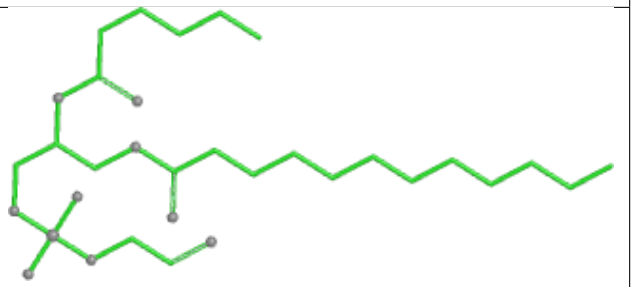
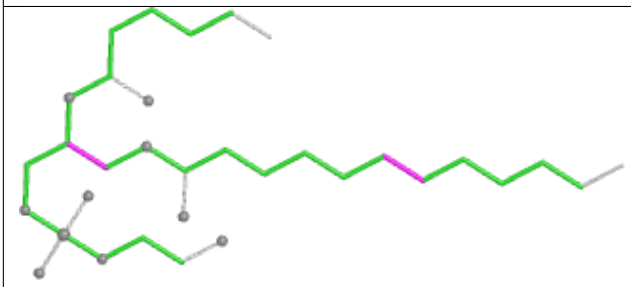
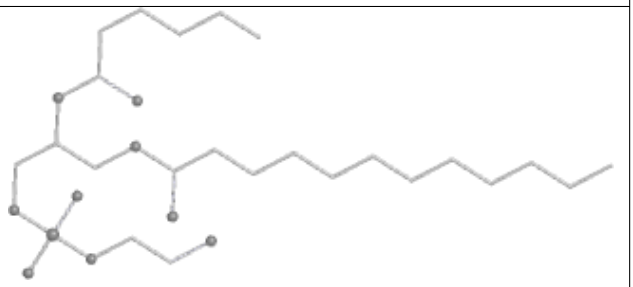


Bond angles

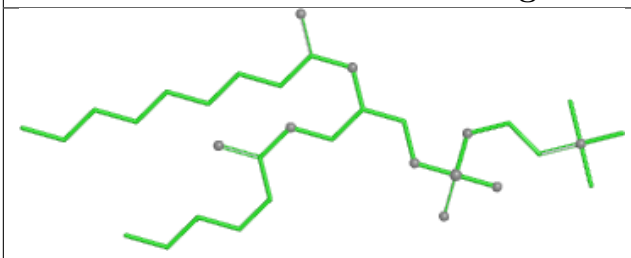


Torsions



Rings

Ligand PC1 1P 401



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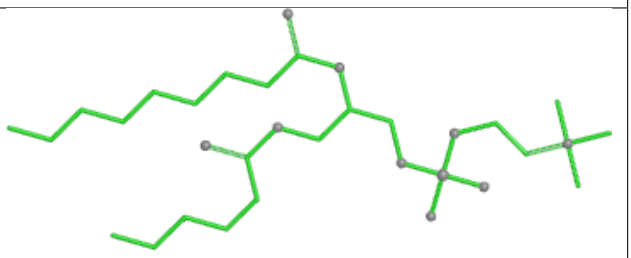
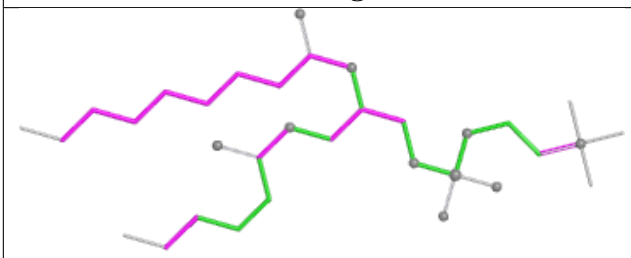


Bond angles



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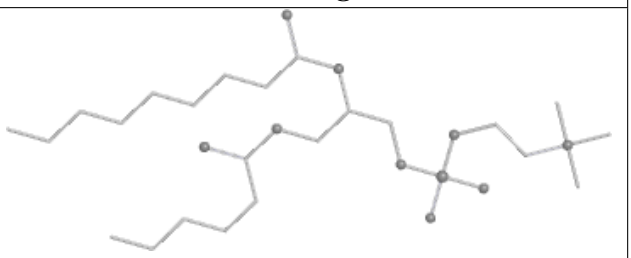
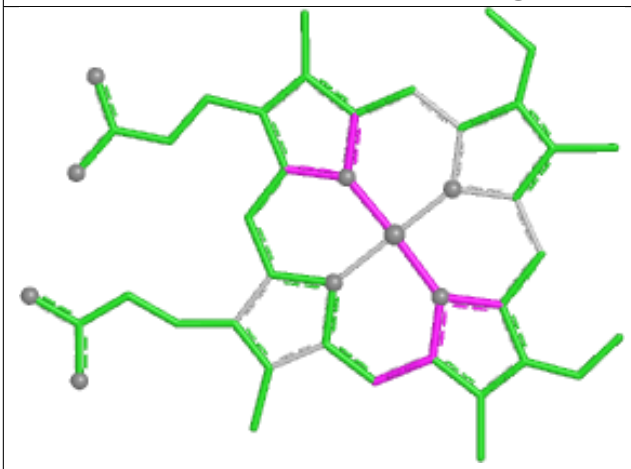
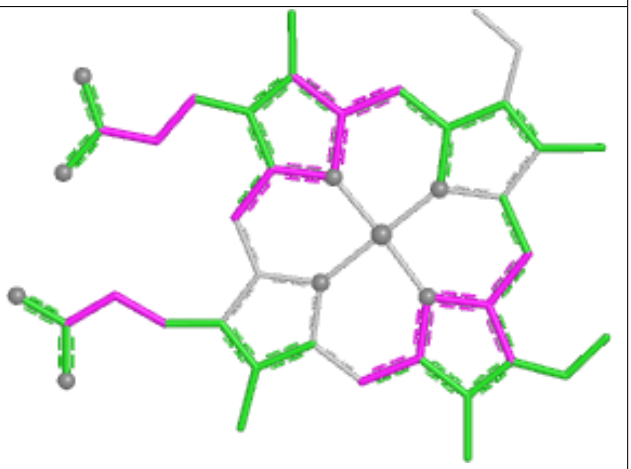


Rings

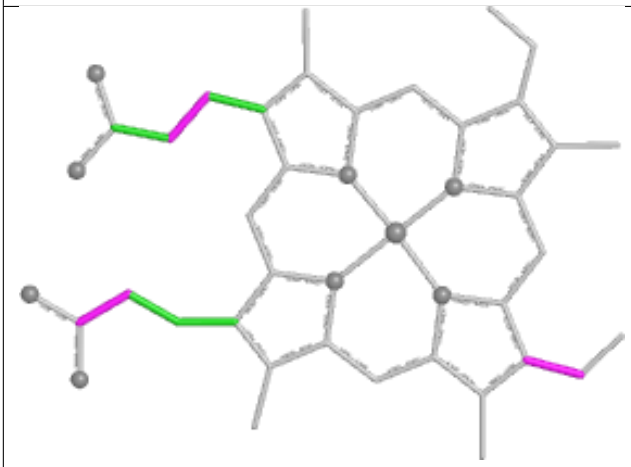
Ligand HEM 3C 501



Bond lengths



Bond angles



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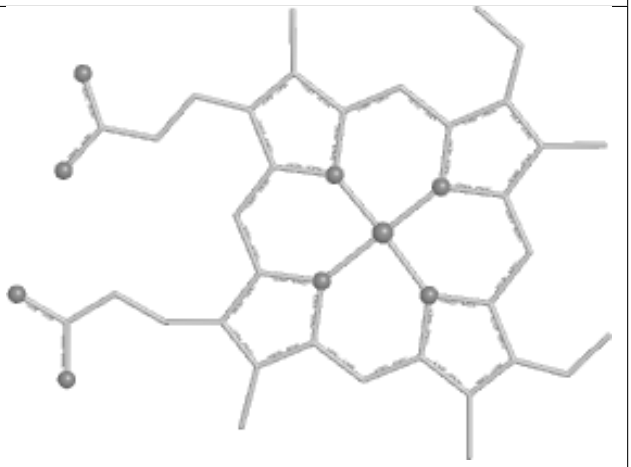
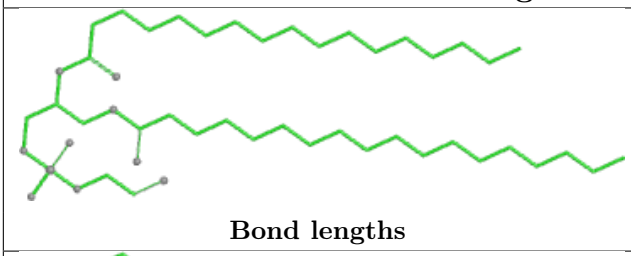


Rings

Ligand 3PE 5M 503



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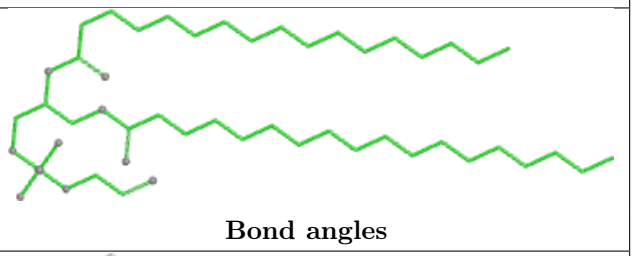
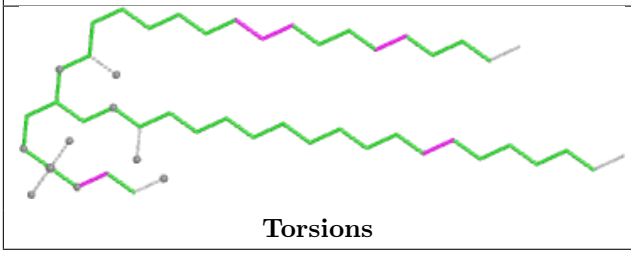


Bond angles



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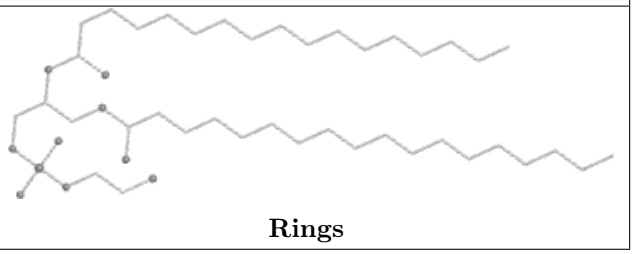
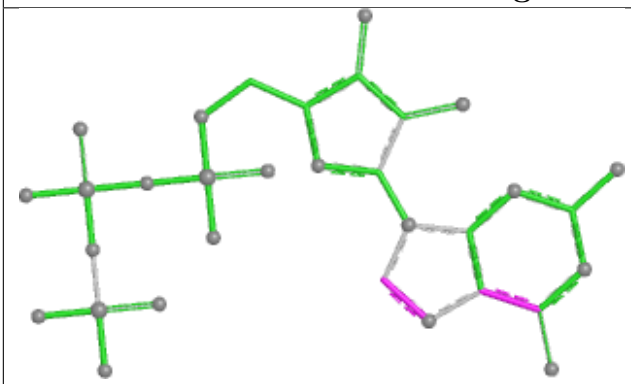
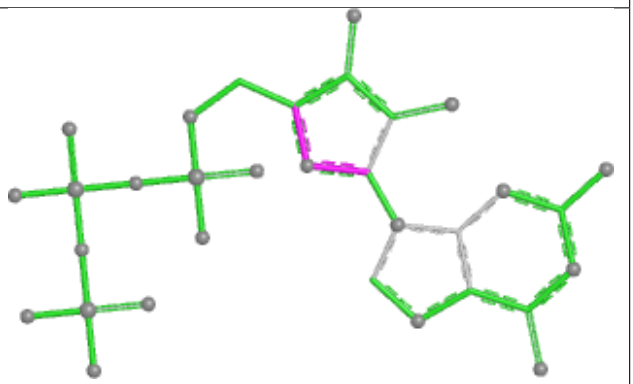


Rings

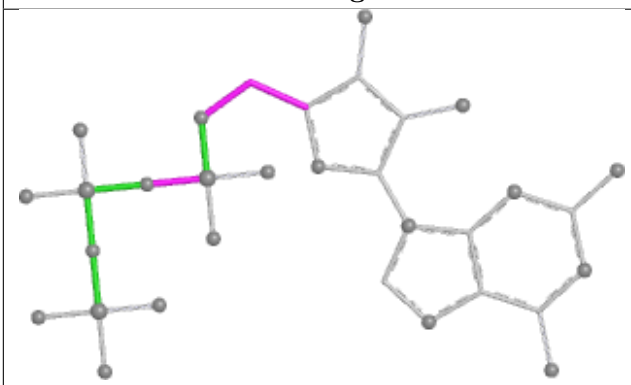
Ligand GTP 1O 401



Bond lengths



Bond angles



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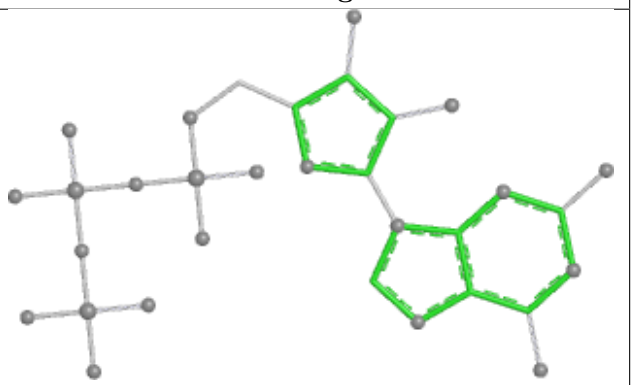
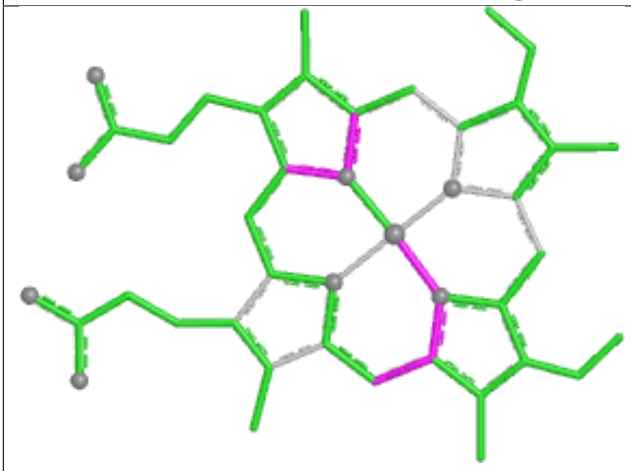


Rings

Ligand HEM 6P 501



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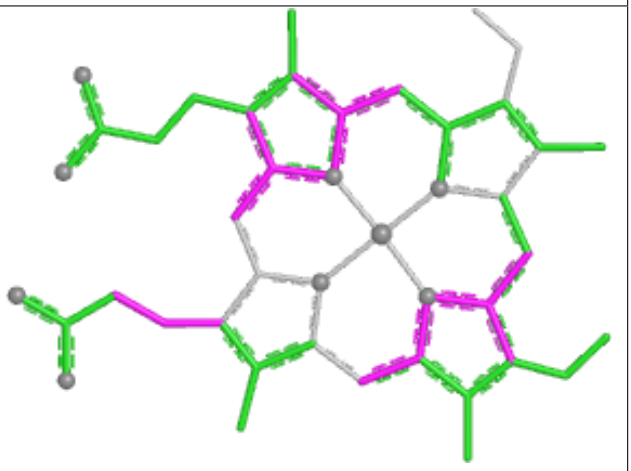
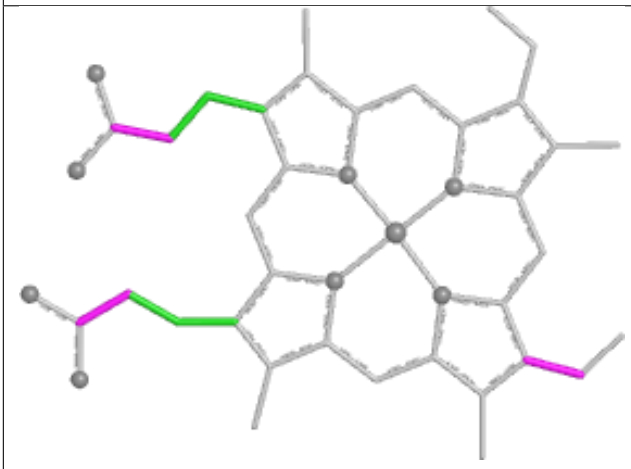


Bond angles



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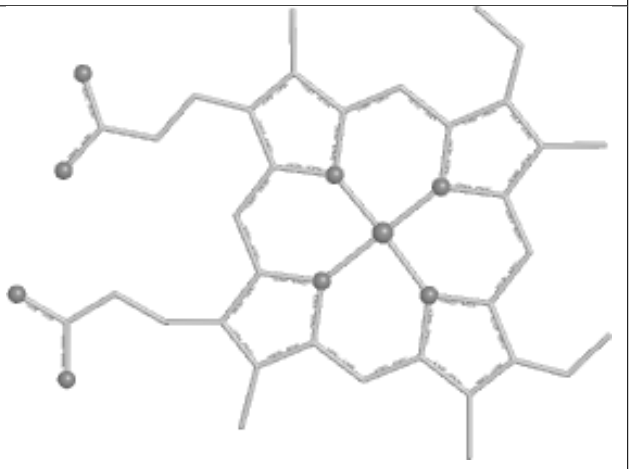
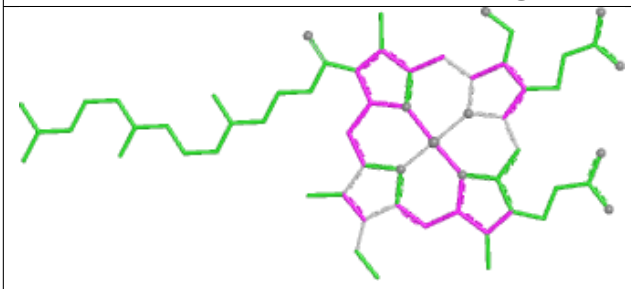
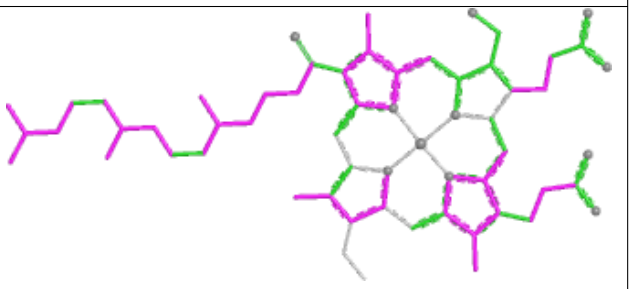


