Full wwPDB EM Validation Report ⓘ

Oct 16, 2024 – 01:15 AM JST

PDB ID	:	8J9H
EMDB ID	:	EMD-36107
Title	:	Cryo-EM structure of Euglena gracilis respiratory complex I, deactive state
Authors	:	Wu, M.C.; He, Z.X.; Tian, H.T.; Hu, Y.Q.; Han, F.Z.; Zhou, L.
Deposited on	:	2023-05-03
Resolution	:	3.11 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:

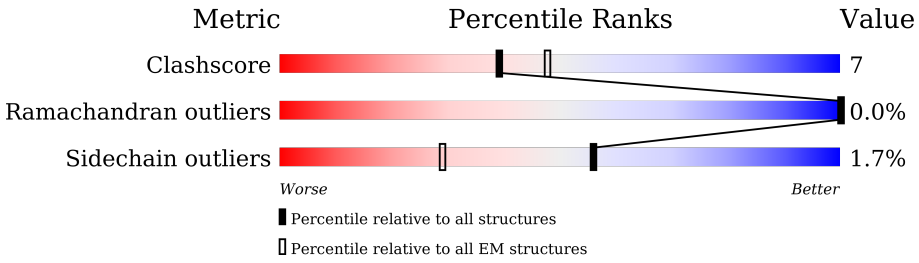
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.11 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%

Mol	Chain	Length	Quality of chain
1	1A	385	74% 17% 9%
2	1B	527	81% 19%
3	2B	142	80% 18% ••
4	4L	171	53% 10% 37%
5	A1	141	81% 16% •
6	A2	193	90% 9% •
7	A3	125	87% 11% ••
8	A5	184	72% 11% • 16%
9	A6	437	82% 15% •

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Mol	Chain	Length	Quality of chain
10	A7	136	85% 15%
11	A8	223	83% 17%
12	A9	489	84% 14%
13	AB	134	56% 10% 34%
14	AL	281	83% 11% 6%
15	AM	198	82% 11% 7%
16	AN	287	94% 6%
17	B2	145	64% 8% 28%
18	B3	62	77% 21%
19	B4	171	84% 15%
20	B5	140	89% 11%
21	B6	91	81% 19%
22	B7	97	79% 21%
23	B8	176	67% 16% 16%
24	B9	158	77% 18%
25	BL	144	89% 11%
26	BM	112	82% 17%
27	C4	185	76% 22%
28	E1	483	78% 16% 7%
29	E2	467	85% 15%
30	E3	434	86% 13%
31	E4	368	79% 16% 5%
32	E5	290	77% 18% 5%
33	E6	371	77% 9% 14%
34	E8	205	80% 19%

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Mol	Chain	Length	Quality of chain
35	EA	126	87% 12%
36	EB	101	88% 12%
37	EC	101	70% 14% 16%
38	ED	151	79% 13% 9%
39	FX	325	53% 19% 27%
40	G1	436	77% 15% 8%
41	G2	267	74% 14% 12%
42	G3	261	85% 15%
43	N1	670	37% 9% 54%
44	N2	300	75% 24%
45	N3	293	32% 8% 59%
45	N6	293	39% 13% 47%
46	N4	478	71% 29%
47	N5	584	69% 30%
48	S2	395	78% 20%
49	S3	277	64% 24% 10%
50	S4	208	74% 16% 9%
51	S5	122	92% 8%
52	S6	147	80% 20%
53	S7	207	82% 15%
54	S8	212	67% 19% 14%
55	U1	12	92% 8%
55	U2	12	92% 8%
56	V1	526	77% 17%
57	V2	225	84% 15%

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Mol	Chain	Length	Quality of chain
58	E7	246	
59	AC	134	

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
61	SF4	S8	297	-	-	X	-
61	SF4	S8	298	-	-	X	-

2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 226135 atoms, of which 112544 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 NDUS1A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	1A	352	5501	1753	2700	488	537	23	0	0

- Molecule 2 is a protein called NDUS1B.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	1B	525	8357	2679	4159	743	765	11	1	0

- Molecule 3 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	2B	140	2059	712	989	172	183	3	0	0

- Molecule 4 is a protein called ND4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	4L	108	1768	606	878	133	145	6	0	0

- Molecule 5 is a protein called NDUFA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	A1	137	2097	684	1026	192	192	3	0	0

- Molecule 6 is a protein called NDUFA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	A2	192	2967	942	1474	267	280	4	0	0

- Molecule 7 is a protein called NDUFA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	A3	124	Total	C	H	N	O	S	0	0
			2089	678	1039	191	175	6		

- Molecule 8 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	A5	154	Total	C	H	N	O	S	0	0
			2509	794	1248	221	244	2		

- Molecule 9 is a protein called NDUFA6.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A6	423	Total	C	H	N	O	S	0	0
			6608	2091	3280	601	632	4		

- Molecule 10 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A7	136	Total	C	H	N	O	S	0	0
			2272	735	1118	219	194	6		

- Molecule 11 is a protein called NDUFA8.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	A8	223	Total	C	H	N	O	S	0	0
			3548	1160	1726	315	334	13		

- Molecule 12 is a protein called NDUFA9.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	A9	484	Total	C	H	N	O	S	0	0
			7679	2449	3850	662	700	18		

- Molecule 13 is a protein called NDUFAB1-alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AB	88	Total	C	H	N	O	S	0	0
			1367	437	673	114	139	4		

- Molecule 14 is a protein called NDUFA12.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	AL	265	Total	C	H	N	O	S	0	0
			4409	1439	2172	414	379	5		

- Molecule 15 is a protein called NDUFA13.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	AM	184	Total	C	H	N	O	S	0	0
			2935	953	1448	264	263	7		

- Molecule 16 is a protein called NDUFA11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	AN	287	Total	C	H	N	O	S	0	0
			4573	1501	2267	396	399	10		

- Molecule 17 is a protein called NDUFB2.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	B2	105	Total	C	H	N	O	S	0	0
			1770	604	857	142	166	1		

- Molecule 18 is a protein called NDUFB3.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	B3	61	Total	C	H	N	O	S	0	0
			758	292	309	88	68	1		

- Molecule 19 is a protein called NDUFB4.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	B4	171	Total	C	H	N	O	S	0	0
			2735	885	1358	250	236	6		

- Molecule 20 is a protein called NDUFB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	B5	140	Total	C	H	N	O	S	0	0
			2181	708	1069	207	195	2		

- Molecule 21 is a protein called NDUFB6.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	B6	91	Total	C	H	N	O	S	0	0
			1520	509	747	132	128	4		

- Molecule 22 is a protein called NDUFB7.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	B7	97	Total	C	H	N	O	S	0	0
			1692	536	835	165	149	7		

- Molecule 23 is a protein called NDUFB8.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	B8	147	Total	C	H	N	O	S	0	0
			2351	804	1127	199	213	8		

- Molecule 24 is a protein called NDUFB9.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	B9	151	Total	C	H	N	O	S	0	0
			2443	795	1207	216	222	3		

- Molecule 25 is a protein called NDUFB10.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	BL	144	Total	C	H	N	O	S	0	0
			2406	786	1179	215	216	10		

- Molecule 26 is a protein called NDUFB11.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	BM	112	Total	C	H	N	O	S	0	0
			1737	577	827	164	167	2		

- Molecule 27 is a protein called NDUFC2.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	C4	183	Total	C	H	N	O	S	0	0
			3062	1000	1517	268	271	6		

- Molecule 28 is a protein called NDUEG1.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	E1	450	Total	C	H	N	O	S	0	0
			7008	2244	3496	601	654	13		

- Molecule 29 is a protein called NDUEG2.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	E2	466	Total	C	H	N	O	S	0	0
			7103	2286	3540	618	655	4		

- Molecule 30 is a protein called NDUEG3.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	E3	432	Total	C	H	N	O	S	0	0
			6518	2071	3263	565	612	7		

- Molecule 31 is a protein called NDUEG4.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	E4	351	Total	C	H	N	O	S	0	0
			5502	1774	2732	477	504	15		

- Molecule 32 is a protein called NDUEG5.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	E5	276	Total	C	H	N	O	S	0	0
			4046	1265	2069	341	369	2		

- Molecule 33 is a protein called NDUEG6.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	E6	318	Total	C	H	N	O	S	0	0
			5228	1703	2554	477	482	12		

- Molecule 34 is a protein called NDUEG8.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	E8	205	Total	C	H	N	O	S	0	0
			3354	1100	1663	288	292	11		

- Molecule 35 is a protein called NDUEG10.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	EA	124	Total	C	H	N	O	S	0	0
			1793	630	832	172	156	3		

- Molecule 36 is a protein called NDUEG11.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	EB	101	Total	C	H	N	O	S	0	0
			1405	473	631	150	144	7		

- Molecule 37 is a protein called NDUEG12.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	EC	85	Total	C	H	N	O	S	0	0
			1323	424	663	116	118	2		

- Molecule 38 is a protein called NDUEG13.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	ED	138	Total	C	H	N	O	S	0	0
			2273	736	1131	205	196	5		

- Molecule 39 is a protein called NDUFX.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	FX	237	Total	C	H	N	O	S	0	0
			3816	1263	1849	338	359	7		

- Molecule 40 is a protein called NDUCA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	G1	403	Total	C	H	N	O	S	0	0
			6146	1979	2999	558	594	16		

- Molecule 41 is a protein called NDUCA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	G2	236	Total	C	H	N	O	S	0	0
			3650	1138	1846	323	338	5		

- Molecule 42 is a protein called NDUCA3.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	G3	261	Total	C	H	N	O	S	0	0
			3905	1226	1944	356	373	6		

- Molecule 43 is a protein called ND1.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	N1	310	Total	C	H	N	O	S	0	0
			5331	1783	2726	380	435	7		

- Molecule 44 is a protein called ND2A.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	N2	296	Total	C	H	N	O	S	0	0
			5101	1725	2589	362	418	7		

- Molecule 45 is a protein called ND3.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	N3	121	Total	C	H	N	O	S	0	0
			2094	720	1057	143	172	2		
45	N6	154	Total	C	H	N	O	S	0	0
			2642	857	1385	187	210	3		

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	N4	478	Total	C	H	N	O	S	0	0
			8215	2743	4214	582	663	13		

- Molecule 47 is a protein called ND5.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	N5	584	Total	C	H	N	O	S	0	0
			9869	3293	5032	711	808	25		

- Molecule 48 is a protein called NDUFS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	S2	394	Total	C	H	N	O	S	0	0
			6274	2041	3101	541	569	22		

- Molecule 49 is a protein called NDUFS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	S3	248	Total	C	H	N	O	S	0	0
			3978	1307	1928	346	384	13		

- Molecule 50 is a protein called NDUFS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	S4	190	Total	C	H	N	O	S	0	0
			3038	956	1502	300	273	7		

- Molecule 51 is a protein called NDUFS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	S5	122	Total	C	H	N	O	S	0	0
			1886	625	895	173	188	5		

- Molecule 52 is a protein called NDUFS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	S6	147	Total	C	H	N	O	S	0	0
			2392	759	1192	225	208	8		

- Molecule 53 is a protein called NDUFS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	S7	201	Total	C	H	N	O	S	0	0
			3045	975	1500	272	284	14		

- Molecule 54 is a protein called NDUFS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	S8	182	Total	C	H	N	O	S	0	0
			2843	915	1392	245	275	16		

- Molecule 55 is a protein called UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U1	12	Total	C	H	N	O	0	0
			76	36	16	12	12		
55	U2	12	Total	C	H	N	O	0	0
			76	36	16	12	12		

- Molecule 56 is a protein called NDUFV1.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	V1	504	Total	C	H	N	O	S	0	0
			7724	2463	3827	680	727	27		

- Molecule 57 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	V2	225	Total	C	H	N	O	S	0	0
			3460	1124	1701	299	319	17		

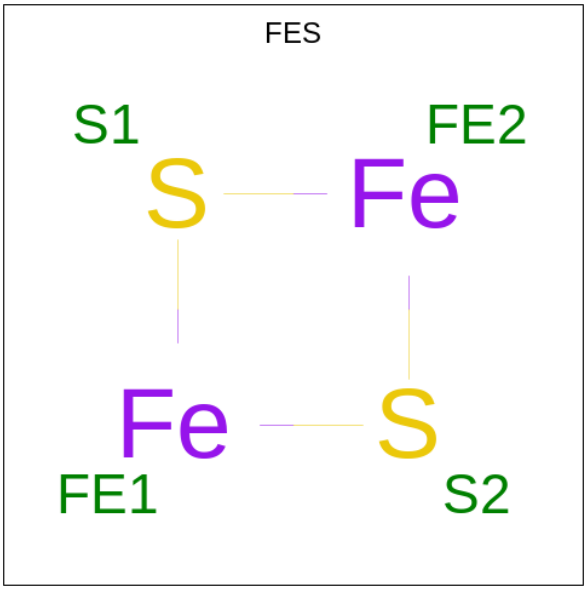
- Molecule 58 is a protein called NDUEG7.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	E7	246	Total	C	H	N	O	S	0	0
			3780	1205	1892	332	344	7		

- Molecule 59 is a protein called NDUFAB1-beta.

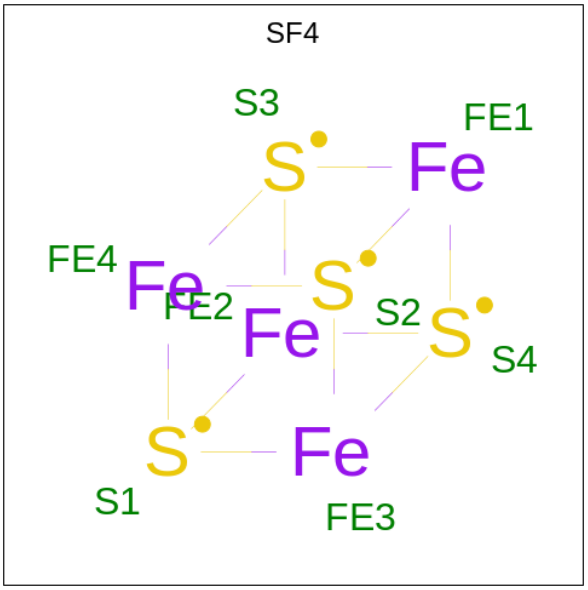
Mol	Chain	Residues	Atoms						AltConf	Trace
59	AC	92	Total	C	H	N	O	S	0	0
			1418	461	697	116	140	4		

- Molecule 60 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
60	1A	1	Total Fe S 4 2 2	0
60	V2	1	Total Fe S 4 2 2	0

- Molecule 61 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

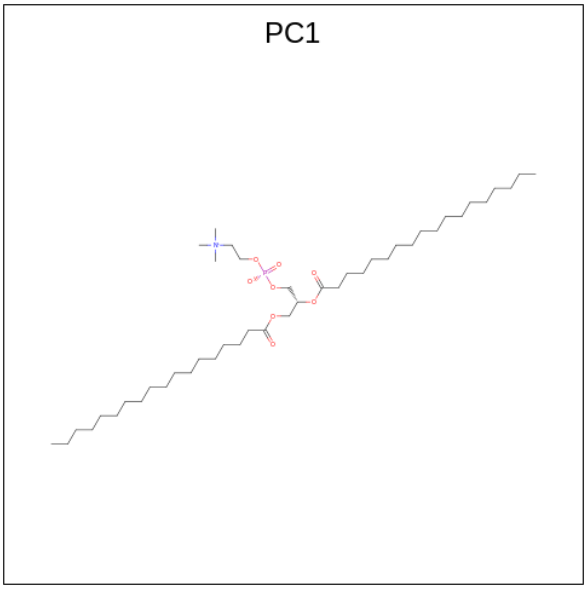


Mol	Chain	Residues	Atoms	AltConf
61	1A	1	Total Fe S 8 4 4	0
61	1A	1	Total Fe S 8 4 4	0
61	S7	1	Total Fe S 8 4 4	0
61	S8	1	Total Fe S 8 4 4	0
61	S8	1	Total Fe S 8 4 4	0
61	V1	1	Total Fe S 8 4 4	0

- Molecule 62 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
62	1A	1	Total K 1 1	0

- Molecule 63 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
63	A1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	A1	1	Total	C	H	N	O	P	0
			67	21	36	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	A9	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	AL	1	Total	C	H	N	O	P	0
			127	40	77	1	8	1	
63	AM	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	AM	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
63	AN	1	Total	C	H	N	O	P	0
			121	38	73	1	8	1	
63	B5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	B5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	C4	1	Total	C	H	N	O	P	0
			88	28	50	1	8	1	
63	E4	1	Total	C	H	N	O	P	0
			130	41	79	1	8	1	

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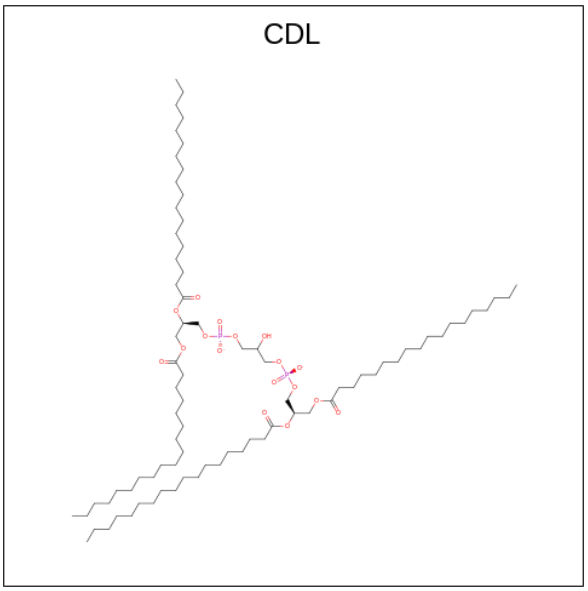
Mol	Chain	Residues	Atoms						AltConf
63	E8	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	E8	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	E8	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	E8	1	Total	C	H	N	O	P	0
			64	20	34	1	8	1	
63	ED	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	N1	1	Total	C	H	N	O	P	0
			124	39	75	1	8	1	
63	N1	1	Total	C	H	N	O	P	0
			94	30	54	1	8	1	
63	N2	1	Total	C	H	N	O	P	0
			85	27	48	1	8	1	
63	N3	1	Total	C	H	N	O	P	0
			103	32	61	1	8	1	
63	N4	1	Total	C	H	N	O	P	0
			91	29	52	1	8	1	
63	N4	1	Total	C	H	N	O	P	0
			73	23	40	1	8	1	
63	N5	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
63	N5	1	Total	C	H	N	O	P	0
			97	31	56	1	8	1	
63	N5	1	Total	C	H	N	O	P	0
			82	26	46	1	8	1	

- Molecule 64 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms					AltConf
64	A3	1	Total	C	H	O	P	0
			118	39	60	17	2	
64	AL	1	Total	C	H	O	P	0
			148	49	80	17	2	
64	AL	1	Total	C	H	O	P	0
			136	45	72	17	2	
64	AL	1	Total	C	H	O	P	0
			154	51	84	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	AM	1	Total	C	H	O	P	0
			163	53	91	17	2	
64	B3	1	Total	C	H	O	P	0
			139	46	74	17	2	
64	B5	1	Total	C	H	O	P	0
			118	39	60	17	2	
64	C4	1	Total	C	H	O	P	0
			235	75	141	17	2	
64	C4	1	Total	C	H	O	P	0
			151	50	82	17	2	
64	E6	1	Total	C	H	O	P	0
			136	45	72	17	2	
64	EA	1	Total	C	H	O	P	0
			121	40	62	17	2	
64	EA	1	Total	C	H	O	P	0
			109	36	54	17	2	

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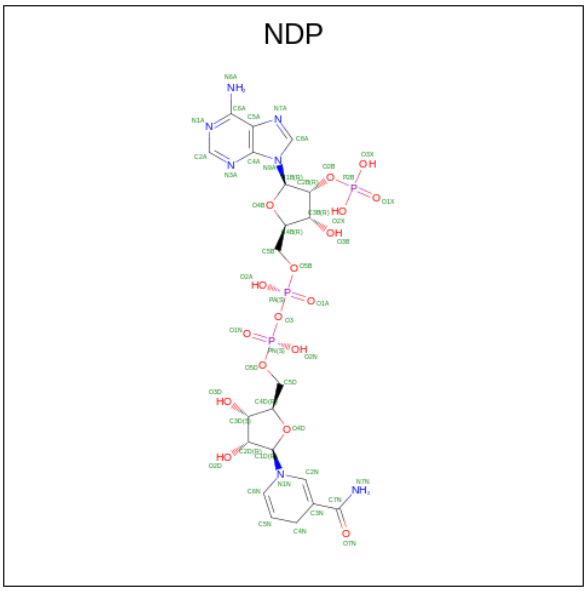
Mol	Chain	Residues	Atoms					AltConf
64	N4	1	Total	C	H	O	P	0
			247	79	149	17	2	
64	N5	1	Total	C	H	O	P	0
			157	51	87	17	2	
64	N5	1	Total	C	H	O	P	0
			229	74	136	17	2	
64	E7	1	Total	C	H	O	P	0
			148	49	80	17	2	

- Molecule 65 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

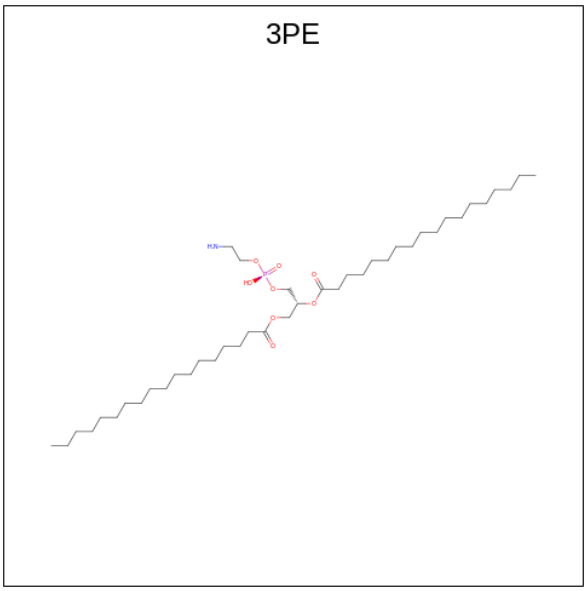


Mol	Chain	Residues	Atoms						AltConf
65	A9	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

- Molecule 66 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (three-letter code: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						AltConf
66	AB	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	
66	AC	1	Total	C	N	O	P	S	0
			36	25	2	7	1	1	

- Molecule 67 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
67	AN	1	Total	C	H	N	O	P	0
			132	41	81	1	8	1	

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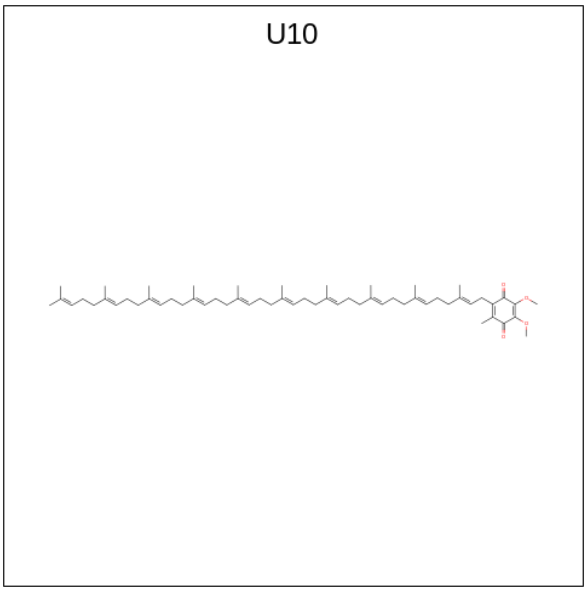
Mol	Chain	Residues	Atoms						AltConf
67	G1	1	Total	C	H	N	O	P	0
			96	30	56	1	8	1	
67	N4	1	Total	C	H	N	O	P	0
			96	31	55	1	8	1	
67	N5	1	Total	C	H	N	O	P	0
			132	41	81	1	8	1	

- Molecule 68 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

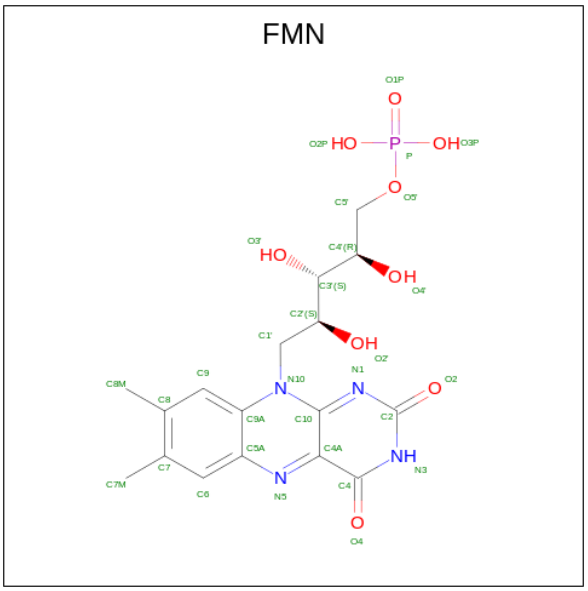


Mol	Chain	Residues	Atoms				AltConf
68	N4	1	Total	C	H	O	0
			98	39	55	4	

- Molecule 69 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
69	S6	1	Total	Zn	0
			1	1	
69	E7	1	Total	Zn	0
			1	1	

- Molecule 70 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



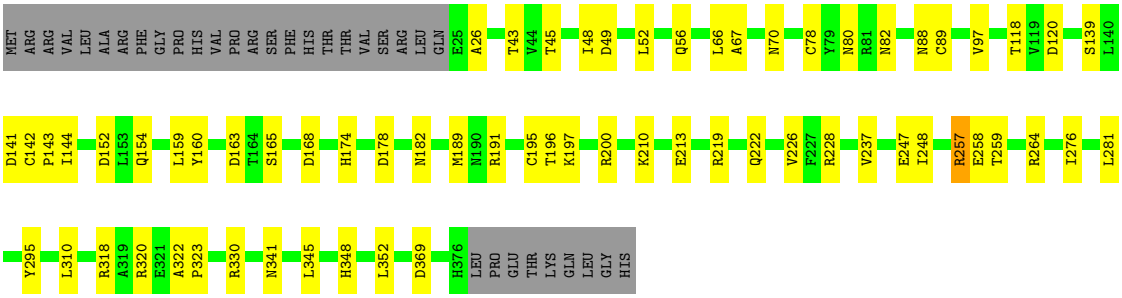
Mol	Chain	Residues	Atoms						AltConf
70	V1	1	Total	C	H	N	O	P	0
			50	17	19	4	9	1	

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. 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. 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.

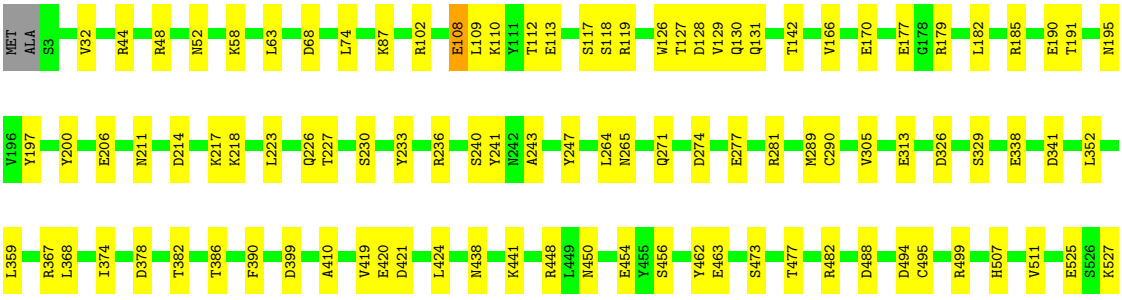
- Molecule 1: NDUS1A

Chain 1A:



- Molecule 2: NDUS1B

Chain 1B:

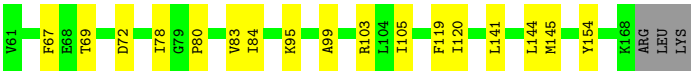


- Molecule 3: NADH dehydrogenase subunit 5

Chain 2B:

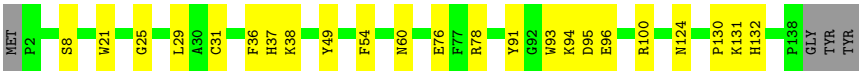
- Molecule 4: ND4L

Chain 4L:



• Molecule 5: NDUFA1

Chain A1:



• Molecule 6: NDUFA2

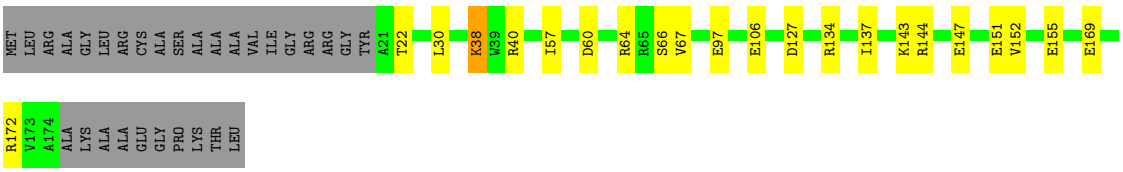
Chain A2:

• Molecule 7: NDUFA3

Chain A3:

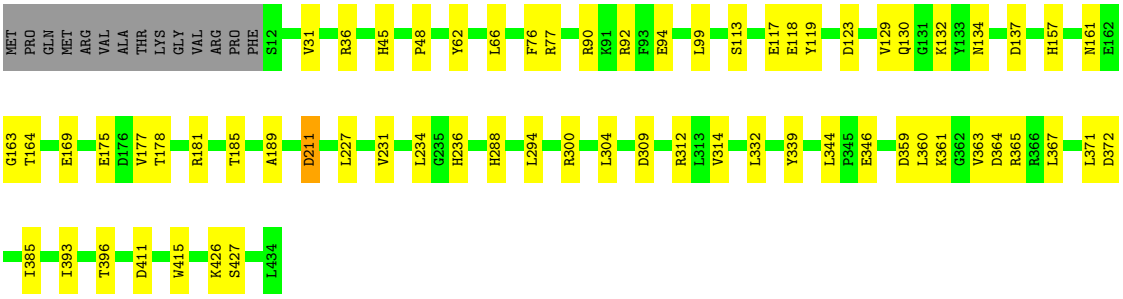
• Molecule 8: NDUFA5

Chain A5:



• Molecule 9: NDUFA6

Chain A6:

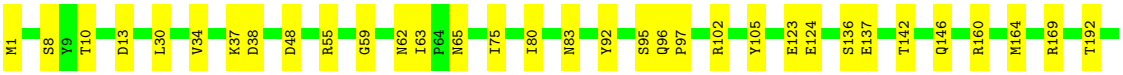


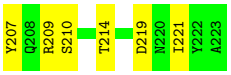
• Molecule 10: NDUFA7

Chain A7:

• Molecule 11: NDUFA8

Chain A8:



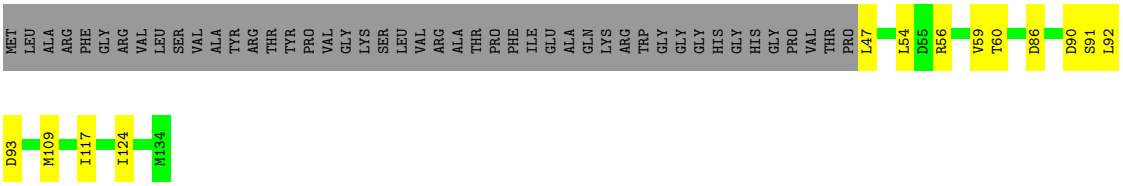


• Molecule 12: NDUFA9

Chain A9:

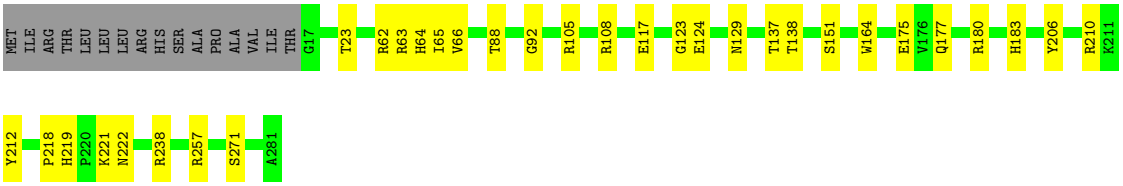
• Molecule 13: NDUFAB1-alpha

Chain AB:



• Molecule 14: NDUFA12

Chain AL:

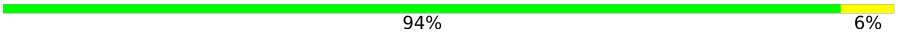


• Molecule 15: NDUFA13

Chain AM:

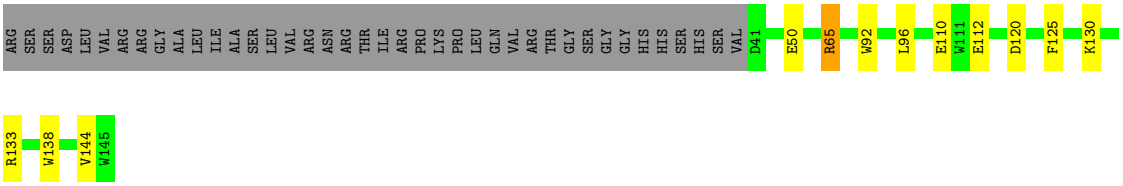
• Molecule 16: NDUFA11

Chain AN:



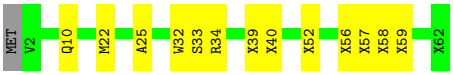
• Molecule 17: NDUFB2

Chain B2:



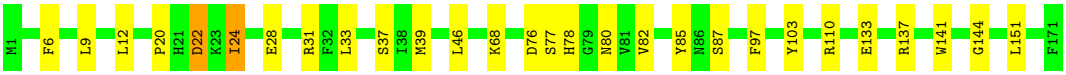
• Molecule 18: NDUFB3

Chain B3:



• Molecule 19: NDUFB4

Chain B4:

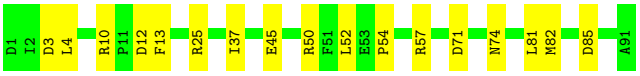


• Molecule 20: NDUFB5

Chain B5:

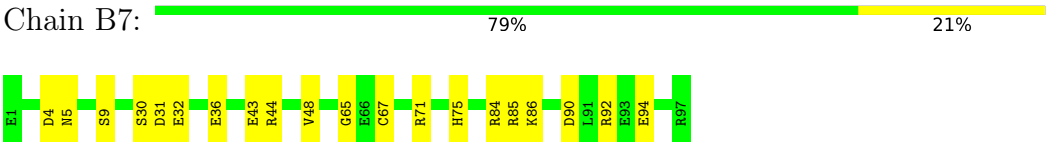
• Molecule 21: NDUFB6

Chain B6:



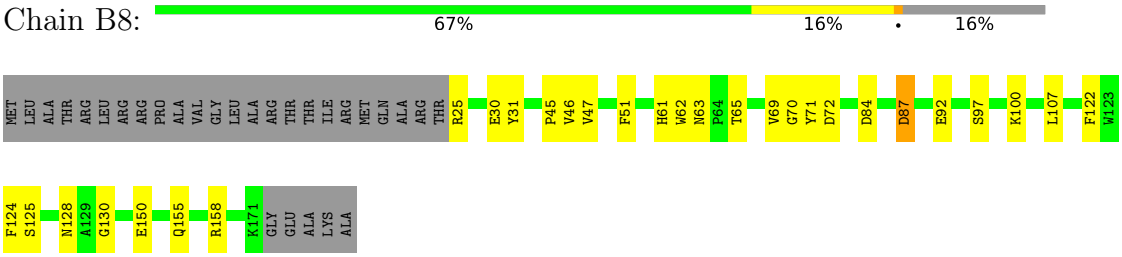
• Molecule 22: NDUFB7

Chain B7:



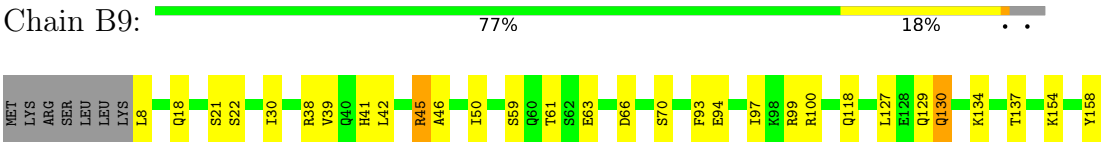
• Molecule 23: NDUFB8

Chain B8:



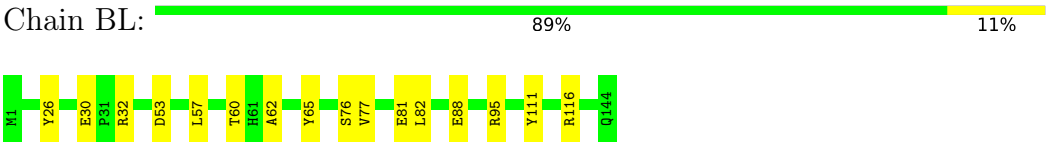
• Molecule 24: NDUFB9

Chain B9:



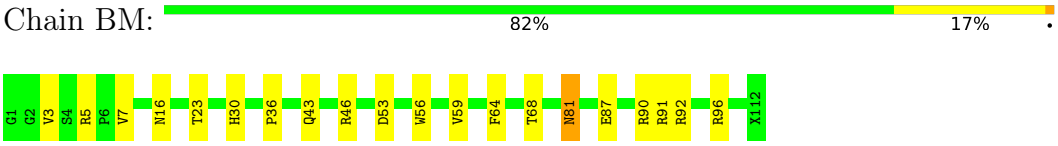
• Molecule 25: NDUFB10

Chain BL:



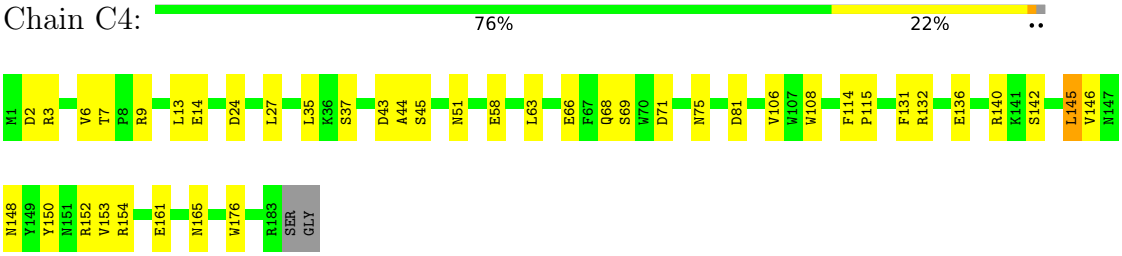
• Molecule 26: NDUFB11

Chain BM:



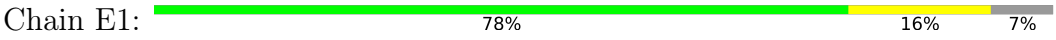
• Molecule 27: NDUFC2

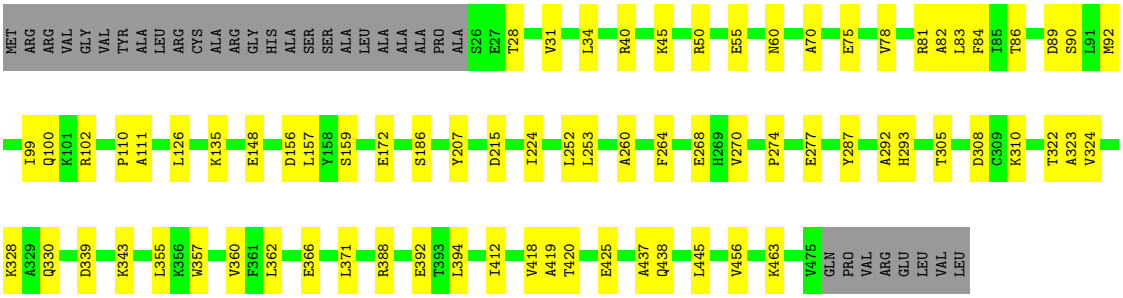
Chain C4:



• Molecule 28: NDUEG1

Chain E1:



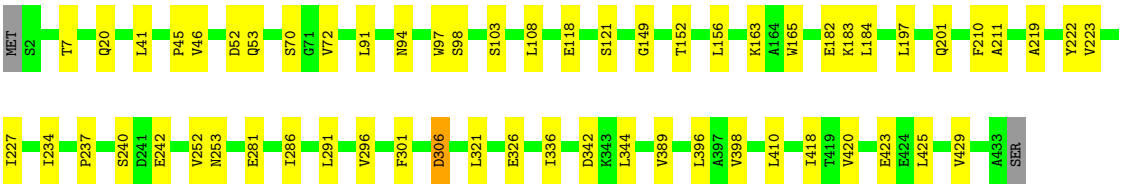


• Molecule 29: NDUEG2

Chain E2:

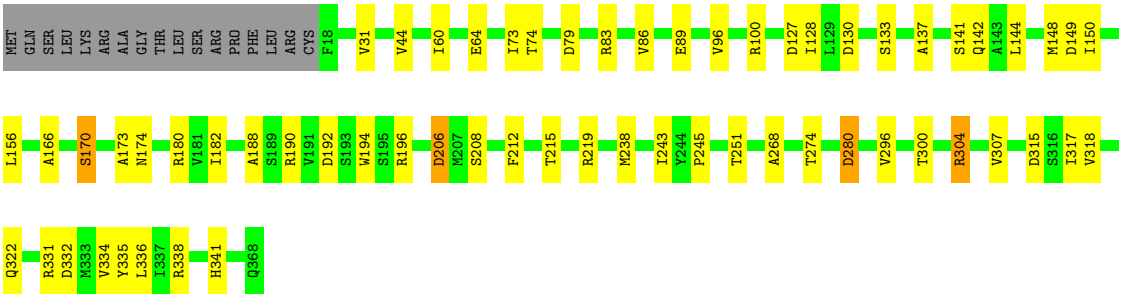
• Molecule 30: NDUEG3

Chain E3:



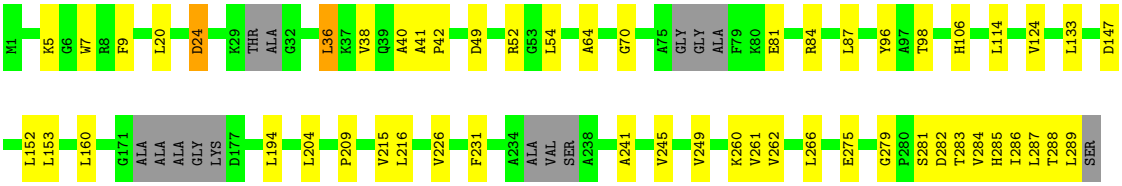
• Molecule 31: NDUEG4

Chain E4:



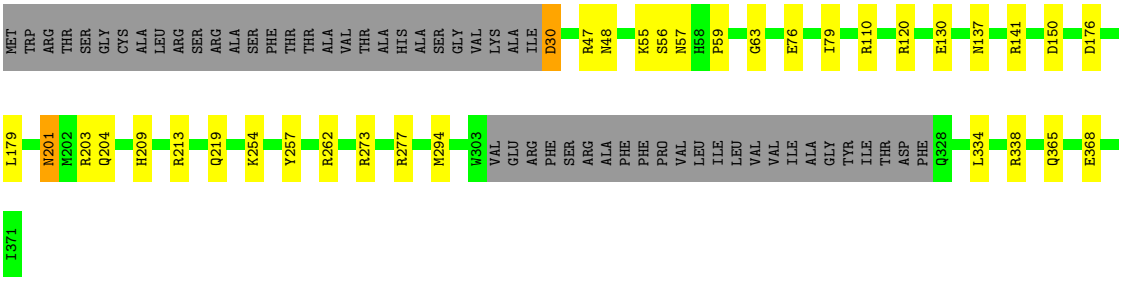
• Molecule 32: NDUEG5

Chain E5:



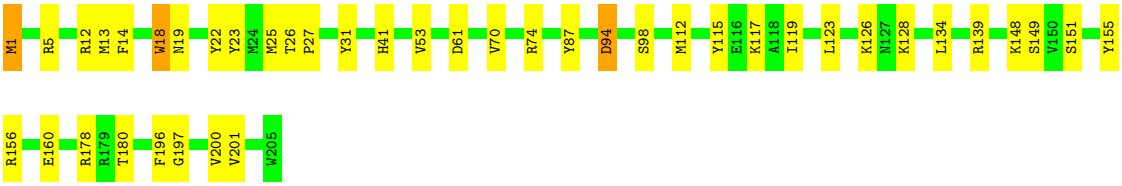
• Molecule 33: NDUEG6

Chain E6:



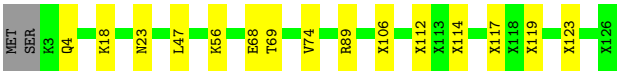
• Molecule 34: NDUEG8

Chain E8:



• Molecule 35: NDUEG10

Chain EA:

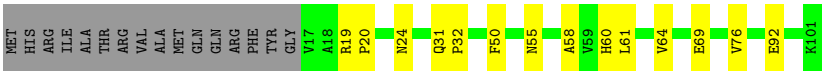


• Molecule 36: NDUEG11

Chain EB:

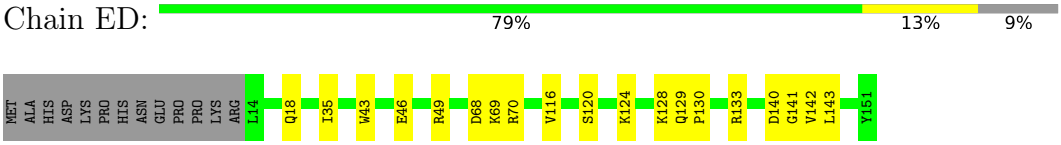
• Molecule 37: NDUEG12

Chain EC:



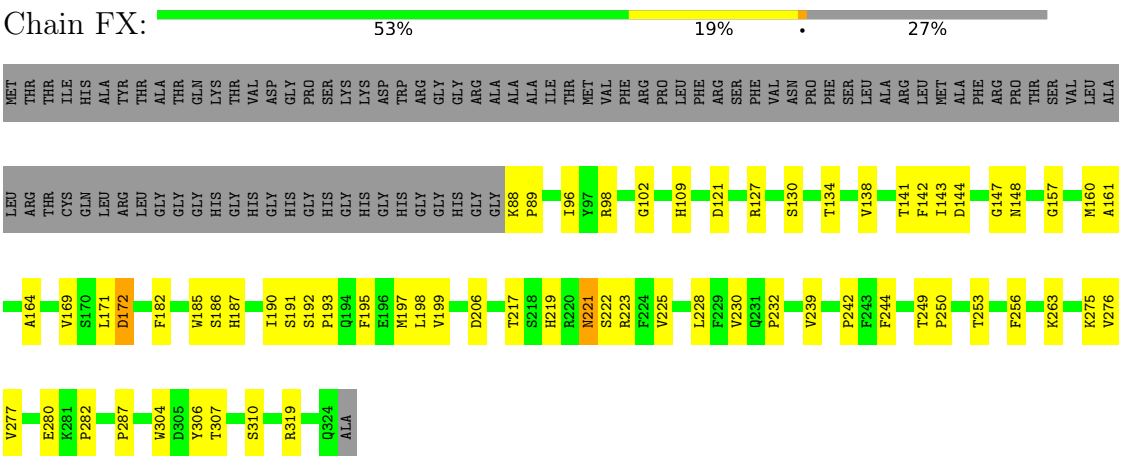
• Molecule 38: NDUEG13

Chain ED:



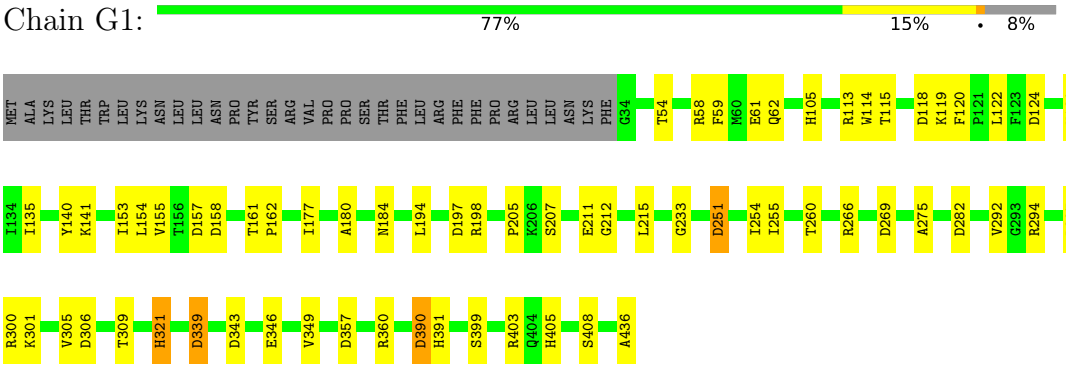
• Molecule 39: NDUFX

Chain FX:



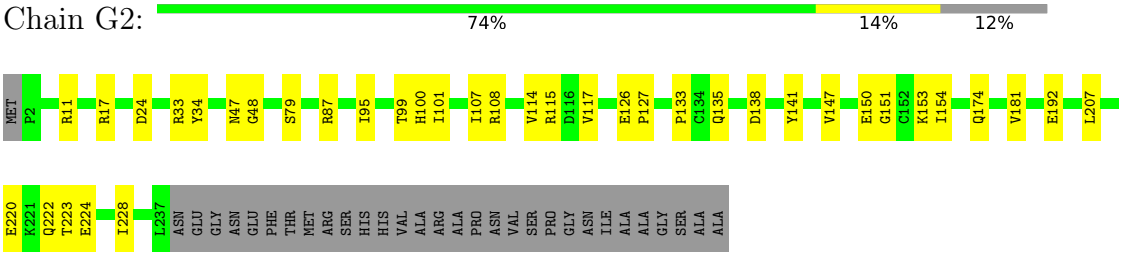
• Molecule 40: NDUCA1

Chain G1:



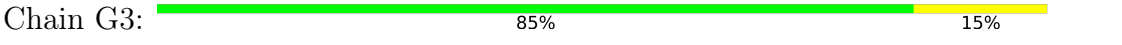
• Molecule 41: NDUCA2

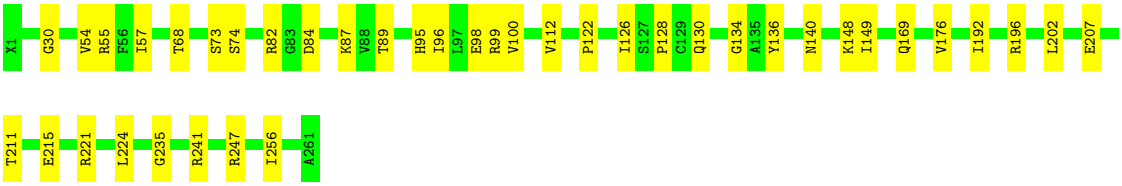
Chain G2:



• Molecule 42: NDUCA3

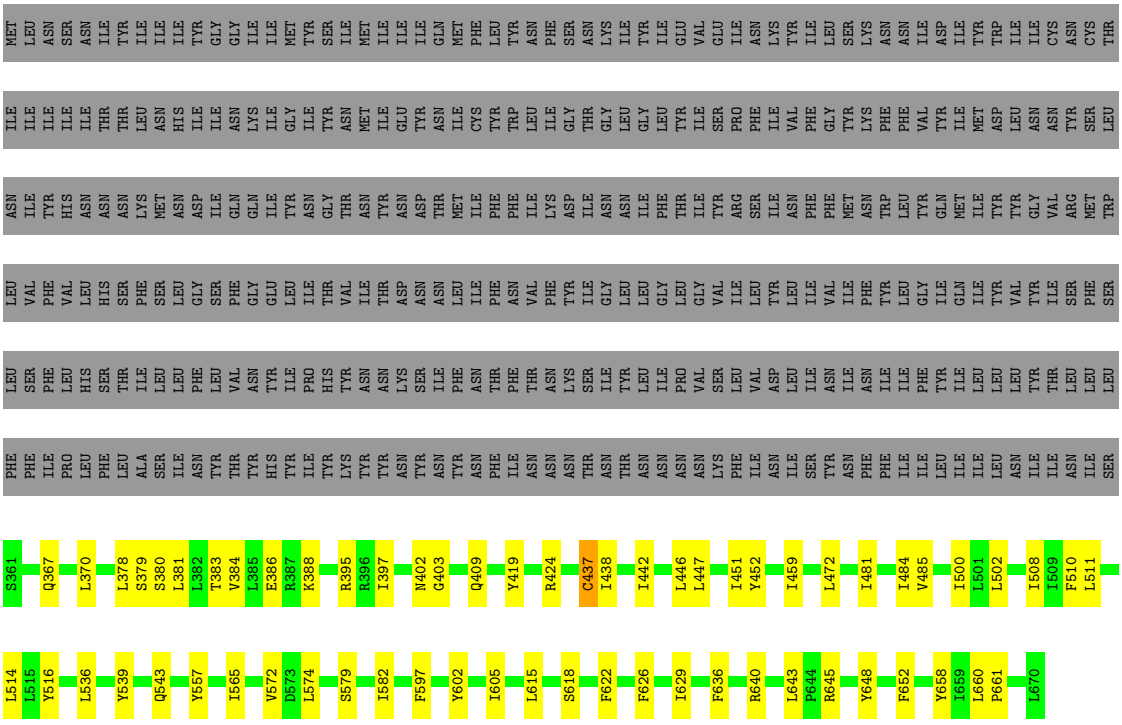
Chain G3:





