



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 03:43 am BST

PDB ID : 8CA5
EMDB ID : EMD-16518
Title : Cryo-EM structure NDUFS4 knockout complex I from *Mus musculus* heart (Class 3).
Authors : Yin, Z.; Bridges, H.R.; Agip, A.N.A.; Hirst, J.
Deposited on : 2023-01-24
Resolution : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, 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 : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

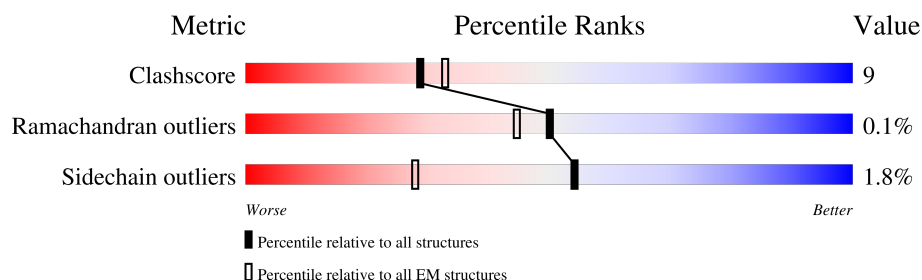
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.






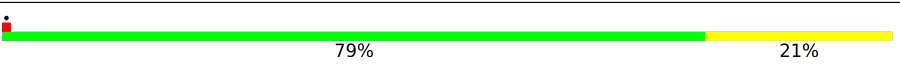
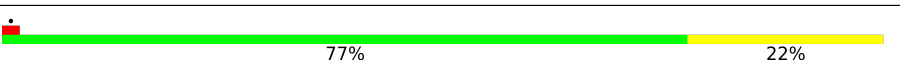

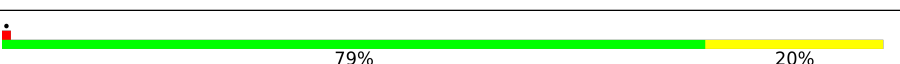
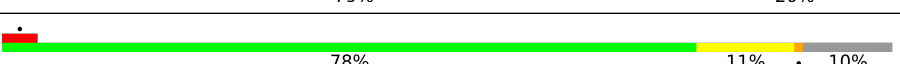
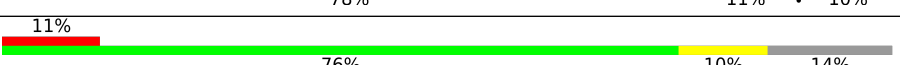


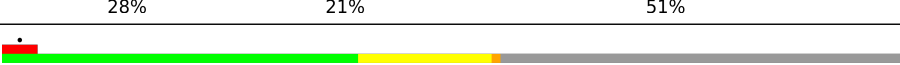
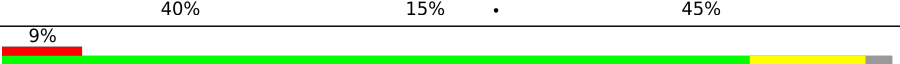
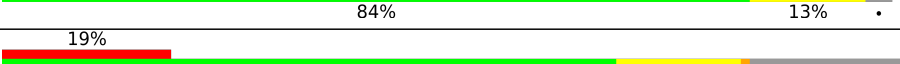



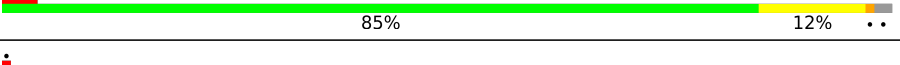
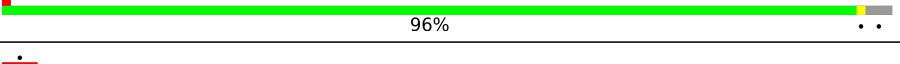
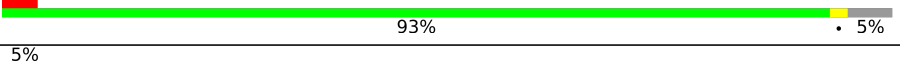
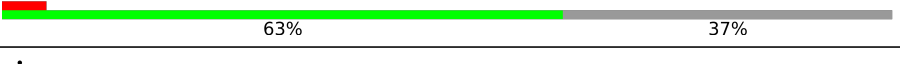
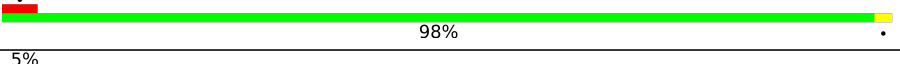
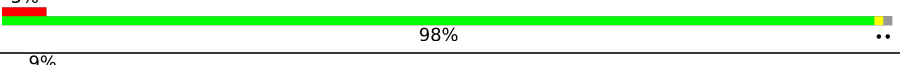
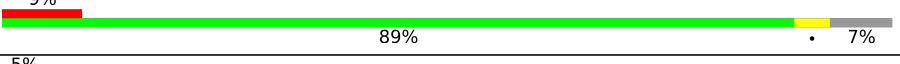

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	t	168	<div> <div>22%</div> <div>62%</div> <div>36%</div> </div>
2	A	115	<div> <div>83%</div> <div>17%</div> </div>
3	B	224	<div> <div>51%</div> <div>18%</div> <div>30%</div> </div>
4	C	263	<div> <div>8%</div> <div>64%</div> <div>15%</div> <div>21%</div> </div>
5	D	463	<div> <div>5%</div> <div>76%</div> <div>17%</div> <div>7%</div> </div>
6	E	248	<div> <div>31%</div> <div>64%</div> <div>20%</div> <div>15%</div> </div>
7	F	464	<div> <div>33%</div> <div>73%</div> <div>19%</div> <div>8%</div> </div>
8	G	727	<div> <div>40%</div> <div>67%</div> <div>27%</div> <div>5%</div> </div>

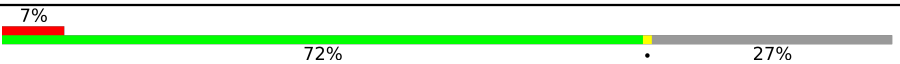


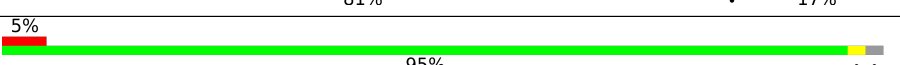
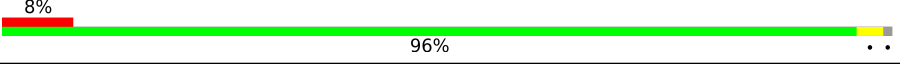
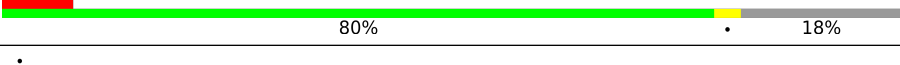
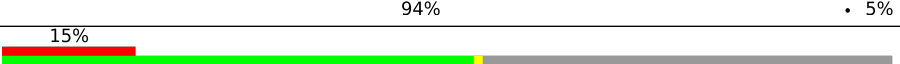
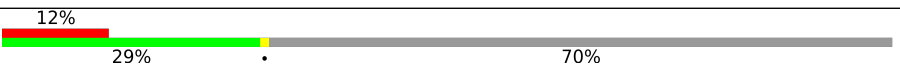
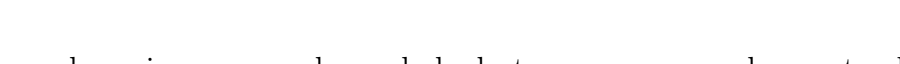
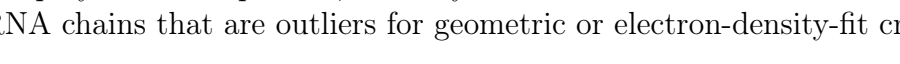
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Mol	Chain	Length	Quality of chain
9	H	318	
10	I	212	
11	J	172	
12	K	98	
13	L	607	
14	M	459	
15	N	345	
16	O	355	
17	P	377	
18	S	99	
19	T	156	
19	U	156	
20	V	116	
21	W	131	
22	X	172	
23	Y	143	
24	Z	144	
25	a	70	
26	b	84	
27	c	76	
28	d	120	
29	e	106	
30	f	57	
31	g	151	
32	h	189	

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Mol	Chain	Length	Quality of chain
33	i	128	
34	j	105	
35	k	104	
36	l	186	
37	m	129	
38	n	179	
39	o	137	
40	p	176	
41	r	113	
42	s	104	

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
43	SF4	B	201	-	-	X	-
43	SF4	G	802	-	-	X	-
43	SF4	I	202	-	-	X	-
46	FES	E	301	-	-	X	-
47	FMN	F	502	-	X	-	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 64198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	t	108	Total	C	N	O	S	0	0
			909	574	160	174	1		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	115	Total	C	N	O	S	0	0
			933	633	133	160	7		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	156	Total	C	N	O	S	0	0
			1247	796	223	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	207	Total	C	N	O	S	0	0
			1721	1111	296	311	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	430	Total	C	N	O	S	0	0
			3463	2215	595	629	24		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	210	Total	C	N	O	S	0	0
			1639	1043	275	310	11		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	428	Total	C	N	O	S	0	0
			3300	2080	589	609	22		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	688	Total	C	N	O	S	0	0
			5248	3294	910	1003	41		

- Molecule 9 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	318	Total	C	N	O	S	0	0
			2540	1706	384	428	22		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	178	Total	C	N	O	S	0	0
			1431	898	245	276	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	171	Total	C	N	O	S	0	0
			1300	874	185	226	15		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

- Molecule 15 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	344	Total	C	N	O	S	0	0
			2696	1791	416	452	37		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	325	Total	C	N	O	S	0	0
			2626	1702	456	461	7		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	82	Total	C	N	O	S	0	0
			594	374	108	110	2		

- Molecule 19 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	76	Total	C	N	O	S	0	0
			611	392	90	124	5		
19	U	86	Total	C	N	O	S	0	0
			692	446	102	139	5		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	109	Total	C	N	O	S	0	0
			935	598	175	156	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 23 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	141	Total	C	N	O	S	0	0
			1167	750	207	202	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	68	Total	C	N	O	S	0	0
			556	360	99	93	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	48	Total	C	N	O	S	0	0
			398	261	69	67	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	120	Total	C	N	O	S	0	0
			996	651	171	165	9		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	105	Total	C	N	O	S	0	0
			877	555	162	152	8		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	53	Total	C	N	O	S	0	0
			456	295	82	77	2		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	h	138	Total	C	N	O	S	0	0
			1162	762	194	203	3		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	93	Total	C	N	O	S	0	0
			778	510	133	132	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	62	Total	C	N	O	S	0	0
			537	355	88	93	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	75	Total	C	N	O	S	0	0
			609	404	103	100	2		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	154	Total	C	N	O	S	0	0
			1294	834	215	234	11		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	m	126	Total	C	N	O	0	0
			1050	676	189	185		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	177	Total	C	N	O	S	0	0
			1534	981	275	267	11		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	113	Total	C	N	O	S	0	0
			979	617	184	170	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	168	Total	C	N	O	S	0	0
			1424	896	256	264	8		

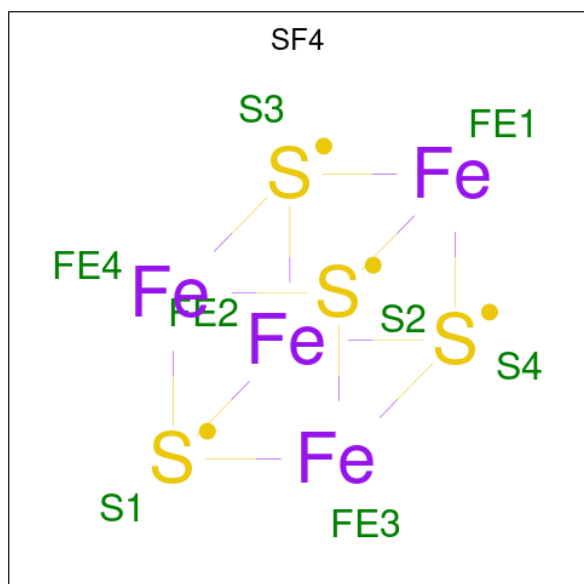
- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	61	Total	C	N	O	S	0	0
			487	311	87	86	3		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

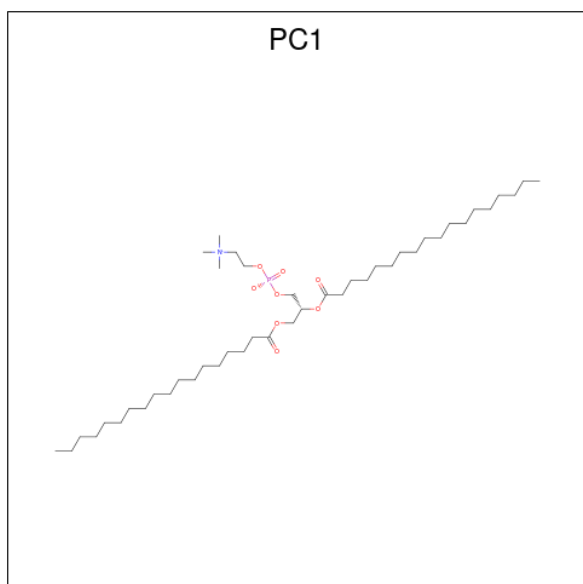
Mol	Chain	Residues	Atoms				AltConf	Trace
42	s	31	Total	C	N	O	0	0
			269	174	45	50		

- Molecule 43 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



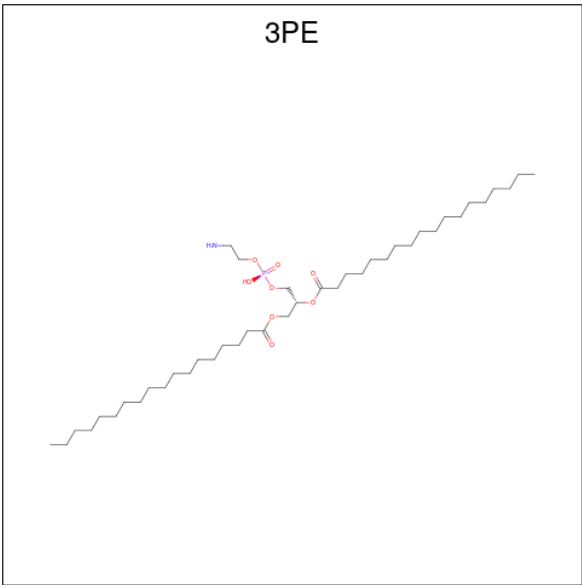
Mol	Chain	Residues	Atoms			AltConf
43	B	1	Total	Fe	S	0
			8	4	4	
43	F	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	

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



Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
44	J	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



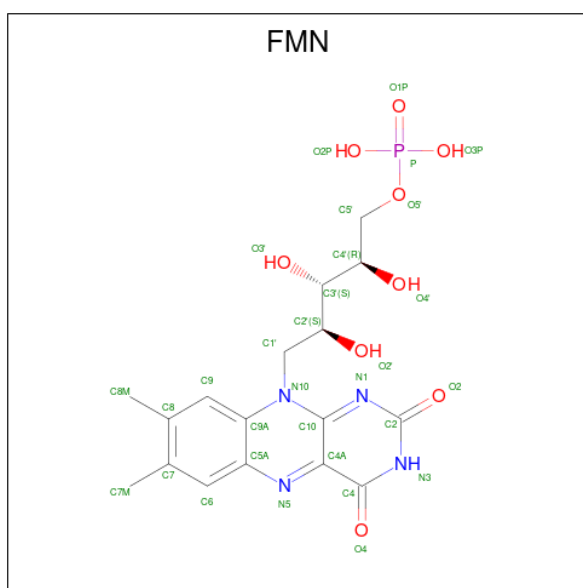
Mol	Chain	Residues	Atoms					AltConf
45	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	H	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	K	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	L	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	M	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	Y	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 46 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



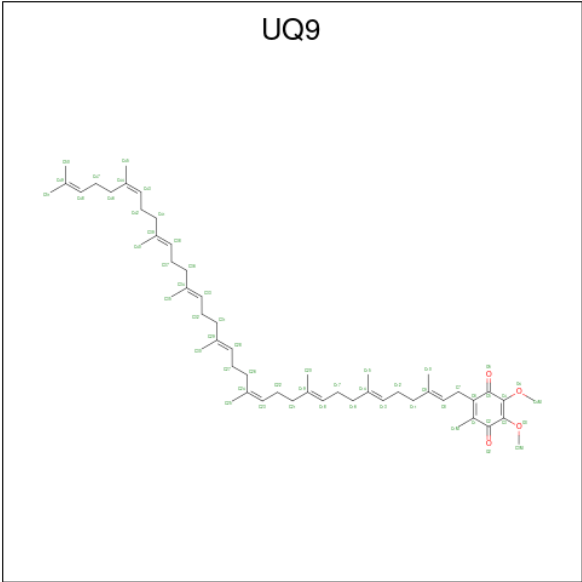
Mol	Chain	Residues	Atoms			AltConf
46	E	1	Total	Fe	S	0
			4	2	2	
46	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



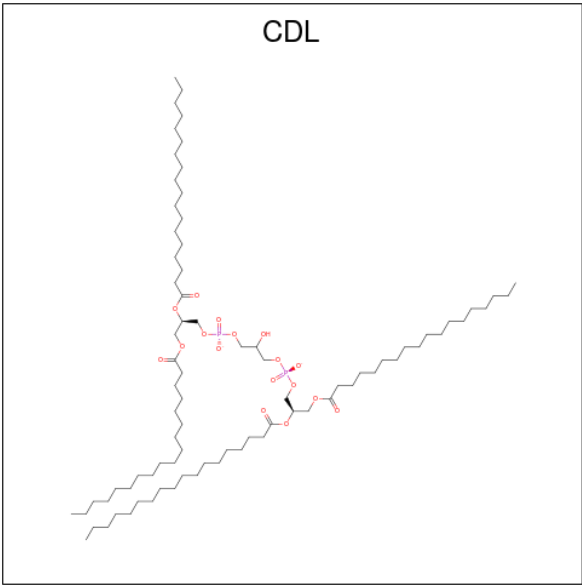
Mol	Chain	Residues	Atoms					AltConf
47	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 48 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$).



Mol	Chain	Residues	Atoms		AltConf
48	H	1	Total	C	0
			45	45	

- Molecule 49 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



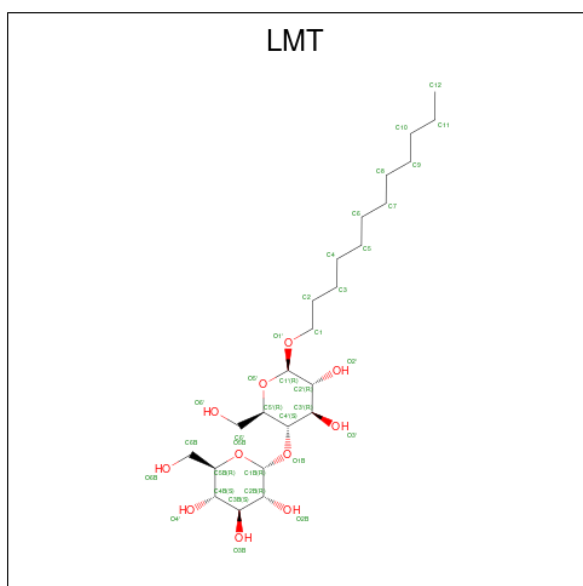
Mol	Chain	Residues	Atoms				AltConf
49	L	1	Total	C	O	P	0
			74	55	17	2	
49	M	1	Total	C	O	P	0
			59	41	16	2	
49	N	1	Total	C	O	P	0
			65	46	17	2	

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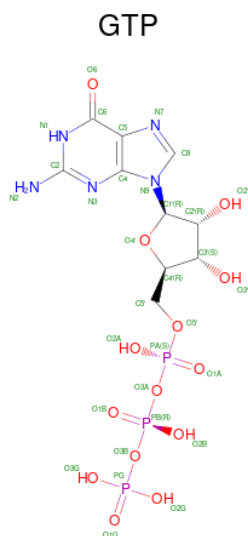
Mol	Chain	Residues	Atoms				AltConf
49	d	1	Total	C	O	P	0
			67	48	17	2	
49	d	1	Total	C	O	P	0
			63	44	17	2	
49	i	1	Total	C	O	P	0
			70	51	17	2	

- Molecule 50 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



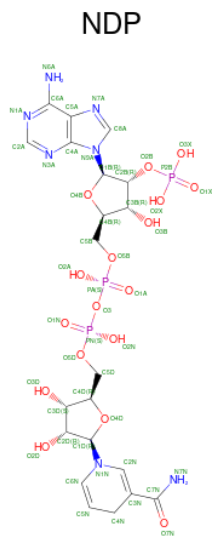
Mol	Chain	Residues	Atoms				AltConf
50	L	1	Total	C	O		0
			35	24	11		
50	L	1	Total	C	O		0
			35	24	11		

- Molecule 51 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
51	O	1	Total 31	C 10	N 5	O 13	P 3	0

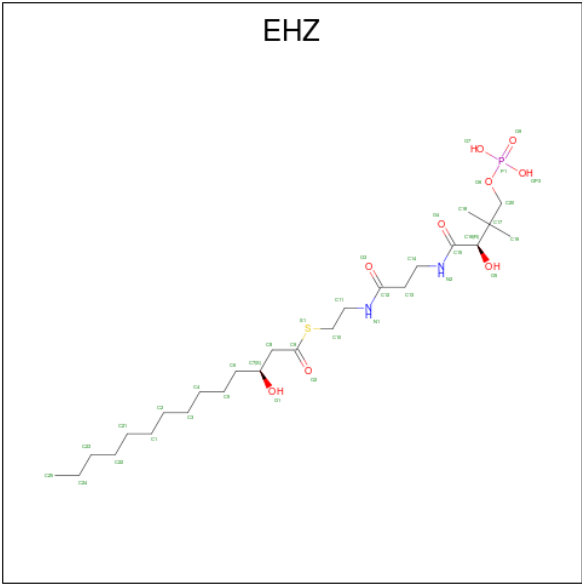
- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 53 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl (3 {S})-3-oxidanyltetradecanethioate (three-letter code: EHZ)

(formula: C₂₅H₄₉N₂O₉PS).

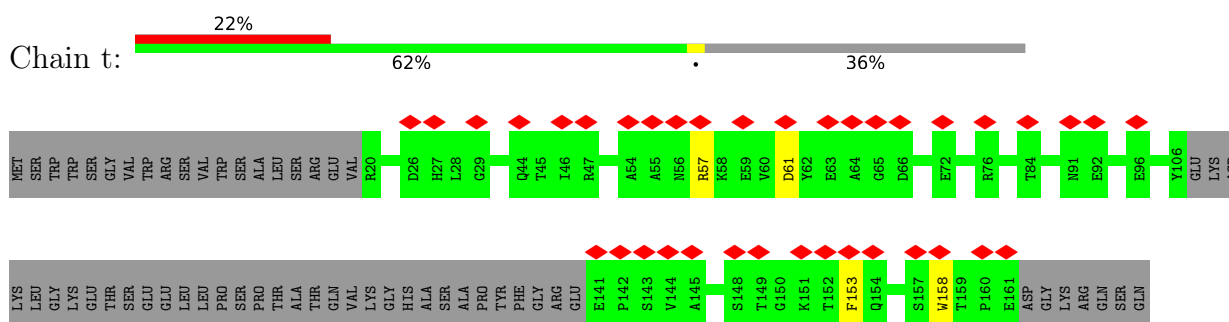


Mol	Chain	Residues	Atoms						AltConf
53	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
53	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

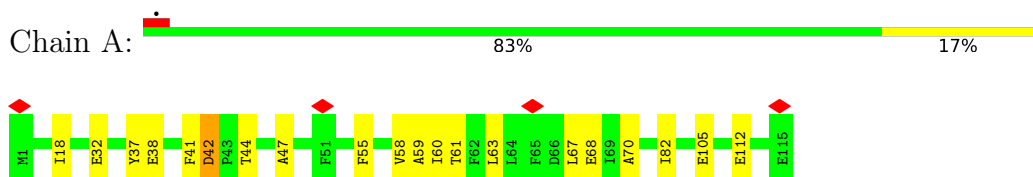
3 Residue-property plots

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

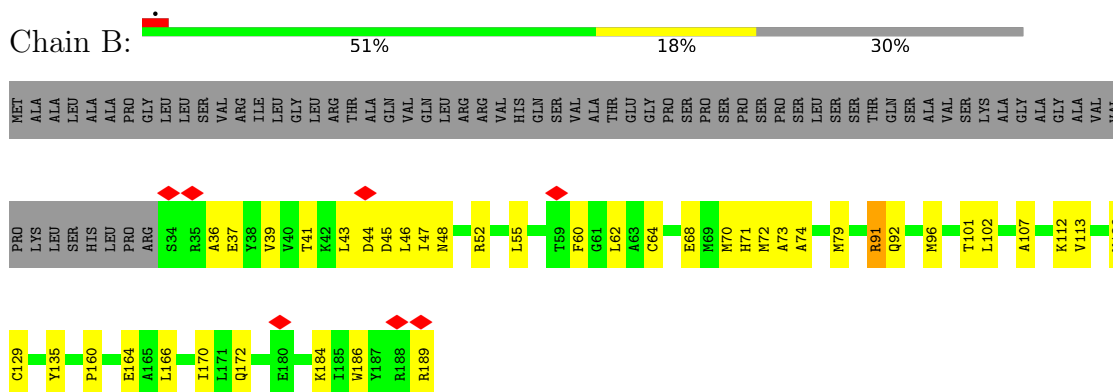
- Molecule 1: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex assembly factor 2



- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

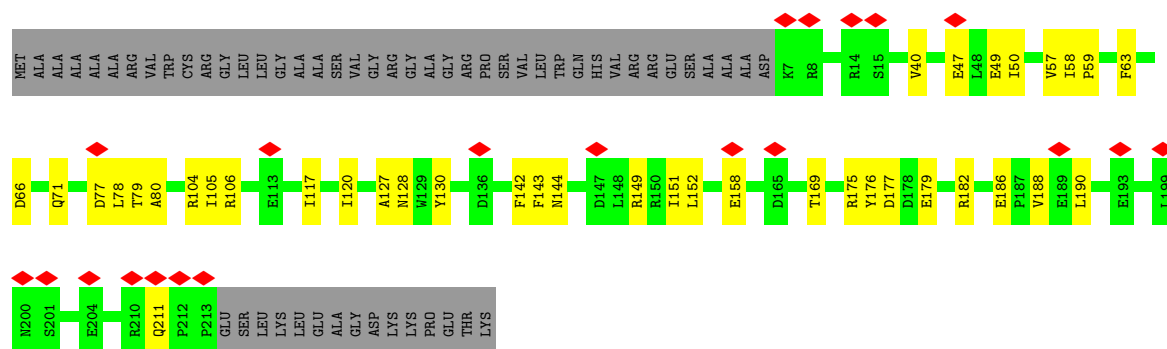


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

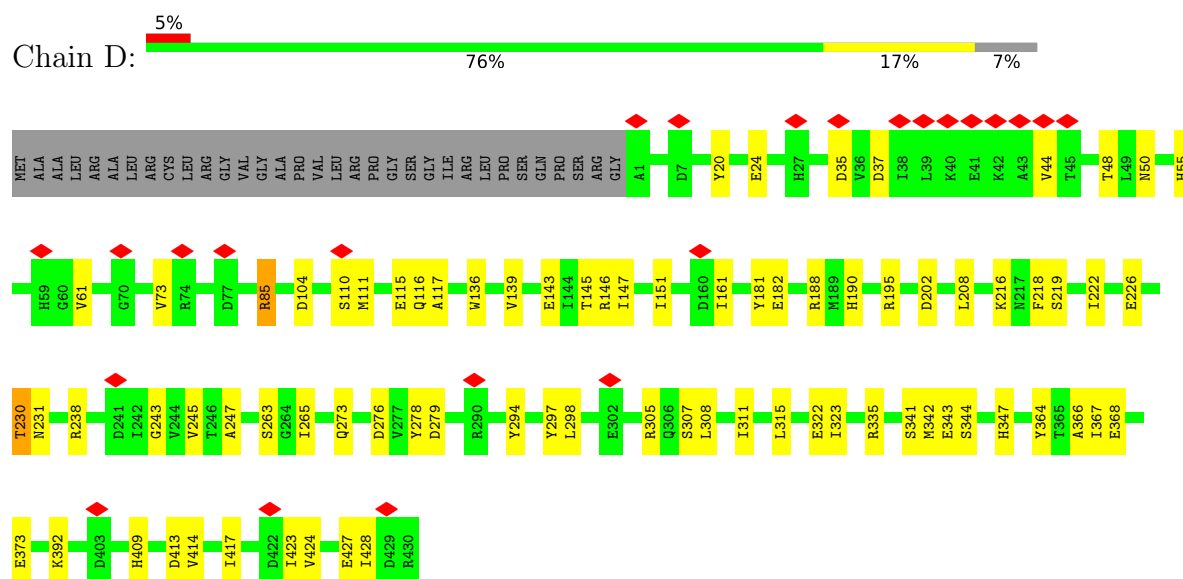


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

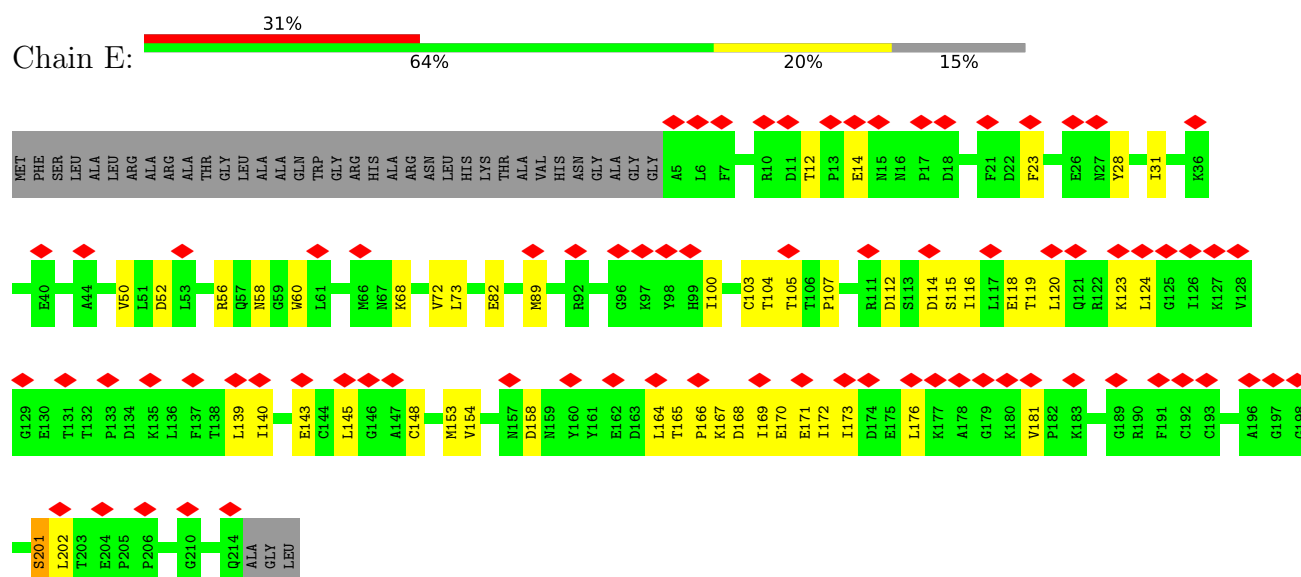




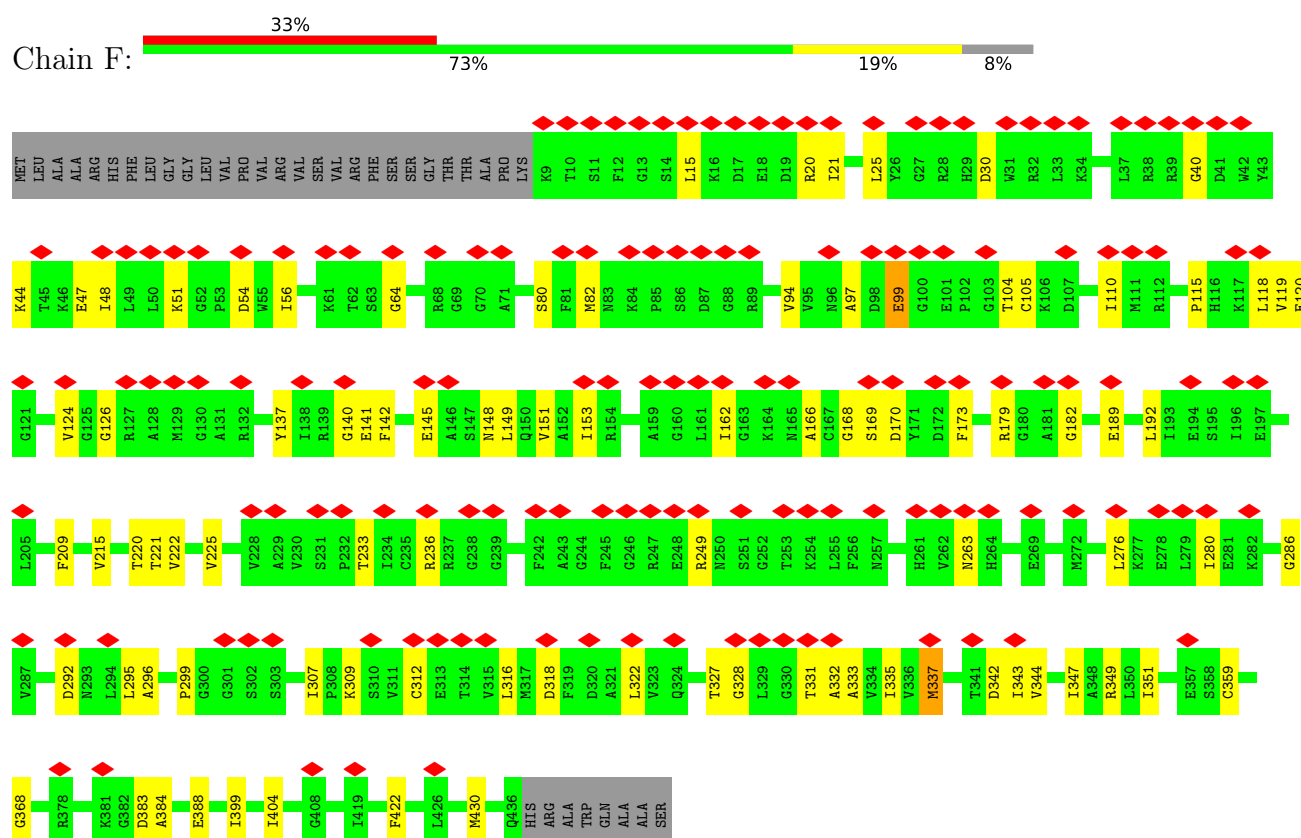
- Molecule 5: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



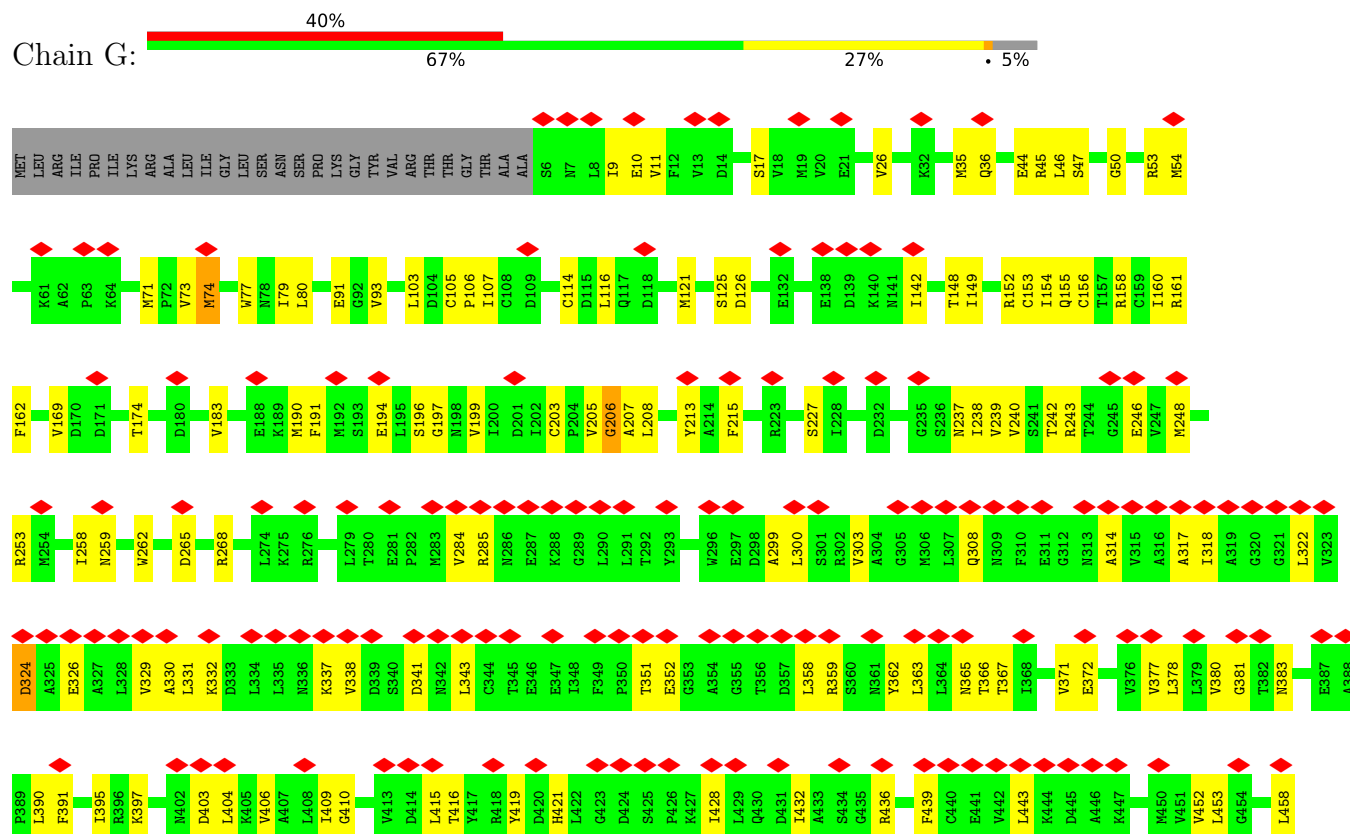
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