Rings

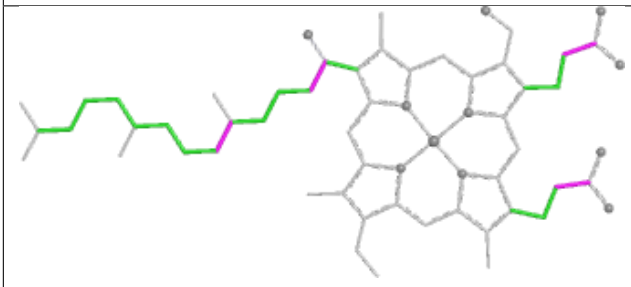
Ligand HEA 8A 606



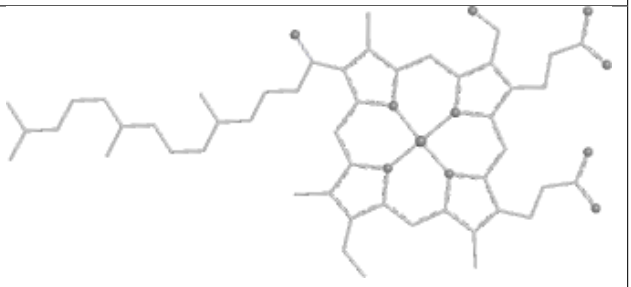
Bond lengths



Bond angles

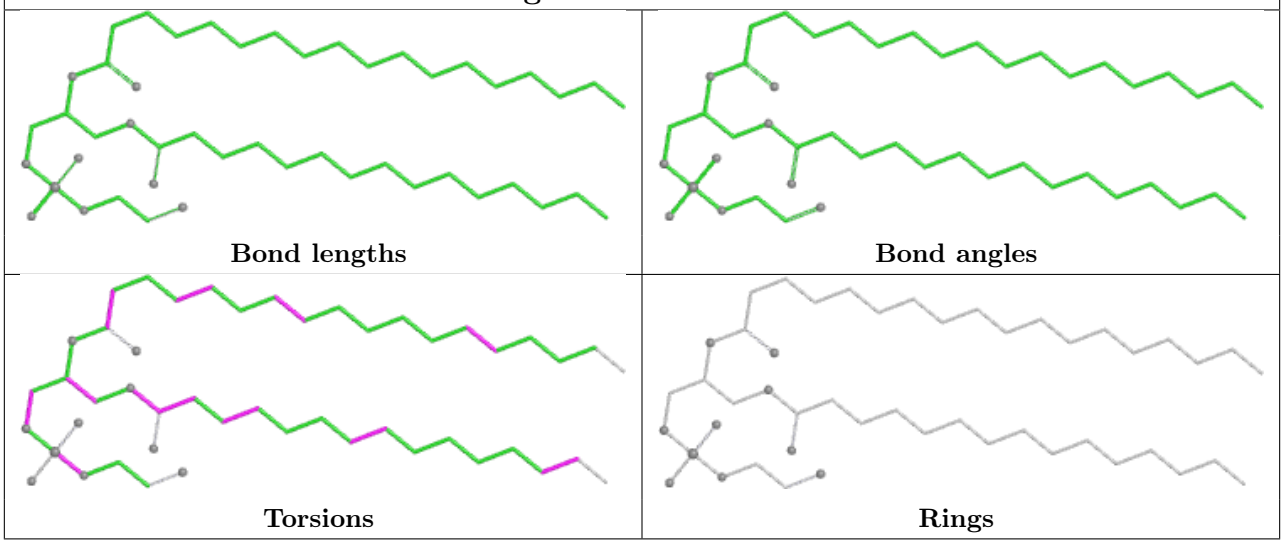


Torsions

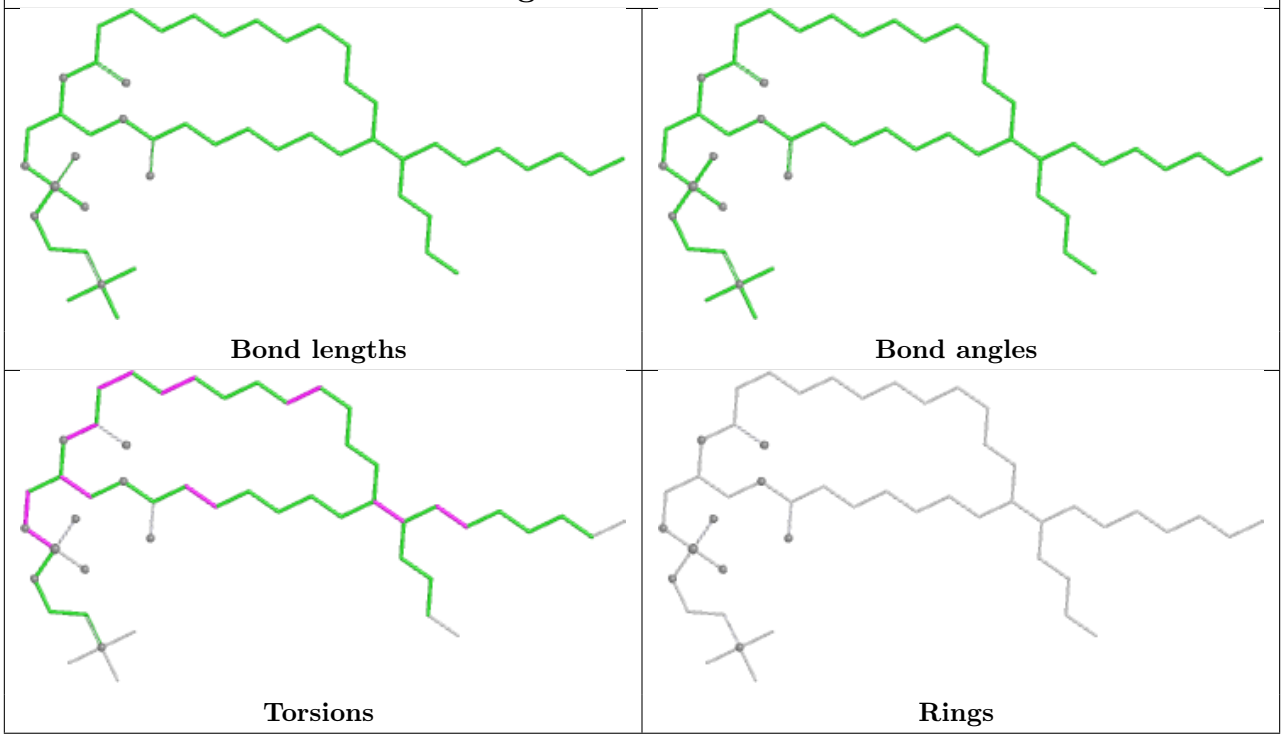


Rings

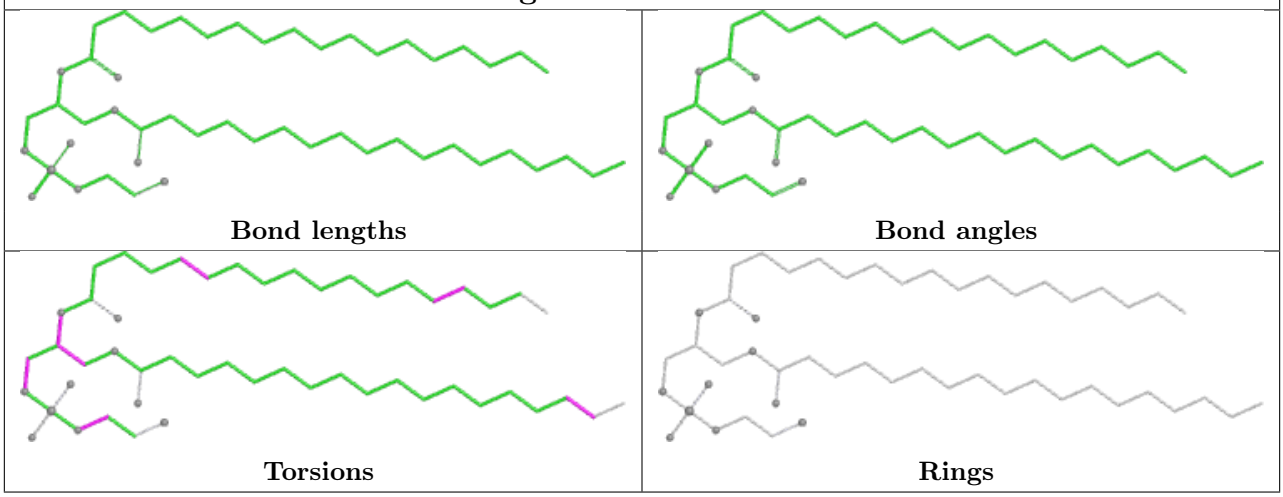
Ligand 3PE 1d 201



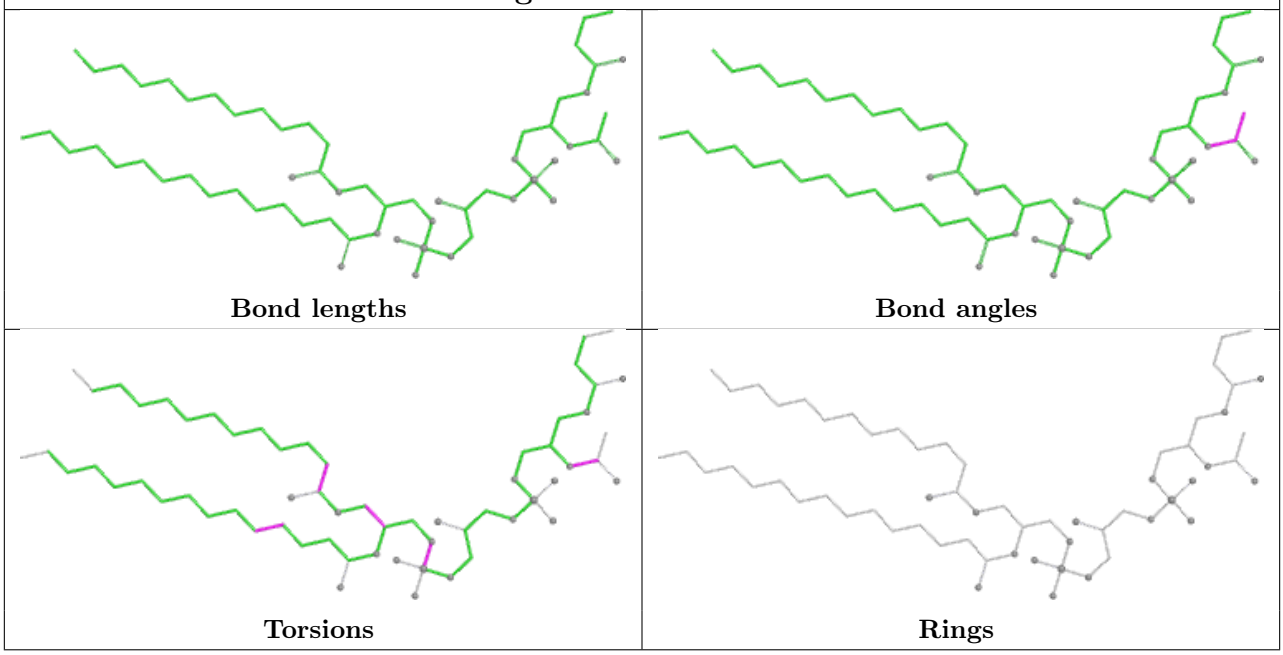
Ligand PSC 8A 611



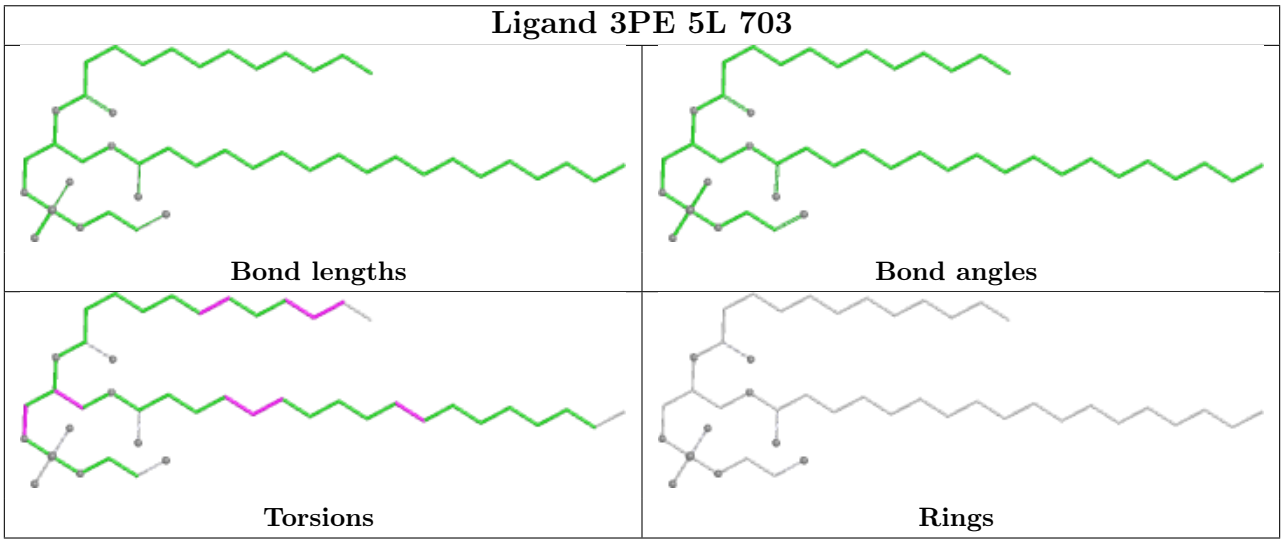
Ligand 3PE 1N 902



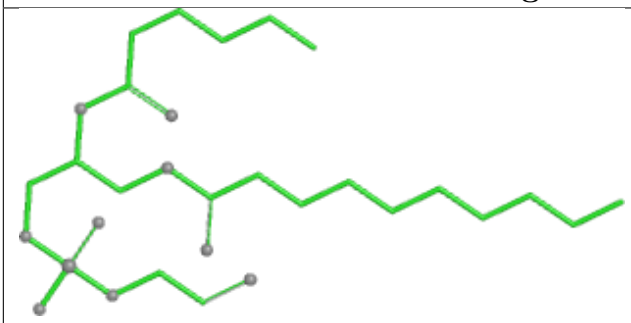
Ligand CDL 5N 903



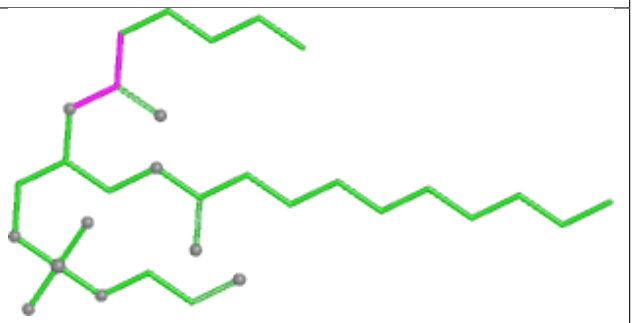
Ligand 3PE 5L 703



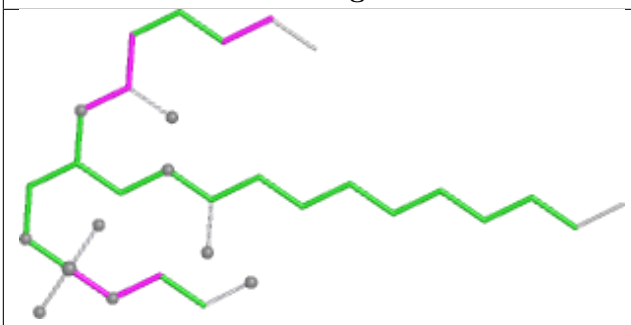
Ligand 3PE 5L 704



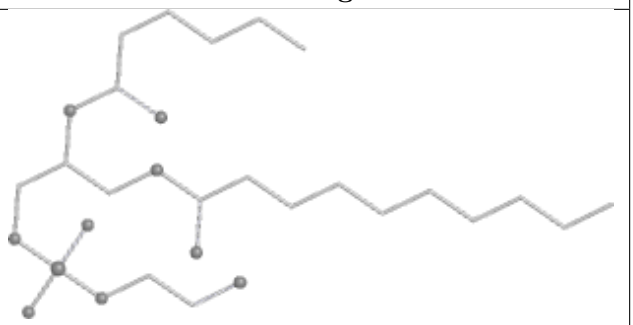
Bond lengths



Bond angles

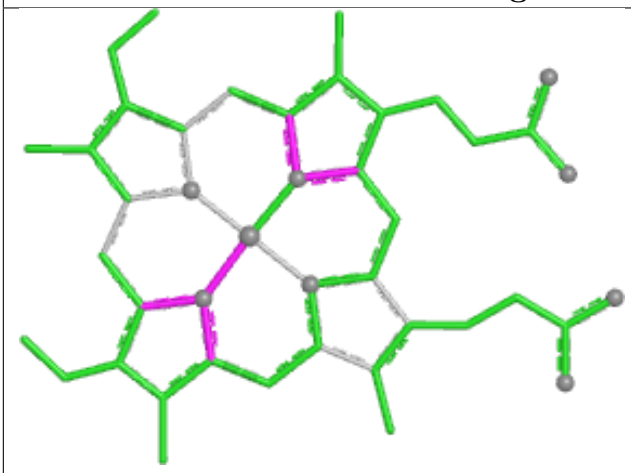


Torsions



Rings

Ligand HEM 3C 502



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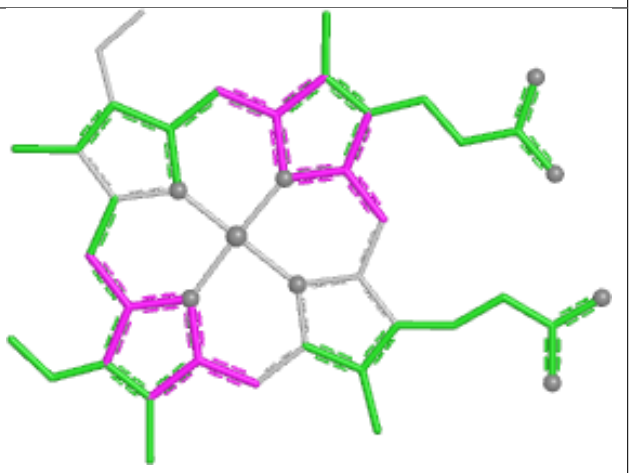
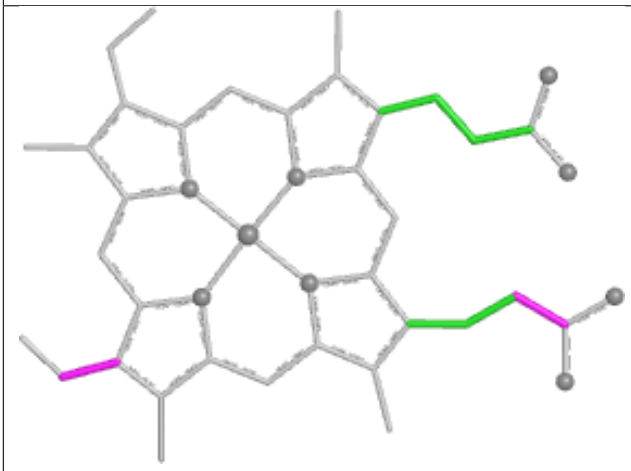
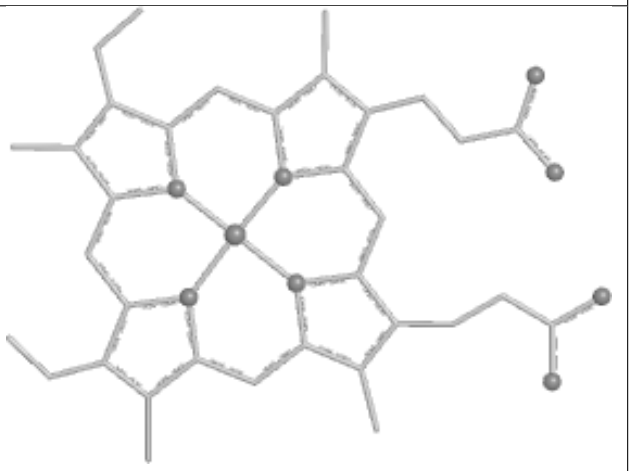