• Molecule 43: ND1

Chain N1:

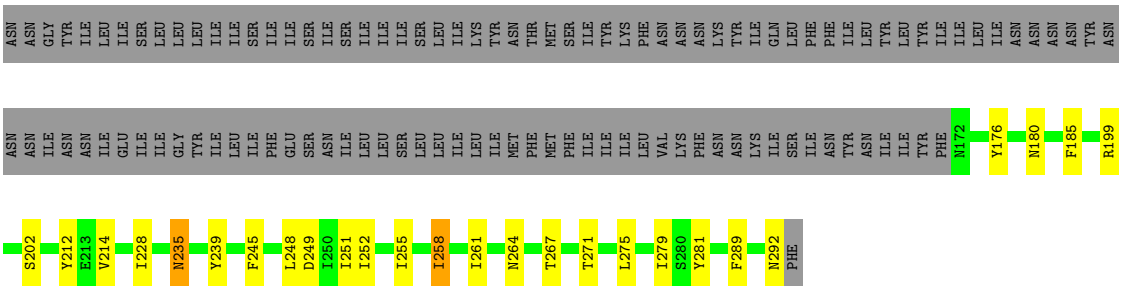


• Molecule 44: ND2A

Chain N2:

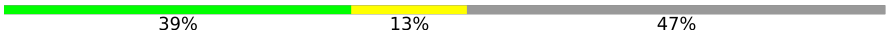
• Molecule 45: ND3

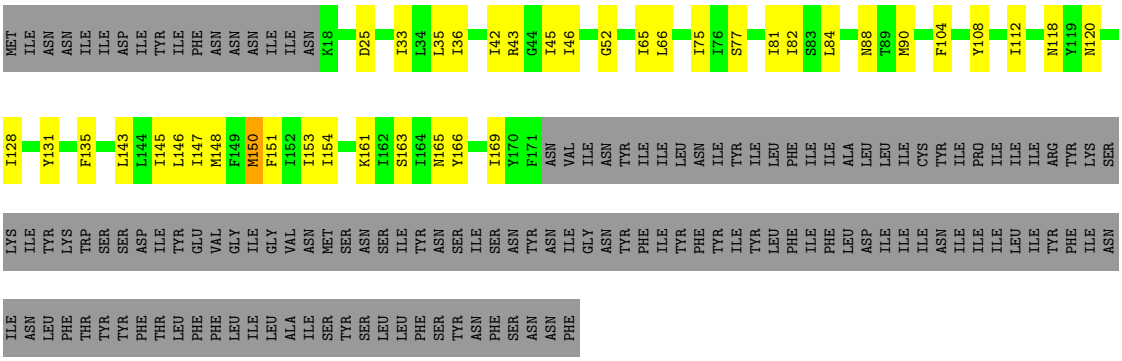
Chain N3:



• Molecule 45: ND3

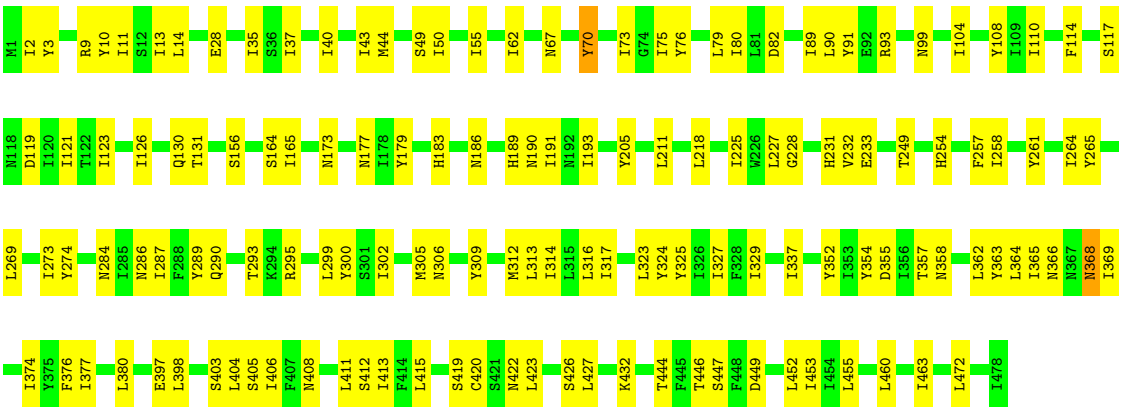
Chain N6:





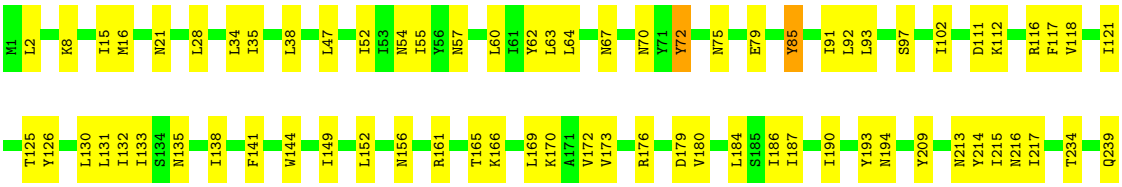
• Molecule 46: NADH-ubiquinone oxidoreductase chain 4

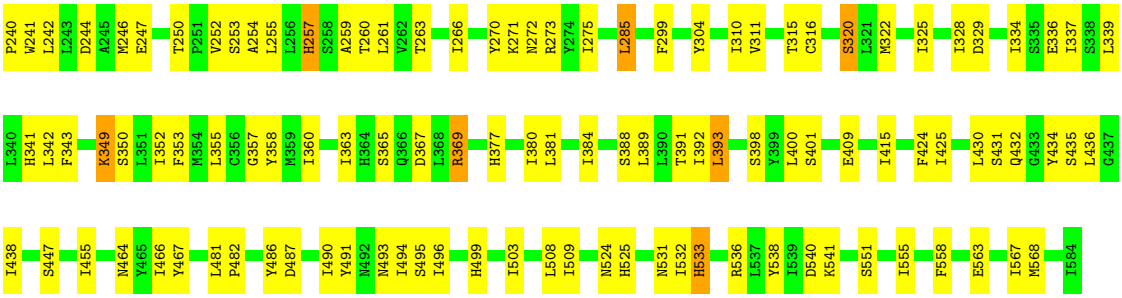
Chain N4:



• Molecule 47: ND5

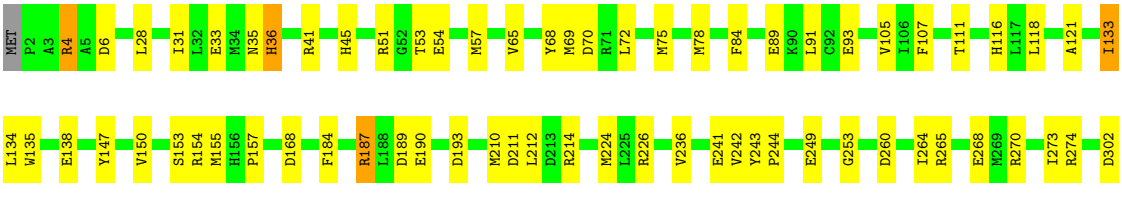
Chain N5:





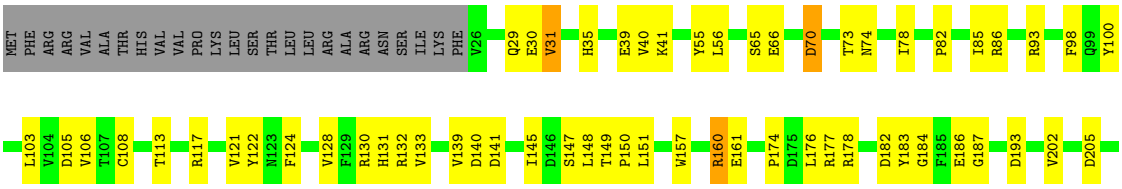
- Molecule 48: NDUFS2

Chain S2:



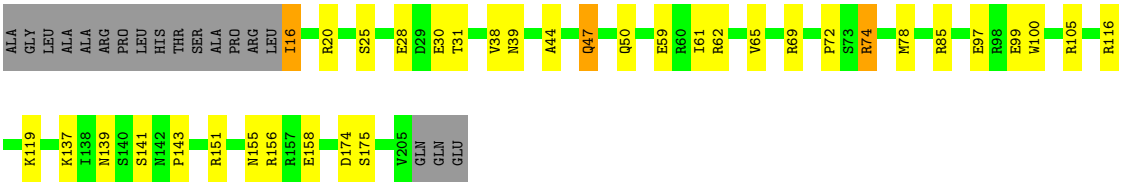
- Molecule 49: NDUFS3

Chain S3:



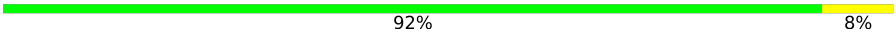
- Molecule 50: NDUFS4

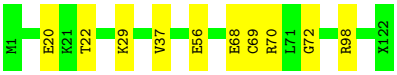
Chain S4:



- Molecule 51: NDUFS5

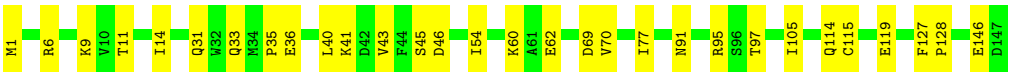
Chain S5:





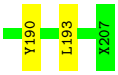
• Molecule 52: NDUFS6

Chain S6:



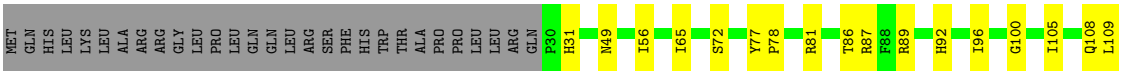
• Molecule 53: NDUFS7

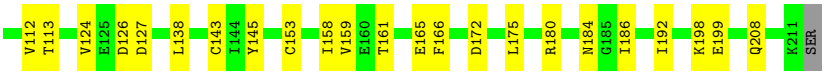
Chain S7:



• Molecule 54: NDUFS8

Chain S8:





• Molecule 55: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

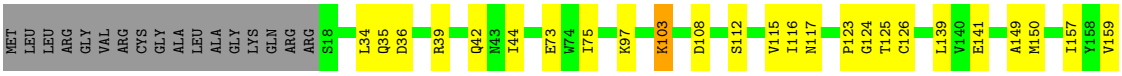
Chain U1:

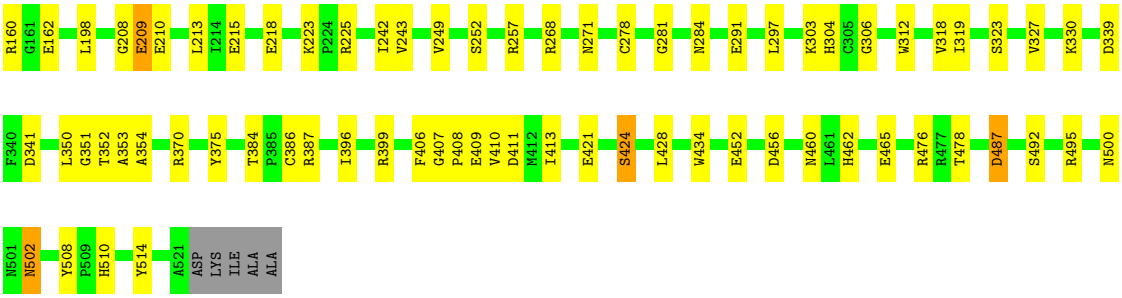
• Molecule 55: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

Chain U2:

• Molecule 56: NDUFV1

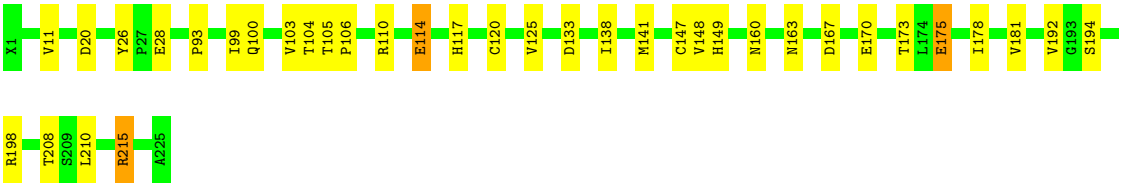
Chain V1:





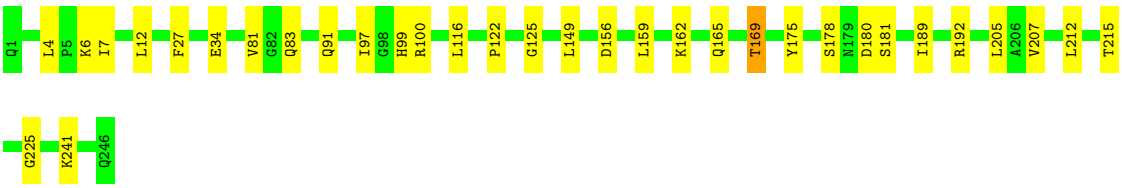
• Molecule 57: NDUFV2

Chain V2:



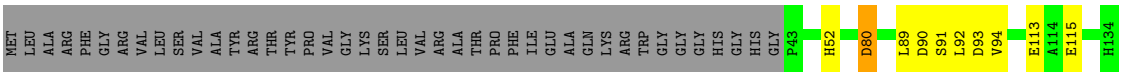
• Molecule 58: NDUEG7

Chain E7:



• Molecule 59: NDUFAB1-beta

Chain AC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	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, 3PE, U10, SF4, FMN, CDL, 2MR, ZMP, FES, NDP, ZN, PC1

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	0.30	0/2858	0.51	0/3878
2	1B	0.29	0/4306	0.50	0/5854
3	2B	0.31	0/958	0.42	0/1306
4	4L	0.31	0/924	0.43	0/1261
5	A1	0.26	0/1108	0.45	0/1511
6	A2	0.26	0/1530	0.49	0/2089
7	A3	0.28	0/1079	0.53	0/1453
8	A5	0.28	0/1282	0.49	0/1737
9	A6	0.26	0/3395	0.49	0/4608
10	A7	0.28	0/1194	0.53	0/1619
11	A8	0.28	0/1879	0.45	0/2543
12	A9	0.29	0/3920	0.50	0/5335
13	AB	0.27	0/704	0.42	0/951
14	AL	0.28	0/2317	0.52	0/3136
15	AM	0.29	0/1533	0.48	0/2079
16	AN	0.28	0/2382	0.47	0/3249
17	B2	0.28	0/947	0.43	0/1291
18	B3	0.29	0/326	0.50	0/441
19	B4	0.30	0/1419	0.48	0/1922
20	B5	0.30	0/1111	0.49	0/1505
21	B6	0.30	0/803	0.47	0/1087
22	B7	0.28	0/877	0.53	0/1172
23	B8	0.31	0/1273	0.43	0/1733
24	B9	0.30	0/1274	0.48	0/1728
25	BL	0.30	0/1266	0.49	0/1710
26	BM	0.31	0/876	0.54	0/1192
27	C4	0.28	0/1592	0.47	0/2158
28	E1	0.27	0/3596	0.47	0/4879
29	E2	0.27	0/3658	0.47	0/4983
30	E3	0.26	0/3320	0.46	0/4520
31	E4	0.27	0/2850	0.47	0/3884
32	E5	0.25	0/2004	0.49	0/2721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	E6	0.26	0/2750	0.46	0/3724
34	E8	0.29	0/1747	0.49	0/2367
35	EA	0.28	0/858	0.45	0/1163
36	EB	0.26	0/650	0.50	0/863
37	EC	0.27	0/676	0.45	0/925
38	ED	0.26	0/1176	0.49	0/1590
39	FX	0.30	0/2035	0.46	0/2763
40	G1	0.30	0/3234	0.50	0/4401
41	G2	0.28	0/1832	0.53	0/2476
42	G3	0.29	0/1957	0.52	0/2646
43	N1	0.29	0/2672	0.44	0/3639
44	N2	0.32	0/2582	0.42	0/3530
45	N3	0.32	0/1068	0.43	0/1456
45	N6	0.28	0/1275	0.43	0/1730
46	N4	0.32	0/4105	0.43	0/5594
47	N5	0.31	0/4963	0.44	0/6758
48	S2	0.32	0/3244	0.52	0/4403
49	S3	0.31	0/2112	0.51	0/2874
50	S4	0.28	0/1573	0.56	0/2107
51	S5	0.27	0/960	0.47	0/1291
52	S6	0.29	0/1232	0.51	0/1659
53	S7	0.30	0/1558	0.50	0/2120
54	S8	0.32	0/1485	0.51	0/2010
56	V1	0.28	0/3990	0.49	0/5394
57	V2	0.29	0/1787	0.47	0/2428
58	E7	0.26	0/1931	0.48	0/2618
59	AC	0.28	0/736	0.42	0/1000
All	All	0.29	0/112749	0.48	0/153064

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2801	2700	2710	45	0
2	1B	4198	4159	4175	71	0
3	2B	1070	989	1008	24	0
4	4L	890	878	880	20	0
5	A1	1071	1026	1030	15	0
6	A2	1493	1474	1478	15	0
7	A3	1050	1039	1041	13	0
8	A5	1261	1248	1251	14	0
9	A6	3328	3280	3293	52	0
10	A7	1154	1118	1123	22	0
11	A8	1822	1726	1736	32	0
12	A9	3829	3850	3857	54	0
13	AB	694	673	677	13	0
14	AL	2237	2172	2180	26	0
15	AM	1487	1448	1452	24	0
16	AN	2306	2267	2275	13	0
17	B2	913	857	858	13	0
18	B3	449	309	311	10	0
19	B4	1377	1358	1364	25	0
20	B5	1112	1069	1075	15	0
21	B6	773	747	751	19	0
22	B7	857	835	841	13	0
23	B8	1224	1127	1136	23	0
24	B9	1236	1207	1212	29	0
25	BL	1227	1179	1185	13	0
26	BM	910	827	830	21	0
27	C4	1545	1517	1519	29	0
28	E1	3512	3496	3510	47	0
29	E2	3563	3540	3554	45	0
30	E3	3255	3263	3279	44	0
31	E4	2770	2732	2742	49	0
32	E5	1977	2069	2075	42	0
33	E6	2674	2554	2562	25	0
34	E8	1691	1663	1668	32	0
35	EA	961	832	837	10	0
36	EB	774	631	636	9	0
37	EC	660	663	666	10	0
38	ED	1142	1131	1134	14	0
39	FX	1967	1849	1858	53	0
40	G1	3147	2999	3015	56	0
41	G2	1804	1846	1850	29	0
42	G3	1961	1944	1950	34	0
43	N1	2605	2726	2729	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	N2	2512	2589	2592	62	0
45	N3	1037	1057	1057	22	0
45	N6	1257	1385	1385	38	0
46	N4	4001	4214	4224	107	0
47	N5	4837	5032	5046	145	0
48	S2	3173	3101	3114	68	0
49	S3	2050	1928	1936	55	0
50	S4	1536	1502	1505	30	0
51	S5	991	895	898	7	0
52	S6	1200	1192	1198	22	0
53	S7	1545	1500	1503	24	0
54	S8	1451	1392	1397	38	0
55	U1	60	16	19	1	0
55	U2	60	16	17	1	0
56	V1	3897	3827	3837	71	0
57	V2	1759	1701	1711	24	0
58	E7	1888	1892	1903	23	0
59	AC	721	697	702	11	0
60	1A	4	0	0	0	0
60	V2	4	0	0	0	0
61	1A	16	0	0	0	0
61	S7	8	0	0	0	0
61	S8	16	0	0	5	0
61	V1	8	0	0	1	0
62	1A	1	0	0	0	0
63	A1	80	111	111	3	0
63	A9	66	80	80	1	0
63	AL	50	77	77	0	0
63	AM	97	148	148	1	0
63	AN	48	73	73	0	0
63	B5	108	176	176	2	0
63	C4	38	50	50	1	0
63	E4	51	79	79	0	0
63	E8	171	250	250	2	0
63	ED	54	88	88	1	0
63	N1	89	129	129	0	0
63	N2	37	48	48	1	0
63	N3	42	61	61	0	0
63	N4	72	92	92	2	0
63	N5	131	190	190	1	0
64	A3	58	60	60	1	0
64	AL	202	236	236	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	AM	216	273	273	10	0
64	B3	65	74	74	1	0
64	B5	58	60	60	1	0
64	C4	163	223	223	1	0
64	E6	64	72	72	0	0
64	E7	68	80	80	0	0
64	EA	114	116	116	1	0
64	N4	98	149	149	4	0
64	N5	163	223	223	4	0
65	A9	48	26	26	3	0
66	AB	36	0	47	6	0
66	AC	36	0	47	15	0
67	AN	51	81	82	0	0
67	G1	40	56	57	2	0
67	N4	41	55	56	0	0
67	N5	51	81	82	0	0
68	N4	43	55	55	5	0
69	E7	1	0	0	0	0
69	S6	1	0	0	0	0
70	V1	31	19	19	0	0
All	All	113591	112544	113046	1574	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 7.