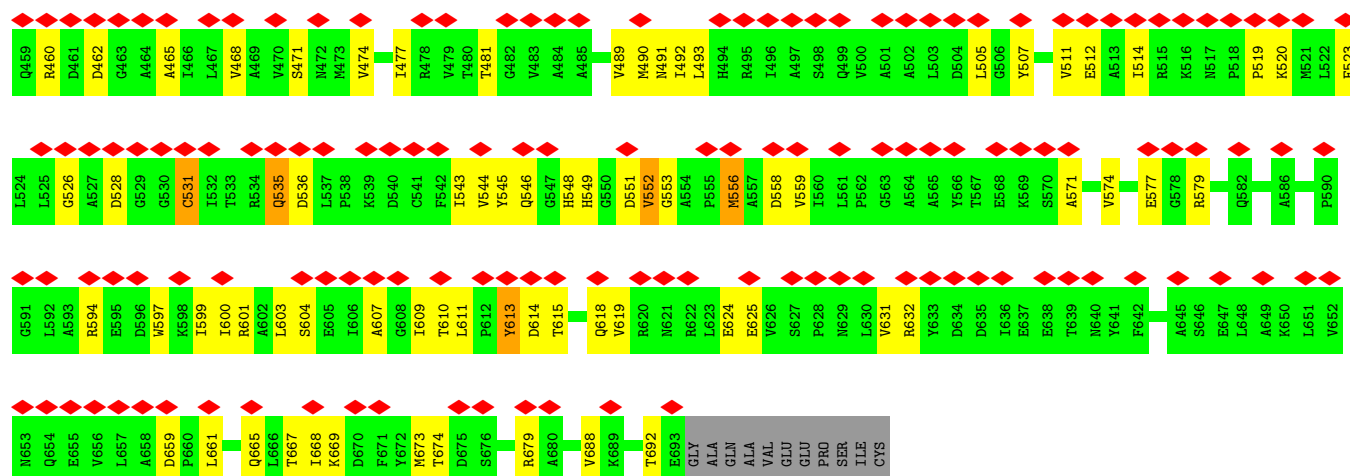


- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

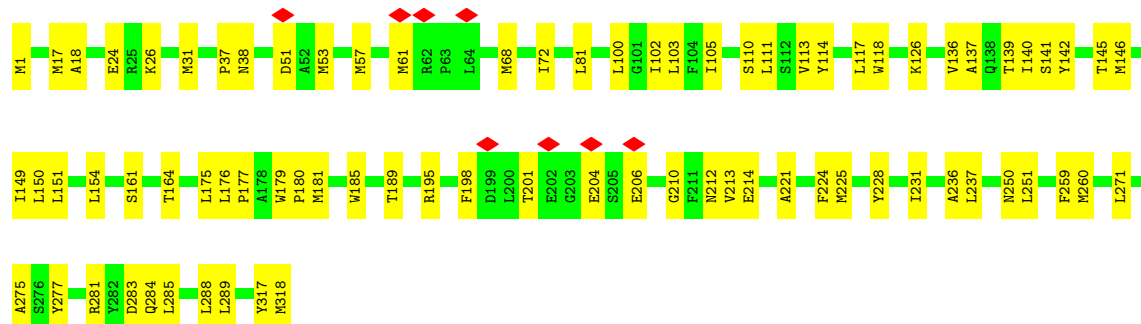
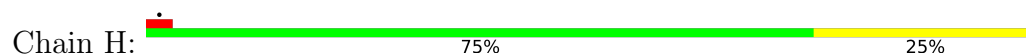


• Molecule 8: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

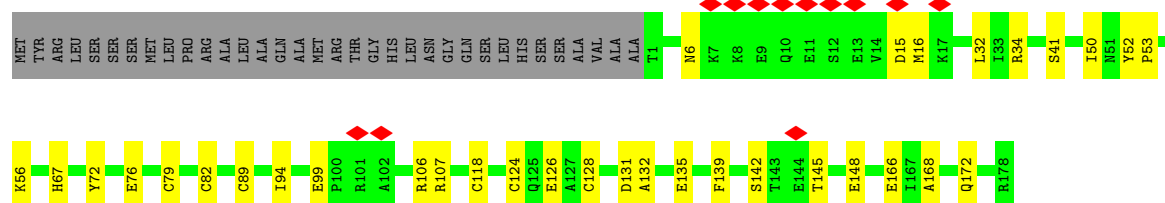




- Molecule 9: NADH-ubiquinone oxidoreductase chain 1

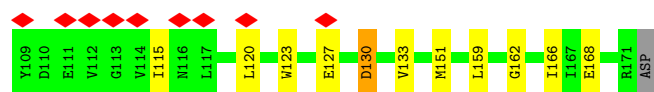


- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

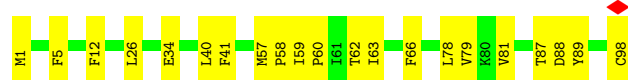
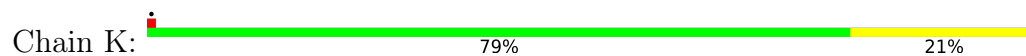


- Molecule 11: NADH-ubiquinone oxidoreductase chain 6

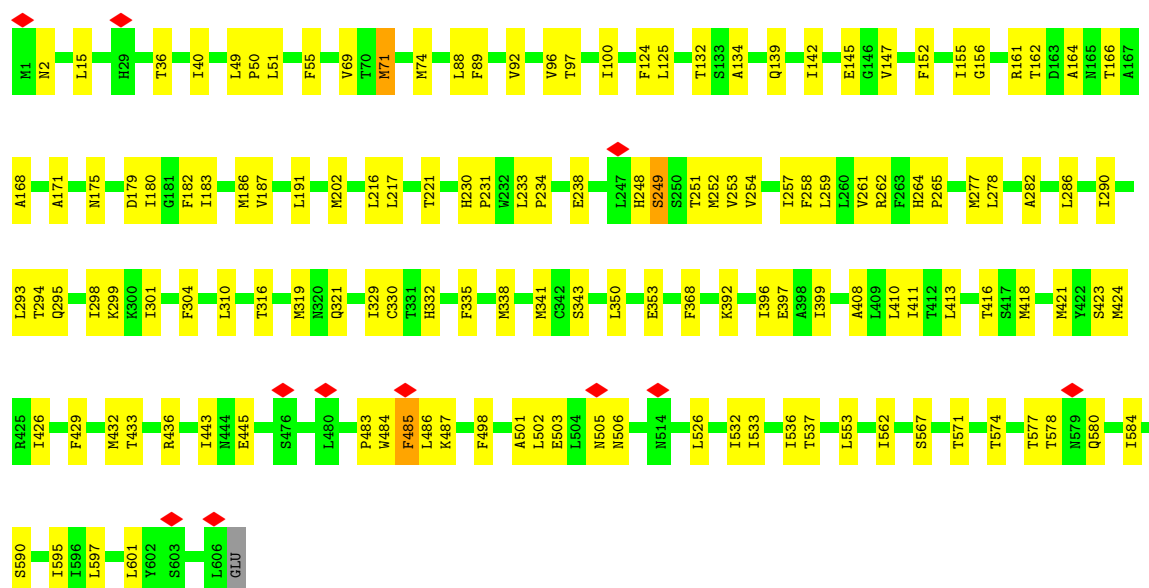
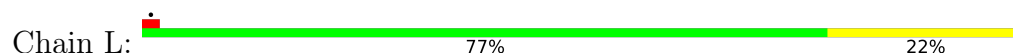




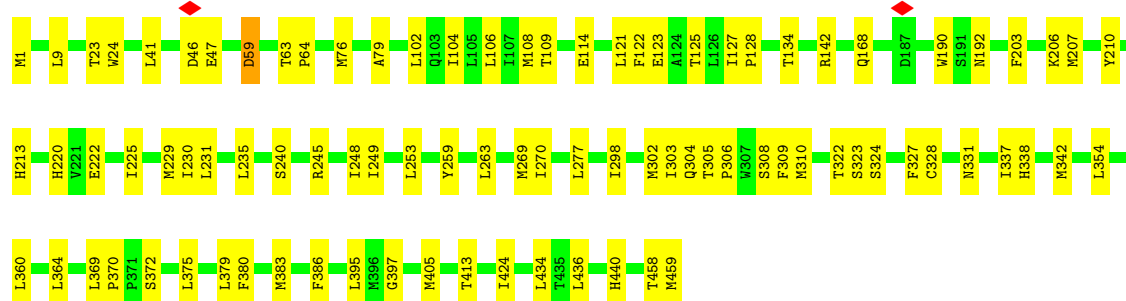
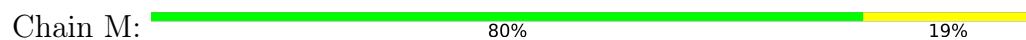
- Molecule 12: NADH-ubiquinone oxidoreductase chain 4L



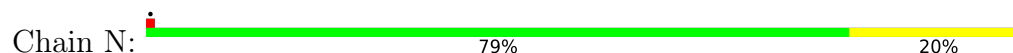
- Molecule 13: NADH-ubiquinone oxidoreductase chain 5

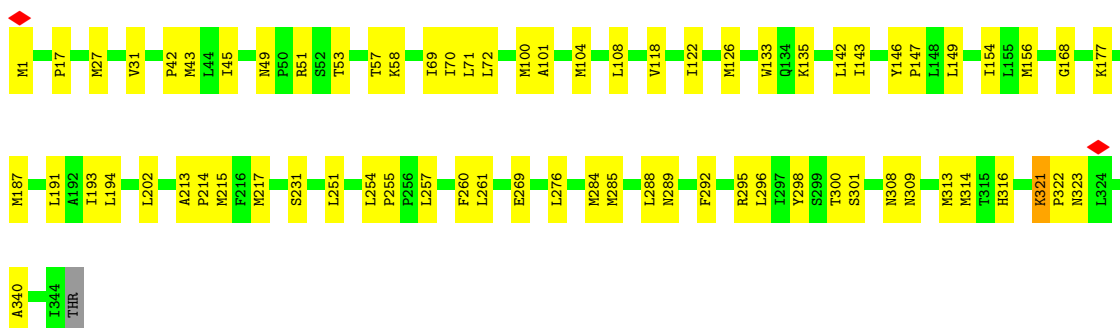


- Molecule 14: NADH-ubiquinone oxidoreductase chain 4



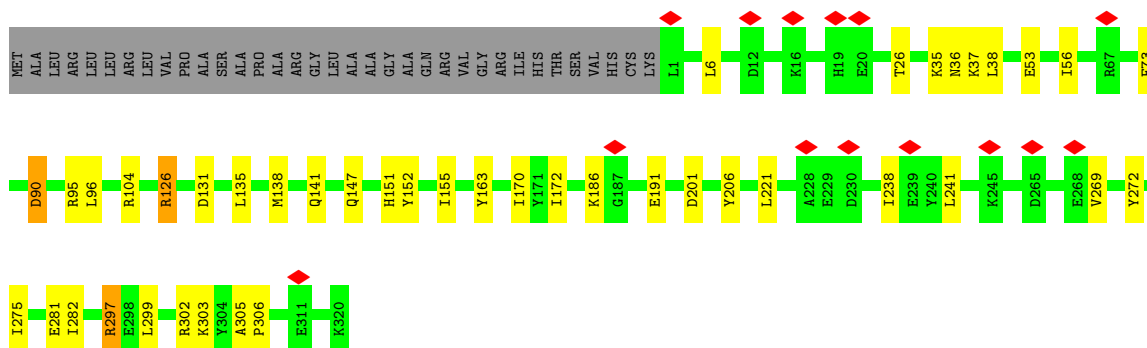
- Molecule 15: NADH-ubiquinone oxidoreductase chain 2





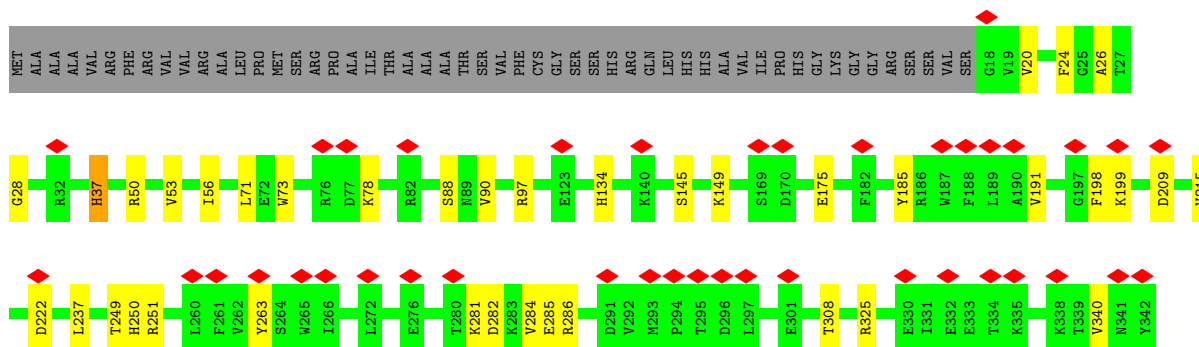
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 78% 11% 10%



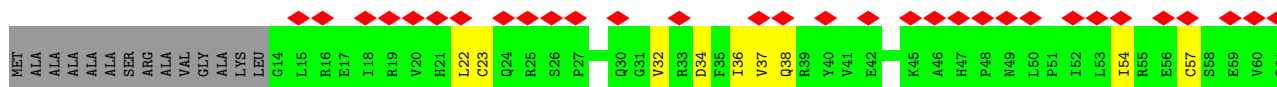
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

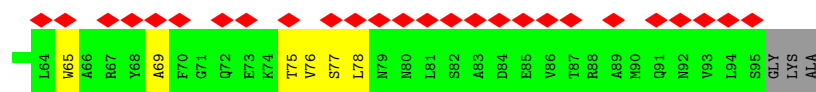
Chain P: 11% 76% 10% 14%



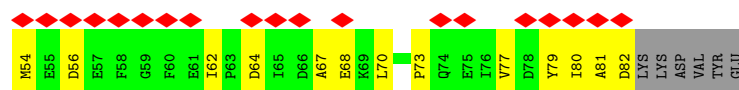
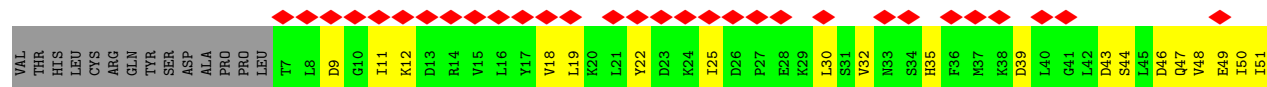
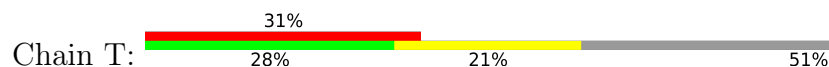
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S: 58% 68% 15% 17%

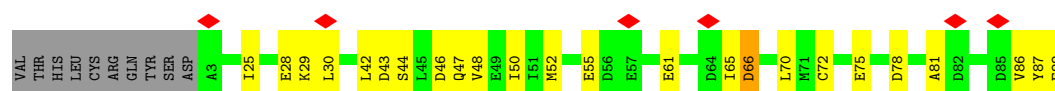




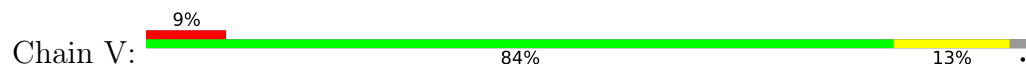
- Molecule 19: Acyl carrier protein, mitochondrial



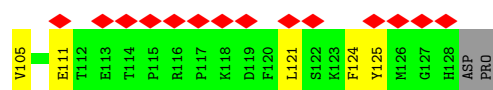
- Molecule 19: Acyl carrier protein, mitochondrial



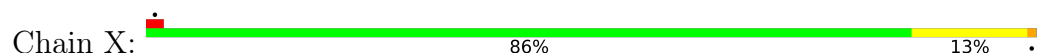
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

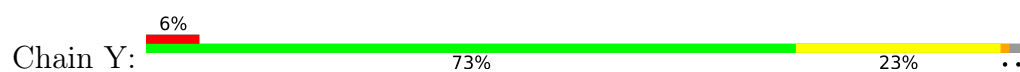


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

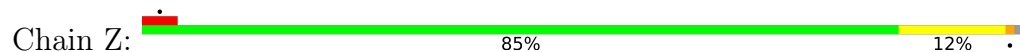




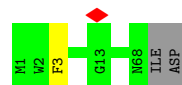
- Molecule 23: MCG5603



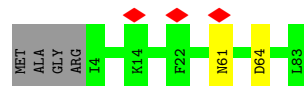
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



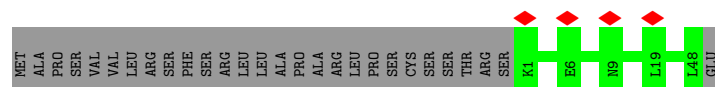
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

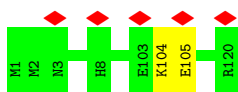


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

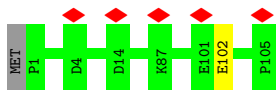


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C2

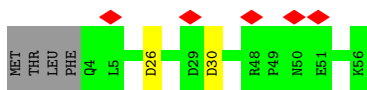
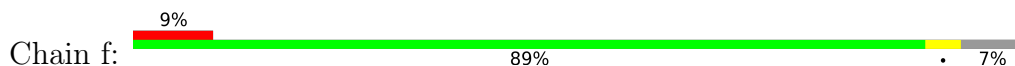




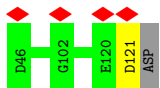
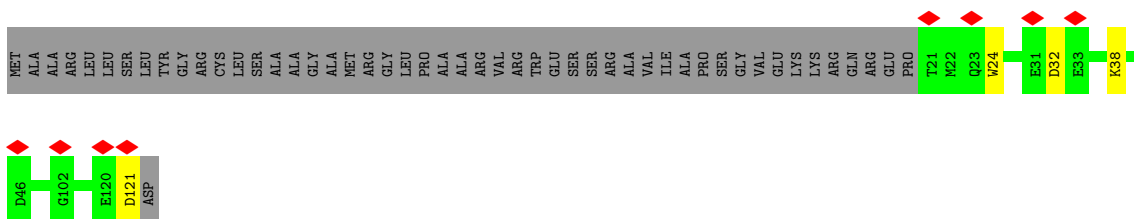
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



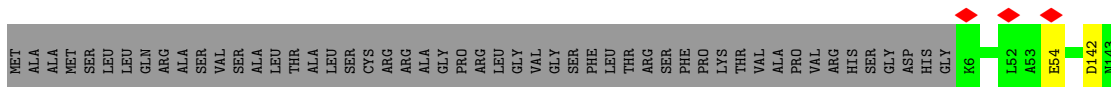
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



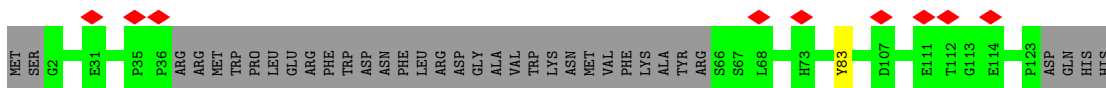
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



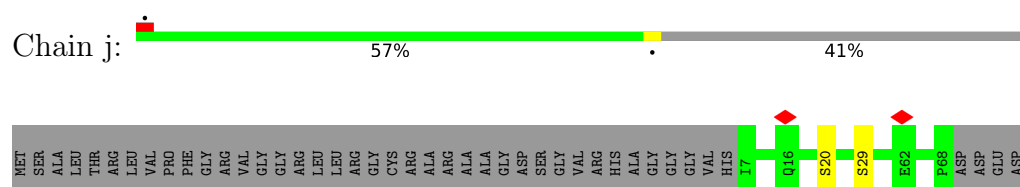
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



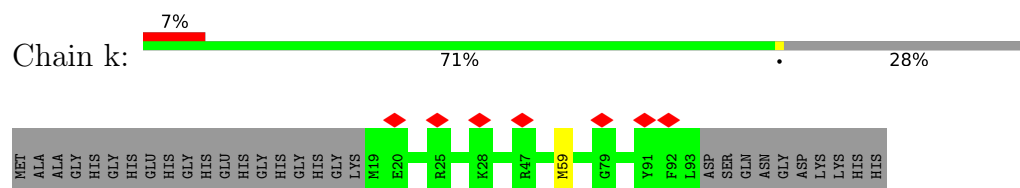
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



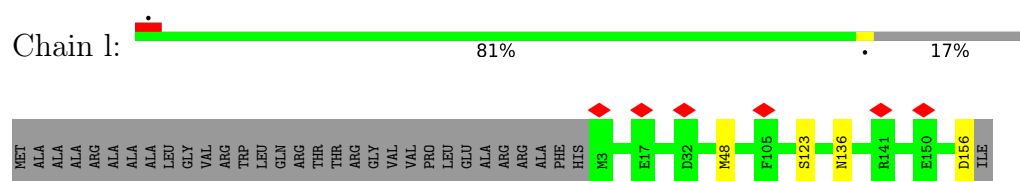
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



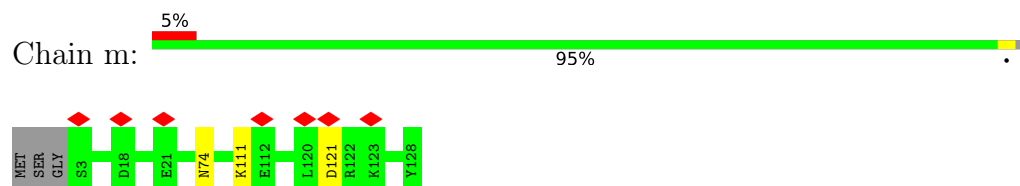
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



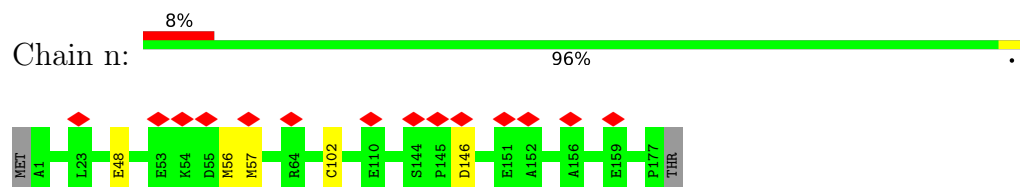
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



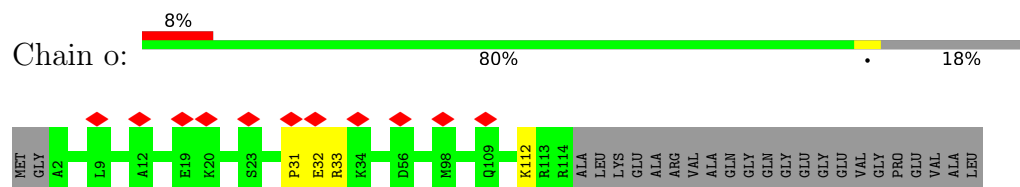
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

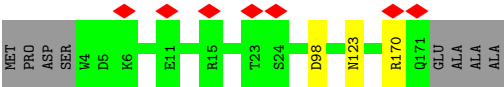


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

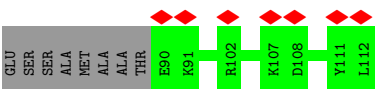
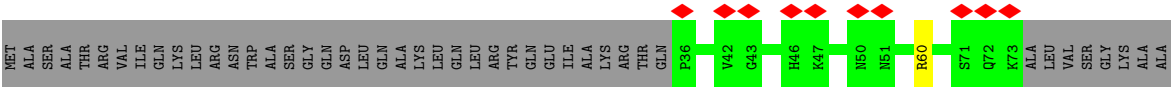


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

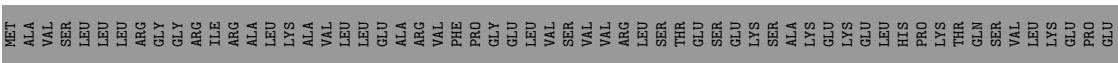




- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10005	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	11.451	Depositor
Minimum map value	-2.901	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.341	Depositor
Recommended contour level	1.7	Depositor
Map size (Å)	608.4, 608.4, 608.4	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.352, 1.352, 1.352	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, FME, SF4, GTP, FMN, CDL, FES, UQ9, EH2, 2MR, 3PE, NDP, 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	t	0.28	0/933	0.54	0/1261
2	A	0.30	0/949	0.46	0/1297
3	B	0.35	0/1278	0.55	0/1730
4	C	0.31	0/1771	0.53	0/2412
5	D	0.31	0/3539	0.51	0/4793
6	E	0.27	0/1679	0.49	0/2288
7	F	0.27	0/3374	0.51	0/4557
8	G	0.28	0/5335	0.52	0/7236
9	H	0.33	0/2607	0.48	0/3564
10	I	0.34	0/1461	0.53	0/1974
11	J	0.34	0/1322	0.48	0/1799
12	K	0.31	0/738	0.48	0/1002
13	L	0.30	0/4913	0.47	0/6686
14	M	0.30	0/3709	0.47	0/5052
15	N	0.30	0/2748	0.48	0/3741
16	O	0.30	0/2674	0.46	0/3626
17	P	0.28	0/2697	0.51	0/3658
18	S	0.25	0/604	0.50	0/827
19	T	0.25	0/620	0.44	0/836
19	U	0.30	0/704	0.46	0/951
20	V	0.28	0/937	0.40	0/1270
21	W	0.27	0/957	0.54	0/1284
22	X	0.30	0/1434	0.50	0/1937
23	Y	0.30	0/1061	0.50	0/1439
24	Z	0.30	0/1198	0.54	0/1616
25	a	0.34	0/569	0.54	0/766
26	b	0.30	0/651	0.42	0/895
27	c	0.31	0/409	0.46	0/555
28	d	0.32	0/1028	0.48	0/1387
29	e	0.30	0/900	0.50	0/1199
30	f	0.28	0/468	0.55	0/630
31	g	0.33	0/878	0.51	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	h	0.32	0/1197	0.50	0/1621
33	i	0.32	0/804	0.51	0/1094
34	j	0.30	0/561	0.46	0/768
35	k	0.33	0/629	0.50	0/851
36	l	0.32	0/1348	0.50	0/1840
37	m	0.31	0/1079	0.54	0/1463
38	n	0.32	0/1589	0.52	0/2152
39	o	0.36	1/1004 (0.1%)	0.69	2/1348 (0.1%)
40	p	0.32	0/1457	0.54	0/1969
41	r	0.27	0/502	0.49	0/680
42	s	0.25	0/277	0.47	0/377
All	All	0.30	1/64592 (0.0%)	0.50	2/87627 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	o	31	PRO	CG-CD	-5.77	1.31	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	o	31	PRO	CA-N-CD	-12.07	94.61	111.50
39	o	31	PRO	N-CD-CG	-8.39	90.61	103.20

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	t	909	0	874	0	0
2	A	933	0	969	21	0
3	B	1247	0	1255	39	0
4	C	1721	0	1680	32	0
5	D	3463	0	3416	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1639	0	1631	44	0
7	F	3300	0	3258	64	0
8	G	5248	0	5236	164	0
9	H	2540	0	2626	68	0
10	I	1431	0	1383	30	0
11	J	1300	0	1315	39	0
12	K	737	0	768	24	0
13	L	4800	0	4985	103	0
14	M	3632	0	3853	69	0
15	N	2696	0	2895	59	0
16	O	2607	0	2566	29	0
17	P	2626	0	2642	23	0
18	S	594	0	543	10	0
19	T	611	0	602	26	0
19	U	692	0	686	15	0
20	V	915	0	954	10	0
21	W	935	0	959	21	0
22	X	1396	0	1383	17	0
23	Y	1037	0	1024	29	0
24	Z	1167	0	1166	15	0
25	a	556	0	568	0	0
26	b	628	0	628	0	0
27	c	398	0	401	0	0
28	d	996	0	1001	0	0
29	e	877	0	871	0	0
30	f	456	0	452	0	0
31	g	850	0	783	0	0
32	h	1162	0	1163	0	0
33	i	778	0	788	0	0
34	j	537	0	495	0	0
35	k	609	0	603	0	0
36	l	1294	0	1186	0	0
37	m	1050	0	1061	0	0
38	n	1534	0	1466	0	0
39	o	979	0	963	0	0
40	p	1424	0	1393	0	0
41	r	487	0	502	0	0
42	s	269	0	256	0	0
43	B	8	0	0	3	0
43	F	8	0	0	0	0
43	G	16	0	0	2	0
43	I	16	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	B	41	0	59	0	0
44	J	42	0	58	2	0
45	D	51	0	82	0	0
45	H	44	0	65	2	0
45	K	33	0	40	0	0
45	L	91	0	136	0	0
45	M	42	0	61	0	0
45	Y	41	0	56	1	0
46	E	4	0	0	2	0
46	G	4	0	0	1	0
47	F	31	0	18	0	0
48	H	45	0	71	6	0
49	L	74	0	92	0	0
49	M	59	0	68	1	0
49	N	65	0	77	0	0
49	d	130	0	151	0	0
49	i	70	0	87	0	0
50	L	70	0	89	1	0
51	O	31	0	10	3	0
52	P	48	0	26	2	0
53	T	37	0	0	1	0
53	U	37	0	0	1	0
All	All	64198	0	64495	907	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 9.