Bond angles

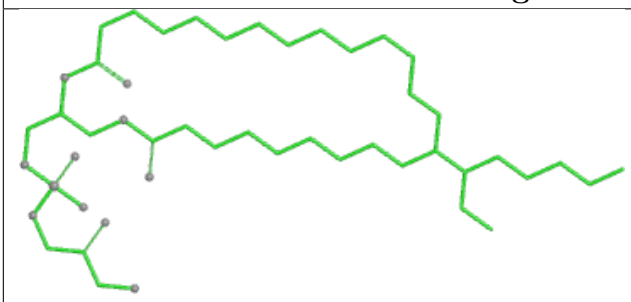


Torsions



Rings

Ligand PGV 8A 601



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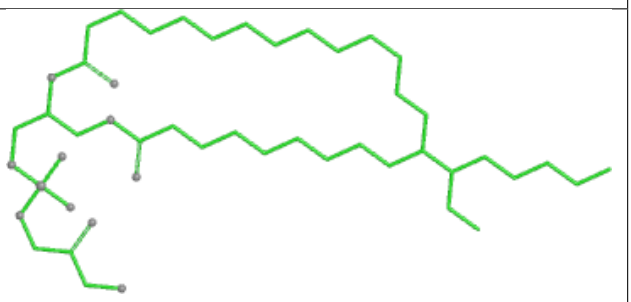
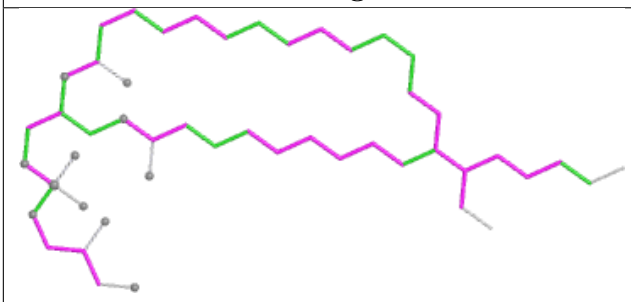


Bond angles



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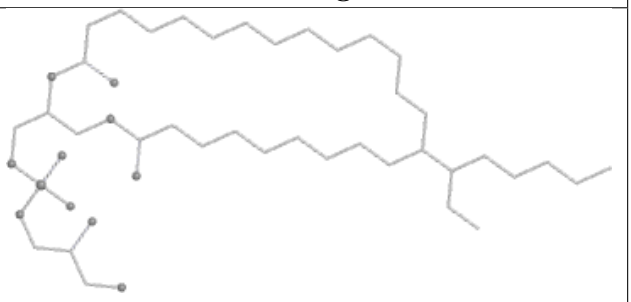
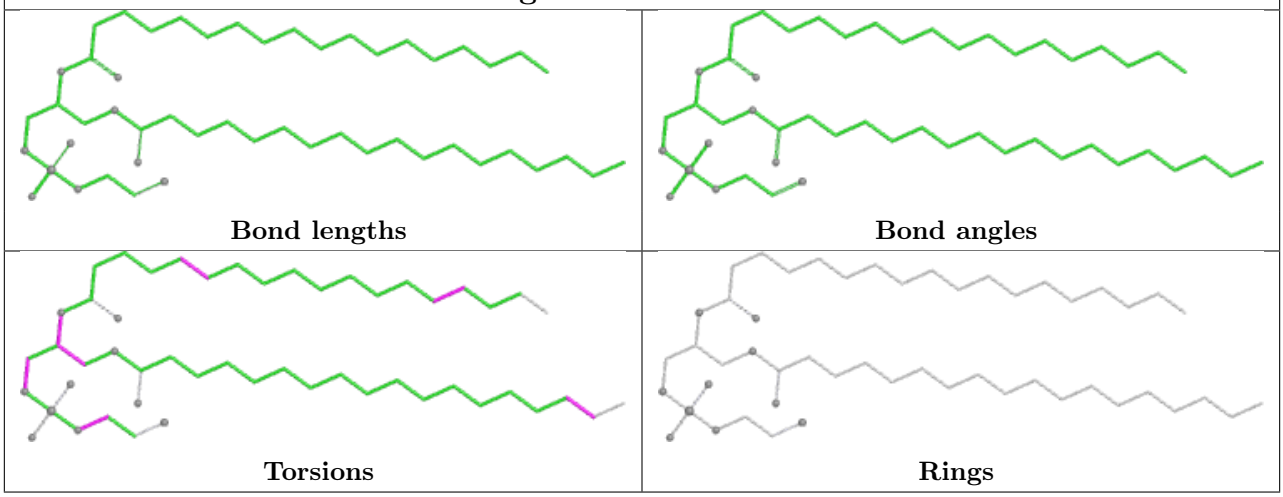
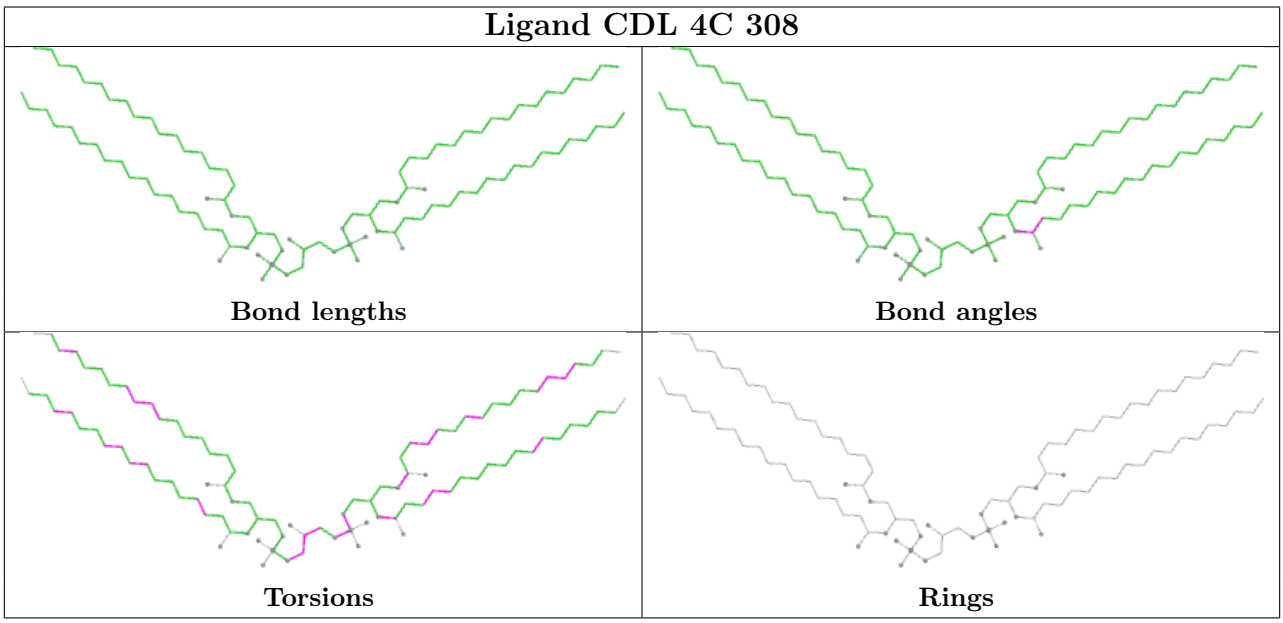


Rings

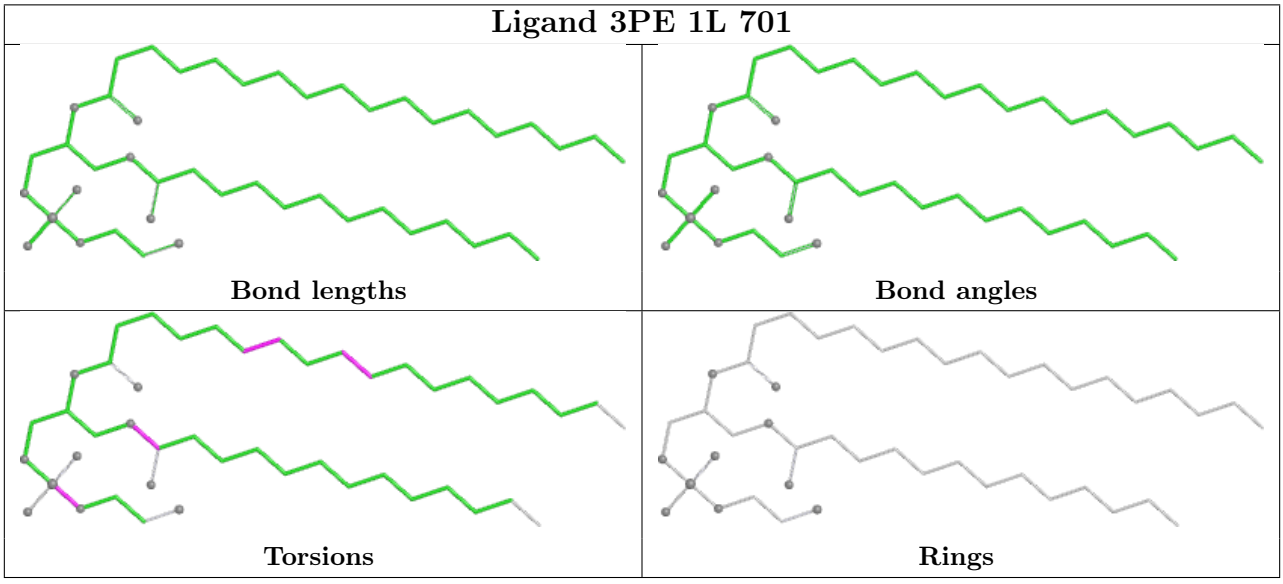
Ligand 3PE 5N 902



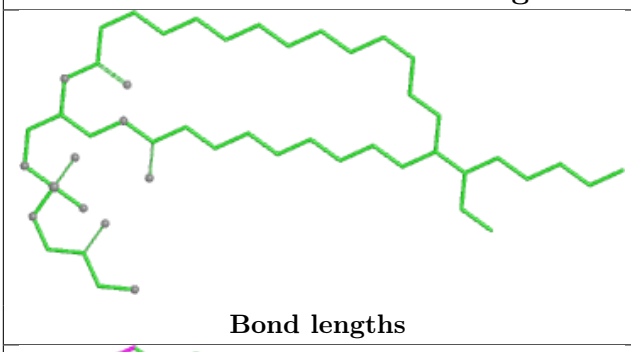
Ligand CDL 4C 308



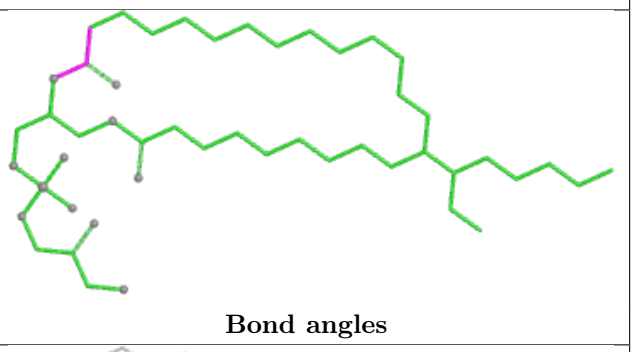
Ligand 3PE 1L 701



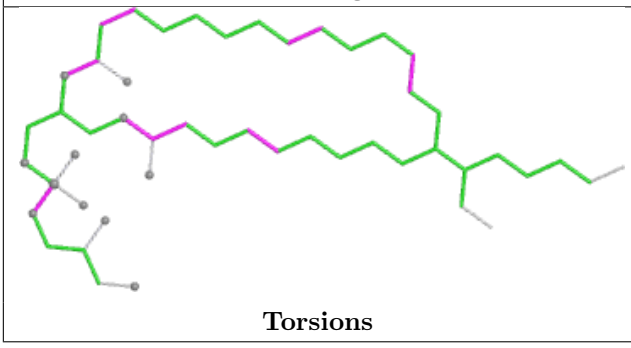
Ligand PGV 4G 101



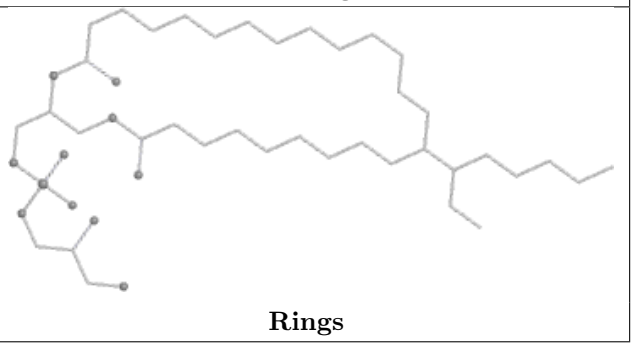
Bond lengths



Bond angles

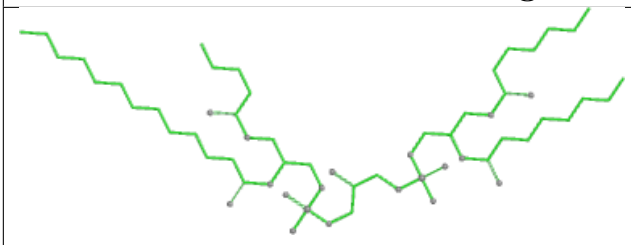


Torsions

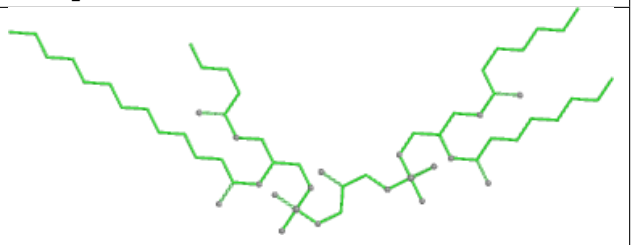


Rings

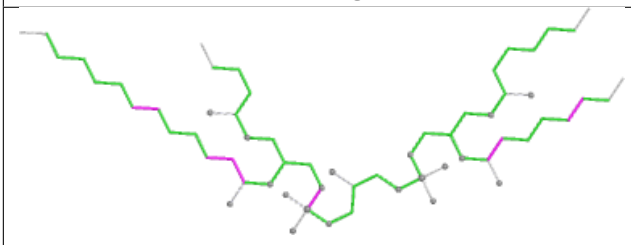
Ligand CDL 1q 201



Bond lengths



Bond angles



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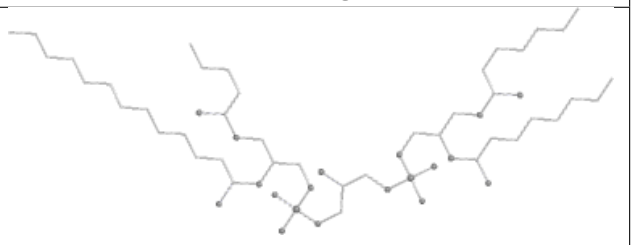
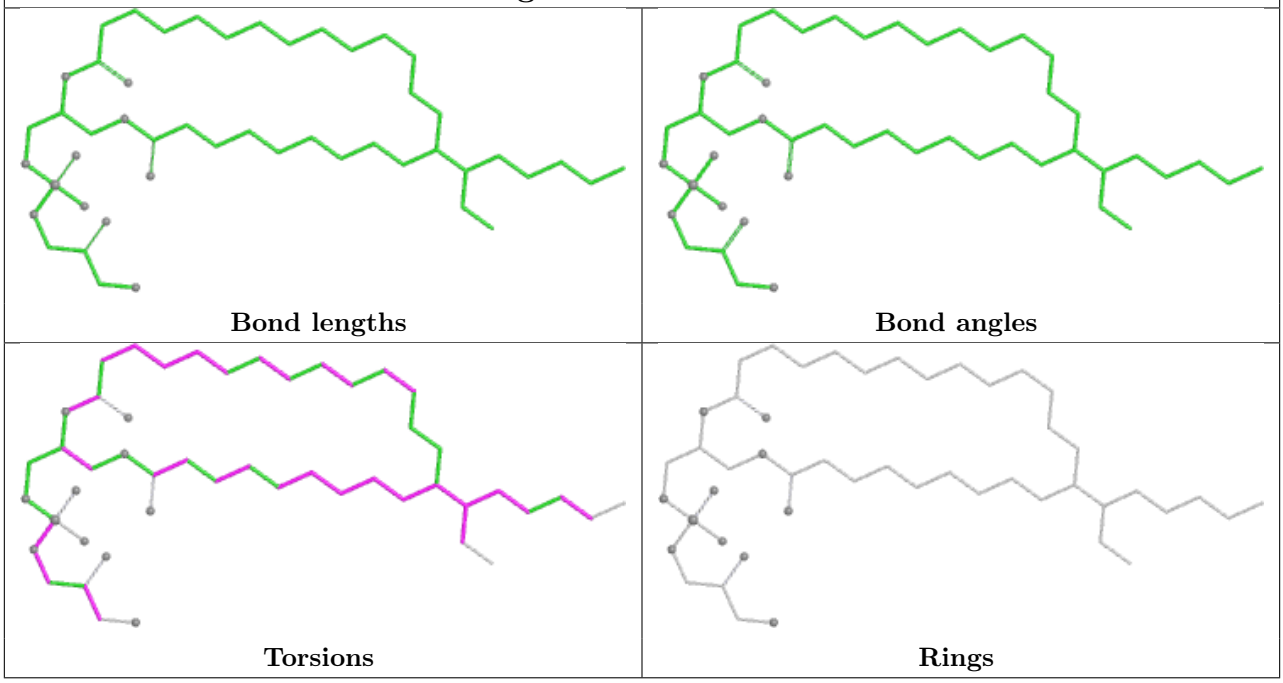
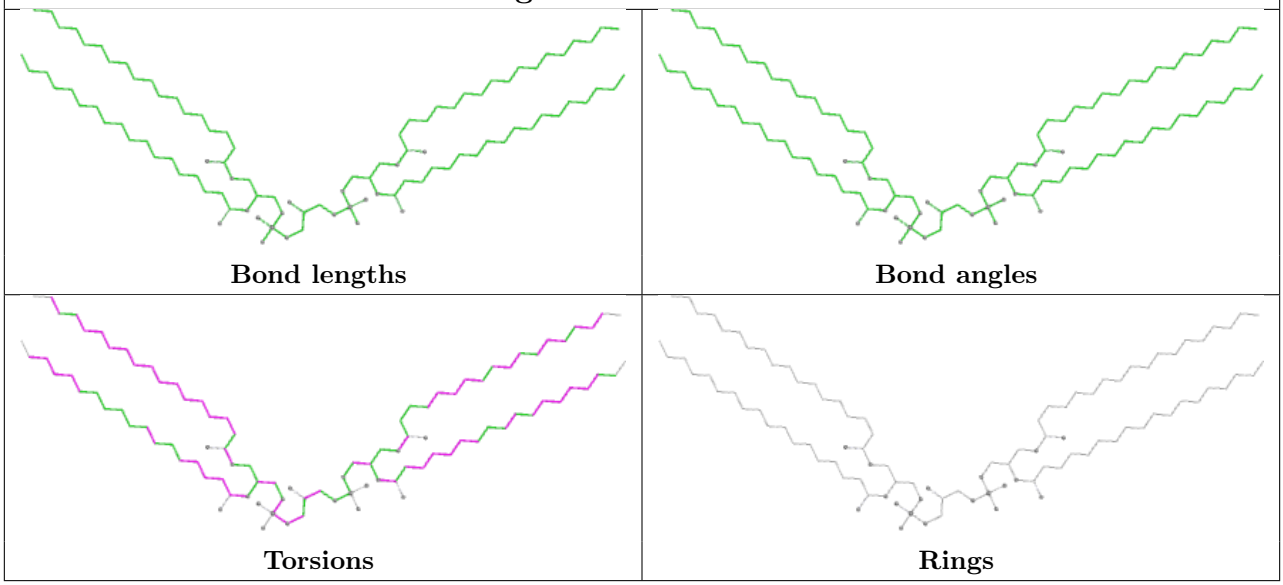