All (1574) 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)
30:E3:222:TYR:HH	37:EC:60:HIS:HE2	1.06	0.99
32:E5:287:LEU:O	32:E5:289:LEU:N	1.97	0.97
10:A7:105:SER:O	49:S3:130:ARG:NH1	2.02	0.93
46:N4:293:THR:HG21	46:N4:365:ILE:HD11	1.50	0.91
7:A3:17:HIS:ND1	31:E4:206:ASP:OD1	2.05	0.90
47:N5:255:LEU:O	47:N5:260:THR:OG1	1.90	0.90
17:B2:120:ASP:OD2	17:B2:130:LYS:NZ	2.04	0.90
9:A6:45:HIS:NE2	9:A6:117:GLU:OE1	2.05	0.89
6:A2:10:SER:OG	30:E3:182:GLU:OE2	1.92	0.88
46:N4:80:ILE:HD11	46:N4:337:ILE:HG23	1.55	0.88
11:A8:214:THR:OG1	11:A8:219:ASP:OD2	1.91	0.87
52:S6:91:ASN:ND2	52:S6:95:ARG:O	2.08	0.87
56:V1:424:SER:OG	61:V1:580:SF4:S2	2.31	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:153:SER:OG	48:S2:155:MET:O	1.93	0.87
13:AB:92:LEU:HD13	66:AB:150:ZMP:H20A	1.58	0.86
46:N4:43:ILE:HD13	46:N4:472:LEU:HD21	1.57	0.86
56:V1:452:GLU:OE2	56:V1:508:TYR:OH	1.93	0.85
48:S2:116:HIS:NE2	48:S2:268:GLU:OE1	2.10	0.84
2:1B:421:ASP:OD2	2:1B:462:TYR:OH	1.96	0.84
17:B2:50:GLU:O	38:ED:70:ARG:NH2	2.11	0.84
7:A3:104:GLU:N	7:A3:104:GLU:OE1	2.11	0.84
14:AL:108:ARG:NH1	43:N1:403:GLY:O	2.10	0.83
34:E8:87:TYR:OH	64:N5:603:CDL:OA4	1.95	0.83
48:S2:111:THR:HG22	48:S2:147:TYR:OH	1.78	0.83
30:E3:53:GLN:NE2	30:E3:94:ASN:OD1	2.11	0.83
52:S6:41:LYS:O	52:S6:45:SER:OG	1.94	0.83
15:AM:74:ARG:NH2	43:N1:516:TYR:O	2.12	0.83
31:E4:238:MET:O	31:E4:304:ARG:NH1	2.11	0.83
49:S3:70:ASP:OD1	49:S3:73:THR:OG1	1.97	0.83
16:AN:248:ILE:O	27:C4:154:ARG:NH2	2.10	0.83
43:N1:514:LEU:O	43:N1:539:TYR:OH	1.96	0.83
41:G2:126:GLU:OE2	41:G2:141:TYR:OH	1.96	0.83
33:E6:254:LYS:NZ	53:S7:40:LEU:O	2.12	0.82
46:N4:67:ASN:N	46:N4:119:ASP:OD2	2.11	0.82
2:1B:399:ASP:OD2	12:A9:102:SER:OG	1.95	0.82
33:E6:120:ARG:NH1	52:S6:69:ASP:OD2	2.12	0.82
33:E6:76:GLU:OE1	33:E6:110:ARG:NH2	2.11	0.82
2:1B:214:ASP:OD2	2:1B:218:LYS:NZ	2.12	0.82
34:E8:123:LEU:O	34:E8:128:LYS:NZ	2.12	0.82
40:G1:133:ARG:NH1	42:G3:215:GLU:OE2	2.12	0.81
47:N5:355:LEU:HD11	47:N5:384:ILE:HG22	1.62	0.81
2:1B:217:LYS:NZ	2:1B:473:SER:OG	2.14	0.81
2:1B:110:LYS:NZ	2:1B:326:ASP:OD2	2.13	0.81
19:B4:85:TYR:OH	67:G1:516:3PE:O14	1.99	0.81
44:N2:32:GLU:N	44:N2:32:GLU:OE1	2.14	0.81
21:B6:57:ARG:NH1	21:B6:82:MET:SD	2.53	0.81
24:B9:66:ASP:OD2	34:E8:41:HIS:NE2	2.14	0.81
24:B9:63:GLU:OE1	34:E8:22:TYR:OH	1.98	0.81
11:A8:13:ASP:OD1	20:B5:115:ASN:ND2	2.13	0.81
12:A9:95:GLU:OE1	50:S4:137:LYS:NZ	2.14	0.81
1:1A:26:ALA:O	2:1B:448:ARG:NE	2.15	0.80
10:A7:46:ALA:O	15:AM:31:ARG:NH1	2.14	0.80
33:E6:137:ASN:OD1	33:E6:141:ARG:NH1	2.15	0.80
27:C4:45:SER:O	27:C4:51:ASN:ND2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:107:PHE:O	48:S2:111:THR:HG23	1.80	0.80
11:A8:63:ILE:O	11:A8:95:SER:OG	1.99	0.80
50:S4:25:SER:OG	50:S4:30:GLU:OE2	1.99	0.80
25:BL:111:TYR:OH	47:N5:193:TYR:O	1.98	0.80
1:1A:165:SER:OG	1:1A:168:ASP:OD1	1.99	0.79
11:A8:102:ARG:NH1	11:A8:221:ILE:O	2.14	0.79
15:AM:46:ARG:NH2	31:E4:192:ASP:OD2	2.16	0.79
30:E3:118:GLU:OE1	30:E3:118:GLU:N	2.15	0.79
14:AL:212:TYR:OH	54:S8:175:LEU:O	1.99	0.79
34:E8:156:ARG:NH2	34:E8:180:THR:O	2.16	0.79
12:A9:230:ARG:NH1	33:E6:150:ASP:OD1	2.15	0.79
31:E4:128:ILE:HD11	31:E4:156:LEU:HD13	1.64	0.78
2:1B:113:GLU:OE2	50:S4:151:ARG:NH2	2.17	0.78
12:A9:161:ARG:NH1	65:A9:559:NDP:O1X	2.17	0.78
27:C4:132:ARG:NH1	27:C4:136:GLU:OE1	2.16	0.78
43:N1:386:GLU:OE2	43:N1:640:ARG:NH1	2.16	0.78
56:V1:411:ASP:OD2	56:V1:510:HIS:NE2	2.16	0.78
40:G1:133:ARG:NH2	40:G1:339:ASP:OD1	2.17	0.78
40:G1:294:ARG:HG2	41:G2:181:VAL:HG21	1.65	0.78
47:N5:97:SER:OG	47:N5:125:THR:HG21	1.84	0.78
40:G1:207:SER:OG	40:G1:233:GLY:O	2.01	0.77
28:E1:172:GLU:OE1	30:E3:183:LYS:NZ	2.17	0.77
46:N4:289:TYR:OH	47:N5:551:SER:OG	1.97	0.77
1:1A:222:GLN:OE1	56:V1:223:LYS:NZ	2.16	0.77
48:S2:226:ARG:NH2	48:S2:268:GLU:OE2	2.16	0.77
32:E5:41:ALA:O	32:E5:287:LEU:O	2.01	0.77
9:A6:132:LYS:NZ	49:S3:184:GLY:O	2.17	0.77
15:AM:47:TYR:OH	48:S2:193:ASP:OD1	2.02	0.77
35:EA:112:UNK:O	35:EA:114:UNK:N	2.18	0.77
29:E2:339:GLU:OE2	29:E2:358:ARG:NH1	2.18	0.76
1:1A:257:ARG:NH1	14:AL:271:SER:OG	2.18	0.76
25:BL:81:GLU:OE2	26:BM:92:ARG:NH1	2.18	0.76
30:E3:222:TYR:OH	37:EC:60:HIS:NE2	2.14	0.76
35:EA:18:LYS:O	35:EA:23:ASN:ND2	2.18	0.76
2:1B:58:LYS:NZ	2:1B:495:CYS:SG	2.56	0.76
29:E2:170:ASP:OD1	29:E2:170:ASP:N	2.18	0.76
38:ED:46:GLU:OE1	38:ED:49:ARG:NH1	2.19	0.76
40:G1:133:ARG:NH2	41:G2:34:TYR:O	2.19	0.76
24:B9:137:THR:HG22	26:BM:23:THR:HG21	1.68	0.76
2:1B:223:LEU:O	2:1B:227:THR:OG1	2.03	0.76
2:1B:118:SER:OG	2:1B:438:ASN:ND2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:G2:150:GLU:OE1	41:G2:150:GLU:N	2.18	0.76
24:B9:70:SER:OG	34:E8:5:ARG:NH2	2.18	0.75
40:G1:211:GLU:OE1	40:G1:211:GLU:N	2.19	0.75
57:V2:160:ASN:OD1	57:V2:163:ASN:ND2	2.19	0.75
27:C4:2:ASP:OD1	27:C4:3:ARG:N	2.19	0.75
33:E6:150:ASP:OD2	33:E6:262:ARG:NH1	2.20	0.75
9:A6:31:VAL:HG11	39:FX:141:THR:HG21	1.67	0.75
12:A9:392:GLU:OE1	12:A9:392:GLU:N	2.18	0.75
22:B7:30:SER:OG	22:B7:32:GLU:OE1	2.04	0.75
58:E7:165:GLN:O	58:E7:169:THR:OG1	2.04	0.75
26:BM:43:GLN:NE2	46:N4:449:ASP:OD1	2.20	0.75
39:FX:130:SER:OG	40:G1:297:ARG:NH2	2.19	0.75
54:S8:198:LYS:NZ	54:S8:199:GLU:OE2	2.19	0.75
2:1B:63:LEU:HD11	2:1B:352:LEU:HD12	1.69	0.74
28:E1:28:THR:O	29:E2:229:ARG:NH1	2.20	0.74
2:1B:102:ARG:O	2:1B:200:TYR:OH	2.04	0.74
14:AL:206:TYR:OH	53:S7:190:TYR:OH	2.03	0.74
56:V1:284:ASN:ND2	56:V1:306:GLY:O	2.20	0.74
46:N4:447:SER:OG	46:N4:449:ASP:OD2	2.05	0.74
12:A9:18:LEU:O	12:A9:50:LYS:NZ	2.17	0.74
33:E6:365:GLN:N	33:E6:365:GLN:OE1	2.20	0.74
12:A9:442:ARG:NH2	43:N1:484:ILE:O	2.20	0.74
18:B3:22:MET:SD	18:B3:34:ARG:NH1	2.60	0.74
46:N4:408:ASN:O	46:N4:412:SER:OG	2.06	0.74
49:S3:174:PRO:O	50:S4:20:ARG:NH1	2.21	0.74
27:C4:71:ASP:O	27:C4:75:ASN:ND2	2.21	0.74
29:E2:187:THR:HG22	29:E2:189:ASP:H	1.52	0.74
47:N5:358:TYR:OH	47:N5:464:ASN:OD1	2.05	0.74
56:V1:421:GLU:OE2	56:V1:434:TRP:NE1	2.20	0.74
24:B9:100:ARG:NH2	34:E8:31:TYR:O	2.21	0.73
39:FX:190:ILE:HG21	39:FX:198:LEU:HD11	1.70	0.73
43:N1:419:TYR:O	45:N3:199:ARG:NH2	2.20	0.73
31:E4:64:GLU:N	31:E4:64:GLU:OE1	2.21	0.73
4:4L:141:LEU:HB3	44:N2:116:VAL:HG11	1.70	0.73
10:A7:134:TYR:OH	31:E4:174:ASN:OD1	2.04	0.73
49:S3:93:ARG:NH1	49:S3:151:LEU:O	2.22	0.73
2:1B:48:ARG:NH1	6:A2:163:ASP:OD1	2.21	0.73
22:B7:67:CYS:SG	22:B7:71:ARG:NH1	2.61	0.73
47:N5:367:ASP:OD2	47:N5:369:ARG:NH1	2.22	0.73
34:E8:13:MET:O	34:E8:23:TYR:OH	2.04	0.73
34:E8:94:ASP:OD1	34:E8:117:LYS:NZ	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A8:92:TYR:OH	11:A8:136:SER:OG	2.03	0.73
5:A1:49:TYR:OH	11:A8:83:ASN:ND2	2.20	0.73
9:A6:92:ARG:HB3	66:AB:150:ZMP:H7A	1.71	0.72
26:BM:87:GLU:OE2	26:BM:91:ARG:NE	2.19	0.72
48:S2:338:GLU:OE2	49:S3:132:ARG:NH2	2.22	0.72
64:A3:201:CDL:OA3	64:A3:201:CDL:O1	2.07	0.72
42:G3:235:GLY:O	45:N6:161:LYS:NZ	2.23	0.72
48:S2:308:GLU:N	48:S2:308:GLU:OE1	2.23	0.72
39:FX:219:HIS:N	39:FX:222:SER:OG	2.23	0.72
56:V1:35:GLN:N	56:V1:35:GLN:OE1	2.22	0.72
2:1B:68:ASP:OD1	6:A2:14:ARG:NH2	2.23	0.72
3:2B:95:SER:OG	23:B8:31:TYR:O	2.08	0.72
11:A8:209:ARG:NH1	15:AM:83:ASP:OD1	2.23	0.72
45:N3:251:ILE:CD1	45:N3:279:ILE:HD11	2.19	0.72
22:B7:84:ARG:NH1	55:U2:7:UNK:O	2.22	0.72
48:S2:105:VAL:HG21	48:S2:242:VAL:HG22	1.72	0.72
25:BL:30:GLU:OE1	25:BL:30:GLU:N	2.22	0.72
16:AN:180:ARG:NH1	39:FX:206:ASP:OD1	2.22	0.71
40:G1:357:ASP:OD2	40:G1:360:ARG:NE	2.23	0.71
56:V1:462:HIS:ND1	56:V1:465:GLU:OE1	2.17	0.71
28:E1:392:GLU:N	28:E1:392:GLU:OE1	2.24	0.71
40:G1:118:ASP:O	40:G1:408:SER:OG	2.04	0.71
2:1B:374:ILE:HG21	2:1B:382:THR:HG21	1.72	0.71
2:1B:87:LYS:NZ	2:1B:240:SER:OG	2.23	0.71
46:N4:9:ARG:NH2	46:N4:70:TYR:OH	2.24	0.71
56:V1:36:ASP:O	57:V2:215:ARG:NH1	2.24	0.71
34:E8:115:TYR:CZ	34:E8:119:ILE:HD11	2.26	0.71
38:ED:18:GLN:N	38:ED:18:GLN:OE1	2.23	0.71
54:S8:165:GLU:N	54:S8:165:GLU:OE1	2.24	0.70
2:1B:277:GLU:O	2:1B:281:ARG:NH2	2.25	0.70
22:B7:94:GLU:OE2	58:E7:100:ARG:NH2	2.23	0.70
7:A3:5:GLU:OE1	10:A7:116:ARG:NH1	2.23	0.70
45:N3:245:PHE:HD2	45:N6:81:ILE:HD11	1.56	0.70
45:N6:163:SER:O	45:N6:165:ASN:ND2	2.25	0.70
5:A1:95:ASP:OD1	11:A8:160:ARG:NH2	2.25	0.70
9:A6:175:GLU:OE2	9:A6:178:THR:OG1	2.09	0.70
47:N5:272:ASN:O	47:N5:275:ILE:HG22	1.92	0.70
1:1A:152:ASP:OD1	49:S3:233:TRP:NE1	2.24	0.70
33:E6:47:ARG:NH1	33:E6:48:ASN:OD1	2.25	0.70
24:B9:21:SER:OG	24:B9:118:GLN:OE1	2.09	0.69
25:BL:88:GLU:OE1	36:EB:79:SER:OG	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AB:109:MET:HE1	13:AB:117:ILE:HD12	1.75	0.69
49:S3:182:ASP:OD1	49:S3:183:TYR:N	2.26	0.69
37:EC:20:PRO:O	37:EC:24:ASN:ND2	2.25	0.69
48:S2:249:GLU:OE1	48:S2:274:ARG:NH1	2.25	0.69
33:E6:55:LYS:NZ	52:S6:46:ASP:OD1	2.21	0.69
47:N5:337:ILE:HD11	47:N5:491:TYR:CG	2.27	0.69
56:V1:249:VAL:O	56:V1:252:SER:OG	2.10	0.69
29:E2:135:THR:OG1	29:E2:440:GLY:O	2.05	0.69
24:B9:18:GLN:NE2	24:B9:22:SER:O	2.26	0.69
48:S2:89:GLU:O	48:S2:93:GLU:N	2.25	0.69
9:A6:45:HIS:ND1	9:A6:113:SER:OG	2.25	0.69
17:B2:92:TRP:CH2	17:B2:96:LEU:HD11	2.28	0.69
21:B6:12:ASP:OD2	47:N5:116:ARG:NH2	2.26	0.69
23:B8:84:ASP:OD1	47:N5:166:LYS:NZ	2.26	0.69
31:E4:180:ARG:NH2	31:E4:274:THR:OG1	2.26	0.69
10:A7:28:GLY:O	14:AL:64:HIS:NE2	2.26	0.69
27:C4:37:SER:OG	27:C4:58:GLU:OE2	2.03	0.69
11:A8:8:SER:OG	44:N2:95:ASN:O	2.11	0.69
56:V1:281:GLY:O	57:V2:110:ARG:NH1	2.26	0.68
1:1A:143:PRO:O	1:1A:264:ARG:NH2	2.27	0.68
48:S2:75:MET:SD	48:S2:118:LEU:HD22	2.33	0.68
47:N5:170:LYS:NZ	47:N5:244:ASP:OD2	2.20	0.68
47:N5:409:GLU:OE1	47:N5:495:SER:OG	2.12	0.68
48:S2:53:THR:HG21	48:S2:72:LEU:HD21	1.75	0.68
31:E4:31:VAL:HG21	48:S2:236:VAL:HG11	1.75	0.68
43:N1:395:ARG:NH2	48:S2:190:GLU:OE1	2.25	0.68
8:A5:38:LYS:NZ	40:G1:391:HIS:O	2.25	0.68
32:E5:81:GLU:OE1	32:E5:81:GLU:N	2.26	0.68
44:N2:126:GLU:N	44:N2:126:GLU:OE1	2.27	0.68
47:N5:2:LEU:HD21	47:N5:133:ILE:HD12	1.74	0.68
64:AM:215:CDL:O1	31:E4:315:ASP:OD2	2.08	0.68
19:B4:24:ILE:O	19:B4:110:ARG:NH1	2.27	0.68
19:B4:133:GLU:OE1	46:N4:274:TYR:OH	2.09	0.68
24:B9:41:HIS:NE2	59:AC:115:GLU:OE2	2.27	0.68
2:1B:264:LEU:HD21	30:E3:344:LEU:HD13	1.76	0.67
48:S2:394:ASP:OD1	48:S2:394:ASP:N	2.26	0.67
57:V2:28:GLU:N	57:V2:28:GLU:OE1	2.27	0.67
8:A5:169:GLU:OE2	8:A5:172:ARG:NH2	2.27	0.67
24:B9:59:SER:OG	34:E8:12:ARG:NH1	2.28	0.67
56:V1:97:LYS:NZ	56:V1:243:VAL:O	2.20	0.67
46:N4:284:ASN:O	46:N4:287:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E1:75:GLU:OE2	28:E1:186:SER:OG	2.12	0.67
47:N5:111:ASP:OD1	47:N5:112:LYS:N	2.28	0.67
33:E6:59:PRO:O	33:E6:203:ARG:NH1	2.28	0.67
6:A2:170:SER:OG	30:E3:326:GLU:OE2	2.11	0.66
12:A9:26:ASN:O	12:A9:26:ASN:ND2	2.28	0.66
24:B9:158:TYR:O	46:N4:446:THR:HG22	1.95	0.66
46:N4:186:ASN:O	46:N4:190:ASN:ND2	2.26	0.66
59:AC:92:LEU:HD21	66:AC:201:ZMP:H19B	1.77	0.66
39:FX:263:LYS:NZ	40:G1:61:GLU:O	2.25	0.66
56:V1:291:GLU:OE2	56:V1:304:HIS:NE2	2.21	0.66
1:1A:88:ASN:OD1	1:1A:89:CYS:N	2.29	0.66
7:A3:53:ARG:NH2	44:N2:25:ILE:O	2.27	0.66
34:E8:156:ARG:NH1	34:E8:160:GLU:OE1	2.29	0.66
9:A6:118:GLU:OE2	49:S3:177:ARG:NE	2.26	0.66
5:A1:78:ARG:NH2	63:A1:203:PC1:O12	2.28	0.66
39:FX:275:LYS:O	39:FX:277:VAL:N	2.27	0.66
41:G2:192:GLU:OE1	41:G2:192:GLU:N	2.29	0.66
7:A3:85:GLN:NE2	11:A8:207:TYR:O	2.29	0.66
56:V1:396:ILE:HB	56:V1:413:ILE:HD13	1.78	0.66
1:1A:318:ARG:NH2	2:1B:494:ASP:OD1	2.29	0.65
43:N1:379:SER:O	43:N1:383:THR:HG23	1.96	0.65
39:FX:185:TRP:O	39:FX:186:SER:OG	2.11	0.65
45:N3:275:LEU:HD23	45:N6:148:MET:SD	2.36	0.65
21:B6:50:ARG:NH2	36:EB:45:HIS:O	2.28	0.65
33:E6:368:GLU:OE1	33:E6:368:GLU:N	2.27	0.65
5:A1:132:HIS:O	15:AM:117:TYR:OH	2.08	0.65
9:A6:426:LYS:O	9:A6:427:SER:OG	2.13	0.65
11:A8:102:ARG:NH2	15:AM:93:CYS:O	2.30	0.65
47:N5:494:ILE:HD13	47:N5:499:HIS:HE1	1.60	0.65
12:A9:463:ASP:OD1	12:A9:464:TYR:N	2.28	0.65
59:AC:80:ASP:N	59:AC:80:ASP:OD1	2.29	0.65
47:N5:393:LEU:HD11	47:N5:432:GLN:CG	2.27	0.65
56:V1:428:LEU:HD23	56:V1:428:LEU:O	1.96	0.65
31:E4:31:VAL:HG21	48:S2:236:VAL:CG1	2.27	0.65
47:N5:246:MET:SD	47:N5:257:HIS:NE2	2.68	0.65
24:B9:50:ILE:HG13	66:AC:201:ZMP:H25A	1.79	0.65
47:N5:92:LEU:HD22	47:N5:343:PHE:HA	1.79	0.65
52:S6:62:GLU:N	52:S6:62:GLU:OE1	2.28	0.65
56:V1:351:GLY:O	56:V1:352:THR:OG1	2.11	0.65
17:B2:112:GLU:O	17:B2:133:ARG:NH2	2.29	0.65
31:E4:180:ARG:NH2	31:E4:268:ALA:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N4:295:ARG:NH1	47:N5:563:GLU:OE2	2.29	0.65
30:E3:149:GLY:O	30:E3:152:THR:OG1	2.13	0.64
9:A6:288:HIS:NE2	9:A6:411:ASP:OD1	2.29	0.64
26:BM:64:PHE:O	26:BM:68:THR:HG23	1.97	0.64
48:S2:241:GLU:O	56:V1:492:SER:OG	2.13	0.64
24:B9:154:LYS:N	26:BM:7:VAL:O	2.31	0.64
31:E4:318:VAL:HG21	31:E4:334:VAL:HG21	1.77	0.64
12:A9:214:SER:HA	53:S7:40:LEU:HD21	1.79	0.64
20:B5:116:LYS:N	27:C4:24:ASP:OD2	2.30	0.64
43:N1:402:ASN:OD1	43:N1:409:GLN:NE2	2.29	0.64
23:B8:150:GLU:N	23:B8:150:GLU:OE1	2.29	0.64
24:B9:99:ARG:NH2	47:N5:531:ASN:OD1	2.30	0.64
11:A8:75:ILE:N	11:A8:137:GLU:OE2	2.31	0.64
46:N4:90:LEU:HD23	46:N4:455:LEU:HD21	1.78	0.64
52:S6:54:ILE:HB	54:S8:186:ILE:HD11	1.80	0.64
24:B9:100:ARG:CD	66:AC:201:ZMP:H25B	2.28	0.64
29:E2:145:GLU:OE1	29:E2:147:LEU:N	2.31	0.64
31:E4:166:ALA:O	31:E4:170:SER:OG	2.15	0.64
47:N5:121:ILE:O	47:N5:125:THR:HG23	1.98	0.64
56:V1:125:THR:HG22	56:V1:354:ALA:HB2	1.80	0.64
58:E7:34:GLU:OE1	58:E7:241:LYS:NZ	2.23	0.64
2:1B:233:TYR:O	2:1B:241:TYR:OH	2.13	0.63
23:B8:25:ARG:NH2	39:FX:172:ASP:OD2	2.31	0.63
46:N4:354:TYR:O	46:N4:358:ASN:N	2.31	0.63
48:S2:189:ASP:OD1	48:S2:270:ARG:NH2	2.31	0.63
56:V1:36:ASP:OD2	57:V2:210:LEU:N	2.30	0.63
57:V2:114:GLU:OE1	57:V2:114:GLU:N	2.31	0.63
54:S8:92:HIS:CE1	61:S8:297:SF4:S4	2.91	0.63
31:E4:196:ARG:N	31:E4:332:ASP:OD1	2.30	0.63
35:EA:47:LEU:HD22	35:EA:56:LYS:HD3	1.80	0.63
44:N2:151:SER:O	44:N2:206:ASN:ND2	2.31	0.63
47:N5:533:HIS:N	64:N5:608:CDL:OB4	2.31	0.63
43:N1:367:GLN:OE1	45:N3:176:TYR:OH	2.15	0.63
47:N5:259:ALA:O	47:N5:260:THR:HG23	1.99	0.63
53:S7:42:GLU:N	53:S7:42:GLU:OE1	2.30	0.63
32:E5:152:LEU:HB2	32:E5:284:VAL:HG11	1.79	0.63
23:B8:25:ARG:NH1	23:B8:30:GLU:OE2	2.32	0.63
42:G3:87:LYS:NZ	42:G3:89:THR:OG1	2.20	0.63
58:E7:178:SER:OG	58:E7:180:ASP:OD1	2.16	0.63
31:E4:219:ARG:NH1	31:E4:280:ASP:OD2	2.32	0.63
44:N2:88:ILE:HG21	45:N6:143:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N4:403:SER:O	46:N4:406:ILE:HG22	1.99	0.63
57:V2:173:THR:OG1	57:V2:175:GLU:OE1	2.09	0.63
25:BL:26:TYR:OH	26:BM:90:ARG:NH2	2.32	0.63
53:S7:85:ALA:O	53:S7:88:ALA:N	2.27	0.63
1:1A:259:THR:HG21	1:1A:295:TYR:O	1.98	0.63
24:B9:46:ALA:HB1	66:AC:201:ZMP:H24A	1.80	0.62
29:E2:4:GLY:O	29:E2:5:THR:OG1	2.17	0.62
44:N2:221:ILE:HD11	44:N2:252:ASN:CG	2.19	0.62
46:N4:368:ASN:ND2	46:N4:444:THR:O	2.31	0.62
47:N5:389:LEU:HD21	47:N5:438:ILE:HD11	1.80	0.62
64:EA:202:CDL:OA3	64:EA:202:CDL:O1	2.17	0.62
36:EB:30:GLN:O	36:EB:35:ARG:NH2	2.32	0.62
8:A5:134:ARG:NH2	8:A5:147:GLU:OE2	2.32	0.62
9:A6:309:ASP:OD1	9:A6:312:ARG:NH2	2.32	0.62
20:B5:104:GLN:N	20:B5:104:GLN:OE1	2.32	0.62
47:N5:393:LEU:HD11	47:N5:432:GLN:HG2	1.81	0.62
45:N6:35:LEU:HD13	45:N6:46:ILE:HG22	1.80	0.62
58:E7:4:LEU:HD12	58:E7:4:LEU:O	2.00	0.62
68:N4:505:U10:H18	68:N4:505:U10:H151	1.82	0.62
1:1A:213:GLU:N	1:1A:213:GLU:OE1	2.33	0.62
11:A8:164:MET:O	11:A8:169:ARG:NH2	2.32	0.62
31:E4:128:ILE:HD11	31:E4:156:LEU:CD1	2.29	0.62
40:G1:113:ARG:NH2	45:N6:166:TYR:OH	2.30	0.62
46:N4:43:ILE:HG12	46:N4:79:LEU:HD22	1.80	0.62
47:N5:494:ILE:HD13	47:N5:499:HIS:CE1	2.34	0.62
2:1B:206:GLU:OE1	2:1B:482:ARG:NH1	2.31	0.62
19:B4:28:GLU:OE1	19:B4:31:ARG:NH2	2.32	0.62
39:FX:172:ASP:OD1	39:FX:172:ASP:N	2.31	0.62
48:S2:265:ARG:NE	48:S2:387:ASP:OD2	2.32	0.62
52:S6:115:CYS:O	52:S6:119:GLU:N	2.32	0.62
10:A7:32:TRP:O	48:S2:187:ARG:NH2	2.29	0.62
18:B3:52:UNK:O	18:B3:56:UNK:N	2.33	0.62
46:N4:43:ILE:HD12	46:N4:44:MET:N	2.14	0.62
48:S2:187:ARG:NH1	48:S2:190:GLU:OE2	2.33	0.62
12:A9:115:ARG:NH1	50:S4:97:GLU:OE2	2.33	0.61
17:B2:110:GLU:O	22:B7:92:ARG:NH1	2.33	0.61
32:E5:282:ASP:O	32:E5:284:VAL:HG13	1.98	0.61
39:FX:121:ASP:OD1	39:FX:127:ARG:NH2	2.33	0.61
57:V2:194:SER:OG	57:V2:198:ARG:O	2.17	0.61
6:A2:6:ARG:NH2	6:A2:135:GLU:OE1	2.32	0.61
11:A8:55:ARG:NH2	11:A8:210:SER:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:FX:161:ALA:N	39:FX:225:VAL:O	2.33	0.61
44:N2:272:TYR:CZ	44:N2:276:ILE:HD11	2.34	0.61
68:N4:505:U10:H151	68:N4:505:U10:C18	2.30	0.61
2:1B:236:ARG:NH2	2:1B:488:ASP:O	2.33	0.61
8:A5:144:ARG:NH1	49:S3:66:GLU:OE2	2.33	0.61
36:EB:89:GLU:N	36:EB:89:GLU:OE1	2.32	0.61
2:1B:441:LYS:HG2	29:E2:25:LEU:HD11	1.82	0.61
4:4L:84:ILE:HG23	45:N6:33:ILE:HD11	1.81	0.61
2:1B:126:TRP:HE1	28:E1:207:TYR:HH	1.49	0.61
5:A1:54:PHE:O	33:E6:338:ARG:NH2	2.29	0.61
29:E2:187:THR:HG21	29:E2:192:ALA:HB3	1.82	0.61
56:V1:126:CYS:SG	57:V2:147:CYS:N	2.72	0.61
2:1B:127:THR:O	2:1B:127:THR:HG23	2.01	0.61
40:G1:141:LYS:NZ	42:G3:211:THR:HG21	2.16	0.61
56:V1:209:GLU:OE1	56:V1:210:GLU:N	2.34	0.61
46:N4:293:THR:HG22	46:N4:362:LEU:HD23	1.83	0.61
47:N5:170:LYS:NZ	47:N5:540:ASP:OD2	2.34	0.61
32:E5:114:LEU:HD11	32:E5:249:VAL:HG22	1.82	0.61
32:E5:241:ALA:O	32:E5:245:VAL:HG23	2.01	0.61
10:A7:36:ASP:OD1	14:AL:62:ARG:NH2	2.32	0.61
63:C4:203:PC1:O12	41:G2:11:ARG:NH1	2.34	0.61
4:4L:84:ILE:CG2	45:N6:33:ILE:HD11	2.31	0.60
9:A6:393:ILE:O	9:A6:396:THR:OG1	2.16	0.60
14:AL:221:LYS:NZ	53:S7:20:VAL:O	2.23	0.60
28:E1:50:ARG:NH1	28:E1:55:GLU:OE1	2.34	0.60
47:N5:311:VAL:O	47:N5:315:THR:HG23	2.01	0.60
10:A7:52:ARG:NH1	48:S2:302:ASP:OD2	2.34	0.60
17:B2:138:TRP:NE1	23:B8:155:GLN:OE1	2.33	0.60
29:E2:116:GLU:OE1	29:E2:116:GLU:N	2.34	0.60
39:FX:221:ASN:O	39:FX:223:ARG:N	2.34	0.60
2:1B:130:GLN:OE1	2:1B:131:GLN:NE2	2.34	0.60
11:A8:62:ASN:ND2	11:A8:62:ASN:O	2.34	0.60
28:E1:305:THR:N	28:E1:308:ASP:OD2	2.33	0.60
30:E3:253:ASN:ND2	32:E5:54:LEU:O	2.34	0.60
47:N5:161:ARG:NH1	47:N5:247:GLU:OE1	2.35	0.60
59:AC:92:LEU:CD2	66:AC:201:ZMP:H19B	2.31	0.60
1:1A:195:CYS:O	1:1A:196:THR:OG1	2.19	0.60
9:A6:304:LEU:HD21	9:A6:385:ILE:HG21	1.82	0.60
18:B3:32:TRP:O	18:B3:33:SER:OG	2.20	0.60
37:EC:60:HIS:O	37:EC:64:VAL:HG23	2.02	0.60
12:A9:194:ARG:NH1	14:AL:219:HIS:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N4:173:ASN:ND2	46:N4:205:TYR:OH	2.30	0.60
46:N4:325:TYR:CE2	46:N4:329:ILE:HD11	2.37	0.60
58:E7:81:VAL:HG23	58:E7:83:GLN:H	1.67	0.60
1:1A:210:LYS:NZ	50:S4:174:ASP:OD2	2.34	0.60
7:A3:22:ASN:OD1	7:A3:23:ARG:NH1	2.33	0.60
46:N4:173:ASN:O	46:N4:177:ASN:ND2	2.33	0.60
56:V1:116:ILE:HG21	56:V1:139:LEU:HD11	1.84	0.60
19:B4:76:ASP:OD1	19:B4:77:SER:N	2.35	0.60
47:N5:260:THR:O	47:N5:263:THR:N	2.33	0.60
1:1A:160:TYR:OH	49:S3:235:ASP:OD1	2.19	0.59
15:AM:187:MET:O	51:S5:98:ARG:NH2	2.34	0.59
26:BM:81:ASN:ND2	47:N5:70:ASN:O	2.35	0.59
48:S2:51:ARG:HG2	53:S7:123:THR:HG21	1.83	0.59
49:S3:186:GLU:N	49:S3:186:GLU:OE1	2.36	0.59
9:A6:181:ARG:NH1	33:E6:176:ASP:OD1	2.35	0.59
28:E1:89:ASP:OD1	28:E1:90:SER:N	2.35	0.59
32:E5:42:PRO:HB3	32:E5:286:ILE:HG22	1.85	0.59
19:B4:20:PRO:O	19:B4:22:ASP:N	2.35	0.59
39:FX:164:ALA:CB	39:FX:171:LEU:HD21	2.32	0.59
48:S2:355:ARG:NH1	49:S3:105:ASP:OD1	2.35	0.59
14:AL:66:VAL:HG11	54:S8:65:ILE:HG22	1.85	0.59
16:AN:105:MET:SD	16:AN:113:LEU:HD12	2.43	0.59
17:B2:65:ARG:NH2	18:B3:39:UNK:O	2.30	0.59
32:E5:49:ASP:OD1	32:E5:52:ARG:NH1	2.34	0.59
37:EC:69:GLU:OE2	37:EC:76:VAL:N	2.34	0.59
44:N2:77:LYS:NZ	45:N3:281:TYR:OH	2.17	0.59
48:S2:31:ILE:HD12	48:S2:45:HIS:CE1	2.37	0.59
49:S3:263:TYR:OH	50:S4:85:ARG:NH1	2.35	0.59
15:AM:52:LYS:NZ	64:AM:216:CDL:OB4	2.32	0.59
66:AC:201:ZMP:H12A	66:AC:201:ZMP:HN2	1.66	0.59
30:E3:156:LEU:HD13	30:E3:184:LEU:HD22	1.84	0.59
43:N1:424:ARG:NH1	45:N3:202:SER:OG	2.36	0.59
46:N4:35:ILE:HG21	46:N4:108:TYR:OH	2.03	0.59
57:V2:20:ASP:OD1	57:V2:26:TYR:OH	2.17	0.59
13:AB:56:ARG:O	13:AB:60:THR:HG23	2.03	0.59
14:AL:210:ARG:NH2	54:S8:172:ASP:OD1	2.31	0.59
8:A5:97:GLU:N	8:A5:97:GLU:OE1	2.36	0.59
19:B4:133:GLU:OE2	19:B4:137:ARG:NE	2.36	0.59
63:B5:203:PC1:O14	26:BM:46:ARG:NH2	2.35	0.59
48:S2:157:PRO:O	54:S8:89:ARG:NH2	2.33	0.59
27:C4:145:LEU:HD12	27:C4:145:LEU:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:FX:144:ASP:O	39:FX:147:GLY:N	2.34	0.58
46:N4:327:ILE:HG22	47:N5:72:TYR:CE2	2.38	0.58
58:E7:7:ILE:O	58:E7:212:LEU:HD12	2.02	0.58
28:E1:260:ALA:HB1	28:E1:292:ALA:HB2	1.85	0.58
52:S6:31:GLN:OE1	52:S6:31:GLN:N	2.36	0.58
1:1A:66:LEU:O	1:1A:70:ASN:ND2	2.36	0.58
47:N5:102:ILE:HG23	47:N5:466:ILE:HD11	1.85	0.58
49:S3:117:ARG:NH2	49:S3:193:ASP:OD1	2.34	0.58
1:1A:43:THR:OG1	1:1A:56:GLN:NE2	2.36	0.58
2:1B:338:GLU:OE2	50:S4:105:ARG:NH1	2.37	0.58
32:E5:36:LEU:HD21	32:E5:70:GLY:HA3	1.83	0.58
28:E1:70:ALA:O	28:E1:102:ARG:NH1	2.36	0.58
32:E5:7:TRP:O	32:E5:96:TYR:HB2	2.02	0.58
40:G1:140:TYR:CE1	42:G3:211:THR:HG22	2.39	0.58
56:V1:73:GLU:OE2	56:V1:103:LYS:NZ	2.37	0.58
2:1B:177:GLU:OE1	2:1B:179:ARG:NH1	2.34	0.58
41:G2:47:ASN:OD1	41:G2:48:GLY:N	2.35	0.58
46:N4:273:ILE:HD12	46:N4:317:ILE:HD13	1.86	0.58
54:S8:161:THR:HG22	54:S8:192:ILE:HD11	1.86	0.58
56:V1:319:ILE:HG12	56:V1:327:VAL:HG12	1.85	0.58
1:1A:348:HIS:NE2	6:A2:176:ASN:O	2.30	0.58
9:A6:364:ASP:OD1	9:A6:365:ARG:N	2.36	0.58
19:B4:9:LEU:HD11	39:FX:253:THR:HG21	1.84	0.58
21:B6:45:GLU:OE2	47:N5:62:TYR:OH	2.17	0.58
23:B8:92:GLU:OE2	23:B8:97:SER:OG	2.14	0.58
24:B9:134:LYS:O	24:B9:137:THR:HG23	2.03	0.58
27:C4:6:VAL:HG22	44:N2:100:THR:OG1	2.04	0.58
40:G1:113:ARG:NH1	40:G1:115:THR:OG1	2.37	0.58
23:B8:87:ASP:OD2	47:N5:541:LYS:NZ	2.37	0.58
39:FX:164:ALA:HB1	39:FX:171:LEU:HD21	1.86	0.58
21:B6:45:GLU:CG	47:N5:64:LEU:HD11	2.34	0.57
3:2B:80:TYR:HB3	3:2B:81:PRO:HD3	1.85	0.57
4:4L:95:LYS:O	4:4L:103:ARG:NH2	2.38	0.57
8:A5:30:LEU:HD22	48:S2:212:LEU:HD22	1.85	0.57
31:E4:190:ARG:NH2	31:E4:341:HIS:O	2.35	0.57
47:N5:169:LEU:O	47:N5:173:VAL:HG23	2.04	0.57
56:V1:312:TRP:O	56:V1:330:LYS:NZ	2.37	0.57
57:V2:99:ILE:HB	57:V2:138:ILE:HD13	1.85	0.57
20:B5:55:TRP:O	20:B5:58:ARG:NH1	2.37	0.57
56:V1:124:GLY:O	56:V1:354:ALA:HB1	2.04	0.57
21:B6:10:ARG:NH1	46:N4:368:ASN:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:G3:112:VAL:HG22	42:G3:128:PRO:HA	1.86	0.57
12:A9:120:THR:OG1	12:A9:195:SER:OG	2.11	0.57
3:2B:54:THR:HG21	64:N4:501:CDL:H792	1.85	0.57
49:S3:82:PRO:HB3	49:S3:139:VAL:HG12	1.86	0.57
52:S6:105:ILE:HD11	52:S6:115:CYS:HB2	1.86	0.57
3:2B:56:ILE:HD12	44:N2:257:PHE:CZ	2.40	0.57
33:E6:334:LEU:O	55:U1:11:UNK:N	2.38	0.57
39:FX:160:MET:SD	39:FX:225:VAL:HG12	2.44	0.57
46:N4:130:GLN:OE1	46:N4:249:THR:HG21	2.04	0.57
47:N5:234:THR:HG21	47:N5:242:LEU:HB2	1.87	0.57
4:4L:69:THR:OG1	4:4L:72:ASP:OD1	2.23	0.57
33:E6:273:ARG:NH1	53:S7:26:LYS:O	2.37	0.57
48:S2:54:GLU:OE1	48:S2:353:ARG:NH2	2.34	0.57
52:S6:6:ARG:NH2	54:S8:208:GLN:O	2.38	0.57
53:S7:116:ASP:OD1	53:S7:116:ASP:N	2.38	0.57
56:V1:410:VAL:O	56:V1:413:ILE:HG22	2.04	0.57
3:2B:57:PHE:CE2	3:2B:61:ILE:HD11	2.40	0.57
9:A6:36:ARG:NH1	48:S2:6:ASP:OD2	2.37	0.57
17:B2:144:VAL:HG13	34:E8:139:ARG:NH2	2.19	0.57
22:B7:65:GLY:N	47:N5:487:ASP:OD2	2.35	0.57
32:E5:5:LYS:O	32:E5:98:THR:N	2.37	0.57
34:E8:70:VAL:HG22	58:E7:205:LEU:HD11	1.87	0.57
9:A6:99:LEU:O	50:S4:47:GLN:NE2	2.35	0.56
12:A9:194:ARG:NH2	14:AL:222:ASN:O	2.38	0.56
34:E8:74:ARG:NH2	58:E7:207:VAL:O	2.37	0.56
48:S2:342:TYR:OH	48:S2:344:GLN:NE2	2.37	0.56
56:V1:218:GLU:OE2	56:V1:225:ARG:NH2	2.37	0.56
46:N4:189:HIS:CD2	46:N4:193:ILE:HD11	2.40	0.56
39:FX:287:PRO:CD	39:FX:307:THR:HG22	2.35	0.56
57:V2:104:THR:HG22	57:V2:105:THR:H	1.70	0.56
39:FX:182:PHE:O	39:FX:217:THR:OG1	2.22	0.56
47:N5:337:ILE:HD11	47:N5:491:TYR:CD1	2.41	0.56
56:V1:384:THR:OG1	56:V1:387:ARG:NH2	2.38	0.56
29:E2:101:PHE:CZ	29:E2:244:ILE:HG22	2.40	0.56
43:N1:481:ILE:O	43:N1:485:VAL:HG22	2.06	0.56
29:E2:240:GLU:N	29:E2:240:GLU:OE1	2.38	0.56
46:N4:352:TYR:CG	46:N4:452:LEU:HD22	2.39	0.56
2:1B:112:THR:O	50:S4:155:ASN:ND2	2.35	0.56
56:V1:406:PHE:O	56:V1:409:GLU:N	2.30	0.56
16:AN:21:SER:OG	16:AN:67:ASP:OD1	2.19	0.56
19:B4:151:LEU:HD22	47:N5:209:TYR:OH	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:EA:74:VAL:HG21	44:N2:15:SER:HA	1.88	0.56
38:ED:116:VAL:HG12	38:ED:116:VAL:O	2.05	0.56
9:A6:123:ASP:OD2	48:S2:45:HIS:NE2	2.39	0.56
15:AM:152:ARG:NH2	15:AM:185:GLU:OE2	2.39	0.56
39:FX:253:THR:HG23	39:FX:304:TRP:HE1	1.70	0.56
1:1A:247:GLU:OE2	1:1A:320:ARG:NH1	2.37	0.56
7:A3:102:GLU:OE2	35:EA:89:ARG:NH2	2.35	0.56
22:B7:44:ARG:HA	22:B7:48:VAL:CG1	2.35	0.56
32:E5:36:LEU:HD23	32:E5:36:LEU:O	2.05	0.56
45:N3:251:ILE:HD11	45:N3:279:ILE:HD11	1.88	0.56
48:S2:72:LEU:HD11	48:S2:356:ILE:HD13	1.87	0.56
10:A7:120:THR:OG1	10:A7:123:TYR:O	2.16	0.55
24:B9:38:ARG:NH2	24:B9:94:GLU:OE1	2.38	0.55
28:E1:425:GLU:OE1	28:E1:463:LYS:N	2.39	0.55
29:E2:147:LEU:HB2	29:E2:251:LEU:HD22	1.88	0.55
47:N5:54:ASN:OD1	47:N5:55:ILE:N	2.39	0.55
32:E5:275:GLU:O	32:E5:279:GLY:N	2.38	0.55
40:G1:113:ARG:NH2	40:G1:119:LYS:O	2.36	0.55
47:N5:315:THR:HG22	47:N5:349:LYS:HG2	1.87	0.55
56:V1:117:ASN:ND2	56:V1:208:GLY:O	2.33	0.55
56:V1:323:SER:HG	56:V1:375:TYR:HH	1.51	0.55
2:1B:32:VAL:HG21	2:1B:359:LEU:HD23	1.87	0.55
22:B7:4:ASP:OD2	22:B7:9:SER:OG	2.13	0.55
5:A1:124:ASN:N	15:AM:194:GLU:OE2	2.34	0.55
28:E1:34:LEU:HD22	28:E1:253:LEU:HD22	1.89	0.55
31:E4:100:ARG:NH2	31:E4:137:ALA:O	2.40	0.55
9:A6:137:ASP:OD2	12:A9:330:ARG:NH2	2.39	0.55
45:N3:261:ILE:HD13	45:N6:128:ILE:HB	1.88	0.55
9:A6:300:ARG:NH2	9:A6:415:TRP:O	2.38	0.55
28:E1:34:LEU:CD2	28:E1:253:LEU:HD22	2.37	0.55
30:E3:423:GLU:OE1	30:E3:423:GLU:N	2.36	0.55
32:E5:84:ARG:NH1	32:E5:114:LEU:O	2.39	0.55
49:S3:264:ASP:OD1	50:S4:151:ARG:NH1	2.40	0.55
12:A9:7:GLU:OE2	12:A9:30:ARG:NH2	2.39	0.55
12:A9:301:ASN:OD1	12:A9:375:ARG:NH2	2.39	0.55
43:N1:447:LEU:HD11	43:N1:472:LEU:HD23	1.89	0.55
19:B4:80:ASN:O	19:B4:82:VAL:HG23	2.06	0.55
29:E2:364:PRO:O	29:E2:400:ARG:NH1	2.39	0.55
41:G2:207:LEU:HD21	42:G3:84:ASP:OD2	2.07	0.55
46:N4:427:LEU:HD11	47:N5:149:ILE:HD11	1.87	0.55
2:1B:329:SER:O	12:A9:94:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B9:130:GLN:HG2	46:N4:444:THR:HG22	1.89	0.55
29:E2:266:GLN:OE1	29:E2:269:ARG:NH2	2.40	0.55
31:E4:318:VAL:HG21	31:E4:334:VAL:CG2	2.36	0.55
48:S2:324:PRO:O	48:S2:345:SER:OG	2.25	0.55
52:S6:40:LEU:HA	52:S6:43:VAL:HG22	1.89	0.55
17:B2:92:TRP:CZ2	17:B2:96:LEU:HD11	2.42	0.54
17:B2:125:PHE:CE2	47:N5:415:ILE:HG22	2.42	0.54
18:B3:10:GLN:OE1	24:B9:61:THR:HG21	2.07	0.54
49:S3:230:GLU:OE2	50:S4:119:LYS:NZ	2.33	0.54
50:S4:69:ARG:NH1	50:S4:143:PRO:O	2.38	0.54
12:A9:239:ARG:NH2	12:A9:339:GLU:OE2	2.41	0.54
39:FX:199:VAL:O	39:FX:223:ARG:NH2	2.40	0.54
41:G2:220:GLU:O	41:G2:223:THR:HG22	2.07	0.54
42:G3:74:SER:OG	42:G3:95:HIS:ND1	2.29	0.54
43:N1:572:VAL:HG12	43:N1:572:VAL:O	2.06	0.54
2:1B:117:SER:OG	2:1B:195:ASN:ND2	2.37	0.54
25:BL:116:ARG:NH1	47:N5:214:TYR:OH	2.40	0.54
30:E3:41:LEU:HD12	30:E3:98:SER:O	2.07	0.54
44:N2:17:ILE:HD11	45:N6:146:LEU:HA	1.88	0.54
45:N6:45:ILE:HD11	45:N6:82:ILE:HG22	1.88	0.54
28:E1:366:GLU:O	28:E1:388:ARG:NH2	2.36	0.54
43:N1:543:GLN:OE1	43:N1:618:SER:N	2.41	0.54
2:1B:420:GLU:HG2	12:A9:89:LEU:HD13	1.89	0.54
46:N4:423:LEU:HD23	47:N5:176:ARG:CZ	2.38	0.54
21:B6:45:GLU:HG3	47:N5:64:LEU:HD11	1.90	0.54
2:1B:226:GLN:NE2	29:E2:29:VAL:O	2.38	0.54
9:A6:119:TYR:CE1	66:AB:150:ZMP:H24A	2.43	0.54
24:B9:100:ARG:HD3	66:AC:201:ZMP:H25B	1.90	0.54
34:E8:126:LYS:O	34:E8:178:ARG:NH2	2.41	0.54
48:S2:355:ARG:NH1	49:S3:106:VAL:O	2.40	0.54
1:1A:345:LEU:HD23	9:A6:367:LEU:HD22	1.90	0.54
63:A1:202:PC1:C1	63:A1:202:PC1:H152	2.38	0.54
46:N4:286:ASN:ND2	47:N5:558:PHE:O	2.38	0.54
47:N5:336:GLU:HG2	47:N5:337:ILE:HD12	1.90	0.54
49:S3:29:GLN:OE1	49:S3:29:GLN:N	2.41	0.54
1:1A:330:ARG:NH2	2:1B:313:GLU:OE2	2.40	0.54
2:1B:454:GLU:OE2	6:A2:58:ARG:NH1	2.39	0.54
12:A9:460:VAL:CG1	40:G1:54:THR:HG23	2.38	0.54
21:B6:52:LEU:O	25:BL:95:ARG:NH1	2.36	0.54
53:S7:184:THR:O	53:S7:187:ALA:N	2.41	0.54
5:A1:76:GLU:OE1	5:A1:93:TRP:NE1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B4:68:LYS:NZ	24:B9:127:LEU:O	2.29	0.53
34:E8:22:TYR:O	34:E8:26:THR:OG1	2.26	0.53
46:N4:90:LEU:HD23	46:N4:455:LEU:CD2	2.38	0.53
4:4L:80:PRO:HD3	45:N6:112:ILE:HD11	1.89	0.53
9:A6:90:ARG:NE	9:A6:94:GLU:OE2	2.39	0.53
12:A9:148:ARG:NH2	65:A9:559:NDP:O3X	2.41	0.53
29:E2:316:LEU:O	29:E2:400:ARG:NH2	2.41	0.53
31:E4:212:PHE:O	31:E4:215:THR:HG23	2.07	0.53
56:V1:44:ILE:HG22	57:V2:210:LEU:HD11	1.91	0.53
1:1A:345:LEU:CD2	9:A6:367:LEU:HD22	2.39	0.53
31:E4:190:ARG:NE	40:G1:436:ALA:O	2.42	0.53
39:FX:134:THR:OG1	40:G1:282:ASP:OD1	2.23	0.53
52:S6:35:PRO:HD3	52:S6:77:ILE:HD11	1.90	0.53
1:1A:352:LEU:HD11	9:A6:360:LEU:CD1	2.39	0.53
13:AB:92:LEU:HD22	66:AB:150:ZMP:H20	1.90	0.53
47:N5:310:ILE:HG21	47:N5:438:ILE:CG2	2.38	0.53
49:S3:35:HIS:ND1	49:S3:39:GLU:OE1	2.37	0.53
16:AN:91:VAL:O	44:N2:169:TYR:OH	2.21	0.53
20:B5:101:GLN:NE2	64:N4:501:CDL:OA3	2.39	0.53
34:E8:14:PHE:O	34:E8:19:ASN:ND2	2.41	0.53
56:V1:456:ASP:OD1	56:V1:476:ARG:NH1	2.37	0.53
58:E7:91:GLN:OE1	58:E7:91:GLN:N	2.42	0.53
20:B5:11:PRO:O	68:N4:505:U10:H302	2.09	0.53
46:N4:269:LEU:HD22	46:N4:313:LEU:HD22	1.91	0.53
47:N5:156:ASN:OD1	47:N5:165:THR:HG22	2.09	0.53
59:AC:92:LEU:CG	66:AC:201:ZMP:H19B	2.39	0.53
9:A6:181:ARG:O	9:A6:185:THR:OG1	2.17	0.53
12:A9:259:TYR:OH	53:S7:43:GLU:OE2	2.24	0.53
15:AM:54:VAL:HG13	64:AM:216:CDL:H532	1.89	0.53
40:G1:251:ASP:N	40:G1:251:ASP:OD1	2.41	0.53
2:1B:119:ARG:NH1	29:E2:19:GLU:OE2	2.37	0.53
16:AN:108:TRP:HZ3	39:FX:307:THR:HG21	1.74	0.53
32:E5:41:ALA:HB3	32:E5:289:LEU:HB3	1.91	0.53
37:EC:50:PHE:O	37:EC:55:ASN:N	2.41	0.53
39:FX:306:TYR:O	39:FX:310:SER:OG	2.06	0.53
46:N4:99:ASN:ND2	68:N4:505:U10:O3	2.40	0.53
49:S3:148:LEU:HD22	49:S3:151:LEU:HD12	1.90	0.53
54:S8:78:PRO:O	54:S8:81:ARG:NE	2.36	0.53
58:E7:12:LEU:HD21	58:E7:212:LEU:HB3	1.90	0.53
48:S2:224:MET:SD	48:S2:386:LEU:HD23	2.48	0.53
51:S5:68:GLU:O	51:S5:72:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N4:173:ASN:OD1	46:N4:177:ASN:ND2	2.42	0.52
47:N5:152:LEU:C	47:N5:152:LEU:HD23	2.30	0.52
53:S7:149:GLY:O	53:S7:153:ASN:ND2	2.42	0.52
1:1A:144:ILE:HG23	54:S8:105:ILE:HD12	1.90	0.52
1:1A:341:ASN:ND2	9:A6:363:VAL:O	2.43	0.52
5:A1:91:TYR:O	5:A1:94:LYS:NZ	2.34	0.52
39:FX:225:VAL:HG11	39:FX:239:VAL:HG11	1.90	0.52
42:G3:96:ILE:HG23	42:G3:100:VAL:HG11	1.91	0.52
9:A6:177:VAL:HG12	9:A6:177:VAL:O	2.10	0.52
14:AL:177:GLN:O	14:AL:180:ARG:NH1	2.35	0.52
20:B5:47:THR:HG22	63:B5:203:PC1:H2E1	1.92	0.52
32:E5:266:LEU:HG	32:E5:289:LEU:HD13	1.92	0.52
46:N4:316:LEU:HD21	46:N4:325:TYR:CZ	2.44	0.52
54:S8:92:HIS:CD2	54:S8:143:CYS:SG	3.02	0.52
15:AM:140:ALA:HA	51:S5:37:VAL:HG21	1.91	0.52
28:E1:277:GLU:OE1	28:E1:277:GLU:N	2.35	0.52
36:EB:60:GLU:HG3	36:EB:68:VAL:HG11	1.91	0.52
46:N4:293:THR:HG22	46:N4:362:LEU:CD2	2.40	0.52
50:S4:156:ARG:NH1	50:S4:158:GLU:OE2	2.41	0.52
16:AN:9:ILE:HA	44:N2:219:LEU:HD22	1.90	0.52
58:E7:12:LEU:HD21	58:E7:212:LEU:CB	2.40	0.52
58:E7:27:PHE:HZ	58:E7:189:ILE:HG21	1.75	0.52
23:B8:70:GLY:HA2	47:N5:555:ILE:HG21	1.92	0.52
27:C4:148:ASN:OD1	27:C4:152:ARG:NH2	2.38	0.52
32:E5:245:VAL:O	32:E5:249:VAL:HG23	2.09	0.52
41:G2:101:ILE:HD13	41:G2:107:ILE:HD12	1.92	0.52
47:N5:567:ILE:HG22	47:N5:567:ILE:O	2.08	0.52
3:2B:34:THR:HG21	3:2B:91:PHE:CZ	2.45	0.52
19:B4:68:LYS:NZ	24:B9:129:GLN:O	2.41	0.52
29:E2:348:ASP:OD1	29:E2:372:ARG:NH2	2.41	0.52
47:N5:486:TYR:CZ	47:N5:490:ILE:HD12	2.44	0.52
51:S5:69:CYS:SG	51:S5:70:ARG:N	2.82	0.52
47:N5:336:GLU:OE1	47:N5:336:GLU:N	2.36	0.52
4:4L:154:TYR:HH	44:N2:129:TRP:HE1	1.57	0.52
29:E2:91:LYS:HD3	29:E2:352:VAL:HG21	1.92	0.52
34:E8:197:GLY:O	34:E8:201:VAL:HG13	2.10	0.52
41:G2:135:GLN:OE1	41:G2:153:LYS:NZ	2.20	0.52
42:G3:98:GLU:OE1	42:G3:98:GLU:N	2.36	0.52
5:A1:100:ARG:NH1	15:AM:168:GLU:OE2	2.43	0.52
13:AB:47:LEU:HD21	39:FX:197:MET:SD	2.50	0.52
18:B3:57:UNK:O	18:B3:59:UNK:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B5:126:GLU:OE1	20:B5:129:ARG:NH2	2.41	0.52
28:E1:86:THR:HG21	28:E1:92:MET:HE2	1.92	0.52
44:N2:98:ASN:O	51:S5:29:LYS:NZ	2.35	0.52
47:N5:52:ILE:HG22	47:N5:52:ILE:O	2.10	0.52
47:N5:144:TRP:NE1	47:N5:179:ASP:OD1	2.36	0.52
7:A3:28:GLN:O	54:S8:31:HIS:NE2	2.39	0.51
31:E4:74:THR:HG1	31:E4:141:SER:HG	1.54	0.51
33:E6:201:ASN:N	33:E6:201:ASN:OD1	2.41	0.51
42:G3:82:ARG:NH1	42:G3:84:ASP:OD2	2.43	0.51
52:S6:70:VAL:HG11	54:S8:100:GLY:O	2.10	0.51
2:1B:108:GLU:CG	2:1B:419:VAL:HG21	2.40	0.51
8:A5:127:ASP:OD1	10:A7:78:ARG:NH2	2.43	0.51
11:A8:146:GLN:OE1	11:A8:146:GLN:N	2.41	0.51
47:N5:389:LEU:CD2	47:N5:438:ILE:HD11	2.40	0.51
48:S2:57:MET:SD	48:S2:354:VAL:HG11	2.50	0.51
21:B6:54:PRO:O	38:ED:128:LYS:NZ	2.33	0.51
40:G1:198:ARG:HH11	42:G3:202:LEU:HD21	1.75	0.51
40:G1:390:ASP:OD1	40:G1:390:ASP:N	2.42	0.51
41:G2:79:SER:OG	41:G2:100:HIS:ND1	2.28	0.51
2:1B:525:GLU:OE1	2:1B:525:GLU:N	2.39	0.51
18:B3:10:GLN:NE2	47:N5:447:SER:O	2.43	0.51
42:G3:54:VAL:HG21	42:G3:57:ILE:HG13	1.91	0.51
45:N3:249:ASP:O	45:N3:252:ILE:HG22	2.11	0.51
7:A3:53:ARG:NH2	44:N2:27:VAL:HG23	2.24	0.51
12:A9:118:VAL:N	12:A9:196:GLN:OE1	2.39	0.51
28:E1:156:ASP:OD2	28:E1:159:SER:OG	2.26	0.51
31:E4:149:ASP:OD1	31:E4:150:ILE:N	2.44	0.51
41:G2:174:GLN:N	41:G2:174:GLN:OE1	2.43	0.51
46:N4:9:ARG:NH1	46:N4:82:ASP:OD2	2.43	0.51
47:N5:285:LEU:HD12	47:N5:285:LEU:O	2.10	0.51
3:2B:86:VAL:HG12	44:N2:238:LEU:HD21	1.93	0.51
44:N2:68:SER:OG	44:N2:79:GLN:NE2	2.42	0.51
56:V1:500:ASN:O	56:V1:502:ASN:N	2.43	0.51
48:S2:241:GLU:N	56:V1:492:SER:OG	2.44	0.51
9:A6:211:ASP:OD1	9:A6:211:ASP:N	2.43	0.51
47:N5:34:LEU:O	47:N5:35:ILE:HD12	2.11	0.51
47:N5:285:LEU:HD13	64:N5:603:CDL:H721	1.92	0.51
54:S8:92:HIS:HE1	61:S8:297:SF4:S4	2.31	0.51
2:1B:271:GLN:O	2:1B:499:ARG:NH2	2.44	0.51
15:AM:57:ARG:NH2	64:AM:217:CDL:OA2	2.44	0.51
19:B4:103:TYR:HE2	23:B8:69:VAL:HG22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B6:71:ASP:OD1	25:BL:95:ARG:NH2	2.43	0.51
22:B7:85:ARG:NH2	23:B8:130:GLY:O	2.40	0.51
28:E1:31:VAL:HG12	28:E1:253:LEU:HD21	1.92	0.51
30:E3:46:VAL:HG22	30:E3:97:TRP:CZ2	2.46	0.51
33:E6:257:TYR:HB2	53:S7:34:ALA:HB1	1.91	0.51
41:G2:114:VAL:HG22	41:G2:114:VAL:O	2.11	0.51
46:N4:89:ILE:HG22	46:N4:104:ILE:HG21	1.92	0.51
12:A9:264:GLU:OE1	12:A9:278:ARG:NH2	2.40	0.51
23:B8:122:PHE:O	23:B8:128:ASN:ND2	2.36	0.51
39:FX:223:ARG:NH2	39:FX:228:LEU:HD21	2.25	0.51
44:N2:81:ILE:CD1	45:N6:153:ILE:HD12	2.40	0.51
46:N4:11:ILE:O	46:N4:14:LEU:N	2.44	0.51
50:S4:174:ASP:OD1	50:S4:175:SER:N	2.44	0.51
6:A2:155:GLU:OE2	30:E3:163:LYS:NZ	2.31	0.50
28:E1:82:ALA:HB3	28:E1:99:ILE:HD13	1.94	0.50
47:N5:239:GLN:N	47:N5:240:PRO:CD	2.74	0.50
1:1A:142:CYS:SG	1:1A:154:GLN:NE2	2.78	0.50
31:E4:79:ASP:OD1	31:E4:79:ASP:N	2.44	0.50
35:EA:117:UNK:C	35:EA:119:UNK:H	2.23	0.50
40:G1:300:ARG:NH1	40:G1:301:LYS:O	2.45	0.50
2:1B:190:GLU:OE2	29:E2:22:VAL:HG11	2.11	0.50
3:2B:87:LEU:HD11	44:N2:242:SER:CB	2.41	0.50
29:E2:224:GLU:N	29:E2:224:GLU:OE1	2.44	0.50
43:N1:388:LYS:NZ	43:N1:397:ILE:O	2.45	0.50
48:S2:362:TYR:OH	49:S3:105:ASP:OD1	2.29	0.50
8:A5:137:ILE:N	49:S3:113:THR:O	2.40	0.50
11:A8:80:ILE:HD13	11:A8:136:SER:OG	2.12	0.50
49:S3:178:ARG:NH2	49:S3:187:GLY:O	2.41	0.50
52:S6:9:LYS:O	52:S6:33:GLN:NE2	2.44	0.50
56:V1:268:ARG:N	56:V1:271:ASN:O	2.44	0.50
58:E7:192:ARG:NH1	58:E7:225:GLY:O	2.43	0.50
59:AC:92:LEU:HG	66:AC:201:ZMP:H19B	1.94	0.50
9:A6:294:LEU:HD12	9:A6:393:ILE:HD11	1.92	0.50
12:A9:460:VAL:HG12	40:G1:54:THR:HG23	1.92	0.50
28:E1:274:PRO:O	28:E1:330:GLN:NE2	2.45	0.50
32:E5:283:THR:HG23	32:E5:283:THR:O	2.12	0.50
39:FX:221:ASN:OD1	39:FX:221:ASN:N	2.45	0.50
40:G1:62:GLN:OE1	48:S2:4:ARG:NE	2.44	0.50
44:N2:92:TYR:O	44:N2:96:ASN:ND2	2.45	0.50
48:S2:105:VAL:HG21	48:S2:242:VAL:CG2	2.41	0.50
48:S2:107:PHE:CZ	48:S2:150:VAL:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B2:125:PHE:CZ	47:N5:415:ILE:HG22	2.47	0.50
46:N4:366:ASN:ND2	46:N4:369:ILE:HG23	2.27	0.50
47:N5:363:ILE:O	47:N5:363:ILE:HG22	2.11	0.50
56:V1:399:ARG:NH1	56:V1:409:GLU:OE1	2.39	0.50
9:A6:314:VAL:HG21	9:A6:332:LEU:HD21	1.93	0.50
19:B4:6:PHE:HD2	19:B4:12:LEU:HD11	1.77	0.50
21:B6:4:LEU:HD13	26:BM:36:PRO:CD	2.42	0.50
21:B6:4:LEU:HD13	26:BM:36:PRO:HD2	1.94	0.50
38:ED:140:ASP:OD1	38:ED:141:GLY:N	2.44	0.50
40:G1:260:THR:OG1	42:G3:140:ASN:ND2	2.42	0.50
41:G2:133:PRO:O	41:G2:151:GLY:N	2.38	0.50
49:S3:140:ASP:OD1	49:S3:141:ASP:N	2.36	0.50
56:V1:75:ILE:HG21	56:V1:149:ALA:HB2	1.94	0.50
56:V1:116:ILE:HD12	56:V1:249:VAL:HG11	1.93	0.50
28:E1:360:VAL:HG11	28:E1:371:LEU:HD23	1.94	0.50
32:E5:124:VAL:O	32:E5:153:LEU:HD21	2.12	0.50
43:N1:582:ILE:HD11	45:N3:214:VAL:CG1	2.41	0.50
47:N5:131:LEU:C	47:N5:131:LEU:HD23	2.31	0.50
48:S2:33:GLU:OE1	48:S2:33:GLU:N	2.43	0.50
59:AC:90:ASP:O	59:AC:94:VAL:HG23	2.12	0.50
4:4L:154:TYR:HH	44:N2:129:TRP:HZ2	1.58	0.50
9:A6:48:PRO:HG2	49:S3:176:LEU:HD22	1.93	0.50
9:A6:361:LYS:NZ	9:A6:372:ASP:OD1	2.44	0.50
13:AB:92:LEU:CD1	66:AB:150:ZMP:H20A	2.36	0.50
64:AM:216:CDL:OA3	31:E4:322:GLN:NE2	2.44	0.50
20:B5:71:VAL:HG21	46:N4:50:ILE:HD11	1.94	0.50
30:E3:118:GLU:HB3	30:E3:296:VAL:HG11	1.92	0.50
30:E3:165:TRP:NE1	30:E3:281:GLU:OE2	2.34	0.50
47:N5:398:SER:O	47:N5:401:SER:OG	2.23	0.50
6:A2:174:PHE:N	9:A6:359:ASP:OD2	2.39	0.49
11:A8:65:ASN:N	11:A8:65:ASN:OD1	2.45	0.49
14:AL:151:SER:OG	64:AL:303:CDL:OB3	2.14	0.49
28:E1:40:ARG:NH2	29:E2:235:ASP:OD2	2.45	0.49
3:2B:5:LEU:HD11	42:G3:224:LEU:HD11	1.94	0.49
11:A8:59:GLY:O	35:EA:123:UNK:N	2.45	0.49
12:A9:468:LEU:HB3	63:A9:560:PC1:H142	1.92	0.49
50:S4:38:VAL:HG23	50:S4:39:ASN:N	2.26	0.49
33:E6:63:GLY:O	33:E6:203:ARG:NH2	2.46	0.49
36:EB:60:GLU:OE2	36:EB:72:ARG:NH1	2.45	0.49
37:EC:19:ARG:NH1	37:EC:92:GLU:OE1	2.39	0.49
52:S6:115:CYS:O	52:S6:119:GLU:CA	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:AC:201:ZMP:H21	66:AC:201:ZMP:O3	2.12	0.49
64:AM:215:CDL:OA4	31:E4:335:TYR:OH	2.25	0.49
39:FX:280:GLU:OE2	39:FX:319:ARG:NH2	2.46	0.49
46:N4:300:TYR:OH	46:N4:426:SER:N	2.46	0.49
47:N5:67:ASN:ND2	47:N5:75:ASN:OD1	2.37	0.49
45:N6:52:GLY:HA3	45:N6:75:ILE:HD13	1.93	0.49
45:N6:147:ILE:O	45:N6:150:MET:HG3	2.13	0.49
49:S3:105:ASP:OD1	49:S3:106:VAL:N	2.46	0.49
9:A6:129:VAL:HG12	9:A6:129:VAL:O	2.12	0.49
28:E1:418:VAL:HG22	28:E1:419:ALA:H	1.76	0.49
44:N2:131:TYR:CZ	44:N2:174:LEU:HD22	2.48	0.49
44:N2:221:ILE:HD11	44:N2:252:ASN:ND2	2.27	0.49
47:N5:360:ILE:HG23	47:N5:365:SER:O	2.13	0.49
56:V1:115:VAL:HG11	56:V1:213:LEU:HD22	1.94	0.49
10:A7:86:LEU:HD23	49:S3:55:TYR:HB2	1.94	0.49
11:A8:30:LEU:O	11:A8:34:VAL:HG13	2.12	0.49
28:E1:45:LYS:NZ	28:E1:293:HIS:O	2.32	0.49
28:E1:148:GLU:OE1	28:E1:148:GLU:N	2.33	0.49
28:E1:339:ASP:OD2	28:E1:343:LYS:NZ	2.46	0.49
34:E8:18:TRP:CZ3	47:N5:436:LEU:HD12	2.46	0.49
43:N1:380:SER:O	43:N1:383:THR:OG1	2.19	0.49
44:N2:171:ILE:N	44:N2:172:PRO:CD	2.76	0.49
46:N4:37:ILE:O	46:N4:40:ILE:HG22	2.13	0.49
47:N5:242:LEU:HD11	47:N5:257:HIS:CE1	2.47	0.49
47:N5:393:LEU:HD11	47:N5:432:GLN:HG3	1.93	0.49
48:S2:184:PHE:CD2	48:S2:273:ILE:HG21	2.47	0.49
56:V1:487:ASP:O	56:V1:492:SER:HA	2.13	0.49
15:AM:54:VAL:HG13	64:AM:216:CDL:C53	2.43	0.49
19:B4:103:TYR:CE2	23:B8:69:VAL:HG22	2.47	0.49
26:BM:56:TRP:HA	26:BM:59:VAL:HG22	1.95	0.49
34:E8:18:TRP:CE3	47:N5:436:LEU:HD12	2.48	0.49
56:V1:157:ILE:HB	56:V1:198:LEU:HD12	1.93	0.49