All (907) 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)
19:T:25:ILE:HD13	19:T:30:LEU:HD22	1.42	0.99
8:G:205:VAL:O	8:G:207:ALA:N	2.05	0.90
14:M:210:TYR:O	14:M:213:HIS:ND1	2.08	0.86
14:M:324:SER:OG	14:M:440:HIS:NE2	2.08	0.86
12:K:40:LEU:HD13	15:N:71:LEU:HD23	1.57	0.85
23:Y:77:VAL:O	23:Y:81:VAL:HG23	1.77	0.84
5:D:145:THR:HG1	5:D:181:TYR:HH	1.21	0.84
8:G:594:ARG:NH1	21:W:124:PHE:O	2.11	0.84
43:B:201:SF4:S1	5:D:190:HIS:CD2	2.71	0.83
7:F:168:GLY:O	7:F:169:SER:OG	1.97	0.83
17:P:97:ARG:NH2	52:P:501:NDP:O3X	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:110:ILE:HG22	7:F:118:LEU:HD11	1.62	0.81
8:G:155:GLN:N	8:G:155:GLN:OE1	2.14	0.81
6:E:12:THR:OG1	6:E:14:GLU:O	1.99	0.81
3:B:172:GLN:OE1	10:I:142:SER:OG	1.98	0.80
22:X:19:VAL:HG22	22:X:23:VAL:HG21	1.63	0.80
13:L:171:ALA:O	13:L:175:ASN:ND2	2.15	0.79
9:H:24:GLU:HA	9:H:271:LEU:HD13	1.65	0.79
8:G:194:GLU:N	8:G:194:GLU:OE1	2.16	0.79
13:L:145:GLU:OE1	14:M:369:LEU:HD12	1.83	0.78
16:O:141:GLN:NE2	16:O:201:ASP:OD2	2.16	0.78
5:D:146:ARG:NH2	5:D:368:GLU:O	2.17	0.78
8:G:44:GLU:N	8:G:44:GLU:OE1	2.16	0.77
8:G:26:VAL:HG13	8:G:79:ILE:HD13	1.66	0.77
45:H:402:3PE:O14	45:H:402:3PE:N	2.12	0.77
8:G:544:VAL:HG23	8:G:559:VAL:HG23	1.67	0.77
13:L:217:LEU:O	13:L:221:THR:HG23	1.84	0.76
3:B:64:CYS:SG	5:D:190:HIS:CE1	2.79	0.76
4:C:158:GLU:N	4:C:158:GLU:OE1	2.18	0.76
8:G:415:LEU:O	8:G:416:THR:OG1	2.04	0.76
7:F:15:LEU:O	7:F:20:ARG:NH1	2.19	0.75
8:G:10:GLU:OE1	8:G:17:SER:OG	2.00	0.75
6:E:139:LEU:O	6:E:140:ILE:HD13	1.85	0.75
16:O:281:GLU:N	16:O:281:GLU:OE1	2.18	0.75
4:C:63:PHE:HA	20:V:89:LEU:HD11	1.68	0.75
13:L:162:THR:O	13:L:166:THR:HG23	1.88	0.74
6:E:201:SER:OG	6:E:202:LEU:N	2.16	0.74
9:H:105:ILE:HG21	9:H:237:LEU:HD11	1.68	0.74
19:T:19:LEU:HB3	19:T:30:LEU:HD21	1.68	0.74
6:E:52:ASP:OD2	7:F:179:ARG:NH2	2.21	0.74
6:E:100:ILE:HG21	6:E:120:LEU:HD11	1.70	0.74
4:C:71:GLN:OE1	20:V:82:GLN:NE2	2.20	0.74
4:C:47:GLU:OE2	4:C:106:ARG:NH2	2.21	0.74
8:G:91:GLU:OE1	8:G:125:SER:N	2.20	0.73
8:G:199:VAL:CG1	8:G:208:LEU:HD11	2.19	0.73
14:M:59:ASP:OD2	14:M:245:ARG:NH2	2.22	0.73
9:H:81:LEU:HD11	9:H:111:LEU:HD23	1.69	0.73
8:G:372:GLU:OE2	8:G:397:LYS:NZ	2.22	0.72
13:L:293:LEU:O	13:L:294:THR:OG1	2.06	0.72
10:I:15:ASP:OD1	10:I:16:MET:N	2.22	0.72
13:L:132:THR:O	13:L:262:ARG:NH2	2.22	0.72
8:G:35:MET:SD	8:G:36:GLN:N	2.63	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:369:LEU:O	14:M:372:SER:OG	2.05	0.72
8:G:199:VAL:HG11	8:G:208:LEU:HD11	1.71	0.72
43:B:201:SF4:S1	5:D:190:HIS:NE2	2.62	0.71
10:I:166:GLU:OE1	10:I:166:GLU:N	2.22	0.71
13:L:161:ARG:NH1	13:L:238:GLU:OE2	2.23	0.70
17:P:50:ARG:NH1	52:P:501:NDP:O3X	2.23	0.70
5:D:343:GLU:N	5:D:343:GLU:OE1	2.24	0.70
13:L:290:ILE:HD13	13:L:418:MET:HE3	1.71	0.70
8:G:458:LEU:HD11	8:G:492:ILE:HD11	1.74	0.70
13:L:251:THR:O	13:L:254:VAL:HG22	1.93	0.69
8:G:453:LEU:HD21	8:G:458:LEU:HD21	1.75	0.69
13:L:424:MET:HA	13:L:424:MET:HE2	1.74	0.69
15:N:108:LEU:CD1	15:N:191:LEU:HD22	2.22	0.69
4:C:66:ASP:HB2	20:V:89:LEU:HD12	1.75	0.69
8:G:688:VAL:O	8:G:692:THR:HG23	1.92	0.69
14:M:190:TRP:CB	23:Y:128:ILE:HD11	2.22	0.69
7:F:292:ASP:O	7:F:309:LYS:NZ	2.26	0.69
8:G:358:LEU:HD13	18:S:54:ILE:HD11	1.75	0.68
8:G:366:THR:O	8:G:367:THR:OG1	2.11	0.68
8:G:674:THR:O	8:G:679:ARG:NH1	2.26	0.68
16:O:38:LEU:HD23	16:O:172:ILE:HD11	1.76	0.68
8:G:318:ILE:HD11	8:G:514:ILE:HG13	1.76	0.67
10:I:94:ILE:HD11	43:I:202:SF4:S1	2.35	0.67
19:T:51:ILE:HD13	19:T:67:ALA:HB1	1.74	0.67
8:G:322:LEU:HD23	8:G:322:LEU:H	1.59	0.67
8:G:324:ASP:HB2	8:G:571:ALA:HB1	1.77	0.67
19:T:46:ASP:OD1	21:W:66:ARG:NH1	2.27	0.67
5:D:424:VAL:HG23	5:D:427:GLU:HG2	1.77	0.67
23:Y:63:THR:O	23:Y:67:ILE:HD12	1.95	0.67
2:A:41:PHE:O	5:D:50:ASN:ND2	2.27	0.67
8:G:174:THR:HG22	8:G:183:VAL:HG22	1.76	0.67
15:N:69:ILE:HD13	15:N:100:MET:HE1	1.75	0.66
23:Y:70:MET:SD	23:Y:101:THR:OG1	2.52	0.66
7:F:384:ALA:HB3	7:F:430:MET:HE1	1.77	0.66
24:Z:35:PHE:O	24:Z:39:ILE:HG12	1.95	0.66
7:F:149:LEU:O	7:F:153:ILE:HG23	1.96	0.66
13:L:433:THR:OG1	13:L:436:ARG:NH1	2.26	0.66
23:Y:105:ARG:O	23:Y:105:ARG:NE	2.24	0.66
9:H:51:ASP:HB3	48:H:401:UQ9:H35B	1.78	0.66
13:L:286:LEU:HD12	13:L:411:ILE:HB	1.77	0.66
5:D:85:2MR:HG2	5:D:85:2MR:HH2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:88:LEU:HD23	13:L:330:CYS:SG	2.36	0.65
17:P:37:HIS:HB3	17:P:215:VAL:HG21	1.78	0.65
6:E:112:ASP:OD1	6:E:115:SER:OG	2.09	0.65
9:H:110:SER:O	9:H:113:VAL:HG12	1.97	0.65
14:M:324:SER:HG	14:M:440:HIS:CD2	2.14	0.65
17:P:185:TYR:HD2	17:P:191:VAL:HG13	1.61	0.64
53:U:201:EHZ:O5	53:U:201:EHZ:O6	2.11	0.64
6:E:165:THR:O	6:E:169:ILE:HD12	1.97	0.64
22:X:20:SER:O	22:X:23:VAL:HG22	1.97	0.64
4:C:50:ILE:HD13	4:C:105:ILE:HD11	1.78	0.64
22:X:23:VAL:HG12	22:X:85:TRP:CG	2.33	0.64
13:L:595:ILE:HD11	15:N:100:MET:CE	2.26	0.64
7:F:342:ASP:OD1	7:F:344:VAL:HG22	1.96	0.64
5:D:373:GLU:OE1	5:D:392:LYS:NZ	2.27	0.64
12:K:98:CYS:O	15:N:177:LYS:NZ	2.30	0.64
8:G:391:PHE:CE2	8:G:395:ILE:HD11	2.33	0.63
8:G:474:VAL:HG22	8:G:489:VAL:HG23	1.79	0.63
13:L:248:HIS:O	13:L:249:SER:OG	2.14	0.63
8:G:284:VAL:HG23	8:G:559:VAL:HG12	1.81	0.63
23:Y:79:ALA:O	23:Y:82:ARG:O	2.17	0.63
5:D:218:PHE:HD2	5:D:308:LEU:HD11	1.63	0.62
6:E:148:CYS:N	7:F:105:CYS:SG	2.72	0.62
10:I:79:CYS:O	10:I:107:ARG:NH1	2.31	0.62
21:W:32:ARG:NH1	21:W:36:GLU:OE2	2.32	0.62
10:I:94:ILE:N	10:I:94:ILE:HD12	2.14	0.62
8:G:474:VAL:CG2	8:G:489:VAL:HG23	2.29	0.62
19:U:43:ASP:OD1	19:U:44:SER:N	2.33	0.62
14:M:190:TRP:CG	23:Y:128:ILE:HD11	2.33	0.62
8:G:160:ILE:HD11	8:G:183:VAL:HG13	1.80	0.62
17:P:249:THR:O	17:P:251:ARG:N	2.32	0.62
8:G:205:VAL:O	8:G:205:VAL:HG23	2.00	0.61
12:K:40:LEU:CD1	15:N:71:LEU:HD23	2.30	0.61
14:M:134:THR:HG21	15:N:298:TYR:HE1	1.63	0.61
23:Y:3:VAL:HG22	23:Y:4:LYS:H	1.65	0.61
13:L:187:VAL:HG12	14:M:383:MET:HG2	1.83	0.61
18:S:65:TRP:CD1	18:S:75:THR:HG23	2.35	0.61
9:H:51:ASP:CB	48:H:401:UQ9:H35B	2.31	0.61
15:N:53:THR:O	15:N:57:THR:HG23	2.01	0.61
6:E:104:THR:O	7:F:349:ARG:NE	2.33	0.61
8:G:381:GLY:HA2	8:G:661:LEU:HD21	1.83	0.61
6:E:105:THR:HG23	46:E:301:FES:S2	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:25:ILE:CD1	19:T:30:LEU:HD22	2.27	0.61
13:L:156:GLY:HA2	13:L:164:ALA:HB1	1.83	0.60
15:N:193:ILE:HD11	15:N:269:GLU:HB3	1.81	0.60
8:G:237:ASN:N	8:G:259:ASN:OD1	2.33	0.60
11:J:123:TRP:CZ3	24:Z:119:LEU:HD12	2.36	0.60
19:U:88:GLU:N	19:U:88:GLU:OE1	2.34	0.60
4:C:149:ARG:HA	21:W:90:MET:CE	2.31	0.60
7:F:104:THR:HG22	7:F:333:ALA:HB2	1.82	0.60
17:P:281:LYS:O	17:P:284:VAL:HG22	2.01	0.60
5:D:111:MET:SD	5:D:111:MET:N	2.73	0.60
9:H:81:LEU:HD11	9:H:111:LEU:CD2	2.31	0.60
9:H:114:TYR:OH	11:J:64:LEU:N	2.34	0.60
4:C:120:ILE:O	4:C:120:ILE:HD12	2.01	0.60
8:G:511:VAL:HG11	8:G:531:CYS:SG	2.42	0.60
23:Y:73:LEU:O	23:Y:77:VAL:HG12	2.02	0.60
9:H:137:ALA:O	9:H:140:ILE:HG22	2.02	0.60
23:Y:41:SER:O	23:Y:56:ARG:NH1	2.35	0.60
7:F:115:PRO:O	7:F:119:VAL:HG23	2.02	0.59
8:G:160:ILE:CD1	8:G:174:THR:HG23	2.31	0.59
8:G:577:GLU:OE2	8:G:579:ARG:NH2	2.35	0.59
3:B:64:CYS:SG	5:D:190:HIS:NE2	2.74	0.59
6:E:103:CYS:SG	6:E:105:THR:HG22	2.42	0.59
6:E:202:LEU:HD21	7:F:25:LEU:CD2	2.33	0.59
8:G:460:ARG:NH2	8:G:462:ASP:OD2	2.34	0.59
24:Z:128:THR:HG23	24:Z:131:GLU:H	1.67	0.59
2:A:68:GLU:HG3	11:J:159:LEU:HD13	1.85	0.59
8:G:324:ASP:OD1	8:G:326:GLU:N	2.36	0.59
11:J:123:TRP:HZ3	24:Z:119:LEU:HD12	1.67	0.59
6:E:107:PRO:HB3	7:F:335:ILE:HD11	1.85	0.59
11:J:32:LEU:HD21	12:K:34:GLU:CD	2.22	0.59
14:M:79:ALA:HB2	14:M:436:LEU:HD11	1.85	0.59
9:H:281:ARG:O	9:H:284:GLN:N	2.36	0.58
22:X:19:VAL:CG2	22:X:23:VAL:HG21	2.33	0.58
5:D:195:ARG:NH2	10:I:126:GLU:OE2	2.36	0.58
15:N:42:PRO:HA	15:N:45:ILE:HG22	1.86	0.58
7:F:21:ILE:HG23	7:F:233:THR:HG21	1.84	0.58
12:K:26:LEU:HD23	12:K:78:LEU:HD12	1.84	0.58
5:D:279:ASP:OD1	5:D:279:ASP:N	2.37	0.58
14:M:46:ASP:OD1	14:M:47:GLU:N	2.37	0.58
19:U:30:LEU:O	19:U:30:LEU:HD23	2.03	0.58
6:E:56:ARG:NH2	6:E:158:ASP:OD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:71:MET:HE3	14:M:310:MET:SD	2.44	0.57
17:P:145:SER:OG	17:P:282:ASP:OD2	2.20	0.57
17:P:282:ASP:O	17:P:286:ARG:HG3	2.04	0.57
11:J:2:ASN:ND2	11:J:3:ASN:OD1	2.37	0.57
11:J:59:TYR:CE1	12:K:34:GLU:OE1	2.57	0.57
2:A:112:GLU:OE1	2:A:112:GLU:N	2.37	0.57
9:H:102:ILE:CD1	9:H:154:LEU:HD11	2.35	0.57
18:S:22:LEU:HD12	18:S:23:CYS:N	2.20	0.57
2:A:67:LEU:O	2:A:70:ALA:HB3	2.03	0.57
8:G:329:VAL:CA	8:G:505:LEU:HD21	2.35	0.56
15:N:122:ILE:HD12	15:N:126:MET:HB3	1.85	0.56
8:G:661:LEU:HD23	8:G:661:LEU:O	2.04	0.56
10:I:145:THR:N	10:I:148:GLU:OE2	2.36	0.56
8:G:511:VAL:O	8:G:511:VAL:HG22	2.05	0.56
13:L:397:GLU:OE2	13:L:487:LYS:NZ	2.35	0.56
16:O:56:ILE:HD11	16:O:96:LEU:CD1	2.35	0.56
20:V:57:MET:SD	20:V:57:MET:N	2.78	0.56
7:F:99:GLU:CD	7:F:104:THR:HG1	2.07	0.56
13:L:100:ILE:HD13	13:L:341:MET:CE	2.35	0.56
13:L:257:ILE:HB	13:L:329:ILE:HD11	1.88	0.56
9:H:118:TRP:CH2	11:J:30:LEU:HD13	2.40	0.56
24:Z:97:MET:SD	24:Z:100:VAL:HG21	2.46	0.56
9:H:117:LEU:HD11	9:H:136:VAL:HG23	1.88	0.56
13:L:278:LEU:HD21	13:L:408:ALA:CB	2.36	0.56
8:G:543:ILE:O	8:G:558:ASP:N	2.35	0.56
9:H:102:ILE:HD13	9:H:154:LEU:HD11	1.87	0.56
16:O:6:LEU:HD12	16:O:6:LEU:O	2.06	0.56
9:H:117:LEU:HD11	9:H:136:VAL:CG2	2.36	0.56
6:E:116:ILE:HD12	6:E:169:ILE:HD11	1.88	0.55
11:J:55:VAL:CG1	12:K:41:PHE:CE2	2.89	0.55
4:C:182:ARG:NH2	21:W:111:GLU:OE2	2.37	0.55
8:G:243:ARG:O	8:G:246:GLU:HG2	2.07	0.55
16:O:104:ARG:NE	16:O:131:ASP:OD1	2.38	0.55
8:G:284:VAL:HG22	8:G:285:ARG:H	1.72	0.55
14:M:303:ILE:HD11	14:M:308:SER:OG	2.05	0.55
13:L:100:ILE:HD13	13:L:341:MET:HE3	1.88	0.55
19:T:11:ILE:HD12	19:T:80:ILE:CG2	2.36	0.55
4:C:40:VAL:HG22	4:C:50:ILE:HG13	1.89	0.55
16:O:163:TYR:OH	16:O:269:VAL:HG13	2.07	0.55
8:G:196:SER:OG	8:G:265:ASP:OD2	2.24	0.55
15:N:284:MET:HA	15:N:284:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:20:TYR:OH	15:N:295:ARG:NH2	2.34	0.54
5:D:116:GLN:NE2	5:D:276:ASP:OD2	2.41	0.54
10:I:53:PRO:O	10:I:56:LYS:NZ	2.40	0.54
19:T:12:LYS:HD2	19:T:77:VAL:HG11	1.88	0.54
19:T:12:LYS:NZ	19:T:32:VAL:HG22	2.22	0.54
6:E:154:VAL:HG22	6:E:164:LEU:HD11	1.90	0.54
9:H:236:ALA:HB1	9:H:259:PHE:HZ	1.71	0.54
9:H:277:TYR:OH	10:I:32:LEU:O	2.23	0.54
12:K:34:GLU:OE2	12:K:34:GLU:C	2.46	0.54
13:L:595:ILE:HD11	15:N:100:MET:HE3	1.87	0.54
14:M:222:GLU:N	14:M:222:GLU:OE1	2.41	0.54
8:G:512:GLU:N	8:G:512:GLU:OE1	2.41	0.54
14:M:207:MET:CB	14:M:298:ILE:HD11	2.38	0.54
12:K:58:PRO:O	12:K:62:THR:HG23	2.08	0.54
18:S:34:ASP:O	18:S:37:VAL:HG12	2.08	0.54
19:T:11:ILE:HD12	19:T:80:ILE:HG21	1.90	0.54
19:U:25:ILE:HD11	19:U:42:LEU:HD11	1.89	0.54
21:W:98:VAL:HG12	21:W:98:VAL:O	2.08	0.54
6:E:114:ASP:O	6:E:118:GLU:HG3	2.08	0.54
13:L:304:PHE:CZ	13:L:526:LEU:HD22	2.43	0.54
5:D:364:TYR:OH	5:D:373:GLU:OE2	2.25	0.54
13:L:350:LEU:HD23	13:L:443:ILE:HD11	1.90	0.54
15:N:300:THR:HG23	15:N:301:SER:N	2.23	0.54
23:Y:70:MET:CE	23:Y:101:THR:OG1	2.56	0.54
4:C:120:ILE:HD11	4:C:127:ALA:HB2	1.89	0.53
8:G:428:ILE:O	8:G:432:ILE:HG13	2.08	0.53
9:H:26:LYS:NZ	9:H:37:PRO:O	2.31	0.53
13:L:424:MET:HA	13:L:424:MET:CE	2.34	0.53
8:G:528:ASP:OD2	8:G:545:TYR:OH	2.25	0.53
15:N:296:LEU:O	15:N:300:THR:HG22	2.07	0.53
19:T:68:GLU:OE2	21:W:35:ARG:NH2	2.41	0.53
8:G:624:GLU:OE2	8:G:632:ARG:NH2	2.41	0.53
14:M:305:THR:O	14:M:308:SER:N	2.41	0.53
17:P:175:GLU:N	17:P:175:GLU:OE1	2.40	0.53
4:C:149:ARG:HA	21:W:90:MET:HE2	1.89	0.53
13:L:286:LEU:HD23	13:L:286:LEU:O	2.09	0.53
16:O:221:LEU:HD11	16:O:241:LEU:HD11	1.91	0.53
22:X:23:VAL:HG12	22:X:85:TRP:CD2	2.44	0.53
8:G:169:VAL:HG11	8:G:191:PHE:CE1	2.43	0.53
17:P:185:TYR:CD2	17:P:191:VAL:HG13	2.43	0.53
13:L:595:ILE:HD11	15:N:100:MET:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:126:MET:SD	3:B:166:LEU:HD22	2.48	0.53
4:C:177:ASP:OD1	4:C:179:GLU:N	2.41	0.53
7:F:384:ALA:HB1	7:F:388:GLU:OE2	2.09	0.53
8:G:53:ARG:N	46:G:803:FES:S1	2.80	0.53
22:X:92:ASN:OD1	22:X:93:MET:N	2.42	0.53
3:B:91:ARG:HE	9:H:61:MET:HE3	1.74	0.53
9:H:126:LYS:H	9:H:126:LYS:HD3	1.74	0.53
14:M:121:LEU:O	14:M:125:THR:HG23	2.08	0.53
14:M:328:CYS:SG	14:M:436:LEU:HD21	2.49	0.53
20:V:18:THR:OG1	20:V:21:GLU:OE1	2.23	0.53
8:G:303:VAL:HG22	8:G:559:VAL:HG21	1.89	0.53
10:I:99:GLU:N	10:I:99:GLU:OE1	2.42	0.52
19:T:19:LEU:CB	19:T:30:LEU:HD21	2.38	0.52
9:H:176:LEU:HB2	9:H:177:PRO:HD3	1.90	0.52
9:H:195:ARG:HD3	9:H:231:ILE:HD11	1.92	0.52
8:G:203:CYS:HB2	43:G:802:SF4:S2	2.49	0.52
3:B:55:LEU:H	3:B:55:LEU:HD23	1.73	0.52
5:D:216:LYS:HA	24:Z:18:ILE:HD11	1.92	0.52
15:N:108:LEU:HD11	15:N:191:LEU:HD22	1.91	0.52
19:U:46:ASP:O	19:U:50:ILE:HG13	2.09	0.52
2:A:59:ALA:HA	9:H:140:ILE:HD11	1.90	0.52
8:G:458:LEU:CD1	8:G:492:ILE:HD11	2.38	0.52
8:G:243:ARG:O	8:G:246:GLU:N	2.30	0.52
11:J:162:GLY:O	11:J:166:ILE:HG12	2.10	0.52
13:L:145:GLU:OE1	14:M:370:PRO:HD2	2.10	0.52
3:B:37:GLU:O	3:B:41:THR:HG23	2.10	0.52
8:G:149:ILE:HD12	8:G:149:ILE:N	2.25	0.52
8:G:154:ILE:HG23	8:G:205:VAL:HG11	1.91	0.52
13:L:282:ALA:HB1	13:L:411:ILE:HD11	1.91	0.52
7:F:118:LEU:HD21	7:F:225:VAL:HB	1.92	0.52
14:M:123:GLU:HG2	15:N:255:PRO:CG	2.39	0.52
21:W:98:VAL:O	21:W:98:VAL:CG1	2.57	0.52
3:B:102:LEU:HD21	3:B:107:ALA:HA	1.90	0.52
16:O:36:ASN:OD1	16:O:37:LYS:N	2.43	0.51
9:H:288:LEU:HD22	9:H:289:LEU:HD12	1.91	0.51
14:M:370:PRO:HG3	14:M:375:LEU:HD13	1.93	0.51
17:P:53:VAL:HA	17:P:56:ILE:HG12	1.91	0.51
3:B:92:GLN:NE2	9:H:212:ASN:O	2.44	0.51
4:C:169:THR:HG21	4:C:190:LEU:HD11	1.91	0.51
6:E:100:ILE:HG21	6:E:120:LEU:CD1	2.39	0.51
16:O:90:ASP:O	16:O:95:ARG:NH2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:202:ASP:N	5:D:323:ILE:HD13	2.25	0.51
8:G:199:VAL:HG12	8:G:208:LEU:HD11	1.93	0.51
16:O:272:TYR:O	16:O:275:ILE:HG23	2.11	0.51
5:D:265:ILE:HD12	5:D:265:ILE:H	1.76	0.51
6:E:120:LEU:HD23	6:E:120:LEU:O	2.10	0.51
7:F:296:ALA:HB1	7:F:307:ILE:O	2.11	0.51
8:G:535:GLN:N	8:G:535:GLN:OE1	2.44	0.51
8:G:659:ASP:OD1	8:G:659:ASP:N	2.43	0.51
10:I:94:ILE:HD12	10:I:94:ILE:H	1.73	0.51
17:P:281:LYS:O	17:P:285:GLU:HG3	2.11	0.51
6:E:145:LEU:HD11	7:F:141:GLU:HG2	1.93	0.51
6:E:167:LYS:O	6:E:171:GLU:HG2	2.10	0.51
8:G:624:GLU:HB2	8:G:631:VAL:HG21	1.91	0.51
13:L:15:LEU:HD22	13:L:125:LEU:HD22	1.93	0.51
7:F:64:GLY:O	7:F:249:ARG:NH2	2.42	0.51
14:M:424:ILE:HG22	14:M:424:ILE:O	2.11	0.51
8:G:284:VAL:HG22	8:G:285:ARG:N	2.25	0.51
10:I:89:CYS:HB2	10:I:94:ILE:HD13	1.93	0.51
13:L:89:PHE:CD2	13:L:132:THR:HG21	2.45	0.51
14:M:127:ILE:HB	14:M:128:PRO:HD3	1.92	0.51
18:S:34:ASP:O	18:S:38:GLN:HG2	2.09	0.51
13:L:578:THR:HG21	15:N:168:GLY:HA2	1.93	0.50
3:B:47:ILE:HD13	9:H:57:MET:HE3	1.94	0.50
5:D:117:ALA:HB2	5:D:367:ILE:HG12	1.93	0.50
5:D:294:TYR:CE2	5:D:298:LEU:HD11	2.46	0.50
7:F:99:GLU:OE2	7:F:104:THR:OG1	2.26	0.50
8:G:338:VAL:HG12	8:G:338:VAL:O	2.11	0.50
13:L:577:THR:O	13:L:580:GLN:NE2	2.44	0.50
13:L:601:LEU:C	13:L:601:LEU:HD23	2.31	0.50
16:O:138:MET:CE	51:O:401:GTP:HN21	2.24	0.50
4:C:175:ARG:NH1	4:C:176:TYR:O	2.45	0.50
4:C:211:GLN:NE2	20:V:114:PRO:O	2.44	0.50
8:G:343:LEU:HD12	8:G:507:TYR:CZ	2.47	0.50
13:L:147:VAL:CG1	13:L:252:MET:HG3	2.42	0.50
14:M:190:TRP:HB2	23:Y:128:ILE:HD11	1.93	0.50
15:N:156:MET:HE2	15:N:156:MET:HA	1.93	0.50
16:O:170:ILE:HD11	16:O:238:ILE:HD11	1.92	0.50
19:U:28:GLU:O	19:U:29:LYS:HB3	2.12	0.50
6:E:120:LEU:HD23	6:E:120:LEU:C	2.31	0.50
8:G:237:ASN:O	8:G:259:ASN:ND2	2.44	0.50
9:H:126:LYS:HD3	9:H:126:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:67:HIS:CE1	43:I:202:SF4:S4	3.04	0.50
12:K:81:VAL:HG21	15:N:57:THR:HG21	1.92	0.50
13:L:142:ILE:HD13	14:M:370:PRO:HB2	1.93	0.50
15:N:108:LEU:HD21	15:N:187:MET:HB3	1.92	0.50
15:N:313:MET:HA	15:N:316:HIS:ND1	2.27	0.50
3:B:36:ALA:HA	3:B:39:VAL:HG12	1.93	0.50
8:G:107:ILE:HA	10:I:106:ARG:NH1	2.27	0.50
6:E:169:ILE:HD12	6:E:169:ILE:H	1.77	0.50
7:F:30:ASP:OD1	7:F:30:ASP:C	3.32	0.50
7:F:318:ASP:O	7:F:322:LEU:HD23	2.12	0.50
11:J:30:LEU:HD21	44:J:201:PC1:H242	1.94	0.50
13:L:597:LEU:HD11	23:Y:36:ILE:HD12	1.94	0.50
21:W:72:ASN:O	21:W:75:VAL:HG22	2.12	0.50
14:M:379:LEU:O	14:M:383:MET:HG3	2.12	0.50
8:G:300:LEU:HD11	8:G:603:LEU:HB2	1.94	0.49
19:T:64:ASP:OD2	21:W:35:ARG:NH1	2.45	0.49
13:L:92:VAL:O	13:L:96:VAL:HG23	2.12	0.49
14:M:9:LEU:HD23	14:M:104:ILE:HD13	1.94	0.49
6:E:72:VAL:HG13	6:E:73:LEU:HD23	1.93	0.49
14:M:102:LEU:HD13	14:M:128:PRO:HB2	1.94	0.49
17:P:26:ALA:O	17:P:28:GLY:N	2.43	0.49
22:X:36:ASP:OD2	22:X:40:LYS:HG2	2.12	0.49
23:Y:88:PRO:HG2	23:Y:128:ILE:HD13	1.94	0.49
5:D:247:ALA:CB	5:D:265:ILE:HD11	2.42	0.49
5:D:247:ALA:HB1	5:D:265:ILE:HD11	1.93	0.49
8:G:439:PHE:CE2	8:G:443:LEU:HD21	2.47	0.49
8:G:625:GLU:HB3	18:S:65:TRP:HZ3	1.77	0.49
19:U:86:VAL:HG13	19:U:87:TYR:N	2.28	0.49
2:A:70:ALA:HB1	11:J:54:MET:HE3	1.95	0.49
3:B:96:MET:CE	3:B:113:VAL:HG23	2.42	0.49
5:D:147:ILE:HD11	5:D:307:SER:CB	2.42	0.49
8:G:330:ALA:CB	8:G:600:ILE:HG21	2.43	0.49
11:J:43:VAL:HG12	11:J:48:GLY:O	2.13	0.49
11:J:92:LEU:HD21	44:J:201:PC1:H371	1.95	0.49
14:M:134:THR:HG21	15:N:298:TYR:CE1	2.46	0.49
3:B:41:THR:HG22	3:B:184:LYS:HD3	1.93	0.49
7:F:148:ASN:O	7:F:151:VAL:HG22	2.13	0.49
13:L:584:ILE:HD11	15:N:58:LYS:HA	1.95	0.49
22:X:6:LEU:HD11	24:Z:86:LEU:HB3	1.94	0.49
8:G:324:ASP:CB	8:G:571:ALA:HB1	2.42	0.49
9:H:213:VAL:HG13	9:H:214:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:63:ILE:HG13	15:N:27:MET:HE3	1.93	0.49
14:M:134:THR:O	14:M:142:ARG:NE	2.44	0.49
5:D:110:SER:HA	5:D:145:THR:CG2	2.43	0.49
7:F:368:GLY:HA3	7:F:399:ILE:HD11	1.95	0.49
13:L:483:PRO:HD2	13:L:486:LEU:HD12	1.95	0.49
17:P:325:ARG:O	17:P:325:ARG:NH1	2.41	0.49
7:F:82:MET:SD	7:F:221:THR:OG1	2.57	0.48
13:L:134:ALA:HB1	13:L:139:GLN:HB3	1.95	0.48
15:N:118:VAL:O	15:N:122:ILE:HG23	2.13	0.48
6:E:82:GLU:OE2	8:G:174:THR:N	2.45	0.48
8:G:169:VAL:HG11	8:G:191:PHE:HE1	1.76	0.48
20:V:20:HIS:O	20:V:24:THR:HG23	2.13	0.48
3:B:47:ILE:HD13	9:H:57:MET:CE	2.44	0.48
6:E:68:LYS:O	6:E:68:LYS:HD3	2.13	0.48
8:G:156:CYS:SG	8:G:158:ARG:HD3	2.53	0.48
8:G:477:ILE:O	8:G:481:THR:OG1	2.29	0.48
13:L:233:LEU:HB3	13:L:234:PRO:HD3	1.95	0.48
14:M:310:MET:HE2	14:M:380:PHE:CG	2.48	0.48
17:P:88:SER:OG	17:P:90:VAL:O	2.31	0.48
5:D:61:VAL:HG23	5:D:61:VAL:O	2.13	0.48
5:D:347:HIS:NE2	8:G:126:ASP:HA	2.28	0.48
8:G:246:GLU:HB2	8:G:248:MET:SD	2.54	0.48
9:H:100:LEU:HD13	9:H:103:LEU:HD12	1.96	0.48
2:A:82:ILE:HG22	2:A:82:ILE:O	2.13	0.48
5:D:143:GLU:OE1	5:D:146:ARG:NH1	2.46	0.48
9:H:139:THR:HG21	11:J:64:LEU:HD22	1.95	0.48
13:L:216:LEU:HD22	13:L:259:LEU:HD21	1.96	0.48
22:X:125:SER:HB3	24:Z:65:GLU:OE1	2.14	0.48
8:G:377:VAL:HG12	8:G:404:LEU:HD21	1.95	0.48
8:G:406:VAL:HG13	8:G:419:TYR:HA	1.93	0.48
8:G:667:THR:HG22	8:G:668:ILE:N	2.28	0.48
9:H:288:LEU:CD2	9:H:289:LEU:HD12	2.44	0.48
16:O:297:ARG:NH1	16:O:302:ARG:O	2.46	0.48
2:A:37:TYR:HB2	3:B:91:ARG:NH1	2.29	0.48
7:F:120:GLU:O	7:F:124:VAL:HG13	2.14	0.48
15:N:135:LYS:HD3	15:N:187:MET:SD	2.54	0.48
15:N:213:ALA:O	15:N:217:MET:HG3	2.14	0.48
16:O:282:ILE:HG22	16:O:282:ILE:O	2.14	0.48
21:W:86:ILE:O	21:W:90:MET:HG3	2.14	0.48
3:B:164:GLU:HG2	10:I:52:TYR:CE1	2.49	0.48
4:C:57:VAL:HG13	4:C:58:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:226:GLU:OE1	5:D:305:ARG:NH2	2.41	0.48
13:L:484:TRP:CE3	13:L:485:PHE:N	2.82	0.48
14:M:207:MET:SD	14:M:240:SER:N	2.87	0.48
6:E:119:THR:HG21	6:E:166:PRO:HB3	1.96	0.48
8:G:365:ASN:O	8:G:367:THR:HG23	2.14	0.48
13:L:89:PHE:CE2	13:L:132:THR:HG21	2.49	0.48
13:L:97:THR:HG21	13:L:125:LEU:HD13	1.96	0.48
3:B:91:ARG:HD2	9:H:61:MET:HE1	1.96	0.47
5:D:423:ILE:HB	5:D:428:ILE:HD11	1.94	0.47
7:F:384:ALA:HB3	7:F:430:MET:CE	2.42	0.47
8:G:452:VAL:CG2	8:G:493:LEU:HD12	2.44	0.47
11:J:6:PHE:CG	11:J:120:LEU:HD21	2.49	0.47
14:M:127:ILE:CG1	15:N:254:LEU:HD23	2.44	0.47
6:E:31:ILE:CD1	6:E:50:VAL:HG22	2.44	0.47
15:N:255:PRO:HA	15:N:260:PHE:CG	2.49	0.47
19:U:55:GLU:HG2	19:U:61:GLU:HA	1.96	0.47
2:A:42:ASP:OD1	3:B:112:LYS:HE3	2.14	0.47
6:E:31:ILE:HD12	6:E:50:VAL:HG22	1.97	0.47
7:F:307:ILE:CG1	7:F:327:THR:HG21	2.44	0.47
13:L:253:VAL:HB	13:L:310:LEU:HD11	1.96	0.47
13:L:571:THR:O	13:L:574:THR:HG22	2.13	0.47
14:M:354:LEU:HD23	14:M:434:LEU:HD22	1.95	0.47
5:D:44:VAL:O	5:D:44:VAL:HG13	2.14	0.47
13:L:2:ASN:OD1	13:L:2:ASN:N	2.42	0.47
13:L:410:LEU:C	13:L:410:LEU:HD23	2.35	0.47
13:L:423:SER:O	13:L:426:ILE:HG22	2.14	0.47
15:N:100:MET:SD	15:N:100:MET:C	2.93	0.47
16:O:53:GLU:OE2	16:O:126:ARG:NH1	2.47	0.47
7:F:215:VAL:HG12	7:F:220:THR:OG1	2.15	0.47
9:H:149:ILE:HG21	9:H:185:TRP:HB2	1.96	0.47
9:H:250:ASN:C	9:H:251:LEU:HD12	2.35	0.47
11:J:93:VAL:O	11:J:97:ILE:HG12	2.15	0.47
13:L:502:LEU:O	13:L:506:ASN:ND2	2.48	0.47
14:M:225:ILE:HD13	14:M:331:ASN:HB2	1.96	0.47
19:U:47:GLN:NE2	19:U:70:LEU:O	2.48	0.47
20:V:37:PHE:O	20:V:44:ARG:NH1	2.48	0.47
5:D:73:VAL:HG21	5:D:414:VAL:HG21	1.96	0.47
7:F:44:LYS:O	7:F:48:ILE:HG13	2.14	0.47
8:G:240:VAL:HG13	8:G:240:VAL:O	2.15	0.47
9:H:31:MET:CE	9:H:275:ALA:HB3	2.45	0.47
9:H:150:LEU:O	9:H:154:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:67:HIS:CD2	10:I:124:CYS:SG	3.07	0.47
11:J:127:GLU:OE1	11:J:127:GLU:HA	2.14	0.47
13:L:353:GLU:HA	13:L:353:GLU:OE1	2.14	0.47
7:F:126:GLY:HA3	7:F:173:PHE:HE1	1.80	0.47
8:G:53:ARG:O	8:G:93:VAL:HG21	2.15	0.47
8:G:215:PHE:HB3	10:I:106:ARG:NE	2.30	0.47
8:G:227:SER:O	8:G:238:ILE:N	2.44	0.47
11:J:32:LEU:HD21	12:K:34:GLU:OE2	2.14	0.47
15:N:308:ASN:OD1	15:N:309:ASN:N	2.48	0.47
14:M:76:MET:HG2	14:M:229:MET:HE2	1.97	0.47
5:D:335:ARG:NH2	10:I:131:ASP:OD1	2.45	0.47
6:E:165:THR:O	6:E:168:ASP:N	2.47	0.47
8:G:303:VAL:CG2	8:G:559:VAL:HG21	2.45	0.47
8:G:465:ALA:O	8:G:468:VAL:HG12	2.15	0.47
8:G:490:MET:SD	8:G:491:ASN:N	2.88	0.47
11:J:32:LEU:HD11	12:K:34:GLU:OE2	2.15	0.47
14:M:309:PHE:HB2	14:M:458:THR:HG21	1.97	0.47
6:E:120:LEU:HD22	6:E:139:LEU:HD22	1.96	0.46
6:E:172:ILE:O	6:E:176:LEU:HG	2.14	0.46
13:L:293:LEU:HD11	13:L:418:MET:HG2	1.97	0.46
19:T:19:LEU:HD23	19:T:50:ILE:HD12	1.97	0.46
2:A:70:ALA:HA	11:J:54:MET:HE1	1.97	0.46
3:B:64:CYS:SG	5:D:190:HIS:HE1	2.32	0.46
7:F:166:ALA:O	7:F:169:SER:OG	2.26	0.46
8:G:190:MET:O	8:G:190:MET:HG2	2.15	0.46
8:G:242:THR:HA	8:G:246:GLU:O	2.15	0.46
11:J:98:MET:SD	11:J:98:MET:C	2.94	0.46
8:G:359:ARG:HB3	8:G:363:LEU:HD12	1.98	0.46
14:M:114:GLU:OE1	22:X:168:PHE:N	2.48	0.46
19:T:35:HIS:O	19:T:39:ASP:HB2	2.15	0.46
5:D:111:MET:O	5:D:115:GLU:HG2	2.15	0.46
8:G:667:THR:HG21	8:G:669:LYS:NZ	2.30	0.46
12:K:41:PHE:CE1	12:K:60:PRO:HB3	2.50	0.46
12:K:57:MET:N	12:K:58:PRO:CD	2.79	0.46
4:C:79:THR:HG22	4:C:80:ALA:H	1.80	0.46
7:F:299:PRO:HG3	7:F:307:ILE:HD12	1.98	0.46
8:G:142:ILE:HG22	8:G:142:ILE:O	2.15	0.46
8:G:308:GLN:OE1	8:G:607:ALA:HB1	2.15	0.46
8:G:383:ASN:ND2	8:G:665:GLN:O	2.49	0.46
8:G:514:ILE:HG23	8:G:519:PRO:CD	2.44	0.46
8:G:601:ARG:NE	8:G:614:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:168:ALA:O	10:I:172:GLN:HG2	2.16	0.46
13:L:36:THR:O	13:L:40:ILE:HG12	2.16	0.46
13:L:152:PHE:CD2	13:L:168:ALA:HB1	2.50	0.46
5:D:143:GLU:O	5:D:147:ILE:HG12	2.15	0.46
8:G:631:VAL:HG12	8:G:631:VAL:O	2.16	0.46
9:H:151:LEU:HD23	9:H:151:LEU:C	2.36	0.46
15:N:276:LEU:C	15:N:276:LEU:HD23	2.36	0.46
19:T:62:ILE:HG22	19:T:67:ALA:HB2	1.97	0.46
22:X:45:CYS:SG	22:X:134:ARG:NE	2.88	0.46
23:Y:79:ALA:O	23:Y:82:ARG:C	2.54	0.46
5:D:322:GLU:OE1	5:D:322:GLU:N	2.46	0.46
8:G:114:CYS:SG	8:G:116:LEU:HB3	2.56	0.46
13:L:316:THR:O	13:L:319:MET:O	2.33	0.46
15:N:261:LEU:HD13	15:N:340:ALA:HB1	1.97	0.46
5:D:55:HIS:NE2	9:H:206:GLU:O	2.49	0.46
7:F:331:THR:O	7:F:332:ALA:HB3	2.16	0.46
8:G:46:LEU:HD21	8:G:162:PHE:HA	1.98	0.46
8:G:153:CYS:SG	8:G:155:GLN:N	2.83	0.46
8:G:526:GLY:N	8:G:546:GLN:O	2.47	0.46
12:K:81:VAL:CG2	15:N:57:THR:HG21	2.45	0.46
13:L:532:ILE:HG23	13:L:533:ILE:N	2.30	0.46
19:U:75:GLU:OE1	19:U:75:GLU:O	2.33	0.46
9:H:181:MET:HA	9:H:181:MET:CE	2.46	0.46
16:O:35:LYS:N	51:O:401:GTP:O3G	2.49	0.46
19:T:70:LEU:HD11	19:T:79:TYR:HD2	1.81	0.46
7:F:189:GLU:H	7:F:189:GLU:CD	2.19	0.45
8:G:11:VAL:HG11	8:G:73:VAL:CG2	2.47	0.45
8:G:47:SER:O	8:G:161:ARG:NH1	2.46	0.45
8:G:443:LEU:O	8:G:481:THR:HG21	2.16	0.45
11:J:151:MET:CG	12:K:62:THR:HG21	2.46	0.45
23:Y:137:PHE:N	23:Y:138:PRO:CD	2.79	0.45
3:B:96:MET:HE1	3:B:113:VAL:HG23	1.98	0.45
5:D:147:ILE:HD11	5:D:307:SER:HB3	1.98	0.45
8:G:613:TYR:HB3	8:G:618:GLN:HB3	1.98	0.45
14:M:23:THR:HG23	14:M:24:TRP:N	2.31	0.45
19:T:18:VAL:HG11	19:T:54:MET:SD	2.57	0.45
20:V:29:LYS:O	20:V:33:ILE:HG12	2.16	0.45
4:C:58:ILE:HB	4:C:59:PRO:HD3	1.97	0.45
4:C:127:ALA:O	4:C:128:ASN:C	2.55	0.45
5:D:245:VAL:HG13	5:D:263:SER:OG	2.17	0.45
5:D:409:HIS:HB3	5:D:413:ASP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:116:ILE:HG23	6:E:169:ILE:HG12	1.98	0.45
8:G:142:ILE:HG22	8:G:191:PHE:HB3	1.99	0.45
9:H:221:ALA:O	9:H:225:MET:HG3	2.16	0.45
48:H:401:UQ9:H23	48:H:401:UQ9:H30	1.97	0.45
11:J:50:PHE:O	11:J:54:MET:HB2	2.16	0.45
11:J:130:ASP:OD1	11:J:130:ASP:N	2.49	0.45
5:D:424:VAL:CG2	5:D:427:GLU:HG2	2.45	0.45
12:K:87:THR:HG1	12:K:89:TYR:HD1	1.64	0.45
13:L:258:PHE:O	13:L:261:VAL:HG12	2.16	0.45
17:P:209:ASP:OD2	17:P:308:THR:OG1	2.20	0.45
19:T:49:GLU:OE2	21:W:66:ARG:NH2	2.50	0.45
3:B:43:LEU:O	3:B:47:ILE:HG12	2.17	0.45
3:B:73:ALA:HA	3:B:79:MET:HG2	1.98	0.45
5:D:151:ILE:HD11	5:D:218:PHE:CZ	2.52	0.45
5:D:414:VAL:O	5:D:417:ILE:HG22	2.17	0.45
9:H:145:THR:HG22	9:H:149:ILE:CD1	2.47	0.45
9:H:198:PHE:CD1	9:H:285:LEU:HD13	2.52	0.45
13:L:71:MET:HE2	14:M:310:MET:CE	2.47	0.45
18:S:32:VAL:O	18:S:36:ILE:HD12	2.16	0.45
18:S:77:SER:C	18:S:78:LEU:HD12	2.37	0.45
2:A:55:PHE:HB2	2:A:58:VAL:CG2	2.46	0.45
7:F:189:GLU:HB3	7:F:222:VAL:HG21	1.97	0.45
8:G:615:THR:O	8:G:619:VAL:HG23	2.16	0.45
10:I:135:GLU:OE2	43:I:202:SF4:S4	2.74	0.45
9:H:236:ALA:HB1	9:H:259:PHE:CZ	2.50	0.45
10:I:128:CYS:HA	43:I:201:SF4:S3	2.57	0.45
14:M:298:ILE:O	14:M:302:MET:HG2	2.16	0.45
5:D:139:VAL:HG23	5:D:278:TYR:CZ	2.51	0.45
8:G:142:ILE:HG13	8:G:148:THR:HG21	1.99	0.45
13:L:69:VAL:HG13	13:L:69:VAL:O	2.17	0.45
13:L:191:LEU:HD12	14:M:386:PHE:HD2	1.82	0.45
17:P:198:PHE:O	17:P:199:LYS:HB2	2.17	0.45
53:T:201:EHZ:O2	53:T:201:EHZ:O1	2.35	0.45
3:B:37:GLU:HA	3:B:37:GLU:OE2	2.17	0.45
3:B:44:ASP:OD1	3:B:48:ASN:ND2	2.50	0.45
7:F:249:ARG:O	7:F:249:ARG:NE	2.40	0.45
9:H:175:LEU:O	9:H:179:TRP:N	2.50	0.45
13:L:230:HIS:N	13:L:231:PRO:CD	2.80	0.45
13:L:536:ILE:HG23	13:L:537:THR:N	2.31	0.45
15:N:213:ALA:HB3	15:N:214:PRO:HD3	1.98	0.45
16:O:26:THR:HG23	16:O:26:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:186:LYS:NZ	16:O:191:GLU:OE2	2.48	0.45
22:X:51:ASP:OD1	22:X:53:ARG:N	2.45	0.45
7:F:307:ILE:HG13	7:F:327:THR:HG21	2.00	0.45
13:L:71:MET:HG3	14:M:459:MET:HE1	1.99	0.45
15:N:156:MET:HA	15:N:156:MET:CE	2.47	0.45
5:D:342:MET:HE1	8:G:103:LEU:HA	1.98	0.44
8:G:197:GLY:HA3	8:G:268:ARG:HD3	1.99	0.44
9:H:17:MET:SD	9:H:17:MET:C	2.96	0.44
13:L:49:LEU:HB3	13:L:50:PRO:CD	2.47	0.44
15:N:255:PRO:O	15:N:257:LEU:N	2.50	0.44
2:A:32:GLU:OE1	2:A:32:GLU:N	2.47	0.44
5:D:143:GLU:OE1	5:D:143:GLU:HA	2.17	0.44
5:D:161:ILE:HG23	5:D:238:ARG:HG2	1.98	0.44
5:D:245:VAL:HG13	5:D:245:VAL:O	2.16	0.44
7:F:40:GLY:O	7:F:236:ARG:NH1	2.48	0.44
8:G:611:LEU:HD23	8:G:613:TYR:HE1	1.81	0.44
9:H:317:TYR:O	9:H:318:MET:CB	2.65	0.44
11:J:44:LEU:HD23	11:J:49:SER:HA	1.98	0.44
3:B:160:PRO:HB3	43:B:201:SF4:S1	2.57	0.44
4:C:143:PHE:O	4:C:144:ASN:OD1	2.36	0.44
8:G:205:VAL:HG22	43:G:802:SF4:S3	2.56	0.44
8:G:330:ALA:HB3	8:G:600:ILE:HG21	1.99	0.44
8:G:359:ARG:CZ	8:G:359:ARG:HB2	2.47	0.44
13:L:179:ASP:O	13:L:179:ASP:OD1	2.35	0.44
17:P:237:LEU:HG	17:P:340:VAL:HG11	1.99	0.44
4:C:175:ARG:NE	4:C:186:GLU:OE2	2.50	0.44
8:G:410:GLY:O	8:G:421:HIS:NE2	2.50	0.44
11:J:133:VAL:HG23	24:Z:67:ARG:CZ	2.48	0.44
14:M:63:THR:OG1	14:M:64:PRO:HD3	2.18	0.44
14:M:122:PHE:CZ	14:M:206:LYS:HD2	2.51	0.44
14:M:322:THR:HG23	14:M:323:SER:N	2.33	0.44
22:X:79:GLU:O	22:X:82:THR:OG1	2.28	0.44
2:A:38:GLU:OE2	9:H:126:LYS:HE2	2.17	0.44
4:C:151:ILE:HG23	4:C:152:LEU:HG	1.99	0.44
6:E:123:LYS:HG2	6:E:173:ILE:HG21	2.00	0.44
9:H:179:TRP:CG	9:H:180:PRO:HD3	2.53	0.44
9:H:224:PHE:CE1	9:H:228:TYR:CE1	3.05	0.44
13:L:368:PHE:HB3	13:L:445:GLU:OE2	2.17	0.44
14:M:305:THR:H	14:M:308:SER:HB2	1.83	0.44
15:N:143:ILE:CD1	15:N:202:LEU:HD21	2.48	0.44
16:O:73:PHE:CE2	16:O:299:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:51:ILE:N	19:T:51:ILE:HD12	3.94	0.44
23:Y:38:SER:HB2	23:Y:57:VAL:HG22	1.98	0.44
4:C:117:ILE:O	4:C:142:PHE:HA	2.18	0.44
7:F:349:ARG:O	7:F:349:ARG:HD3	2.17	0.44
11:J:73:MET:CE	12:K:79:VAL:HA	2.48	0.44
13:L:319:MET:O	13:L:321:GLN:N	2.51	0.44
14:M:270:ILE:HD12	14:M:395:LEU:HD22	1.99	0.44
2:A:63:LEU:HD21	11:J:65:VAL:HB	2.00	0.44
2:A:70:ALA:HB2	11:J:58:ILE:HD11	1.98	0.44
9:H:145:THR:HG22	9:H:149:ILE:HD11	2.00	0.44
12:K:59:ILE:HB	12:K:60:PRO:HD3	2.00	0.44
16:O:56:ILE:HD11	16:O:96:LEU:HD11	2.00	0.44
23:Y:41:SER:OG	45:Y:401:3PE:O12	2.36	0.44
8:G:471:SER:O	8:G:474:VAL:HG12	2.18	0.44
13:L:124:PHE:HE1	13:L:147:VAL:HG13	1.83	0.44
13:L:392:LYS:O	13:L:396:ILE:HG12	2.18	0.44
15:N:255:PRO:HA	15:N:260:PHE:HB2	1.99	0.44
8:G:44:GLU:HG2	8:G:45:ARG:HD2	2.00	0.43
9:H:53:MET:O	9:H:57:MET:SD	2.76	0.43
14:M:207:MET:HB3	14:M:298:ILE:HD11	2.00	0.43
14:M:305:THR:OG1	14:M:306:PRO:HD2	2.17	0.43
14:M:342:MET:HG2	14:M:413:THR:HG21	2.00	0.43
15:N:142:LEU:HB3	15:N:194:LEU:HD21	1.99	0.43
16:O:151:HIS:CE1	16:O:155:ILE:HD11	2.53	0.43
17:P:134:HIS:HB2	17:P:149:LYS:CD	2.48	0.43
3:B:55:LEU:HD23	3:B:55:LEU:N	2.33	0.43
5:D:104:ASP:HB3	5:D:190:HIS:HA	2.00	0.43
8:G:332:LYS:HA	8:G:343:LEU:HD13	1.99	0.43
14:M:259:TYR:O	14:M:263:LEU:HG	2.18	0.43
15:N:146:TYR:N	15:N:147:PRO:CD	2.82	0.43
15:N:215:MET:HE3	15:N:251:LEU:HD12	2.00	0.43
15:N:285:MET:CE	15:N:288:LEU:HD12	2.48	0.43
15:N:321:LYS:N	15:N:322:PRO:CD	2.81	0.43
17:P:71:LEU:HD12	17:P:71:LEU:O	2.18	0.43
4:C:104:ARG:NH1	5:D:273:GLN:OE1	2.52	0.43
8:G:378:LEU:HD11	8:G:409:ILE:HG13	2.00	0.43
13:L:282:ALA:CB	13:L:411:ILE:HD11	2.48	0.43
23:Y:17:THR:HG22	23:Y:18:GLN:N	2.34	0.43
6:E:116:ILE:HG23	6:E:169:ILE:CD1	2.49	0.43
7:F:48:ILE:HG22	7:F:56:ILE:HD11	2.00	0.43
11:J:17:LEU:HD12	11:J:17:LEU:N	4.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:27:LEU:HD12	21:W:27:LEU:N	2.33	0.43
21:W:37:LEU:O	21:W:37:LEU:HD12	2.18	0.43
22:X:124:LEU:HB2	24:Z:65:GLU:OE2	2.18	0.43
3:B:126:MET:HE1	3:B:166:LEU:HD22	2.01	0.43
3:B:186:TRP:O	3:B:189:ARG:HB3	2.18	0.43
5:D:208:LEU:HD22	5:D:315:LEU:HD23	1.99	0.43
7:F:404:ILE:HD11	8:G:50:GLY:O	2.18	0.43
9:H:68:MET:HG2	9:H:72:ILE:HD12	2.00	0.43
22:X:82:THR:HA	22:X:85:TRP:CD1	2.54	0.43
8:G:317:ALA:CB	8:G:331:LEU:HD21	2.49	0.43
8:G:452:VAL:HA	8:G:491:ASN:OD1	2.19	0.43
8:G:551:ASP:O	8:G:552:VAL:HB	2.19	0.43
11:J:56:PHE:O	11:J:60:LEU:HG	2.18	0.43
8:G:54:MET:HA	8:G:93:VAL:HG11	2.00	0.43
19:U:81:ALA:HB1	19:U:86:VAL:CG1	2.48	0.43
7:F:94:VAL:HG11	7:F:192:LEU:HD22	2.01	0.43
7:F:110:ILE:CG2	7:F:118:LEU:HD11	2.40	0.43
8:G:74:MET:SD	8:G:77:TRP:NE1	2.91	0.43
8:G:105:CYS:HB2	8:G:106:PRO:HD3	2.01	0.43
8:G:604:SER:CB	8:G:611:LEU:HD13	2.49	0.43
15:N:289:ASN:HA	15:N:292:PHE:CE2	2.53	0.43
23:Y:17:THR:HG22	23:Y:18:GLN:H	1.83	0.43
9:H:24:GLU:CA	9:H:271:LEU:HD13	2.41	0.43
16:O:147:GLN:OE1	16:O:147:GLN:N	2.52	0.43
5:D:341:SER:O	5:D:344:SER:OG	2.34	0.43
7:F:263:ASN:ND2	7:F:286:GLY:O	2.52	0.43
8:G:574:VAL:HG23	8:G:579:ARG:O	2.19	0.43
8:G:599:ILE:HD13	21:W:124:PHE:CZ	2.54	0.43
9:H:141:SER:OG	9:H:142:TYR:N	2.52	0.43
14:M:106:LEU:HA	14:M:109:THR:OG1	2.19	0.43
15:N:49:ASN:O	15:N:53:THR:HG23	2.18	0.43
16:O:26:THR:O	16:O:26:THR:CG2	2.67	0.43
48:H:401:UQ9:C16	48:H:401:UQ9:H20	2.47	0.42
13:L:332:HIS:HA	13:L:335:PHE:CE2	2.54	0.42
23:Y:4:LYS:O	23:Y:7:PHE:N	2.47	0.42
4:C:77:ASP:OD1	5:D:392:LYS:HG3	2.19	0.42
5:D:147:ILE:HD11	5:D:307:SER:HB2	2.02	0.42
13:L:429:PHE:O	13:L:436:ARG:NH2	2.52	0.42
19:U:75:GLU:OE1	19:U:78:ASP:HB2	2.19	0.42
3:B:72:MET:HE3	3:B:170:ILE:HG13	2.02	0.42
5:D:347:HIS:CG	8:G:121:MET:HE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:54:ASP:N	7:F:54:ASP:OD1	2.51	0.42
8:G:324:ASP:OD1	8:G:326:GLU:HB2	2.20	0.42
8:G:329:VAL:N	8:G:505:LEU:HD21	2.34	0.42
8:G:337:LYS:HD3	8:G:609:ILE:HG23	2.01	0.42
8:G:362:TYR:O	8:G:362:TYR:CD2	2.72	0.42
13:L:286:LEU:HD23	13:L:286:LEU:C	2.39	0.42
15:N:149:LEU:HD13	15:N:154:ILE:HD11	2.01	0.42
19:U:48:VAL:O	19:U:52:MET:HG3	2.19	0.42
7:F:97:ALA:HB3	7:F:137:TYR:O	2.20	0.42
8:G:299:ALA:O	8:G:303:VAL:HG23	2.19	0.42
8:G:359:ARG:HA	8:G:362:TYR:CE1	2.54	0.42
9:H:17:MET:SD	9:H:18:ALA:N	2.92	0.42
12:K:12:PHE:CE1	15:N:72:LEU:HD22	2.55	0.42
14:M:76:MET:SD	14:M:230:ILE:HB	2.59	0.42
14:M:304:GLN:O	14:M:304:GLN:HG3	2.19	0.42
16:O:151:HIS:NE2	16:O:155:ILE:HD11	2.34	0.42
3:B:91:ARG:HE	9:H:61:MET:CE	2.31	0.42
4:C:78:LEU:HB3	4:C:130:TYR:HB3	2.02	0.42
7:F:316:LEU:O	7:F:318:ASP:N	2.50	0.42
14:M:277:LEU:HD21	14:M:405:MET:HB3	2.00	0.42
5:D:37:ASP:OD2	15:N:51:ARG:NE	2.50	0.42
6:E:143:GLU:HA	6:E:143:GLU:OE1	2.19	0.42
6:E:202:LEU:HD12	6:E:202:LEU:O	2.19	0.42
7:F:337:MET:HE3	7:F:343:ILE:HD11	2.02	0.42
11:J:106:LEU:HD12	11:J:115:ILE:HD13	2.01	0.42
12:K:41:PHE:CE1	12:K:60:PRO:CB	3.02	0.42
14:M:192:ASN:HB3	14:M:253:LEU:HD11	2.01	0.42
14:M:248:ILE:HG23	14:M:249:ILE:HG23	2.00	0.42
15:N:43:MET:HE2	15:N:43:MET:HA	3.67	0.42
24:Z:97:MET:CE	24:Z:100:VAL:HG21	2.49	0.42
6:E:23:PHE:HB2	6:E:28:TYR:CZ	2.55	0.42
8:G:544:VAL:CG2	8:G:559:VAL:HG23	2.44	0.42
8:G:597:TRP:HA	8:G:600:ILE:HG22	2.02	0.42
11:J:73:MET:HE3	12:K:79:VAL:HA	2.02	0.42
13:L:97:THR:HG21	13:L:125:LEU:CD1	2.49	0.42
13:L:418:MET:HA	13:L:421:MET:HG3	2.02	0.42
13:L:501:ALA:O	13:L:505:ASN:OD1	2.38	0.42
20:V:8:THR:OG1	20:V:13:LEU:O	2.38	0.42
21:W:121:LEU:O	21:W:125:TYR:CD1	2.72	0.42
7:F:140:GLY:HA2	7:F:179:ARG:HG2	2.02	0.42
8:G:351:THR:O	8:G:351:THR:OG1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:185:TRP:O	9:H:189:THR:HG23	2.20	0.42
10:I:50:ILE:O	10:I:52:TYR:N	2.53	0.42
13:L:145:GLU:CD	14:M:369:LEU:HD12	2.40	0.42
13:L:217:LEU:HD13	13:L:277:MET:HG2	2.02	0.42
14:M:41:LEU:HB3	14:M:63:THR:HG22	2.02	0.42
14:M:230:ILE:HG23	14:M:231:LEU:N	2.34	0.42
23:Y:125:LEU:HD23	23:Y:125:LEU:HA	1.93	0.42
5:D:243:GLY:HA3	5:D:417:ILE:HD13	2.02	0.42
6:E:31:ILE:HD12	6:E:50:VAL:HG13	2.01	0.42
7:F:168:GLY:C	7:F:169:SER:HG	2.23	0.42
8:G:213:TYR:O	8:G:213:TYR:CG	2.73	0.42
8:G:239:VAL:HG23	8:G:253:ARG:HB2	2.01	0.42
13:L:202:MET:HA	13:L:202:MET:CE	2.49	0.42
14:M:108:MET:HB3	14:M:121:LEU:HD13	2.01	0.42
24:Z:11:PRO:HD3	24:Z:15:TYR:CZ	2.55	0.42
3:B:71:HIS:O	3:B:74:ALA:HB3	2.19	0.42
6:E:107:PRO:HB2	46:E:301:FES:S2	2.60	0.42
8:G:673:MET:HG3	8:G:688:VAL:HG21	2.02	0.42
4:C:182:ARG:NH1	21:W:111:GLU:OE2	2.53	0.41
6:E:58:ASN:O	6:E:60:TRP:N	2.50	0.41
6:E:124:LEU:HD11	6:E:173:ILE:HG12	2.02	0.41
8:G:11:VAL:HG11	8:G:73:VAL:HG21	2.01	0.41
8:G:152:ARG:HD2	8:G:206:GLY:O	2.20	0.41
13:L:182:PHE:O	13:L:186:MET:HG3	2.20	0.41
13:L:264:HIS:N	13:L:265:PRO:HD2	2.35	0.41
14:M:220:HIS:ND1	14:M:327:PHE:CZ	2.88	0.41
19:T:12:LYS:HZ3	19:T:32:VAL:HG22	1.84	0.41
19:T:73:PRO:O	19:T:77:VAL:HG13	2.20	0.41
3:B:52:ARG:O	3:B:55:LEU:HD22	2.21	0.41
5:D:307:SER:O	5:D:311:ILE:HG12	2.19	0.41
7:F:47:GLU:O	7:F:51:LYS:HG3	2.20	0.41
7:F:192:LEU:HD23	7:F:192:LEU:O	2.21	0.41
7:F:295:LEU:HD11	7:F:422:PHE:CE1	2.55	0.41
8:G:160:ILE:HD11	8:G:174:THR:HG23	2.01	0.41
8:G:314:ALA:O	8:G:520:LYS:N	2.52	0.41
9:H:38:ASN:OD1	9:H:38:ASN:C	2.59	0.41
13:L:155:ILE:HG22	13:L:156:GLY:N	2.36	0.41
17:P:78:LYS:HD3	17:P:78:LYS:N	2.36	0.41
19:U:65:ILE:HG23	19:U:66:ASP:N	2.35	0.41
3:B:62:LEU:N	3:B:62:LEU:HD12	2.35	0.41
7:F:142:PHE:HB3	7:F:145:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:260:MET:SD	9:H:260:MET:C	2.99	0.41
48:H:401:UQ9:H35A	48:H:401:UQ9:C38	2.51	0.41
17:P:20:VAL:O	17:P:88:SER:OG	2.38	0.41
2:A:47:ALA:HB2	9:H:126:LYS:HD2	2.02	0.41
7:F:383:ASP:O	7:F:384:ALA:HB2	2.20	0.41
8:G:632:ARG:NH1	18:S:57:CYS:SG	2.93	0.41
13:L:567:SER:HB2	50:L:705:LMT:O2'	2.20	0.41
19:T:44:SER:O	19:T:48:VAL:HG23	2.20	0.41
19:T:81:ALA:O	19:T:82:ASP:C	2.58	0.41
22:X:14:VAL:HG22	22:X:15:GLU:N	2.36	0.41
23:Y:136:LEU:HD23	23:Y:136:LEU:H	1.86	0.41
3:B:101:THR:OG1	3:B:129:CYS:SG	2.72	0.41
8:G:262:TRP:HB2	8:G:390:LEU:HD21	2.02	0.41
8:G:452:VAL:HG22	8:G:493:LEU:HD12	2.01	0.41
8:G:553:GLY:O	8:G:556:MET:SD	2.79	0.41
11:J:19:LEU:O	11:J:19:LEU:HD23	2.20	0.41
13:L:484:TRP:CZ3	13:L:485:PHE:HB3	2.56	0.41
2:A:60:ILE:HD12	11:J:166:ILE:HB	2.03	0.41
3:B:46:LEU:HD21	9:H:53:MET:CE	2.51	0.41
3:B:164:GLU:HB3	10:I:139:PHE:CE1	2.55	0.41
8:G:371:VAL:HG21	8:G:391:PHE:CE1	2.55	0.41
45:H:402:3PE:HN2	45:H:402:3PE:P	2.33	0.41
13:L:298:ILE:HG23	13:L:299:LYS:N	2.36	0.41
16:O:305:ALA:O	16:O:306:PRO:C	2.59	0.41
19:T:9:ASP:OD1	19:T:9:ASP:C	2.58	0.41
19:T:22:TYR:CG	19:T:50:ILE:HD11	2.56	0.41
6:E:89:MET:CE	7:F:182:GLY:N	2.84	0.41
13:L:251:THR:O	13:L:252:MET:C	2.59	0.41
15:N:17:PRO:HG2	15:N:133:TRP:NE1	2.36	0.41
21:W:97:LYS:O	21:W:98:VAL:HB	2.21	0.41
9:H:150:LEU:HD21	9:H:185:TRP:CZ3	2.56	0.41
11:J:52:GLY:O	11:J:55:VAL:HG22	2.20	0.41
13:L:49:LEU:HB3	13:L:50:PRO:HD3	2.02	0.41
13:L:503:GLU:OE2	13:L:503:GLU:C	2.59	0.41
24:Z:138:GLY:O	24:Z:141:TRP:O	2.38	0.41
3:B:68:GLU:OE1	5:D:188:ARG:NH1	2.54	0.41
5:D:230:THR:HG22	5:D:231:ASN:N	2.36	0.41
5:D:247:ALA:HA	5:D:265:ILE:HD11	2.02	0.41
7:F:119:VAL:HG12	7:F:162:ILE:HD11	2.03	0.41
7:F:347:ILE:O	7:F:351:ILE:HG12	2.20	0.41
8:G:160:ILE:HD13	8:G:174:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:322:LEU:HD23	8:G:322:LEU:N	2.32	0.41
8:G:609:ILE:HG22	8:G:610:THR:N	2.36	0.41
8:G:611:LEU:HD23	8:G:613:TYR:CE1	2.56	0.41
10:I:72:TYR:N	10:I:76:GLU:O	2.50	0.41
10:I:145:THR:OG1	10:I:148:GLU:OE2	2.24	0.41
12:K:66:PHE:CZ	15:N:31:VAL:HG13	2.55	0.41
13:L:179:ASP:OD1	13:L:183:ILE:HD12	2.21	0.41
13:L:295:GLN:O	13:L:301:ILE:HD11	2.21	0.41
13:L:590:SER:HB3	23:Y:44:LEU:HD21	2.03	0.41
15:N:45:ILE:O	15:N:45:ILE:HG23	2.20	0.41
19:U:86:VAL:HG13	19:U:87:TYR:H	1.86	0.41
2:A:44:THR:HG1	5:D:48:THR:HG1	1.67	0.41
7:F:327:THR:OG1	7:F:328:GLY:N	2.53	0.41
9:H:179:TRP:N	9:H:180:PRO:CD	2.84	0.41
13:L:413:LEU:O	13:L:416:THR:OG1	2.29	0.41
49:M:502:CDL:OB4	16:O:303:LYS:NZ	2.54	0.41
21:W:44:GLU:HA	21:W:44:GLU:OE1	2.21	0.41
21:W:54:LEU:HD11	21:W:105:VAL:HG11	2.03	0.41
23:Y:96:CYS:O	23:Y:100:LEU:HG	2.21	0.41
3:B:70:MET:HG3	48:H:401:UQ9:H10A	2.03	0.40
5:D:245:VAL:HG13	5:D:263:SER:HG	1.87	0.40
5:D:366:ALA:HB1	5:D:373:GLU:HG2	2.03	0.40
8:G:80:LEU:HD12	8:G:80:LEU:HA	1.97	0.40
8:G:154:ILE:CG2	8:G:205:VAL:HG11	2.51	0.40
9:H:161:SER:HG	9:H:164:THR:HG1	1.66	0.40
9:H:237:LEU:HD23	9:H:237:LEU:HA	1.97	0.40
10:I:128:CYS:SG	10:I:132:ALA:N	2.86	0.40
13:L:578:THR:CG2	15:N:168:GLY:HA2	2.51	0.40
19:T:25:ILE:HB	19:T:30:LEU:HD13	2.03	0.40
22:X:28:ALA:O	22:X:32:GLY:N	2.47	0.40
24:Z:61:ILE:O	24:Z:65:GLU:HG2	2.21	0.40
3:B:45:ASP:OD1	3:B:45:ASP:C	2.59	0.40
4:C:79:THR:HG22	4:C:80:ALA:N	2.36	0.40
5:D:335:ARG:NH1	10:I:126:GLU:O	2.54	0.40
7:F:276:LEU:O	7:F:280:ILE:HG22	2.22	0.40
7:F:296:ALA:HB3	7:F:337:MET:CE	2.51	0.40
8:G:258:ILE:HG13	8:G:259:ASN:H	1.87	0.40
8:G:329:VAL:HA	8:G:505:LEU:HD21	2.02	0.40
8:G:380:VAL:HG12	8:G:409:ILE:HD12	2.03	0.40
9:H:201:THR:O	9:H:210:GLY:HA3	2.21	0.40
11:J:168:GLU:OE1	15:N:1:FME:SD	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:51:LEU:HD21	13:L:55:PHE:CE2	2.56	0.40
13:L:180:ILE:HD12	14:M:397:GLY:CA	2.51	0.40
14:M:231:LEU:HA	14:M:235:LEU:HD12	2.03	0.40
14:M:337:ILE:O	14:M:338:HIS:C	2.59	0.40
15:N:70:ILE:HG13	15:N:101:ALA:HB1	2.04	0.40
16:O:138:MET:HE1	51:O:401:GTP:HN21	1.87	0.40
18:S:75:THR:HG22	18:S:76:VAL:N	2.37	0.40
23:Y:96:CYS:HA	23:Y:116:CYS:HA	2.04	0.40
2:A:59:ALA:HA	9:H:140:ILE:CD1	2.51	0.40
4:C:158:GLU:O	4:C:158:GLU:CG	2.70	0.40
6:E:181:VAL:O	6:E:181:VAL:HG23	2.21	0.40
8:G:390:LEU:HD23	8:G:390:LEU:HA	1.94	0.40
8:G:436:ARG:HA	8:G:436:ARG:NE	2.36	0.40
10:I:6:ASN:O	10:I:6:ASN:CG	2.60	0.40
11:J:80:GLU:OE1	11:J:80:GLU:N	2.45	0.40
14:M:360:LEU:O	14:M:364:LEU:HG	2.22	0.40
16:O:135:LEU:HD22	16:O:152:TYR:CD1	2.56	0.40
23:Y:86:ASP:OD1	23:Y:86:ASP:O	2.38	0.40
24:Z:29:LEU:HD12	24:Z:29:LEU:HA	1.95	0.40
4:C:177:ASP:OD1	4:C:177:ASP:C	2.58	0.40
8:G:9:ILE:HG22	8:G:11:VAL:HG13	2.02	0.40
10:I:52:TYR:CG	10:I:53:PRO:N	2.90	0.40
13:L:161:ARG:CZ	13:L:238:GLU:OE2	2.68	0.40
13:L:396:ILE:HA	13:L:399:ILE:HG22	2.04	0.40
13:L:445:GLU:O	13:L:445:GLU:HG3	2.21	0.40
2:A:18:ILE:HD13	2:A:18:ILE:HA	2.51	0.40
2:A:61:THR:HG21	2:A:105:GLU:OE1	2.21	0.40
4:C:188:VAL:O	4:C:188:VAL:HG13	2.21	0.40
5:D:136:TRP:O	5:D:139:VAL:HG12	2.21	0.40
5:D:219:SER:O	5:D:222:ILE:HG22	2.21	0.40
13:L:553:LEU:HD12	13:L:553:LEU:H	1.87	0.40
14:M:203:PHE:O	14:M:207:MET:HG2	2.22	0.40
17:P:286:ARG:NH1	17:P:286:ARG:HB3	2.36	0.40
23:Y:30:GLY:O	23:Y:64:ALA:HB1	2.22	0.40
23:Y:127:LYS:HE3	23:Y:131:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	t	104/168 (62%)	93 (89%)	10 (10%)	1 (1%)	13	46
2	A	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
3	B	154/224 (69%)	143 (93%)	11 (7%)	0	100	100
4	C	205/263 (78%)	196 (96%)	9 (4%)	0	100	100
5	D	427/463 (92%)	402 (94%)	25 (6%)	0	100	100
6	E	208/248 (84%)	190 (91%)	18 (9%)	0	100	100
7	F	426/464 (92%)	397 (93%)	29 (7%)	0	100	100
8	G	686/727 (94%)	637 (93%)	47 (7%)	2 (0%)	37	70
9	H	316/318 (99%)	292 (92%)	24 (8%)	0	100	100
10	I	176/212 (83%)	171 (97%)	5 (3%)	0	100	100
11	J	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
12	K	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
13	L	604/607 (100%)	567 (94%)	35 (6%)	2 (0%)	37	70
14	M	457/459 (100%)	442 (97%)	15 (3%)	0	100	100
15	N	342/345 (99%)	330 (96%)	12 (4%)	0	100	100
16	O	318/355 (90%)	307 (96%)	11 (4%)	0	100	100
17	P	323/377 (86%)	302 (94%)	20 (6%)	1 (0%)	37	70
18	S	80/99 (81%)	75 (94%)	4 (5%)	1 (1%)	10	41
19	T	74/156 (47%)	73 (99%)	1 (1%)	0	100	100
19	U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
20	V	110/116 (95%)	106 (96%)	4 (4%)	0	100	100
21	W	107/131 (82%)	101 (94%)	5 (5%)	1 (1%)	14	48
22	X	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
23	Y	138/143 (96%)	130 (94%)	8 (6%)	0	100	100
24	Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	a	66/70 (94%)	63 (96%)	3 (4%)	0	100	100
26	b	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
27	c	46/76 (60%)	45 (98%)	1 (2%)	0	100	100
28	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
29	e	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
30	f	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
31	g	99/151 (66%)	94 (95%)	5 (5%)	0	100	100
32	h	136/189 (72%)	135 (99%)	1 (1%)	0	100	100
33	i	89/128 (70%)	84 (94%)	5 (6%)	0	100	100
34	j	60/105 (57%)	57 (95%)	3 (5%)	0	100	100
35	k	73/104 (70%)	72 (99%)	1 (1%)	0	100	100
36	l	152/186 (82%)	142 (93%)	10 (7%)	0	100	100
37	m	124/129 (96%)	118 (95%)	6 (5%)	0	100	100
38	n	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
39	o	111/137 (81%)	102 (92%)	8 (7%)	1 (1%)	14	48
40	p	166/176 (94%)	160 (96%)	6 (4%)	0	100	100
41	r	57/113 (50%)	53 (93%)	4 (7%)	0	100	100
42	s	29/104 (28%)	26 (90%)	3 (10%)	0	100	100
All	All	7758/8946 (87%)	7335 (94%)	414 (5%)	9 (0%)	50	80