Rings

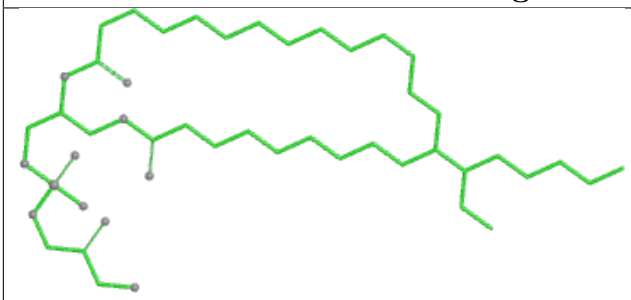
Ligand PGV 8J 101



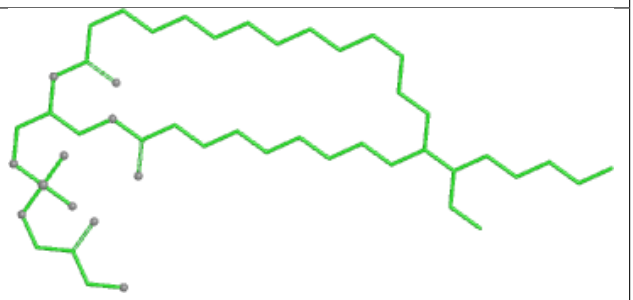
Ligand CDL 8D 201



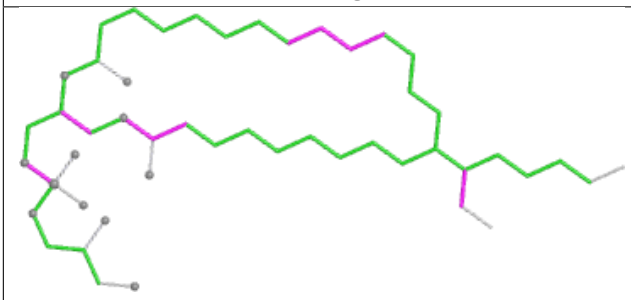
Ligand PGV 4A 601



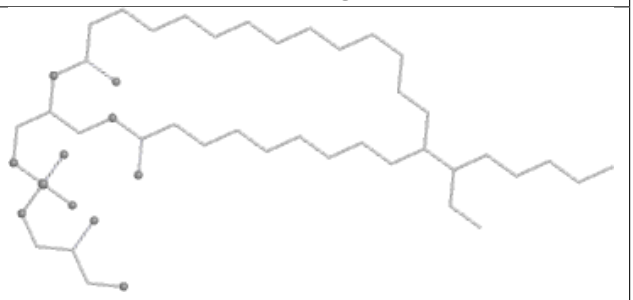
Bond lengths



Bond angles

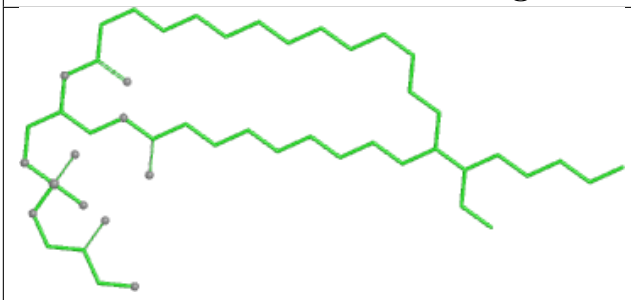


Torsions



Rings

Ligand PGV 4A 602



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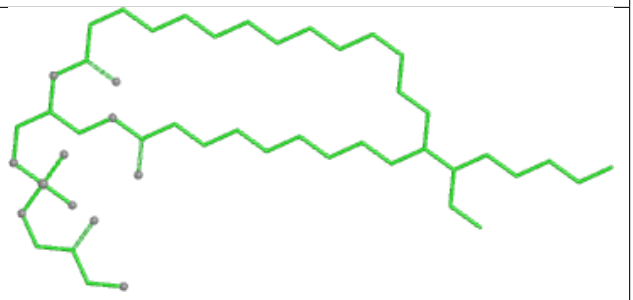

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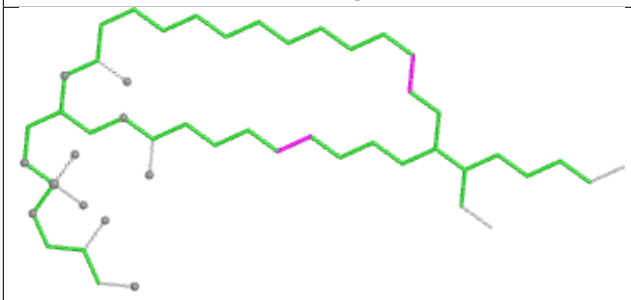

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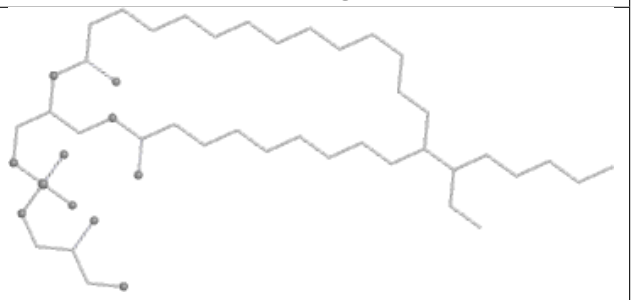
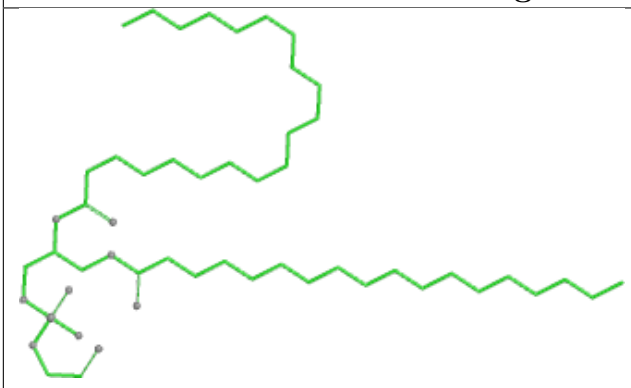


Rings

Ligand PEK 8C 306



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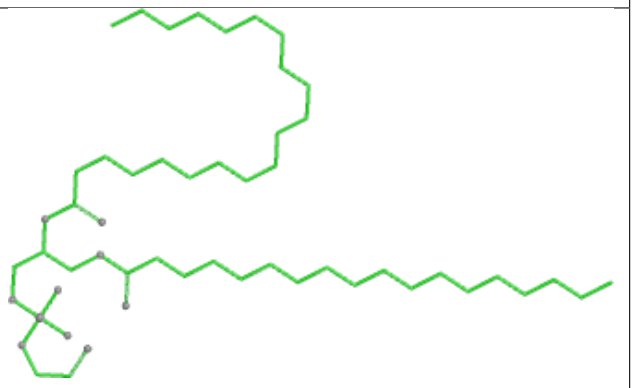
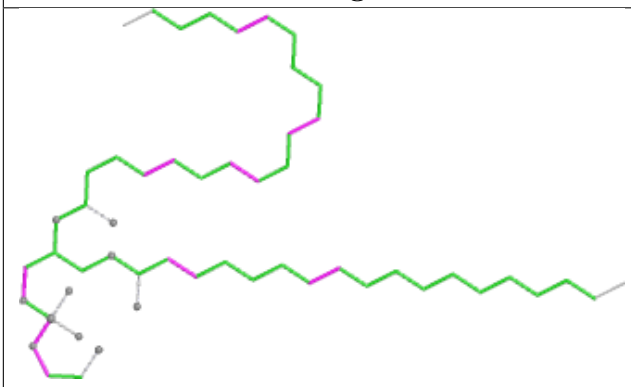


Bond angles



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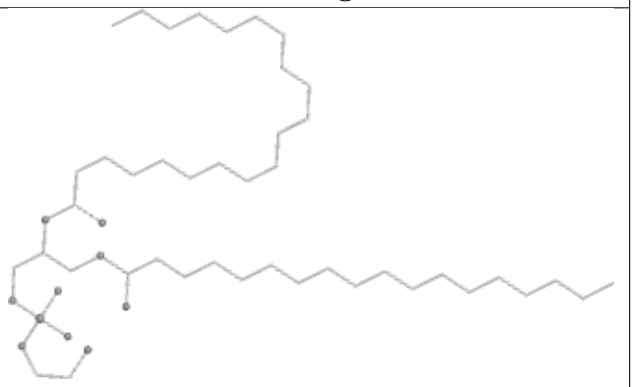
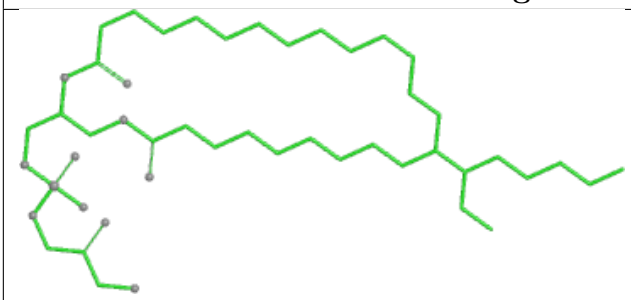


Rings

Ligand PGV 8B 301



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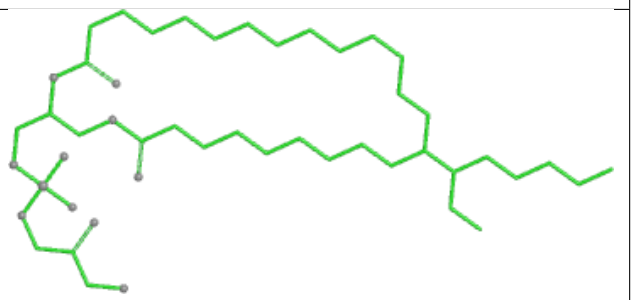
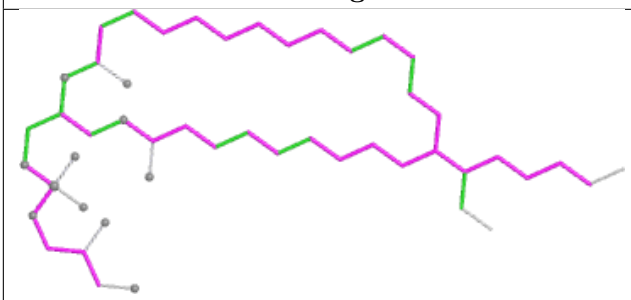


Bond angles



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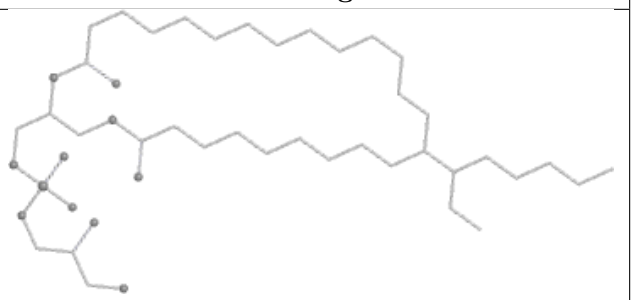
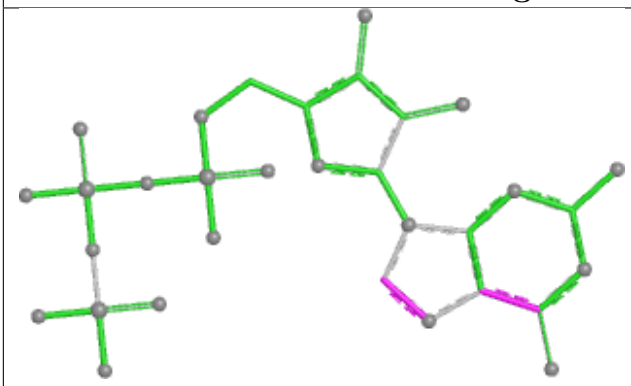


Rings

Ligand GTP 5O 401



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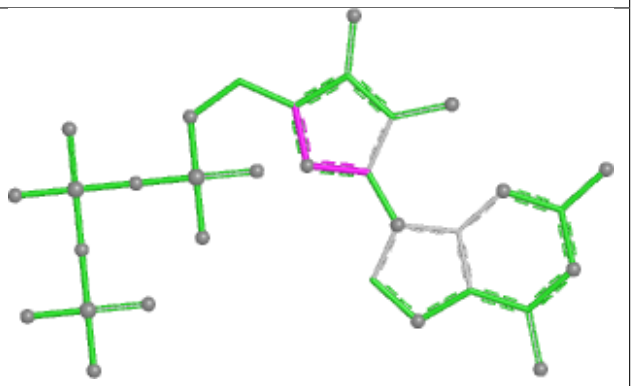
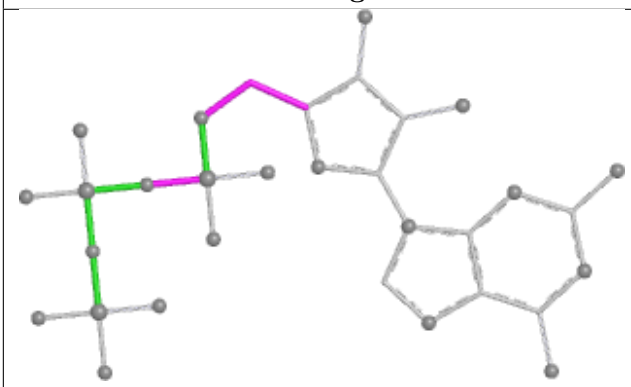


Bond angles



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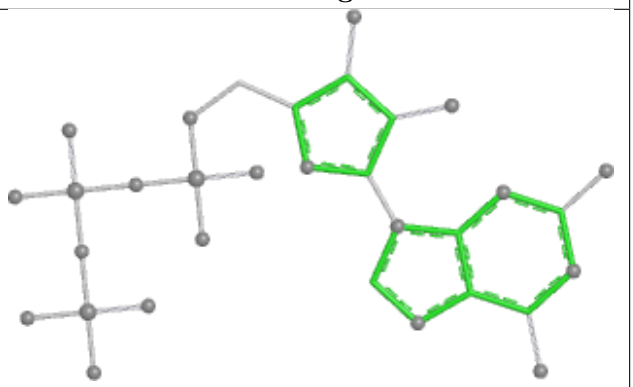
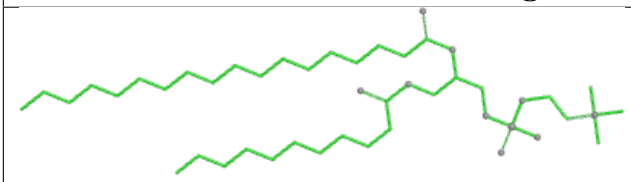


Rings

Ligand PC1 1h 202



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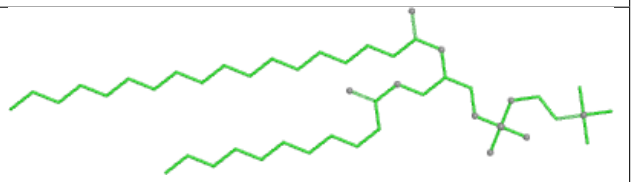
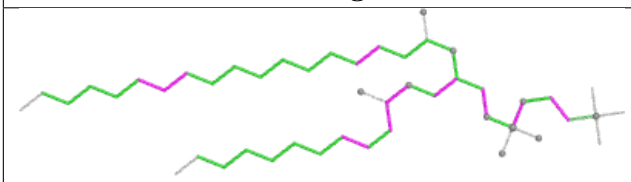


Bond angles



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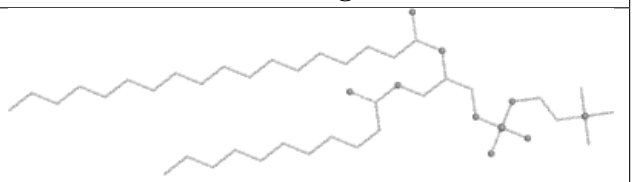
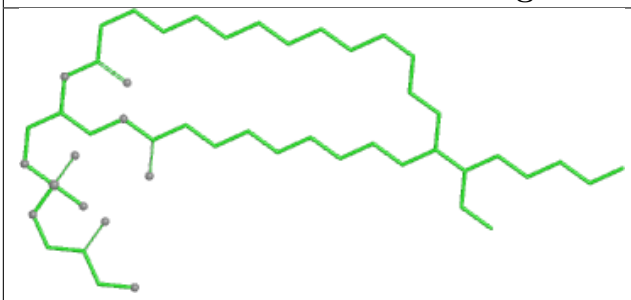


Rings

Ligand PGV 4J 101



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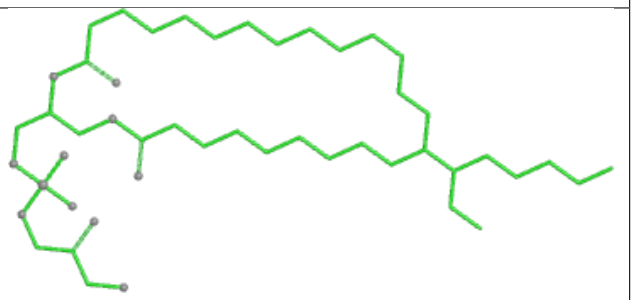
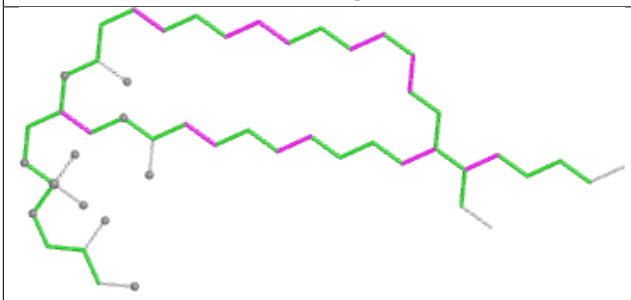