5:A1:31:CYS:SG	43:N1:370:LEU:HD12	2.53	0.49
7:A3:37:LEU:O	7:A3:48:ARG:NH2	2.42	0.49
12:A9:287:ASP:OD2	12:A9:290:THR:OG1	2.31	0.49
30:E3:219:ALA:O	30:E3:223:VAL:HG23	2.13	0.49
31:E4:127:ASP:O	31:E4:130:ASP:N	2.43	0.49
63:N5:601:PC1:O13	63:N5:601:PC1:H143	2.12	0.49
56:V1:160:ARG:NH2	56:V1:162:GLU:OE1	2.46	0.49
14:AL:105:ARG:NE	64:AL:303:CDL:OB3	2.46	0.49
50:S4:38:VAL:HG23	50:S4:39:ASN:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:S8:158:ILE:HG23	54:S8:158:ILE:O	2.12	0.49
56:V1:487:ASP:OD2	56:V1:495:ARG:NE	2.43	0.49
12:A9:93:LEU:HB3	50:S4:141:SER:HB3	1.95	0.49
12:A9:246:ILE:HD11	12:A9:408:PRO:HA	1.95	0.49
23:B8:63:ASN:ND2	23:B8:65:THR:OG1	2.41	0.49
30:E3:418:ILE:HG22	30:E3:420:VAL:HG13	1.95	0.49
39:FX:138:VAL:HG22	39:FX:232:PRO:HA	1.93	0.49
44:N2:108:ILE:HD12	44:N2:142:ILE:HG21	1.94	0.49
47:N5:209:TYR:O	47:N5:213:ASN:ND2	2.40	0.49
2:1B:108:GLU:HG2	2:1B:419:VAL:HG21	1.95	0.48
4:4L:141:LEU:HD11	45:N6:150:MET:HE1	1.95	0.48
11:A8:210:SER:N	15:AM:86:ASP:OD2	2.46	0.48
19:B4:97:PHE:HD2	46:N4:364:LEU:HD21	1.77	0.48
9:A6:339:TYR:HB2	9:A6:344:LEU:HD12	1.96	0.48
18:B3:39:UNK:O	18:B3:40:UNK:CB	2.61	0.48
40:G1:59:PHE:O	42:G3:247:ARG:NH1	2.46	0.48
40:G1:212:GLY:O	42:G3:99:ARG:NE	2.46	0.48
52:S6:127:PHE:N	52:S6:128:PRO:CD	2.76	0.48
1:1A:174:HIS:O	1:1A:174:HIS:ND1	2.45	0.48
29:E2:125:ALA:O	29:E2:129:VAL:HG23	2.14	0.48
47:N5:132:ILE:O	47:N5:271:LYS:NZ	2.39	0.48
2:1B:166:VAL:HG21	2:1B:182:LEU:HD12	1.95	0.48
3:2B:63:ILE:HD13	44:N2:260:ILE:HD13	1.95	0.48
4:4L:99:ALA:HA	42:G3:256:ILE:HD11	1.95	0.48
45:N3:267:THR:HG21	45:N6:135:PHE:O	2.14	0.48
47:N5:102:ILE:CG2	47:N5:466:ILE:HD11	2.43	0.48
47:N5:328:ILE:HG22	47:N5:328:ILE:O	2.13	0.48
48:S2:210:MET:SD	48:S2:214:ARG:NH1	2.87	0.48
3:2B:79:LEU:HD11	63:N2:301:PC1:H2A1	1.94	0.48
10:A7:112:HIS:CD2	31:E4:31:VAL:HG13	2.48	0.48
25:BL:53:ASP:OD1	25:BL:57:LEU:N	2.45	0.48
32:E5:36:LEU:HD22	32:E5:87:LEU:HD11	1.96	0.48
41:G2:223:THR:HG23	41:G2:224:GLU:HG2	1.96	0.48
43:N1:442:ILE:HD11	45:N3:185:PHE:HA	1.96	0.48
44:N2:50:ILE:HD11	44:N2:87:ILE:HD11	1.95	0.48
47:N5:525:HIS:HB3	58:E7:4:LEU:HD23	1.96	0.48
43:N1:446:LEU:HD12	45:N3:180:ASN:ND2	2.29	0.48
1:1A:276:ILE:HG22	1:1A:281:LEU:HD23	1.96	0.48
5:A1:38:LYS:NZ	5:A1:96:GLU:OE1	2.37	0.48
10:A7:69:ILE:O	10:A7:69:ILE:HG23	2.13	0.48
20:B5:129:ARG:NH1	51:S5:22:THR:OG1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E3:108:LEU:HD12	30:E3:108:LEU:N	2.28	0.48
33:E6:56:SER:OG	33:E6:57:ASN:ND2	2.47	0.48
43:N1:579:SER:OG	43:N1:645:ARG:NH1	2.47	0.48
49:S3:106:VAL:HG22	49:S3:122:TYR:CD1	2.48	0.48
2:1B:185:ARG:NH1	28:E1:215:ASP:OD2	2.43	0.48
46:N4:43:ILE:HG22	46:N4:75:ILE:HG23	1.96	0.48
48:S2:350:LEU:HD11	50:S4:116:ARG:NE	2.28	0.48
12:A9:136:LEU:HD11	12:A9:199:PHE:CE1	2.49	0.48
32:E5:64:ALA:O	32:E5:96:TYR:N	2.46	0.48
41:G2:95:ILE:HG23	41:G2:99:THR:HG21	1.95	0.48
47:N5:380:ILE:HG23	47:N5:381:LEU:N	2.29	0.48
52:S6:115:CYS:O	52:S6:119:GLU:HA	2.14	0.48
54:S8:108:GLN:N	61:S8:298:SF4:S1	2.78	0.48
54:S8:112:VAL:O	54:S8:112:VAL:HG22	2.14	0.48
2:1B:507:HIS:O	2:1B:511:VAL:HG23	2.13	0.48
4:4L:67:PHE:O	27:C4:13:LEU:N	2.40	0.48
5:A1:36:PHE:CG	43:N1:459:ILE:HD11	2.49	0.48
8:A5:57:ILE:O	8:A5:64:ARG:NH1	2.38	0.48
29:E2:154:ARG:O	29:E2:157:VAL:HG23	2.13	0.48
30:E3:286:ILE:HG13	30:E3:291:LEU:HD23	1.95	0.48
30:E3:389:VAL:CG2	30:E3:398:VAL:HG21	2.44	0.48
36:EB:95:ASP:OD1	36:EB:96:ARG:N	2.44	0.48
39:FX:192:SER:HB3	39:FX:193:PRO:HD3	1.96	0.48
40:G1:292:VAL:HG22	40:G1:299:LEU:HB2	1.96	0.48
13:AB:60:THR:HG22	13:AB:124:ILE:HG21	1.96	0.47
64:AM:215:CDL:O1	31:E4:338:ARG:NH2	2.39	0.47
16:AN:258:PRO:HG2	20:B5:91:ILE:HG21	1.95	0.47
33:E6:30:ASP:OD1	33:E6:30:ASP:N	2.47	0.47
40:G1:153:ILE:HG23	40:G1:162:PRO:HD2	1.96	0.47
43:N1:451:ILE:HD13	43:N1:536:LEU:HD11	1.96	0.47
1:1A:120:ASP:N	1:1A:120:ASP:OD1	2.47	0.47
2:1B:463:GLU:OE1	2:1B:463:GLU:N	2.47	0.47
3:2B:59:TYR:CE1	44:N2:267:LEU:HD22	2.48	0.47
16:AN:108:TRP:CZ3	39:FX:307:THR:HG21	2.49	0.47
46:N4:264:ILE:HG22	46:N4:265:TYR:N	2.28	0.47
46:N4:377:ILE:HG23	46:N4:460:LEU:HD11	1.95	0.47
2:1B:341:ASP:N	2:1B:341:ASP:OD1	2.47	0.47
6:A2:2:ALA:N	30:E3:201:GLN:O	2.47	0.47
30:E3:425:LEU:O	30:E3:429:VAL:HG23	2.14	0.47
38:ED:142:VAL:HG23	38:ED:143:LEU:N	2.28	0.47
47:N5:270:TYR:CE2	47:N5:339:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A6:31:VAL:CG1	39:FX:141:THR:HG21	2.42	0.47
63:AM:220:PC1:H143	31:E4:194:TRP:CZ3	2.48	0.47
27:C4:142:SER:O	27:C4:146:VAL:HG22	2.15	0.47
31:E4:296:VAL:O	31:E4:300:THR:HG22	2.14	0.47
40:G1:254:ILE:C	40:G1:255:ILE:HD12	2.35	0.47
9:A6:90:ARG:NH2	13:AB:93:ASP:OD1	2.47	0.47
28:E1:264:PHE:CE2	28:E1:270:VAL:HG21	2.50	0.47
32:E5:281:SER:OG	32:E5:283:THR:HG22	2.13	0.47
47:N5:92:LEU:HD21	47:N5:259:ALA:HB2	1.95	0.47
47:N5:310:ILE:HG21	47:N5:438:ILE:HG21	1.97	0.47
54:S8:159:VAL:HG11	54:S8:192:ILE:HD12	1.96	0.47
2:1B:74:LEU:HD22	2:1B:390:PHE:HZ	1.80	0.47
24:B9:30:ILE:HD13	24:B9:42:LEU:HD21	1.96	0.47
29:E2:60:ARG:NH1	29:E2:184:THR:OG1	2.46	0.47
31:E4:336:LEU:HD23	31:E4:336:LEU:O	2.15	0.47
40:G1:343:ASP:OD1	41:G2:33:ARG:NH2	2.43	0.47
47:N5:246:MET:HE1	47:N5:253:SER:HB3	1.97	0.47
48:S2:121:ALA:HB1	48:S2:133:ILE:HA	1.97	0.47
56:V1:159:VAL:CG2	56:V1:198:LEU:HD11	2.44	0.47
66:AC:201:ZMP:H12A	66:AC:201:ZMP:N2	2.30	0.47
1:1A:226:VAL:O	1:1A:228:ARG:N	2.47	0.47
2:1B:367:ARG:NE	30:E3:410:LEU:O	2.42	0.47
10:A7:126:ARG:NH2	15:AM:38:GLY:O	2.47	0.47
28:E1:81:ARG:NE	28:E1:126:LEU:O	2.46	0.47
28:E1:310:LYS:NZ	52:S6:146:GLU:OE1	2.37	0.47
29:E2:40:TYR:HA	29:E2:43:VAL:HG22	1.97	0.47
31:E4:130:ASP:OD2	31:E4:133:SER:OG	2.32	0.47
32:E5:38:VAL:HG11	32:E5:41:ALA:HB2	1.96	0.47
34:E8:148:LYS:O	34:E8:149:SER:OG	2.19	0.47
39:FX:143:ILE:HG21	39:FX:244:PHE:CD2	2.50	0.47
46:N4:258:ILE:HD11	46:N4:312:MET:SD	2.55	0.47
46:N4:398:LEU:HD11	47:N5:138:ILE:HD11	1.97	0.47
47:N5:131:LEU:HD23	47:N5:131:LEU:O	2.15	0.47
45:N6:45:ILE:HD11	45:N6:82:ILE:CG2	2.44	0.47
48:S2:33:GLU:HB2	48:S2:41:ARG:HB3	1.96	0.47
50:S4:65:VAL:O	50:S4:139:ASN:N	2.48	0.47
52:S6:97:THR:HG22	52:S6:97:THR:O	2.14	0.47
54:S8:159:VAL:HG11	54:S8:192:ILE:HG23	1.96	0.47
54:S8:159:VAL:CG1	54:S8:192:ILE:HD12	2.44	0.47
58:E7:212:LEU:O	58:E7:215:THR:OG1	2.26	0.47
1:1A:45:THR:HB	1:1A:52:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A2:102:GLN:O	12:A9:78:LYS:NZ	2.36	0.47
7:A3:55:ALA:HB3	43:N1:658:TYR:HA	1.96	0.47
26:BM:96:ARG:NH2	36:EB:39:ASP:OD1	2.48	0.47
27:C4:13:LEU:HD23	27:C4:14:GLU:N	2.30	0.47
27:C4:43:ASP:O	27:C4:44:ALA:HB3	2.15	0.47
47:N5:60:LEU:HD22	47:N5:135:ASN:OD1	2.14	0.47
47:N5:388:SER:O	47:N5:391:THR:OG1	2.31	0.47
48:S2:253:GLY:H	48:S2:264:ILE:HD11	1.80	0.47
53:S7:76:SER:OG	53:S7:78:TRP:NE1	2.48	0.47
56:V1:319:ILE:CG1	56:V1:327:VAL:HG12	2.45	0.47
11:A8:10:THR:HG22	20:B5:105:VAL:HG13	1.97	0.47
31:E4:188:ALA:HB1	31:E4:336:LEU:HD21	1.97	0.47
37:EC:69:GLU:HG2	37:EC:76:VAL:HG23	1.96	0.47
42:G3:68:THR:HB	42:G3:87:LYS:HZ3	1.80	0.47
46:N4:40:ILE:HD12	46:N4:43:ILE:HD11	1.97	0.47
46:N4:110:ILE:CG2	46:N4:126:ILE:HG23	2.45	0.47
2:1B:170:GLU:N	2:1B:170:GLU:OE1	2.48	0.47
14:AL:175:GLU:OE2	15:AM:31:ARG:NH2	2.47	0.47
40:G1:292:VAL:HG21	67:G1:516:3PE:H332	1.96	0.47
48:S2:211:ASP:OD1	48:S2:211:ASP:N	2.43	0.47
8:A5:152:VAL:HG21	12:A9:65:THR:HG22	1.97	0.46
27:C4:148:ASN:O	27:C4:152:ARG:NE	2.45	0.46
29:E2:293:SER:HG	29:E2:317:PHE:HD2	1.63	0.46
30:E3:52:ASP:OD1	30:E3:240:SER:OG	2.32	0.46
30:E3:306:ASP:OD1	30:E3:306:ASP:N	2.48	0.46
34:E8:53:VAL:HG12	34:E8:61:ASP:CG	2.35	0.46
63:ED:201:PC1:H132	63:ED:201:PC1:O13	2.15	0.46
47:N5:126:TYR:CE2	47:N5:130:LEU:HD11	2.50	0.46
21:B6:37:ILE:HD12	47:N5:15:ILE:HD11	1.96	0.46
22:B7:36:GLU:OE1	38:ED:133:ARG:NH2	2.48	0.46
29:E2:424:ASP:OD1	29:E2:425:ASP:N	2.48	0.46
43:N1:381:LEU:HA	43:N1:384:VAL:HG12	1.97	0.46
43:N1:605:ILE:HD11	43:N1:636:PHE:CE2	2.50	0.46
47:N5:117:PHE:CZ	47:N5:252:VAL:HG23	2.50	0.46
49:S3:202:VAL:CG2	53:S7:165:VAL:HG22	2.45	0.46
56:V1:487:ASP:OD1	56:V1:487:ASP:N	2.48	0.46
2:1B:109:LEU:HD21	2:1B:197:TYR:CZ	2.51	0.46
19:B4:33:LEU:HD21	19:B4:39:MET:HB2	1.97	0.46
64:B5:201:CDL:OA3	26:BM:46:ARG:NH1	2.44	0.46
56:V1:271:ASN:ND2	56:V1:341:ASP:OD2	2.45	0.46
11:A8:1:MET:HE2	44:N2:195:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:G3:148:LYS:C	42:G3:149:ILE:HD12	2.36	0.46
29:E2:287:LEU:HD12	29:E2:454:LEU:HD12	1.97	0.46
49:S3:85:ILE:HD11	49:S3:122:TYR:CD2	2.50	0.46
56:V1:213:LEU:O	56:V1:213:LEU:HD23	2.16	0.46
56:V1:407:GLY:O	56:V1:410:VAL:N	2.49	0.46
9:A6:163:GLY:N	9:A6:169:GLU:OE1	2.40	0.46
10:A7:109:TRP:CZ2	49:S3:128:VAL:HG22	2.50	0.46
44:N2:248:ILE:O	44:N2:252:ASN:ND2	2.46	0.46
12:A9:85:SER:HA	12:A9:92:ARG:O	2.15	0.46
12:A9:276:ILE:N	12:A9:276:ILE:HD12	2.30	0.46
21:B6:81:LEU:HD11	38:ED:124:LYS:HD3	1.98	0.46
46:N4:374:ILE:HD11	46:N4:453:ILE:HG13	1.98	0.46
47:N5:16:MET:SD	47:N5:28:LEU:HD13	2.56	0.46
12:A9:288:ASN:O	12:A9:292:LEU:HD12	2.15	0.46
13:AB:60:THR:HG22	13:AB:124:ILE:HD13	1.97	0.46
31:E4:182:ILE:HD12	31:E4:182:ILE:N	2.31	0.46
32:E5:7:TRP:HB2	32:E5:96:TYR:CB	2.46	0.46
46:N4:258:ILE:HD12	46:N4:261:TYR:CE2	2.51	0.46
45:N6:42:ILE:HD12	45:N6:43:ARG:N	2.30	0.46
52:S6:54:ILE:HG21	54:S8:96:ILE:HG12	1.98	0.46
13:AB:54:LEU:HD23	13:AB:59:VAL:HG22	1.98	0.46
28:E1:50:ARG:NH2	28:E1:89:ASP:OD2	2.44	0.46
32:E5:204:LEU:HD21	32:E5:231:PHE:HB2	1.98	0.46
39:FX:142:PHE:HB3	39:FX:169:VAL:HG21	1.98	0.46
43:N1:602:TYR:HA	43:N1:605:ILE:HG22	1.98	0.46
44:N2:146:LEU:C	44:N2:146:LEU:HD23	2.36	0.46
1:1A:49:ASP:OD2	1:1A:118:THR:OG1	2.34	0.46
19:B4:6:PHE:CD2	19:B4:12:LEU:HD11	2.50	0.46
28:E1:83:LEU:HD13	28:E1:126:LEU:HD12	1.97	0.46
37:EC:58:ALA:HA	37:EC:61:LEU:HD12	1.97	0.46
41:G2:17:ARG:NH1	42:G3:30:GLY:O	2.47	0.46
43:N1:543:GLN:NE2	43:N1:615:LEU:O	2.49	0.46
1:1A:341:ASN:O	1:1A:345:LEU:HG	2.16	0.45
2:1B:52:ASN:ND2	2:1B:265:ASN:OD1	2.45	0.45
2:1B:368:LEU:HD21	30:E3:410:LEU:HD13	1.97	0.45
8:A5:155:GLU:OE1	12:A9:68:ARG:NH2	2.48	0.45
23:B8:100:LYS:NZ	47:N5:538:TYR:OH	2.40	0.45
28:E1:268:GLU:OE1	28:E1:322:THR:OG1	2.19	0.45
46:N4:121:ILE:HG23	64:N4:501:CDL:H801	1.98	0.45
46:N4:232:VAL:HG23	46:N4:233:GLU:HG2	1.97	0.45
47:N5:254:ALA:HB2	47:N5:353:PHE:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S7:104:TYR:CD2	53:S7:193:LEU:HD21	2.50	0.45
6:A2:26:PRO:O	6:A2:27:GLU:HB3	2.16	0.45
19:B4:78:HIS:O	19:B4:80:ASN:ND2	2.48	0.45
23:B8:72:ASP:O	46:N4:432:LYS:NZ	2.49	0.45
34:E8:196:PHE:O	34:E8:200:VAL:HG22	2.17	0.45
40:G1:105:HIS:CE1	42:G3:241:ARG:HE	2.34	0.45
40:G1:194:LEU:HD22	40:G1:215:LEU:HD12	1.98	0.45
44:N2:215:ILE:O	44:N2:219:LEU:HG	2.16	0.45
9:A6:134:ASN:HD21	66:AB:150:ZMP:H24	1.81	0.45
21:B6:85:ASP:OD1	38:ED:120:SER:OG	2.25	0.45
27:C4:114:PHE:HB2	27:C4:115:PRO:HD3	1.97	0.45
29:E2:353:THR:HG22	29:E2:354:ALA:N	2.31	0.45
39:FX:144:ASP:OD1	39:FX:148:ASN:HB2	2.16	0.45
46:N4:62:ILE:HG23	46:N4:62:ILE:O	2.16	0.45
46:N4:419:SER:O	46:N4:422:ASN:HB2	2.17	0.45
49:S3:139:VAL:HG11	49:S3:145:ILE:HB	1.97	0.45
3:2B:49:TYR:CG	44:N2:281:ILE:HG13	2.51	0.45
11:A8:124:GLU:OE1	11:A8:124:GLU:N	2.42	0.45
27:C4:161:GLU:OE1	27:C4:165:ASN:ND2	2.46	0.45
29:E2:280:ALA:HB1	29:E2:286:SER:HB3	1.98	0.45
30:E3:211:ALA:HB2	30:E3:227:ILE:HD13	1.98	0.45
32:E5:260:LYS:C	32:E5:284:VAL:O	2.55	0.45
36:EB:30:GLN:OE1	36:EB:31:CYS:N	2.41	0.45
38:ED:68:ASP:OD1	38:ED:69:LYS:N	2.49	0.45
47:N5:341:HIS:CE1	47:N5:400:LEU:HD11	2.52	0.45
47:N5:434:TYR:CD1	47:N5:435:SER:N	2.85	0.45
1:1A:258:GLU:OE2	14:AL:238:ARG:NH2	2.36	0.45
11:A8:30:LEU:O	11:A8:34:VAL:HG22	2.17	0.45
45:N3:258:ILE:HD13	45:N3:271:THR:HG21	1.99	0.45
46:N4:211:LEU:HA	46:N4:254:HIS:CE1	2.52	0.45
46:N4:228:GLY:O	46:N4:232:VAL:HG13	2.16	0.45
47:N5:47:LEU:HB2	47:N5:91:ILE:HD11	1.98	0.45
14:AL:23:THR:O	14:AL:23:THR:HG22	2.16	0.45
44:N2:171:ILE:HD12	44:N2:247:THR:OG1	2.16	0.45
46:N4:191:ILE:HD11	46:N4:257:PHE:CE2	2.52	0.45
46:N4:302:ILE:O	46:N4:306:ASN:ND2	2.37	0.45
47:N5:355:LEU:HD11	47:N5:384:ILE:CG2	2.39	0.45
56:V1:215:GLU:OE2	56:V1:225:ARG:NE	2.34	0.45
1:1A:78:CYS:O	1:1A:200:ARG:NH2	2.41	0.45
1:1A:139:SER:OG	1:1A:141:ASP:OD1	2.29	0.45
1:1A:163:ASP:OD1	10:A7:55:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A6:99:LEU:HD21	50:S4:50:GLN:HG3	1.98	0.45
29:E2:421:LEU:HD11	29:E2:465:THR:OG1	2.17	0.45
31:E4:318:VAL:HG23	31:E4:331:ARG:HG2	1.99	0.45
33:E6:130:GLU:OE2	33:E6:213:ARG:NH2	2.49	0.45
43:N1:500:ILE:HG21	45:N6:84:LEU:HB2	1.97	0.45
43:N1:626:PHE:O	43:N1:629:ILE:HG13	2.16	0.45
45:N3:228:ILE:HD12	45:N3:228:ILE:N	2.32	0.45
47:N5:393:LEU:HD13	47:N5:393:LEU:O	2.15	0.45
48:S2:75:MET:CE	48:S2:118:LEU:HD13	2.47	0.45
48:S2:78:MET:HB2	48:S2:111:THR:HG21	1.98	0.45
49:S3:234:ASP:OD1	49:S3:235:ASP:N	2.49	0.45
56:V1:42:GLN:O	57:V2:210:LEU:HD13	2.17	0.45
59:AC:93:ASP:N	59:AC:93:ASP:OD1	2.50	0.45
12:A9:202:ILE:HD13	12:A9:224:LEU:HD21	1.99	0.45
17:B2:112:GLU:OE1	23:B8:158:ARG:NH1	2.50	0.45
19:B4:9:LEU:CD1	39:FX:253:THR:HG21	2.47	0.45
44:N2:58:LEU:HD22	44:N2:87:ILE:HG12	1.98	0.45
46:N4:357:THR:CG2	46:N4:369:ILE:HD13	2.47	0.45
47:N5:425:ILE:HG23	47:N5:509:ILE:HD13	1.98	0.45
12:A9:80:THR:HG22	12:A9:81:GLU:N	2.32	0.45
25:BL:82:LEU:C	25:BL:82:LEU:HD23	2.37	0.45
27:C4:27:LEU:HB3	27:C4:35:LEU:HD21	1.99	0.45
29:E2:217:VAL:HG11	29:E2:268:LEU:CD1	2.47	0.45
46:N4:352:TYR:CD2	46:N4:452:LEU:HD22	2.51	0.45
66:AC:201:ZMP:H4	66:AC:201:ZMP:H1	1.81	0.45
28:E1:324:VAL:HG23	28:E1:355:LEU:CD1	2.47	0.45
40:G1:405:HIS:O	45:N6:169:ILE:HG22	2.17	0.45
56:V1:303:LYS:NZ	57:V2:208:THR:O	2.50	0.45
15:AM:54:VAL:HG12	64:AM:215:CDL:HA31	1.98	0.44
27:C4:150:TYR:HA	27:C4:153:VAL:HG12	1.99	0.44
39:FX:249:THR:N	39:FX:250:PRO:HD2	2.32	0.44
43:N1:508:ILE:HG12	45:N3:248:LEU:HB3	1.98	0.44
44:N2:39:PHE:HA	44:N2:69:THR:HG21	1.98	0.44
57:V2:149:HIS:HB3	57:V2:170:GLU:HB3	1.98	0.44
11:A8:37:LYS:O	35:EA:106:UNK:N	2.51	0.44
12:A9:215:PHE:O	53:S7:48:GLN:NE2	2.48	0.44
14:AL:257:ARG:CD	54:S8:124:VAL:HG11	2.47	0.44
29:E2:348:ASP:HB3	29:E2:359:LEU:HD11	1.99	0.44
39:FX:157:GLY:N	39:FX:230:VAL:O	2.40	0.44
46:N4:227:LEU:HD22	46:N4:231:HIS:CE1	2.52	0.44
46:N4:314:ILE:HG21	46:N4:404:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N5:34:LEU:C	47:N5:35:ILE:HD12	2.38	0.44
45:N6:65:ILE:HG23	45:N6:66:LEU:N	2.33	0.44
49:S3:160:ARG:NH1	49:S3:177:ARG:O	2.50	0.44
57:V2:178:ILE:HA	57:V2:181:VAL:HG22	1.98	0.44
3:2B:59:TYR:CE1	3:2B:63:ILE:HG21	2.53	0.44
12:A9:202:ILE:HD13	12:A9:224:LEU:CD2	2.48	0.44
21:B6:3:ASP:OD2	59:AC:52:HIS:NE2	2.50	0.44
23:B8:46:VAL:HG23	23:B8:47:VAL:N	2.32	0.44
28:E1:324:VAL:HG23	28:E1:355:LEU:HD11	2.00	0.44
32:E5:24:ASP:OD1	32:E5:24:ASP:N	2.49	0.44
32:E5:87:LEU:N	32:E5:87:LEU:HD12	2.32	0.44
43:N1:502:LEU:HD21	43:N1:574:LEU:HD12	2.00	0.44
2:1B:129:VAL:HG12	2:1B:129:VAL:O	2.17	0.44
26:BM:3:VAL:O	41:G2:115:ARG:NH2	2.50	0.44
29:E2:9:THR:HG22	29:E2:10:GLY:N	2.32	0.44
32:E5:262:VAL:H	32:E5:285:HIS:HB2	1.82	0.44
40:G1:155:VAL:HG11	42:G3:221:ARG:NH2	2.32	0.44
41:G2:181:VAL:HG23	42:G3:176:VAL:HG21	1.99	0.44
43:N1:582:ILE:HD13	45:N3:212:TYR:HE2	1.83	0.44
46:N4:405:SER:OG	47:N5:187:ILE:HD12	2.17	0.44
56:V1:34:LEU:O	56:V1:39:ARG:NH1	2.45	0.44
56:V1:150:MET:CE	56:V1:242:ILE:HG21	2.48	0.44
56:V1:150:MET:SD	56:V1:242:ILE:HG21	2.58	0.44
24:B9:100:ARG:HD2	66:AC:201:ZMP:H25B	2.00	0.44
26:BM:16:ASN:N	26:BM:16:ASN:OD1	2.50	0.44
28:E1:323:ALA:HB2	28:E1:357:TRP:CE2	2.53	0.44
30:E3:252:VAL:HG11	32:E5:209:PRO:HG3	2.00	0.44
31:E4:251:THR:HG23	31:E4:251:THR:O	2.18	0.44
40:G1:275:ALA:HB1	41:G2:147:VAL:HG11	1.99	0.44
47:N5:466:ILE:HG23	47:N5:467:TYR:N	2.33	0.44
2:1B:177:GLU:HG3	2:1B:477:THR:HG21	1.99	0.44
11:A8:142:THR:HG21	11:A8:192:THR:HG21	1.99	0.44
12:A9:28:PRO:O	12:A9:59:VAL:HG22	2.17	0.44
16:AN:247:TYR:O	16:AN:271:TYR:OH	2.22	0.44
24:B9:39:VAL:HG21	66:AC:201:ZMP:H11	1.99	0.44
30:E3:103:SER:HB3	30:E3:108:LEU:HD11	1.99	0.44
31:E4:170:SER:O	31:E4:173:ALA:HB3	2.17	0.44
32:E5:285:HIS:O	32:E5:286:ILE:HG23	2.18	0.44
33:E6:294:MET:SD	53:S7:52:ARG:NE	2.91	0.44
39:FX:88:LYS:N	39:FX:89:PRO:HD2	2.32	0.44
43:N1:511:LEU:O	43:N1:511:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N5:310:ILE:HD13	47:N5:438:ILE:HG22	1.99	0.44
56:V1:123:PRO:O	57:V2:147:CYS:SG	2.75	0.44
3:2B:67:ASN:N	3:2B:67:ASN:OD1	2.51	0.44
3:2B:109:ILE:O	3:2B:109:ILE:HG23	2.18	0.44
8:A5:67:VAL:HG22	8:A5:106:GLU:OE2	2.18	0.44
9:A6:189:ALA:HB2	33:E6:219:GLN:HG3	1.98	0.44
14:AL:65:ILE:HG23	14:AL:66:VAL:HG13	2.00	0.44
24:B9:8:LEU:HD23	39:FX:96:ILE:HA	1.98	0.44
48:S2:395:ARG:NH2	49:S3:161:GLU:OE1	2.50	0.44
53:S7:118:ILE:HD12	53:S7:139:MET:HE2	1.99	0.44
54:S8:180:ARG:NH1	54:S8:184:ASN:OD1	2.50	0.44
56:V1:456:ASP:O	56:V1:460:ASN:ND2	2.45	0.44
58:E7:122:PRO:O	58:E7:125:GLY:N	2.48	0.44
5:A1:21:TRP:CE3	43:N1:378:LEU:HD22	2.53	0.44
11:A8:105:TYR:OH	15:AM:104:GLN:NE2	2.50	0.44
22:B7:43:GLU:O	22:B7:48:VAL:HG12	2.18	0.44
40:G1:124:ASP:OD1	40:G1:403:ARG:NH2	2.37	0.44
40:G1:130:HIS:NE2	40:G1:346:GLU:OE1	2.51	0.44
40:G1:305:VAL:O	40:G1:309:THR:HG23	2.18	0.44
42:G3:149:ILE:HD12	42:G3:149:ILE:N	2.32	0.44
44:N2:214:ILE:HG23	44:N2:256:LEU:HD21	1.98	0.44
46:N4:131:THR:HG21	46:N4:164:SER:CB	2.48	0.44
47:N5:263:THR:HB	47:N5:342:LEU:HD11	2.00	0.44
56:V1:159:VAL:HG21	56:V1:198:LEU:HD11	2.00	0.44
3:2B:57:PHE:HB2	3:2B:77:PHE:CE1	2.53	0.44
4:4L:144:LEU:HD12	45:N6:154:ILE:HD11	2.00	0.44
11:A8:96:GLN:HB3	11:A8:97:PRO:HD3	1.99	0.44
41:G2:154:ILE:HD12	41:G2:154:ILE:N	2.33	0.44
47:N5:217:ILE:N	47:N5:217:ILE:HD12	2.32	0.44
56:V1:370:ARG:NH1	57:V2:103:VAL:O	2.41	0.44
2:1B:289:MET:SD	2:1B:305:VAL:HG13	2.58	0.43
4:4L:105:ILE:HG22	45:N6:36:ILE:HD11	2.00	0.43
7:A3:53:ARG:HH22	44:N2:27:VAL:HG23	1.83	0.43
11:A8:1:MET:N	44:N2:199:ASN:OD1	2.51	0.43
24:B9:30:ILE:HD13	24:B9:42:LEU:CD2	2.48	0.43
31:E4:336:LEU:HD23	31:E4:336:LEU:C	2.38	0.43
43:N1:582:ILE:HD11	45:N3:214:VAL:HG12	2.00	0.43
49:S3:157:TRP:HE1	50:S4:16:ILE:HG23	1.83	0.43
2:1B:166:VAL:HG21	2:1B:182:LEU:CD1	2.48	0.43
10:A7:54:GLU:OE2	15:AM:28:ARG:NH2	2.48	0.43
20:B5:23:ILE:HG13	41:G2:114:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BL:77:VAL:HG21	26:BM:87:GLU:HG2	2.01	0.43
32:E5:261:VAL:HA	32:E5:285:HIS:HA	1.99	0.43
39:FX:98:ARG:N	59:AC:113:GLU:OE2	2.44	0.43
40:G1:157:ASP:OD1	40:G1:157:ASP:N	2.50	0.43
42:G3:98:GLU:O	42:G3:122:PRO:HA	2.18	0.43
44:N2:17:ILE:HD13	45:N6:145:ILE:HG22	2.00	0.43
46:N4:43:ILE:HD13	46:N4:472:LEU:CD2	2.39	0.43
46:N4:117:SER:OG	46:N4:123:ILE:HD12	2.18	0.43
46:N4:324:TYR:O	46:N4:327:ILE:HG12	2.19	0.43
47:N5:190:ILE:O	47:N5:194:ASN:HA	2.17	0.43
4:4L:119:PHE:HE1	45:N6:131:TYR:HH	1.66	0.43
13:AB:86:ASP:OD1	13:AB:86:ASP:N	2.49	0.43
22:B7:75:HIS:HB3	47:N5:494:ILE:HD12	2.00	0.43
26:BM:5:ARG:HG3	40:G1:305:VAL:HG11	2.00	0.43
28:E1:135:LYS:O	28:E1:157:LEU:HD12	2.18	0.43
30:E3:197:LEU:C	30:E3:197:LEU:HD12	2.38	0.43
45:N3:255:ILE:HA	45:N3:258:ILE:HG22	2.00	0.43
46:N4:110:ILE:HG23	46:N4:126:ILE:HG23	2.01	0.43
47:N5:93:LEU:HD13	47:N5:259:ALA:O	2.18	0.43
52:S6:11:THR:HA	52:S6:14:ILE:HD13	2.01	0.43
52:S6:114:GLN:N	52:S6:114:GLN:OE1	2.51	0.43
57:V2:175:GLU:O	57:V2:178:ILE:HG13	2.18	0.43
58:E7:4:LEU:HD13	58:E7:6:LYS:O	2.18	0.43
2:1B:128:ASP:OD1	2:1B:128:ASP:N	2.51	0.43
10:A7:26:VAL:HG12	15:AM:52:LYS:HD2	1.99	0.43
16:AN:237:PRO:HG2	27:C4:153:VAL:HG23	2.00	0.43
30:E3:242:GLU:OE1	30:E3:242:GLU:N	2.43	0.43
32:E5:7:TRP:HB2	32:E5:96:TYR:HB3	2.00	0.43
40:G1:58:ARG:NE	40:G1:61:GLU:OE1	2.37	0.43
46:N4:55:ILE:HG22	63:N4:502:PC1:H321	2.00	0.43
46:N4:73:ILE:N	46:N4:73:ILE:HD12	2.33	0.43
56:V1:350:LEU:HD11	56:V1:353:ALA:HB2	2.01	0.43
30:E3:45:PRO:HB2	30:E3:70:SER:HB2	2.00	0.43
31:E4:73:ILE:HD12	31:E4:96:VAL:HG13	2.01	0.43
40:G1:114:TRP:CE3	44:N2:30:ILE:HD13	2.53	0.43
46:N4:314:ILE:HG21	46:N4:404:LEU:HD11	2.00	0.43
47:N5:8:LYS:NZ	47:N5:38:LEU:HD12	2.34	0.43
53:S7:90:GLU:HG2	53:S7:183:PRO:O	2.19	0.43
1:1A:52:LEU:HD22	12:A9:32:LEU:HD12	1.99	0.43
4:4L:145:MET:HE2	44:N2:116:VAL:HG13	2.00	0.43
9:A6:77:ARG:NH2	12:A9:434:ASP:O	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:E1:86:THR:HG21	28:E1:92:MET:CE	2.49	0.43
30:E3:321:LEU:HD12	30:E3:321:LEU:N	2.34	0.43
31:E4:128:ILE:HD13	31:E4:148:MET:HE1	2.01	0.43
31:E4:144:LEU:HD12	31:E4:173:ALA:HB2	2.01	0.43
33:E6:277:ARG:NH1	53:S7:27:GLN:O	2.44	0.43
63:E8:301:PC1:H152	64:N5:603:CDL:OB4	2.19	0.43
46:N4:290:GLN:O	46:N4:362:LEU:HD12	2.18	0.43
46:N4:323:LEU:O	46:N4:327:ILE:HG23	2.19	0.43
45:N6:25:ASP:OD1	45:N6:25:ASP:N	2.51	0.43
51:S5:56:GLU:N	51:S5:56:GLU:OE1	2.51	0.43
2:1B:127:THR:O	2:1B:127:THR:CG2	2.66	0.43
27:C4:176:TRP:HE3	46:N4:183:HIS:HE2	1.67	0.43
29:E2:101:PHE:CE1	29:E2:244:ILE:HG22	2.54	0.43
29:E2:422:SER:OG	29:E2:424:ASP:OD1	2.36	0.43
39:FX:144:ASP:HB3	39:FX:169:VAL:HG22	2.00	0.43
42:G3:55:ARG:N	42:G3:73:SER:O	2.52	0.43
46:N4:413:ILE:HG12	47:N5:184:LEU:HD22	1.99	0.43
48:S2:168:ASP:O	54:S8:87:ARG:NH2	2.47	0.43
49:S3:74:ASN:O	49:S3:131:HIS:NE2	2.52	0.43
1:1A:322:ALA:N	1:1A:323:PRO:HD2	2.33	0.43
2:1B:48:ARG:NE	30:E3:336:ILE:HD13	2.34	0.43
28:E1:328:LYS:HB2	28:E1:362:LEU:HD23	2.01	0.43
29:E2:320:HIS:O	29:E2:321:HIS:CG	2.72	0.43
43:N1:643:LEU:HD21	54:S8:56:ILE:HG23	2.01	0.43
56:V1:396:ILE:HG21	56:V1:413:ILE:HB	2.01	0.43
30:E3:91:LEU:HD12	30:E3:91:LEU:N	2.34	0.43
39:FX:98:ARG:HD2	39:FX:102:GLY:O	2.19	0.43
39:FX:190:ILE:HG12	39:FX:223:ARG:O	2.19	0.43
46:N4:305:MET:N	46:N4:305:MET:SD	2.92	0.43
47:N5:117:PHE:HZ	47:N5:252:VAL:HG23	1.83	0.43
48:S2:51:ARG:CD	53:S7:123:THR:HG21	2.49	0.43
54:S8:77:TYR:CG	54:S8:78:PRO:HA	2.54	0.43
56:V1:396:ILE:CB	56:V1:413:ILE:HD13	2.46	0.43
2:1B:386:THR:HA	30:E3:396:LEU:HD21	2.00	0.43
10:A7:54:GLU:OE2	15:AM:28:ARG:NH1	2.50	0.43
19:B4:37:SER:OG	19:B4:46:LEU:O	2.37	0.43
23:B8:124:PHE:CZ	47:N5:496:ILE:HB	2.52	0.43
24:B9:46:ALA:HB2	24:B9:97:ILE:HD11	2.01	0.43
39:FX:250:PRO:O	39:FX:253:THR:HG22	2.19	0.43
46:N4:420:CYS:SG	47:N5:180:VAL:HG22	2.59	0.43
56:V1:141:GLU:OE2	56:V1:257:ARG:NH1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:E7:97:ILE:HG21	58:E7:116:LEU:HD13	2.01	0.43
2:1B:274:ASP:OD1	2:1B:274:ASP:N	2.51	0.42
4:4L:83:VAL:HG11	45:N6:104:PHE:HZ	1.84	0.42
9:A6:227:LEU:O	9:A6:231:VAL:HG23	2.18	0.42
19:B4:24:ILE:HG22	19:B4:110:ARG:HH11	1.84	0.42
40:G1:135:ILE:HD13	40:G1:349:VAL:HG21	2.00	0.42
46:N4:114:PHE:HB2	46:N4:126:ILE:HG21	2.00	0.42
46:N4:191:ILE:HD11	46:N4:257:PHE:CD2	2.54	0.42
46:N4:460:LEU:HD23	46:N4:463:ILE:HD11	2.01	0.42
47:N5:216:ASN:OD1	47:N5:216:ASN:N	2.48	0.42
47:N5:377:HIS:ND1	47:N5:455:ILE:HG21	2.34	0.42
50:S4:61:ILE:O	50:S4:61:ILE:HG23	2.19	0.42
50:S4:72:PRO:O	50:S4:74:ARG:NH1	2.52	0.42
1:1A:197:LYS:HB3	1:1A:248:ILE:CG2	2.49	0.42
12:A9:121:VAL:HG11	12:A9:133:VAL:HG23	2.00	0.42
32:E5:215:VAL:HG23	32:E5:215:VAL:O	2.19	0.42
42:G3:130:GLN:OE1	42:G3:148:LYS:NZ	2.52	0.42
68:N4:505:U10:H303	68:N4:505:U10:H261	2.02	0.42
47:N5:316:CYS:O	47:N5:320:SER:OG	2.34	0.42
3:2B:81:PRO:HB2	46:N4:165:ILE:HD11	2.01	0.42
9:A6:164:THR:O	9:A6:164:THR:HG22	2.19	0.42
24:B9:45:ARG:HG2	24:B9:97:ILE:HG21	2.02	0.42
28:E1:78:VAL:HG22	28:E1:224:ILE:HG23	2.00	0.42
28:E1:412:ILE:O	28:E1:420:THR:HG23	2.19	0.42
43:N1:383:THR:HG22	43:N1:602:TYR:CG	2.54	0.42
46:N4:91:TYR:OH	46:N4:355:ASP:OD2	2.34	0.42
47:N5:28:LEU:HD11	47:N5:118:VAL:HG11	2.02	0.42
47:N5:352:ILE:HD12	47:N5:392:ILE:HG21	2.00	0.42
48:S2:69:MET:HG3	48:S2:84:PHE:HB2	2.01	0.42
54:S8:92:HIS:CE1	61:S8:297:SF4:S2	3.11	0.42
54:S8:126:ASP:OD1	54:S8:127:ASP:N	2.44	0.42
54:S8:153:CYS:HB2	54:S8:158:ILE:HG22	2.01	0.42
56:V1:297:LEU:HD21	56:V1:318:VAL:HG11	2.01	0.42
29:E2:26:LEU:N	29:E2:27:PRO:CD	2.83	0.42
29:E2:69:ARG:NH2	29:E2:155:LEU:O	2.47	0.42
40:G1:154:LEU:HD12	40:G1:177:ILE:HG12	2.01	0.42
40:G1:306:ASP:O	40:G1:309:THR:OG1	2.30	0.42
47:N5:259:ALA:HA	47:N5:263:THR:HG21	2.01	0.42
45:N6:33:ILE:HA	45:N6:36:ILE:HG22	2.01	0.42
49:S3:31:VAL:HG21	49:S3:40:VAL:HG21	2.00	0.42
58:E7:81:VAL:HG11	58:E7:149:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:E7:159:LEU:HD23	58:E7:159:LEU:C	2.40	0.42
10:A7:109:TRP:HZ2	49:S3:128:VAL:HG22	1.85	0.42
26:BM:53:ASP:OD1	26:BM:53:ASP:N	2.44	0.42
34:E8:151:SER:O	34:E8:155:TYR:N	2.43	0.42
48:S2:28:LEU:HD22	48:S2:390:PHE:CZ	2.54	0.42
14:AL:117:GLU:OE1	14:AL:117:GLU:N	2.49	0.42
31:E4:128:ILE:HD13	31:E4:148:MET:CE	2.49	0.42
40:G1:197:ASP:OD1	40:G1:198:ARG:N	2.53	0.42
43:N1:510:PHE:CE2	43:N1:514:LEU:HD11	2.54	0.42
44:N2:10:ILE:HG22	44:N2:14:ILE:HD12	2.01	0.42
46:N4:14:LEU:HD11	63:N4:502:PC1:H362	2.01	0.42
49:S3:56:LEU:HD21	49:S3:78:ILE:HD11	2.02	0.42
66:AC:201:ZMP:H3A	66:AC:201:ZMP:H6	1.45	0.42
1:1A:178:ASP:OD1	1:1A:189:MET:N	2.47	0.42
5:A1:25:GLY:O	5:A1:29:LEU:HG	2.20	0.42
63:A1:202:PC1:H152	63:A1:202:PC1:H11	2.01	0.42
14:AL:124:GLU:HA	14:AL:129:ASN:O	2.20	0.42
27:C4:66:GLU:O	27:C4:69:SER:OG	2.32	0.42
34:E8:1:MET:SD	59:AC:89:LEU:HD13	2.59	0.42
47:N5:57:ASN:HB3	47:N5:85:TYR:HD2	1.85	0.42
48:S2:35:ASN:O	48:S2:36:HIS:HB3	2.20	0.42
56:V1:478:THR:O	56:V1:514:TYR:OH	2.29	0.42
2:1B:410:ALA:HB1	6:A2:95:PHE:HB2	2.01	0.42
26:BM:53:ASP:OD2	46:N4:93:ARG:NE	2.52	0.42
27:C4:106:VAL:HG21	27:C4:108:TRP:CZ2	2.55	0.42
41:G2:126:GLU:HB3	41:G2:127:PRO:HD2	2.00	0.42
44:N2:254:TYR:OH	44:N2:275:THR:OG1	2.20	0.42
56:V1:407:GLY:N	56:V1:408:PRO:HD2	2.34	0.42
4:4L:72:ASP:OD1	4:4L:72:ASP:N	2.53	0.42
9:A6:157:HIS:NE2	9:A6:161:ASN:OD1	2.53	0.42
17:B2:144:VAL:HG22	34:E8:139:ARG:NH1	2.35	0.42
18:B3:25:ALA:O	38:ED:35:ILE:HG22	2.20	0.42
22:B7:86:LYS:NZ	22:B7:90:ASP:OD1	2.49	0.42
39:FX:253:THR:HG23	39:FX:304:TRP:NE1	2.35	0.42
40:G1:184:ASN:O	40:G1:205:PRO:HA	2.20	0.42
42:G3:169:GLN:OE1	42:G3:169:GLN:N	2.53	0.42
44:N2:150:LEU:HD13	44:N2:153:LEU:HD12	2.00	0.42
47:N5:328:ILE:O	47:N5:328:ILE:CG2	2.68	0.42
58:E7:156:ASP:OD2	58:E7:162:LYS:NZ	2.40	0.42
9:A6:90:ARG:NH1	13:AB:93:ASP:OD1	2.53	0.42
9:A6:294:LEU:CD1	9:A6:393:ILE:HD11	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AB:90:ASP:OD1	13:AB:91:SER:N	2.49	0.42
23:B8:87:ASP:OD1	23:B8:87:ASP:N	2.52	0.42
28:E1:438:GLN:HB3	28:E1:445:LEU:HD11	2.02	0.42
31:E4:74:THR:OG1	31:E4:141:SER:OG	2.33	0.42
34:E8:26:THR:N	34:E8:27:PRO:CD	2.83	0.42
47:N5:322:MET:O	47:N5:325:ILE:HG22	2.20	0.42
47:N5:334:ILE:HG23	47:N5:334:ILE:O	2.19	0.42
47:N5:393:LEU:HD21	47:N5:432:GLN:HA	2.01	0.42
48:S2:357:ARG:O	48:S2:357:ARG:HG3	2.20	0.42
4:4L:78:ILE:HG21	4:4L:120:ILE:HG21	2.02	0.41
12:A9:78:LYS:NZ	12:A9:83:GLN:O	2.46	0.41
14:AL:137:THR:OG1	14:AL:138:THR:N	2.53	0.41
28:E1:252:LEU:HD21	28:E1:287:TYR:CZ	2.55	0.41
40:G1:141:LYS:NZ	42:G3:207:GLU:OE2	2.49	0.41
40:G1:211:GLU:OE2	41:G2:87:ARG:NH1	2.53	0.41
40:G1:269:ASP:OD1	40:G1:269:ASP:N	2.53	0.41
41:G2:181:VAL:HG23	42:G3:176:VAL:CG2	2.50	0.41
42:G3:126:ILE:N	42:G3:126:ILE:HD12	2.35	0.41
46:N4:131:THR:HG21	46:N4:164:SER:HB2	2.01	0.41
49:S3:86:ARG:NE	49:S3:147:SER:O	2.42	0.41
53:S7:79:PRO:HA	53:S7:117:LEU:O	2.20	0.41
1:1A:276:ILE:HG22	1:1A:281:LEU:CD2	2.50	0.41
1:1A:369:ASP:HA	9:A6:234:LEU:HD13	2.02	0.41
2:1B:378:ASP:O	2:1B:382:THR:HG23	2.19	0.41
11:A8:142:THR:CG2	11:A8:192:THR:HG21	2.49	0.41
14:AL:88:THR:O	14:AL:92:GLY:N	2.50	0.41
16:AN:86:ARG:NH1	16:AN:121:TYR:OH	2.53	0.41
23:B8:45:PRO:HB3	23:B8:62:TRP:CE2	2.55	0.41
42:G3:136:TYR:CD2	42:G3:192:ILE:HG23	2.55	0.41
44:N2:81:ILE:HD11	45:N6:153:ILE:HD12	2.01	0.41
44:N2:131:TYR:CE2	44:N2:174:LEU:HD22	2.55	0.41
47:N5:491:TYR:OH	47:N5:493:ASN:ND2	2.52	0.41
48:S2:75:MET:SD	48:S2:118:LEU:HD13	2.59	0.41
57:V2:105:THR:HB	57:V2:106:PRO:HD3	2.02	0.41
4:4L:144:LEU:HD11	45:N6:151:PHE:CZ	2.55	0.41
6:A2:27:GLU:HA	6:A2:30:ALA:HB3	2.02	0.41
8:A5:22:THR:O	8:A5:22:THR:HG23	2.20	0.41
9:A6:62:TYR:CZ	9:A6:66:LEU:HD11	2.56	0.41
9:A6:178:THR:HB	33:E6:179:LEU:HD13	2.02	0.41
23:B8:71:TYR:O	46:N4:363:TYR:OH	2.37	0.41
30:E3:286:ILE:CG1	30:E3:291:LEU:HD23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:S2:243:TYR:N	48:S2:244:PRO:HD2	2.36	0.41
3:2B:75:LEU:HD13	44:N2:221:ILE:HG21	2.02	0.41
19:B4:144:GLY:O	47:N5:216:ASN:ND2	2.53	0.41
27:C4:63:LEU:HD11	27:C4:140:ARG:NH1	2.36	0.41
28:E1:437:ALA:HB2	28:E1:456:VAL:HG13	2.03	0.41
29:E2:417:GLU:OE1	29:E2:417:GLU:N	2.53	0.41
46:N4:299:LEU:HD23	46:N4:302:ILE:HD12	2.03	0.41
45:N6:46:ILE:HD12	45:N6:46:ILE:N	2.35	0.41
54:S8:86:THR:OG1	54:S8:199:GLU:OE2	2.38	0.41
54:S8:109:LEU:O	54:S8:113:THR:HG22	2.20	0.41
3:2B:48:ASN:ND2	3:2B:126:UNK:O	2.53	0.41
6:A2:45:LEU:HD22	49:S3:272:PRO:HD2	2.02	0.41
64:B3:102:CDL:OB3	38:ED:43:TRP:NE1	2.42	0.41
19:B4:141:TRP:CG	63:E8:302:PC1:H133	2.56	0.41
40:G1:120:PHE:O	40:G1:122:LEU:N	2.52	0.41
46:N4:225:ILE:HG23	47:N5:568:MET:SD	2.60	0.41
46:N4:411:LEU:O	46:N4:415:LEU:HG	2.20	0.41
47:N5:250:THR:HG21	47:N5:357:GLY:HA2	2.02	0.41
47:N5:266:ILE:HD12	47:N5:266:ILE:N	2.36	0.41
47:N5:299:PHE:CE1	47:N5:430:LEU:HD11	2.55	0.41
48:S2:135:TRP:O	48:S2:138:GLU:HG3	2.20	0.41
49:S3:149:THR:N	49:S3:150:PRO:HD2	2.36	0.41
49:S3:205:ASP:O	49:S3:209:SER:N	2.52	0.41
50:S4:59:GLU:OE2	50:S4:62:ARG:NH2	2.45	0.41
56:V1:396:ILE:CG2	56:V1:413:ILE:HD13	2.50	0.41
12:A9:158:MET:N	53:S7:66:SER:OG	2.54	0.41
12:A9:200:ASN:ND2	12:A9:200:ASN:O	2.54	0.41
28:E1:100:GLN:NE2	28:E1:287:TYR:OH	2.52	0.41
31:E4:243:ILE:HD12	31:E4:307:VAL:HG21	2.02	0.41
31:E4:245:PRO:HG2	31:E4:317:ILE:HD13	2.02	0.41
32:E5:260:LYS:HB2	32:E5:284:VAL:H	1.84	0.41
34:E8:112:MET:SD	34:E8:134:LEU:HD21	2.61	0.41
44:N2:81:ILE:HD12	45:N6:153:ILE:HD12	2.02	0.41
47:N5:63:LEU:HD11	47:N5:79:GLU:HB3	2.02	0.41
49:S3:103:LEU:HD21	49:S3:106:VAL:CG2	2.51	0.41
50:S4:99:GLU:HG2	50:S4:100:TRP:N	2.35	0.41
57:V2:167:ASP:HB3	57:V2:192:VAL:HG13	2.01	0.41
2:1B:142:THR:HG21	50:S4:158:GLU:OE1	2.21	0.41
10:A7:107:PHE:CE2	10:A7:109:TRP:HA	2.55	0.41
12:A9:260:LYS:NZ	65:A9:559:NDP:O2D	2.42	0.41
26:BM:53:ASP:OD2	46:N4:93:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:E3:45:PRO:HD3	30:E3:121:SER:HB2	2.02	0.41
34:E8:115:TYR:CE2	34:E8:119:ILE:HD11	2.55	0.41
41:G2:117:VAL:HG22	41:G2:133:PRO:HA	2.03	0.41
44:N2:214:ILE:HG22	44:N2:218:PHE:CE2	2.56	0.41
14:AL:210:ARG:NH1	54:S8:172:ASP:OD1	2.54	0.41
16:AN:245:MET:O	27:C4:152:ARG:NH1	2.46	0.41
21:B6:12:ASP:OD1	21:B6:13:PHE:N	2.52	0.41
30:E3:156:LEU:CD1	30:E3:184:LEU:HD22	2.49	0.41
34:E8:25:MET:SD	47:N5:532:ILE:HG21	2.61	0.41
39:FX:171:LEU:HB3	39:FX:186:SER:HA	2.03	0.41
44:N2:122:ILE:N	44:N2:122:ILE:HD12	2.36	0.41
47:N5:241:TRP:HH2	47:N5:261:LEU:HD23	1.86	0.41
47:N5:329:ASP:HA	47:N5:334:ILE:HG22	2.03	0.41
49:S3:193:ASP:OD1	49:S3:193:ASP:N	2.51	0.41
54:S8:161:THR:HA	54:S8:192:ILE:HD11	2.02	0.41
57:V2:11:VAL:HG11	57:V2:93:PRO:HG3	2.02	0.41
1:1A:48:ILE:HD13	1:1A:67:ALA:HB2	2.03	0.41
2:1B:243:ALA:O	2:1B:247:TYR:N	2.53	0.41
3:2B:63:ILE:C	3:2B:63:ILE:HD12	2.41	0.41
10:A7:112:HIS:CD2	31:E4:31:VAL:HG22	2.56	0.41
11:A8:10:THR:HG22	20:B5:105:VAL:CG1	2.50	0.41
64:AM:217:CDL:OB3	54:S8:49:ASN:ND2	2.53	0.41
21:B6:13:PHE:O	47:N5:21:ASN:ND2	2.54	0.41
25:BL:65:TYR:OH	46:N4:49:SER:O	2.38	0.41
27:C4:63:LEU:O	27:C4:68:GLN:NE2	2.50	0.41
32:E5:9:PHE:HB3	32:E5:20:LEU:HD23	2.02	0.41
35:EA:4:GLN:OE1	44:N2:184:ASN:ND2	2.53	0.41
39:FX:191:SER:O	39:FX:195:PHE:HB2	2.21	0.41
42:G3:134:GLY:O	42:G3:196:ARG:NH2	2.51	0.41
43:N1:437:CYS:SG	43:N1:438:ILE:N	2.93	0.41
43:N1:660:LEU:HB3	43:N1:661:PRO:HD3	2.03	0.41
46:N4:89:ILE:CG2	46:N4:104:ILE:HG21	2.51	0.41
47:N5:431:SER:HA	47:N5:434:TYR:CE2	2.55	0.41
47:N5:481:LEU:N	47:N5:482:PRO:CD	2.84	0.41
48:S2:134:LEU:H	48:S2:134:LEU:HD12	1.86	0.41
49:S3:30:GLU:OE1	49:S3:246:TYR:OH	2.32	0.41
49:S3:98:PHE:CD1	49:S3:98:PHE:N	2.87	0.41
49:S3:100:TYR:CE2	49:S3:133:VAL:HG13	2.56	0.41
54:S8:153:CYS:HA	61:S8:298:SF4:S3	2.61	0.41
1:1A:97:VAL:HG12	1:1A:97:VAL:O	2.21	0.41
2:1B:44:ARG:O	2:1B:44:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2B:57:PHE:CZ	3:2B:61:ILE:HD11	2.56	0.41
14:AL:123:GLY:HA3	14:AL:164:TRP:CZ2	2.56	0.41
27:C4:7:THR:HG23	27:C4:7:THR:O	2.21	0.41
32:E5:133:LEU:HD12	32:E5:160:LEU:HB3	2.03	0.41
32:E5:194:LEU:CD1	32:E5:226:VAL:HG11	2.51	0.41
39:FX:256:PHE:HB3	39:FX:282:PRO:HB3	2.02	0.41
44:N2:171:ILE:HD11	44:N2:248:ILE:HG13	2.01	0.41
45:N3:235:ASN:OD1	45:N3:235:ASN:N	2.53	0.41
46:N4:13:ILE:HG12	46:N4:35:ILE:HD13	2.02	0.41
47:N5:141:PHE:HB2	47:N5:186:ILE:HD11	2.03	0.41
47:N5:215:ILE:HG23	47:N5:216:ASN:N	2.35	0.41
47:N5:424:PHE:N	47:N5:424:PHE:CD1	2.89	0.41
50:S4:31:THR:O	50:S4:31:THR:HG22	2.20	0.41
56:V1:108:ASP:OD1	56:V1:108:ASP:N	2.53	0.41
4:4L:83:VAL:HG11	45:N6:104:PHE:CZ	2.56	0.40
9:A6:76:PHE:O	9:A6:130:GLN:NE2	2.54	0.40
12:A9:142:THR:HG21	14:AL:218:PRO:CG	2.51	0.40
19:B4:24:ILE:HG23	23:B8:61:HIS:O	2.22	0.40
20:B5:94:ARG:CZ	46:N4:179:TYR:OH	2.69	0.40
25:BL:60:THR:HG22	25:BL:62:ALA:H	1.86	0.40
29:E2:424:ASP:HA	29:E2:452:LYS:CE	2.51	0.40
30:E3:237:PRO:HG3	32:E5:216:LEU:HD22	2.03	0.40
31:E4:83:ARG:HA	31:E4:86:VAL:HG22	2.03	0.40
34:E8:98:SER:OG	34:E8:117:LYS:NZ	2.54	0.40
39:FX:187:HIS:O	39:FX:242:PRO:HD3	2.21	0.40
41:G2:222:GLN:HA	41:G2:228:ILE:HD12	2.03	0.40
43:N1:565:ILE:HG12	43:N1:572:VAL:HG11	2.03	0.40
44:N2:157:PHE:HA	44:N2:160:TYR:HB2	2.03	0.40
47:N5:503:ILE:HD12	47:N5:508:LEU:HD11	2.02	0.40
48:S2:270:ARG:O	48:S2:273:ILE:HG12	2.21	0.40
49:S3:232:GLU:HG3	50:S4:78:MET:HB3	2.03	0.40
1:1A:182:ASN:OD1	1:1A:237:VAL:HB	2.21	0.40
2:1B:191:THR:O	2:1B:227:THR:HG22	2.21	0.40
18:B3:58:UNK:O	18:B3:59:UNK:C	2.69	0.40
28:E1:110:PRO:O	28:E1:111:ALA:HB3	2.21	0.40
29:E2:331:ARG:NH1	29:E2:401:PRO:O	2.54	0.40
39:FX:287:PRO:HD3	39:FX:307:THR:HG22	2.02	0.40
48:S2:65:VAL:O	48:S2:68:TYR:HB2	2.22	0.40
48:S2:241:GLU:O	56:V1:492:SER:CB	2.69	0.40
49:S3:124:PHE:HB2	49:S3:133:VAL:HG23	2.03	0.40
57:V2:148:VAL:HG23	57:V2:149:HIS:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:E7:180:ASP:OD1	58:E7:181:SER:N	2.54	0.40
2:1B:63:LEU:CD1	2:1B:352:LEU:HD12	2.45	0.40
3:2B:58:LEU:HD12	64:N4:501:CDL:H831	2.04	0.40
5:A1:130:PRO:O	5:A1:131:LYS:HB3	2.20	0.40
8:A5:143:LYS:NZ	8:A5:151:GLU:OE2	2.29	0.40
12:A9:256:PHE:O	12:A9:260:LYS:HG3	2.22	0.40
12:A9:309:THR:OG1	12:A9:310:TYR:N	2.54	0.40
21:B6:74:ASN:ND2	38:ED:130:PRO:O	2.52	0.40
28:E1:252:LEU:HD12	28:E1:394:LEU:HD11	2.02	0.40
30:E3:72:VAL:HG12	30:E3:121:SER:HB3	2.04	0.40
30:E3:210:PHE:HZ	30:E3:234:ILE:HD12	1.87	0.40
32:E5:40:ALA:HA	32:E5:289:LEU:N	2.36	0.40
40:G1:321:HIS:ND1	40:G1:321:HIS:C	2.75	0.40
44:N2:50:ILE:HD12	44:N2:62:ILE:HG21	2.03	0.40
45:N6:118:ASN:OD1	45:N6:120:ASN:ND2	2.54	0.40
45:N6:151:PHE:O	45:N6:154:ILE:HG13	2.21	0.40
48:S2:72:LEU:CD1	48:S2:356:ILE:HD13	2.51	0.40
49:S3:73:THR:O	49:S3:74:ASN:HB2	2.21	0.40
49:S3:106:VAL:HG22	49:S3:122:TYR:HD1	1.86	0.40
54:S8:145:TYR:HH	54:S8:166:PHE:HZ	1.66	0.40
2:1B:424:LEU:HB2	12:A9:89:LEU:HD11	2.03	0.40
27:C4:114:PHE:CZ	64:C4:202:CDL:OA7	2.74	0.40
29:E2:28:LEU:HD12	29:E2:29:VAL:HG23	2.03	0.40
35:EA:68:GLU:O	35:EA:69:THR:HG23	2.22	0.40
44:N2:174:LEU:HD23	44:N2:175:TYR:CE1	2.57	0.40
45:N3:239:TYR:OH	45:N6:88:ASN:ND2	2.43	0.40
46:N4:218:LEU:HD13	46:N4:309:TYR:CE1	2.55	0.40
48:S2:91:LEU:HD23	48:S2:323:ILE:CG2	2.52	0.40
1:1A:80:ASN:ND2	1:1A:82:ASN:OD1	2.53	0.40
2:1B:450:ASN:HA	2:1B:456:SER:OG	2.22	0.40
3:2B:68:ILE:O	3:2B:71:ILE:N	2.55	0.40
7:A3:70:TYR:N	7:A3:71:PRO:HD2	2.36	0.40
9:A6:367:LEU:O	9:A6:371:LEU:HG	2.22	0.40
12:A9:398:ILE:HG12	12:A9:402:LEU:HD12	2.03	0.40
27:C4:9:ARG:NH2	44:N2:147:ILE:O	2.49	0.40
31:E4:44:VAL:HG23	31:E4:60:ILE:HD11	2.03	0.40
37:EC:31:GLN:N	37:EC:32:PRO:HD2	2.37	0.40
40:G1:162:PRO:HA	40:G1:180:ALA:O	2.21	0.40
44:N2:293:ASN:OD1	44:N2:294:ASN:N	2.54	0.40
46:N4:2:ILE:HG23	46:N4:3:TYR:N	2.36	0.40
46:N4:376:PHE:CE2	46:N4:380:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:N4:376:PHE:CZ	46:N4:380:LEU:HD11	2.57	0.40
47:N5:393:LEU:CD2	47:N5:432:GLN:HA	2.52	0.40
50:S4:44:ALA:HB3	50:S4:47:GLN:HG3	2.03	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	350/385 (91%)	335 (96%)	15 (4%)	0	100	100
2	1B	523/527 (99%)	501 (96%)	22 (4%)	0	100	100
3	2B	112/142 (79%)	103 (92%)	9 (8%)	0	100	100
4	4L	106/171 (62%)	104 (98%)	2 (2%)	0	100	100
5	A1	135/141 (96%)	124 (92%)	11 (8%)	0	100	100
6	A2	190/193 (98%)	186 (98%)	4 (2%)	0	100	100
7	A3	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
8	A5	152/184 (83%)	149 (98%)	3 (2%)	0	100	100
9	A6	421/437 (96%)	405 (96%)	16 (4%)	0	100	100
10	A7	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
11	A8	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
12	A9	482/489 (99%)	463 (96%)	19 (4%)	0	100	100
13	AB	86/134 (64%)	83 (96%)	3 (4%)	0	100	100
14	AL	263/281 (94%)	248 (94%)	15 (6%)	0	100	100
15	AM	182/198 (92%)	175 (96%)	7 (4%)	0	100	100
16	AN	285/287 (99%)	281 (99%)	4 (1%)	0	100	100
17	B2	103/145 (71%)	103 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	B3	32/62 (52%)	31 (97%)	1 (3%)	0	100	100
19	B4	169/171 (99%)	154 (91%)	15 (9%)	0	100	100
20	B5	132/140 (94%)	130 (98%)	2 (2%)	0	100	100
21	B6	89/91 (98%)	89 (100%)	0	0	100	100
22	B7	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
23	B8	145/176 (82%)	133 (92%)	12 (8%)	0	100	100
24	B9	149/158 (94%)	140 (94%)	9 (6%)	0	100	100
25	BL	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
26	BM	99/112 (88%)	98 (99%)	1 (1%)	0	100	100
27	C4	181/185 (98%)	174 (96%)	7 (4%)	0	100	100
28	E1	448/483 (93%)	434 (97%)	14 (3%)	0	100	100
29	E2	464/467 (99%)	445 (96%)	19 (4%)	0	100	100
30	E3	430/434 (99%)	420 (98%)	10 (2%)	0	100	100
31	E4	349/368 (95%)	338 (97%)	11 (3%)	0	100	100
32	E5	266/290 (92%)	245 (92%)	20 (8%)	1 (0%)	30	61
33	E6	314/371 (85%)	310 (99%)	4 (1%)	0	100	100
34	E8	203/205 (99%)	191 (94%)	12 (6%)	0	100	100
35	EA	96/126 (76%)	92 (96%)	4 (4%)	0	100	100
36	EB	73/101 (72%)	72 (99%)	1 (1%)	0	100	100
37	EC	83/101 (82%)	77 (93%)	6 (7%)	0	100	100
38	ED	136/151 (90%)	130 (96%)	6 (4%)	0	100	100
39	FX	235/325 (72%)	224 (95%)	10 (4%)	1 (0%)	30	61
40	G1	401/436 (92%)	380 (95%)	21 (5%)	0	100	100
41	G2	234/267 (88%)	218 (93%)	16 (7%)	0	100	100
42	G3	253/261 (97%)	235 (93%)	18 (7%)	0	100	100
43	N1	308/670 (46%)	289 (94%)	19 (6%)	0	100	100
44	N2	294/300 (98%)	279 (95%)	15 (5%)	0	100	100
45	N3	119/293 (41%)	115 (97%)	4 (3%)	0	100	100
45	N6	152/293 (52%)	146 (96%)	6 (4%)	0	100	100
46	N4	476/478 (100%)	461 (97%)	15 (3%)	0	100	100
47	N5	582/584 (100%)	552 (95%)	30 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
48	S2	391/395 (99%)	369 (94%)	21 (5%)	1 (0%)	37 67
49	S3	246/277 (89%)	235 (96%)	11 (4%)	0	100 100
50	S4	188/208 (90%)	174 (93%)	14 (7%)	0	100 100
51	S5	110/122 (90%)	108 (98%)	2 (2%)	0	100 100
52	S6	145/147 (99%)	137 (94%)	8 (6%)	0	100 100
53	S7	195/207 (94%)	182 (93%)	13 (7%)	0	100 100
54	S8	180/212 (85%)	176 (98%)	4 (2%)	0	100 100
56	V1	502/526 (95%)	478 (95%)	24 (5%)	0	100 100
57	V2	220/225 (98%)	211 (96%)	9 (4%)	0	100 100
58	E7	244/246 (99%)	238 (98%)	6 (2%)	0	100 100
59	AC	90/134 (67%)	88 (98%)	2 (2%)	0	100 100
All	All	13527/15237 (89%)	12943 (96%)	581 (4%)	3 (0%)	100 100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	E5	288	THR
48	S2	36	HIS
39	FX	276	VAL