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	G	206	GLY
8	G	552	VAL
17	P	250	HIS
39	o	32	GLU
13	L	249	SER
18	S	69	ALA
13	L	562	ILE
21	W	98	VAL
1	t	158	TRP

5.3.2 Protein sidechains ⓘ

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	t	96/147 (65%)	93 (97%)	3 (3%)	35	56
2	A	103/103 (100%)	102 (99%)	1 (1%)	73	81
3	B	132/185 (71%)	129 (98%)	3 (2%)	45	64
4	C	189/227 (83%)	188 (100%)	1 (0%)	86	90
5	D	370/394 (94%)	365 (99%)	5 (1%)	62	75
6	E	183/206 (89%)	180 (98%)	3 (2%)	58	73
7	F	343/370 (93%)	336 (98%)	7 (2%)	50	68
8	G	567/610 (93%)	553 (98%)	14 (2%)	42	62
9	H	279/279 (100%)	276 (99%)	3 (1%)	70	79
10	I	152/178 (85%)	148 (97%)	4 (3%)	41	61
11	J	136/137 (99%)	133 (98%)	3 (2%)	47	65
12	K	87/87 (100%)	85 (98%)	2 (2%)	45	64
13	L	548/549 (100%)	541 (99%)	7 (1%)	65	76
14	M	414/414 (100%)	411 (99%)	3 (1%)	81	86
15	N	306/307 (100%)	301 (98%)	5 (2%)	58	73
16	O	284/309 (92%)	280 (99%)	4 (1%)	62	75
17	P	286/325 (88%)	281 (98%)	5 (2%)	56	72
18	S	56/80 (70%)	56 (100%)	0	100	100
19	T	70/135 (52%)	67 (96%)	3 (4%)	25	49
19	U	79/135 (58%)	77 (98%)	2 (2%)	42	62
20	V	100/102 (98%)	99 (99%)	1 (1%)	73	81
21	W	103/114 (90%)	103 (100%)	0	100	100
22	X	153/154 (99%)	151 (99%)	2 (1%)	65	76
23	Y	105/107 (98%)	103 (98%)	2 (2%)	52	70
24	Z	122/123 (99%)	120 (98%)	2 (2%)	58	73
25	a	58/60 (97%)	57 (98%)	1 (2%)	56	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	b	71/73 (97%)	69 (97%)	2 (3%)	38	59
27	c	42/67 (63%)	42 (100%)	0	100	100
28	d	107/107 (100%)	105 (98%)	2 (2%)	52	70
29	e	93/94 (99%)	92 (99%)	1 (1%)	70	79
30	f	49/53 (92%)	47 (96%)	2 (4%)	26	50
31	g	92/129 (71%)	88 (96%)	4 (4%)	25	49
32	h	123/162 (76%)	121 (98%)	2 (2%)	58	73
33	i	88/120 (73%)	87 (99%)	1 (1%)	70	79
34	j	58/87 (67%)	56 (97%)	2 (3%)	32	55
35	k	58/78 (74%)	57 (98%)	1 (2%)	56	72
36	l	139/161 (86%)	135 (97%)	4 (3%)	37	59
37	m	112/114 (98%)	109 (97%)	3 (3%)	40	60
38	n	162/164 (99%)	157 (97%)	5 (3%)	35	56
39	o	106/121 (88%)	104 (98%)	2 (2%)	52	70
40	p	153/158 (97%)	150 (98%)	3 (2%)	50	68
41	r	57/96 (59%)	56 (98%)	1 (2%)	54	71
42	s	31/95 (33%)	30 (97%)	1 (3%)	34	56
All	All	6862/7716 (89%)	6740 (98%)	122 (2%)	54	71