Bond angles



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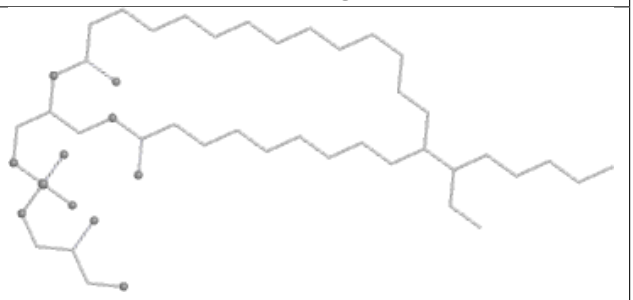
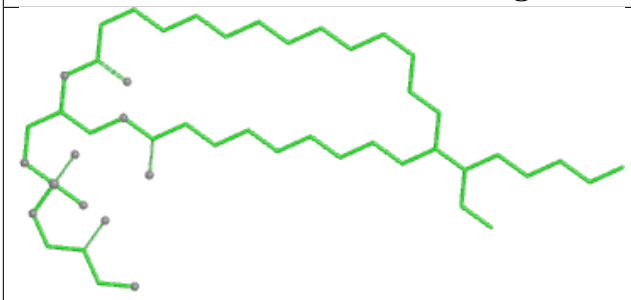


Rings

Ligand PGV 8C 305



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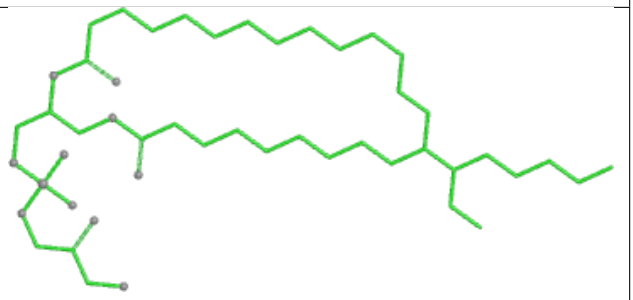
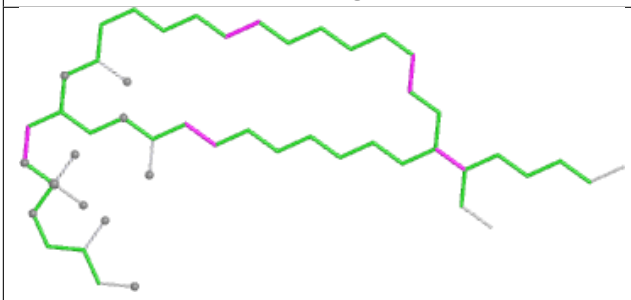
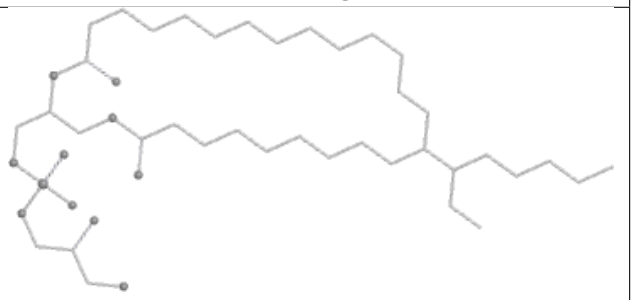


Bond angles

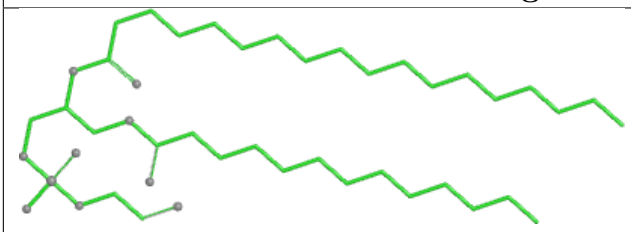


Torsions



Rings

Ligand 3PE 5L 701



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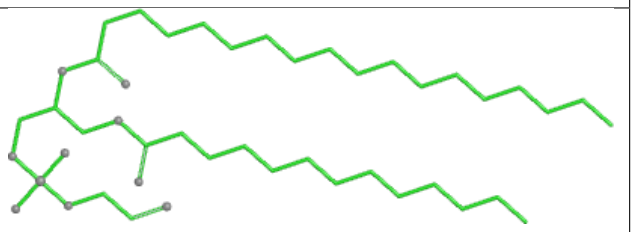
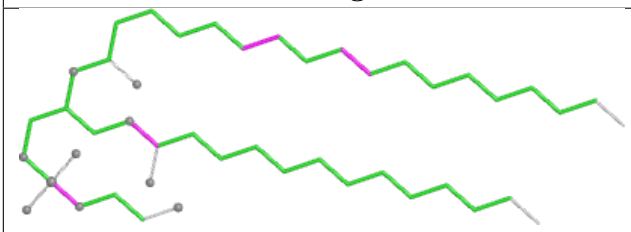
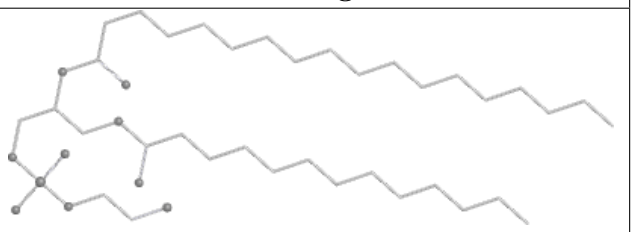


Bond angles

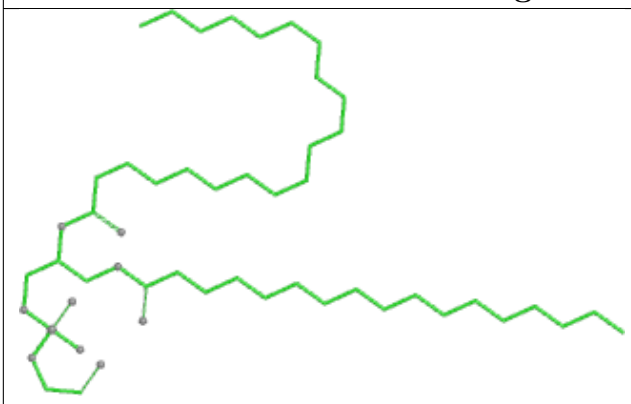


Torsions



Rings

Ligand PEK 8C 307



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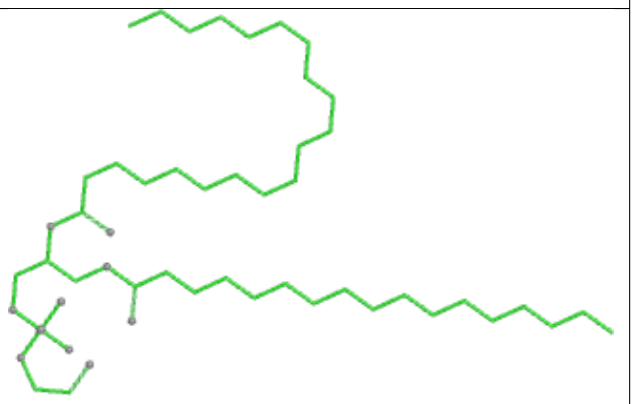
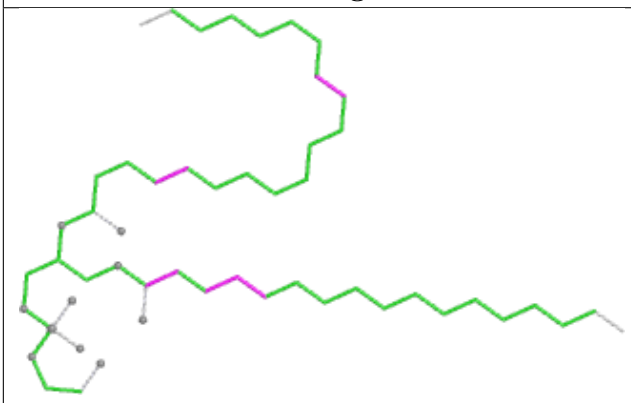


Bond angles



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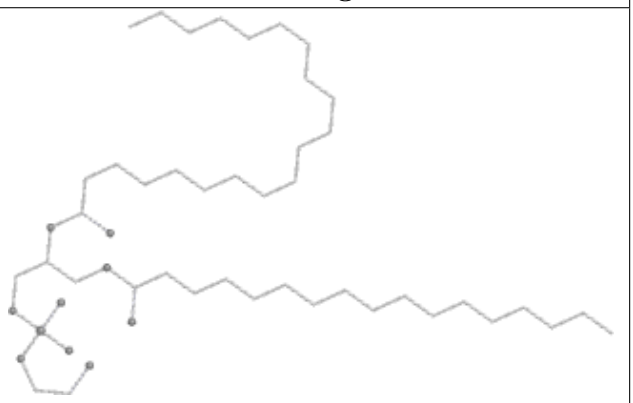
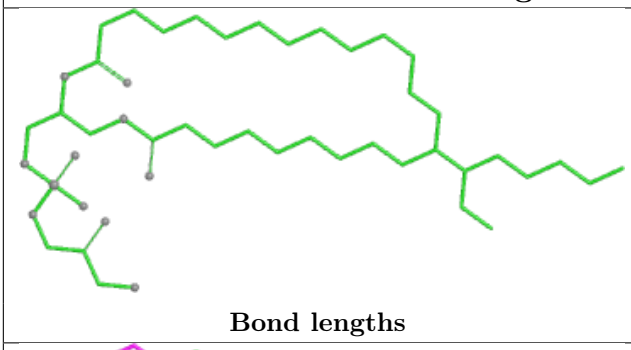


Rings

Ligand PGV 8L 101



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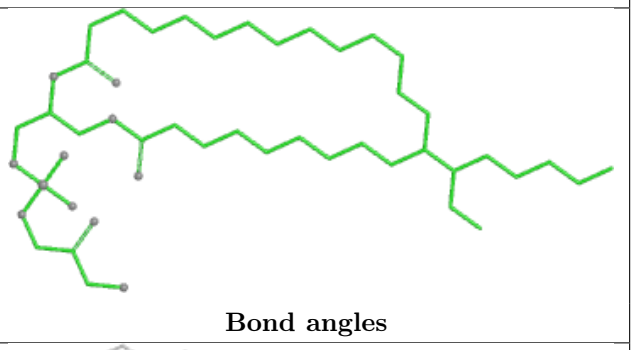

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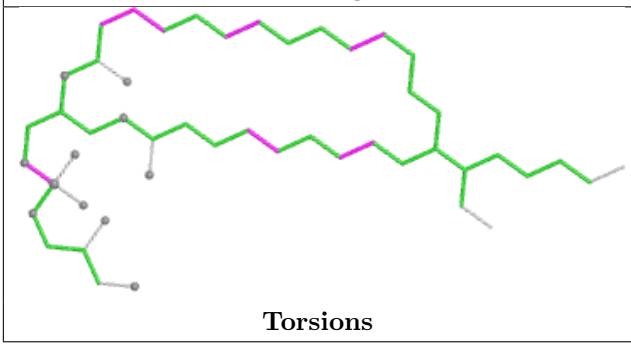

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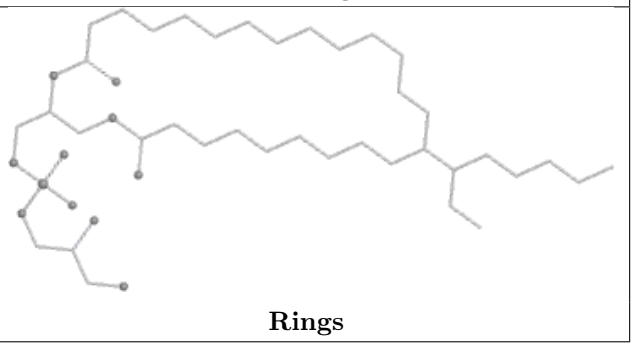
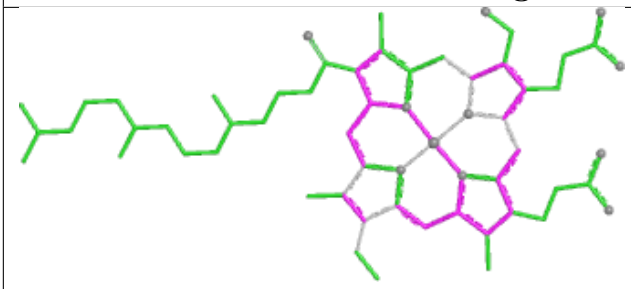


Rings

Ligand HEA 8A 605



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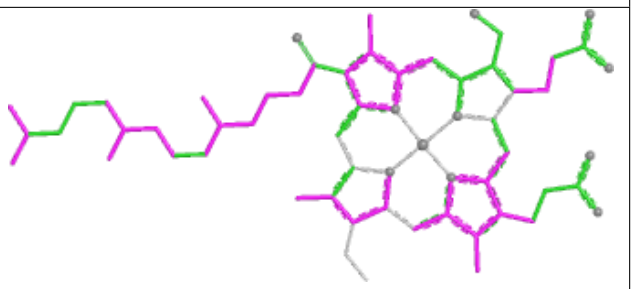
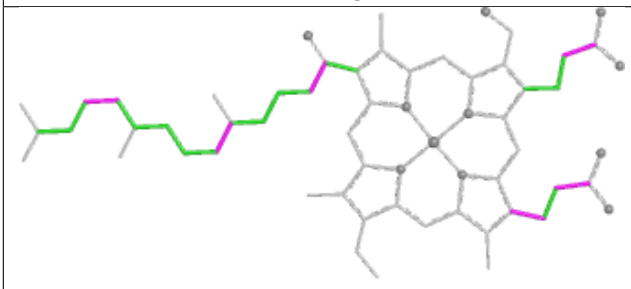


Bond angles



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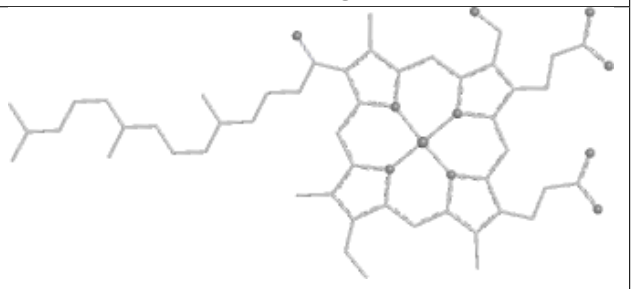
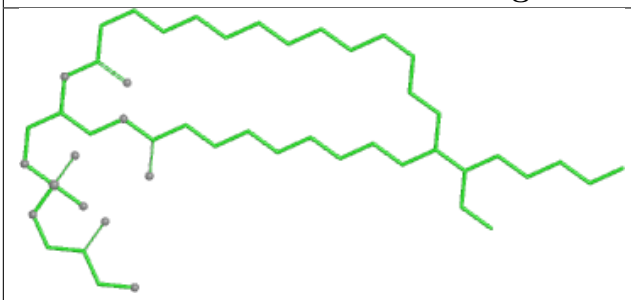


Rings

Ligand PGV 8A 603



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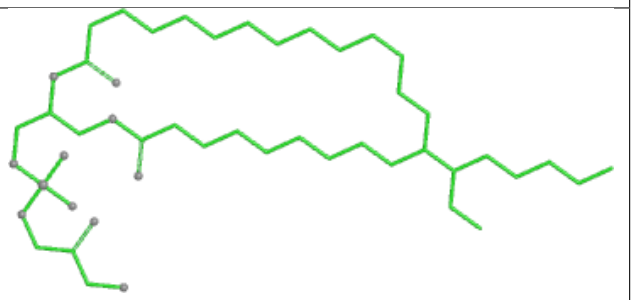
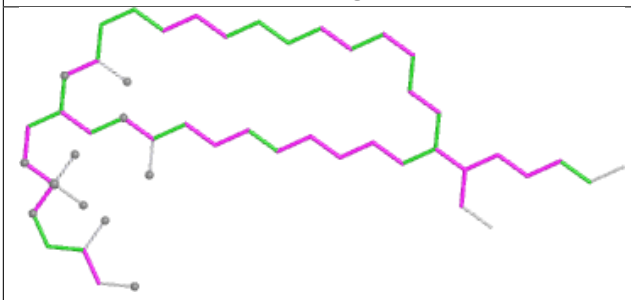


Bond angles



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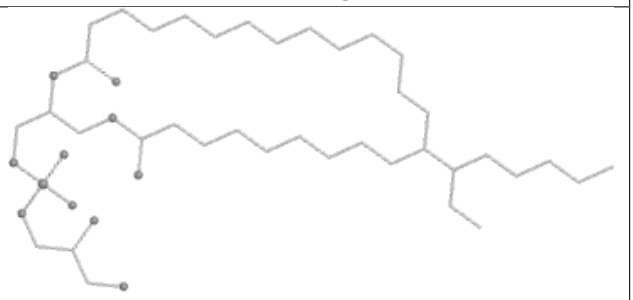
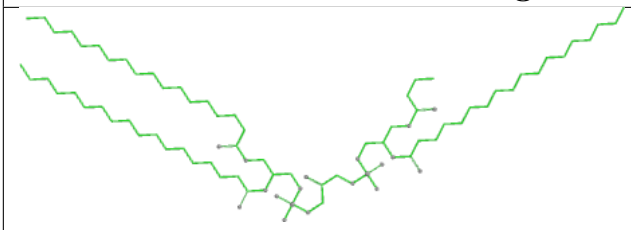


Rings

Ligand CDL 1X 201



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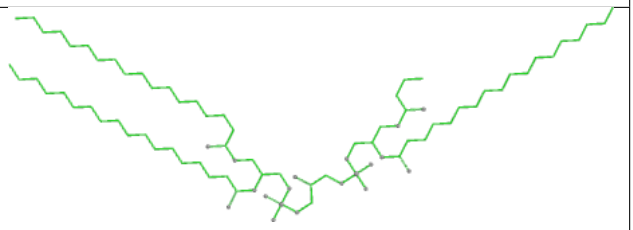
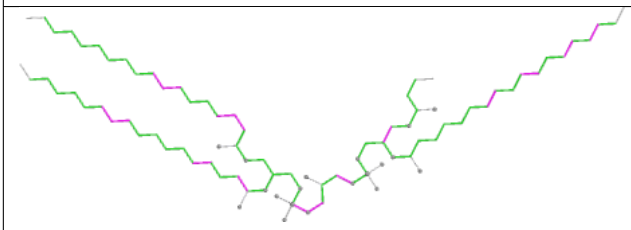
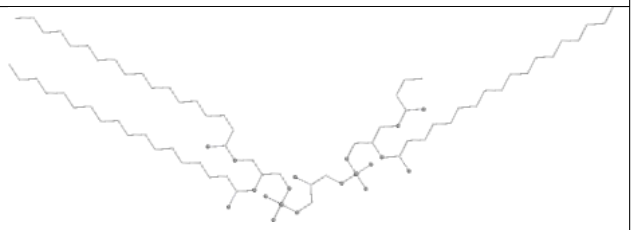