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	310/340 (91%)	305 (98%)	5 (2%)	58 77
2	1B	453/454 (100%)	448 (99%)	5 (1%)	70 83
3	2B	109/111 (98%)	105 (96%)	4 (4%)	29 57
4	4L	96/151 (64%)	96 (100%)	0	100 100
5	A1	115/118 (98%)	112 (97%)	3 (3%)	41 66
6	A2	159/160 (99%)	158 (99%)	1 (1%)	84 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A3	104/104 (100%)	102 (98%)	2 (2%)	52	73
8	A5	134/152 (88%)	130 (97%)	4 (3%)	36	62
9	A6	346/358 (97%)	343 (99%)	3 (1%)	75	87
10	A7	119/119 (100%)	118 (99%)	1 (1%)	79	89
11	A8	196/196 (100%)	193 (98%)	3 (2%)	60	78
12	A9	420/424 (99%)	417 (99%)	3 (1%)	81	90
13	AB	79/114 (69%)	79 (100%)	0	100	100
14	AL	228/242 (94%)	226 (99%)	2 (1%)	75	87
15	AM	156/168 (93%)	155 (99%)	1 (1%)	84	91
16	AN	241/241 (100%)	239 (99%)	2 (1%)	79	89
17	B2	97/131 (74%)	96 (99%)	1 (1%)	73	85
18	B3	30/31 (97%)	30 (100%)	0	100	100
19	B4	144/144 (100%)	141 (98%)	3 (2%)	48	71
20	B5	108/108 (100%)	108 (100%)	0	100	100
21	B6	82/82 (100%)	81 (99%)	1 (1%)	67	82
22	B7	93/93 (100%)	91 (98%)	2 (2%)	47	69
23	B8	127/148 (86%)	123 (97%)	4 (3%)	35	61
24	B9	132/139 (95%)	129 (98%)	3 (2%)	45	68
25	BL	132/132 (100%)	130 (98%)	2 (2%)	60	78
26	BM	93/93 (100%)	91 (98%)	2 (2%)	47	69
27	C4	166/167 (99%)	163 (98%)	3 (2%)	54	75
28	E1	381/404 (94%)	379 (100%)	2 (0%)	86	92
29	E2	379/380 (100%)	375 (99%)	4 (1%)	70	83
30	E3	339/341 (99%)	334 (98%)	5 (2%)	60	78
31	E4	302/317 (95%)	295 (98%)	7 (2%)	45	68
32	E5	200/205 (98%)	196 (98%)	4 (2%)	50	72
33	E6	272/314 (87%)	267 (98%)	5 (2%)	54	75
34	E8	179/179 (100%)	176 (98%)	3 (2%)	56	76
35	EA	84/86 (98%)	84 (100%)	0	100	100
36	EB	70/70 (100%)	70 (100%)	0	100	100
37	EC	73/86 (85%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	ED	121/133 (91%)	120 (99%)	1 (1%)	79 89
39	FX	212/276 (77%)	209 (99%)	3 (1%)	62 79
40	G1	333/365 (91%)	325 (98%)	8 (2%)	44 68
41	G2	192/214 (90%)	189 (98%)	3 (2%)	58 77
42	G3	202/202 (100%)	202 (100%)	0	100 100
43	N1	295/639 (46%)	288 (98%)	7 (2%)	44 68
44	N2	285/289 (99%)	280 (98%)	5 (2%)	54 75
45	N3	116/281 (41%)	111 (96%)	5 (4%)	25 53
45	N6	147/281 (52%)	143 (97%)	4 (3%)	40 65
46	N4	455/455 (100%)	448 (98%)	7 (2%)	60 78
47	N5	546/546 (100%)	531 (97%)	15 (3%)	40 65
48	S2	335/336 (100%)	328 (98%)	7 (2%)	48 71
49	S3	224/250 (90%)	216 (96%)	8 (4%)	30 58
50	S4	159/172 (92%)	155 (98%)	4 (2%)	42 67
51	S5	102/102 (100%)	101 (99%)	1 (1%)	73 85
52	S6	130/130 (100%)	127 (98%)	3 (2%)	45 68
53	S7	165/171 (96%)	162 (98%)	3 (2%)	54 75
54	S8	160/187 (86%)	158 (99%)	2 (1%)	65 80
56	V1	412/427 (96%)	403 (98%)	9 (2%)	47 69
57	V2	190/190 (100%)	181 (95%)	9 (5%)	22 50
58	E7	192/192 (100%)	189 (98%)	3 (2%)	58 77
59	AC	80/111 (72%)	78 (98%)	2 (2%)	42 67
All	All	11801/13051 (90%)	11602 (98%)	199 (2%)	56 76