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	t	57	ARG
1	t	61	ASP
1	t	153	PHE
2	A	42	ASP
3	B	60	PHE
3	B	91	ARG
3	B	135	TYR
4	C	49	GLU
5	D	24	GLU
5	D	35	ASP
5	D	182	GLU
5	D	230	THR
5	D	297	TYR
6	E	153	MET

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Mol	Chain	Res	Type
6	E	170	GLU
6	E	201	SER
7	F	80	SER
7	F	99	GLU
7	F	170	ASP
7	F	209	PHE
7	F	312	CYS
7	F	337	MET
7	F	359	CYS
8	G	71	MET
8	G	74	MET
8	G	324	ASP
8	G	341	ASP
8	G	352	GLU
8	G	403	ASP
8	G	523	PHE
8	G	531	CYS
8	G	535	GLN
8	G	536	ASP
8	G	548	HIS
8	G	549	HIS
8	G	556	MET
8	G	613	TYR
9	H	146	MET
9	H	204	GLU
9	H	283	ASP
10	I	34	ARG
10	I	41	SER
10	I	82	CYS
10	I	118	CYS
11	J	9	SER
11	J	24	SER
11	J	130	ASP
12	K	5	PHE
12	K	88	ASP
13	L	71	MET
13	L	74	MET
13	L	338	MET
13	L	343	SER
13	L	432	MET
13	L	485	PHE
13	L	498	PHE

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Mol	Chain	Res	Type
14	M	59	ASP
14	M	168	GLN
14	M	269	MET
15	N	104	MET
15	N	231	SER
15	N	314	MET
15	N	321	LYS
15	N	323	ASN
16	O	90	ASP
16	O	126	ARG
16	O	206	TYR
16	O	297	ARG
17	P	24	PHE
17	P	37	HIS
17	P	73	TRP
17	P	222	ASP
17	P	263	TYR
19	T	43	ASP
19	T	47	GLN
19	T	56	ASP
19	U	66	ASP
19	U	72	CYS
20	V	109	ASN
22	X	47	TRP
22	X	125	SER
23	Y	4	LYS
23	Y	137	PHE
24	Z	9	MET
24	Z	97	MET
25	a	3	PHE
26	b	61	ASN
26	b	64	ASP
28	d	104	LYS
28	d	105	GLU
29	e	102	GLU
30	f	26	ASP
30	f	30	ASP
31	g	24	TRP
31	g	32	ASP
31	g	38	LYS
31	g	121	ASP
32	h	54	GLU

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Mol	Chain	Res	Type
32	h	142	ASP
33	i	83	TYR
34	j	20	SER
34	j	29	SER
35	k	59	MET
36	l	48	MET
36	l	123	SER
36	l	136	ASN
36	l	156	ASP
37	m	74	ASN
37	m	111	LYS
37	m	121	ASP
38	n	48	GLU
38	n	56	MET
38	n	57	MET
38	n	102	CYS
38	n	146	ASP
39	o	33	ARG
39	o	112	LYS
40	p	98	ASP
40	p	123	ASN
40	p	170	ARG
41	r	60	ARG
42	s	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	t	22	HIS
4	C	71	GLN
6	E	55	GLN
6	E	91	ASN
7	F	224	ASN
7	F	283	HIS
7	F	402	HIS
8	G	629	ASN
9	H	292	ASN
10	I	172	GLN
13	L	136	ASN
13	L	175	ASN
13	L	295	GLN
13	L	506	ASN

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Mol	Chain	Res	Type
14	M	103	GLN
14	M	144	ASN
14	M	430	HIS
15	N	172	GLN
15	N	273	ASN
17	P	103	ASN
18	S	61	GLN
20	V	40	HIS
20	V	82	GLN
22	X	123	GLN
24	Z	134	ASN
26	b	10	ASN
27	c	9	ASN
29	e	44	HIS
29	e	76	HIS
29	e	96	HIS
31	g	117	GLN
32	h	108	GLN
36	l	54	GLN
36	l	71	ASN
38	n	13	GLN
38	n	32	HIS
40	p	58	ASN
40	p	103	ASN
40	p	123	ASN
41	r	109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	M	1	14	8,9,10	1.02	1 (12%)	7,9,11	0.76	0
13	FME	L	1	13	8,9,10	0.96	0	7,9,11	0.65	0
15	FME	N	1	15	8,9,10	0.95	0	7,9,11	0.83	0
9	FME	H	1	9	8,9,10	0.90	0	7,9,11	1.28	1 (14%)
11	FME	J	1	11	8,9,10	0.94	0	7,9,11	1.06	1 (14%)
5	2MR	D	85	5	10,12,13	1.85	1 (10%)	5,13,15	4.62	3 (60%)
2	FME	A	1	2	8,9,10	0.99	0	7,9,11	0.76	0
12	FME	K	1	12	8,9,10	0.94	0	7,9,11	1.23	1 (14%)

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
14	FME	M	1	14	-	1/7/9/11	-
13	FME	L	1	13	-	1/7/9/11	-
15	FME	N	1	15	-	2/7/9/11	-
9	FME	H	1	9	-	4/7/9/11	-
11	FME	J	1	11	-	3/7/9/11	-
5	2MR	D	85	5	-	5/10/13/15	-
2	FME	A	1	2	-	1/7/9/11	-
12	FME	K	1	12	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	85	2MR	CZ-NE	5.24	1.45	1.34
14	M	1	FME	CA-N	-2.04	1.43	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	85	2MR	NE-CZ-NH2	8.82	127.57	119.48
5	D	85	2MR	CD-NE-CZ	4.58	131.98	123.41
5	D	85	2MR	CG-CD-NE	2.58	119.58	112.21
9	H	1	FME	CA-N-CN	2.57	126.78	122.82
12	K	1	FME	C-CA-N	2.55	114.33	109.73
11	J	1	FME	C-CA-N	2.09	113.51	109.73

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	85	2MR	N-CA-CB-CG
5	D	85	2MR	O-C-CA-CB
5	D	85	2MR	CG-CD-NE-CZ
9	H	1	FME	O1-CN-N-CA
9	H	1	FME	CB-CA-N-CN
11	J	1	FME	O1-CN-N-CA
11	J	1	FME	N-CA-CB-CG
12	K	1	FME	N-CA-CB-CG
5	D	85	2MR	NE-CD-CG-CB
2	A	1	FME	CB-CG-SD-CE
9	H	1	FME	C-CA-CB-CG
15	N	1	FME	N-CA-CB-CG
9	H	1	FME	CB-CG-SD-CE
5	D	85	2MR	C-CA-CB-CG
11	J	1	FME	C-CA-CB-CG
12	K	1	FME	C-CA-CB-CG
14	M	1	FME	N-CA-CB-CG
12	K	1	FME	CB-CA-N-CN
13	L	1	FME	CB-CA-N-CN
15	N	1	FME	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	1	FME	1	0
5	D	85	2MR	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	FMN	F	502	-	33,33,33	4.61	19 (57%)	48,50,50	4.78	24 (50%)
43	SF4	I	201	10	0,12,12	-	-	-		
46	FES	E	301	6	0,4,4	-	-	-		
53	EHZ	T	201	19	29,36,37	1.88	5 (17%)	35,44,47	1.44	3 (8%)
45	3PE	M	501	-	41,41,50	0.95	4 (9%)	44,46,55	1.07	2 (4%)
51	GTP	O	401	-	26,33,34	2.65	10 (38%)	32,52,54	1.63	9 (28%)
45	3PE	D	501	-	50,50,50	0.85	3 (6%)	53,55,55	1.09	2 (3%)
45	3PE	L	701	-	48,48,50	0.87	2 (4%)	51,53,55	1.04	2 (3%)
50	LMT	L	704	-	36,36,36	1.15	5 (13%)	47,47,47	1.03	2 (4%)
52	NDP	P	501	-	45,52,52	2.22	4 (8%)	53,80,80	1.76	13 (24%)
49	CDL	d	201	-	66,66,99	1.09	7 (10%)	72,78,111	1.21	4 (5%)
43	SF4	G	802	8	0,12,12	-	-	-		
45	3PE	H	402	-	43,43,50	0.91	4 (9%)	46,48,55	1.22	3 (6%)
50	LMT	L	705	-	36,36,36	1.18	6 (16%)	47,47,47	0.94	2 (4%)
43	SF4	G	801	8	0,12,12	-	-	-		
43	SF4	I	202	10	0,12,12	-	-	-		
46	FES	G	803	8	0,4,4	-	-	-		
49	CDL	L	702	-	73,73,99	1.05	7 (9%)	79,85,111	1.13	5 (6%)
53	EHZ	U	201	19	29,36,37	1.87	5 (17%)	35,44,47	1.59	5 (14%)
49	CDL	d	202	-	62,62,99	1.12	7 (11%)	68,74,111	1.12	4 (5%)
43	SF4	B	201	3,5	0,12,12	-	-	-		
49	CDL	i	201	-	69,69,99	1.06	7 (10%)	75,81,111	1.15	4 (5%)
45	3PE	L	703	-	41,41,50	0.95	4 (9%)	44,46,55	1.07	2 (4%)
49	CDL	N	401	-	64,64,99	1.11	7 (10%)	70,76,111	1.16	4 (5%)
45	3PE	Y	401	-	40,40,50	0.95	4 (10%)	43,45,55	1.02	2 (4%)
48	UQ9	H	401	-	44,44,58	0.83	0	52,52,73	2.22	22 (42%)
49	CDL	M	502	-	58,58,99	1.08	4 (6%)	63,69,111	1.06	3 (4%)
44	PC1	J	201	-	41,41,53	1.42	6 (14%)	47,49,61	1.11	3 (6%)
45	3PE	K	201	-	32,32,50	1.04	4 (12%)	35,37,55	1.15	2 (5%)
44	PC1	B	202	-	40,40,53	1.42	6 (15%)	46,48,61	1.06	2 (4%)
43	SF4	F	501	7	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	FMN	F	502	-	-	6/18/18/18	0/3/3/3
43	SF4	I	201	10	-	-	0/6/5/5
46	FES	E	301	6	-	-	0/1/1/1
53	EHZ	T	201	19	-	12/42/44/45	-
45	3PE	M	501	-	-	16/45/45/54	-
51	GTP	O	401	-	-	3/18/34/38	0/3/3/3
45	3PE	D	501	-	-	24/54/54/54	-
45	3PE	L	701	-	-	20/52/52/54	-
50	LMT	L	704	-	-	11/21/61/61	0/2/2/2
52	NDP	P	501	-	-	10/30/77/77	0/5/5/5
49	CDL	d	201	-	-	25/77/77/110	-
43	SF4	G	802	8	-	-	0/6/5/5
45	3PE	H	402	-	-	19/47/47/54	-
50	LMT	L	705	-	-	12/21/61/61	0/2/2/2
43	SF4	G	801	8	-	-	0/6/5/5
53	EHZ	U	201	19	-	18/42/44/45	-
49	CDL	L	702	-	-	31/84/84/110	-
43	SF4	I	202	10	-	-	0/6/5/5
46	FES	G	803	8	-	-	0/1/1/1
49	CDL	d	202	-	-	39/73/73/110	-
43	SF4	B	201	3,5	-	-	0/6/5/5
49	CDL	i	201	-	-	37/80/80/110	-
45	3PE	L	703	-	-	18/45/45/54	-
49	CDL	N	401	-	-	41/75/75/110	-
45	3PE	Y	401	-	-	12/44/44/54	-
48	UQ9	H	401	-	-	17/50/50/81	-
49	CDL	M	502	-	-	42/67/67/110	-
44	PC1	J	201	-	-	17/45/45/57	-
45	3PE	K	201	-	-	16/36/36/54	-
44	PC1	B	202	-	-	18/44/44/57	-
43	SF4	F	501	7	-	-	0/6/5/5

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.25	1.82	1.59
47	F	502	FMN	C6-C5A	11.39	1.57	1.40
47	F	502	FMN	C9A-C5A	10.35	1.58	1.41
47	F	502	FMN	C9-C8	-9.90	1.25	1.39
47	F	502	FMN	O2-C2	8.78	1.40	1.24
47	F	502	FMN	O4-C4	8.43	1.39	1.23
51	O	401	GTP	O6-C6	8.32	1.40	1.23
47	F	502	FMN	C8-C7	-6.79	1.24	1.40
53	U	201	EHZ	C15-N2	6.09	1.46	1.33
53	T	201	EHZ	C15-N2	5.99	1.46	1.33
47	F	502	FMN	C4A-C4	5.96	1.66	1.44
53	T	201	EHZ	C12-N1	5.82	1.46	1.33
53	U	201	EHZ	C12-N1	5.64	1.46	1.33
47	F	502	FMN	C2-N3	-5.34	1.26	1.39
47	F	502	FMN	C4A-N5	4.71	1.39	1.30
51	O	401	GTP	C2-N2	4.68	1.45	1.34
51	O	401	GTP	C2-N1	4.45	1.48	1.37
52	P	501	NDP	PN-O5D	4.12	1.76	1.59
51	O	401	GTP	C2-N3	4.04	1.43	1.33
44	B	202	PC1	O31-C31	3.69	1.44	1.33
44	J	201	PC1	O31-C31	3.67	1.44	1.33
44	B	202	PC1	O21-C21	3.55	1.44	1.34
44	J	201	PC1	O21-C21	3.53	1.44	1.34
47	F	502	FMN	C8M-C8	3.39	1.57	1.51
47	F	502	FMN	C4A-C10	3.28	1.53	1.44
52	P	501	NDP	O2B-C2B	-3.13	1.32	1.44
47	F	502	FMN	C9A-N10	2.99	1.46	1.41
45	L	701	3PE	O21-C2	-2.84	1.39	1.46
50	L	704	LMT	O3'-C3'	-2.76	1.36	1.43
53	T	201	EHZ	C9-S1	2.74	1.82	1.76
53	U	201	EHZ	C9-S1	2.74	1.82	1.76
49	d	202	CDL	OB8-CB7	2.73	1.41	1.33
45	D	501	3PE	O21-C2	-2.69	1.39	1.46
49	L	702	CDL	OB8-CB7	2.68	1.41	1.33
49	d	201	CDL	OB8-CB7	2.68	1.41	1.33
49	i	201	CDL	OB8-CB7	2.67	1.41	1.33
50	L	705	LMT	O3'-C3'	-2.67	1.36	1.43
49	M	502	CDL	OB6-CB5	2.66	1.41	1.34
49	i	201	CDL	OA6-CA4	-2.65	1.40	1.46
51	O	401	GTP	C5-C6	-2.64	1.42	1.47
50	L	705	LMT	O2'-C2'	-2.63	1.36	1.43
49	N	401	CDL	OA6-CA4	-2.62	1.40	1.46
49	M	502	CDL	OB8-CB7	2.61	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	N	401	CDL	OB8-CB7	2.60	1.40	1.33
49	L	702	CDL	OB6-CB4	-2.60	1.40	1.46
45	L	703	3PE	O21-C2	-2.59	1.40	1.46
49	N	401	CDL	OB6-CB4	-2.58	1.40	1.46
49	i	201	CDL	OB6-CB5	2.57	1.41	1.34
50	L	704	LMT	O2'-C2'	-2.56	1.37	1.43
44	B	202	PC1	O21-C2	-2.55	1.40	1.46
49	d	202	CDL	OB6-CB4	-2.53	1.40	1.46
51	O	401	GTP	C1'-N9	-2.52	1.41	1.49
47	F	502	FMN	C10-N1	2.51	1.38	1.33
45	L	701	3PE	O31-C31	2.49	1.40	1.33
49	d	202	CDL	OA8-CA7	2.49	1.40	1.33
45	H	402	3PE	O31-C31	2.48	1.40	1.33
47	F	502	FMN	P-O2P	-2.47	1.45	1.54
49	i	201	CDL	OA8-CA7	2.47	1.40	1.33
49	d	201	CDL	OB6-CB5	2.47	1.41	1.34
44	J	201	PC1	O21-C2	-2.46	1.40	1.46
45	L	703	3PE	O31-C31	2.46	1.40	1.33
45	M	501	3PE	O21-C2	-2.45	1.40	1.46
49	M	502	CDL	OA8-CA7	2.45	1.40	1.33
49	L	702	CDL	OA8-CA7	2.45	1.40	1.33
51	O	401	GTP	O4'-C1'	2.44	1.47	1.42
49	N	401	CDL	OA8-CA7	2.43	1.40	1.33
45	K	201	3PE	O21-C2	-2.43	1.40	1.46
53	T	201	EHZ	O4-C15	-2.43	1.18	1.23
49	L	702	CDL	OA6-CA4	-2.42	1.40	1.46
45	Y	401	3PE	O21-C2	-2.41	1.40	1.46
50	L	704	LMT	O3B-C3B	-2.40	1.37	1.43
50	L	704	LMT	O2B-C2B	-2.40	1.37	1.43
49	d	201	CDL	OA6-CA4	-2.39	1.40	1.46
47	F	502	FMN	P-O3P	-2.39	1.45	1.54
50	L	705	LMT	O2B-C2B	-2.38	1.37	1.43
45	M	501	3PE	O31-C31	2.37	1.40	1.33
49	N	401	CDL	OB6-CB5	2.36	1.41	1.34
49	d	201	CDL	OA8-CA6	-2.35	1.39	1.45
49	d	202	CDL	OB6-CB5	2.34	1.40	1.34
47	F	502	FMN	C5A-N5	2.34	1.44	1.39
49	d	202	CDL	OA6-CA4	-2.34	1.40	1.46
50	L	705	LMT	O3B-C3B	-2.33	1.37	1.43
49	d	201	CDL	OA8-CA7	2.32	1.40	1.33
53	U	201	EHZ	O4-C15	-2.32	1.18	1.23
45	H	402	3PE	O21-C2	-2.31	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	O	401	GTP	C2'-C3'	-2.31	1.46	1.52
49	d	201	CDL	OA6-CA5	2.31	1.40	1.34
45	D	501	3PE	O31-C3	-2.30	1.39	1.45
49	d	201	CDL	OB6-CB4	-2.30	1.40	1.46
45	K	201	3PE	O31-C31	2.29	1.40	1.33
45	Y	401	3PE	O31-C31	2.29	1.40	1.33
49	L	702	CDL	OB6-CB5	2.29	1.40	1.34
44	B	202	PC1	P-O11	2.28	1.68	1.59
47	F	502	FMN	C1'-C2'	2.27	1.55	1.52
44	B	202	PC1	C22-C21	2.25	1.57	1.50
44	J	201	PC1	P-O11	2.24	1.68	1.59
51	O	401	GTP	PG-O2G	-2.23	1.46	1.54
49	L	702	CDL	OA8-CA6	-2.21	1.40	1.45
53	U	201	EHZ	O3-C12	-2.21	1.18	1.23
45	K	201	3PE	O21-C21	2.21	1.40	1.34
47	F	502	FMN	C7M-C7	2.20	1.55	1.51
44	J	201	PC1	C22-C21	2.19	1.57	1.50
45	Y	401	3PE	O31-C3	-2.18	1.40	1.45
47	F	502	FMN	O4'-C4'	-2.18	1.38	1.43
45	D	501	3PE	O31-C31	2.18	1.39	1.33
49	i	201	CDL	OA8-CA6	-2.18	1.40	1.45
49	N	401	CDL	OA8-CA6	-2.16	1.40	1.45
51	O	401	GTP	PG-O3G	-2.16	1.46	1.54
45	Y	401	3PE	O21-C21	2.15	1.40	1.34
50	L	705	LMT	O4'-C4B	-2.15	1.37	1.43
49	i	201	CDL	OA6-CA5	2.15	1.40	1.34
49	L	702	CDL	OA6-CA5	2.14	1.40	1.34
53	T	201	EHZ	O3-C12	-2.14	1.18	1.23
44	B	202	PC1	P-O13	2.14	1.68	1.59
49	d	202	CDL	OA6-CA5	2.13	1.40	1.34
50	L	704	LMT	O4'-C4B	-2.13	1.38	1.43
45	M	501	3PE	O31-C3	-2.12	1.40	1.45
44	J	201	PC1	P-O13	2.12	1.67	1.59
45	M	501	3PE	O21-C21	2.12	1.40	1.34
49	d	202	CDL	OA8-CA6	-2.11	1.40	1.45
49	i	201	CDL	OB6-CB4	-2.11	1.41	1.46
52	P	501	NDP	C7N-N7N	2.11	1.39	1.33
45	H	402	3PE	O21-C21	2.09	1.40	1.34
49	M	502	CDL	OA8-CA6	-2.09	1.40	1.45
45	H	402	3PE	O31-C3	-2.09	1.40	1.45
45	L	703	3PE	O31-C3	-2.06	1.40	1.45
49	N	401	CDL	OA6-CA5	2.05	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	L	705	LMT	O1'-C1'	-2.03	1.36	1.40
45	K	201	3PE	O31-C3	-2.03	1.40	1.45
45	L	703	3PE	O21-C21	2.01	1.40	1.34

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	F	502	FMN	C6-C5A-N5	15.23	145.09	118.51
47	F	502	FMN	C4-C4A-N5	14.85	139.36	118.23
47	F	502	FMN	C6-C5A-C9A	-11.94	102.05	118.94
47	F	502	FMN	C5A-N5-C4A	9.67	134.14	118.07
47	F	502	FMN	C9A-C5A-N5	-8.81	112.86	122.43
47	F	502	FMN	C9A-N10-C10	8.08	133.35	120.77
52	P	501	NDP	PN-O3-PA	-7.31	107.75	132.83
47	F	502	FMN	C10-N1-C2	6.62	130.14	116.90
47	F	502	FMN	C5A-C9A-N10	-6.58	111.16	117.95
47	F	502	FMN	C10-C4A-N5	-5.87	112.39	124.86
48	H	401	UQ9	C35-C34-C36	5.78	124.99	115.27
47	F	502	FMN	C4-C4A-C10	-5.09	108.25	116.79
49	d	201	CDL	OA6-CA5-C11	5.07	122.42	111.50
53	U	201	EHZ	C8-C9-S1	4.95	119.75	113.63
53	T	201	EHZ	C8-C9-S1	4.62	119.34	113.63
49	M	502	CDL	OB6-CB5-C51	4.55	121.31	111.50
44	J	201	PC1	O21-C21-C22	4.49	121.19	111.50
45	L	703	3PE	O21-C21-C22	4.48	121.16	111.50
49	L	702	CDL	OA6-CA5-C11	4.46	121.12	111.50
45	H	402	3PE	O21-C21-C22	4.18	120.51	111.50
45	K	201	3PE	O21-C21-C22	4.10	120.34	111.50
45	Y	401	3PE	O21-C21-C22	4.02	120.17	111.50
44	B	202	PC1	O21-C21-C22	4.01	120.15	111.50
49	d	201	CDL	OB6-CB5-C51	3.98	120.09	111.50
49	N	401	CDL	OB6-CB5-C51	3.95	120.02	111.50
49	d	202	CDL	OA6-CA5-C11	3.94	119.99	111.50
47	F	502	FMN	C9-C9A-N10	3.88	127.08	121.84
45	M	501	3PE	O21-C21-C22	3.88	119.85	111.50
49	i	201	CDL	OA6-CA5-C11	3.86	119.83	111.50
49	N	401	CDL	OA6-CA5-C11	3.86	119.82	111.50
48	H	401	UQ9	C32-C31-C29	-3.85	100.32	112.98
48	H	401	UQ9	C37-C38-C39	-3.78	118.57	127.66
48	H	401	UQ9	C16-C17-C18	3.77	124.28	111.88
48	H	401	UQ9	C22-C23-C24	-3.77	118.57	127.66
45	D	501	3PE	O21-C21-C22	3.71	119.50	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	H	401	UQ9	C7-C8-C9	-3.70	118.07	126.57
49	i	201	CDL	OB6-CB5-C51	3.70	119.47	111.50
45	H	402	3PE	O31-C31-C32	3.68	123.45	111.91
48	H	401	UQ9	C22-C21-C19	-3.62	101.07	112.98
48	H	401	UQ9	C40-C39-C41	3.61	121.35	115.27
49	L	702	CDL	OB6-CB5-C51	3.38	118.78	111.50
51	O	401	GTP	C2-N1-C6	-3.26	119.10	125.10
49	d	202	CDL	OB6-CB5-C51	3.24	118.49	111.50
45	L	701	3PE	O21-C21-C22	3.24	118.48	111.50
52	P	501	NDP	O2B-P2B-O1X	-3.22	96.97	109.39
49	d	202	CDL	OB8-CB7-C71	3.12	121.69	111.91
51	O	401	GTP	PB-O3B-PG	-3.11	122.16	132.83
51	O	401	GTP	C5-C6-N1	3.10	119.43	113.95
51	O	401	GTP	PA-O3A-PB	-3.02	122.47	132.83
52	P	501	NDP	PA-O5B-C5B	-2.99	104.13	121.68
48	H	401	UQ9	C42-C43-C44	-2.97	120.50	127.66
45	K	201	3PE	O31-C31-C32	2.96	121.19	111.91
49	i	201	CDL	OA8-CA7-C31	2.94	121.12	111.91
50	L	704	LMT	C1'-O5'-C5'	-2.92	107.95	113.69
53	U	201	EHZ	C14-C13-C12	-2.91	107.50	112.36
47	F	502	FMN	C9A-C9-C8	2.91	125.15	119.30
48	H	401	UQ9	C32-C33-C34	-2.91	120.66	127.66
49	M	502	CDL	OB8-CB7-C71	2.88	120.94	111.91
53	U	201	EHZ	C19-C17-C16	2.81	113.69	108.82
49	N	401	CDL	OA8-CA7-C31	2.81	120.71	111.91
49	L	702	CDL	OB8-CB7-C71	2.80	120.71	111.91
51	O	401	GTP	O3G-PG-O3B	2.79	114.00	104.64
48	H	401	UQ9	C50-C49-C51	2.79	120.77	114.60
47	F	502	FMN	C4A-C10-N1	-2.77	118.29	124.73
51	O	401	GTP	O2G-PG-O3B	2.77	113.94	104.64
47	F	502	FMN	O2P-P-O5'	2.73	114.00	106.73
48	H	401	UQ9	C36-C34-C33	-2.71	115.62	121.12
45	D	501	3PE	O31-C31-C32	2.71	120.42	111.91
47	F	502	FMN	O3P-P-O5'	2.71	113.95	106.73
52	P	501	NDP	PN-O5D-C5D	-2.71	105.81	121.68
45	L	701	3PE	O31-C31-C32	2.70	120.39	111.91
49	d	201	CDL	OB8-CB7-C71	2.70	120.38	111.91
47	F	502	FMN	O5'-P-O1P	2.68	114.00	106.47
49	i	201	CDL	OB8-CB7-C71	2.67	120.27	111.91
49	d	201	CDL	OA8-CA7-C31	2.65	120.24	111.91
49	d	202	CDL	OA8-CA7-C31	2.62	120.12	111.91
48	H	401	UQ9	C21-C22-C23	-2.60	103.33	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	F	502	FMN	C1'-N10-C9A	-2.60	116.19	120.51
52	P	501	NDP	O3X-P2B-O2X	2.58	117.50	107.64
53	T	201	EHZ	C10-S1-C9	2.58	109.89	101.87
45	M	501	3PE	O31-C31-C32	2.55	119.91	111.91
49	N	401	CDL	OB8-CB7-C71	2.54	119.87	111.91
48	H	401	UQ9	C17-C18-C19	-2.53	121.56	127.66
47	F	502	FMN	N10-C10-N1	2.53	125.61	118.35
48	H	401	UQ9	C31-C29-C28	-2.51	116.03	121.12
44	B	202	PC1	O31-C31-C32	2.51	119.79	111.91
49	L	702	CDL	OA8-CA7-C31	2.51	119.78	111.91
48	H	401	UQ9	C12-C11-C9	-2.51	104.73	112.98
48	H	401	UQ9	C20-C19-C18	-2.48	117.31	123.68
48	H	401	UQ9	C17-C16-C14	-2.47	104.85	112.98
48	H	401	UQ9	C20-C19-C21	2.47	119.42	115.27
44	J	201	PC1	O31-C31-C32	2.46	119.63	111.91
52	P	501	NDP	C2A-N1A-C6A	-2.46	114.55	118.75
52	P	501	NDP	C3N-C2N-N1N	-2.44	119.62	123.10
50	L	705	LMT	C3'-C4'-C5'	-2.41	105.41	110.93
47	F	502	FMN	C5A-C6-C7	2.40	125.11	120.71
49	M	502	CDL	OA8-CA7-C31	2.36	119.32	111.91
47	F	502	FMN	C9-C8-C7	2.33	123.00	119.67
52	P	501	NDP	O2N-PN-O1N	2.32	123.69	112.24
45	Y	401	3PE	O31-C31-C32	2.31	119.17	111.91
47	F	502	FMN	C4-N3-C2	2.29	129.87	125.64
47	F	502	FMN	C5'-C4'-C3'	-2.29	107.79	112.20
47	F	502	FMN	C6-C7-C8	2.27	122.92	119.67
53	U	201	EHZ	C16-C15-N2	2.25	121.06	116.58
47	F	502	FMN	O4-C4-C4A	-2.23	120.69	126.60
53	U	201	EHZ	C10-S1-C9	2.20	108.73	101.87
51	O	401	GTP	O2A-PA-O1A	-2.19	101.43	112.24
49	L	702	CDL	CB4-OB6-CB5	-2.17	112.44	117.79
53	T	201	EHZ	C13-C12-N1	2.17	120.08	116.42
45	L	703	3PE	O31-C31-C32	2.17	118.71	111.91
45	H	402	3PE	O31-C31-O32	-2.16	118.14	123.59
50	L	705	LMT	C1'-O5'-C5'	-2.13	109.50	113.69
52	P	501	NDP	C5B-C4B-C3B	-2.12	107.22	115.18
52	P	501	NDP	O5D-PN-O1N	-2.12	100.77	109.07
51	O	401	GTP	O2B-PB-O1B	-2.10	101.84	112.24
52	P	501	NDP	O4B-C4B-C3B	2.09	109.25	105.11
44	J	201	PC1	C2-O21-C21	-2.09	112.65	117.79
48	H	401	UQ9	C27-C28-C29	-2.05	122.72	127.66
50	L	704	LMT	O1'-C1'-C2'	2.05	111.50	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	H	401	UQ9	C45-C44-C46	2.04	118.71	115.27
48	H	401	UQ9	C46-C47-C48	-2.04	105.17	111.88
51	O	401	GTP	O6-C6-C5	-2.03	120.41	124.37
52	P	501	NDP	C5D-C4D-C3D	-2.02	107.61	115.18
52	P	501	NDP	C3B-C2B-C1B	-2.01	99.12	102.89

There are no chirality outliers.

All (464) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	202	PC1	C11-O13-P-O11
44	B	202	PC1	C1-O11-P-O14
44	B	202	PC1	C12-C11-O13-P
44	B	202	PC1	O13-C11-C12-N
44	B	202	PC1	O11-C1-C2-O21
44	B	202	PC1	C22-C21-O21-C2
44	J	201	PC1	C1-O11-P-O13
45	H	402	3PE	C11-O13-P-O14
45	H	402	3PE	O32-C31-O31-C3
45	H	402	3PE	C32-C31-O31-C3
45	H	402	3PE	C22-C21-O21-C2
45	K	201	3PE	C1-O11-P-O12
45	K	201	3PE	C1-O11-P-O14
45	L	703	3PE	C1-O11-P-O14
45	L	703	3PE	C22-C21-O21-C2
45	M	501	3PE	C11-O13-P-O11
45	M	501	3PE	C11-O13-P-O14
45	M	501	3PE	O11-C1-C2-O21
45	M	501	3PE	C22-C21-O21-C2
45	Y	401	3PE	C1-O11-P-O14
47	F	502	FMN	C5'-O5'-P-O2P
47	F	502	FMN	C5'-O5'-P-O3P
48	H	401	UQ9	C45-C44-C46-C47
48	H	401	UQ9	C43-C44-C46-C47
49	L	702	CDL	CA2-OA2-PA1-OA3
49	L	702	CDL	CA2-OA2-PA1-OA4
49	L	702	CDL	CA2-OA2-PA1-OA5
49	L	702	CDL	OB5-CB3-CB4-OB6
49	L	702	CDL	C51-CB5-OB6-CB4
49	M	502	CDL	CA2-OA2-PA1-OA3
49	M	502	CDL	CA2-OA2-PA1-OA4
49	M	502	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
49	M	502	CDL	CA3-OA5-PA1-OA3
49	M	502	CDL	CB2-OB2-PB2-OB3
49	M	502	CDL	CB3-OB5-PB2-OB3
49	N	401	CDL	CA2-C1-CB2-OB2
49	N	401	CDL	C1-CA2-OA2-PA1
49	N	401	CDL	CA3-OA5-PA1-OA3
49	N	401	CDL	CA3-OA5-PA1-OA4
49	N	401	CDL	CB2-OB2-PB2-OB3
49	N	401	CDL	OB7-CB5-OB6-CB4
49	N	401	CDL	C51-CB5-OB6-CB4
49	d	201	CDL	CB2-OB2-PB2-OB3
49	d	201	CDL	CB2-OB2-PB2-OB4
49	d	201	CDL	CB2-OB2-PB2-OB5
49	d	201	CDL	CB3-OB5-PB2-OB2
49	d	201	CDL	C51-CB5-OB6-CB4
49	d	202	CDL	C1-CA2-OA2-PA1
49	d	202	CDL	CA2-OA2-PA1-OA3
49	d	202	CDL	CA3-OA5-PA1-OA3
49	d	202	CDL	CB2-OB2-PB2-OB3
49	d	202	CDL	CB2-OB2-PB2-OB4
49	d	202	CDL	CB2-OB2-PB2-OB5
49	i	201	CDL	CA2-OA2-PA1-OA3
49	i	201	CDL	CA2-OA2-PA1-OA4
49	i	201	CDL	CB2-OB2-PB2-OB3
49	i	201	CDL	CB2-OB2-PB2-OB4
49	i	201	CDL	CB3-OB5-PB2-OB3
49	i	201	CDL	C51-CB5-OB6-CB4
50	L	704	LMT	O5B-C1B-O1B-C4'
50	L	704	LMT	C2'-C1'-O1'-C1
50	L	704	LMT	O5'-C1'-O1'-C1
50	L	705	LMT	C2'-C1'-O1'-C1
50	L	705	LMT	O5'-C1'-O1'-C1
51	O	401	GTP	C5'-O5'-PA-O1A
52	P	501	NDP	C5B-O5B-PA-O3
52	P	501	NDP	C3B-C4B-C5B-O5B
53	T	201	EHZ	C6-C7-C8-C9
53	T	201	EHZ	S1-C10-C11-N1
53	T	201	EHZ	C16-C17-C20-O6
53	T	201	EHZ	C19-C17-C20-O6
53	U	201	EHZ	S1-C10-C11-N1
53	U	201	EHZ	C12-C13-C14-N2
53	U	201	EHZ	C16-C15-N2-C14