Bond angles

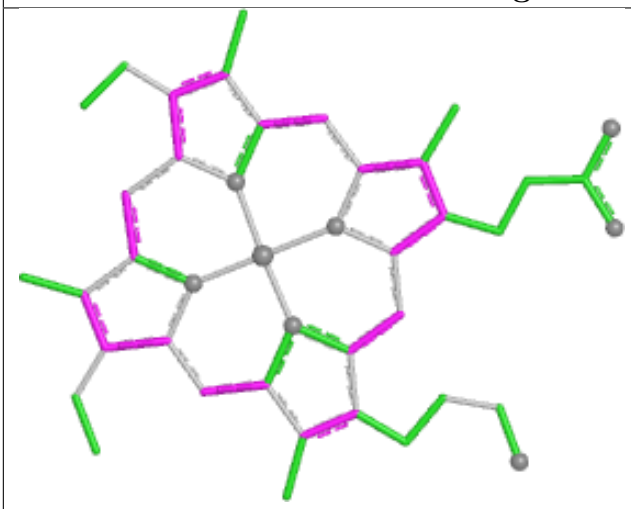


Torsions

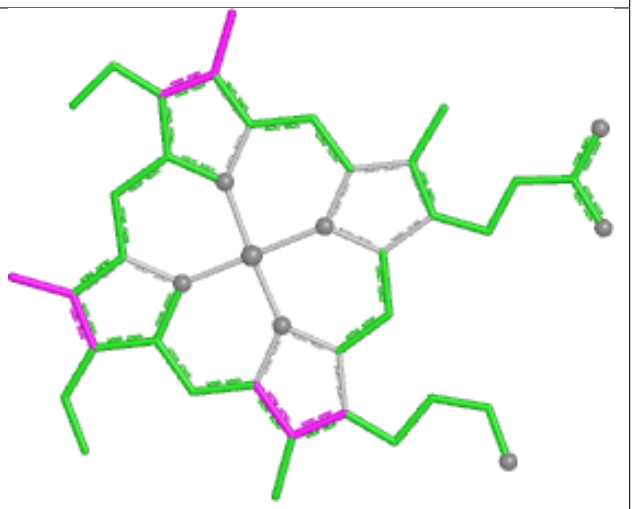


Rings

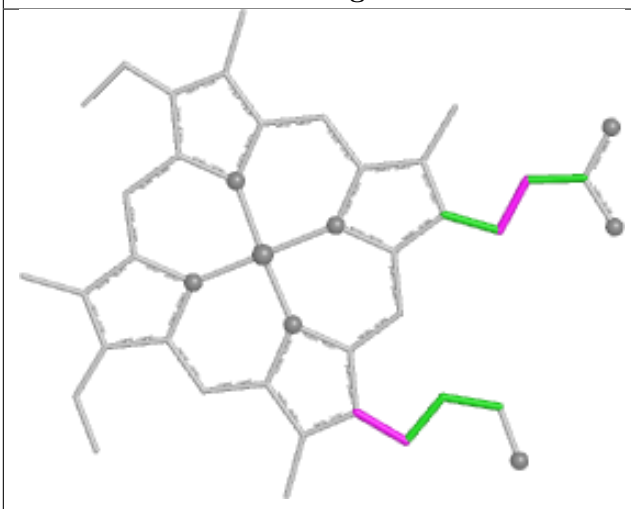
Ligand HEC 6D 501



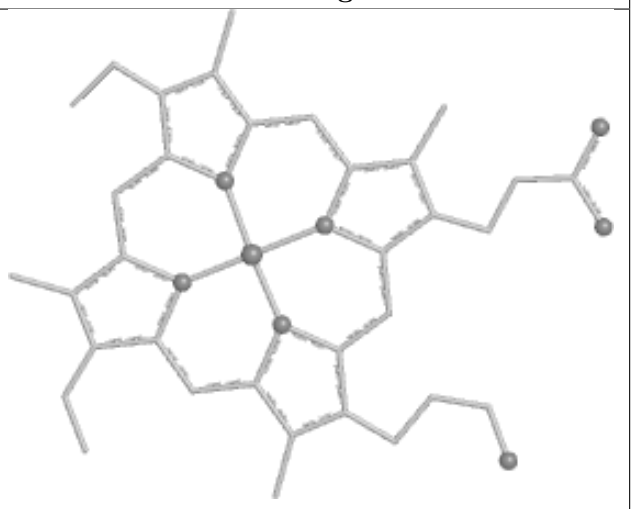
Bond lengths



Bond angles

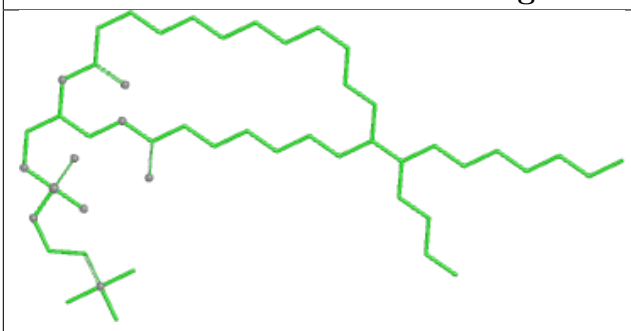


Torsions

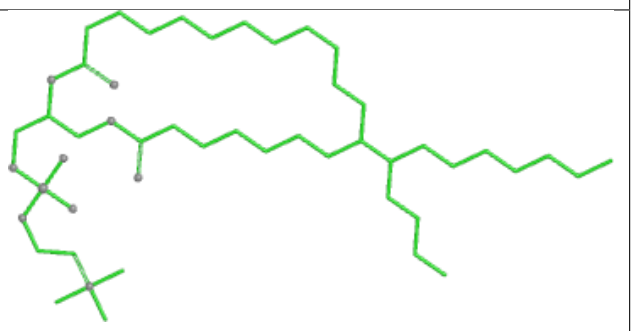


Rings

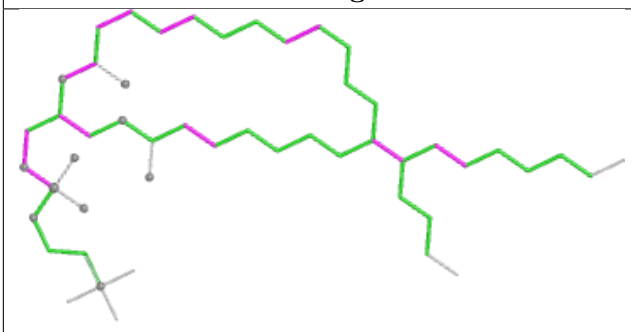
Ligand PSC 4B 303



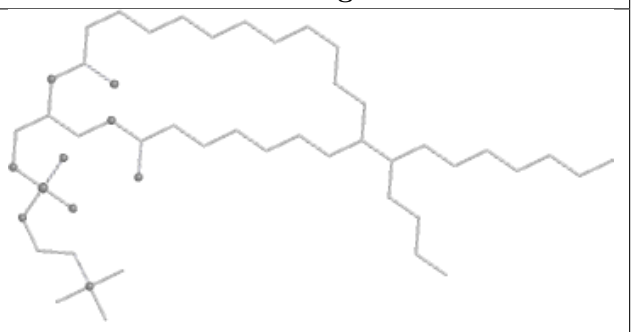
Bond lengths



Bond angles

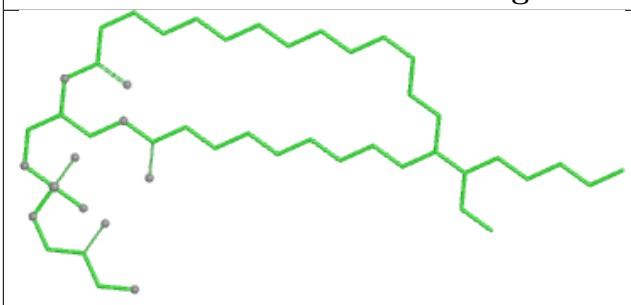


Torsions



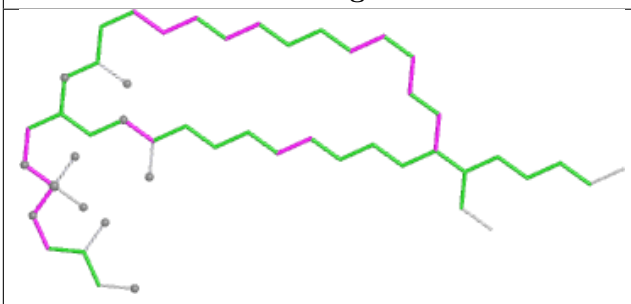
Rings

Ligand PGV 4K 101

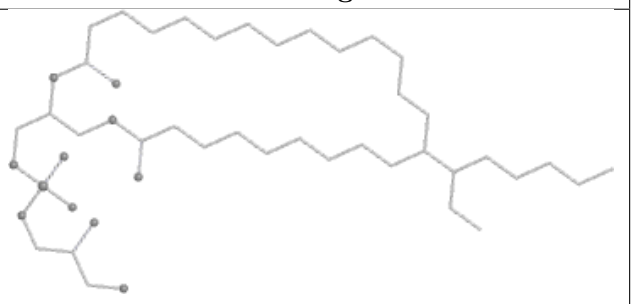


Bond lengths

Bond angles

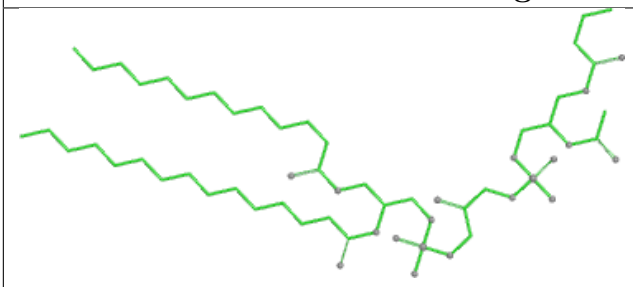


Torsions

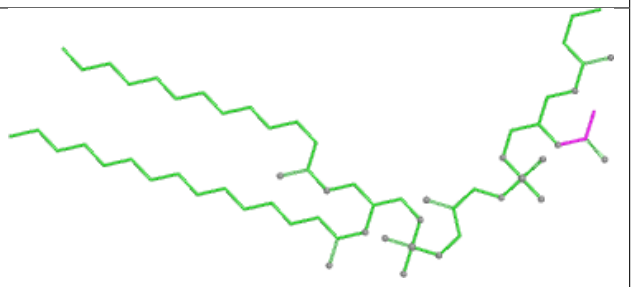


Rings

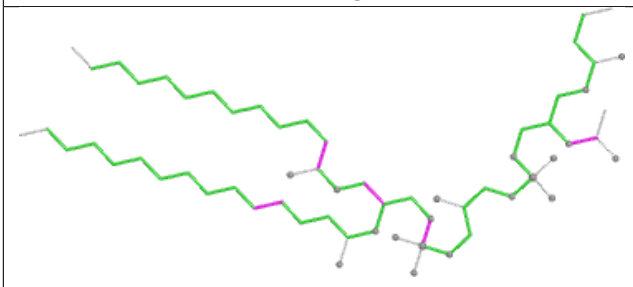
Ligand CDL 1N 903



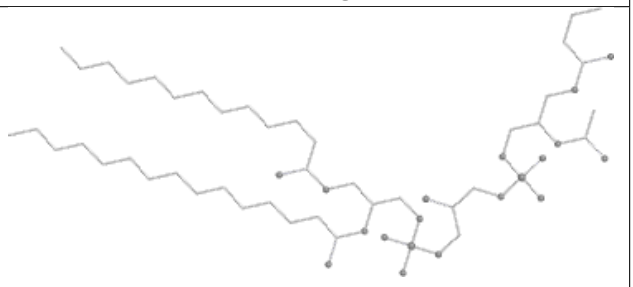
Bond lengths



Bond angles

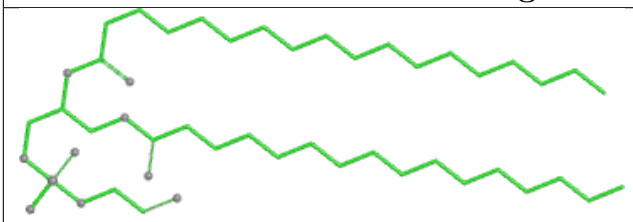


Torsions

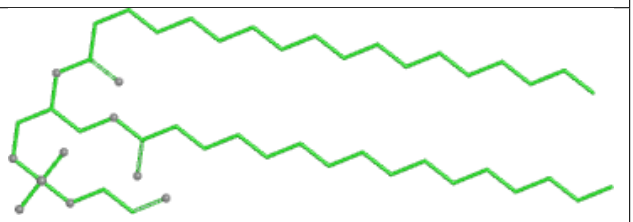


Rings

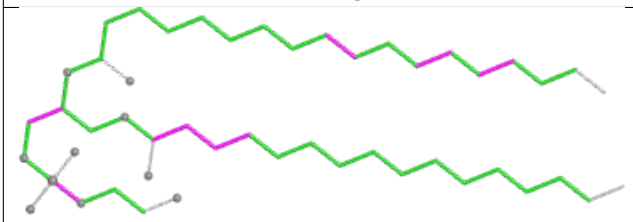
Ligand 3PE 5N 901



Bond lengths

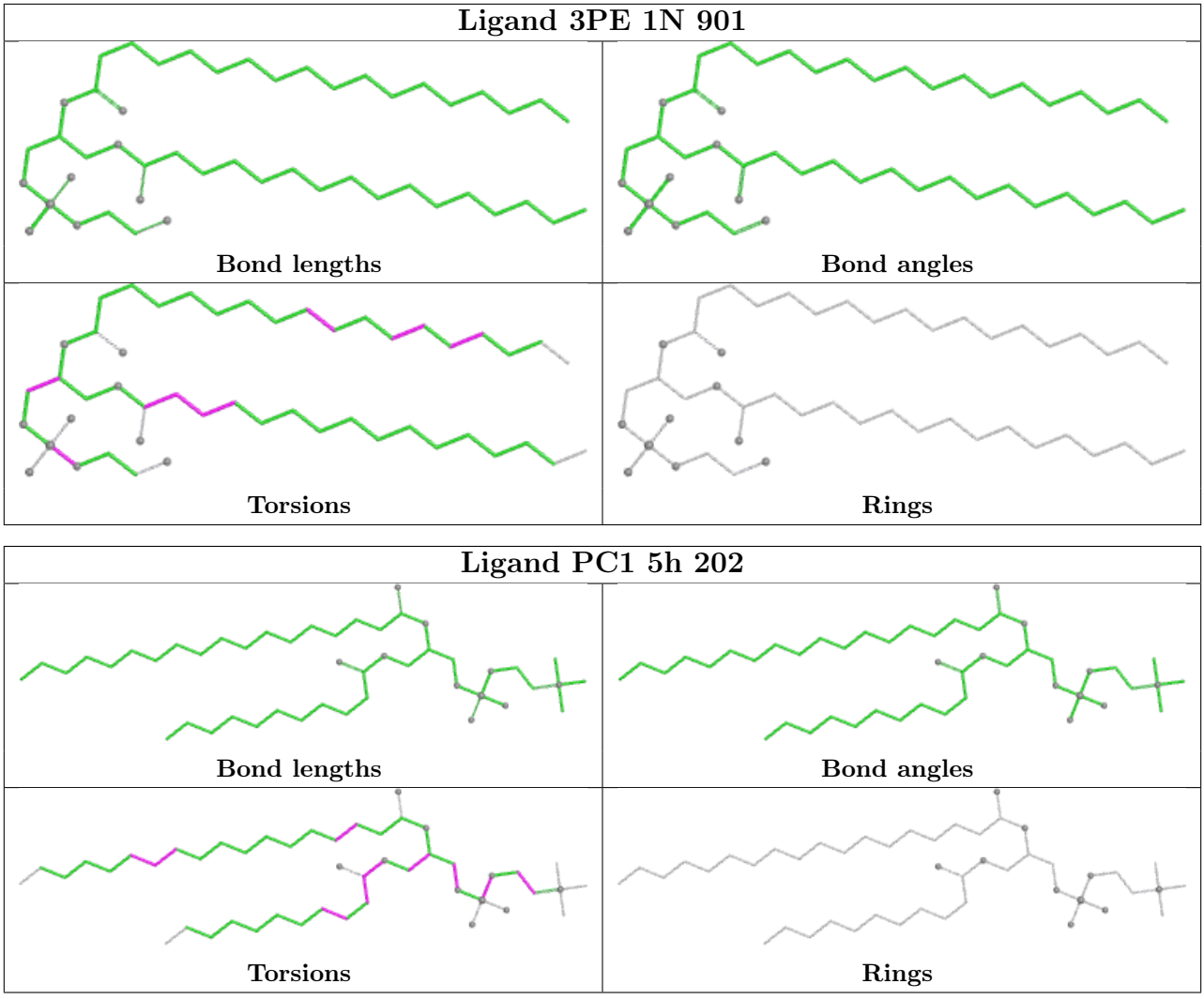


Bond angles



Torsions

Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	1B	6
1	1A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1A	1:FME	C	2:ASN	N	3.48

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1B	103:VAL	C	104:TYR	N	2.65
1	1B	60:MET	C	61:HIS	N	2.47
1	1B	100:LEU	C	101:ARG	N	2.08
1	1B	57:VAL	C	58:GLU	N	1.93
1	1B	95:LYS	C	96:MET	N	1.89
1	1B	92:LEU	C	93:THR	N	0.77

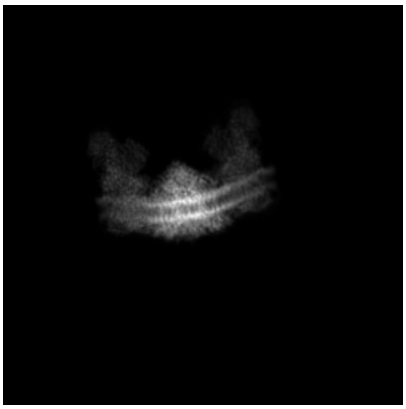
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42233. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

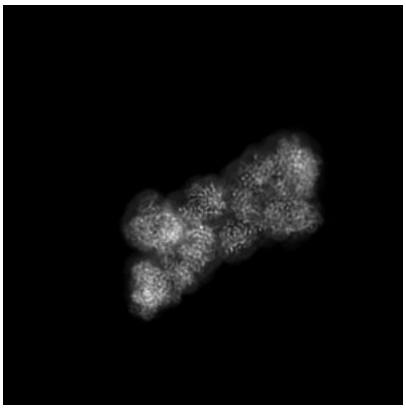
6.1 Orthogonal projections

6.1.1 Primary map



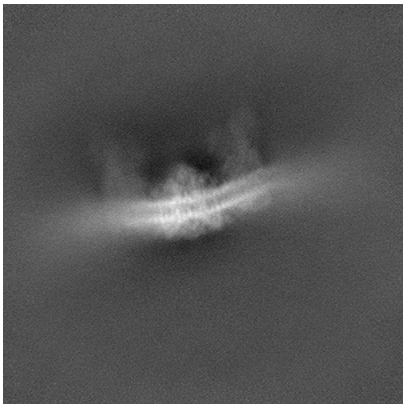
X

Y

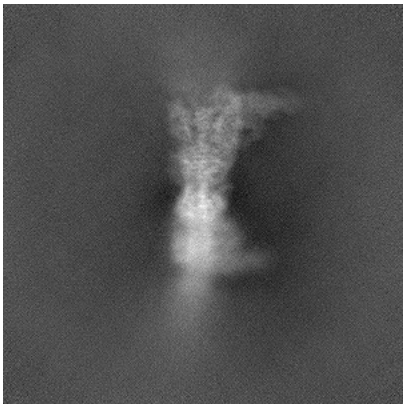


Z

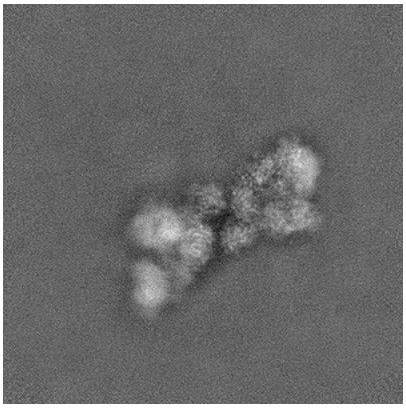
6.1.2 Raw map



X



Y



Z

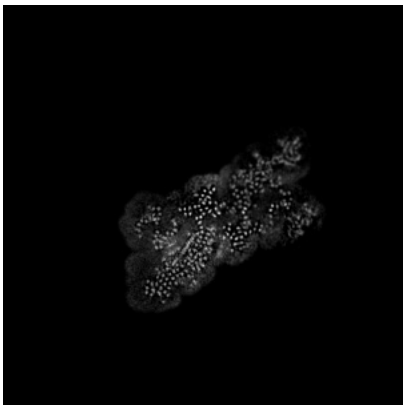
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