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	159	LEU
1	1A	191	ARG
1	1A	219	ARG
1	1A	257	ARG
1	1A	310	LEU
2	1B	108	GLU
2	1B	211	ASN

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Mol	Chain	Res	Type
2	1B	230	SER
2	1B	290	CYS
2	1B	527	LYS
3	2B	5	LEU
3	2B	33	TYR
3	2B	66	ASN
3	2B	67	ASN
5	A1	8	SER
5	A1	37	HIS
5	A1	60	ASN
6	A2	118	ASP
7	A3	15	THR
7	A3	53	ARG
8	A5	38	LYS
8	A5	40	ARG
8	A5	60	ASP
8	A5	66	SER
9	A6	211	ASP
9	A6	236	HIS
9	A6	346	GLU
10	A7	22	GLN
11	A8	38	ASP
11	A8	48	ASP
11	A8	123	GLU
12	A9	190	GLN
12	A9	392	GLU
12	A9	436	MET
14	AL	63	ARG
14	AL	183	HIS
15	AM	87	ASP
16	AN	14	SER
16	AN	256	CYS
17	B2	65	ARG
19	B4	22	ASP
19	B4	24	ILE
19	B4	87	SER
21	B6	25	ARG
22	B7	5	ASN
22	B7	31	ASP
23	B8	51	PHE
23	B8	87	ASP
23	B8	107	LEU

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Mol	Chain	Res	Type
23	B8	125	SER
24	B9	45	ARG
24	B9	93	PHE
24	B9	130	GLN
25	BL	32	ARG
25	BL	76	SER
26	BM	30	HIS
26	BM	81	ASN
27	C4	81	ASP
27	C4	131	PHE
27	C4	145	LEU
28	E1	60	ASN
28	E1	84	PHE
29	E2	135	THR
29	E2	170	ASP
29	E2	325	THR
29	E2	400	ARG
30	E3	7	THR
30	E3	20	GLN
30	E3	301	PHE
30	E3	306	ASP
30	E3	342	ASP
31	E4	89	GLU
31	E4	142	GLN
31	E4	170	SER
31	E4	206	ASP
31	E4	208	SER
31	E4	280	ASP
31	E4	304	ARG
32	E5	24	ASP
32	E5	36	LEU
32	E5	106	HIS
32	E5	147	ASP
33	E6	30	ASP
33	E6	79	ILE
33	E6	201	ASN
33	E6	204	GLN
33	E6	209	HIS
34	E8	1	MET
34	E8	18	TRP
34	E8	94	ASP
38	ED	129	GLN

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Mol	Chain	Res	Type
39	FX	109	HIS
39	FX	172	ASP
39	FX	221	ASN
40	G1	158	ASP
40	G1	161	THR
40	G1	251	ASP
40	G1	266	ARG
40	G1	321	HIS
40	G1	339	ASP
40	G1	390	ASP
40	G1	399	SER
41	G2	24	ASP
41	G2	108	ARG
41	G2	138	ASP
43	N1	437	CYS
43	N1	452	TYR
43	N1	557	TYR
43	N1	597	PHE
43	N1	622	PHE
43	N1	648	TYR
43	N1	652	PHE
44	N2	44	PHE
44	N2	96	ASN
44	N2	155	SER
44	N2	230	PHE
44	N2	268	PHE
45	N3	235	ASN
45	N3	258	ILE
45	N3	264	ASN
45	N3	289	PHE
45	N3	292	ASN
46	N4	10	TYR
46	N4	28	GLU
46	N4	70	TYR
46	N4	76	TYR
46	N4	156	SER
46	N4	368	ASN
46	N4	397	GLU
47	N5	72	TYR
47	N5	85	TYR
47	N5	172	VAL
47	N5	257	HIS

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Mol	Chain	Res	Type
47	N5	273	ARG
47	N5	285	LEU
47	N5	304	TYR
47	N5	320	SER
47	N5	349	LYS
47	N5	350	SER
47	N5	369	ARG
47	N5	393	LEU
47	N5	524	ASN
47	N5	533	HIS
47	N5	536	ARG
45	N6	77	SER
45	N6	90	MET
45	N6	108	TYR
45	N6	150	MET
48	S2	4	ARG
48	S2	70	ASP
48	S2	133	ILE
48	S2	187	ARG
48	S2	260	ASP
48	S2	357	ARG
48	S2	394	ASP
49	S3	31	VAL
49	S3	41	LYS
49	S3	65	SER
49	S3	70	ASP
49	S3	108	CYS
49	S3	121	VAL
49	S3	160	ARG
49	S3	247	ASP
50	S4	16	ILE
50	S4	28	GLU
50	S4	47	GLN
50	S4	74	ARG
51	S5	20	GLU
52	S6	1	MET
52	S6	36	GLU
52	S6	60	LYS
53	S7	42	GLU
53	S7	86	CYS
53	S7	157	TYR
54	S8	72	SER

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Mol	Chain	Res	Type
54	S8	138	LEU
56	V1	103	LYS
56	V1	112	SER
56	V1	209	GLU
56	V1	278	CYS
56	V1	339	ASP
56	V1	386	CYS
56	V1	424	SER
56	V1	487	ASP
56	V1	502	ASN
57	V2	100	GLN
57	V2	114	GLU
57	V2	117	HIS
57	V2	120	CYS
57	V2	125	VAL
57	V2	133	ASP
57	V2	141	MET
57	V2	175	GLU
57	V2	215	ARG
58	E7	99	HIS
58	E7	169	THR
58	E7	175	TYR
59	AC	80	ASP
59	AC	91	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	56	GLN
1	1A	80	ASN
1	1A	82	ASN
1	1A	128	GLN
1	1A	194	HIS
1	1A	260	ASN
1	1A	304	GLN
1	1A	326	ASN
2	1B	33	ASN
2	1B	149	ASN
2	1B	155	HIS
2	1B	157	HIS
2	1B	242	ASN
2	1B	315	ASN

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Mol	Chain	Res	Type
2	1B	481	GLN
2	1B	500	HIS
2	1B	507	HIS
3	2B	3	ASN
3	2B	26	ASN
3	2B	98	ASN
3	2B	102	ASN
4	4L	66	GLN
5	A1	60	ASN
5	A1	67	GLN
5	A1	121	HIS
6	A2	12	HIS
6	A2	113	HIS
6	A2	115	HIS
7	A3	28	GLN
7	A3	34	ASN
9	A6	107	HIS
9	A6	350	GLN
10	A7	22	GLN
10	A7	56	GLN
10	A7	92	GLN
10	A7	124	GLN
11	A8	23	HIS
11	A8	27	GLN
11	A8	52	HIS
11	A8	54	HIS
11	A8	83	ASN
11	A8	96	GLN
11	A8	134	HIS
11	A8	182	GLN
12	A9	79	GLN
12	A9	154	HIS
12	A9	165	GLN
12	A9	174	GLN
12	A9	288	ASN
12	A9	368	GLN
12	A9	401	HIS
14	AL	20	GLN
14	AL	107	GLN
14	AL	201	HIS
14	AL	219	HIS
15	AM	25	GLN

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Mol	Chain	Res	Type
15	AM	73	GLN
15	AM	104	GLN
16	AN	20	HIS
16	AN	154	GLN
16	AN	156	GLN
17	B2	119	HIS
19	B4	69	GLN
19	B4	92	HIS
20	B5	100	GLN
22	B7	5	ASN
23	B8	61	HIS
23	B8	63	ASN
23	B8	91	GLN
23	B8	113	ASN
23	B8	156	GLN
24	B9	20	GLN
24	B9	112	ASN
25	BL	3	GLN
26	BM	99	GLN
28	E1	177	GLN
28	E1	192	GLN
28	E1	204	ASN
28	E1	223	HIS
28	E1	395	ASN
29	E2	20	GLN
29	E2	58	ASN
29	E2	153	HIS
29	E2	201	ASN
29	E2	344	GLN
30	E3	20	GLN
30	E3	99	GLN
30	E3	232	HIS
30	E3	303	ASN
30	E3	313	HIS
30	E3	355	GLN
30	E3	365	GLN
31	E4	59	HIS
31	E4	146	ASN
32	E5	264	HIS
33	E6	49	GLN
33	E6	57	ASN
33	E6	184	ASN

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Mol	Chain	Res	Type
33	E6	222	GLN
34	E8	19	ASN
35	EA	49	HIS
37	EC	97	HIS
38	ED	89	GLN
38	ED	139	HIS
39	FX	124	HIS
39	FX	133	GLN
39	FX	166	GLN
40	G1	105	HIS
40	G1	148	ASN
40	G1	191	HIS
40	G1	333	ASN
40	G1	404	GLN
40	G1	413	ASN
41	G2	36	HIS
42	G3	140	ASN
43	N1	402	ASN
43	N1	409	GLN
43	N1	426	ASN
43	N1	440	ASN
43	N1	476	HIS
44	N2	4	ASN
44	N2	6	ASN
44	N2	28	ASN
44	N2	40	ASN
44	N2	43	ASN
44	N2	55	ASN
44	N2	75	ASN
44	N2	76	ASN
44	N2	79	GLN
44	N2	82	HIS
44	N2	89	ASN
44	N2	208	ASN
44	N2	209	HIS
44	N2	294	ASN
45	N3	172	ASN
45	N3	180	ASN
45	N3	219	ASN
45	N3	264	ASN
46	N4	48	GLN
46	N4	71	ASN

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Mol	Chain	Res	Type
46	N4	112	ASN
46	N4	189	HIS
46	N4	209	ASN
46	N4	231	HIS
46	N4	254	HIS
46	N4	304	HIS
46	N4	321	ASN
46	N4	339	HIS
46	N4	366	ASN
47	N5	17	ASN
47	N5	49	ASN
47	N5	95	ASN
47	N5	235	GLN
47	N5	345	HIS
47	N5	366	GLN
47	N5	453	HIS
47	N5	493	ASN
47	N5	499	HIS
47	N5	524	ASN
47	N5	525	HIS
47	N5	533	HIS
47	N5	553	HIS
47	N5	572	HIS
45	N6	159	ASN
45	N6	165	ASN
48	S2	36	HIS
48	S2	50	HIS
48	S2	115	ASN
48	S2	278	GLN
48	S2	309	ASN
48	S2	344	GLN
48	S2	372	GLN
49	S3	99	GLN
49	S3	153	HIS
49	S3	173	HIS
49	S3	208	ASN
50	S4	39	ASN
50	S4	139	ASN
51	S5	75	GLN
52	S6	98	HIS
52	S6	136	GLN
53	S7	27	GLN

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Mol	Chain	Res	Type
53	S7	31	GLN
53	S7	37	GLN
53	S7	159	HIS
54	S8	70	GLN
54	S8	108	GLN
56	V1	50	GLN
56	V1	502	ASN
57	V2	121	HIS
57	V2	149	HIS
58	E7	1	GLN
58	E7	83	GLN
58	E7	166	HIS
59	AC	110	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
48	2MR	S2	154	48	10,12,13	2.43	2 (20%)	5,13,15	0.89	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
48	2MR	S2	154	48	-	2/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	S2	154	2MR	CZ-NH2	5.18	1.44	1.33
48	S2	154	2MR	CZ-NE	5.07	1.45	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	S2	154	2MR	CG-CD-NE-CZ
48	S2	154	2MR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 64 ligands modelled in this entry, 3 are monoatomic - leaving 61 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	$\#\|Z\| > 2$
63	PC1	N1	702	-	39,39,53	0.34	0	45,47,61	0.29	0
70	FMN	V1	579	-	33,33,33	0.27	0	48,50,50	0.38	0
61	SF4	S8	298	54	0,12,12	-	-	-		
64	CDL	A3	201	-	57,57,99	0.39	0	63,69,111	0.35	0
63	PC1	E8	302	-	53,53,53	0.30	0	59,61,61	0.29	0
64	CDL	B3	102	-	64,64,99	0.37	0	70,76,111	0.35	0
63	PC1	N4	503	-	32,32,53	0.36	0	38,40,61	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
63	PC1	N5	606	-	35,35,53	0.35	0	41,43,61	0.30	0
67	3PE	G1	516	-	39,39,50	0.34	0	42,44,55	0.30	0
67	3PE	AN	302	-	50,50,50	0.30	0	53,55,55	0.29	0
63	PC1	C4	203	-	37,37,53	0.34	0	43,45,61	0.30	0
61	SF4	1A	403	1	0,12,12	-	-	-		
68	U10	N4	505	-	43,43,63	2.42	15 (34%)	52,55,79	1.65	15 (28%)
63	PC1	B5	203	-	53,53,53	0.30	0	59,61,61	0.32	0
63	PC1	AM	220	-	47,47,53	0.31	0	53,55,61	0.26	0
64	CDL	E7	301	-	67,67,99	0.36	0	73,79,111	0.30	0
61	SF4	1A	402	1	0,12,12	-	-	-		
64	CDL	AL	302	-	67,67,99	0.36	0	73,79,111	0.31	0
64	CDL	AL	304	-	69,69,99	0.36	0	75,81,111	0.32	0
64	CDL	N5	608	-	92,92,99	0.31	0	98,104,111	0.29	0
63	PC1	ED	201	-	53,53,53	0.30	0	59,61,61	0.29	0
63	PC1	A1	203	-	30,30,53	0.37	0	36,38,61	0.33	0
63	PC1	A1	202	-	48,48,53	0.32	0	54,56,61	0.31	0
63	PC1	E8	301	-	53,53,53	0.30	0	59,61,61	0.29	0
64	CDL	AL	303	-	63,63,99	0.37	0	69,75,111	0.31	0
64	CDL	B5	201	-	57,57,99	0.39	0	63,69,111	0.34	0
61	SF4	V1	580	56	0,12,12	-	-	-		
64	CDL	EA	202	-	54,54,99	0.40	0	60,66,111	0.34	0
67	3PE	N4	504	-	40,40,50	0.34	0	43,45,55	0.31	0
66	ZMP	AB	150	13	29,35,36	0.69	1 (3%)	34,42,45	0.80	1 (2%)
61	SF4	S7	301	53	0,12,12	-	-	-		
64	CDL	C4	202	-	93,93,99	0.32	0	99,105,111	0.30	0
63	PC1	A9	560	-	32,32,53	0.37	0	38,40,61	0.34	0
63	PC1	E4	401	-	50,50,53	0.30	0	56,58,61	0.31	0
63	PC1	E8	304	-	29,29,53	0.38	0	35,37,61	0.35	0
63	PC1	N2	301	-	36,36,53	0.35	0	42,44,61	0.33	0
64	CDL	N4	501	-	97,97,99	0.31	0	103,109,111	0.27	0
64	CDL	N5	603	-	69,69,99	0.35	0	75,81,111	0.32	0
64	CDL	EA	201	-	58,58,99	0.39	0	64,70,111	0.33	0
63	PC1	AM	218	-	48,48,53	0.31	0	54,56,61	0.28	0
63	PC1	E8	303	-	32,32,53	0.36	0	38,40,61	0.35	0
63	PC1	AN	301	-	47,47,53	0.32	0	53,55,61	0.30	0
63	PC1	N1	701	-	48,48,53	0.30	0	54,56,61	0.28	0
60	FES	V2	301	57	0,4,4	-	-	-		
64	CDL	C4	204	-	68,68,99	0.35	0	74,80,111	0.31	0
63	PC1	A9	561	-	32,32,53	0.36	0	38,40,61	0.34	0
65	NDP	A9	559	-	45,52,52	0.53	0	53,80,80	0.57	1 (1%)
60	FES	1A	401	1	0,4,4	-	-	-		
61	SF4	S8	297	54	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
63	PC1	B5	202	-	53,53,53	0.30	0	59,61,61	0.32	0
64	CDL	E6	431	-	63,63,99	0.37	0	69,75,111	0.32	0
64	CDL	AM	216	-	71,71,99	0.35	0	77,83,111	0.33	0
67	3PE	N5	607	-	50,50,50	0.31	0	53,55,55	0.30	0
63	PC1	N5	605	-	40,40,53	0.33	0	46,48,61	0.29	0
63	PC1	AL	301	-	49,49,53	0.31	0	55,57,61	0.29	0
63	PC1	N3	301	-	41,41,53	0.33	0	47,49,61	0.33	0
63	PC1	N4	502	-	38,38,53	0.34	0	44,46,61	0.32	0
63	PC1	N5	601	-	53,53,53	0.30	0	59,61,61	0.30	0
66	ZMP	AC	201	59	29,35,36	0.68	1 (3%)	34,42,45	0.81	1 (2%)
64	CDL	AM	215	-	71,71,99	0.35	0	77,83,111	0.30	0
64	CDL	AM	217	-	71,71,99	0.36	0	77,83,111	0.33	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
63	PC1	N1	702	-	-	11/43/43/57	-
70	FMN	V1	579	-	-	2/18/18/18	0/3/3/3
61	SF4	S8	298	54	-	-	0/6/5/5
64	CDL	A3	201	-	-	6/68/68/110	-
63	PC1	E8	302	-	-	17/57/57/57	-
64	CDL	B3	102	-	-	11/75/75/110	-
63	PC1	N4	503	-	-	6/36/36/57	-
63	PC1	N5	606	-	-	10/39/39/57	-
67	3PE	G1	516	-	-	8/43/43/54	-
67	3PE	AN	302	-	-	10/54/54/54	-
63	PC1	C4	203	-	-	11/41/41/57	-
61	SF4	1A	403	1	-	-	0/6/5/5
68	U10	N4	505	-	-	8/39/63/87	0/1/1/1
63	PC1	B5	203	-	-	16/57/57/57	-
63	PC1	AM	220	-	-	9/51/51/57	-
64	CDL	E7	301	-	-	19/78/78/110	-
64	CDL	AL	302	-	-	9/78/78/110	-
64	CDL	AL	304	-	-	25/80/80/110	-
64	CDL	N5	608	-	-	17/103/103/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	SF4	1A	402	1	-	-	0/6/5/5
63	PC1	ED	201	-	-	8/57/57/57	-
63	PC1	A1	203	-	-	6/34/34/57	-
63	PC1	A1	202	-	-	15/52/52/57	-
63	PC1	E8	301	-	-	12/57/57/57	-
64	CDL	AL	303	-	-	11/74/74/110	-
64	CDL	B5	201	-	-	14/68/68/110	-
61	SF4	V1	580	56	-	-	0/6/5/5
64	CDL	EA	202	-	-	16/65/65/110	-
67	3PE	N4	504	-	-	10/44/44/54	-
66	ZMP	AB	150	13	-	14/40/42/43	-
64	CDL	C4	202	-	-	20/104/104/110	-
61	SF4	S7	301	53	-	-	0/6/5/5
63	PC1	A9	560	-	-	12/36/36/57	-
63	PC1	E4	401	-	-	13/54/54/57	-
63	PC1	E8	304	-	-	11/33/33/57	-
63	PC1	N2	301	-	-	9/40/40/57	-
64	CDL	N4	501	-	-	23/108/108/110	-
64	CDL	N5	603	-	-	12/80/80/110	-
64	CDL	EA	201	-	-	13/69/69/110	-
63	PC1	AM	218	-	-	21/52/52/57	-
63	PC1	E8	303	-	-	8/36/36/57	-
63	PC1	AN	301	-	-	12/51/51/57	-
63	PC1	N1	701	-	-	15/52/52/57	-
60	FES	V2	301	57	-	-	0/1/1/1
64	CDL	C4	204	-	-	12/79/79/110	-
63	PC1	A9	561	-	-	9/36/36/57	-
65	NDP	A9	559	-	-	5/30/77/77	0/5/5/5
67	3PE	N5	607	-	-	16/54/54/54	-
63	PC1	B5	202	-	-	16/57/57/57	-
64	CDL	E6	431	-	-	23/74/74/110	-
60	FES	1A	401	1	-	-	0/1/1/1
64	CDL	AM	216	-	-	18/82/82/110	-
61	SF4	S8	297	54	-	-	0/6/5/5
63	PC1	N5	605	-	-	13/44/44/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	PC1	AL	301	-	-	9/53/53/57	-
63	PC1	N3	301	-	-	10/45/45/57	-
63	PC1	N4	502	-	-	16/42/42/57	-
63	PC1	N5	601	-	-	9/57/57/57	-
66	ZMP	AC	201	59	-	23/40/42/43	-
64	CDL	AM	215	-	-	16/82/82/110	-
64	CDL	AM	217	-	-	22/82/82/110	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	N4	505	U10	C6-C1	10.32	1.54	1.35
68	N4	505	U10	C4-C3	4.21	1.53	1.36
68	N4	505	U10	C7-C8	3.11	1.55	1.50
68	N4	505	U10	C7-C6	2.88	1.56	1.51
68	N4	505	U10	C26-C24	2.66	1.56	1.51
68	N4	505	U10	C31-C29	2.59	1.56	1.51
68	N4	505	U10	C16-C14	2.55	1.56	1.51
66	AC	201	ZMP	C9-C10	-2.50	1.48	1.50
66	AB	150	ZMP	C9-C10	-2.50	1.48	1.50
68	N4	505	U10	C6-C5	2.46	1.53	1.46
68	N4	505	U10	O5-C5	-2.42	1.18	1.23
68	N4	505	U10	C21-C19	2.41	1.56	1.51
68	N4	505	U10	C11-C9	2.31	1.56	1.51
68	N4	505	U10	O2-C2	-2.27	1.18	1.23
68	N4	505	U10	O3-C3M	-2.16	1.40	1.45
68	N4	505	U10	C27-C28	2.09	1.57	1.50
68	N4	505	U10	C36-C34	2.07	1.55	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	N4	505	U10	C7-C8-C9	-3.67	120.69	126.79
68	N4	505	U10	C30-C29-C31	3.52	121.19	115.27
68	N4	505	U10	C22-C23-C24	-3.17	120.03	127.66
68	N4	505	U10	C15-C14-C16	3.03	120.38	115.27
68	N4	505	U10	C25-C24-C26	2.88	120.11	115.27
68	N4	505	U10	C20-C19-C21	2.78	119.95	115.27
68	N4	505	U10	C17-C18-C19	-2.62	121.35	127.66
68	N4	505	U10	C12-C13-C14	-2.56	121.49	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
68	N4	505	U10	C10-C9-C11	2.44	119.38	115.27
68	N4	505	U10	C1M-C1-C6	-2.39	120.50	124.40
66	AB	150	ZMP	C15-C14-C13	-2.36	108.42	112.36
65	A9	559	NDP	C5A-C6A-N6A	2.30	123.84	120.35
68	N4	505	U10	C15-C14-C13	-2.26	117.87	123.68
68	N4	505	U10	C27-C28-C29	-2.25	122.24	127.66
68	N4	505	U10	C36-C34-C35	2.10	119.24	114.60
68	N4	505	U10	C7-C6-C5	2.09	120.99	118.48
66	AC	201	ZMP	C15-C14-C13	-2.07	108.91	112.36
68	N4	505	U10	C27-C26-C24	-2.02	106.34	112.98

There are no chirality outliers.

All (687) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	A1	203	PC1	C11-O13-P-O12
63	A1	203	PC1	C11-O13-P-O14
63	A1	203	PC1	C1-O11-P-O12
63	A9	560	PC1	C1-O11-P-O12
63	A9	560	PC1	C1-O11-P-O14
63	A9	560	PC1	C1-O11-P-O13
63	A9	561	PC1	C11-O13-P-O14
63	A9	561	PC1	C1-O11-P-O12
63	A9	561	PC1	C1-O11-P-O14
63	AM	218	PC1	C1-O11-P-O14
63	AM	220	PC1	C1-O11-P-O14
63	AN	301	PC1	C11-O13-P-O11
63	AN	301	PC1	C1-O11-P-O14
63	B5	202	PC1	C11-O13-P-O11
63	B5	202	PC1	C1-O11-P-O13
63	B5	202	PC1	O13-C11-C12-N
63	B5	203	PC1	C1-O11-P-O12
63	B5	203	PC1	C1-O11-P-O14
63	C4	203	PC1	C11-O13-P-O11
63	E4	401	PC1	C11-O13-P-O12
63	E8	302	PC1	C1-O11-P-O12
63	E8	304	PC1	C1-O11-P-O14
63	E8	304	PC1	C1-O11-P-O13
63	ED	201	PC1	C11-O13-P-O11
63	N1	701	PC1	C1-O11-P-O13
63	N1	702	PC1	C1-O11-P-O12
63	N2	301	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
63	N2	301	PC1	O13-C11-C12-N
63	N3	301	PC1	C1-O11-P-O13
63	N4	502	PC1	C11-O13-P-O14
63	N4	502	PC1	C1-O11-P-O12
63	N5	601	PC1	C11-O13-P-O14
63	N5	605	PC1	C11-O13-P-O12
63	N5	606	PC1	C1-O11-P-O14
64	AL	303	CDL	OB6-CB4-CB6-OB8
64	AL	304	CDL	CA2-OA2-PA1-OA4
64	AL	304	CDL	CB3-OB5-PB2-OB2
64	AM	215	CDL	CA3-OA5-PA1-OA3
64	AM	215	CDL	CB3-OB5-PB2-OB2
64	AM	215	CDL	OB5-CB3-CB4-OB6
64	AM	216	CDL	CA2-OA2-PA1-OA4
64	AM	217	CDL	CA3-OA5-PA1-OA4
64	AM	217	CDL	CB2-OB2-PB2-OB3
64	AM	217	CDL	CB2-OB2-PB2-OB4
64	AM	217	CDL	CB2-OB2-PB2-OB5
64	AM	217	CDL	CB3-OB5-PB2-OB3
64	B3	102	CDL	CA2-OA2-PA1-OA3
64	B3	102	CDL	CA3-OA5-PA1-OA3
64	B3	102	CDL	CA3-OA5-PA1-OA4
64	B3	102	CDL	CB3-OB5-PB2-OB4
64	B5	201	CDL	CB3-OB5-PB2-OB3
64	B5	201	CDL	CB3-OB5-PB2-OB4
64	C4	202	CDL	CA2-OA2-PA1-OA3
64	C4	202	CDL	CA2-OA2-PA1-OA4
64	C4	202	CDL	CA2-OA2-PA1-OA5
64	C4	202	CDL	CA3-OA5-PA1-OA2
64	C4	204	CDL	CA2-OA2-PA1-OA3
64	C4	204	CDL	CA3-OA5-PA1-OA2
64	C4	204	CDL	CA3-OA5-PA1-OA3
64	C4	204	CDL	CA3-OA5-PA1-OA4
64	E6	431	CDL	CA2-OA2-PA1-OA3
64	E6	431	CDL	CA3-OA5-PA1-OA3
64	E6	431	CDL	CA3-OA5-PA1-OA4
64	EA	201	CDL	CA2-OA2-PA1-OA3
64	EA	201	CDL	C1-CB2-OB2-PB2
64	EA	201	CDL	CB3-OB5-PB2-OB3
64	EA	201	CDL	CB3-OB5-PB2-OB4
64	EA	202	CDL	CB3-OB5-PB2-OB4
64	N4	501	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
64	N4	501	CDL	CA2-OA2-PA1-OA4
64	N5	603	CDL	CB2-OB2-PB2-OB3
64	N5	603	CDL	CB2-OB2-PB2-OB4
64	N5	608	CDL	O1-C1-CB2-OB2
64	E7	301	CDL	C1-CA2-OA2-PA1
64	E7	301	CDL	CA3-OA5-PA1-OA2
64	E7	301	CDL	OB5-CB3-CB4-OB6
65	A9	559	NDP	C2N-C3N-C7N-N7N
66	AB	150	ZMP	S1-C11-C12-N1
66	AB	150	ZMP	C7-C8-C9-C10
66	AC	201	ZMP	C19-C18-C21-O5
66	AC	201	ZMP	C17-C18-C21-O5
66	AC	201	ZMP	O4-C17-C18-C21
66	AC	201	ZMP	C16-C17-C18-C21
66	AC	201	ZMP	O4-C17-C18-C19
66	AC	201	ZMP	C16-C17-C18-C19
66	AC	201	ZMP	O4-C17-C18-C20
66	AC	201	ZMP	C16-C17-C18-C20
67	AN	302	3PE	C11-O13-P-O11
67	AN	302	3PE	C11-O13-P-O14
67	AN	302	3PE	O13-C11-C12-N
67	N4	504	3PE	C11-O13-P-O14
67	N5	607	3PE	C11-O13-P-O14
67	N5	607	3PE	O13-C11-C12-N
68	N4	505	U10	C1-C6-C7-C8
68	N4	505	U10	C5-C6-C7-C8
68	N4	505	U10	C28-C29-C31-C32
68	N4	505	U10	C30-C29-C31-C32
70	V1	579	FMN	N10-C1'-C2'-O2'
70	V1	579	FMN	N10-C1'-C2'-C3'
66	AB	150	ZMP	C14-C13-N1-C12
66	AC	201	ZMP	C14-C13-N1-C12
66	AC	201	ZMP	C3-C4-C5-C6
64	E6	431	CDL	O1-C1-CA2-OA2
66	AC	201	ZMP	C5-C6-C7-C8
64	A3	201	CDL	C1-CA2-OA2-PA1
64	AL	302	CDL	CB4-CB3-OB5-PB2
66	AB	150	ZMP	O2-C13-N1-C12
66	AC	201	ZMP	O2-C13-N1-C12
64	B3	102	CDL	CA7-C31-C32-C33
64	AL	304	CDL	CB2-C1-CA2-OA2
64	E6	431	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
63	N3	301	PC1	C11-C12-N-C15
65	A9	559	NDP	O4D-C1D-N1N-C6N
64	N5	608	CDL	CB5-C51-C52-C53
64	AL	304	CDL	O1-C1-CA2-OA2
63	N1	702	PC1	O21-C2-C3-O31
63	B5	202	PC1	C21-C22-C23-C24
63	B5	202	PC1	C31-C32-C33-C34
63	N5	605	PC1	C21-C22-C23-C24
64	A3	201	CDL	CA5-C11-C12-C13
63	B5	202	PC1	C24-C25-C26-C27
63	A1	202	PC1	C11-C12-N-C13
63	N1	701	PC1	C11-C12-N-C15
63	N3	301	PC1	C11-C12-N-C13
64	AL	302	CDL	CB5-C51-C52-C53
64	AM	217	CDL	CB5-C51-C52-C53
64	N4	501	CDL	CA5-C11-C12-C13
67	G1	516	3PE	C21-C22-C23-C24
63	A1	202	PC1	C11-O13-P-O11
63	A1	202	PC1	C1-O11-P-O13
63	A1	203	PC1	C11-O13-P-O11
63	A1	203	PC1	C1-O11-P-O13
63	A9	561	PC1	C1-O11-P-O13
63	AM	220	PC1	C1-O11-P-O13
63	AN	301	PC1	C1-O11-P-O13
63	B5	203	PC1	C1-O11-P-O13
63	E4	401	PC1	C11-O13-P-O11
63	E8	301	PC1	C11-O13-P-O11
63	E8	301	PC1	C1-O11-P-O13
63	E8	302	PC1	C1-O11-P-O13
63	E8	303	PC1	C1-O11-P-O13
63	N1	702	PC1	C1-O11-P-O13
63	N2	301	PC1	C1-O11-P-O13
63	N4	502	PC1	C11-O13-P-O11
63	N4	502	PC1	C1-O11-P-O13
63	N5	601	PC1	C11-O13-P-O11
63	N5	605	PC1	C1-O11-P-O13
63	N5	606	PC1	C1-O11-P-O13
64	AL	303	CDL	CA2-OA2-PA1-OA5
64	AL	304	CDL	CA2-OA2-PA1-OA5
64	AM	215	CDL	CB2-OB2-PB2-OB5
64	AM	217	CDL	CA3-OA5-PA1-OA2
64	AM	217	CDL	CB3-OB5-PB2-OB2