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Mol	Chain	Res	Type	Atoms
53	U	201	EHZ	C15-C16-C17-C18
53	U	201	EHZ	C15-C16-C17-C19
53	U	201	EHZ	C15-C16-C17-C20
53	U	201	EHZ	O5-C16-C17-C18
53	U	201	EHZ	O5-C16-C17-C19
53	U	201	EHZ	O5-C16-C17-C20
53	U	201	EHZ	O2-C9-S1-C10
53	U	201	EHZ	C8-C9-S1-C10
45	D	501	3PE	O32-C31-O31-C3
49	i	201	CDL	OB9-CB7-OB8-CB6
45	L	701	3PE	C2-C3-O31-C31
49	L	702	CDL	OB9-CB7-OB8-CB6
49	d	202	CDL	OA9-CA7-OA8-CA6
49	d	202	CDL	OB9-CB7-OB8-CB6
49	i	201	CDL	OA9-CA7-OA8-CA6
44	B	202	PC1	O22-C21-O21-C2
45	H	402	3PE	O22-C21-O21-C2
45	L	703	3PE	O22-C21-O21-C2
45	M	501	3PE	O22-C21-O21-C2
49	L	702	CDL	OB7-CB5-OB6-CB4
49	M	502	CDL	OB7-CB5-OB6-CB4
49	d	201	CDL	OB7-CB5-OB6-CB4
45	D	501	3PE	C32-C31-O31-C3
49	L	702	CDL	C71-CB7-OB8-CB6
49	d	202	CDL	C31-CA7-OA8-CA6
49	d	202	CDL	C71-CB7-OB8-CB6
49	i	201	CDL	C31-CA7-OA8-CA6
49	i	201	CDL	C71-CB7-OB8-CB6
49	M	502	CDL	C51-CB5-OB6-CB4
49	N	401	CDL	OB9-CB7-OB8-CB6
49	d	201	CDL	C31-CA7-OA8-CA6
49	d	201	CDL	C71-CB7-OB8-CB6
49	i	201	CDL	OB7-CB5-OB6-CB4
49	M	502	CDL	OB9-CB7-OB8-CB6
49	M	502	CDL	O1-C1-CB2-OB2
49	N	401	CDL	O1-C1-CA2-OA2
49	N	401	CDL	O1-C1-CB2-OB2
49	d	202	CDL	O1-C1-CA2-OA2
44	J	201	PC1	C32-C31-O31-C3
49	N	401	CDL	C71-CB7-OB8-CB6
49	d	201	CDL	OA9-CA7-OA8-CA6
49	d	201	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
53	U	201	EHZ	O4-C15-N2-C14
49	N	401	CDL	C11-CA5-OA6-CA4
49	d	202	CDL	C78-C79-C80-C81
49	N	401	CDL	CA7-C31-C32-C33
52	P	501	NDP	O4D-C4D-C5D-O5D
49	M	502	CDL	C71-CB7-OB8-CB6
50	L	704	LMT	O5'-C5'-C6'-O6'
49	N	401	CDL	CA4-CA3-OA5-PA1
48	H	401	UQ9	C35-C34-C36-C37
48	H	401	UQ9	C33-C34-C36-C37
44	J	201	PC1	O32-C31-O31-C3
48	H	401	UQ9	C39-C41-C42-C43
48	H	401	UQ9	C29-C31-C32-C33
48	H	401	UQ9	C19-C21-C22-C23
48	H	401	UQ9	C14-C16-C17-C18
49	i	201	CDL	C11-CA5-OA6-CA4
49	M	502	CDL	CB2-C1-CA2-OA2
49	M	502	CDL	OA5-CA3-CA4-CA6
44	B	202	PC1	C32-C31-O31-C3
45	L	701	3PE	C32-C31-O31-C3
49	M	502	CDL	O1-C1-CA2-OA2
49	M	502	CDL	OA5-CA3-CA4-OA6
49	d	201	CDL	CB5-C51-C52-C53
44	B	202	PC1	O32-C31-O31-C3
49	N	401	CDL	OA7-CA5-OA6-CA4
50	L	705	LMT	O5B-C5B-C6B-O6B
50	L	705	LMT	O5'-C5'-C6'-O6'
44	B	202	PC1	C21-C22-C23-C24
49	L	702	CDL	CB5-C51-C52-C53
52	P	501	NDP	O4B-C4B-C5B-O5B
45	D	501	3PE	C21-C22-C23-C24
45	L	701	3PE	O32-C31-O31-C3
53	U	201	EHZ	C5-C6-C7-C8
48	H	401	UQ9	C9-C11-C12-C13
49	i	201	CDL	OA7-CA5-OA6-CA4
49	N	401	CDL	C71-C72-C73-C74
45	D	501	3PE	C22-C21-O21-C2
45	D	501	3PE	C1-O11-P-O13
45	K	201	3PE	C1-O11-P-O13
45	L	703	3PE	C1-O11-P-O13
45	M	501	3PE	C1-O11-P-O13
49	L	702	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
49	M	502	CDL	CA3-OA5-PA1-OA2
49	M	502	CDL	CB2-OB2-PB2-OB5
49	N	401	CDL	CA2-OA2-PA1-OA5
49	N	401	CDL	CA3-OA5-PA1-OA2
49	N	401	CDL	CB2-OB2-PB2-OB5
49	i	201	CDL	CA2-OA2-PA1-OA5
49	i	201	CDL	CA3-OA5-PA1-OA2
49	i	201	CDL	CB2-OB2-PB2-OB5
49	d	202	CDL	CB5-C51-C52-C53
49	d	202	CDL	CB2-C1-CA2-OA2
45	D	501	3PE	O22-C21-O21-C2
52	P	501	NDP	C3D-C4D-C5D-O5D
49	N	401	CDL	C75-C76-C77-C78
53	T	201	EHZ	C18-C17-C20-O6
45	H	402	3PE	C3-C2-O21-C21
49	i	201	CDL	CB3-CB4-OB6-CB5
49	L	702	CDL	C52-C53-C54-C55
49	M	502	CDL	C53-C54-C55-C56
45	D	501	3PE	C31-C32-C33-C34
49	i	201	CDL	CB5-C51-C52-C53
45	L	703	3PE	C25-C26-C27-C28
49	d	202	CDL	C75-C76-C77-C78
53	U	201	EHZ	C2-C3-C4-C5
45	M	501	3PE	C3B-C3C-C3D-C3E
49	M	502	CDL	OA6-CA4-CA6-OA8
45	H	402	3PE	C34-C35-C36-C37
50	L	705	LMT	C6-C7-C8-C9
49	N	401	CDL	C83-C84-C85-C86
49	d	201	CDL	C31-C32-C33-C34
50	L	704	LMT	C11-C10-C9-C8
44	B	202	PC1	C37-C38-C39-C3A
45	D	501	3PE	C25-C26-C27-C28
49	d	202	CDL	C71-C72-C73-C74
45	Y	401	3PE	C33-C34-C35-C36
49	L	702	CDL	C77-C78-C79-C80
45	D	501	3PE	C37-C38-C39-C3A
49	N	401	CDL	C51-C52-C53-C54
48	H	401	UQ9	C25-C24-C26-C27
48	H	401	UQ9	C23-C24-C26-C27
49	L	702	CDL	C11-CA5-OA6-CA4
49	M	502	CDL	CB5-C51-C52-C53
50	L	704	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	i	201	CDL	C20-C21-C22-C23
53	T	201	EHZ	C5-C6-C7-O1
49	d	202	CDL	CA5-C11-C12-C13
49	L	702	CDL	OA7-CA5-OA6-CA4
49	L	702	CDL	C75-C76-C77-C78
45	D	501	3PE	C2D-C2E-C2F-C2G
49	L	702	CDL	C14-C15-C16-C17
44	J	201	PC1	C27-C28-C29-C2A
49	N	401	CDL	C78-C79-C80-C81
49	i	201	CDL	C51-C52-C53-C54
53	T	201	EHZ	C3-C4-C5-C6
44	B	202	PC1	C3C-C3D-C3E-C3F
45	M	501	3PE	C37-C38-C39-C3A
49	d	202	CDL	CA7-C31-C32-C33
49	M	502	CDL	C31-CA7-OA8-CA6
45	D	501	3PE	C3C-C3D-C3E-C3F
49	N	401	CDL	C53-C54-C55-C56
50	L	705	LMT	C5-C6-C7-C8
49	i	201	CDL	CA5-C11-C12-C13
49	M	502	CDL	CA3-CA4-CA6-OA8
49	d	201	CDL	C57-C58-C59-C60
45	K	201	3PE	C22-C21-O21-C2
49	d	202	CDL	C11-CA5-OA6-CA4
45	D	501	3PE	C3A-C3B-C3C-C3D
45	L	701	3PE	C27-C28-C29-C2A
49	i	201	CDL	C72-C73-C74-C75
45	L	703	3PE	C24-C25-C26-C27
49	i	201	CDL	O1-C1-CB2-OB2
49	d	202	CDL	OA7-CA5-OA6-CA4
44	J	201	PC1	O21-C2-C3-O31
45	L	701	3PE	C32-C33-C34-C35
45	D	501	3PE	C32-C33-C34-C35
49	M	502	CDL	C55-C56-C57-C58
45	K	201	3PE	C32-C31-O31-C3
45	H	402	3PE	C11-O13-P-O11
49	M	502	CDL	CB3-OB5-PB2-OB2
49	d	202	CDL	CA2-OA2-PA1-OA5
49	d	202	CDL	CA3-OA5-PA1-OA2
49	i	201	CDL	CB3-OB5-PB2-OB2
45	M	501	3PE	C3A-C3B-C3C-C3D
45	L	701	3PE	O11-C1-C2-C3
45	M	501	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
49	d	201	CDL	C55-C56-C57-C58
45	K	201	3PE	C2-C3-O31-C31
44	J	201	PC1	C1-C2-C3-O31
45	K	201	3PE	C1-C2-C3-O31
45	L	703	3PE	C33-C34-C35-C36
49	N	401	CDL	CB3-CB4-CB6-OB8
49	d	202	CDL	CB3-CB4-CB6-OB8
44	J	201	PC1	C31-C32-C33-C34
45	M	501	3PE	C35-C36-C37-C38
49	N	401	CDL	CA5-C11-C12-C13
49	M	502	CDL	OA9-CA7-OA8-CA6
53	U	201	EHZ	C5-C6-C7-O1
49	d	201	CDL	CB3-CB4-OB6-CB5
47	F	502	FMN	C5'-O5'-P-O1P
49	M	502	CDL	C31-C32-C33-C34
49	N	401	CDL	C76-C77-C78-C79
45	L	701	3PE	C22-C23-C24-C25
49	N	401	CDL	OA6-CA4-CA6-OA8
45	L	703	3PE	C22-C23-C24-C25
45	K	201	3PE	O22-C21-O21-C2
44	B	202	PC1	C35-C36-C37-C38
50	L	705	LMT	C2B-C1B-O1B-C4'
53	T	201	EHZ	C5-C6-C7-C8
45	H	402	3PE	C32-C33-C34-C35
50	L	704	LMT	C4B-C5B-C6B-O6B
44	B	202	PC1	O11-C1-C2-C3
49	L	702	CDL	OB5-CB3-CB4-CB6
49	d	202	CDL	OA5-CA3-CA4-CA6
50	L	705	LMT	O5B-C1B-O1B-C4'
49	L	702	CDL	C73-C74-C75-C76
45	K	201	3PE	O32-C31-O31-C3
44	B	202	PC1	C3F-C3G-C3H-C3I
49	d	201	CDL	C1-CA2-OA2-PA1
49	M	502	CDL	C51-C52-C53-C54
44	J	201	PC1	C37-C38-C39-C3A
49	M	502	CDL	C75-C76-C77-C78
44	J	201	PC1	C33-C34-C35-C36
49	M	502	CDL	CB3-CB4-CB6-OB8
49	N	401	CDL	CA3-CA4-CA6-OA8
49	i	201	CDL	CB3-CB4-CB6-OB8
44	B	202	PC1	C1-O11-P-O13
49	d	201	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
50	L	704	LMT	C4'-C5'-C6'-O6'
45	L	701	3PE	O11-C1-C2-O21
44	J	201	PC1	C34-C35-C36-C37
49	L	702	CDL	OB6-CB4-CB6-OB8
49	M	502	CDL	OB6-CB4-CB6-OB8
45	H	402	3PE	C36-C37-C38-C39
49	M	502	CDL	CA2-C1-CB2-OB2
49	d	202	CDL	CA2-C1-CB2-OB2
49	M	502	CDL	C52-C51-CB5-OB6
45	D	501	3PE	C2-C1-O11-P
49	N	401	CDL	C1-CB2-OB2-PB2
49	N	401	CDL	C84-C85-C86-C87
53	U	201	EHZ	C21-C1-C2-C3
53	T	201	EHZ	O2-C9-S1-C10
49	L	702	CDL	C55-C56-C57-C58
45	D	501	3PE	O11-C1-C2-C3
49	M	502	CDL	OB5-CB3-CB4-CB6
49	d	201	CDL	C54-C55-C56-C57
45	L	701	3PE	C26-C27-C28-C29
44	J	201	PC1	C22-C23-C24-C25
45	L	701	3PE	C34-C35-C36-C37
49	d	202	CDL	CA6-CA4-OA6-CA5
53	T	201	EHZ	C8-C9-S1-C10
45	D	501	3PE	O11-C1-C2-O21
45	K	201	3PE	O31-C31-C32-C33
52	P	501	NDP	C2D-C1D-N1N-C6N
49	N	401	CDL	CB2-C1-CA2-OA2
53	T	201	EHZ	O1-C7-C8-C9
45	K	201	3PE	O21-C2-C3-O31
49	i	201	CDL	OB6-CB4-CB6-OB8
49	M	502	CDL	C58-C59-C60-C61
49	N	401	CDL	C79-C80-C81-C82
45	H	402	3PE	C38-C39-C3A-C3B
50	L	704	LMT	C4-C5-C6-C7
45	Y	401	3PE	C32-C31-O31-C3
49	d	202	CDL	CB3-OB5-PB2-OB2
49	d	202	CDL	O1-C1-CB2-OB2
49	L	702	CDL	C1-CA2-OA2-PA1
44	J	201	PC1	C1-O11-P-O12
45	D	501	3PE	C1-O11-P-O12
45	D	501	3PE	C1-O11-P-O14
45	H	402	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
45	L	701	3PE	C1-O11-P-O14
45	L	703	3PE	C1-O11-P-O12
45	M	501	3PE	C1-O11-P-O12
45	M	501	3PE	C1-O11-P-O14
49	L	702	CDL	CB2-OB2-PB2-OB3
49	M	502	CDL	CA3-OA5-PA1-OA4
49	M	502	CDL	CB2-OB2-PB2-OB4
49	M	502	CDL	CB3-OB5-PB2-OB4
49	N	401	CDL	CA2-OA2-PA1-OA3
49	N	401	CDL	CA2-OA2-PA1-OA4
49	d	202	CDL	CA2-OA2-PA1-OA4
49	i	201	CDL	CA3-OA5-PA1-OA4
52	P	501	NDP	C5B-O5B-PA-O2A
49	d	202	CDL	C76-C77-C78-C79
44	J	201	PC1	C24-C25-C26-C27
45	D	501	3PE	C12-C11-O13-P
45	H	402	3PE	C12-C11-O13-P
45	L	703	3PE	C12-C11-O13-P
48	H	401	UQ9	C20-C19-C21-C22
45	H	402	3PE	O11-C1-C2-O21
45	L	701	3PE	C2F-C2G-C2H-C2I
45	L	703	3PE	O21-C21-C22-C23
44	J	201	PC1	O13-C11-C12-N
45	Y	401	3PE	O32-C31-O31-C3
45	L	701	3PE	O21-C21-C22-C23
49	d	201	CDL	C52-C53-C54-C55
45	M	501	3PE	C22-C23-C24-C25
52	P	501	NDP	O4D-C1D-N1N-C6N
45	D	501	3PE	C3F-C3G-C3H-C3I
45	L	703	3PE	C1-C2-O21-C21
49	L	702	CDL	CA6-CA4-OA6-CA5
49	M	502	CDL	CB6-CB4-OB6-CB5
50	L	705	LMT	O1'-C1-C2-C3
45	L	701	3PE	C2-C1-O11-P
49	M	502	CDL	C1-CB2-OB2-PB2
45	M	501	3PE	C3D-C3E-C3F-C3G
49	N	401	CDL	OB6-CB4-CB6-OB8
49	d	202	CDL	OB6-CB4-CB6-OB8
45	D	501	3PE	C11-O13-P-O11
45	L	701	3PE	C11-O13-P-O11
45	Y	401	3PE	C1-O11-P-O13
45	Y	401	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
49	d	201	CDL	CA3-OA5-PA1-OA2
49	d	202	CDL	C51-C52-C53-C54
50	L	705	LMT	C4B-C5B-C6B-O6B
50	L	705	LMT	C4'-C5'-C6'-O6'
45	H	402	3PE	C33-C34-C35-C36
49	d	202	CDL	C80-C81-C82-C83
49	d	202	CDL	CB7-C71-C72-C73
45	Y	401	3PE	C2-C1-O11-P
48	H	401	UQ9	C11-C12-C13-C14
49	N	401	CDL	C81-C82-C83-C84
49	L	702	CDL	C56-C57-C58-C59
49	L	702	CDL	C71-C72-C73-C74
49	i	201	CDL	C17-C18-C19-C20
50	L	704	LMT	C5'-C4'-O1B-C1B
50	L	704	LMT	C3-C4-C5-C6
53	U	201	EHZ	C19-C17-C20-O6
45	L	703	3PE	C3-C2-O21-C21
49	d	201	CDL	C51-C52-C53-C54
45	L	701	3PE	C1-O11-P-O13
52	P	501	NDP	C2D-C1D-N1N-C2N
49	i	201	CDL	C73-C74-C75-C76
49	d	202	CDL	C32-C33-C34-C35
48	H	401	UQ9	C15-C14-C16-C17
49	L	702	CDL	CA7-C31-C32-C33
49	M	502	CDL	CA4-CA6-OA8-CA7
45	L	701	3PE	C28-C29-C2A-C2B
49	M	502	CDL	C56-C57-C58-C59
47	F	502	FMN	O2'-C2'-C3'-C4'
51	O	401	GTP	PB-O3A-PA-O1A
47	F	502	FMN	O2'-C2'-C3'-O3'
45	M	501	3PE	C32-C33-C34-C35
49	L	702	CDL	CB3-CB4-CB6-OB8
48	H	401	UQ9	C18-C19-C21-C22
49	d	202	CDL	OA5-CA3-CA4-OA6
44	J	201	PC1	C35-C36-C37-C38
53	T	201	EHZ	C21-C22-C23-C24
45	H	402	3PE	O11-C1-C2-C3
49	N	401	CDL	OA5-CA3-CA4-CA6
49	N	401	CDL	OB5-CB3-CB4-CB6
49	N	401	CDL	C12-C11-CA5-OA6
49	L	702	CDL	C54-C55-C56-C57
44	J	201	PC1	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
45	Y	401	3PE	O31-C31-C32-C33
49	i	201	CDL	C12-C11-CA5-OA6
48	H	401	UQ9	C13-C14-C16-C17
45	Y	401	3PE	C35-C36-C37-C38
49	i	201	CDL	C19-C20-C21-C22
49	M	502	CDL	C52-C51-CB5-OB7
45	K	201	3PE	O21-C21-C22-C23
52	P	501	NDP	O4D-C1D-N1N-C2N
45	K	201	3PE	O11-C1-C2-C3
49	i	201	CDL	C32-C31-CA7-OA8
45	L	701	3PE	O21-C2-C3-O31
49	d	201	CDL	C32-C31-CA7-OA8
49	i	201	CDL	C52-C51-CB5-OB6
45	D	501	3PE	O31-C31-C32-C33
45	H	402	3PE	O31-C31-C32-C33
44	B	202	PC1	C32-C33-C34-C35
49	d	202	CDL	C12-C11-CA5-OA6
45	L	701	3PE	C36-C37-C38-C39
51	O	401	GTP	O4'-C4'-C5'-O5'
45	L	703	3PE	C21-C22-C23-C24
45	D	501	3PE	C29-C2A-C2B-C2C
49	N	401	CDL	C12-C11-CA5-OA7
49	i	201	CDL	C12-C11-CA5-OA7
45	K	201	3PE	O22-C21-C22-C23
44	B	202	PC1	C1-C2-C3-O31
45	Y	401	3PE	C24-C25-C26-C27
45	Y	401	3PE	O32-C31-C32-C33
49	d	201	CDL	C52-C51-CB5-OB6
45	L	703	3PE	C2-C1-O11-P
45	H	402	3PE	C1-O11-P-O14
45	L	701	3PE	C11-O13-P-O14
49	d	202	CDL	CB3-OB5-PB2-OB3
49	i	201	CDL	CB3-OB5-PB2-OB4
45	D	501	3PE	O32-C31-C32-C33
49	i	201	CDL	C32-C31-CA7-OA9
45	L	703	3PE	O13-C11-C12-N
49	L	702	CDL	C78-C79-C80-C81
45	Y	401	3PE	O21-C21-C22-C23
53	U	201	EHZ	C1-C2-C3-C4
49	i	201	CDL	C52-C51-CB5-OB7
45	K	201	3PE	C12-C11-O13-P
45	L	703	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
49	L	702	CDL	C12-C13-C14-C15
50	L	705	LMT	C11-C10-C9-C8
48	H	401	UQ9	C16-C17-C18-C19
45	H	402	3PE	O32-C31-C32-C33
49	d	202	CDL	C12-C11-CA5-OA7
45	K	201	3PE	O11-C1-C2-O21
47	F	502	FMN	N10-C1'-C2'-O2'
49	L	702	CDL	C13-C14-C15-C16
49	d	201	CDL	C32-C31-CA7-OA9
44	J	201	PC1	O21-C21-C22-C23
49	d	201	CDL	C52-C51-CB5-OB7
45	L	703	3PE	O31-C31-C32-C33

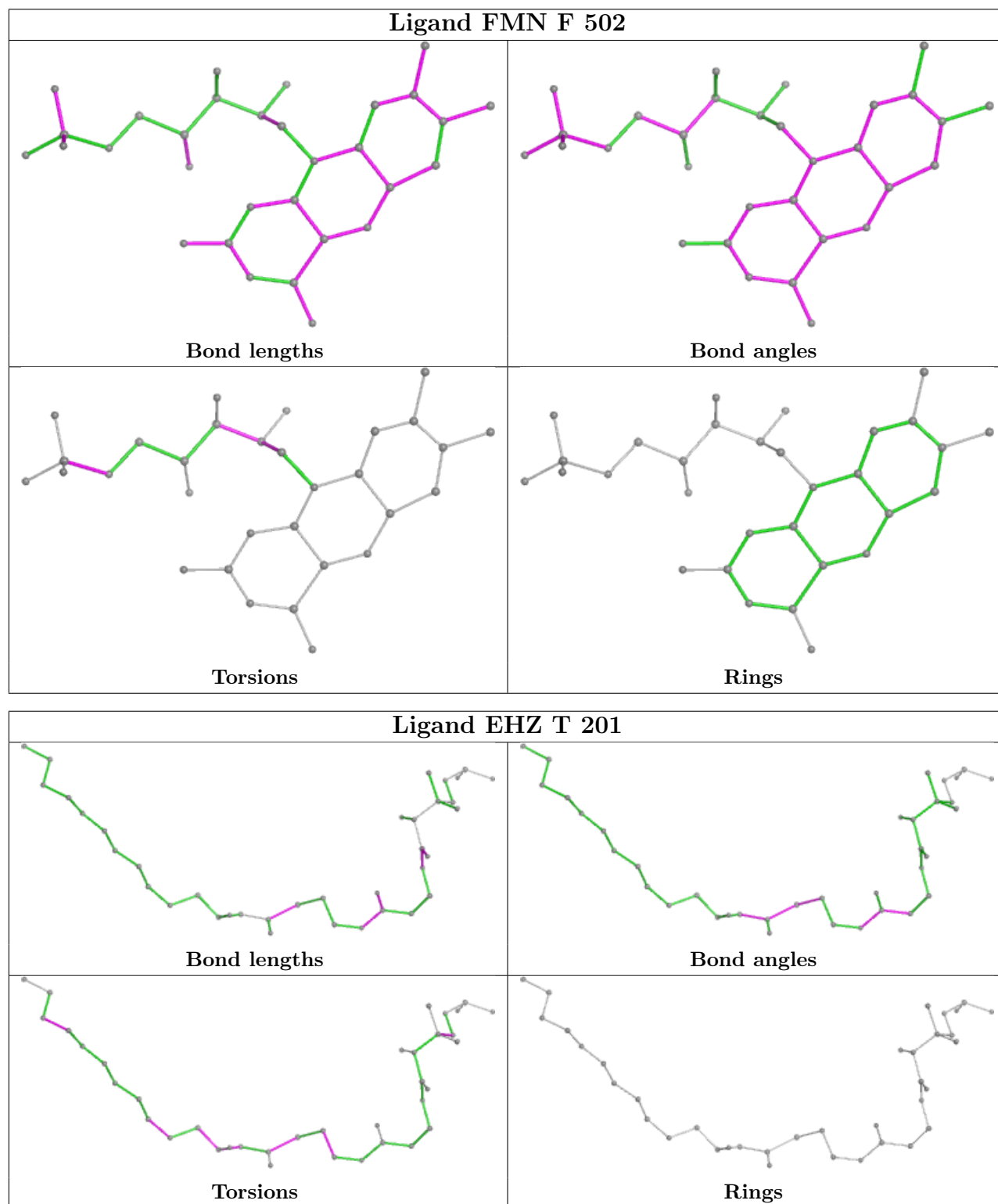
There are no ring outliers.

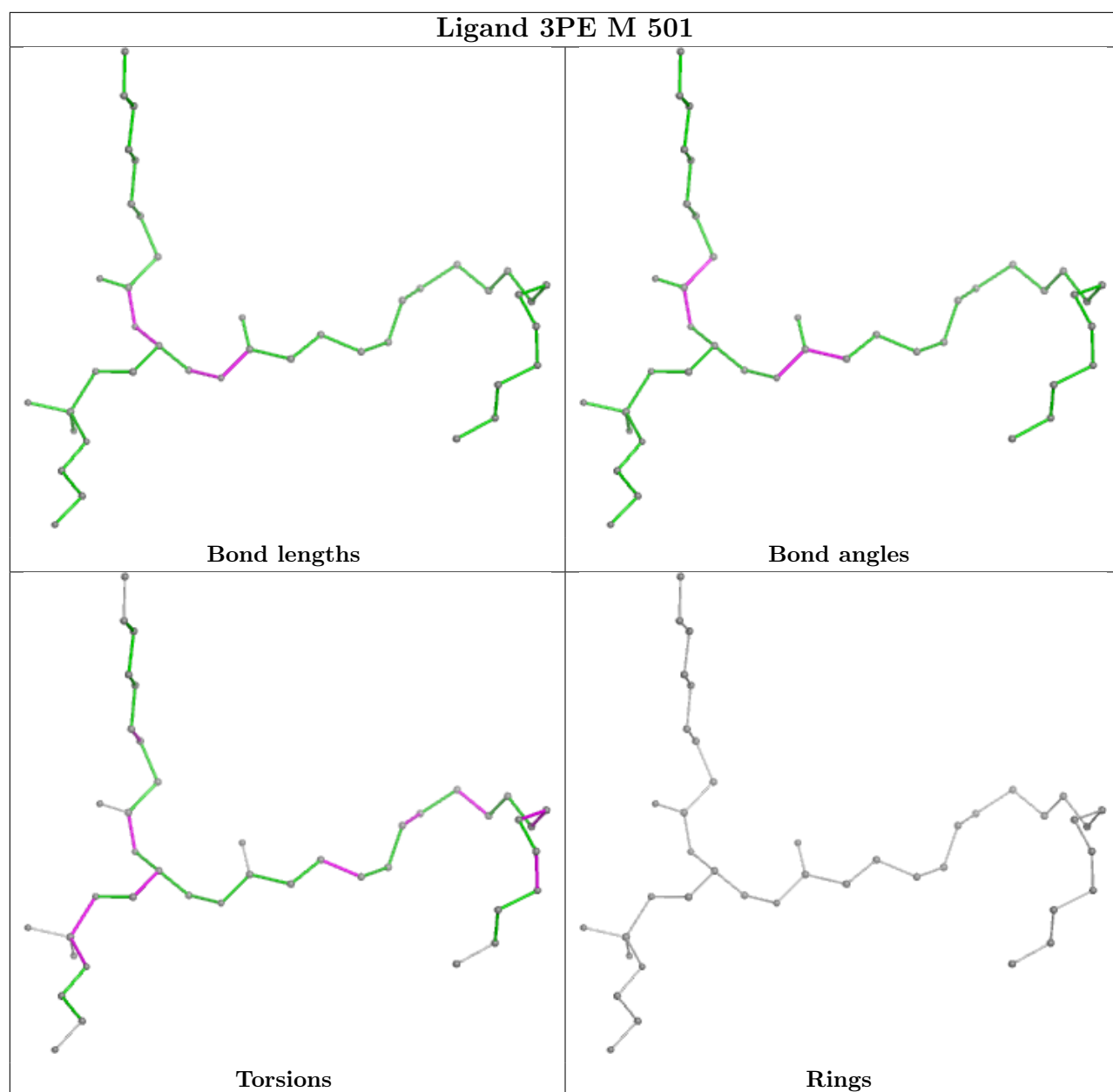
16 monomers are involved in 32 short contacts:

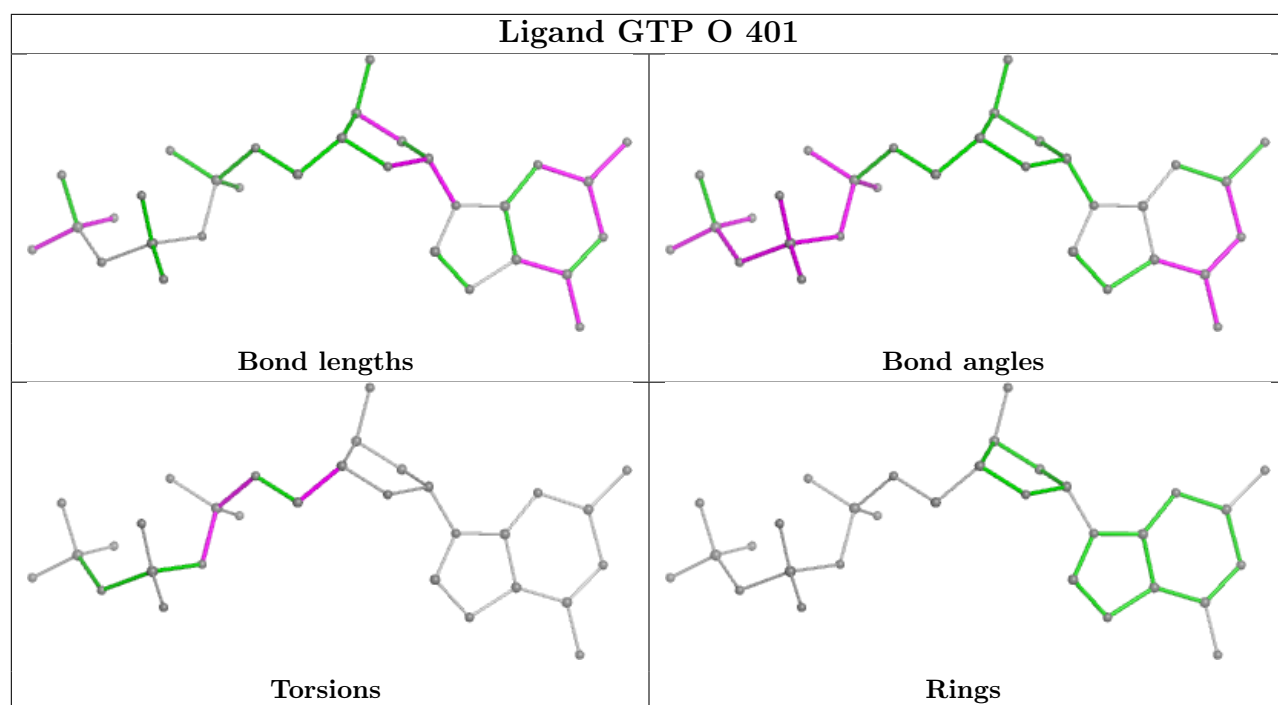
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	I	201	SF4	1	0
46	E	301	FES	2	0
53	T	201	EHZ	1	0
51	O	401	GTP	3	0
52	P	501	NDP	2	0
43	G	802	SF4	2	0
45	H	402	3PE	2	0
50	L	705	LMT	1	0
43	I	202	SF4	3	0
46	G	803	FES	1	0
53	U	201	EHZ	1	0
43	B	201	SF4	3	0
45	Y	401	3PE	1	0
48	H	401	UQ9	6	0
49	M	502	CDL	1	0
44	J	201	PC1	2	0

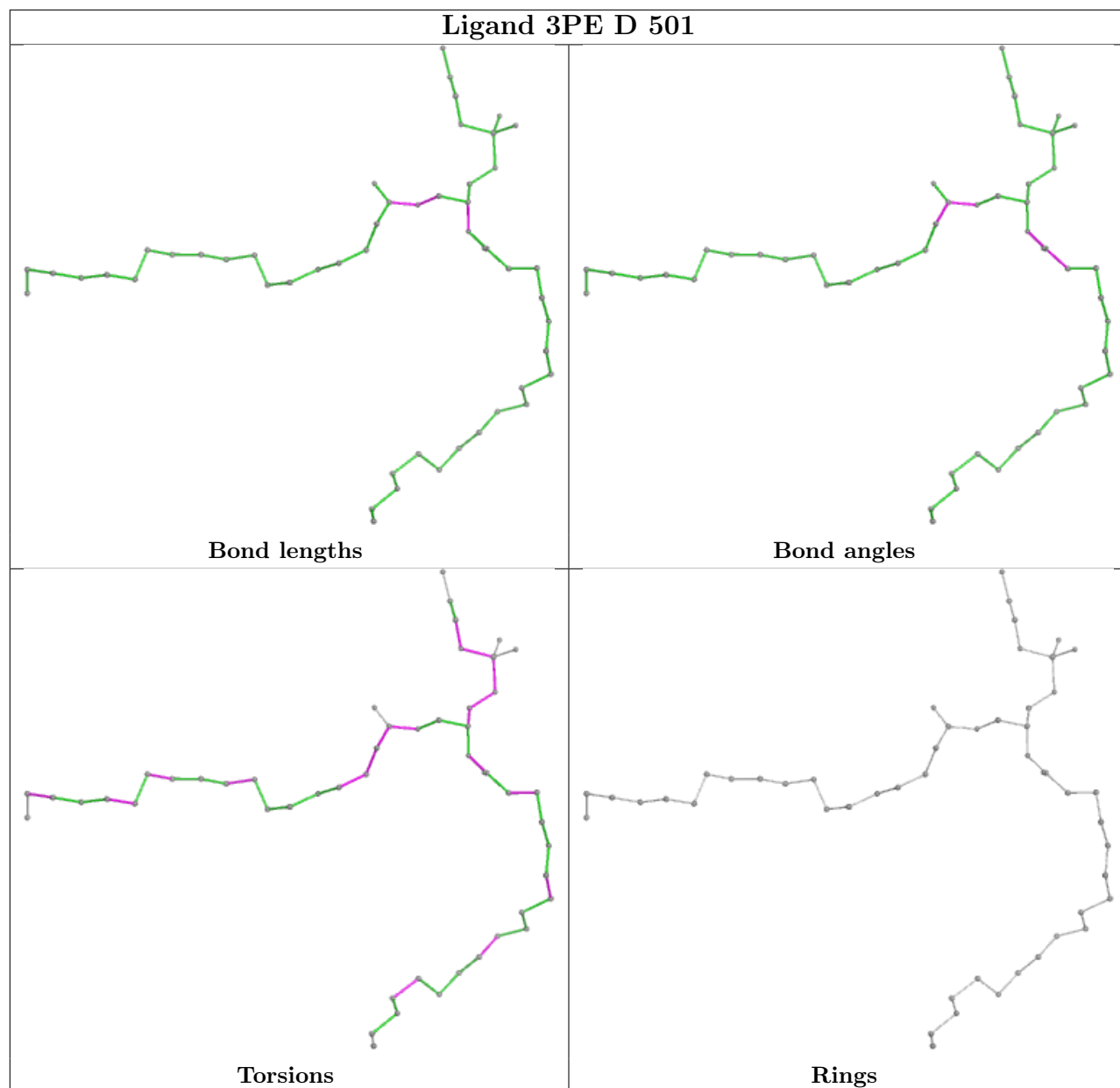
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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