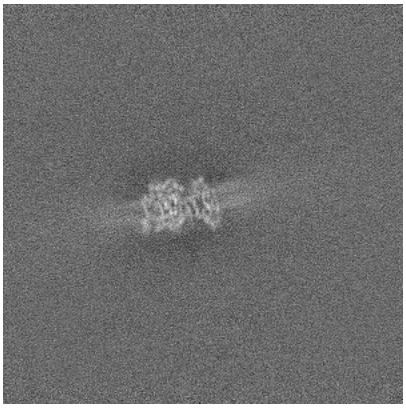
X Index: 256

Y Index: 256

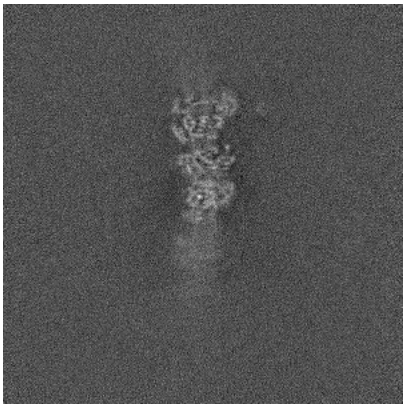


Z Index: 256

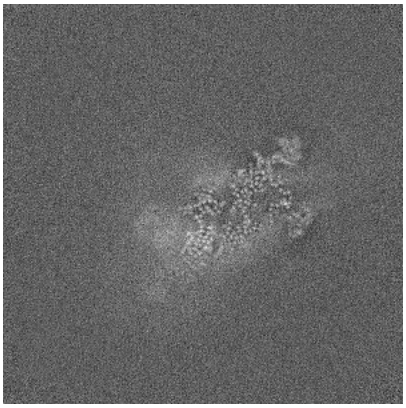
6.2.2 Raw map



X Index: 256



Y Index: 256



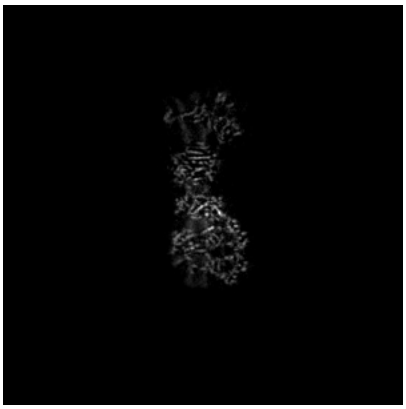
Z Index: 256

The images above show central slices of the map in three orthogonal directions.

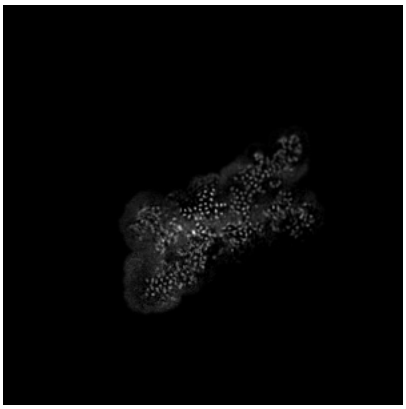
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 252

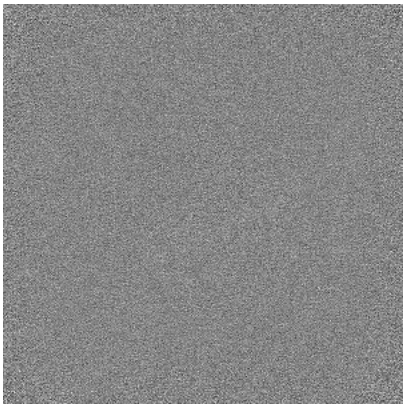


Y Index: 222

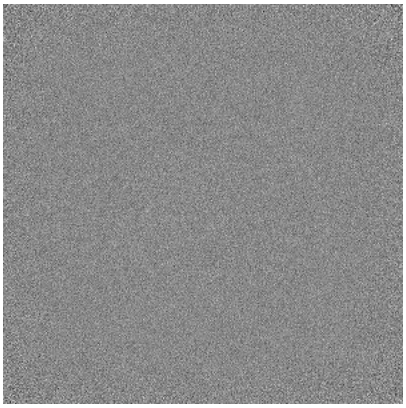


Z Index: 260

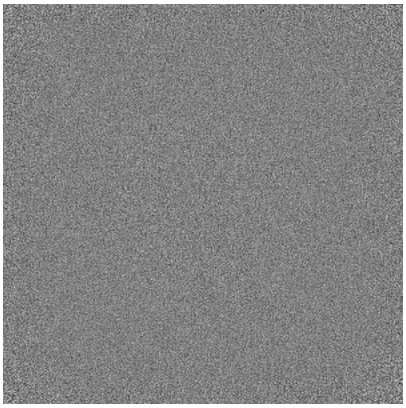
6.3.2 Raw map



X Index: 0



Y Index: 0

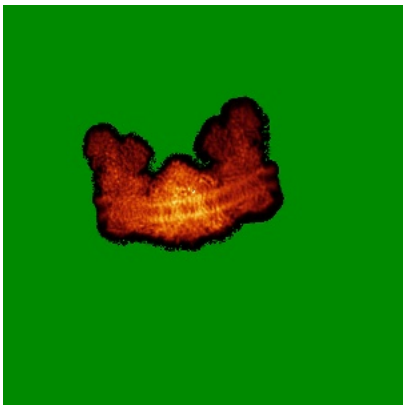


Z Index: 0

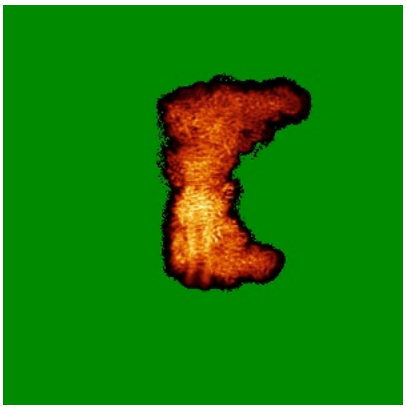
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

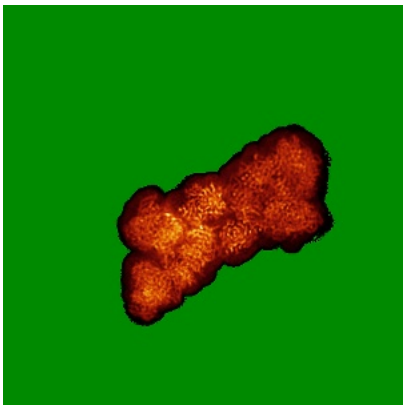
6.4.1 Primary map



X

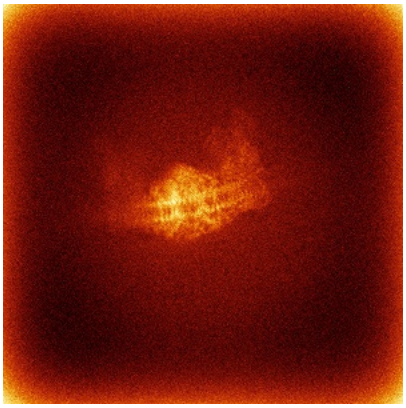


Y

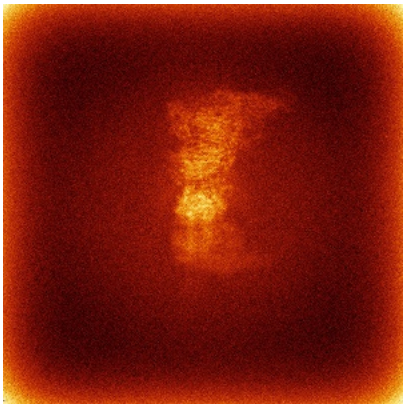


Z

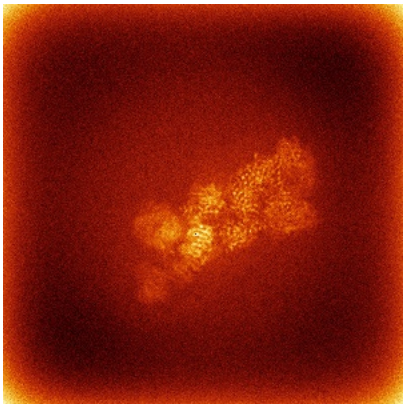
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

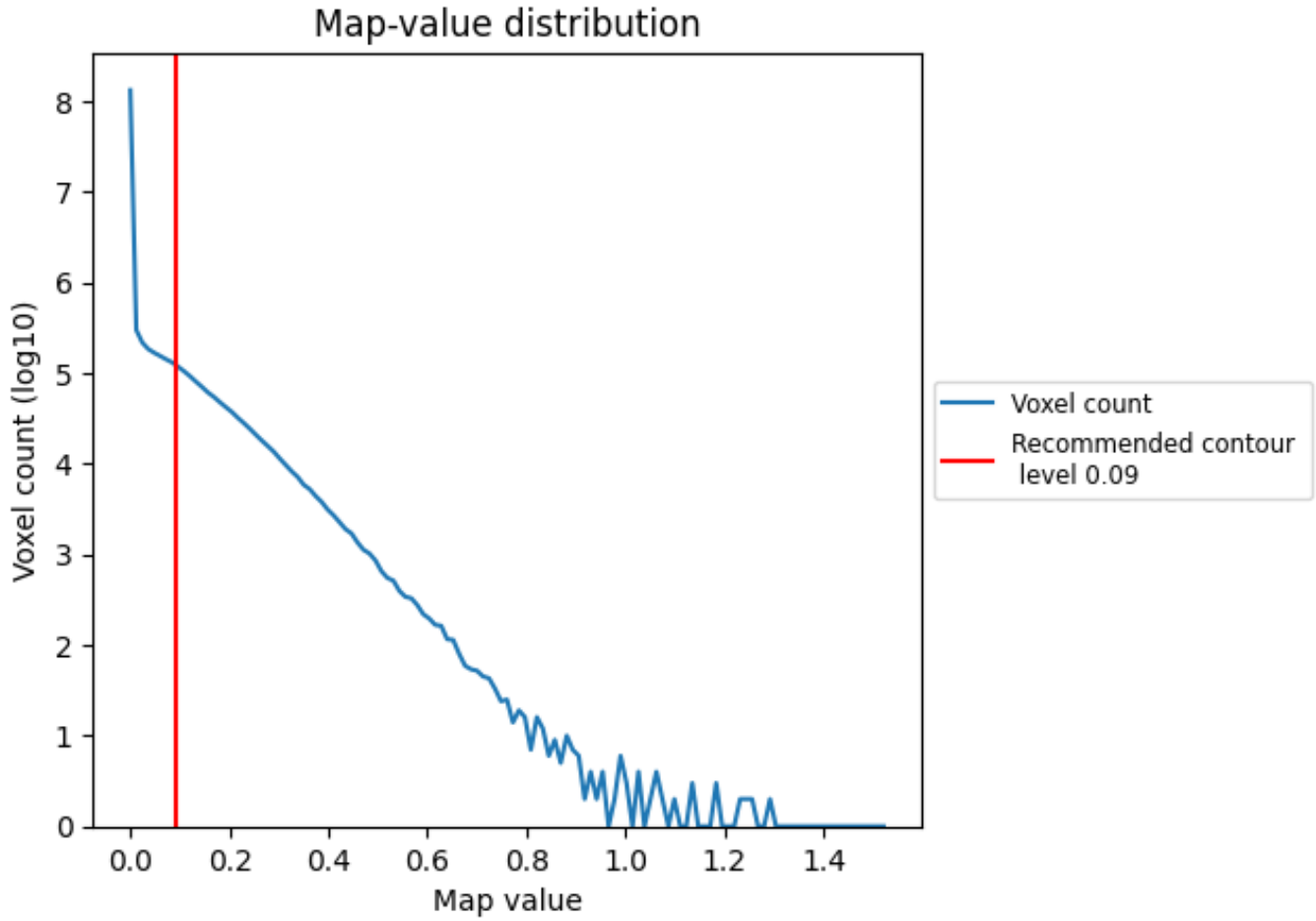
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

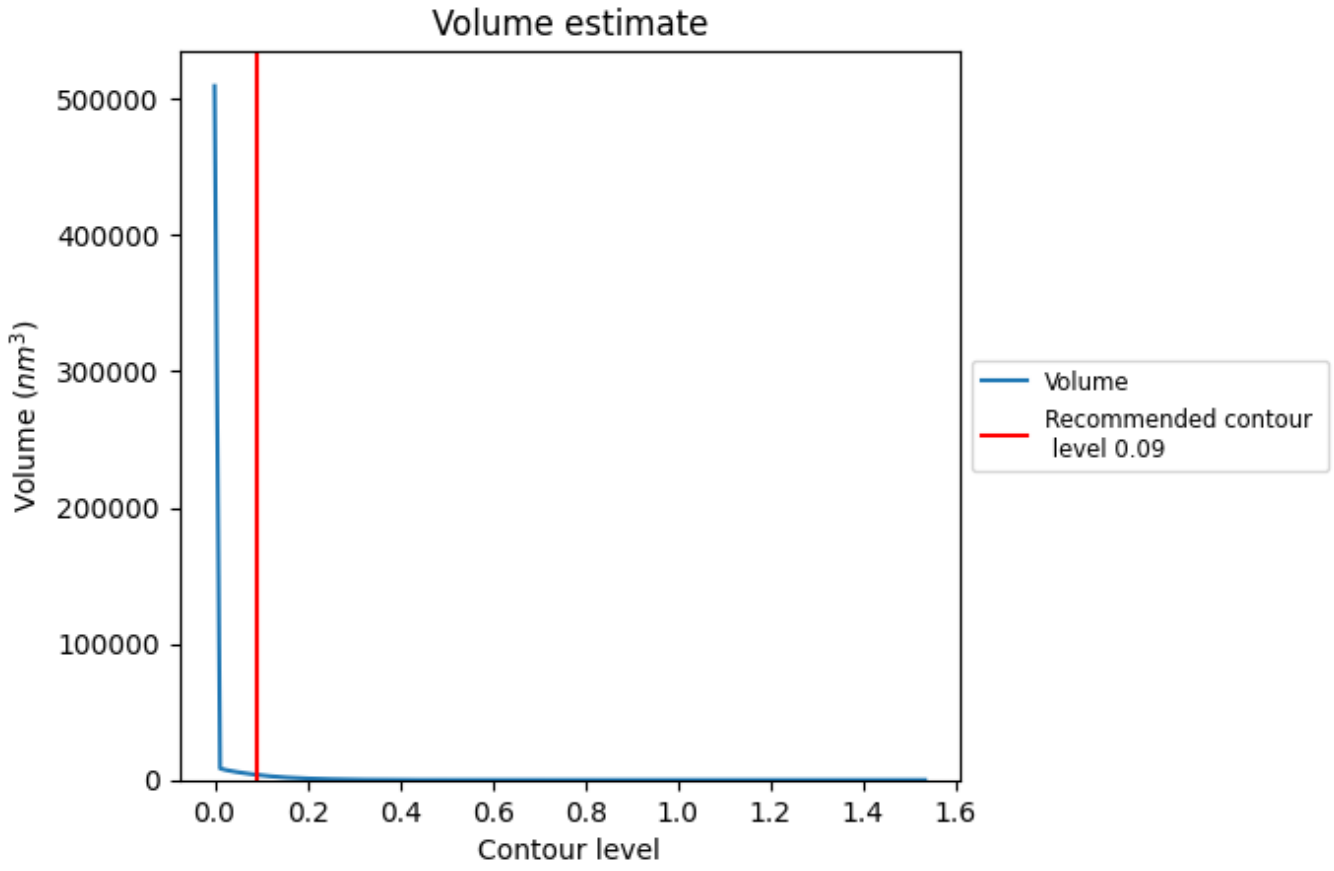
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

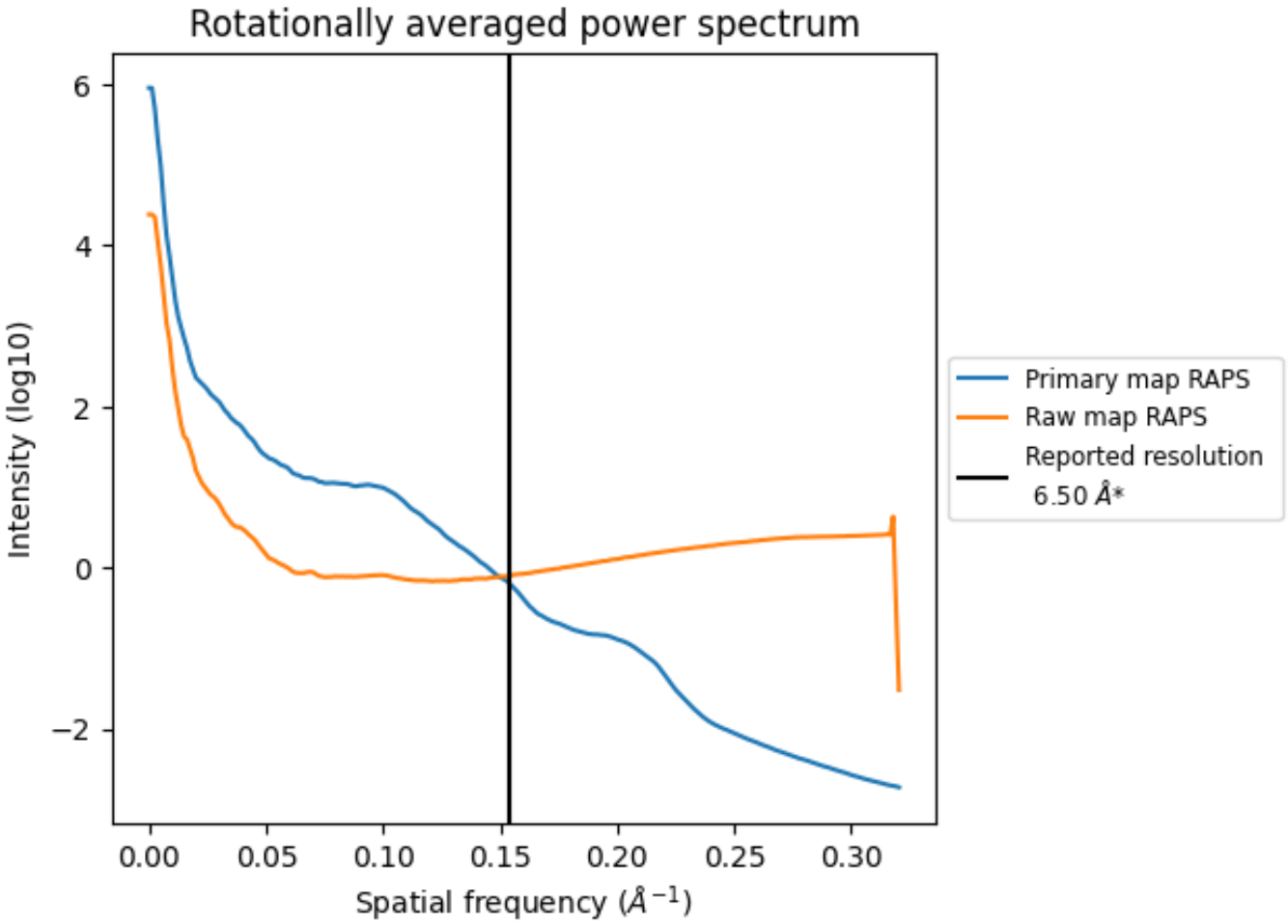
7.2 Volume estimate



The volume at the recommended contour level is 3822 nm^3; this corresponds to an approximate mass of 3453 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