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Mol	Chain	Res	Type	Atoms
64	B3	102	CDL	CA3-OA5-PA1-OA2
64	B3	102	CDL	CB3-OB5-PB2-OB2
64	B5	201	CDL	CA3-OA5-PA1-OA2
64	B5	201	CDL	CB3-OB5-PB2-OB2
64	C4	204	CDL	CA2-OA2-PA1-OA5
64	E6	431	CDL	CA2-OA2-PA1-OA5
64	E6	431	CDL	CA3-OA5-PA1-OA2
64	EA	201	CDL	CB3-OB5-PB2-OB2
64	EA	202	CDL	CB3-OB5-PB2-OB2
64	N4	501	CDL	CA2-OA2-PA1-OA5
64	N4	501	CDL	CB3-OB5-PB2-OB2
64	N5	603	CDL	CA3-OA5-PA1-OA2
64	N5	603	CDL	CB2-OB2-PB2-OB5
64	E7	301	CDL	CA2-OA2-PA1-OA5
67	N4	504	3PE	C11-O13-P-O11
67	N5	607	3PE	C1-O11-P-O13
67	N5	607	3PE	C11-O13-P-O11
64	C4	202	CDL	CB7-C71-C72-C73
64	N5	608	CDL	CA2-C1-CB2-OB2
63	N3	301	PC1	C26-C27-C28-C29
63	B5	202	PC1	C26-C27-C28-C29
64	AL	304	CDL	C11-C12-C13-C14
66	AC	201	ZMP	C20-C18-C21-O5
63	C4	203	PC1	C21-C22-C23-C24
66	AB	150	ZMP	C6-C7-C8-C9
63	E8	304	PC1	C2-C1-O11-P
63	AM	218	PC1	C24-C25-C26-C27
64	B3	102	CDL	C51-C52-C53-C54
64	N4	501	CDL	C53-C54-C55-C56
66	AB	150	ZMP	C2-C3-C4-C5
64	AL	302	CDL	C32-C33-C34-C35
63	ED	201	PC1	C21-C22-C23-C24
63	AM	218	PC1	C25-C26-C27-C28
63	A9	561	PC1	C32-C33-C34-C35
66	AC	201	ZMP	C2-C3-C4-C5
63	B5	203	PC1	C2E-C2F-C2G-C2H
67	G1	516	3PE	C29-C2A-C2B-C2C
63	ED	201	PC1	C24-C25-C26-C27
64	AM	216	CDL	C37-C38-C39-C40
66	AB	150	ZMP	C3-C4-C5-C6
63	A1	202	PC1	C11-C12-N-C15
63	E8	304	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
64	AL	303	CDL	C51-C52-C53-C54
64	C4	202	CDL	C51-C52-C53-C54
64	N4	501	CDL	C19-C20-C21-C22
64	N4	501	CDL	C38-C39-C40-C41
63	N1	701	PC1	C37-C38-C39-C3A
63	N5	601	PC1	C31-C32-C33-C34
63	AM	220	PC1	C23-C24-C25-C26
63	N5	601	PC1	C32-C33-C34-C35
64	EA	202	CDL	CA3-CA4-CA6-OA8
64	AL	302	CDL	C35-C36-C37-C38
64	C4	202	CDL	C61-C62-C63-C64
66	AB	150	ZMP	C1-C2-C3-C4
63	AN	301	PC1	C35-C36-C37-C38
64	AM	217	CDL	C33-C34-C35-C36
63	E4	401	PC1	C33-C34-C35-C36
63	A1	202	PC1	C11-C12-N-C14
63	N3	301	PC1	C11-C12-N-C14
64	C4	204	CDL	CA5-C11-C12-C13
64	N5	608	CDL	CA7-C31-C32-C33
63	AM	220	PC1	C2C-C2D-C2E-C2F
64	AL	304	CDL	C13-C14-C15-C16
63	N1	701	PC1	C2B-C2C-C2D-C2E
64	AL	303	CDL	CB7-C71-C72-C73
64	EA	202	CDL	C53-C54-C55-C56
67	G1	516	3PE	C25-C26-C27-C28
64	B5	201	CDL	C55-C56-C57-C58
63	N1	702	PC1	C27-C28-C29-C2A
63	B5	203	PC1	C2C-C2D-C2E-C2F
63	A9	560	PC1	C2-C3-O31-C31
63	AM	218	PC1	C11-C12-N-C13
63	N1	701	PC1	C11-C12-N-C14
63	AM	218	PC1	C37-C38-C39-C3A
63	ED	201	PC1	C3B-C3C-C3D-C3E
63	AM	220	PC1	C27-C28-C29-C2A
63	E8	302	PC1	C22-C23-C24-C25
64	A3	201	CDL	C71-C72-C73-C74
63	A9	561	PC1	C11-O13-P-O11
63	N5	605	PC1	C11-O13-P-O11
64	N5	608	CDL	CA2-OA2-PA1-OA5
63	C4	203	PC1	C2-C1-O11-P
64	N4	501	CDL	C78-C79-C80-C81
66	AC	201	ZMP	C1-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
64	EA	202	CDL	OB5-CB3-CB4-CB6
64	E7	301	CDL	OA5-CA3-CA4-CA6
64	AM	216	CDL	CB7-C71-C72-C73
63	N4	502	PC1	C34-C35-C36-C37
63	A1	202	PC1	C22-C23-C24-C25
63	AM	218	PC1	C35-C36-C37-C38
67	AN	302	3PE	C27-C28-C29-C2A
64	C4	204	CDL	C11-C12-C13-C14
64	N5	608	CDL	C42-C43-C44-C45
63	E8	304	PC1	C11-C12-N-C13
63	N1	701	PC1	C11-C12-N-C13
63	B5	203	PC1	C1-C2-C3-O31
63	N4	502	PC1	C1-C2-C3-O31
64	AL	302	CDL	CA3-CA4-CA6-OA8
64	AL	303	CDL	CB3-CB4-CB6-OB8
64	AL	304	CDL	CB3-CB4-CB6-OB8
64	AM	216	CDL	CA3-CA4-CA6-OA8
63	AM	218	PC1	C39-C3A-C3B-C3C
67	N5	607	3PE	C35-C36-C37-C38
63	B5	202	PC1	C3B-C3C-C3D-C3E
64	A3	201	CDL	C52-C53-C54-C55
67	N5	607	3PE	C22-C23-C24-C25
66	AC	201	ZMP	O3-C16-C17-O4
64	N4	501	CDL	CA7-C31-C32-C33
63	N2	301	PC1	C24-C25-C26-C27
64	E6	431	CDL	C15-C16-C17-C18
64	AL	304	CDL	C14-C15-C16-C17
63	N5	605	PC1	C11-C12-N-C13
63	AM	220	PC1	C31-C32-C33-C34
63	E8	301	PC1	C31-C32-C33-C34
63	N4	502	PC1	C31-C32-C33-C34
64	N5	608	CDL	C17-C18-C19-C20
63	N2	301	PC1	C25-C26-C27-C28
63	E8	304	PC1	C11-C12-N-C14
63	B5	202	PC1	O11-C1-C2-C3
63	E4	401	PC1	O11-C1-C2-C3
64	AM	215	CDL	OB5-CB3-CB4-CB6
64	AM	216	CDL	OB5-CB3-CB4-CB6
64	AM	217	CDL	OA5-CA3-CA4-CA6
64	C4	202	CDL	OB5-CB3-CB4-CB6
64	E6	431	CDL	OB5-CB3-CB4-CB6
64	E7	301	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
63	AL	301	PC1	C2A-C2B-C2C-C2D
63	N2	301	PC1	C27-C28-C29-C2A
64	EA	202	CDL	CB7-C71-C72-C73
63	A1	203	PC1	C21-C22-C23-C24
63	ED	201	PC1	C28-C29-C2A-C2B
64	B5	201	CDL	C71-C72-C73-C74
63	A9	560	PC1	C2-C1-O11-P
63	B5	202	PC1	C2-C1-O11-P
63	N1	702	PC1	C2-C1-O11-P
63	N3	301	PC1	C2-C1-O11-P
64	EA	202	CDL	C1-CA2-OA2-PA1
66	AC	201	ZMP	S1-C11-C12-N1
64	C4	202	CDL	C59-C60-C61-C62
63	A1	202	PC1	C25-C26-C27-C28
63	A9	560	PC1	C1-C2-C3-O31
63	N1	702	PC1	C1-C2-C3-O31
64	EA	201	CDL	CB3-CB4-CB6-OB8
64	E7	301	CDL	CB3-CB4-CB6-OB8
63	N1	701	PC1	C2C-C2D-C2E-C2F
64	AM	217	CDL	C31-C32-C33-C34
66	AB	150	ZMP	N2-C16-C17-C18
63	AM	218	PC1	C11-C12-N-C14
63	AM	218	PC1	C11-O13-P-O11
64	E6	431	CDL	CB2-OB2-PB2-OB5
67	G1	516	3PE	C1-O11-P-O13
63	E4	401	PC1	C28-C29-C2A-C2B
63	E4	401	PC1	O11-C1-C2-O21
64	AM	217	CDL	OA5-CA3-CA4-OA6
64	C4	202	CDL	OB5-CB3-CB4-OB6
64	EA	202	CDL	OB5-CB3-CB4-OB6
64	N4	501	CDL	C83-C84-C85-C86
63	B5	203	PC1	O21-C2-C3-O31
64	AM	216	CDL	OA6-CA4-CA6-OA8
67	N4	504	3PE	O31-C31-C32-C33
63	AL	301	PC1	C2-C1-O11-P
63	N4	503	PC1	C2-C1-O11-P
64	AL	303	CDL	C1-CA2-OA2-PA1
64	AL	303	CDL	CA4-CA3-OA5-PA1
63	AN	301	PC1	C3A-C3B-C3C-C3D
64	AL	304	CDL	OB5-CB3-CB4-CB6
66	AC	201	ZMP	C6-C7-C8-C9
63	N5	601	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
64	N5	603	CDL	C58-C59-C60-C61
66	AC	201	ZMP	C22-C23-C24-C25
63	E4	401	PC1	C1-C2-C3-O31
64	AL	304	CDL	C1-CA2-OA2-PA1
64	E6	431	CDL	CA4-CA3-OA5-PA1
64	E6	431	CDL	CA3-CA4-CA6-OA8
64	N4	501	CDL	CA4-CA3-OA5-PA1
64	AM	216	CDL	OB5-CB3-CB4-OB6
64	E6	431	CDL	OB5-CB3-CB4-OB6
63	A9	560	PC1	O21-C2-C3-O31
63	AL	301	PC1	O21-C2-C3-O31
63	AM	218	PC1	O21-C2-C3-O31
63	E4	401	PC1	O21-C2-C3-O31
64	AL	302	CDL	OA6-CA4-CA6-OA8
64	E6	431	CDL	OA6-CA4-CA6-OA8
64	E6	431	CDL	OB6-CB4-CB6-OB8
63	E4	401	PC1	C21-C22-C23-C24
63	C4	203	PC1	C11-C12-N-C15
63	N5	605	PC1	C11-C12-N-C15
65	A9	559	NDP	C2B-O2B-P2B-O3X
63	N1	702	PC1	C33-C34-C35-C36
64	E7	301	CDL	C72-C73-C74-C75
64	AL	304	CDL	C31-C32-C33-C34
63	B5	203	PC1	C34-C35-C36-C37
63	C4	203	PC1	C24-C25-C26-C27
64	E7	301	CDL	C32-C33-C34-C35
64	AL	304	CDL	CB5-C51-C52-C53
64	AM	215	CDL	C56-C57-C58-C59
64	EA	201	CDL	CA2-OA2-PA1-OA5
64	EA	202	CDL	CA2-OA2-PA1-OA5
64	N5	603	CDL	CA2-OA2-PA1-OA5
63	AM	218	PC1	C2-C1-O11-P
64	AM	217	CDL	CA4-CA3-OA5-PA1
64	E6	431	CDL	C1-CB2-OB2-PB2
63	A1	202	PC1	C11-O13-P-O14
63	A1	202	PC1	C1-O11-P-O12
63	A1	202	PC1	C1-O11-P-O14
63	A9	561	PC1	C11-O13-P-O12
63	AM	218	PC1	C11-O13-P-O12
63	AM	220	PC1	C1-O11-P-O12
63	AN	301	PC1	C11-O13-P-O12
63	AN	301	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
63	B5	202	PC1	C11-O13-P-O12
63	B5	202	PC1	C1-O11-P-O12
63	C4	203	PC1	C11-O13-P-O12
63	C4	203	PC1	C11-O13-P-O14
63	C4	203	PC1	C11-C12-N-C13
63	E4	401	PC1	C11-O13-P-O14
63	E8	301	PC1	C11-O13-P-O14
63	E8	303	PC1	C1-O11-P-O14
63	ED	201	PC1	C11-O13-P-O12
63	N1	701	PC1	C1-O11-P-O12
63	N3	301	PC1	C1-O11-P-O12
63	N4	502	PC1	C11-O13-P-O12
63	N5	601	PC1	C11-O13-P-O12
63	N5	605	PC1	C11-O13-P-O14
63	N5	605	PC1	C1-O11-P-O14
63	N5	606	PC1	C1-O11-P-O12
64	AL	303	CDL	CA2-OA2-PA1-OA3
64	AL	304	CDL	CB3-OB5-PB2-OB4
64	AM	215	CDL	CB2-OB2-PB2-OB3
64	AM	215	CDL	CB2-OB2-PB2-OB4
64	AM	215	CDL	CB3-OB5-PB2-OB4
64	AM	217	CDL	CB3-OB5-PB2-OB4
64	B5	201	CDL	CA3-OA5-PA1-OA3
64	C4	202	CDL	CA3-OA5-PA1-OA3
64	C4	202	CDL	CA3-OA5-PA1-OA4
64	C4	204	CDL	CA2-OA2-PA1-OA4
64	N4	501	CDL	CB3-OB5-PB2-OB3
64	N4	501	CDL	CB3-OB5-PB2-OB4
64	N5	603	CDL	CA3-OA5-PA1-OA3
64	N5	603	CDL	CA3-OA5-PA1-OA4
64	E7	301	CDL	CA2-OA2-PA1-OA3
64	E7	301	CDL	CA3-OA5-PA1-OA4
67	N4	504	3PE	C11-O13-P-O12
67	N5	607	3PE	C1-O11-P-O12
67	N5	607	3PE	C1-O11-P-O14
67	N5	607	3PE	C11-O13-P-O12
63	ED	201	PC1	O11-C1-C2-C3
63	N1	701	PC1	O11-C1-C2-C3
64	C4	204	CDL	OB5-CB3-CB4-CB6
63	B5	203	PC1	C3B-C3C-C3D-C3E
63	A1	202	PC1	C31-C32-C33-C34
67	N4	504	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
64	N4	501	CDL	C76-C77-C78-C79
63	B5	202	PC1	C12-C11-O13-P
63	E8	304	PC1	C12-C11-O13-P
64	B5	201	CDL	CA5-C11-C12-C13
63	E8	302	PC1	C39-C3A-C3B-C3C
63	B5	203	PC1	C24-C25-C26-C27
64	C4	202	CDL	C17-C18-C19-C20
63	B5	202	PC1	O11-C1-C2-O21
63	E8	302	PC1	O11-C1-C2-O21
63	ED	201	PC1	O11-C1-C2-O21
64	AL	304	CDL	OB5-CB3-CB4-OB6
64	C4	204	CDL	OB5-CB3-CB4-OB6
63	AN	301	PC1	O31-C31-C32-C33
64	AL	304	CDL	CB7-C71-C72-C73
63	E8	302	PC1	C11-C12-N-C14
63	N5	606	PC1	C11-C12-N-C15
63	A9	560	PC1	O13-C11-C12-N
63	A9	561	PC1	O13-C11-C12-N
63	AL	301	PC1	C1-C2-C3-O31
63	AM	218	PC1	C1-C2-C3-O31
63	AN	301	PC1	O13-C11-C12-N
63	E8	301	PC1	O13-C11-C12-N
63	E8	303	PC1	O13-C11-C12-N
63	E8	304	PC1	O13-C11-C12-N
63	N1	702	PC1	O13-C11-C12-N
63	N4	502	PC1	O13-C11-C12-N
63	N4	503	PC1	O13-C11-C12-N
63	N5	606	PC1	O13-C11-C12-N
64	E6	431	CDL	CB3-CB4-CB6-OB8
63	N4	502	PC1	O21-C2-C3-O31
64	AL	304	CDL	OB6-CB4-CB6-OB8
64	EA	201	CDL	OB6-CB4-CB6-OB8
64	EA	202	CDL	OA6-CA4-CA6-OA8
64	E7	301	CDL	OB6-CB4-CB6-OB8
63	A9	560	PC1	C32-C33-C34-C35
63	AM	218	PC1	C22-C23-C24-C25
66	AB	150	ZMP	O3-C16-C17-O4
63	E8	301	PC1	C27-C28-C29-C2A
67	N4	504	3PE	C36-C37-C38-C39
63	AM	218	PC1	C11-C12-N-C15
63	N5	605	PC1	C11-C12-N-C14
67	AN	302	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
63	AL	301	PC1	C31-C32-C33-C34
64	E7	301	CDL	CA7-C31-C32-C33
63	A1	202	PC1	C24-C25-C26-C27
64	C4	202	CDL	C38-C39-C40-C41
63	N1	701	PC1	O31-C31-C32-C33
63	AL	301	PC1	C3-C2-O21-C21
63	B5	202	PC1	C1-C2-O21-C21
63	N2	301	PC1	C1-C2-O21-C21
64	E6	431	CDL	CA6-CA4-OA6-CA5
64	E6	431	CDL	CB6-CB4-OB6-CB5
64	AL	304	CDL	CA7-C31-C32-C33
63	E8	301	PC1	C35-C36-C37-C38
64	AM	216	CDL	CB4-CB3-OB5-PB2
63	N1	701	PC1	O11-C1-C2-O21
64	E7	301	CDL	OA5-CA3-CA4-OA6
63	E8	302	PC1	C2C-C2D-C2E-C2F
63	B5	203	PC1	C3C-C3D-C3E-C3F
68	N4	505	U10	C24-C26-C27-C28
63	N2	301	PC1	C11-O13-P-O11
63	N4	503	PC1	C1-O11-P-O13
64	AL	304	CDL	CA3-OA5-PA1-OA2
64	AM	216	CDL	CB3-OB5-PB2-OB2
64	AM	217	CDL	CA2-OA2-PA1-OA5
64	C4	204	CDL	CB2-OB2-PB2-OB5
64	EA	202	CDL	CB2-OB2-PB2-OB5
64	N5	603	CDL	CB3-OB5-PB2-OB2
64	N5	608	CDL	CA3-OA5-PA1-OA2
63	E8	303	PC1	C1-C2-C3-O31
64	C4	202	CDL	C39-C40-C41-C42
64	EA	201	CDL	CB4-CB3-OB5-PB2
63	N5	606	PC1	C24-C25-C26-C27
64	N4	501	CDL	C73-C74-C75-C76
67	AN	302	3PE	C2C-C2D-C2E-C2F
63	B5	203	PC1	C21-C22-C23-C24
63	B5	203	PC1	C2A-C2B-C2C-C2D
66	AB	150	ZMP	C22-C23-C24-C25
63	B5	203	PC1	C25-C26-C27-C28
64	N4	501	CDL	C16-C17-C18-C19
63	E4	401	PC1	C11-C12-N-C13
63	E8	302	PC1	C11-C12-N-C13
63	N5	606	PC1	C11-C12-N-C14
68	N4	505	U10	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
64	AM	216	CDL	C31-C32-C33-C34
64	C4	202	CDL	C77-C78-C79-C80
66	AC	201	ZMP	O3-C16-C17-C18
63	N5	605	PC1	C23-C24-C25-C26
67	N5	607	3PE	C2-C1-O11-P
63	C4	203	PC1	C11-C12-N-C14
63	AM	220	PC1	C25-C26-C27-C28
63	AM	218	PC1	C3C-C3D-C3E-C3F
63	B5	203	PC1	C35-C36-C37-C38
63	E8	302	PC1	C3A-C3B-C3C-C3D
63	N3	301	PC1	C1-C2-C3-O31
64	N5	608	CDL	CA3-CA4-CA6-OA8
66	AC	201	ZMP	N2-C16-C17-C18
64	AM	217	CDL	C15-C16-C17-C18
63	A9	560	PC1	C1-C2-O21-C21
63	AN	301	PC1	C1-C2-O21-C21
63	N4	502	PC1	C3-C2-O21-C21
64	AL	304	CDL	CB3-CB4-OB6-CB5
64	AL	304	CDL	CB6-CB4-OB6-CB5
64	AM	216	CDL	CA6-CA4-OA6-CA5
64	AM	217	CDL	CA3-CA4-OA6-CA5
64	AM	215	CDL	C15-C16-C17-C18
63	N5	606	PC1	C11-C12-N-C13
63	N1	701	PC1	C2A-C2B-C2C-C2D
63	E8	301	PC1	C29-C2A-C2B-C2C
66	AC	201	ZMP	C4-C5-C6-C7
64	E6	431	CDL	C1-CA2-OA2-PA1
63	E8	301	PC1	C24-C25-C26-C27
64	N4	501	CDL	C22-C23-C24-C25
64	B5	201	CDL	OB5-CB3-CB4-OB6
67	N4	504	3PE	O11-C1-C2-O21
64	C4	202	CDL	C72-C71-CB7-OB8
66	AB	150	ZMP	C1-C22-C23-C24
63	N1	702	PC1	C32-C33-C34-C35
67	AN	302	3PE	C38-C39-C3A-C3B
63	E8	302	PC1	C11-C12-N-C15
66	AC	201	ZMP	C12-C11-S1-C10
63	E8	303	PC1	O21-C2-C3-O31
64	N5	608	CDL	OA6-CA4-CA6-OA8
63	AL	301	PC1	C2D-C2E-C2F-C2G
66	AB	150	ZMP	C5-C6-C7-C8
64	AL	302	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
64	AM	216	CDL	C42-C43-C44-C45
64	B3	102	CDL	C35-C36-C37-C38
63	E8	304	PC1	O11-C1-C2-O21
63	E8	302	PC1	C3D-C3E-C3F-C3G
67	AN	302	3PE	C34-C35-C36-C37
63	E8	304	PC1	O11-C1-C2-C3
67	N4	504	3PE	O11-C1-C2-C3
63	N2	301	PC1	O21-C21-C22-C23
68	N4	505	U10	C29-C31-C32-C33
63	E8	303	PC1	O31-C31-C32-C33
63	N4	502	PC1	O21-C21-C22-C23
63	N5	605	PC1	O21-C21-C22-C23
64	N5	608	CDL	C12-C11-CA5-OA6
63	N5	606	PC1	C35-C36-C37-C38
64	N5	608	CDL	C1-CB2-OB2-PB2
63	B5	203	PC1	C38-C39-C3A-C3B
63	N4	503	PC1	C36-C37-C38-C39
63	N3	301	PC1	C11-O13-P-O11
64	B3	102	CDL	CA2-OA2-PA1-OA5
64	B5	201	CDL	CB2-OB2-PB2-OB5
64	E7	301	CDL	CB3-OB5-PB2-OB2
63	AN	301	PC1	C32-C33-C34-C35
64	N4	501	CDL	C54-C55-C56-C57
63	N4	502	PC1	C11-C12-N-C13
64	AL	303	CDL	C12-C11-CA5-OA6
64	AL	304	CDL	C12-C11-CA5-OA6
67	AN	302	3PE	C29-C2A-C2B-C2C
64	A3	201	CDL	C11-C12-C13-C14
63	N1	701	PC1	O21-C21-C22-C23
63	A1	202	PC1	C1-C2-O21-C21
63	B5	202	PC1	C3-C2-O21-C21
64	AM	216	CDL	CA3-CA4-OA6-CA5
64	AM	217	CDL	CB3-CB4-OB6-CB5
64	EA	202	CDL	CA6-CA4-OA6-CA5
64	AM	215	CDL	C14-C15-C16-C17
64	B3	102	CDL	C34-C35-C36-C37
64	N5	603	CDL	C52-C53-C54-C55
63	AM	218	PC1	O21-C21-C22-C23
64	EA	201	CDL	C52-C51-CB5-OB6
63	E8	302	PC1	C35-C36-C37-C38
64	AL	304	CDL	C72-C71-CB7-OB8
64	AM	217	CDL	C72-C71-CB7-OB8

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Mol	Chain	Res	Type	Atoms
64	B5	201	CDL	C12-C11-CA5-OA6
64	EA	201	CDL	C72-C71-CB7-OB8
64	C4	204	CDL	C53-C54-C55-C56
68	N4	505	U10	C2-C3-O3-C3M
67	N4	504	3PE	C2-C1-O11-P
67	G1	516	3PE	C34-C35-C36-C37
64	AM	215	CDL	C12-C11-CA5-OA6
64	C4	202	CDL	O1-C1-CB2-OB2
63	C4	203	PC1	O31-C31-C32-C33
64	C4	202	CDL	OA5-CA3-CA4-CA6
67	N5	607	3PE	O11-C1-C2-C3
64	N4	501	CDL	C34-C35-C36-C37
63	N5	606	PC1	O31-C31-C32-C33
64	A3	201	CDL	OB6-CB4-CB6-OB8
64	AL	302	CDL	OB6-CB4-CB6-OB8
63	AN	301	PC1	C24-C25-C26-C27
63	A1	202	PC1	C33-C34-C35-C36
63	E4	401	PC1	C11-C12-N-C15
65	A9	559	NDP	C2B-O2B-P2B-O2X
64	AM	215	CDL	C52-C51-CB5-OB6
64	E6	431	CDL	C52-C51-CB5-OB6
64	AM	216	CDL	C32-C33-C34-C35
63	N1	702	PC1	O21-C21-C22-C23
67	AN	302	3PE	C2B-C2C-C2D-C2E
65	A9	559	NDP	O4B-C4B-C5B-O5B
63	E8	302	PC1	C38-C39-C3A-C3B
64	B5	201	CDL	C12-C11-CA5-OA7
63	E8	301	PC1	C28-C29-C2A-C2B
63	E4	401	PC1	C11-C12-N-C14
64	N5	608	CDL	C12-C11-CA5-OA7
63	N5	601	PC1	C35-C36-C37-C38
63	E8	302	PC1	C36-C37-C38-C39
63	AL	301	PC1	C27-C28-C29-C2A
63	N5	605	PC1	C33-C34-C35-C36
64	AM	217	CDL	C72-C71-CB7-OB9
64	EA	201	CDL	C52-C51-CB5-OB7
64	EA	201	CDL	C72-C71-CB7-OB9
63	N4	503	PC1	C32-C33-C34-C35
64	C4	202	CDL	C13-C14-C15-C16
63	C4	203	PC1	O32-C31-C32-C33
64	AL	304	CDL	C12-C11-CA5-OA7
64	AL	302	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
63	AM	220	PC1	O21-C21-C22-C23
63	E8	302	PC1	O31-C31-C32-C33
63	E8	303	PC1	O32-C31-C32-C33
63	N1	701	PC1	O22-C21-C22-C23
63	N4	502	PC1	O22-C21-C22-C23
64	AM	215	CDL	C12-C11-CA5-OA7
63	A9	561	PC1	C2-C1-O11-P
64	B5	201	CDL	C1-CA2-OA2-PA1
63	N5	601	PC1	C28-C29-C2A-C2B
63	N1	702	PC1	O22-C21-C22-C23
63	N5	605	PC1	O22-C21-C22-C23
64	AL	303	CDL	C12-C11-CA5-OA7
63	AL	301	PC1	C1-O11-P-O14
63	E8	301	PC1	C1-O11-P-O14
63	E8	303	PC1	C11-O13-P-O14
64	AL	303	CDL	CA3-OA5-PA1-OA3
64	AM	216	CDL	CA2-OA2-PA1-OA3
64	AM	216	CDL	CB3-OB5-PB2-OB3
64	B5	201	CDL	CB2-OB2-PB2-OB3
64	N5	603	CDL	CB3-OB5-PB2-OB3
64	N5	608	CDL	CA2-OA2-PA1-OA3
64	N5	608	CDL	CA3-OA5-PA1-OA3
67	G1	516	3PE	C1-O11-P-O12
64	N4	501	CDL	C80-C81-C82-C83
67	N4	504	3PE	O32-C31-C32-C33
63	N4	502	PC1	O31-C31-C32-C33
64	AM	216	CDL	C71-C72-C73-C74
63	AM	218	PC1	O22-C21-C22-C23
64	E6	431	CDL	C52-C51-CB5-OB7
64	N5	603	CDL	C56-C57-C58-C59
67	N5	607	3PE	C2C-C2D-C2E-C2F
64	AL	304	CDL	C72-C71-CB7-OB9
64	E7	301	CDL	C75-C76-C77-C78
67	N5	607	3PE	C3B-C3C-C3D-C3E
64	N4	501	CDL	C59-C60-C61-C62
63	E8	304	PC1	C22-C23-C24-C25
63	A1	202	PC1	C3-C2-O21-C21
63	A9	560	PC1	C3-C2-O21-C21
63	E8	301	PC1	C12-C11-O13-P
64	AM	217	CDL	CA6-CA4-OA6-CA5
64	AM	217	CDL	CB6-CB4-OB6-CB5
64	E6	431	CDL	CB3-CB4-OB6-CB5

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Mol	Chain	Res	Type	Atoms
64	EA	202	CDL	CA3-CA4-OA6-CA5
66	AB	150	ZMP	O3-C16-C17-C18
67	G1	516	3PE	C12-C11-O13-P
64	EA	202	CDL	O1-C1-CA2-OA2
64	AM	215	CDL	C52-C51-CB5-OB7
64	AM	215	CDL	C72-C71-CB7-OB8
64	EA	202	CDL	C32-C31-CA7-OA8
64	N4	501	CDL	C12-C11-CA5-OA6
64	N5	608	CDL	C52-C51-CB5-OB6
64	E7	301	CDL	C12-C11-CA5-OA6
64	E7	301	CDL	C32-C31-CA7-OA8
67	N5	607	3PE	O31-C31-C32-C33
63	AM	218	PC1	C21-C22-C23-C24
64	AM	216	CDL	C1-CB2-OB2-PB2
63	AM	218	PC1	O32-C31-C32-C33
63	E8	302	PC1	O32-C31-C32-C33
67	N5	607	3PE	C23-C24-C25-C26
63	A9	560	PC1	O31-C31-C32-C33
63	AM	218	PC1	O31-C31-C32-C33
63	N3	301	PC1	O21-C21-C22-C23
64	N5	608	CDL	C41-C42-C43-C44
64	E7	301	CDL	C32-C31-CA7-OA9
63	N4	503	PC1	O31-C31-C32-C33
64	EA	202	CDL	C32-C31-CA7-OA9
63	N5	601	PC1	C11-C12-N-C13
63	N1	701	PC1	C23-C24-C25-C26
63	N4	502	PC1	O32-C31-C32-C33
67	N5	607	3PE	O32-C31-C32-C33
63	E8	302	PC1	C3C-C3D-C3E-C3F
67	G1	516	3PE	O31-C31-C32-C33

There are no ring outliers.

32 monomers are involved in 76 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	S8	298	SF4	2	0
64	A3	201	CDL	1	0
63	E8	302	PC1	1	0
64	B3	102	CDL	1	0
67	G1	516	3PE	2	0
63	C4	203	PC1	1	0
68	N4	505	U10	5	0

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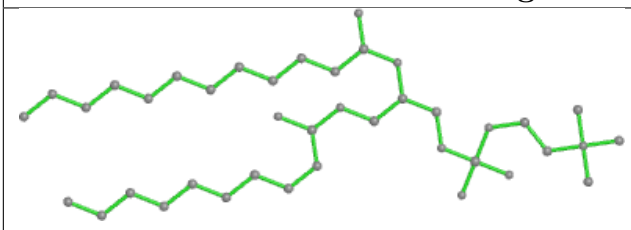
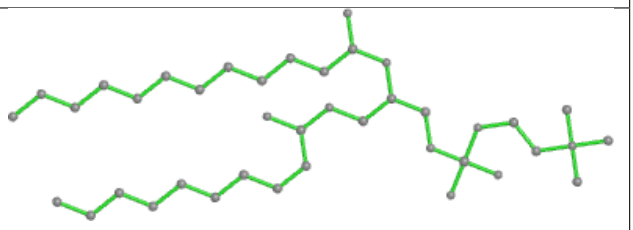
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	B5	203	PC1	2	0
63	AM	220	PC1	1	0
64	N5	608	CDL	1	0
63	ED	201	PC1	1	0
63	A1	203	PC1	1	0
63	A1	202	PC1	2	0
63	E8	301	PC1	1	0
64	AL	303	CDL	2	0
64	B5	201	CDL	1	0
61	V1	580	SF4	1	0
64	EA	202	CDL	1	0
66	AB	150	ZMP	6	0
64	C4	202	CDL	1	0
63	A9	560	PC1	1	0
63	N2	301	PC1	1	0
64	N4	501	CDL	4	0
64	N5	603	CDL	3	0
65	A9	559	NDP	3	0
61	S8	297	SF4	3	0
64	AM	216	CDL	4	0
63	N4	502	PC1	2	0
63	N5	601	PC1	1	0
66	AC	201	ZMP	15	0
64	AM	215	CDL	4	0
64	AM	217	CDL	2	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.

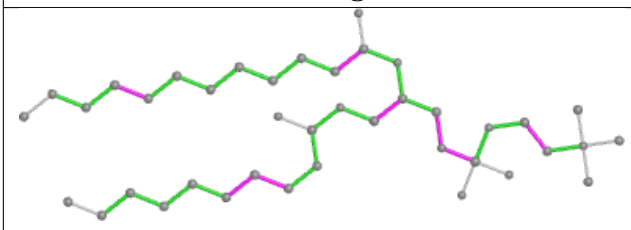
Ligand PC1 N1 702



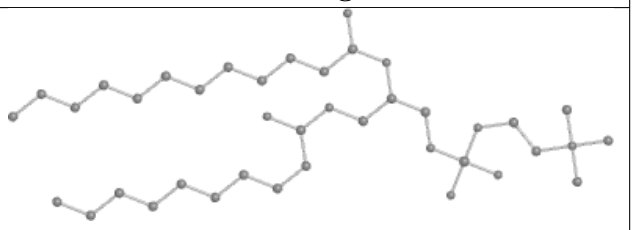
Bond lengths



Bond angles

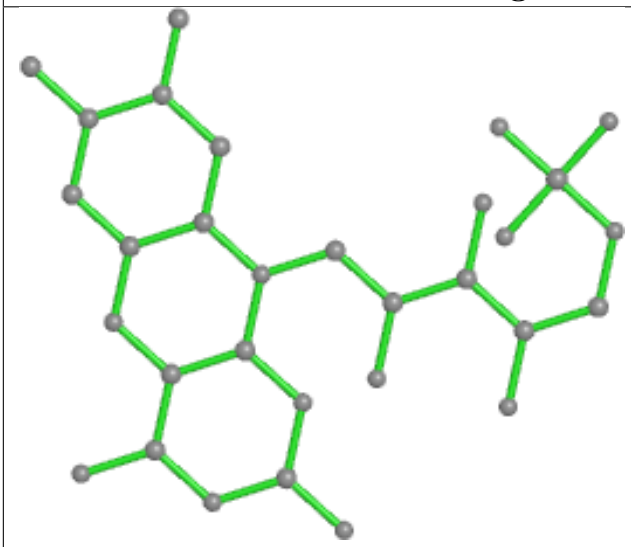


Torsions

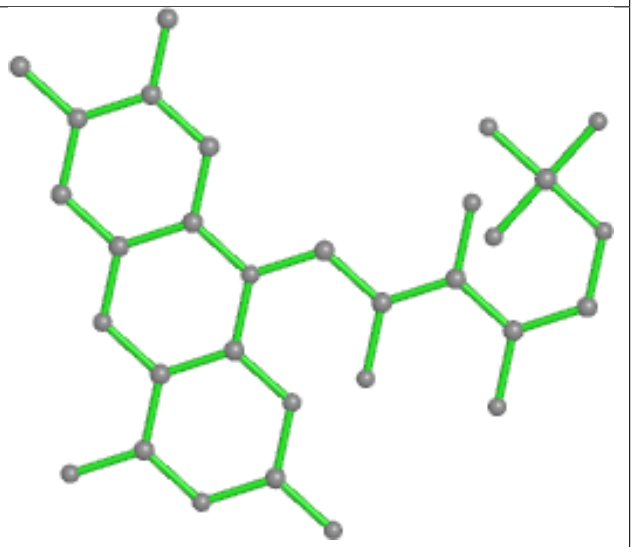


Rings

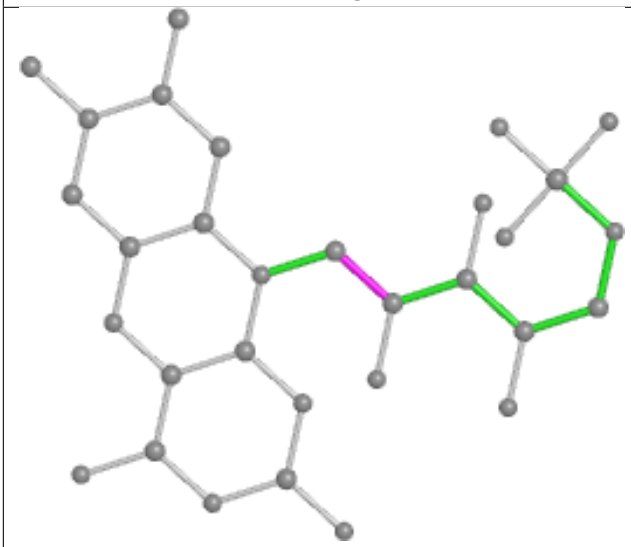
Ligand FMN V1 579



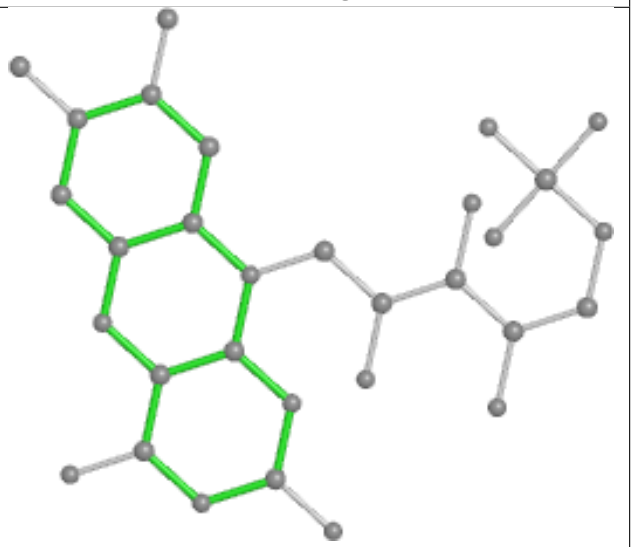
Bond lengths



Bond angles

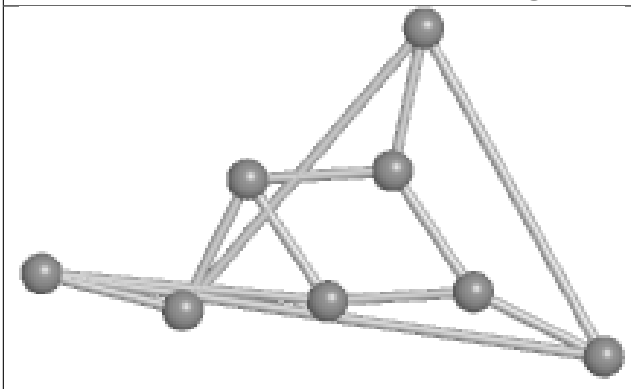


Torsions

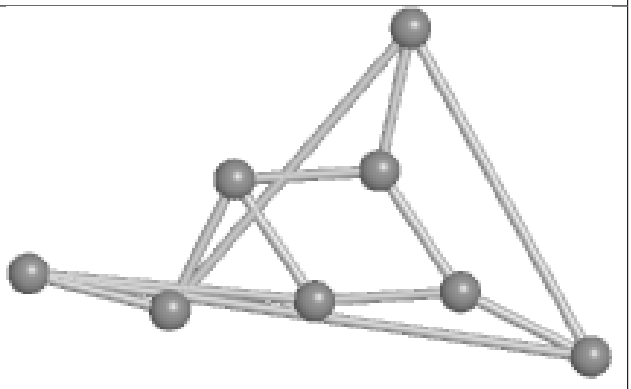


Rings

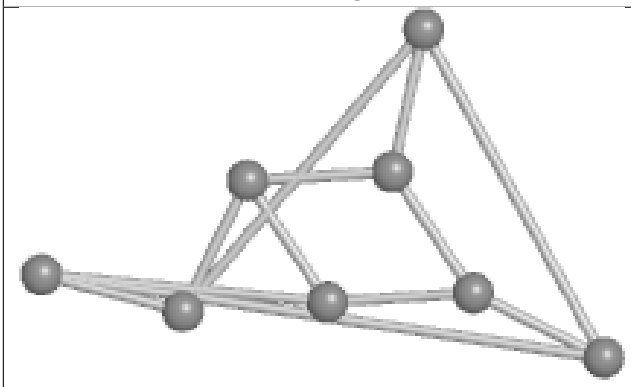
Ligand SF4 S8 298



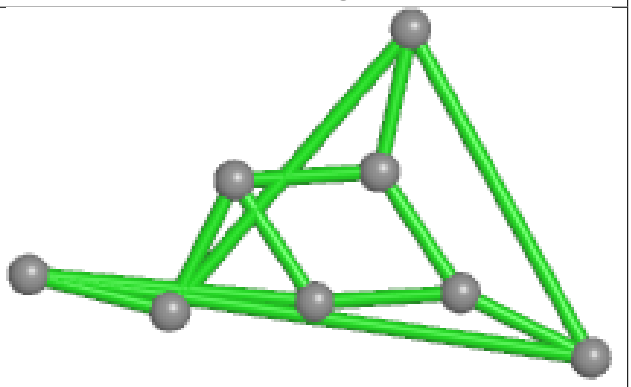
Bond lengths



Bond angles

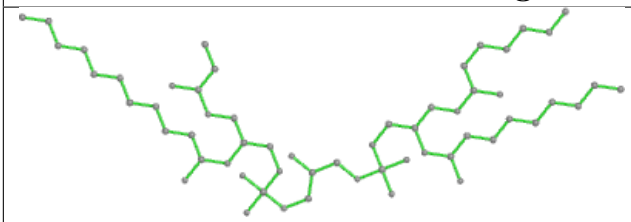


Torsions

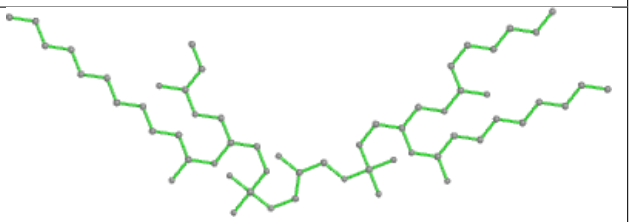


Rings

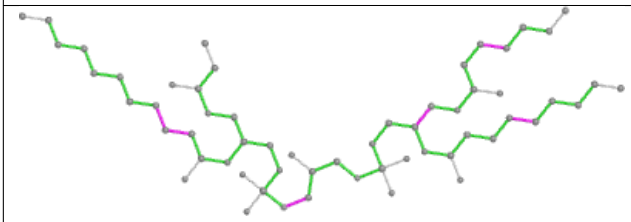
Ligand CDL A3 201



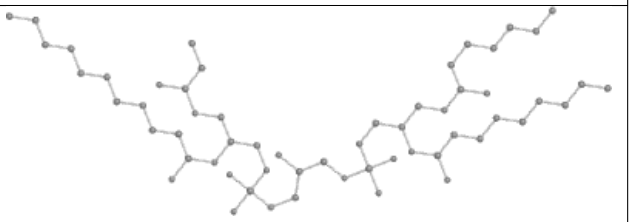
Bond lengths



Bond angles

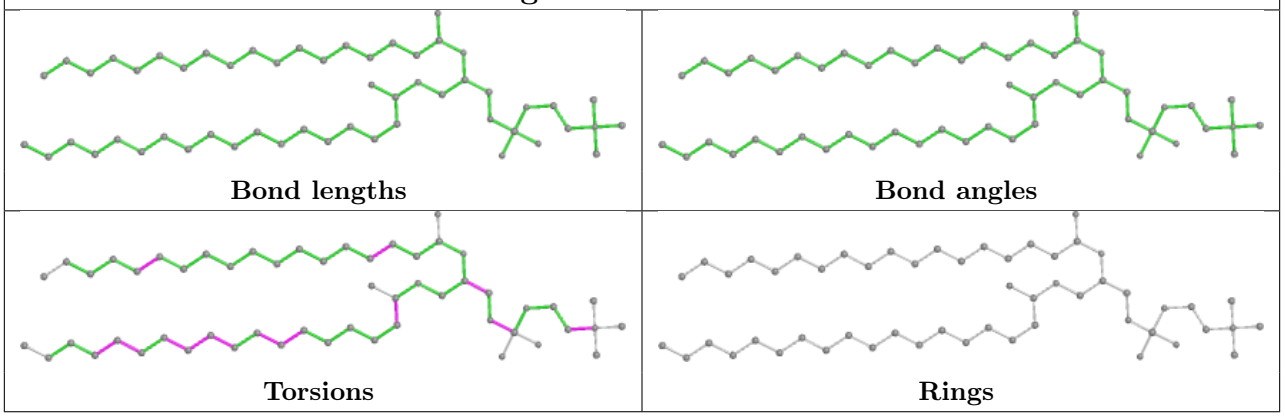


Torsions

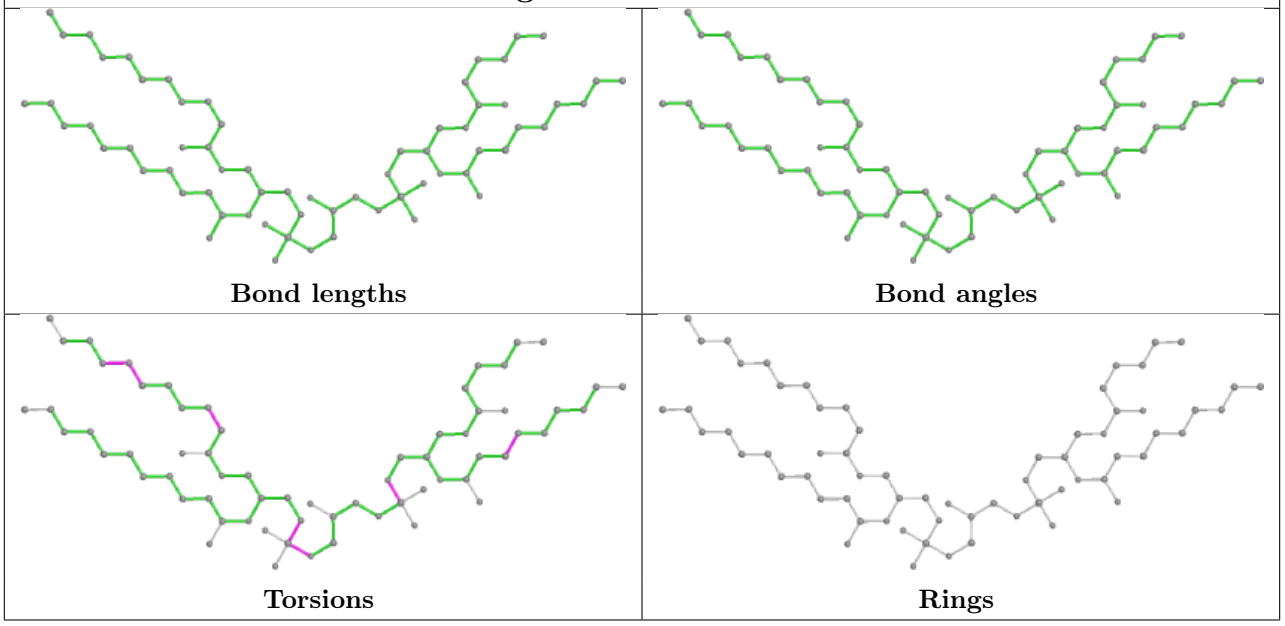


Rings

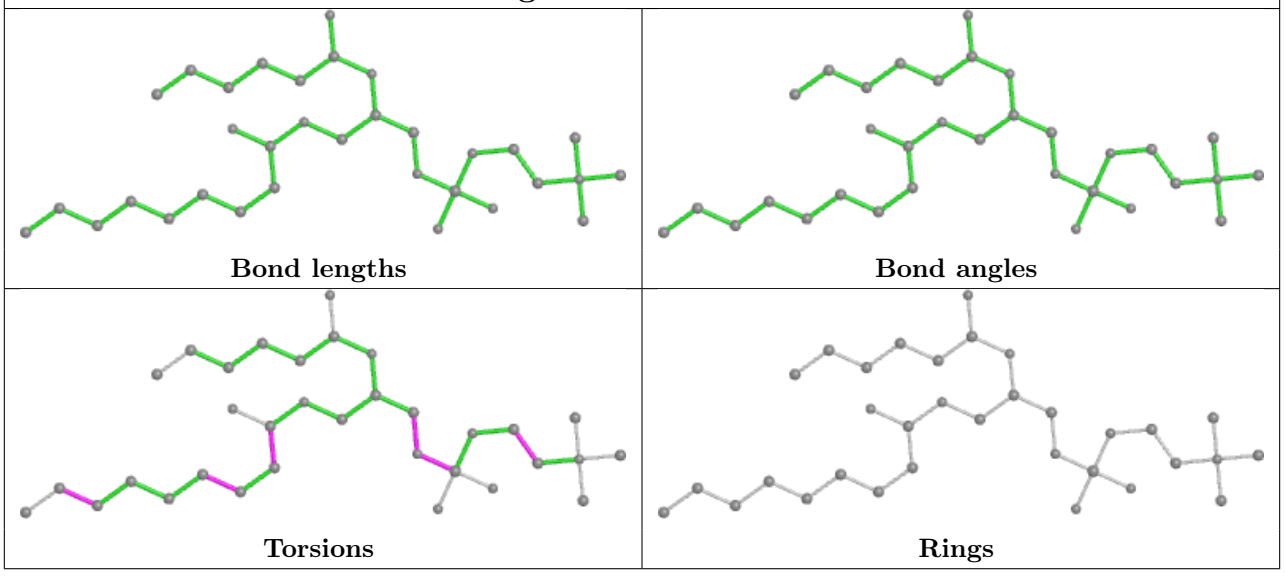
Ligand PC1 E8 302



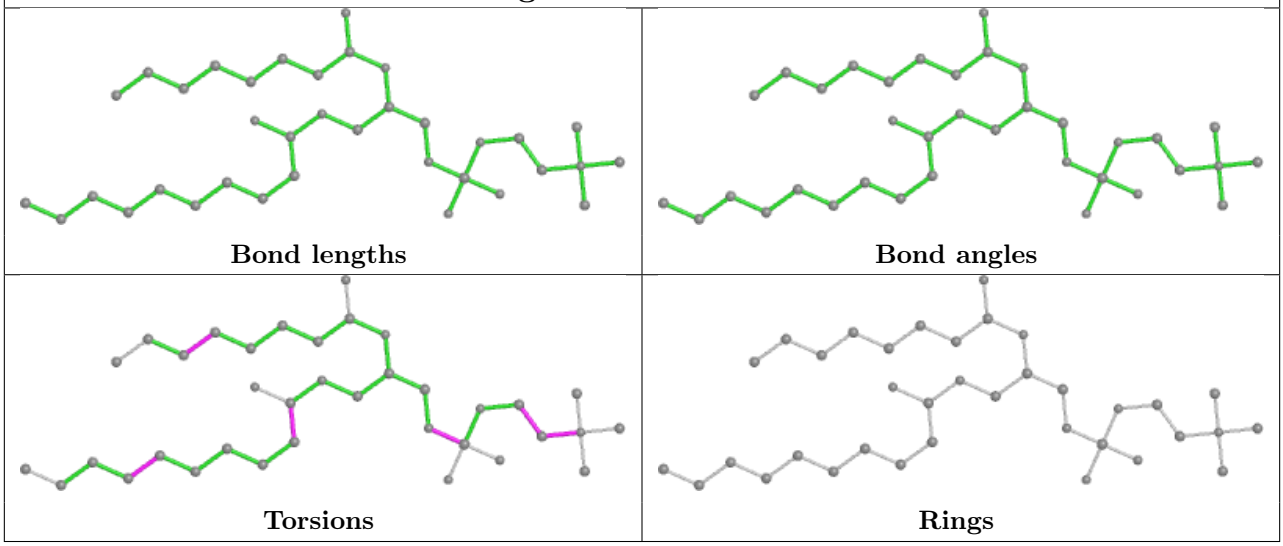
Ligand CDL B3 102



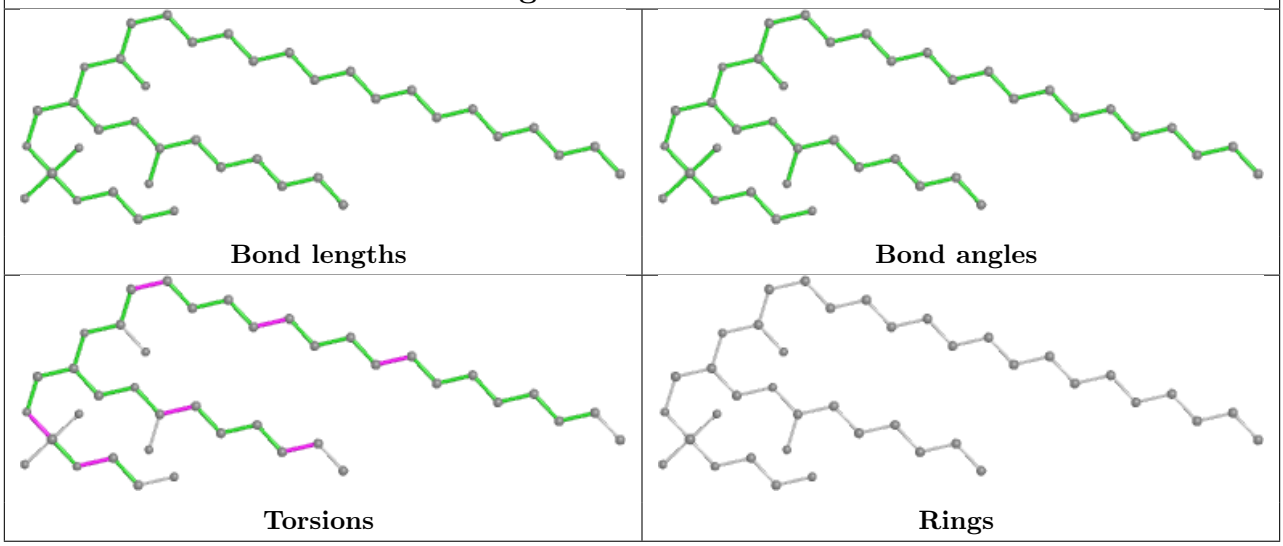
Ligand PC1 N4 503



Ligand PC1 N5 606



Ligand 3PE G1 516



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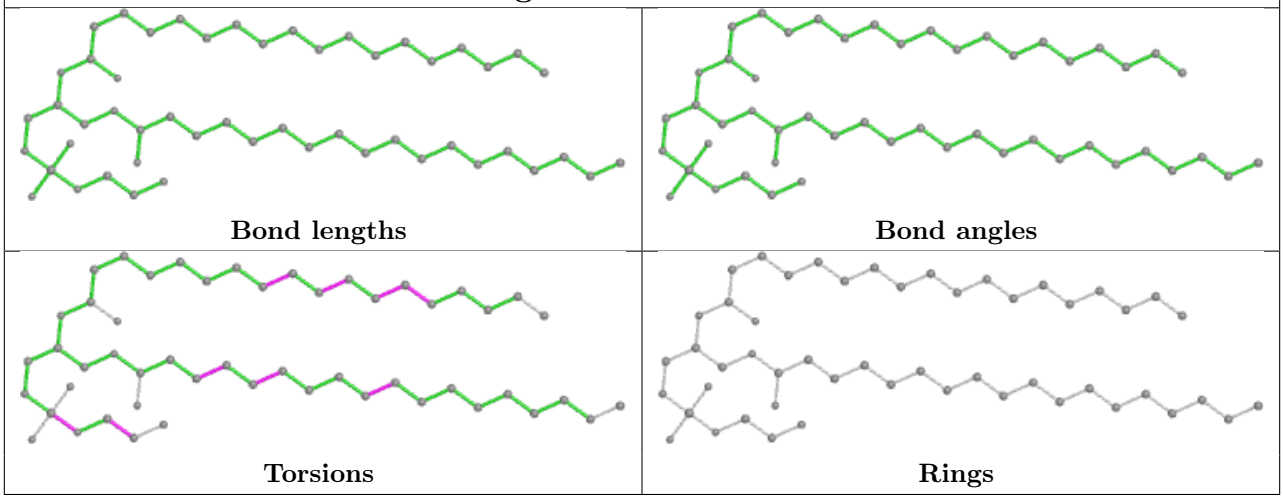
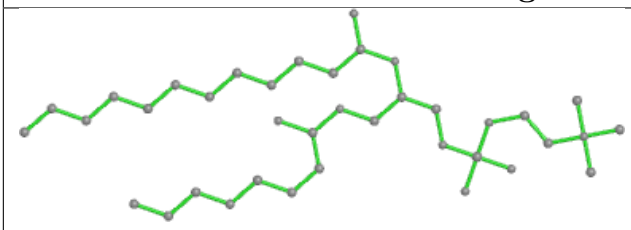
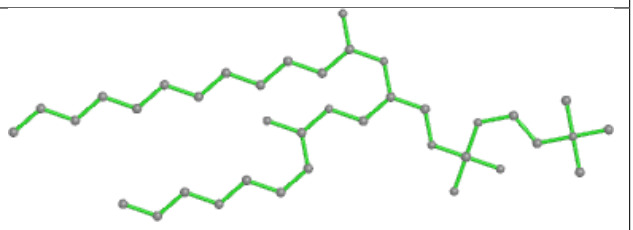