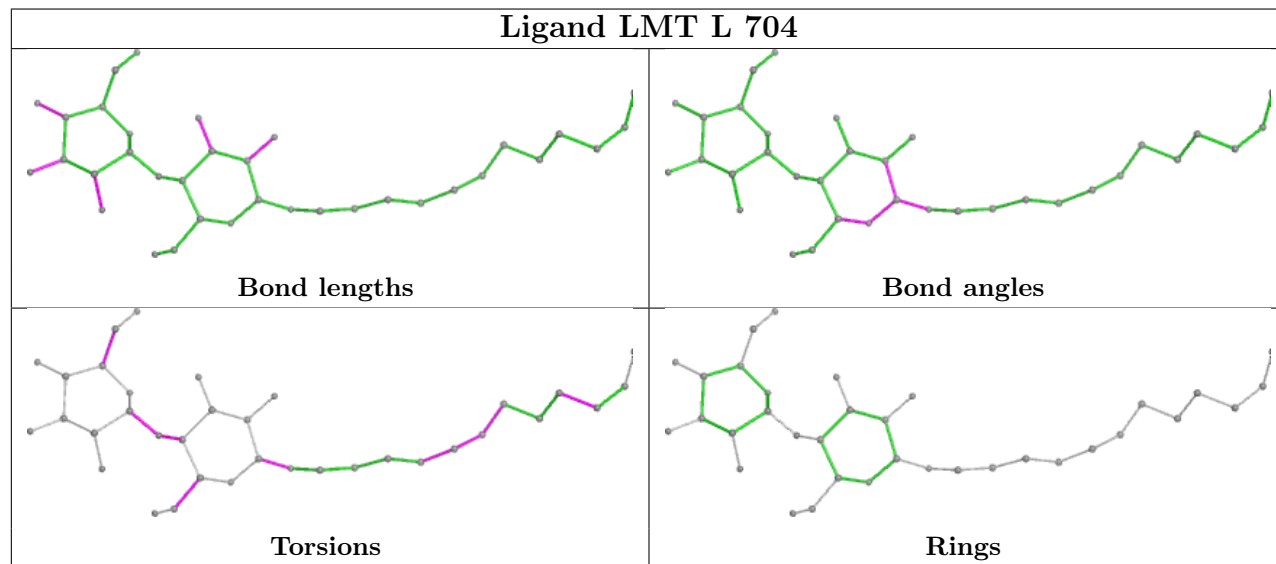
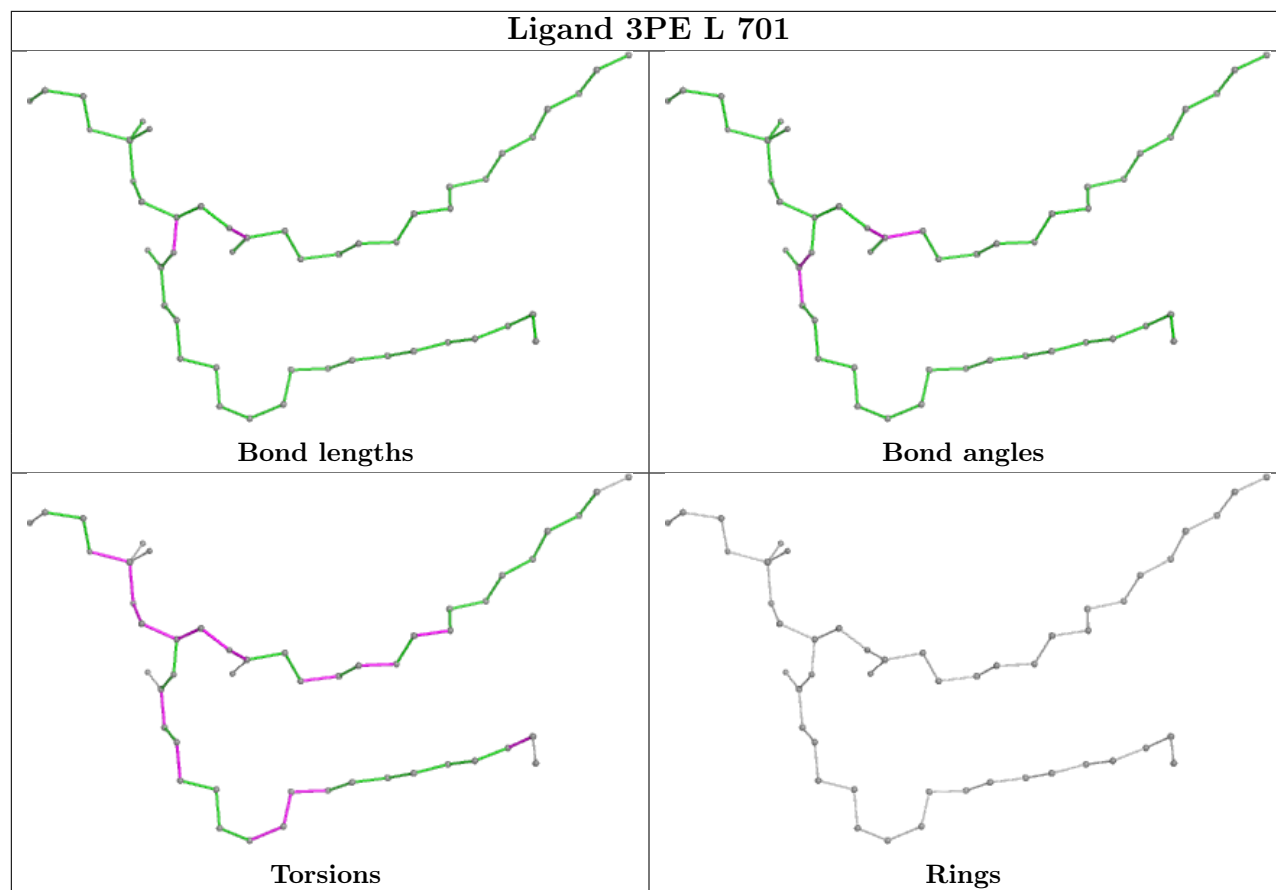
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

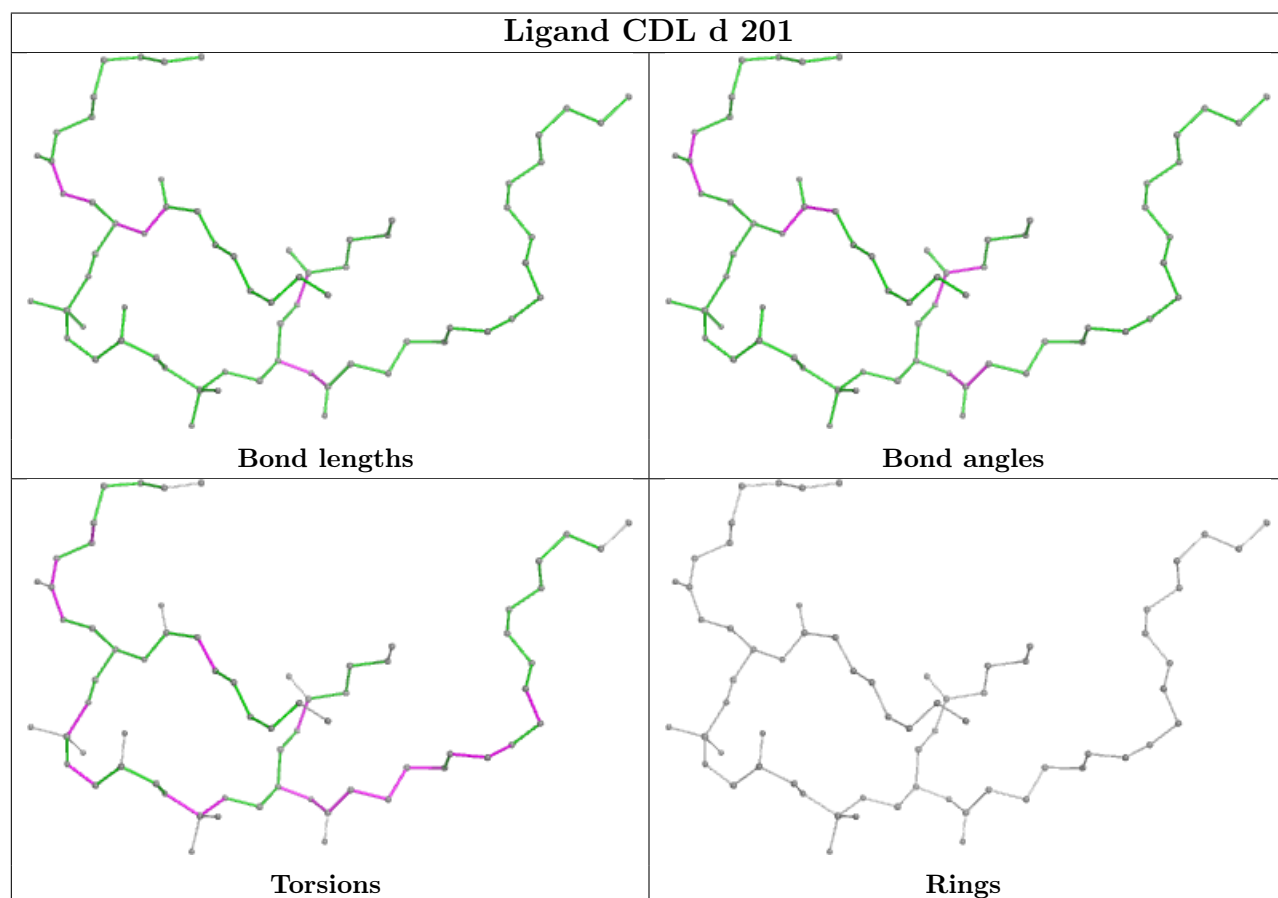
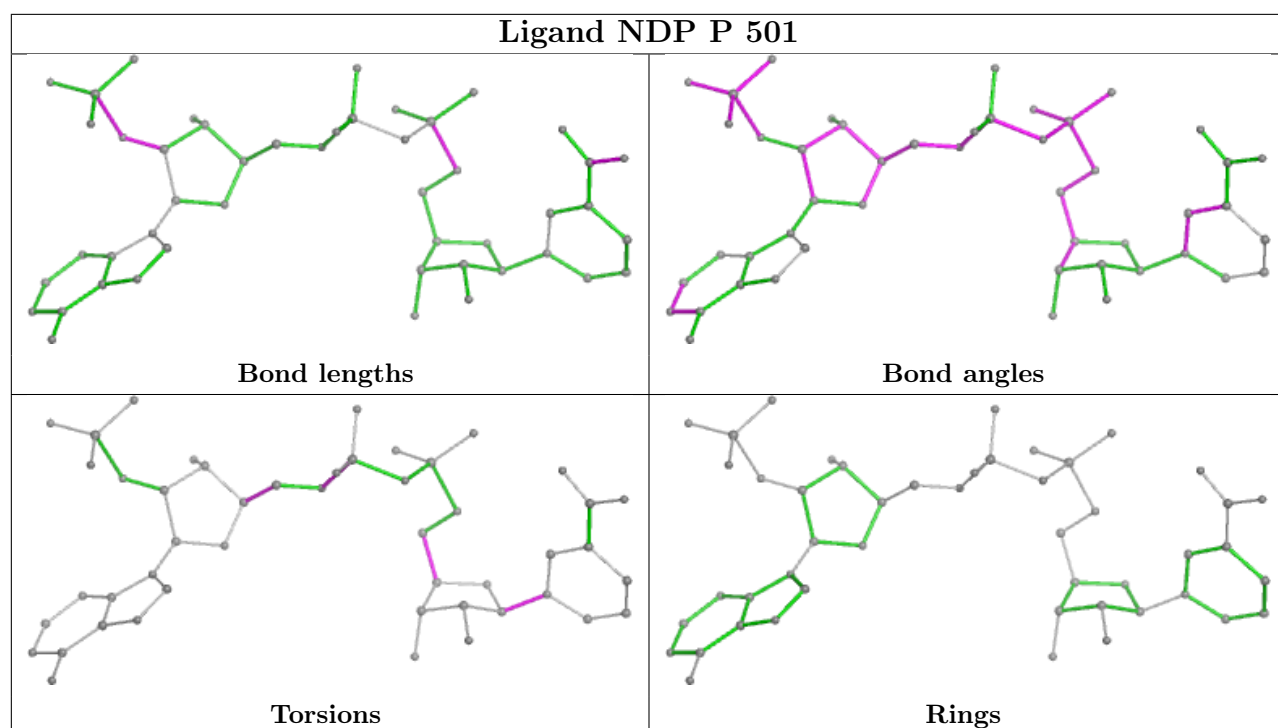


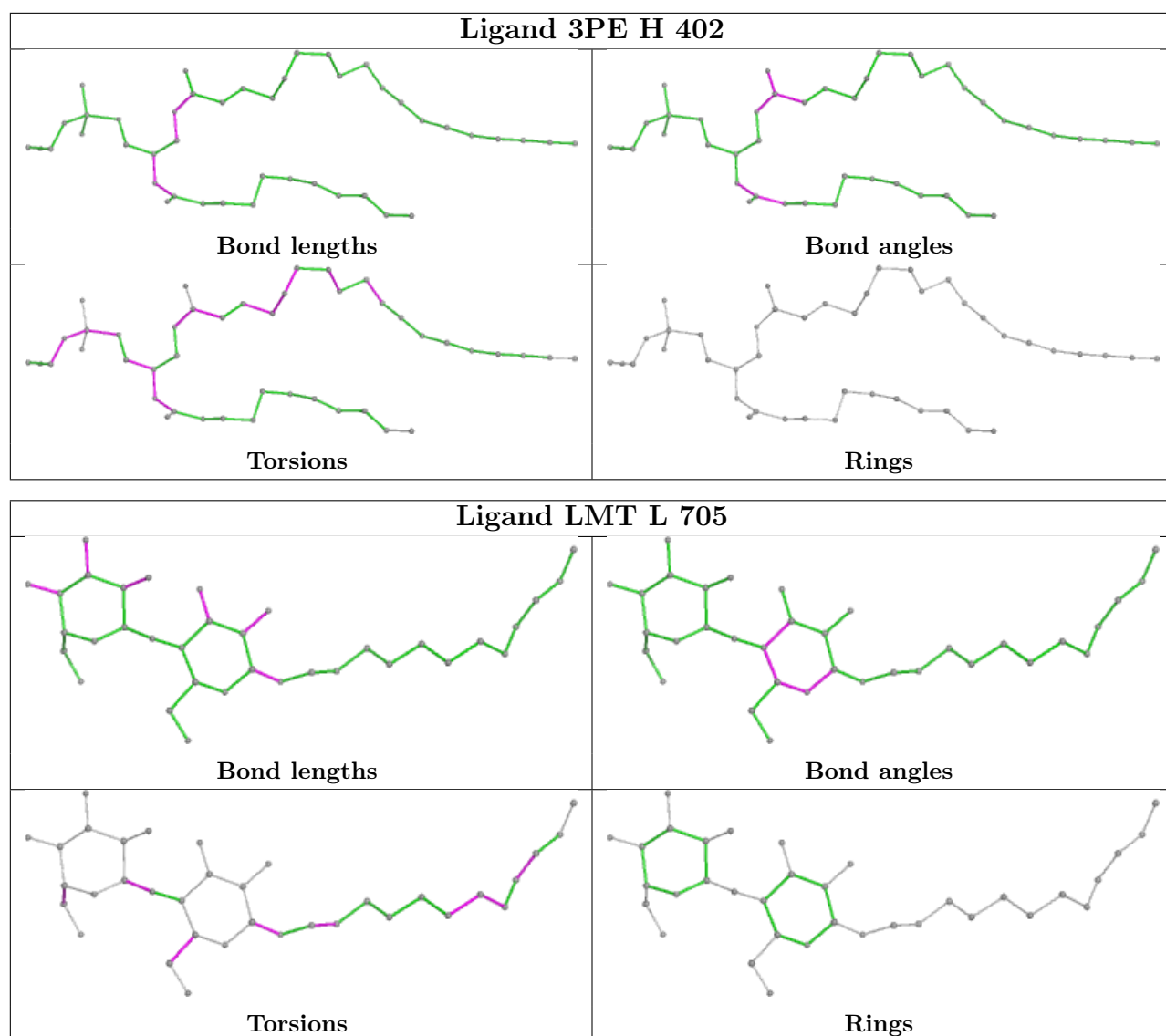


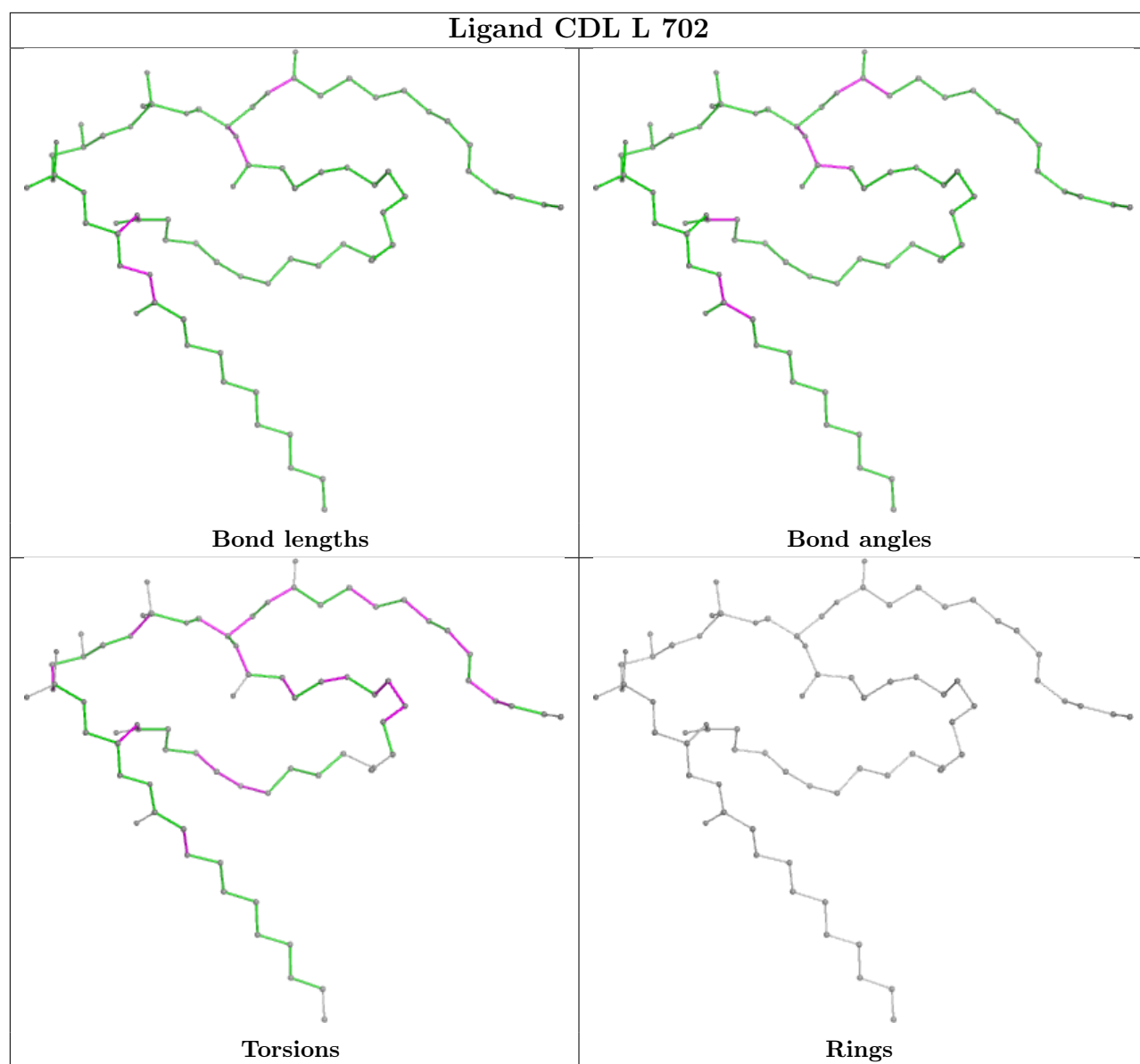


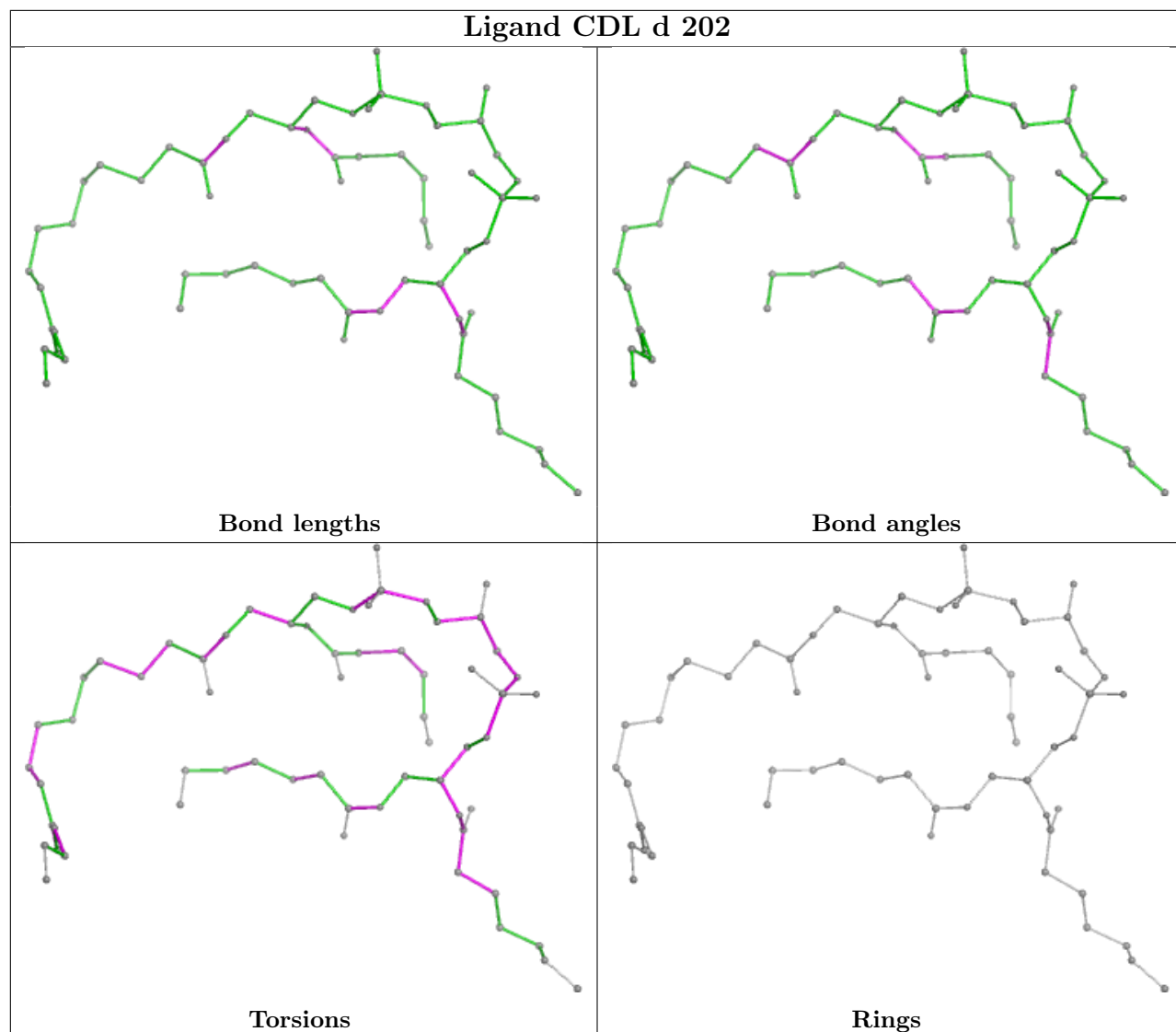
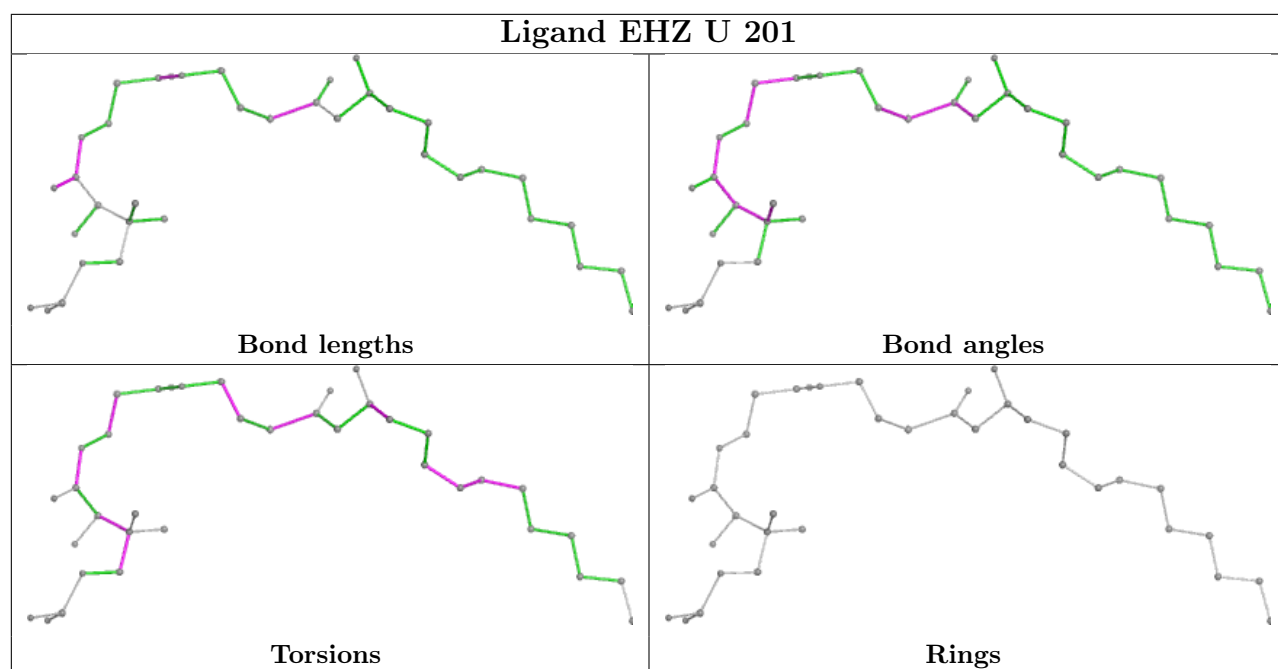


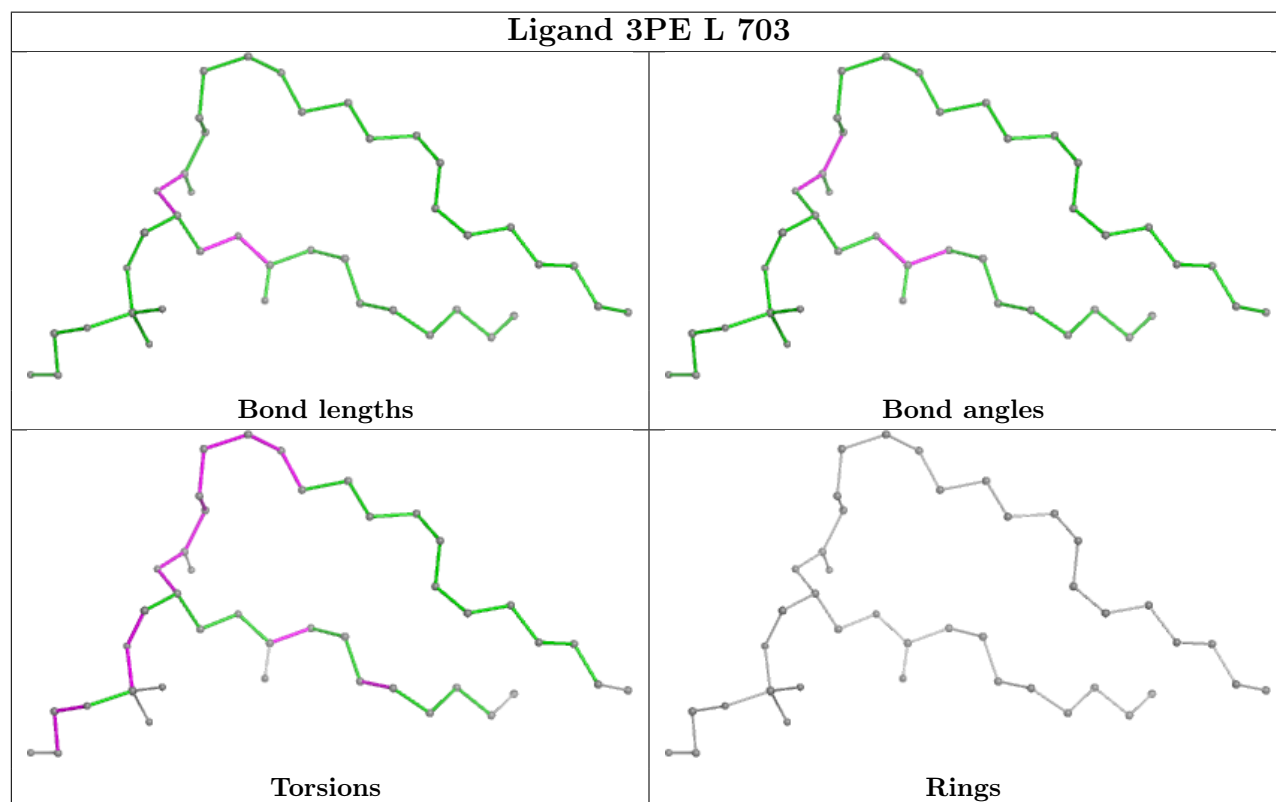
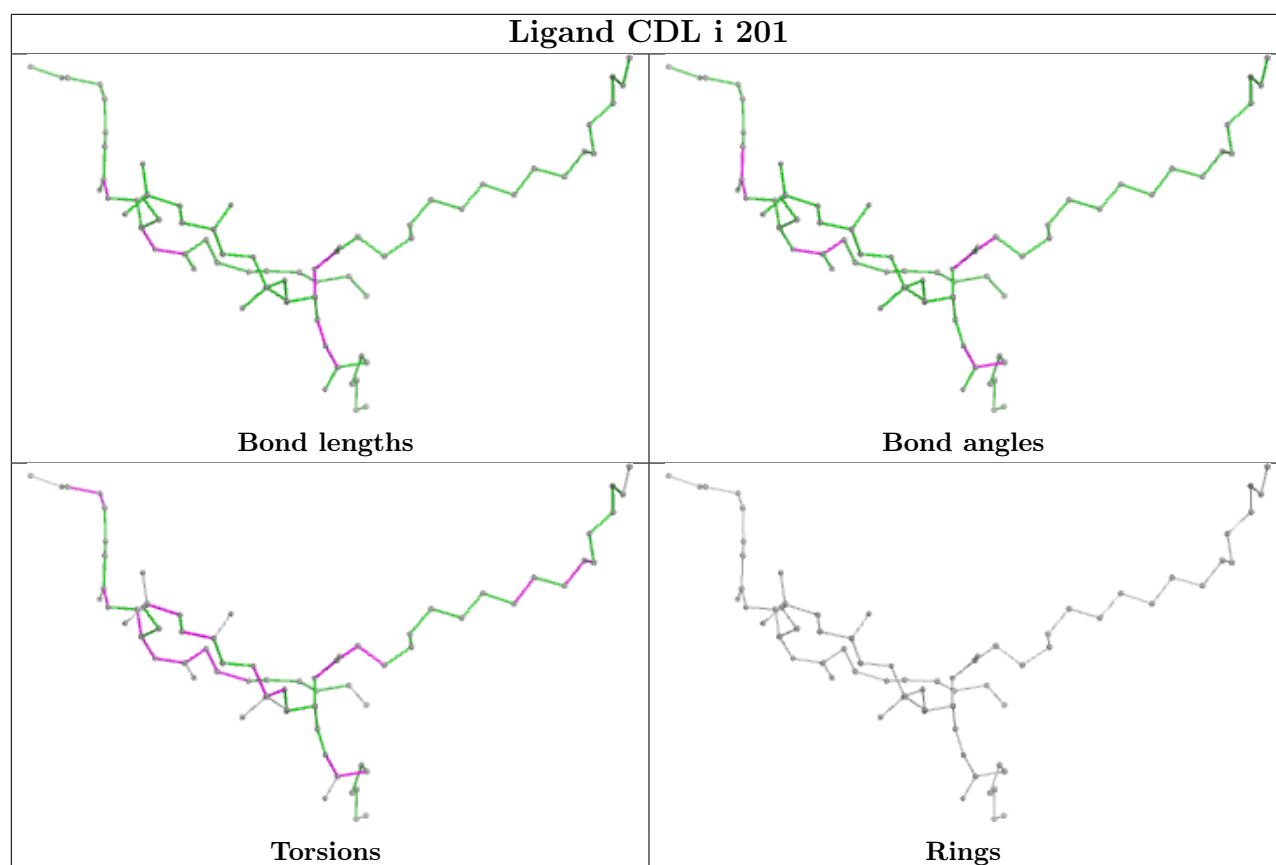


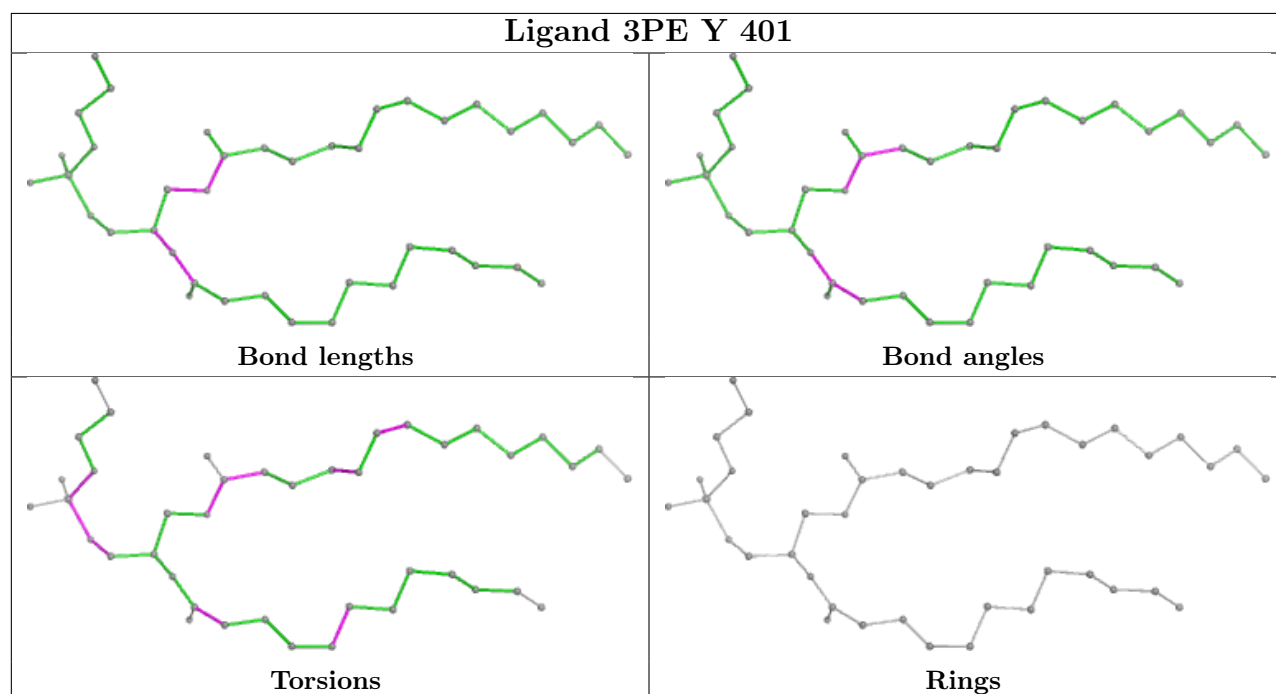
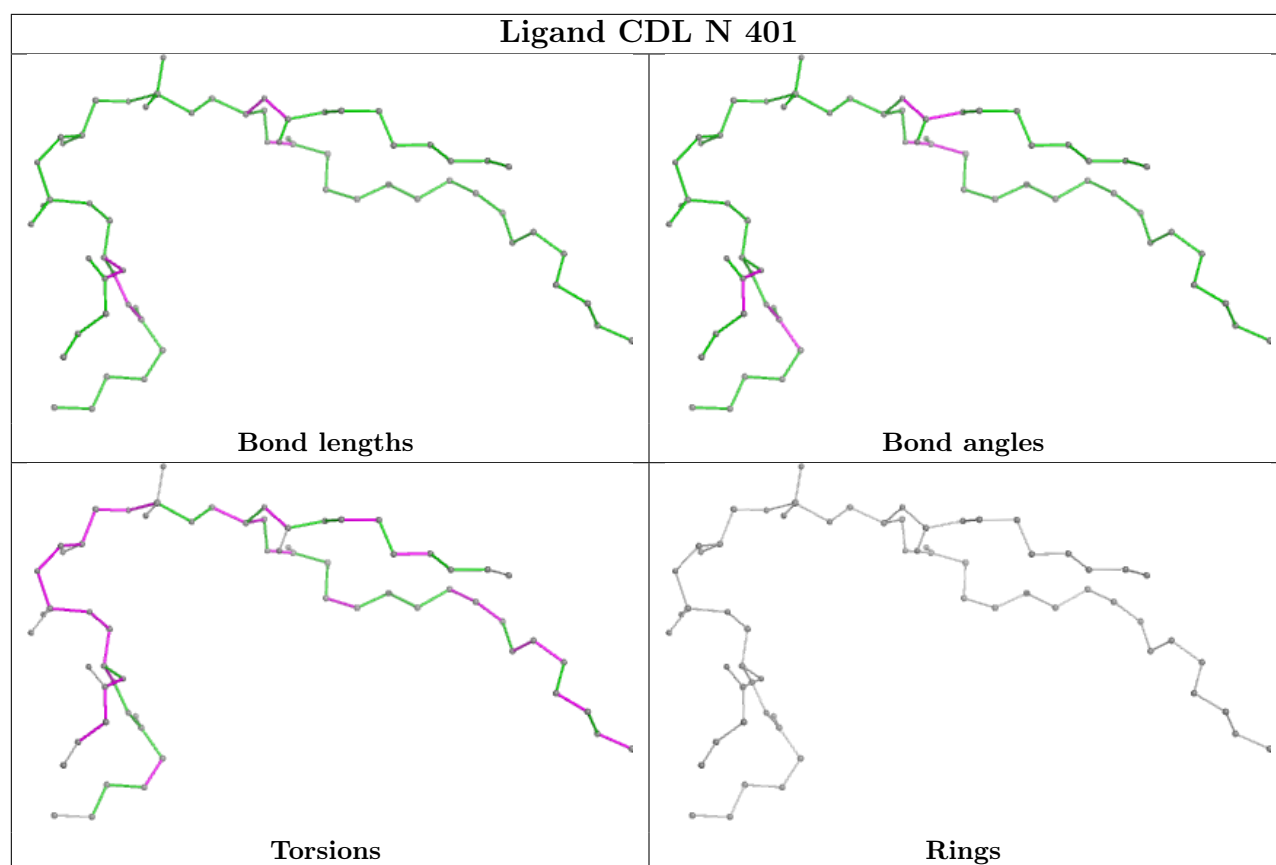