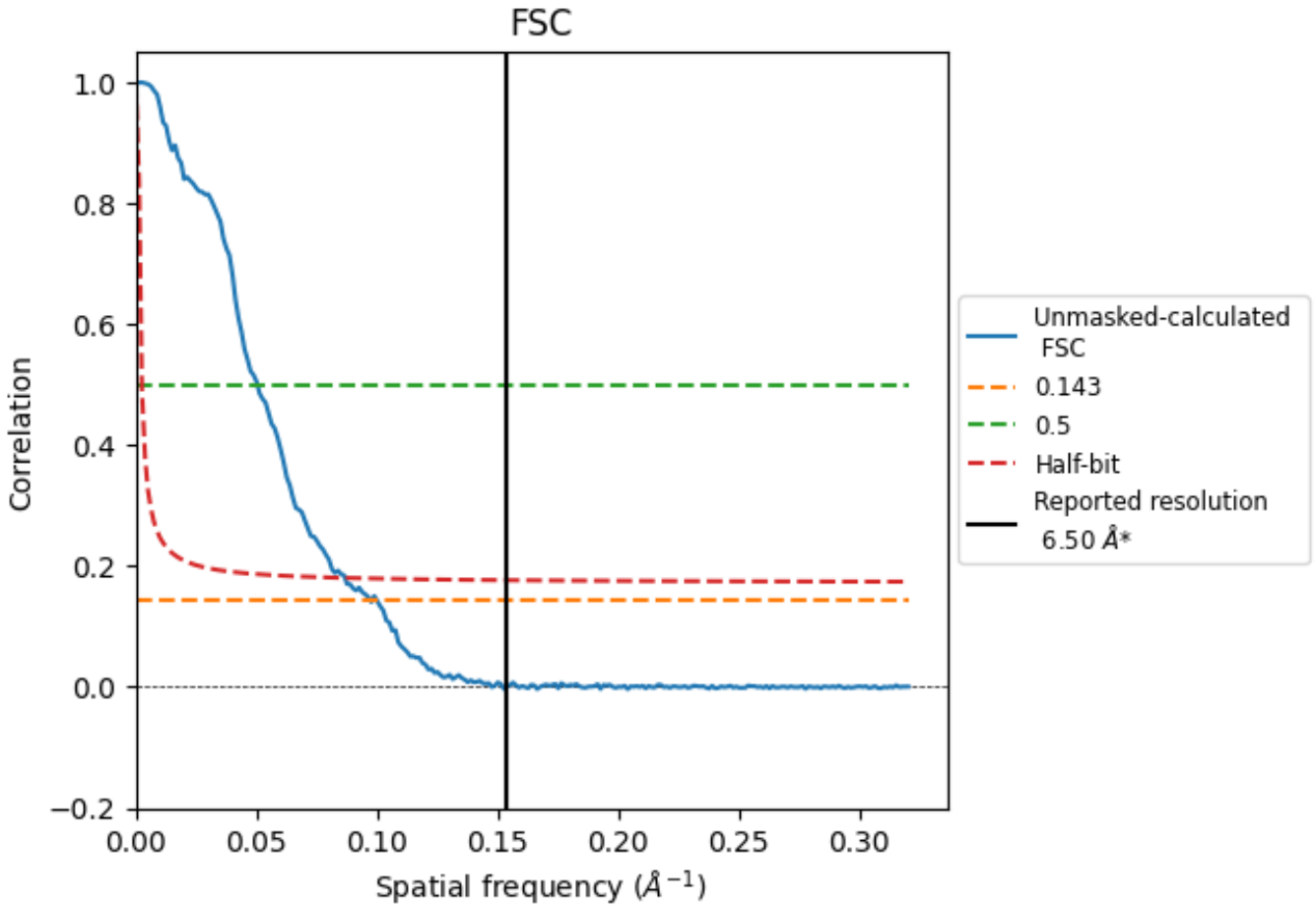


*Reported resolution corresponds to spatial frequency of 0.154 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.154 Å^{-1}

8.2 Resolution estimates (i)

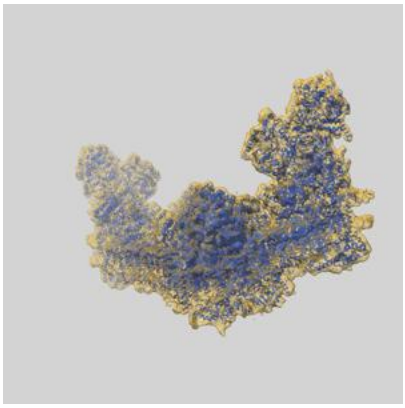
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	10.28	19.84	11.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.28 differs from the reported value 6.5 by more than 10 %

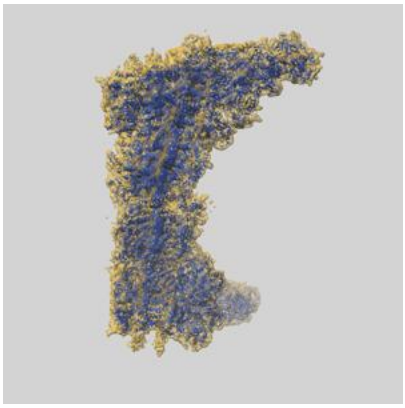
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42233 and PDB model 8UGR. Per-residue inclusion information can be found in section 3 on page 43.

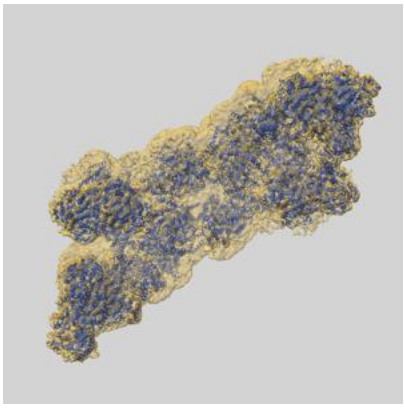
9.1 Map-model overlay



X



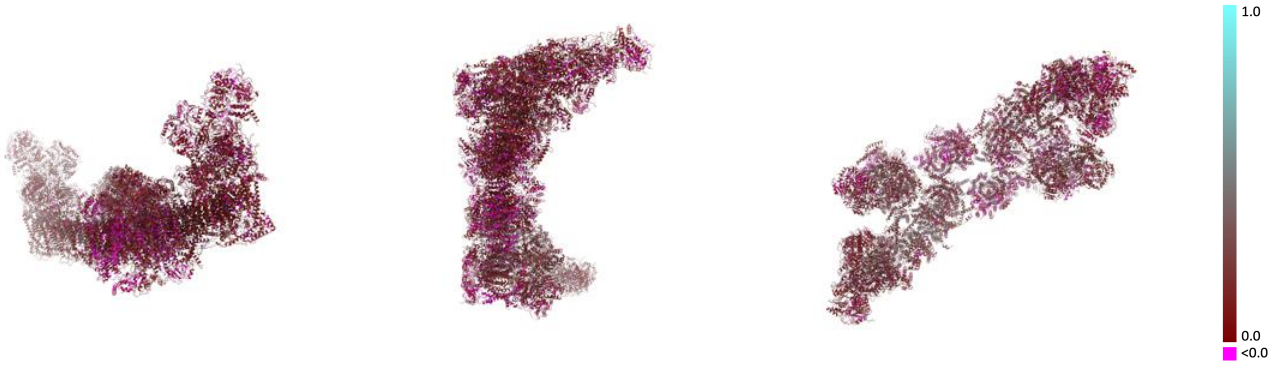
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

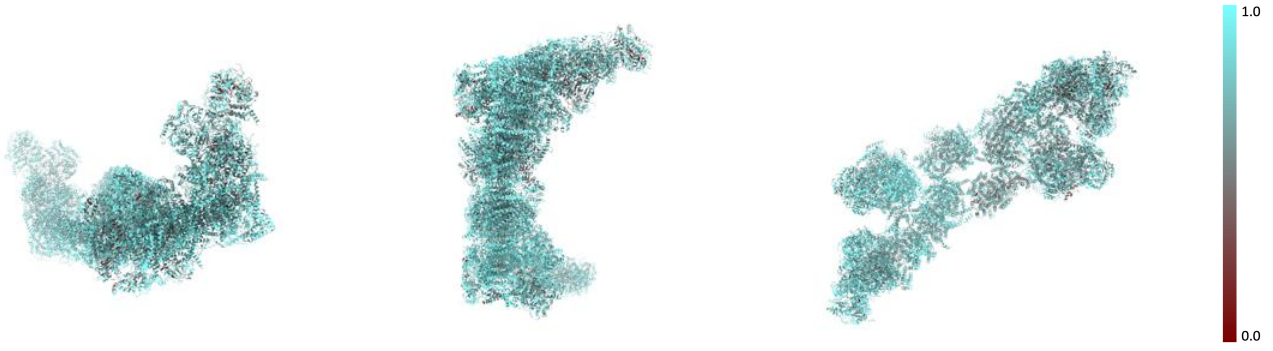
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

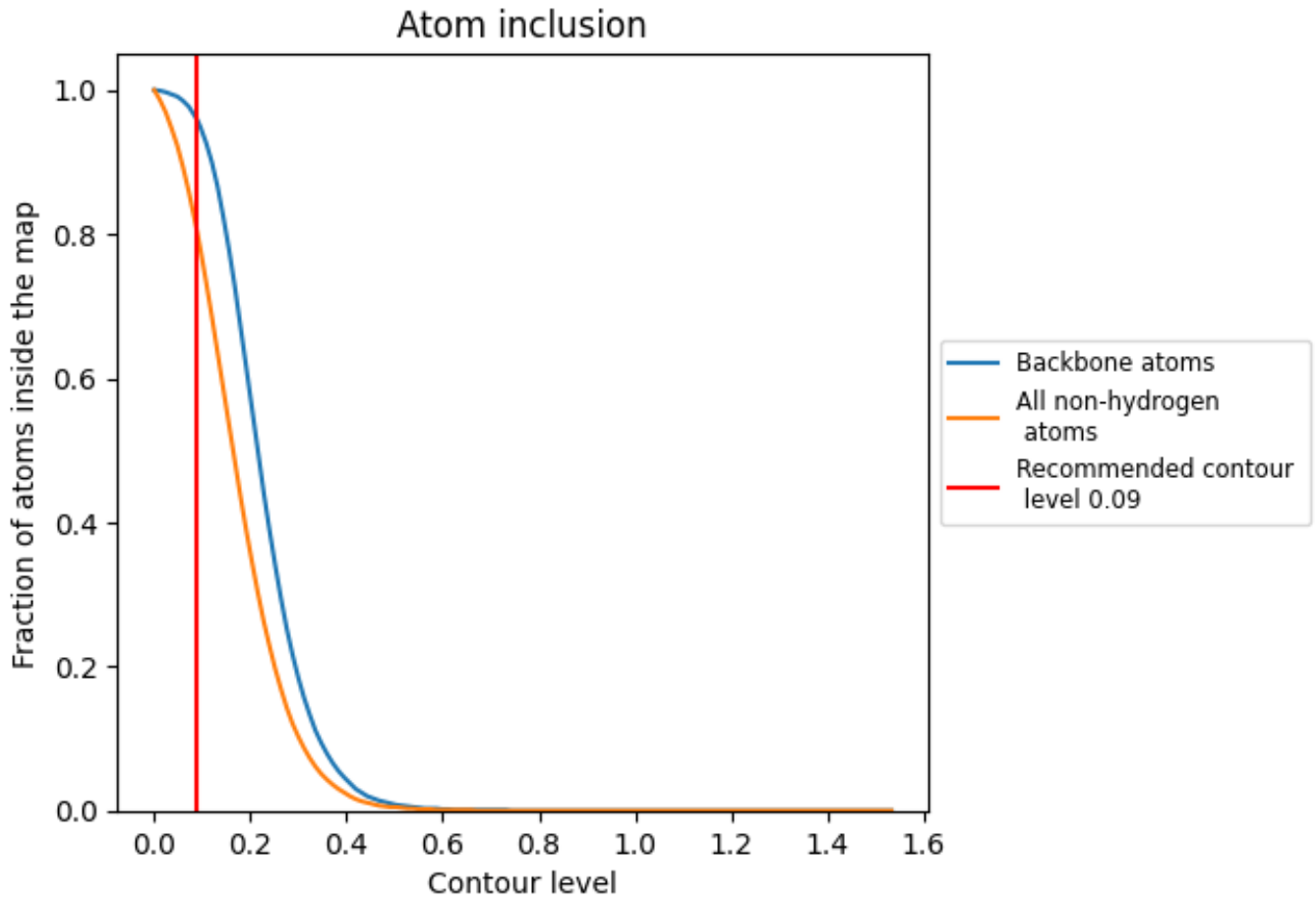
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8010	0.1600
1A	0.7750	0.1960
1B	0.8030	0.2300
1C	0.7990	0.2210
1D	0.7980	0.2060
1E	0.8330	0.2090
1F	0.8100	0.1760
1G	0.8230	0.2080
1H	0.8240	0.1890
1I	0.8180	0.2150
1J	0.8360	0.1710
1K	0.8320	0.1910
1L	0.9050	0.1890
1M	0.8980	0.2170
1N	0.8670	0.2260
1O	0.8950	0.1900
1P	0.8360	0.1990
1Q	0.7380	0.2270
1R	0.8660	0.2540
1S	0.7940	0.1900
1T	0.8320	0.1770
1U	0.9030	0.1810
1V	0.7730	0.1780
1W	0.7940	0.2150
1X	0.8810	0.2170
1Y	0.9370	0.1820
1Z	0.8740	0.2100
1a	0.9140	0.2150
1b	0.9000	0.2010
1c	0.8970	0.2090
1d	0.8930	0.2160
1e	0.8860	0.2410
1f	0.9190	0.2100
1g	0.9130	0.2140
1h	0.9140	0.2170

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Chain	Atom inclusion	Q-score
1i	0.9000	0.1900
1j	0.9060	0.1840
1k	0.9460	0.1840
1l	0.9510	0.2200
1m	0.9510	0.2050
1n	0.9330	0.1890
1o	0.9470	0.1720
1p	0.9470	0.2290
1q	0.8680	0.2290
1r	0.8720	0.2390
1s	0.8570	0.1980
3A	0.7850	0.1450
3B	0.8380	0.1860
3C	0.8960	0.2350
3D	0.7500	0.0640
3E	0.8070	0.0930
3F	0.7830	0.0970
3G	0.9240	0.2530
3H	0.9080	0.2290
3I	0.5460	0.0970
3J	0.8320	0.0520
3N	0.9560	0.2470
3O	0.9140	0.2620
3P	0.9240	0.1540
3Q	0.9270	0.1420
3R	0.8590	0.1180
3S	0.9270	0.1930
3T	0.9700	0.1980
3U	0.9730	0.1630
3V	0.8280	0.1040
3W	0.9740	0.1440
3X	0.9540	0.0710
3Y	0.8370	0.1400
4A	0.7520	0.0940
4B	0.7360	0.0870
4C	0.7760	0.0760
4D	0.8200	0.1170
4E	0.7670	0.1020
4F	0.7570	0.1150
4G	0.9230	0.0980
4H	0.7550	0.1060
4I	0.8330	0.1040

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Chain	Atom inclusion	Q-score
4J	0.8820	0.1400
4K	0.9410	0.1290
4L	0.8350	0.1060
4M	0.8940	0.1470
4N	0.7210	0.1040
5A	0.6350	0.1250
5B	0.7630	0.1540
5C	0.6670	0.1480
5D	0.6810	0.1290
5E	0.6880	0.1480
5F	0.6680	0.1040
5G	0.7200	0.1450
5H	0.7410	0.1400
5I	0.7430	0.1400
5J	0.7850	0.1320
5K	0.7740	0.1440
5L	0.7720	0.1170
5M	0.7660	0.1390
5N	0.7650	0.1480
5O	0.7860	0.1540
5P	0.7960	0.1530
5Q	0.6140	0.1500
5R	0.8280	0.1840
5S	0.7200	0.1460
5T	0.6610	0.1300
5U	0.6450	0.1200
5V	0.6690	0.1340
5W	0.7070	0.1700
5X	0.8580	0.1590
5Y	0.8100	0.1470
5Z	0.8100	0.1520
5a	0.8800	0.1540
5b	0.8470	0.1620
5c	0.8370	0.1710
5d	0.7980	0.1620
5e	0.8850	0.1810
5f	0.8620	0.1810
5g	0.7860	0.1680
5h	0.8290	0.1570
5i	0.8060	0.1430
5j	0.7770	0.1340
5k	0.8330	0.1680

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Chain	Atom inclusion	Q-score
5l	0.8180	0.1470
5m	0.7910	0.1490
5n	0.7600	0.1410
5o	0.8730	0.1290
5p	0.8710	0.1700
5q	0.8340	0.1840
5r	0.7520	0.1750
5s	0.7280	0.1300
6A	0.7950	0.1940
6B	0.7630	0.2100
6C	0.7630	0.1870
6D	0.8430	0.1830
6E	0.6680	0.0550
6F	0.5410	0.0580
6G	0.5580	0.0190
6H	0.6470	0.0480
6I	0.4020	0.0390
6J	0.8980	0.1760
6N	0.7960	0.1940
6O	0.7720	0.2160
6P	0.7230	0.1030
6Q	0.7240	0.1020
6R	0.6710	0.0900
6S	0.7410	0.1510
6T	0.8250	0.1220
6U	0.7980	0.1470
6V	0.4880	0.0860
6W	0.7990	0.1180
6X	0.7280	0.0690
6Y	0.8520	0.2060
8A	0.7250	0.1360
8B	0.6710	0.0610
8C	0.6230	0.0460
8D	0.7240	0.0870
8E	0.6030	0.0610
8F	0.6090	0.0830
8G	0.8320	0.0910
8H	0.7130	0.0840
8I	0.7510	0.0870
8J	0.7880	0.1010
8K	0.8520	0.1050
8L	0.7250	0.0950

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Chain	Atom inclusion	Q-score
8M	0.8340	0.1150
8N	0.6810	0.0830