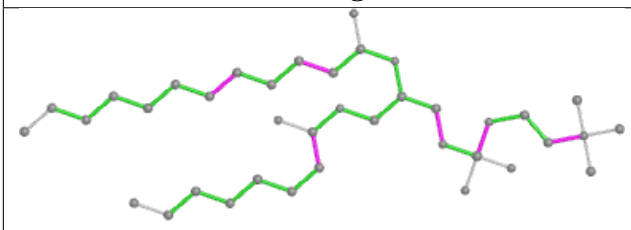
Ligand PC1 C4 203



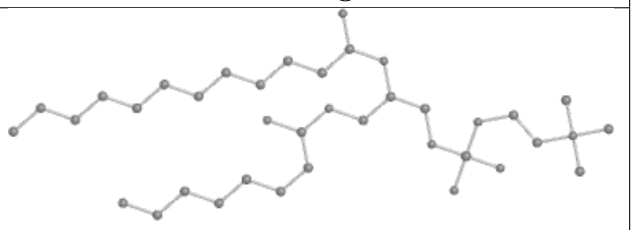
Bond lengths



Bond angles

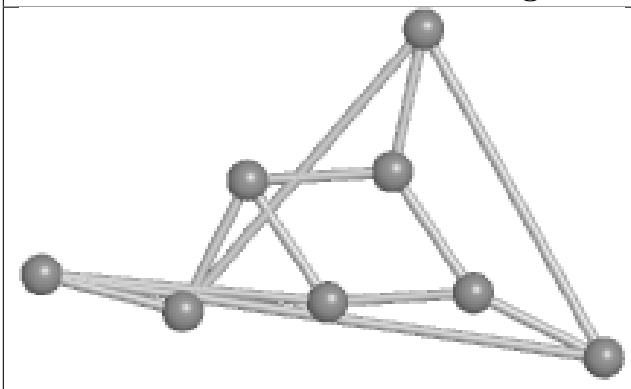


Torsions

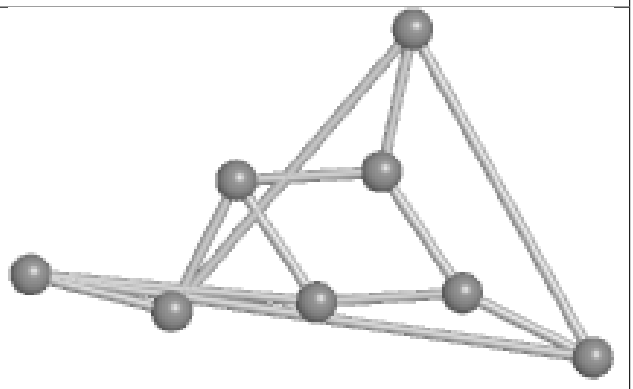


Rings

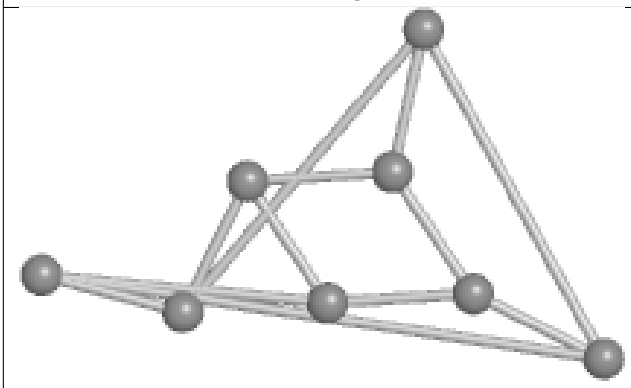
Ligand SF4 1A 403



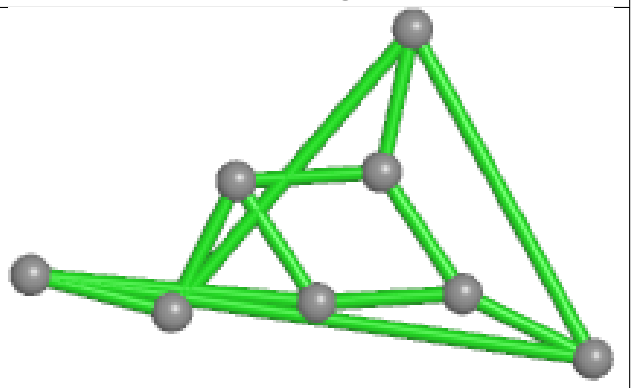
Bond lengths



Bond angles

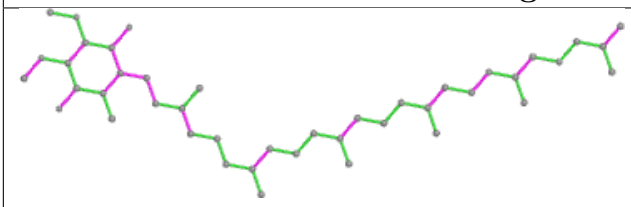


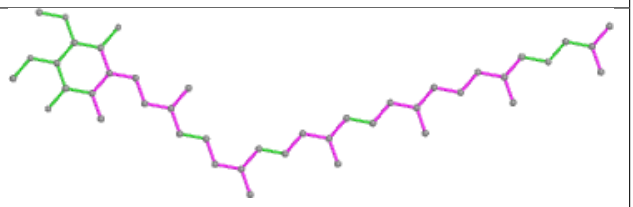
Torsions

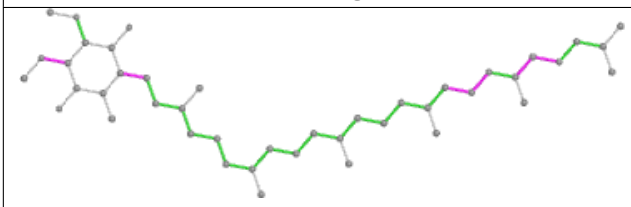


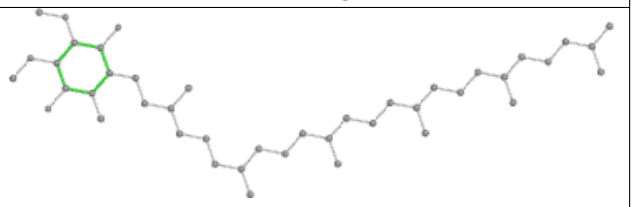
Rings

Ligand U10 N4 505

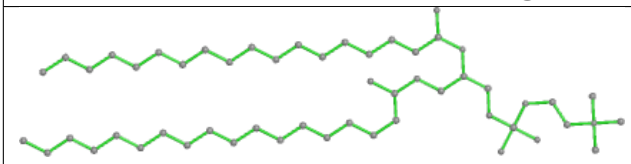

Bond lengths

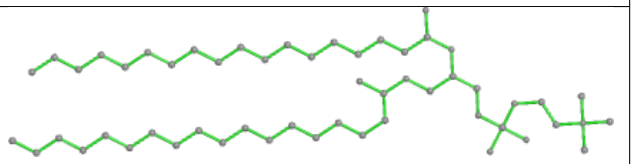

Bond angles

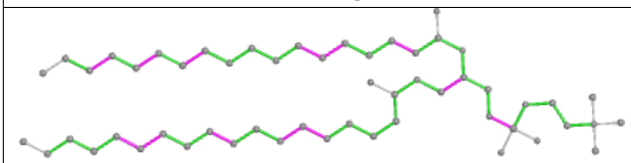

Torsions

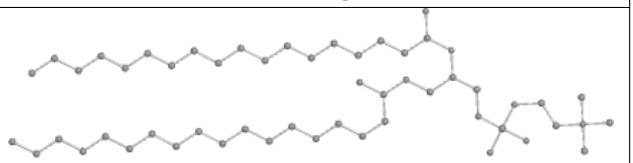

Rings

Ligand PC1 B5 203

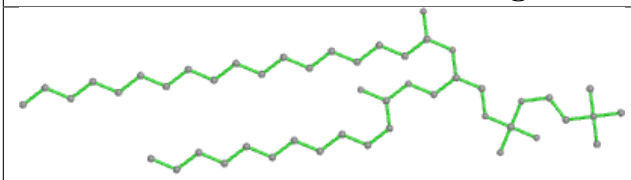

Bond lengths

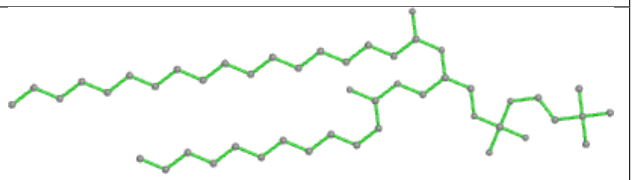

Bond angles

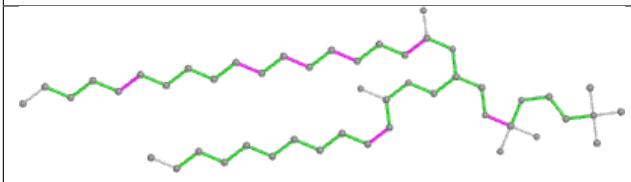

Torsions

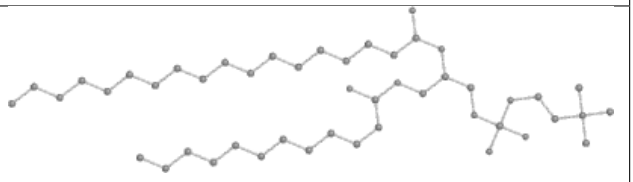

Rings

Ligand PC1 AM 220

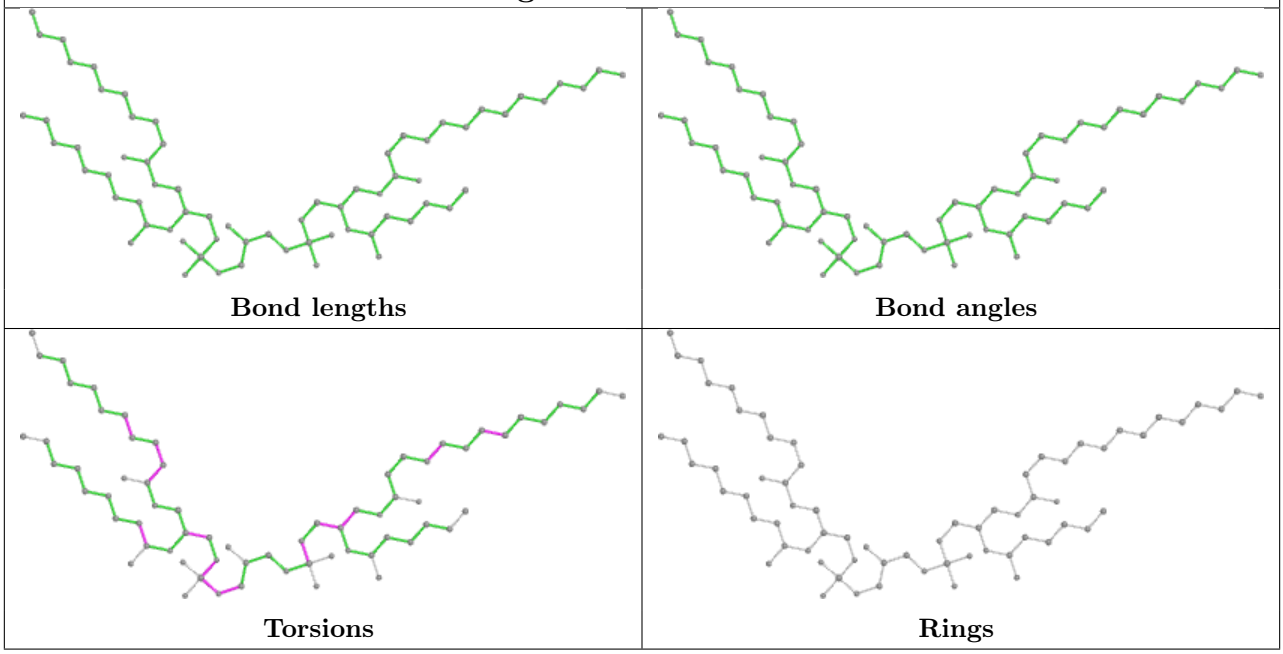

Bond lengths


Bond angles

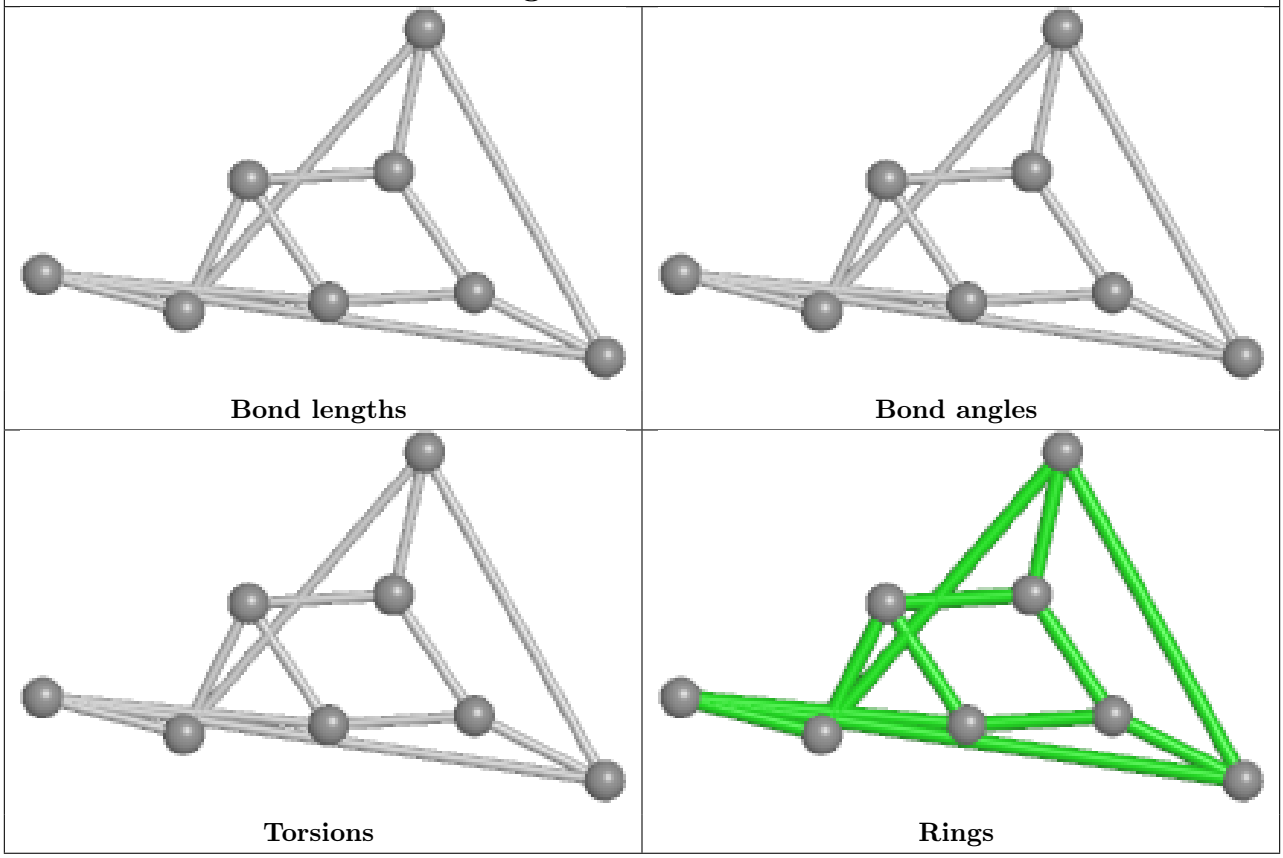

Torsions


Rings

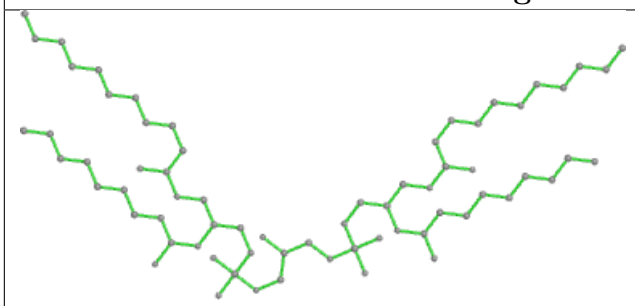
Ligand CDL E7 301



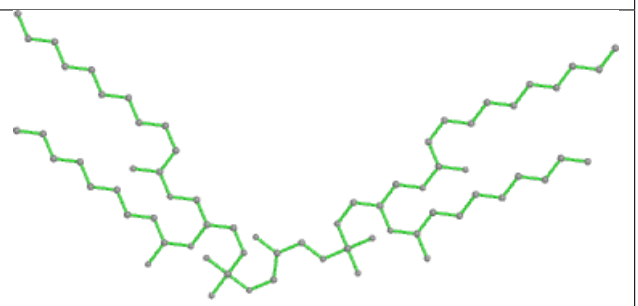
Ligand SF4 1A 402



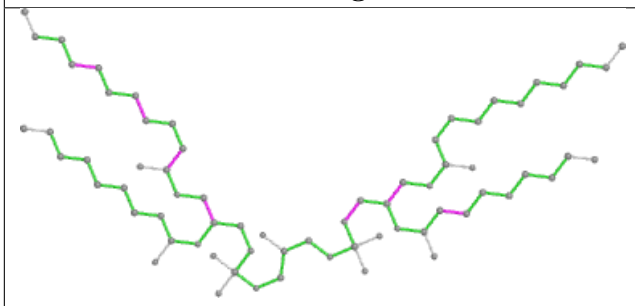
Ligand CDL AL 302



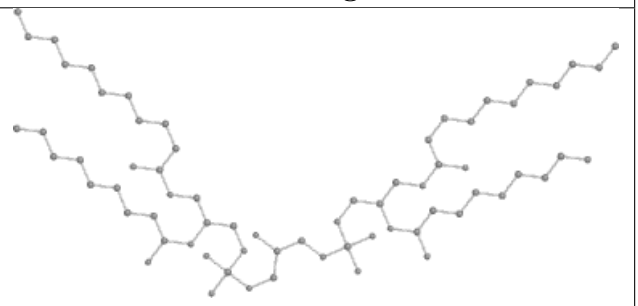
Bond lengths



Bond angles

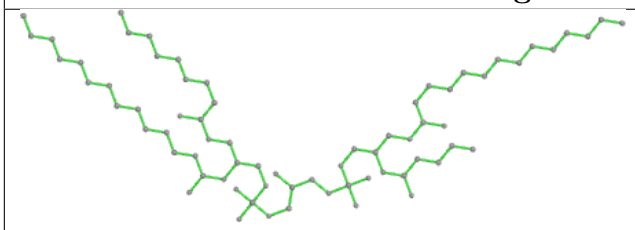


Torsions

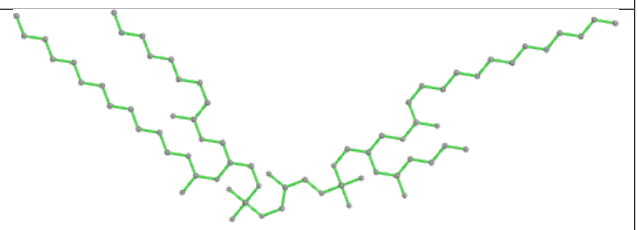


Rings

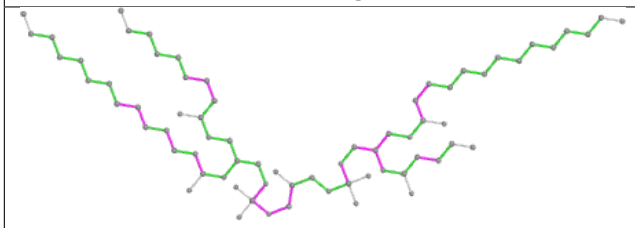
Ligand CDL AL 304



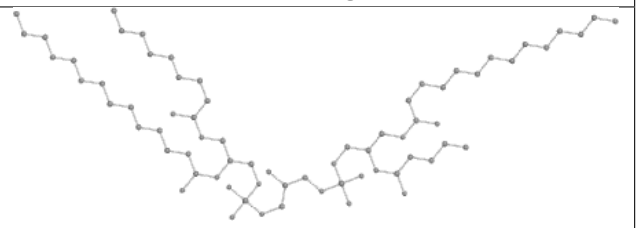
Bond lengths



Bond angles

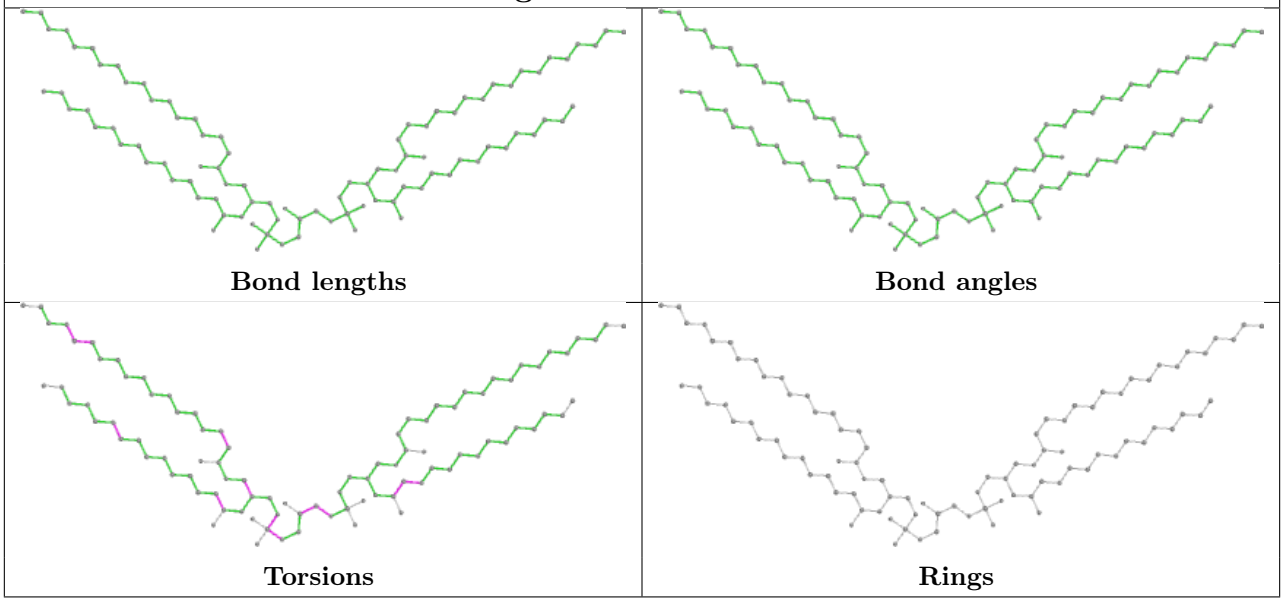


Torsions

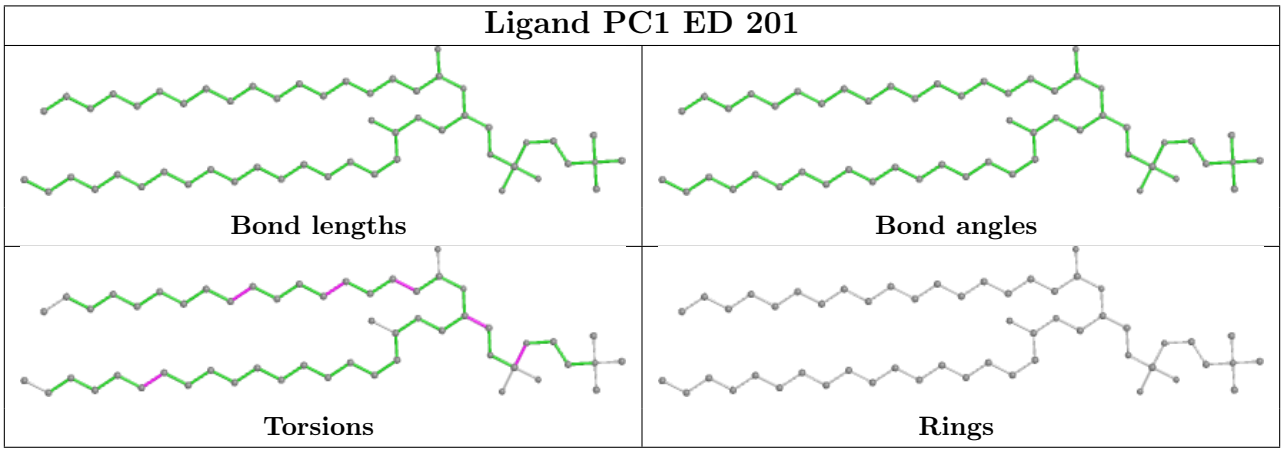


Rings

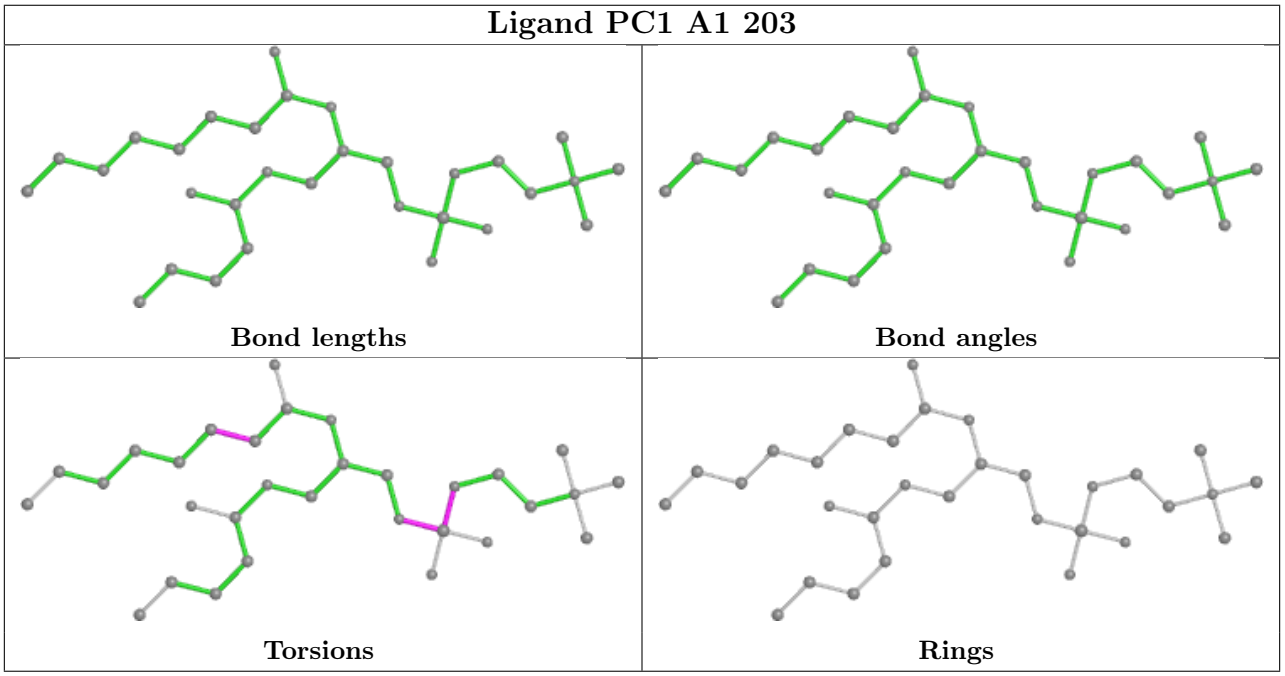
Ligand CDL N5 608



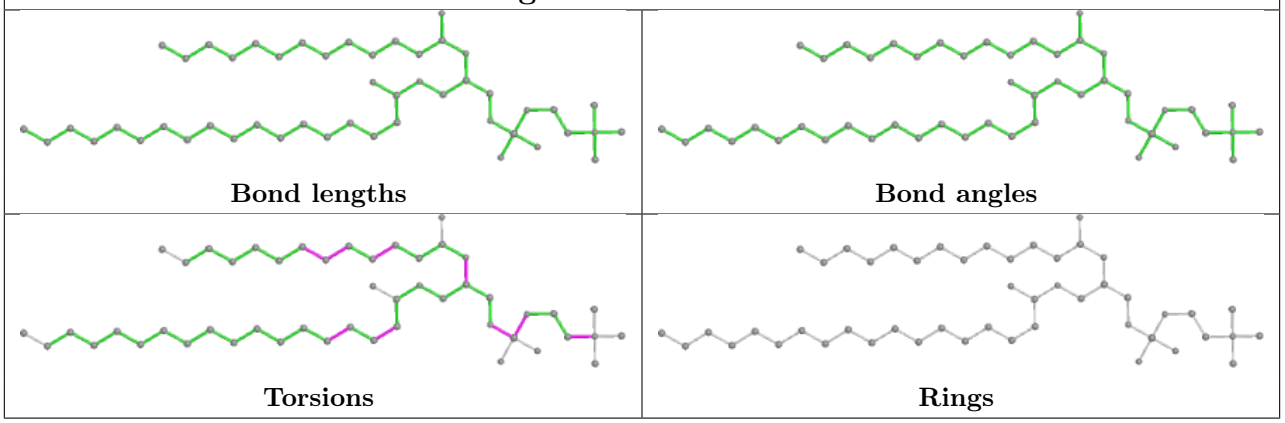
Ligand PC1 ED 201



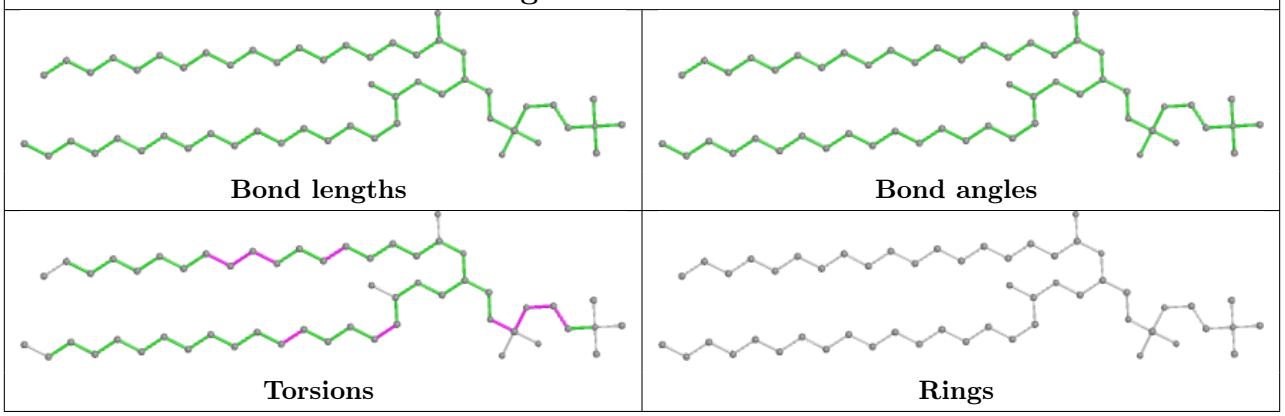
Ligand PC1 A1 203



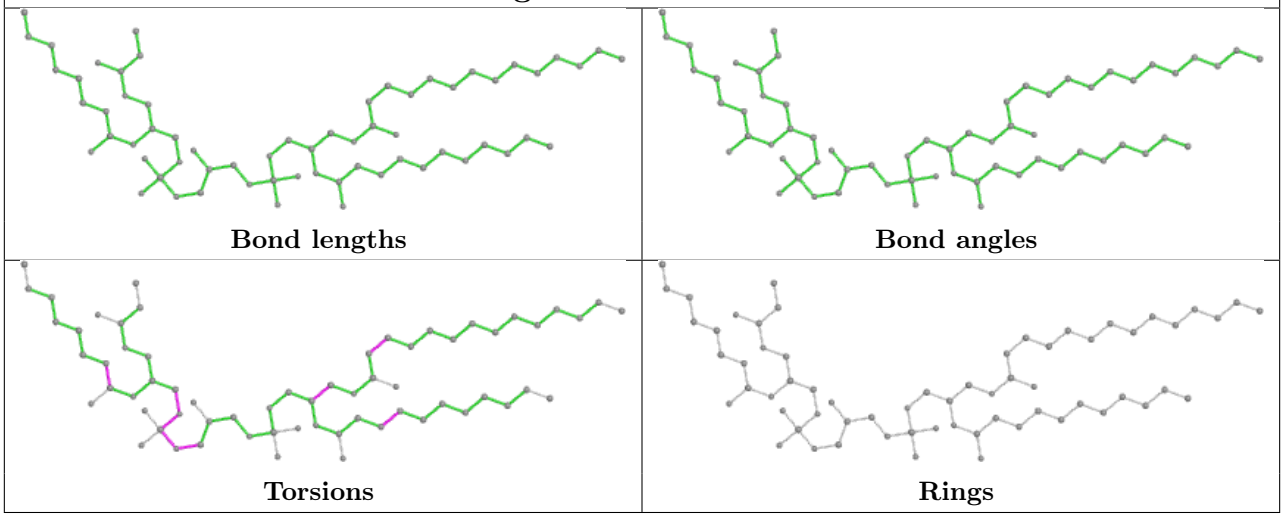
Ligand PC1 A1 202



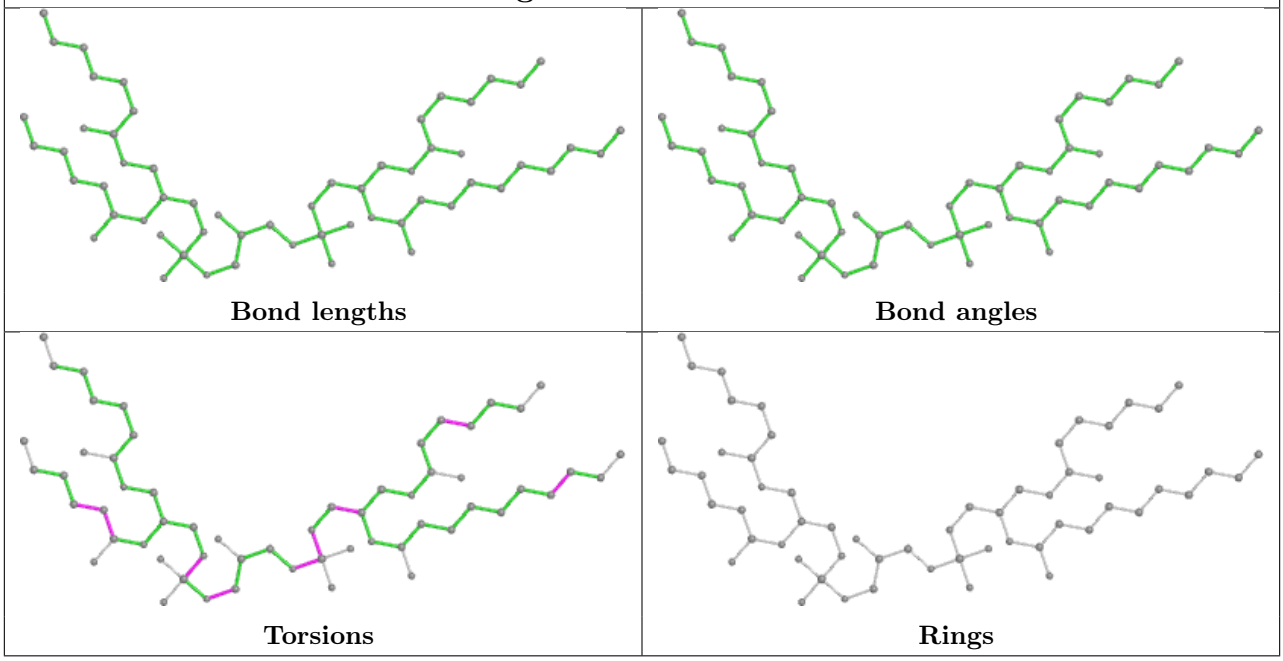
Ligand PC1 E8 301



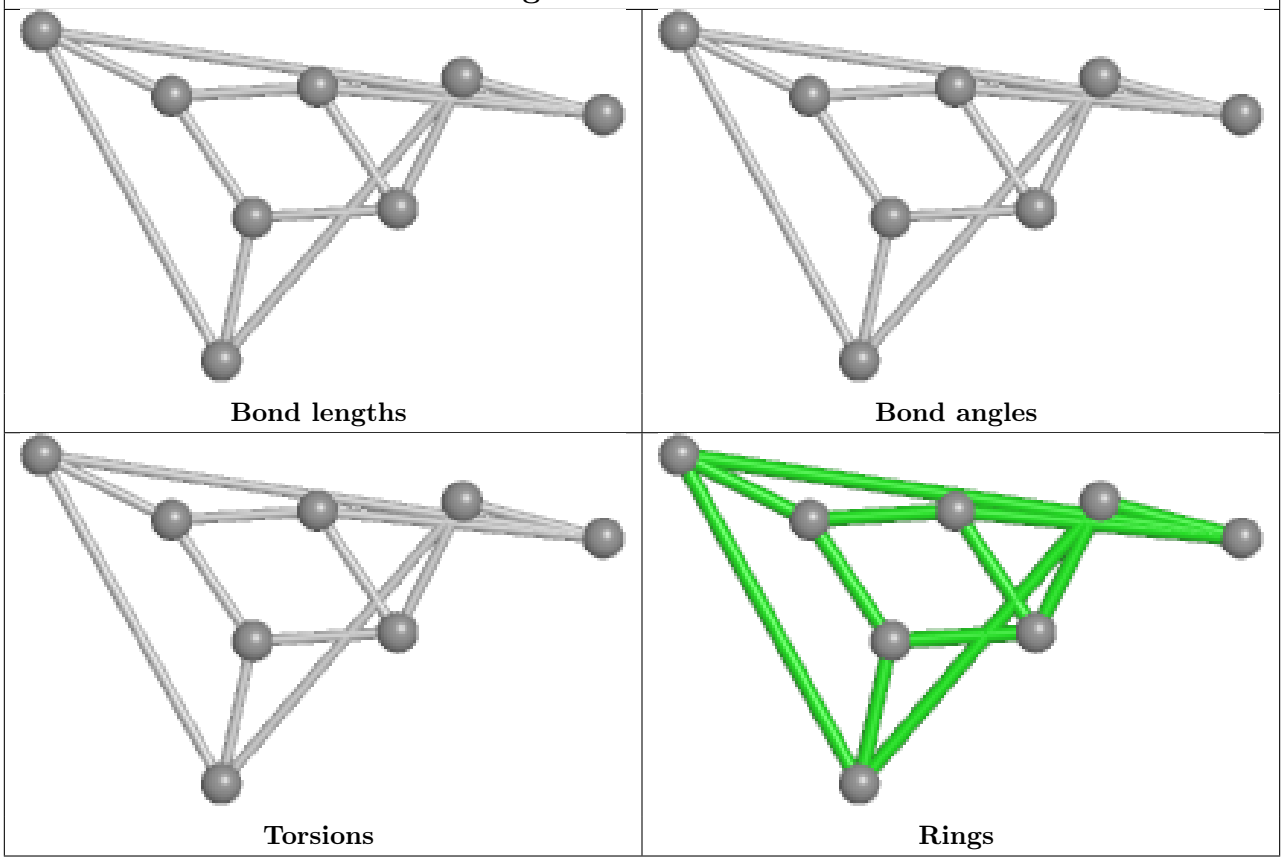
Ligand CDL AL 303



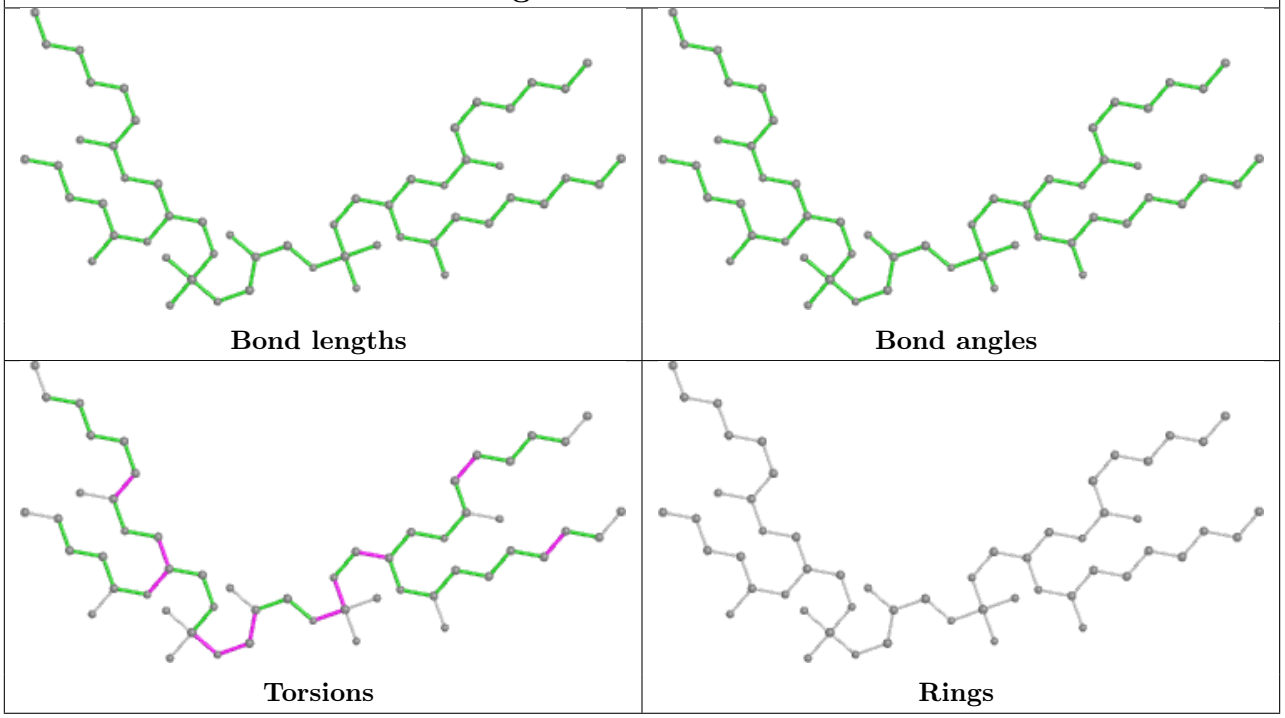
Ligand CDL B5 201



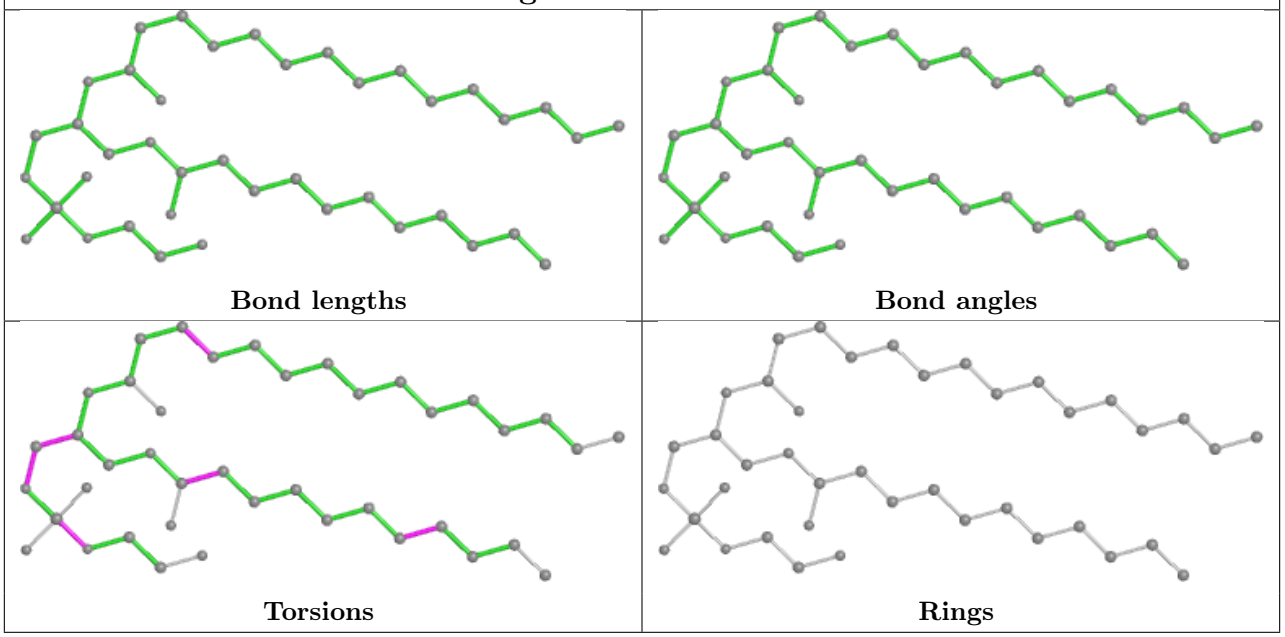
Ligand SF4 V1 580



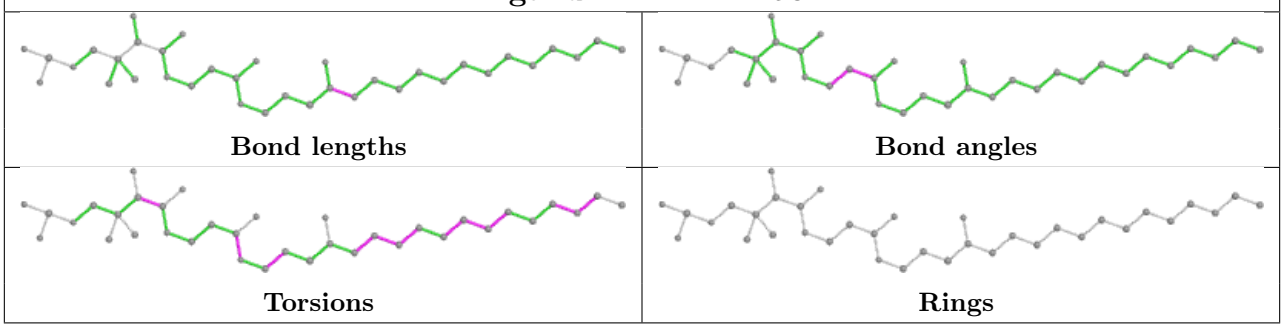
Ligand CDL EA 202



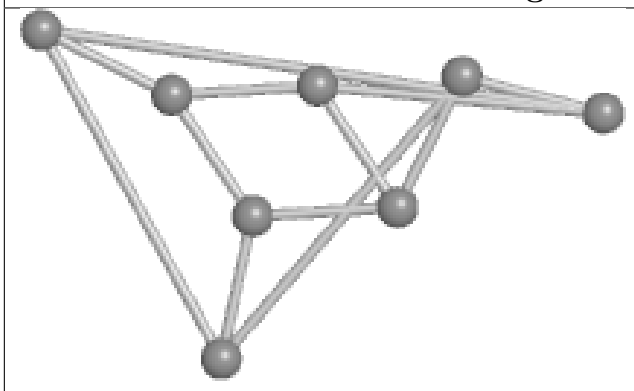
Ligand 3PE N4 504



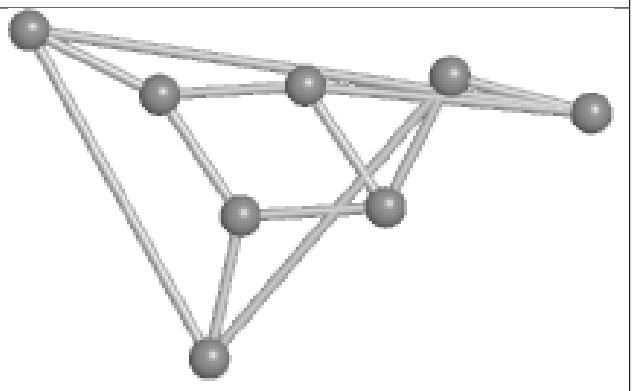
Ligand ZMP AB 150



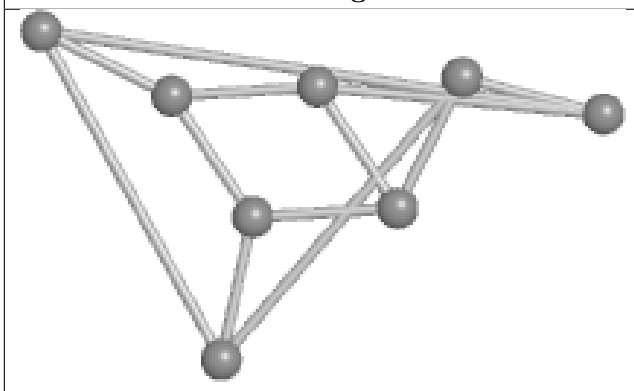
Ligand SF4 S7 301



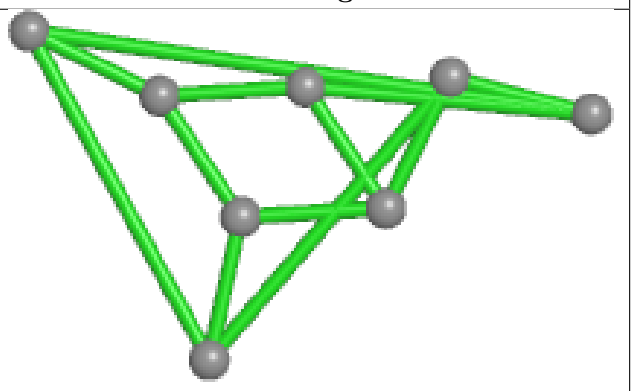
Bond lengths



Bond angles

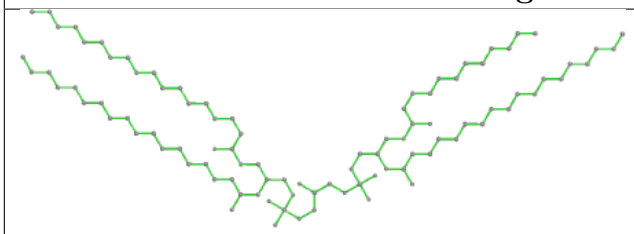


Torsions

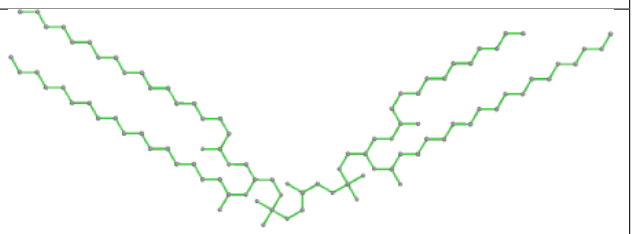


Rings

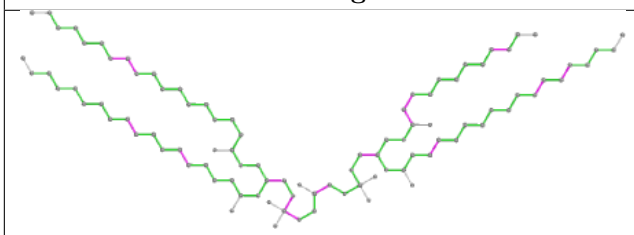
Ligand CDL C4 202



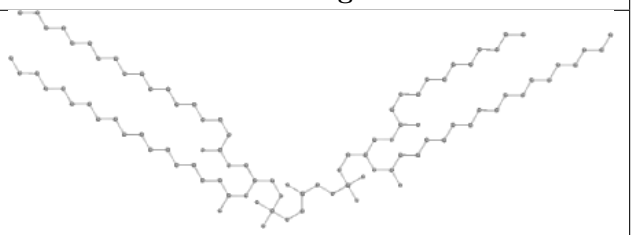
Bond lengths



Bond angles

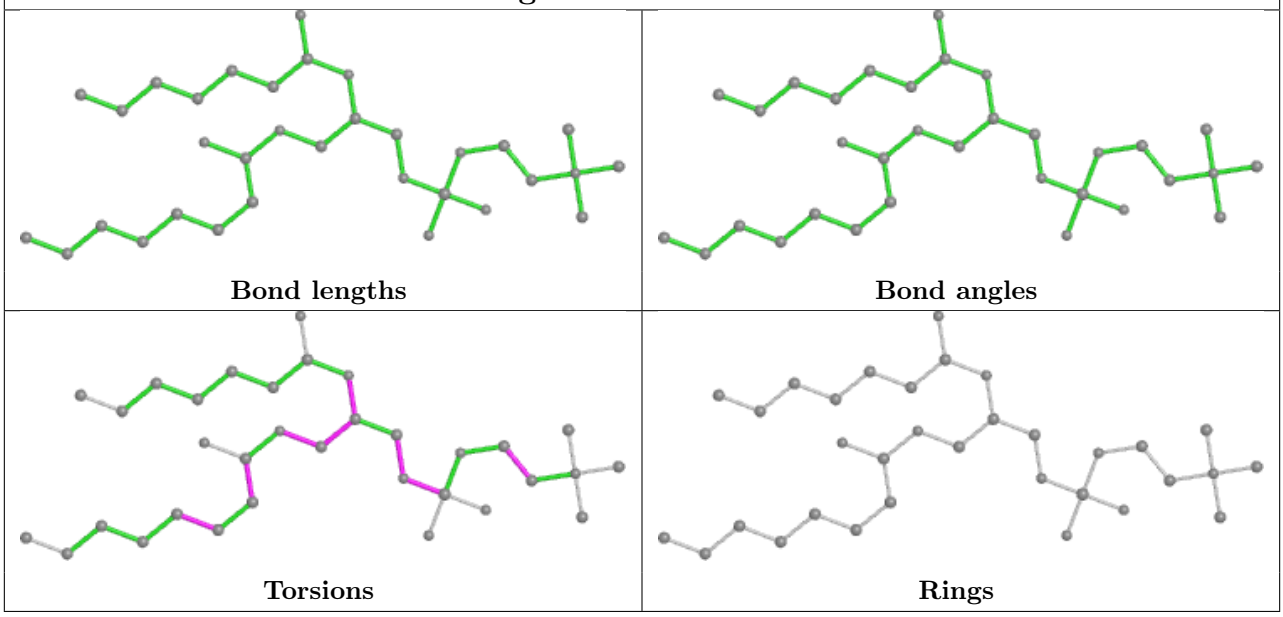


Torsions

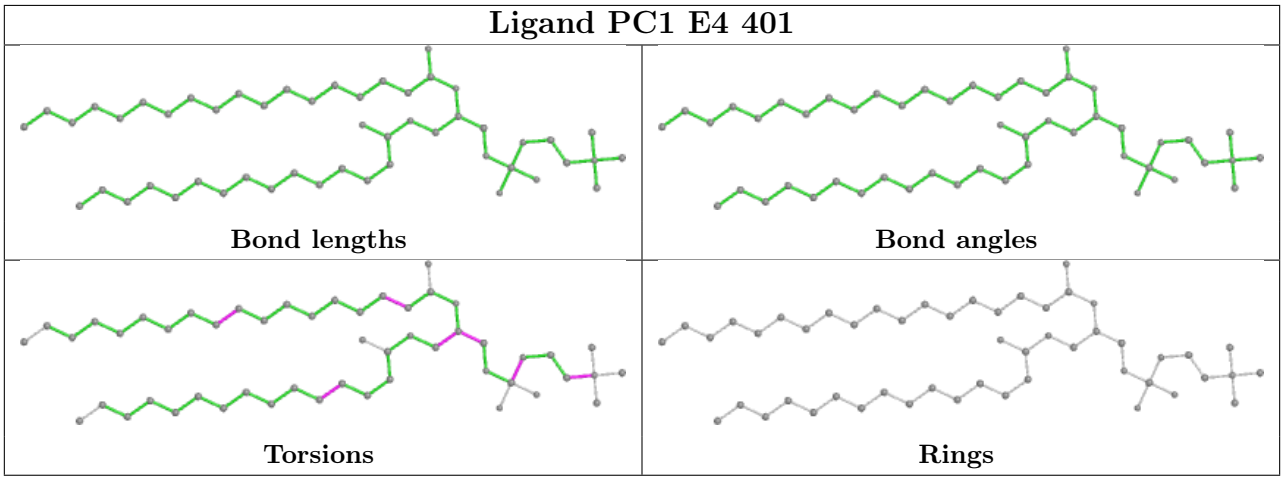


Rings

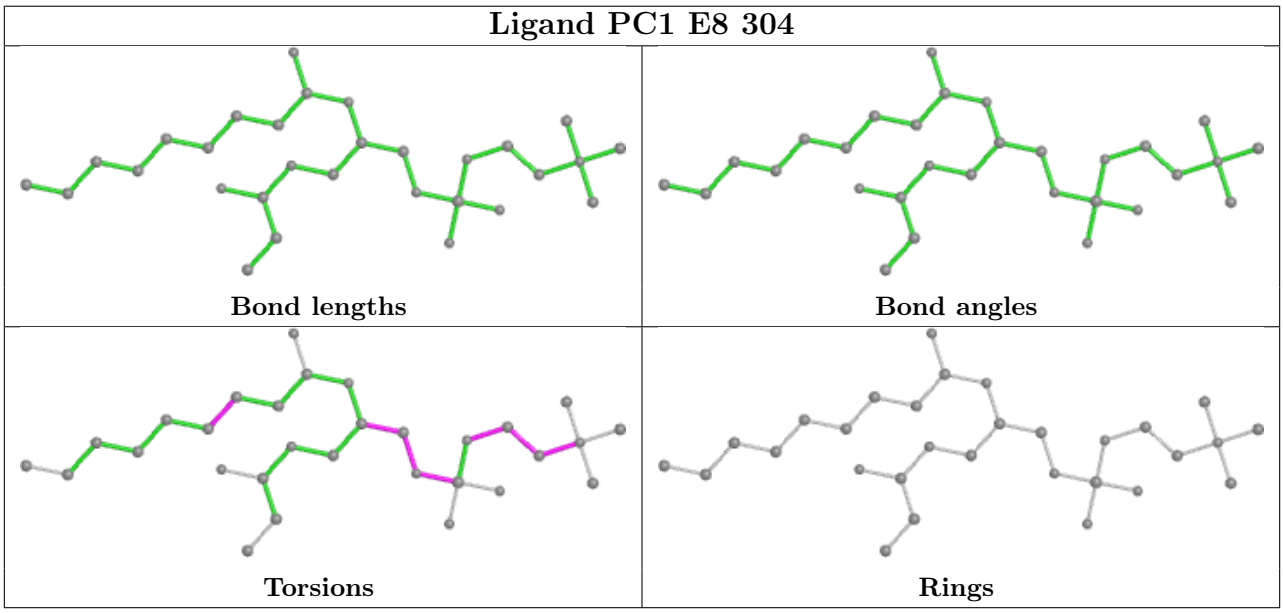
Ligand PC1 A9 560



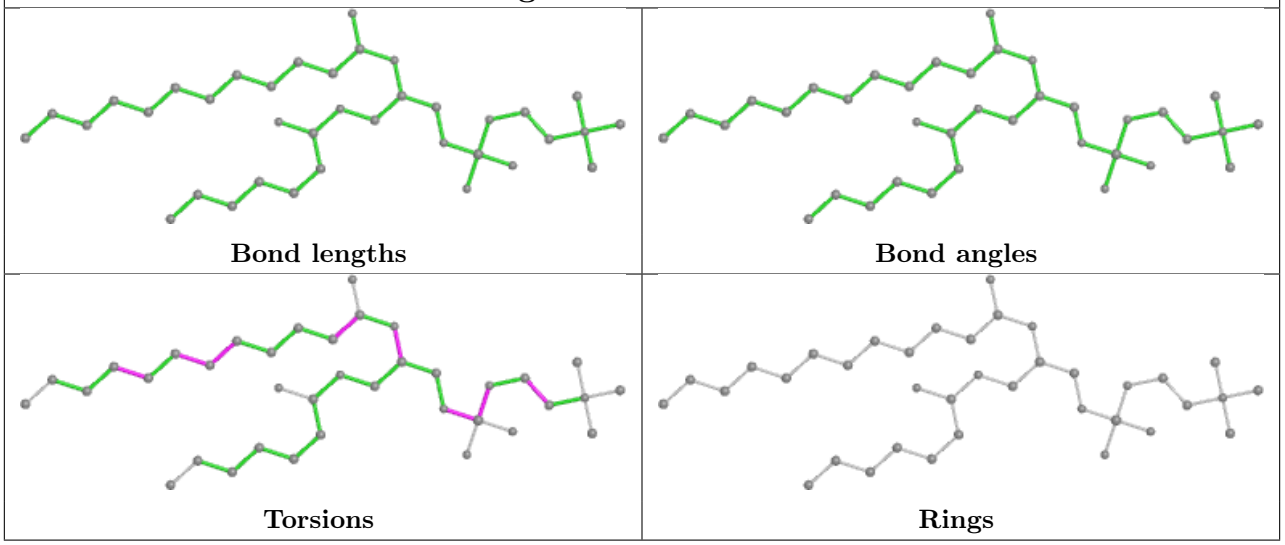
Ligand PC1 E4 401



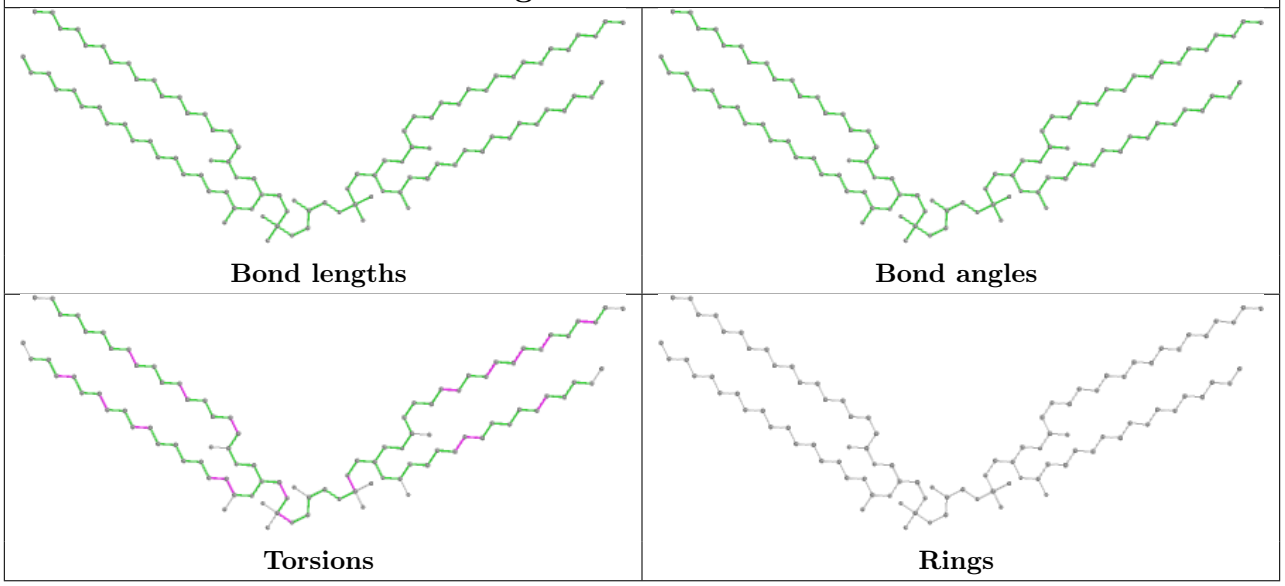
Ligand PC1 E8 304



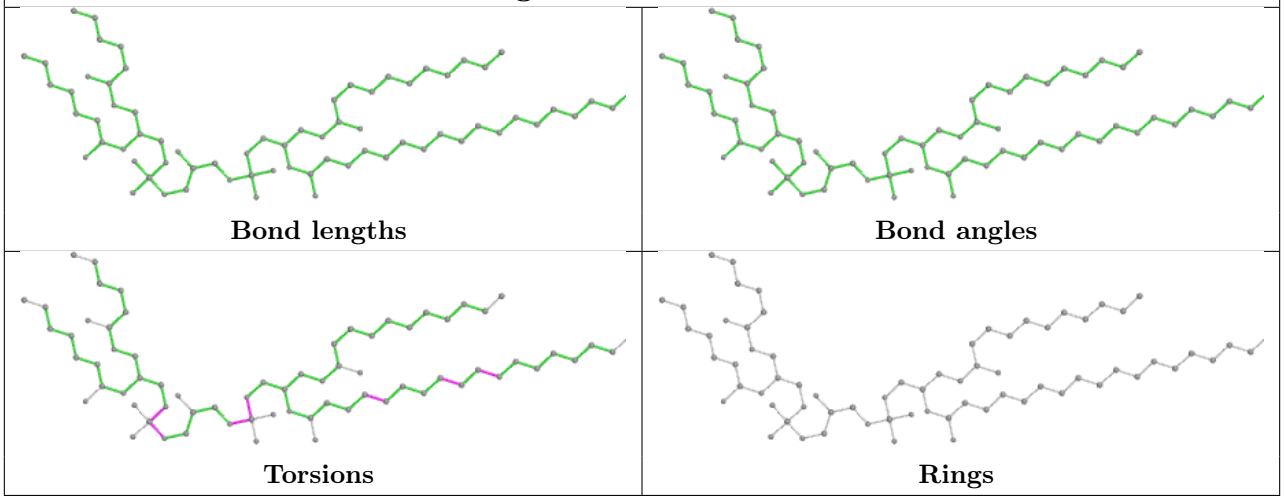
Ligand PC1 N2 301



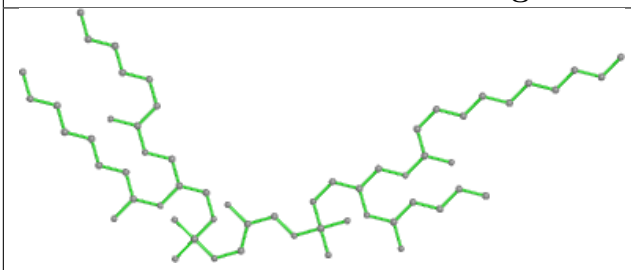
Ligand CDL N4 501



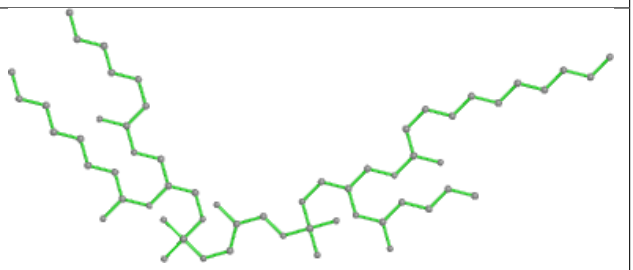
Ligand CDL N5 603



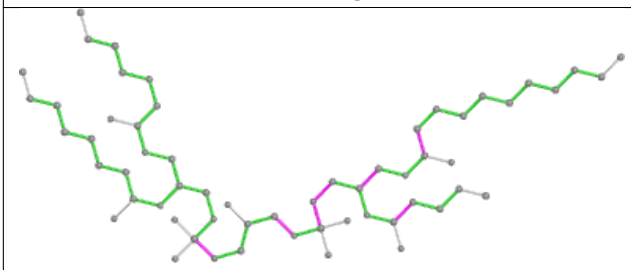
Ligand CDL EA 201



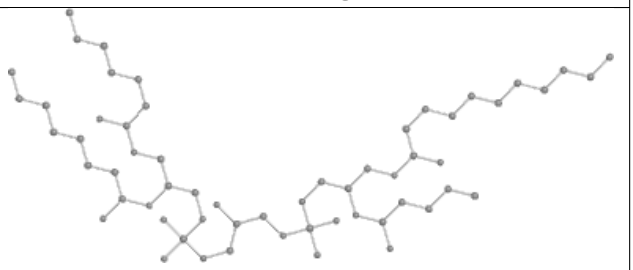
Bond lengths



Bond angles

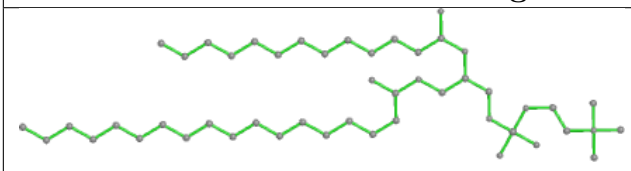


Torsions

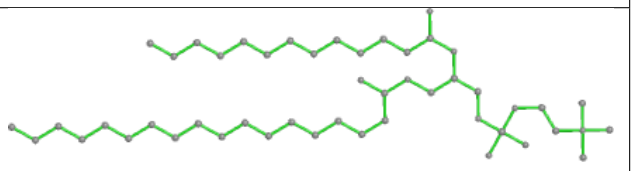


Rings

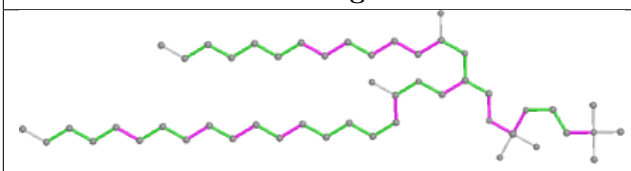
Ligand PC1 AM 218



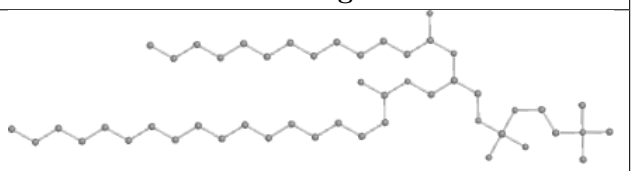
Bond lengths



Bond angles

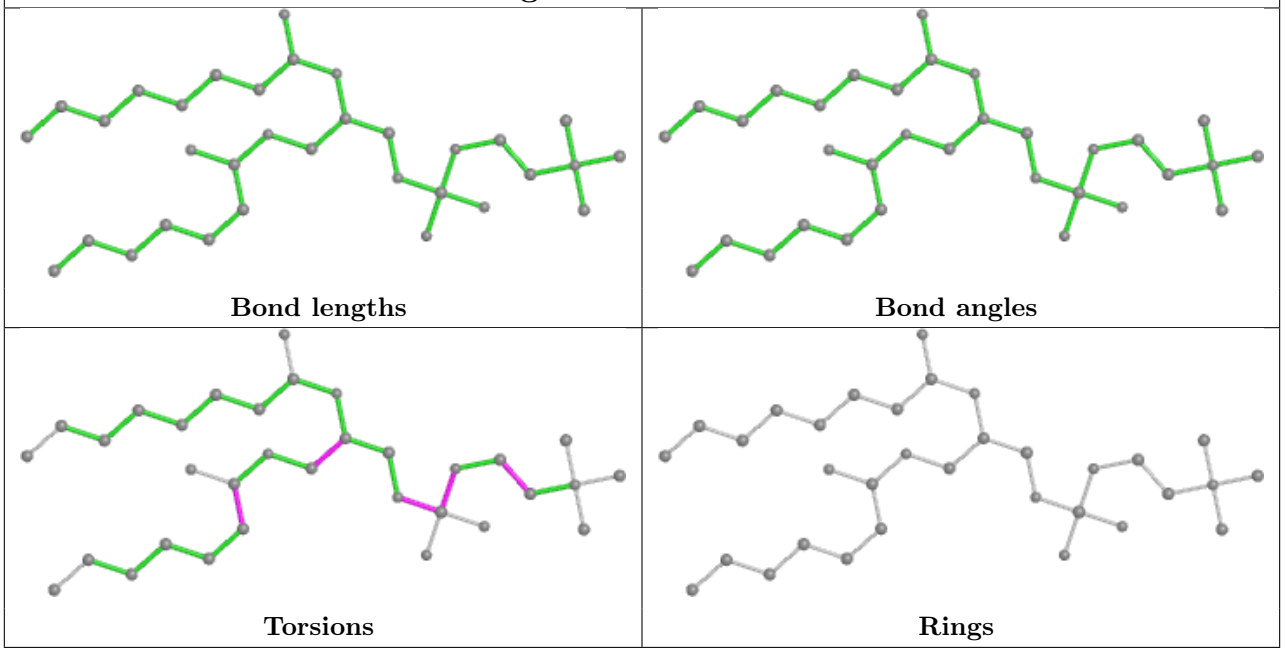


Torsions

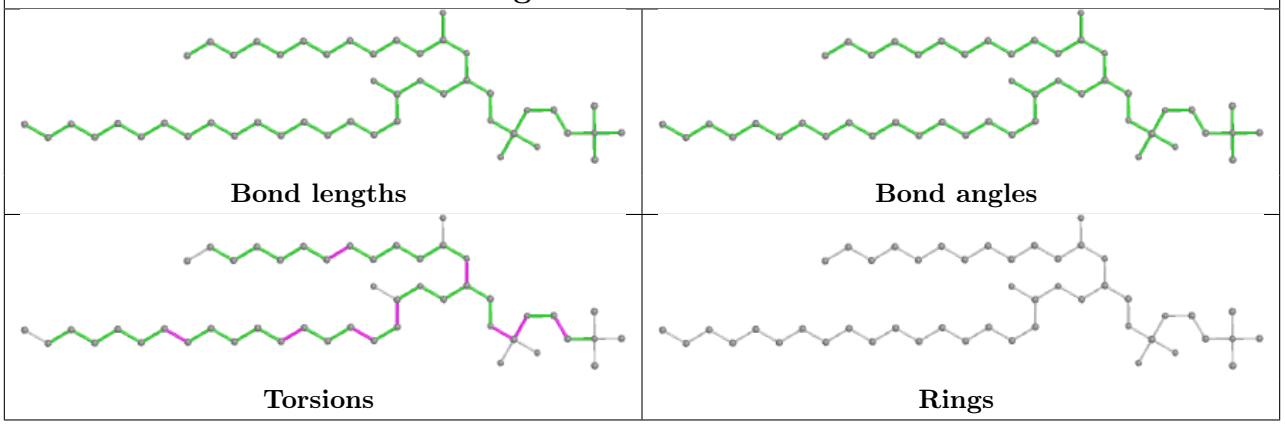


Rings

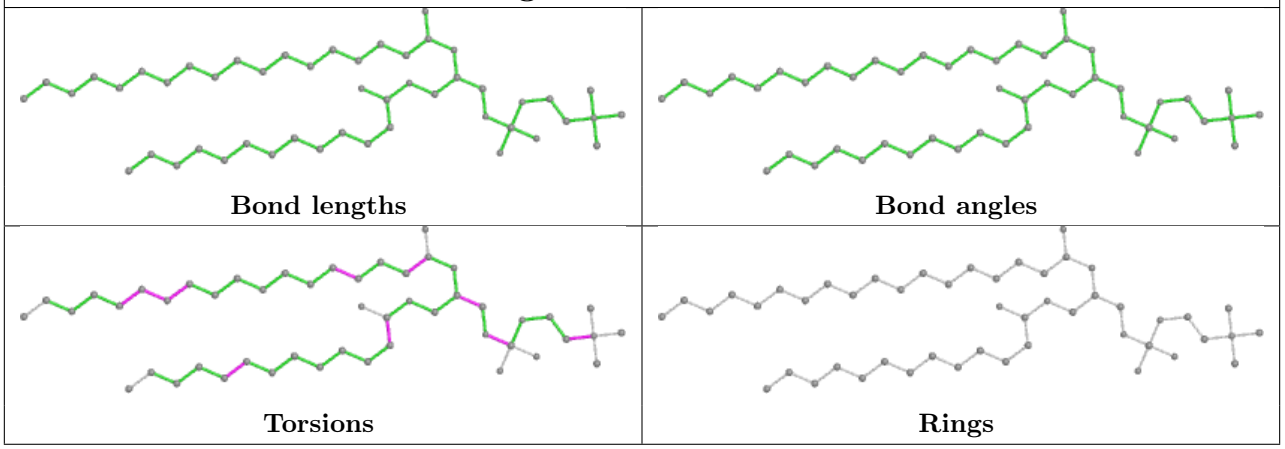
Ligand PC1 E8 303



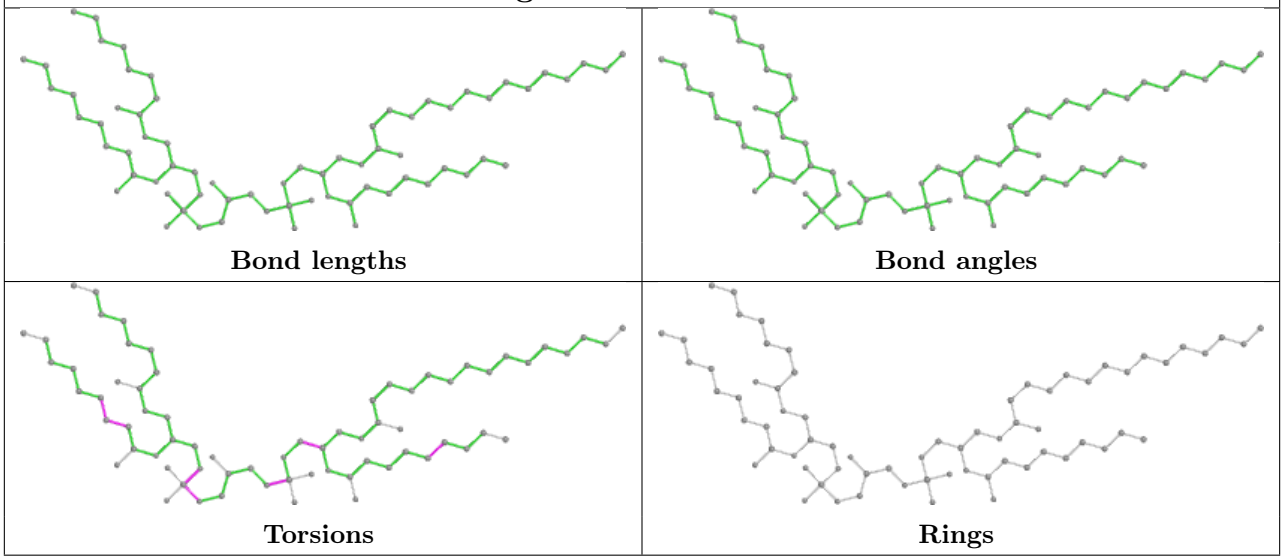
Ligand PC1 AN 301



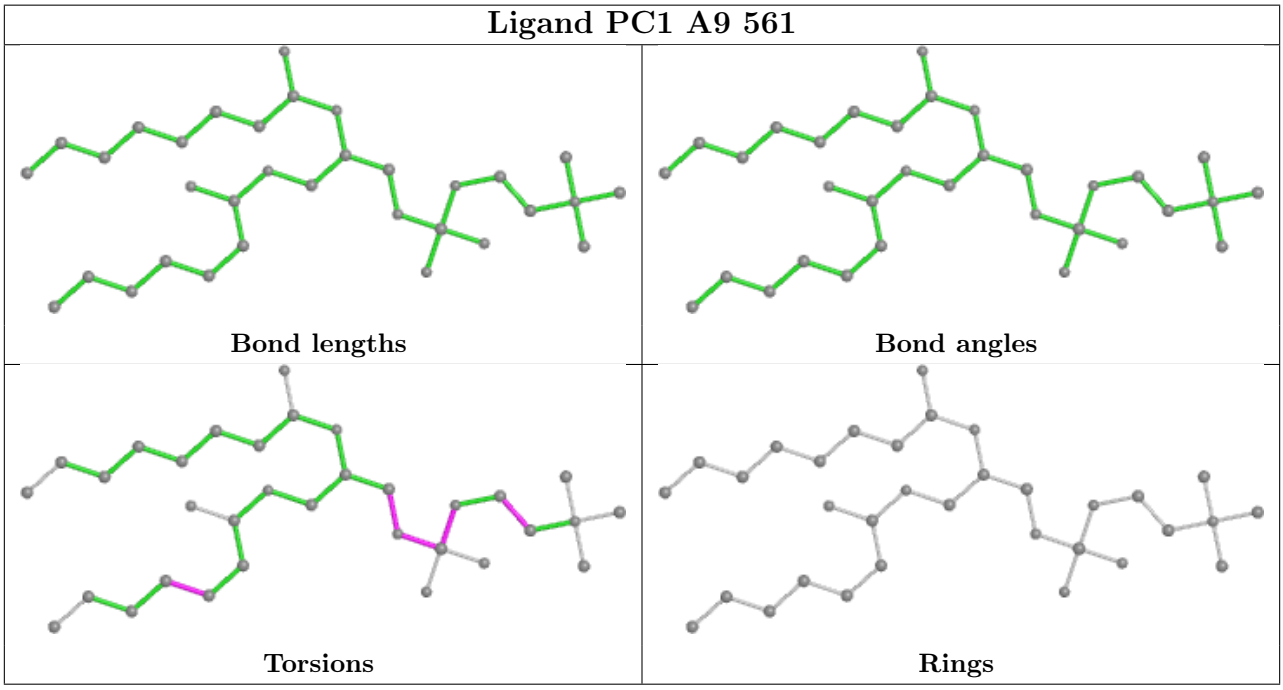
Ligand PC1 N1 701



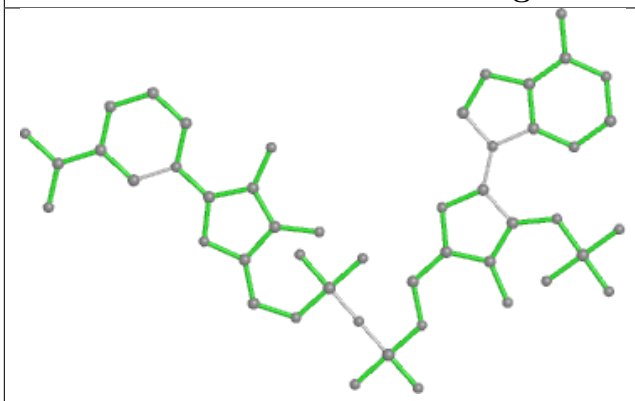
Ligand CDL C4 204



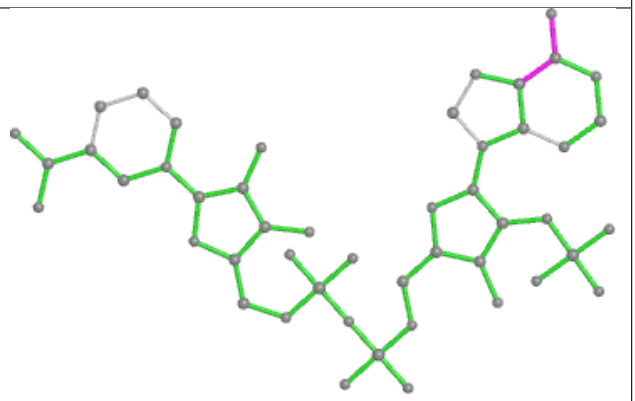
Ligand PC1 A9 561



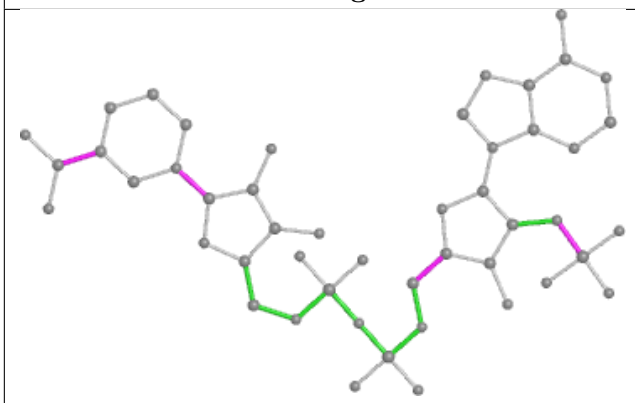
Ligand NDP A9 559



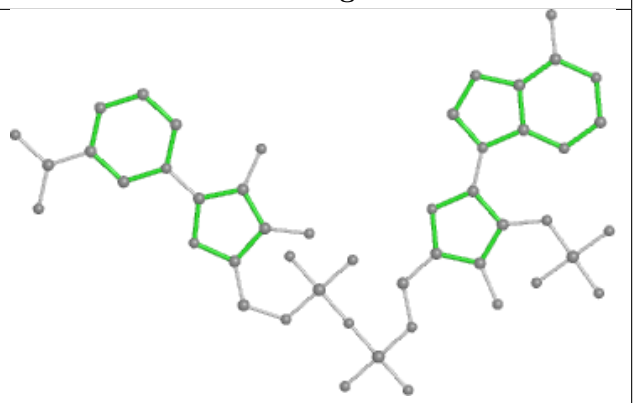
Bond lengths



Bond angles

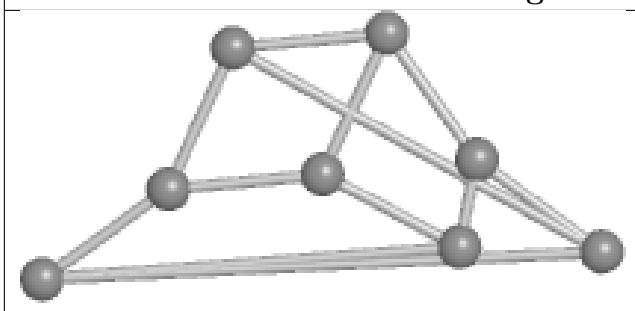


Torsions

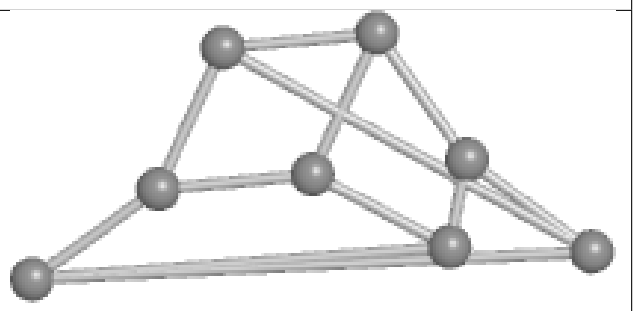


Rings

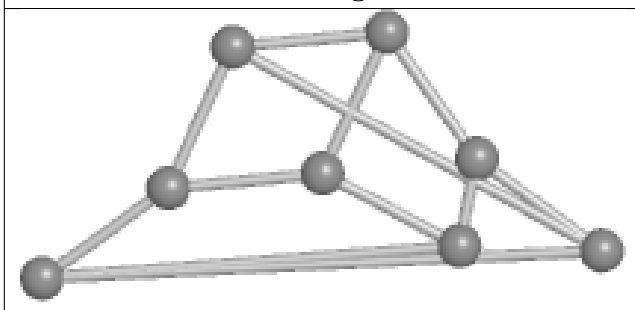
Ligand SF4 S8 297



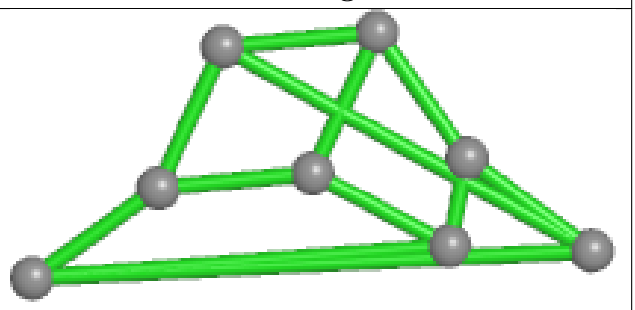
Bond lengths



Bond angles

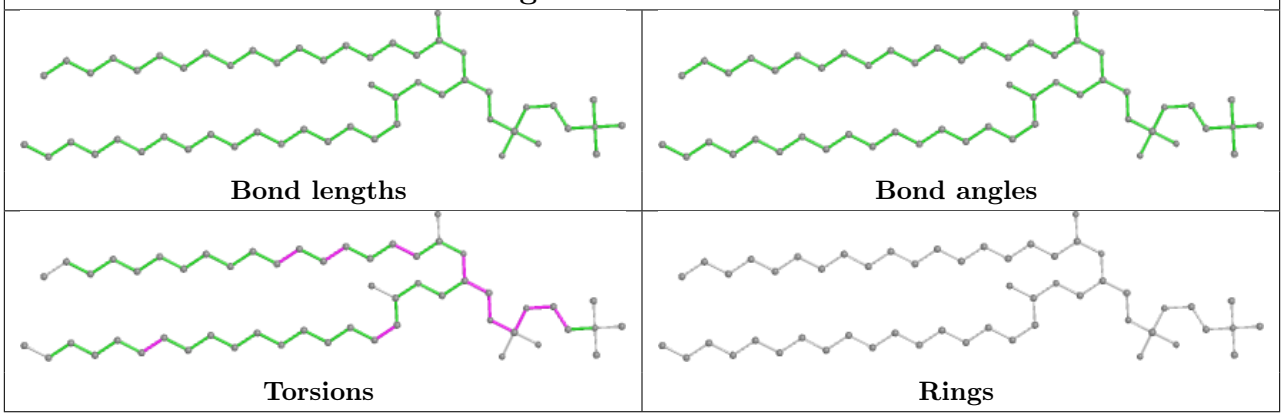


Torsions

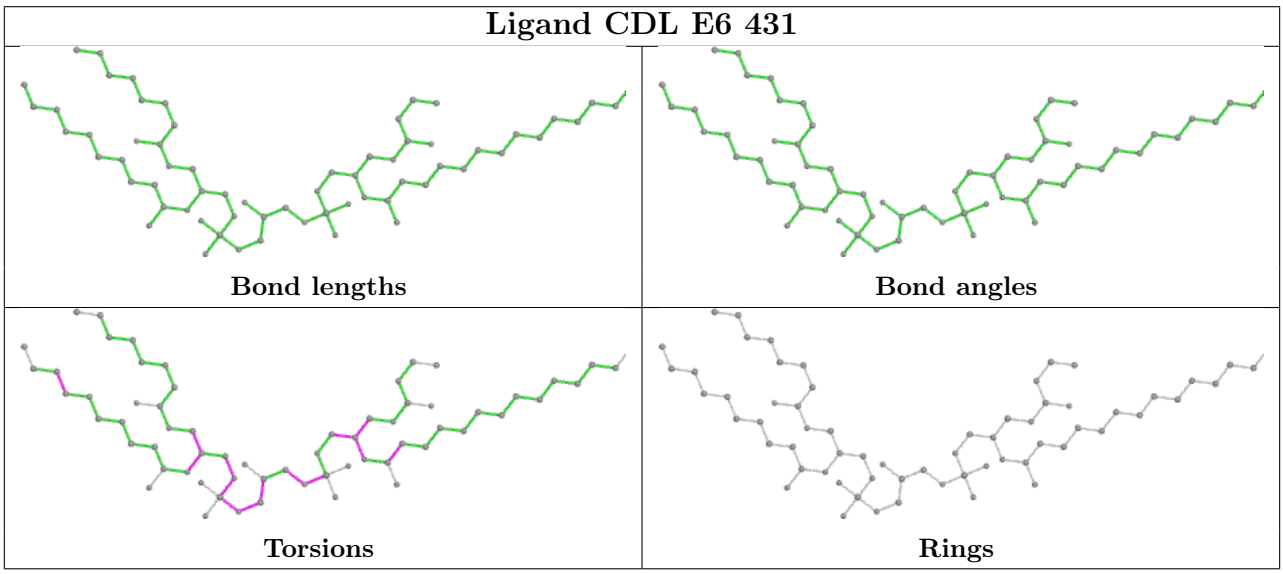


Rings

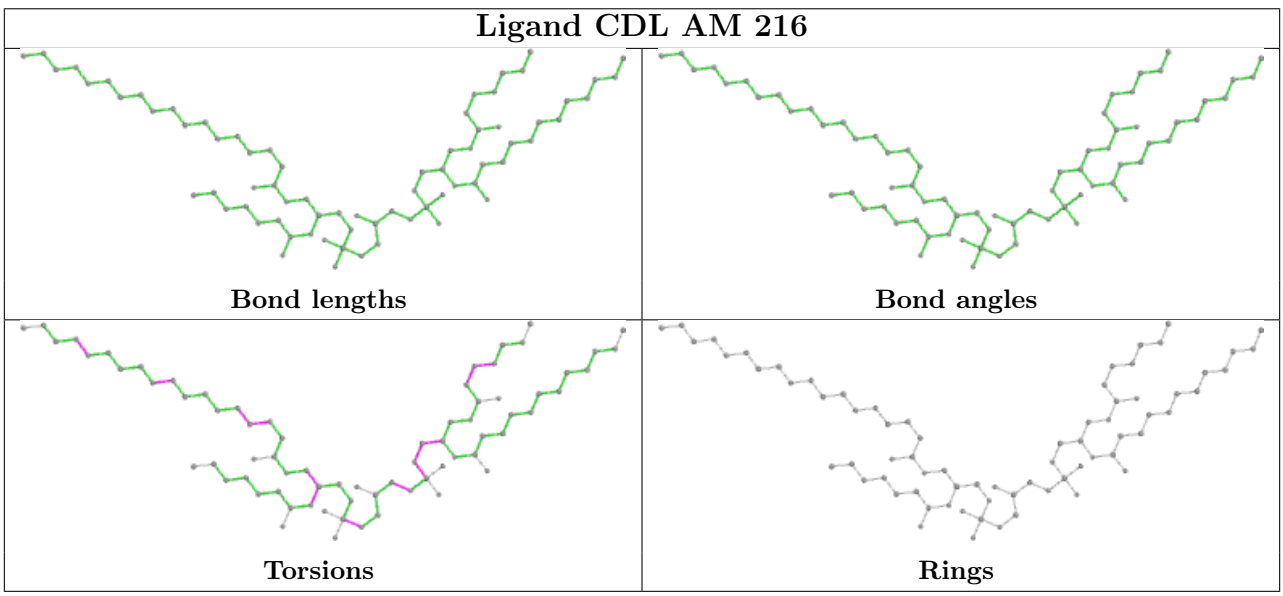
Ligand PC1 B5 202



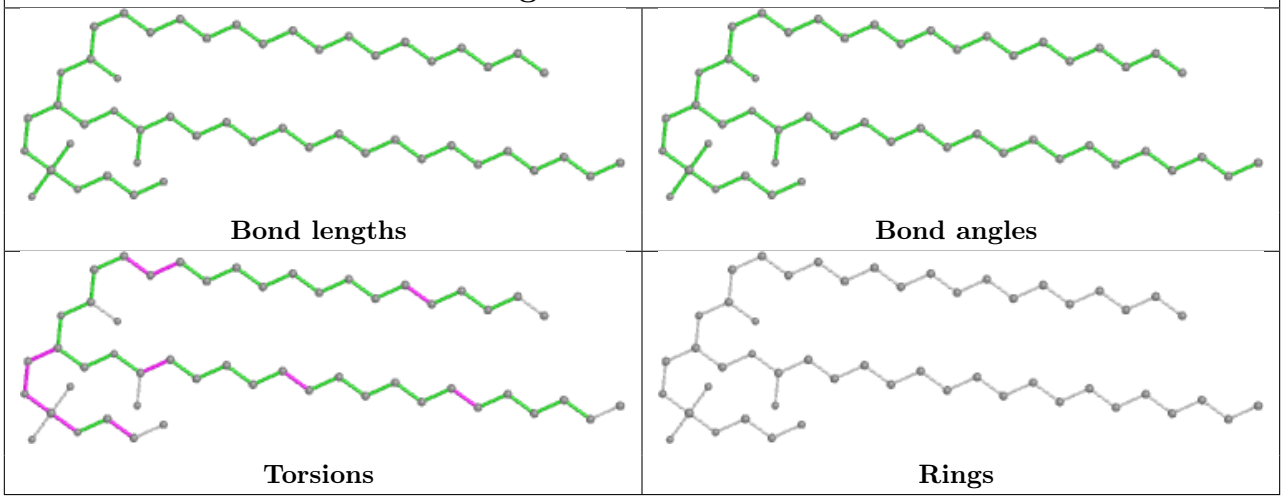
Ligand CDL E6 431



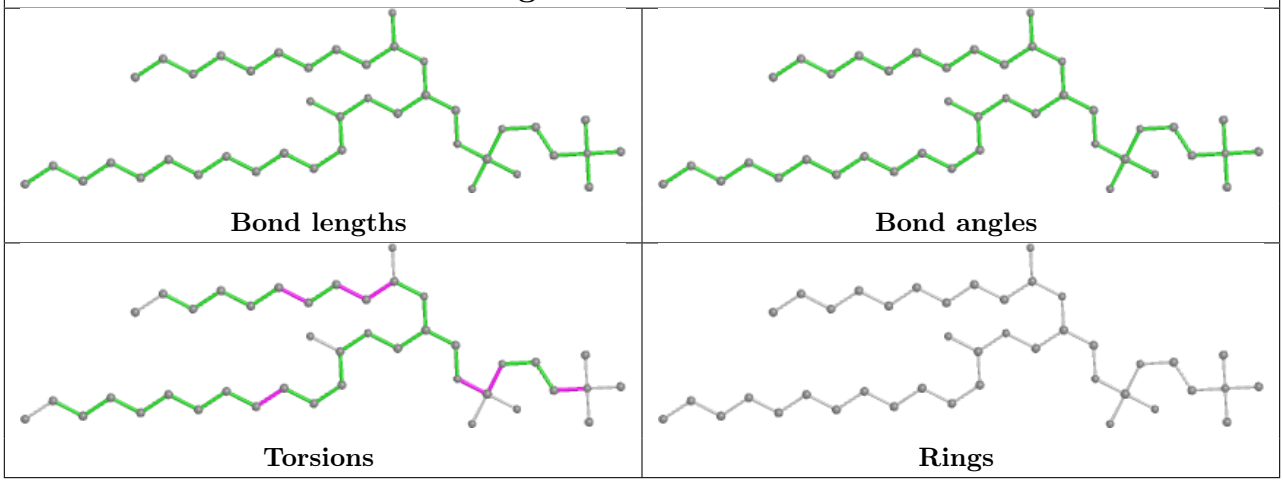
Ligand CDL AM 216



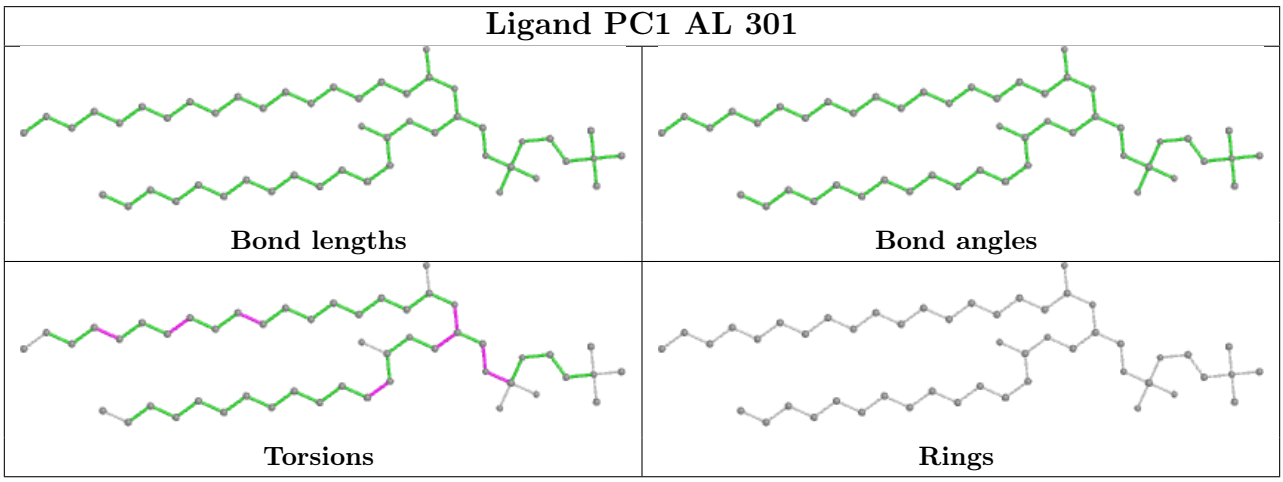
Ligand 3PE N5 607



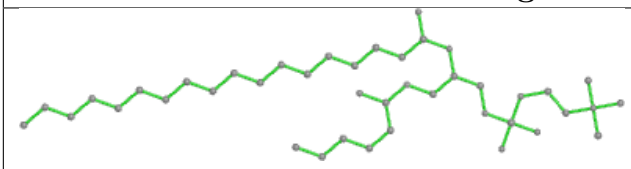
Ligand PC1 N5 605



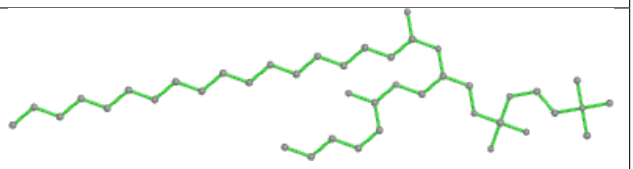
Ligand PC1 AL 301



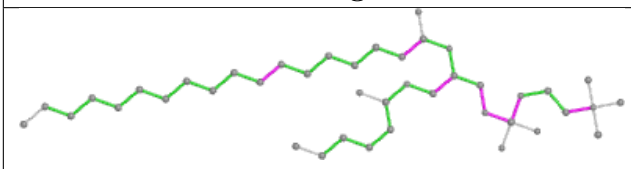
Ligand PC1 N3 301



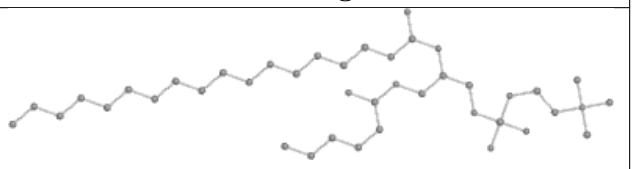
Bond lengths



Bond angles

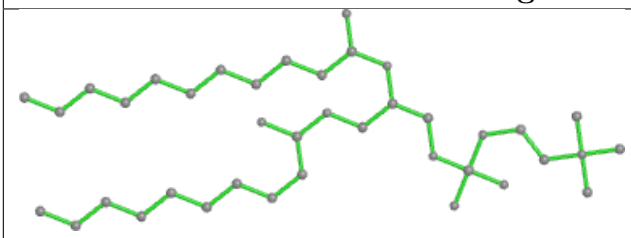


Torsions

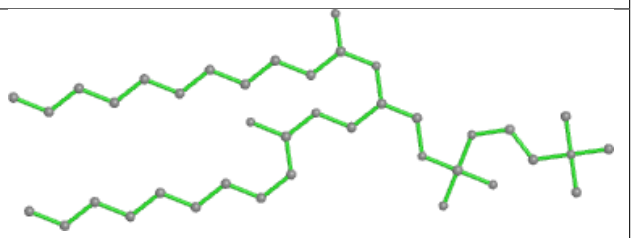


Rings

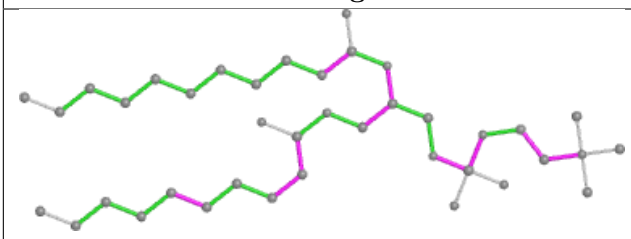
Ligand PC1 N4 502



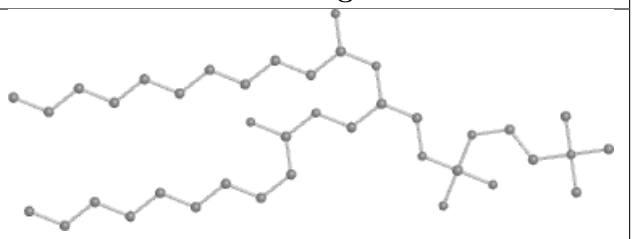
Bond lengths



Bond angles

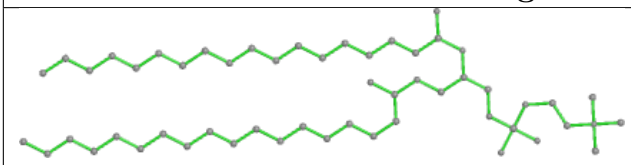


Torsions

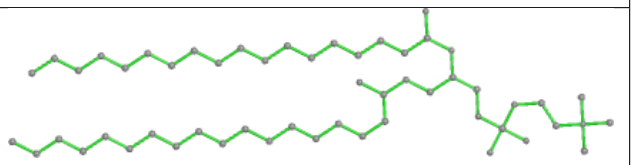


Rings

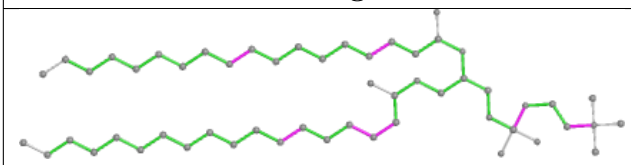
Ligand PC1 N5 601



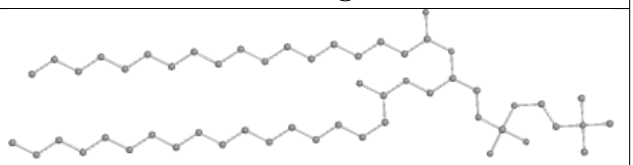
Bond lengths



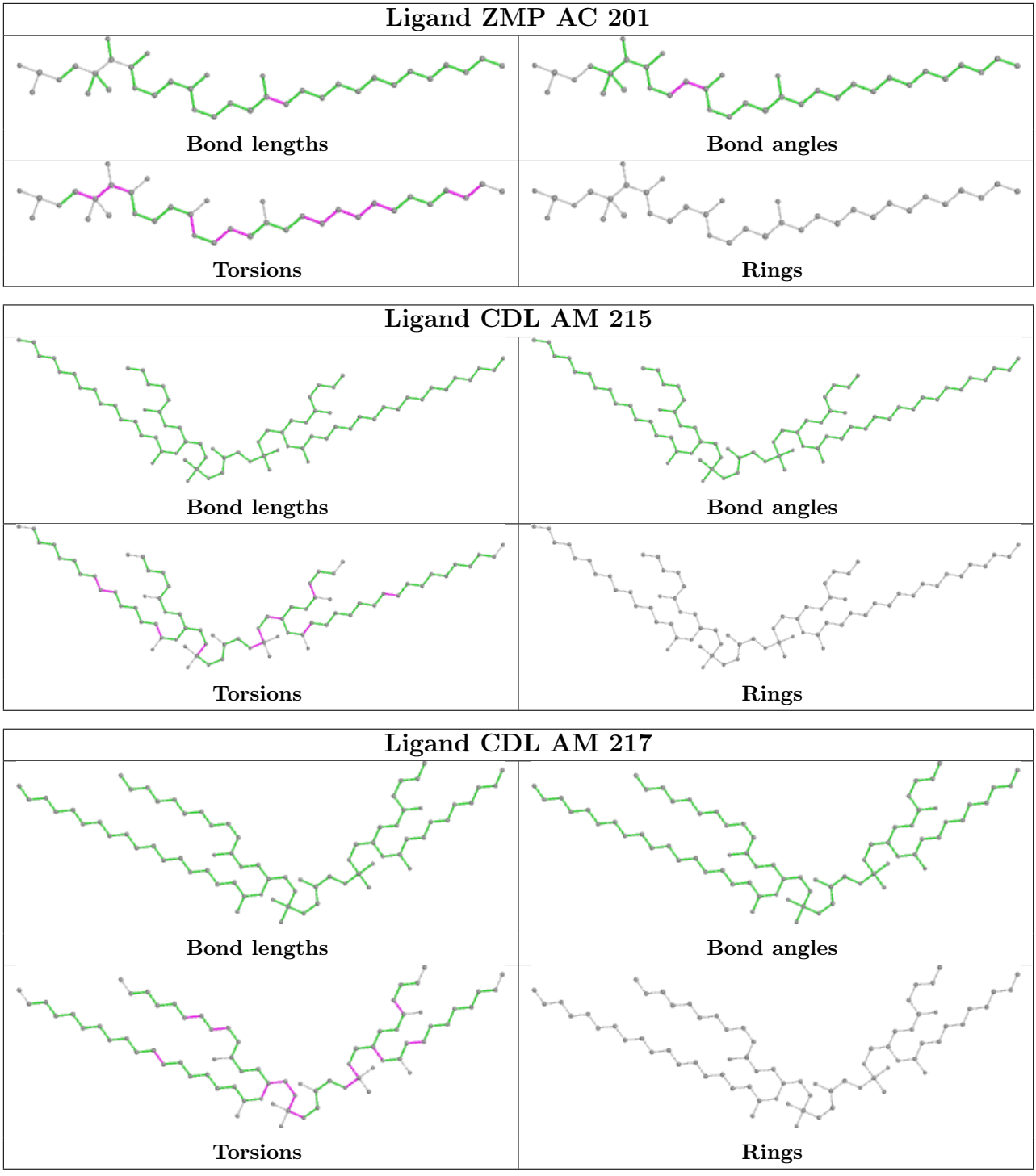
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.