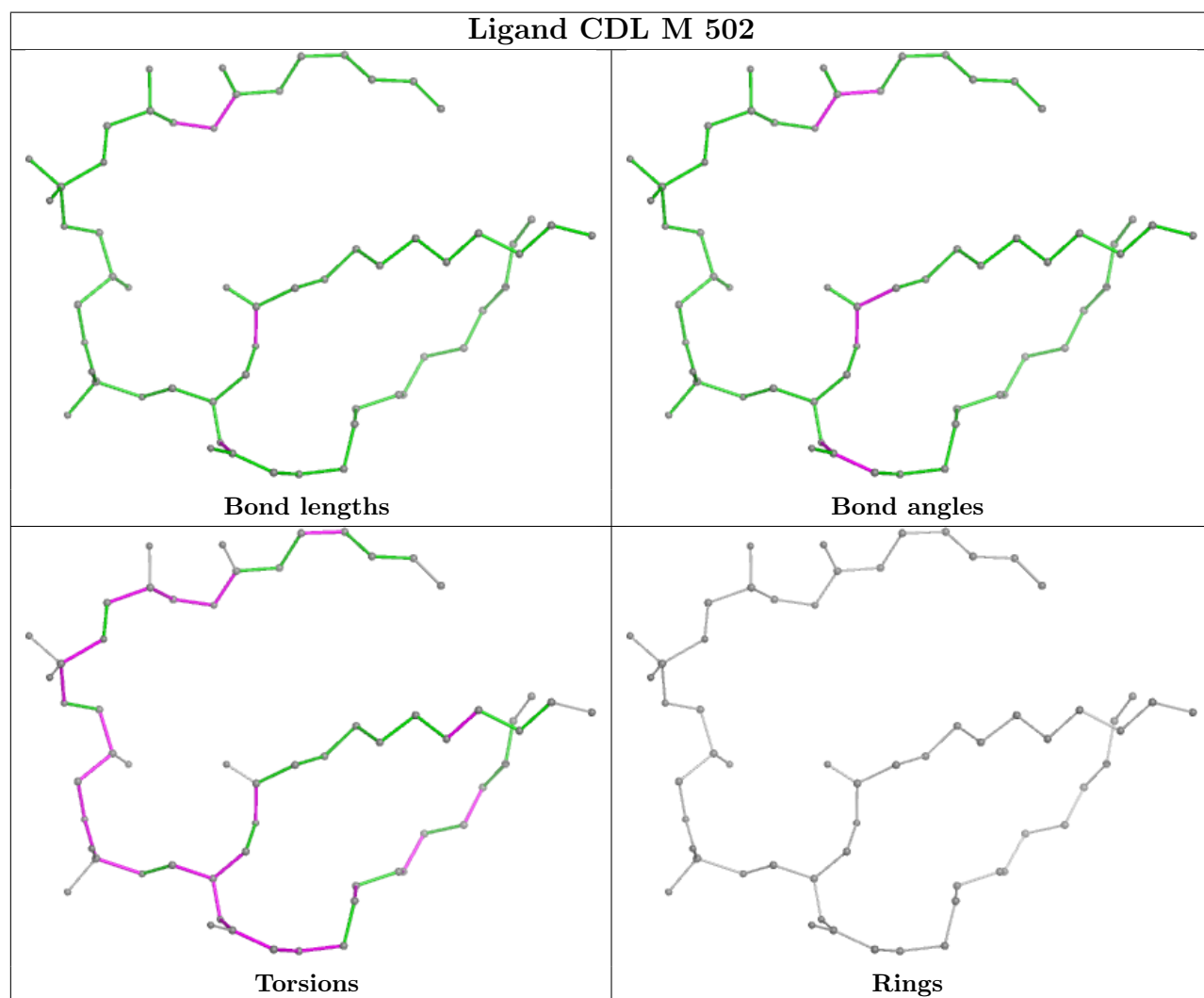
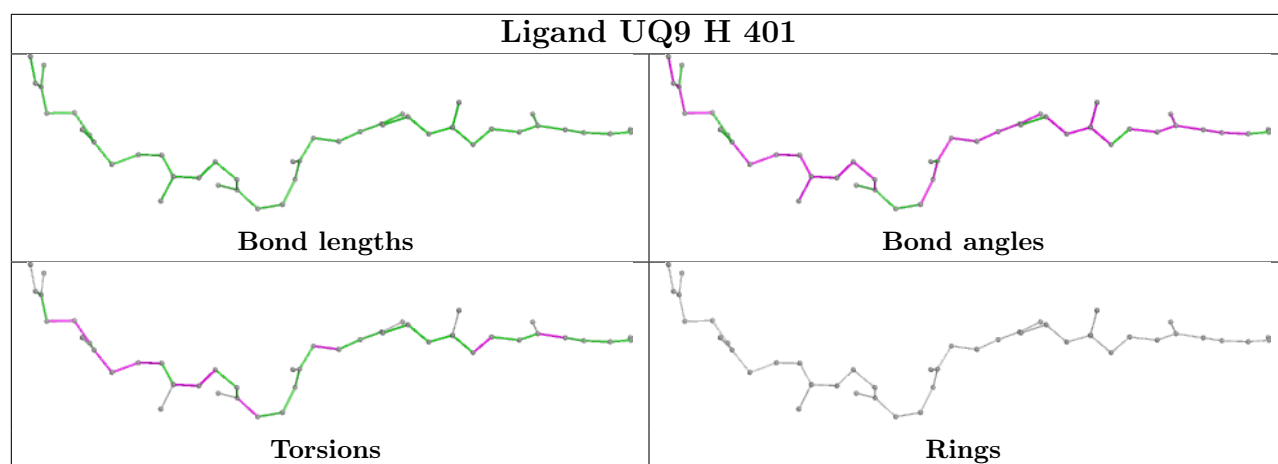


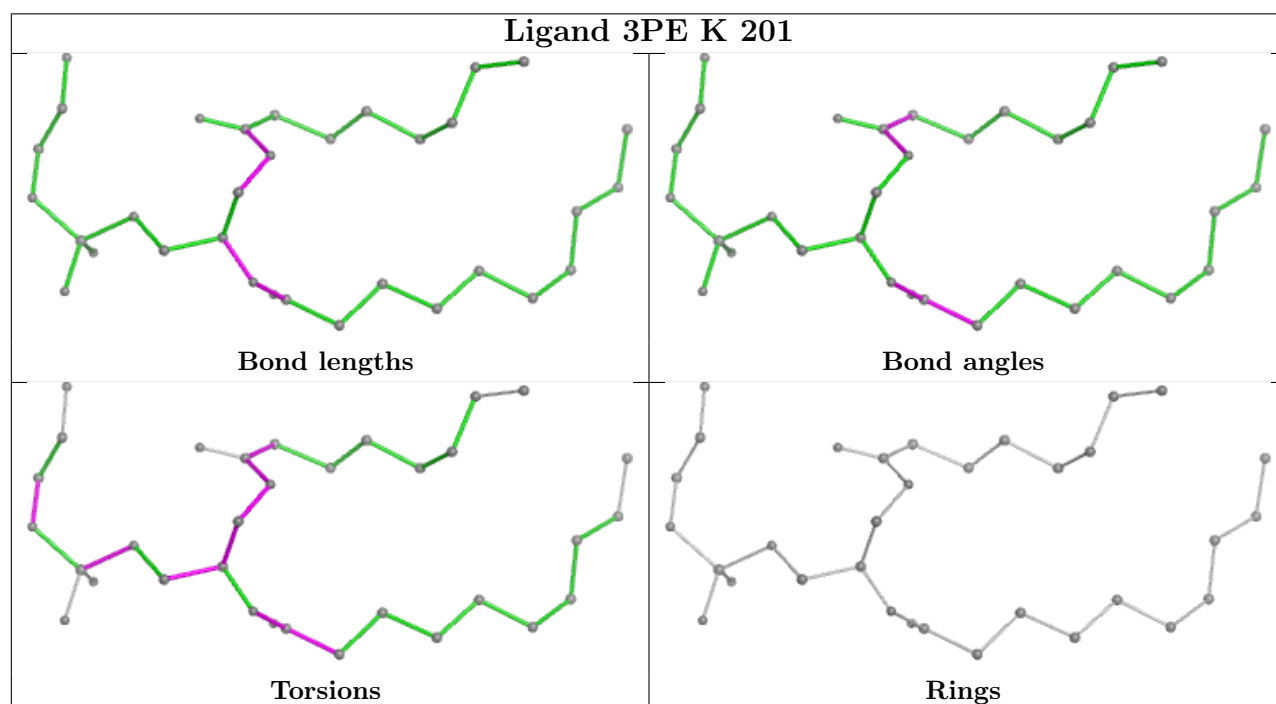
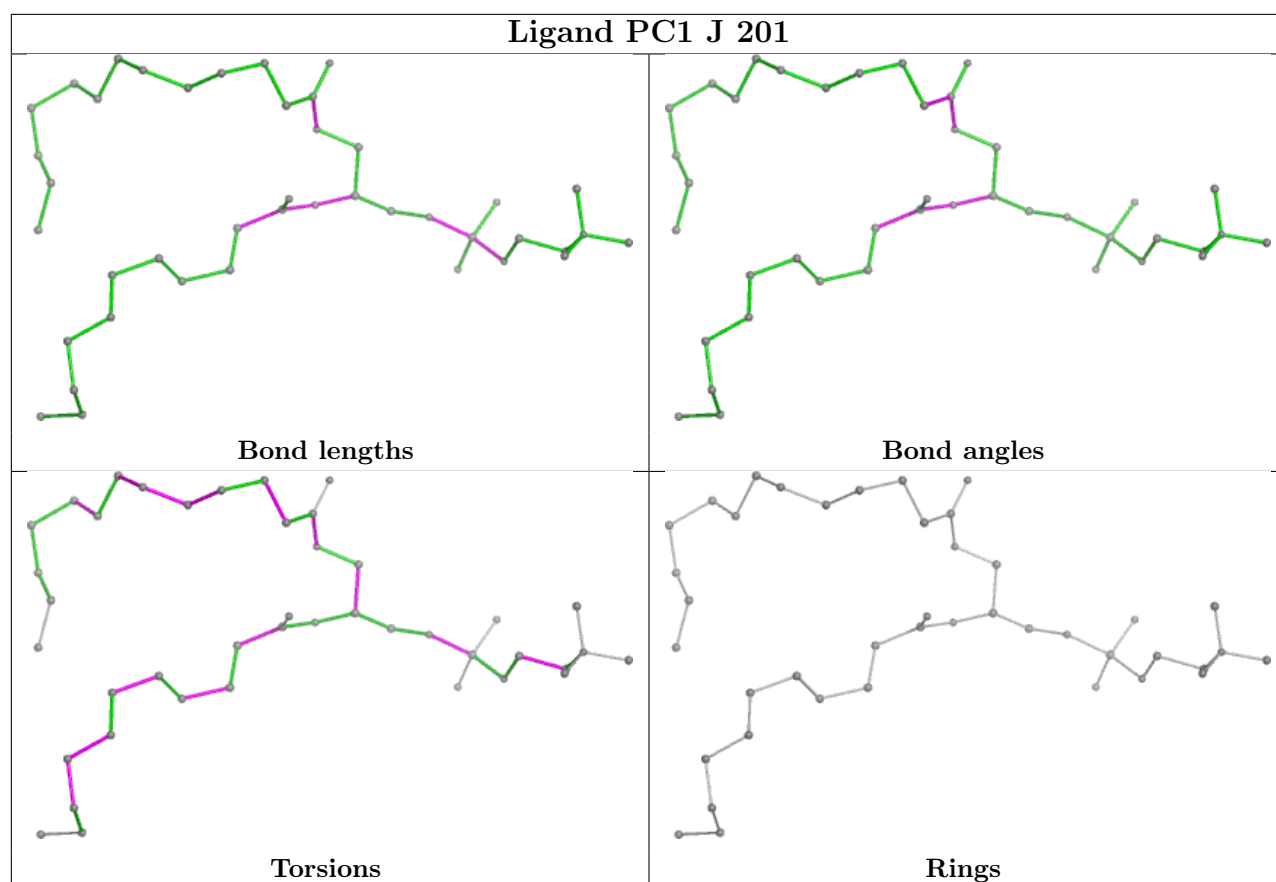


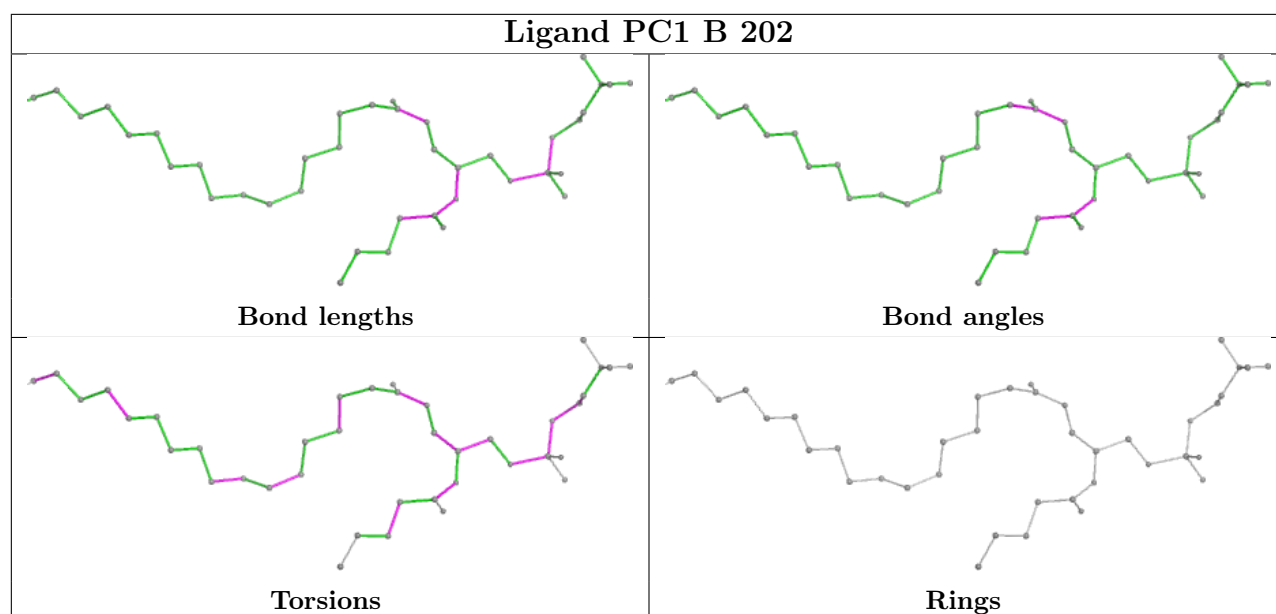












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

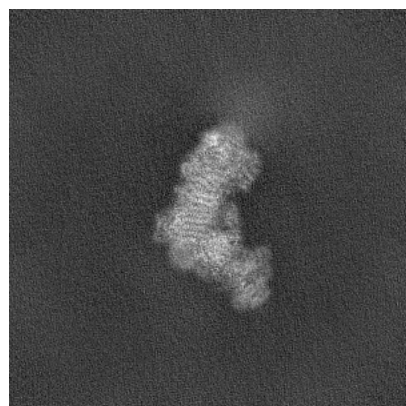
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16518. These allow visual inspection of the internal detail of the map and identification of artifacts.

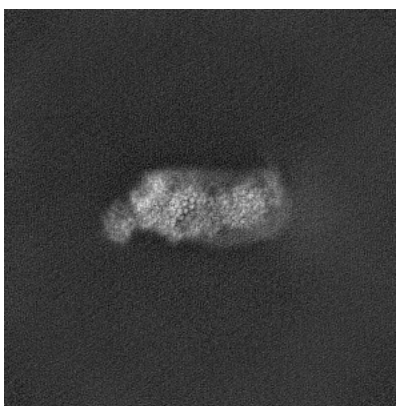
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

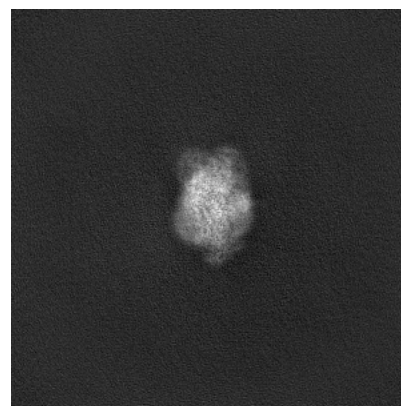
6.1.1 Primary map



X

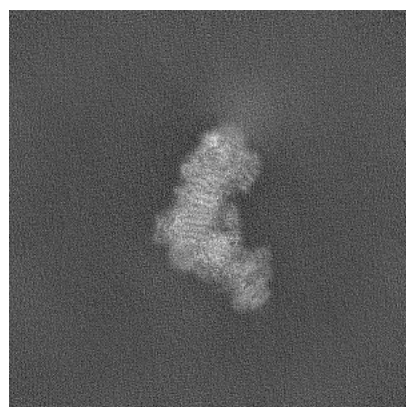


Y

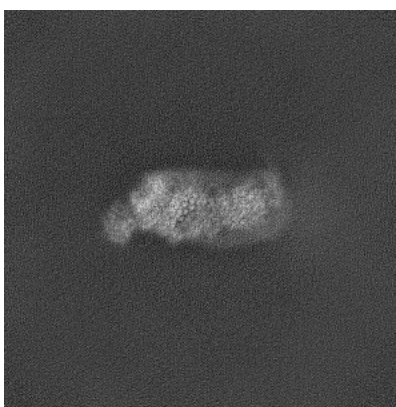


Z

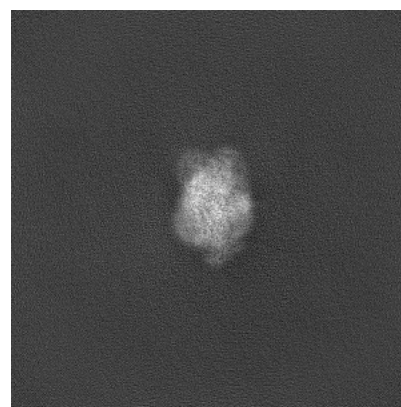
6.1.2 Raw map



X



Y

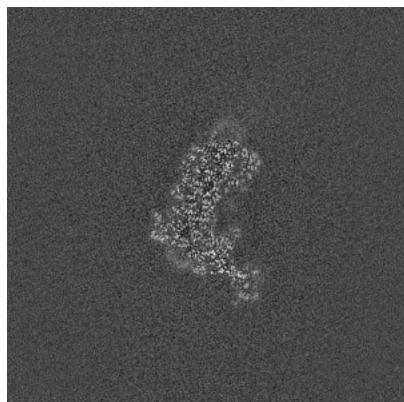


Z

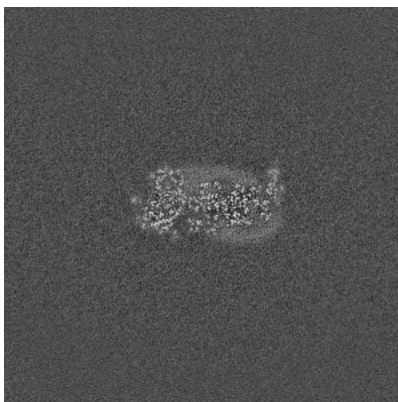
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 225

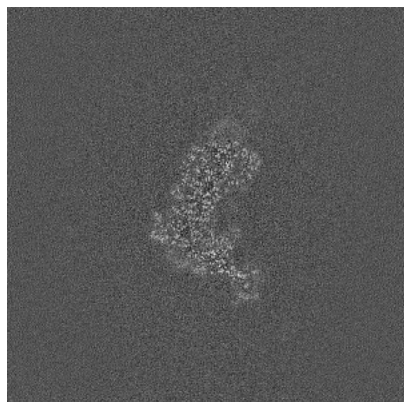


Y Index: 225

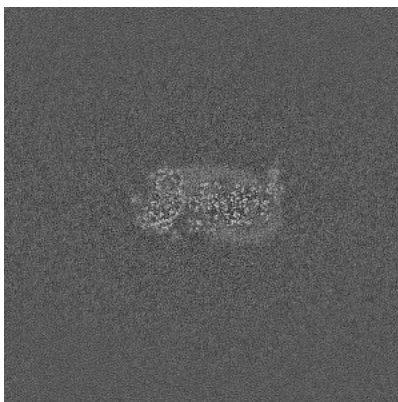


Z Index: 225

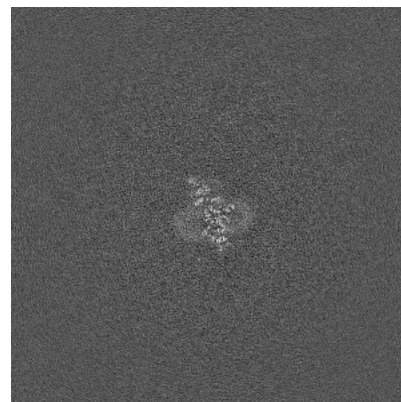
6.2.2 Raw map



X Index: 225



Y Index: 225

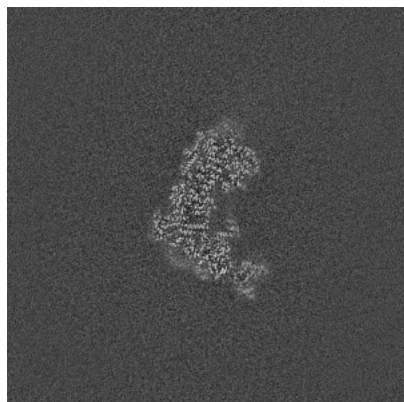


Z Index: 225

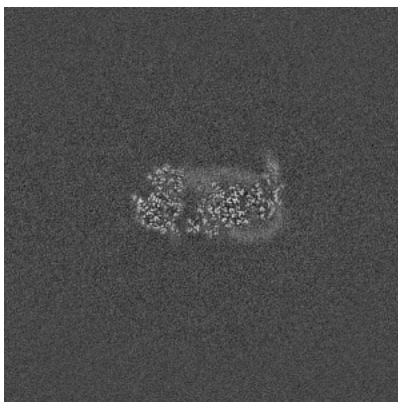
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

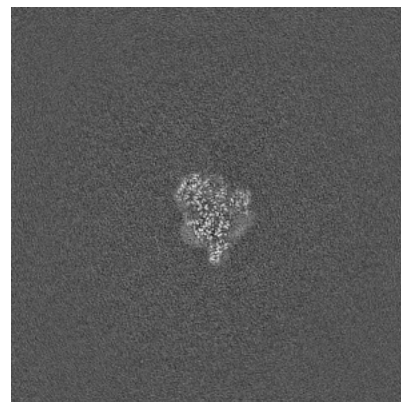
6.3.1 Primary map



X Index: 230

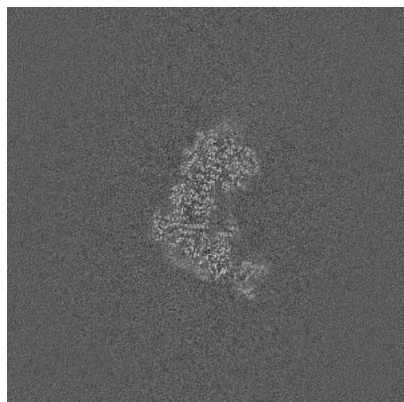


Y Index: 229

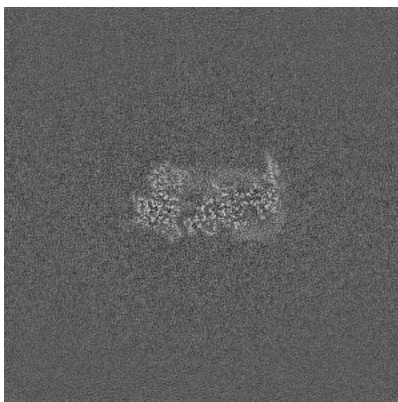


Z Index: 190

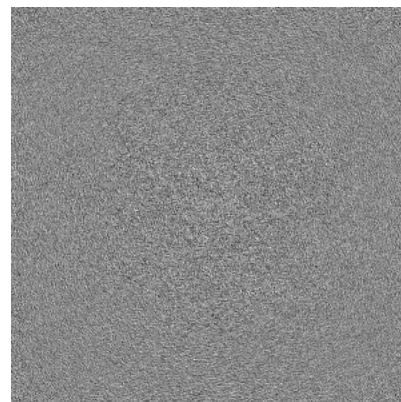
6.3.2 Raw map



X Index: 230



Y Index: 231

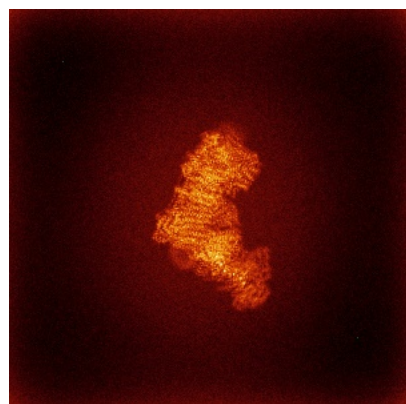


Z Index: 0

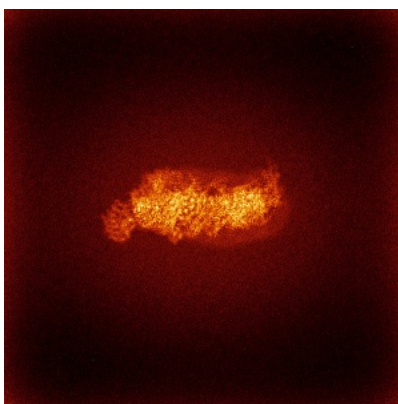
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

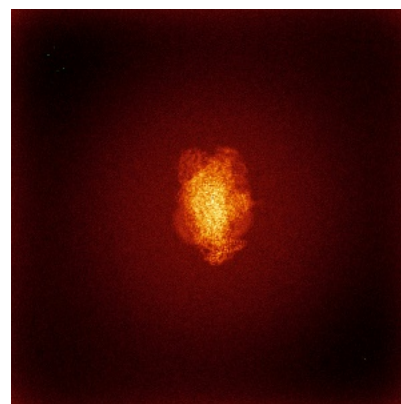
6.4.1 Primary map



X

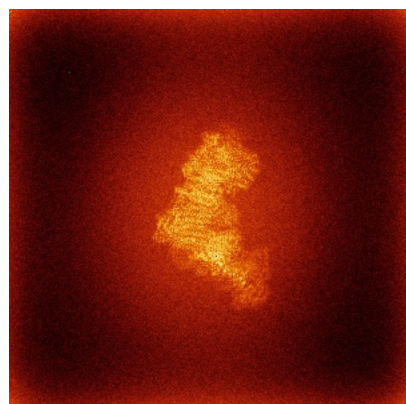


Y

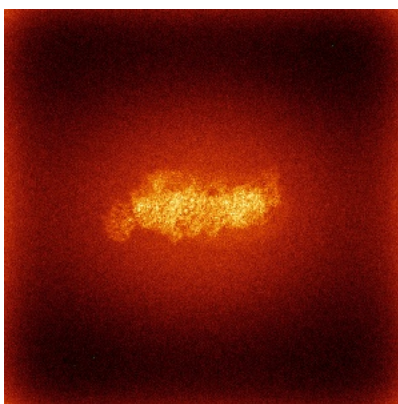


Z

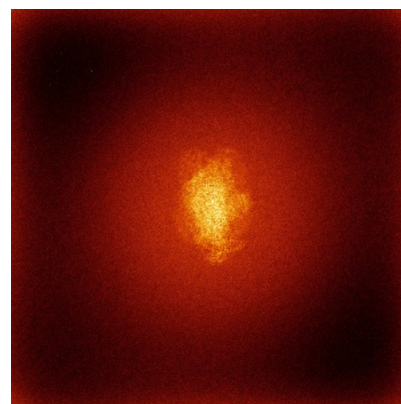
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

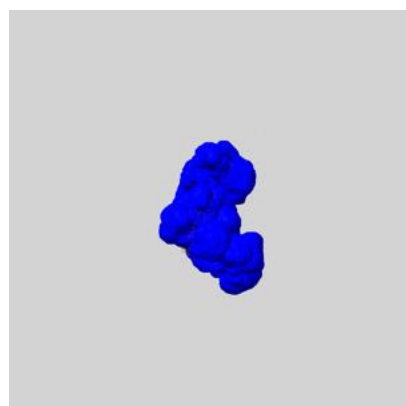
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

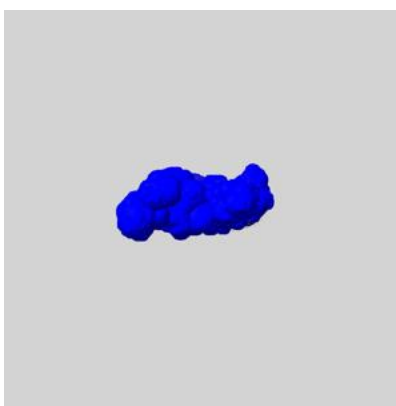
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

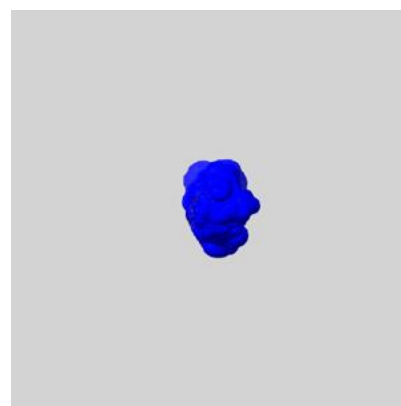
6.6.1 emd_16518_msk_1.map [i](#)



X



Y

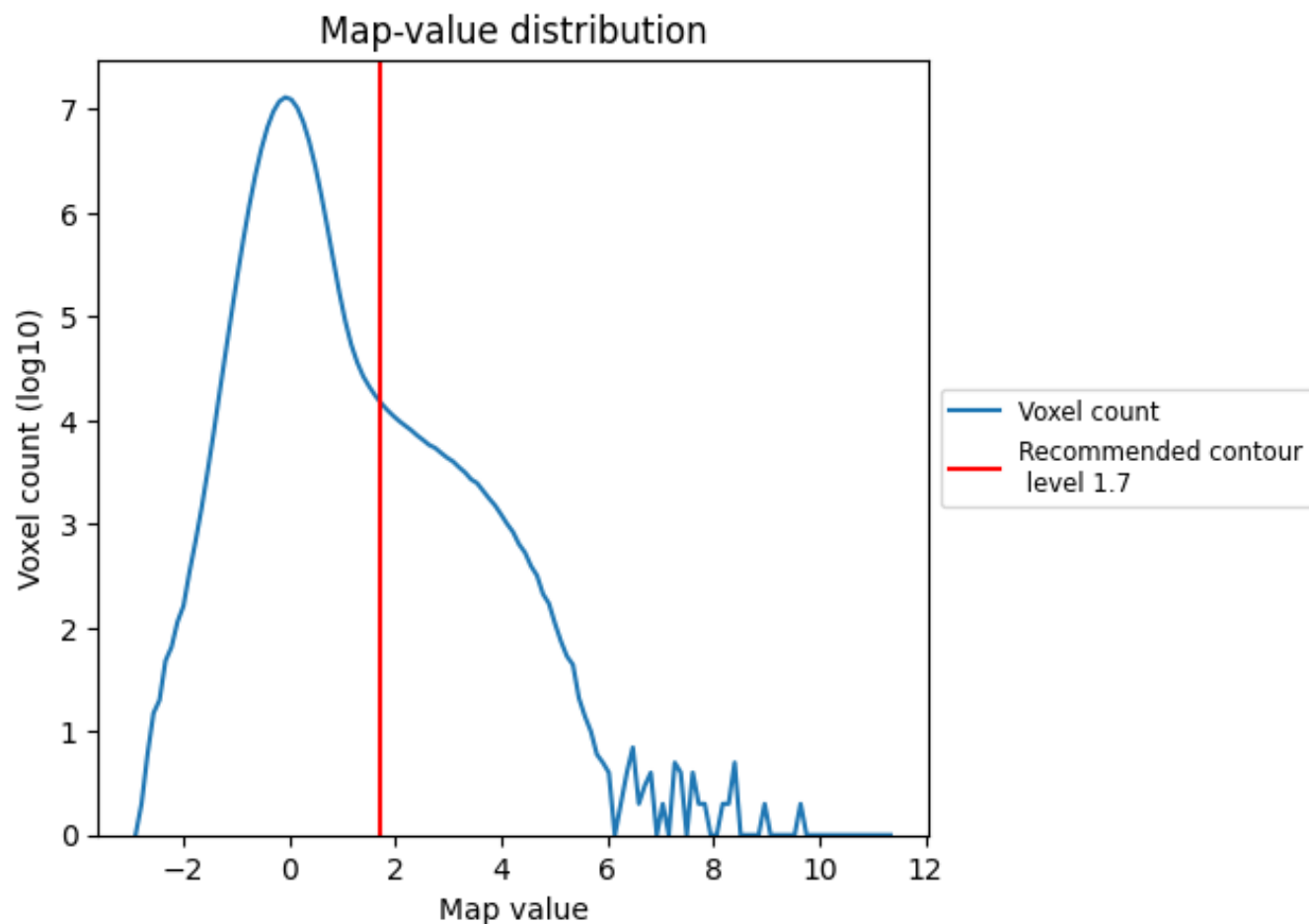


Z

7 Map analysis [i](#)

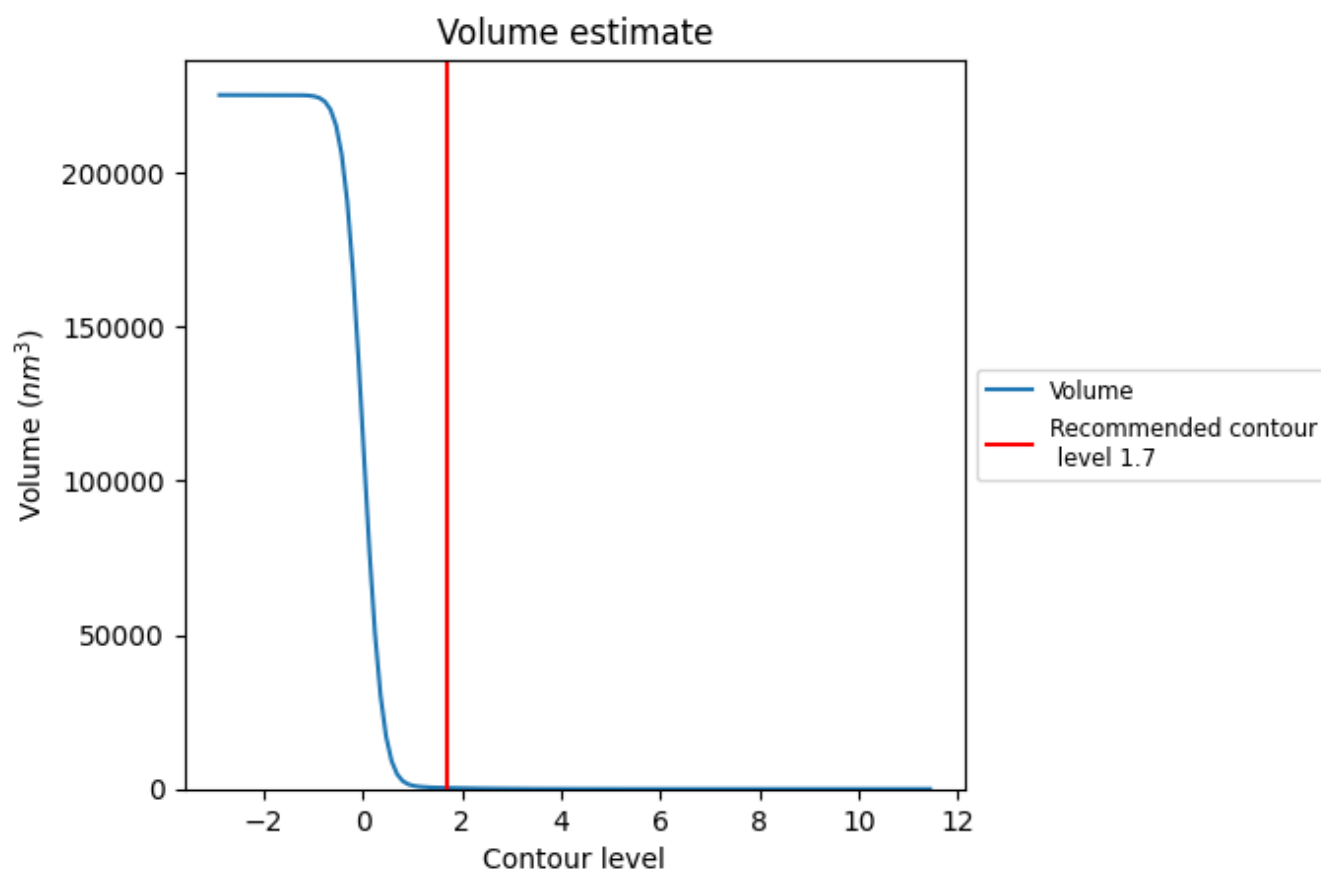
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

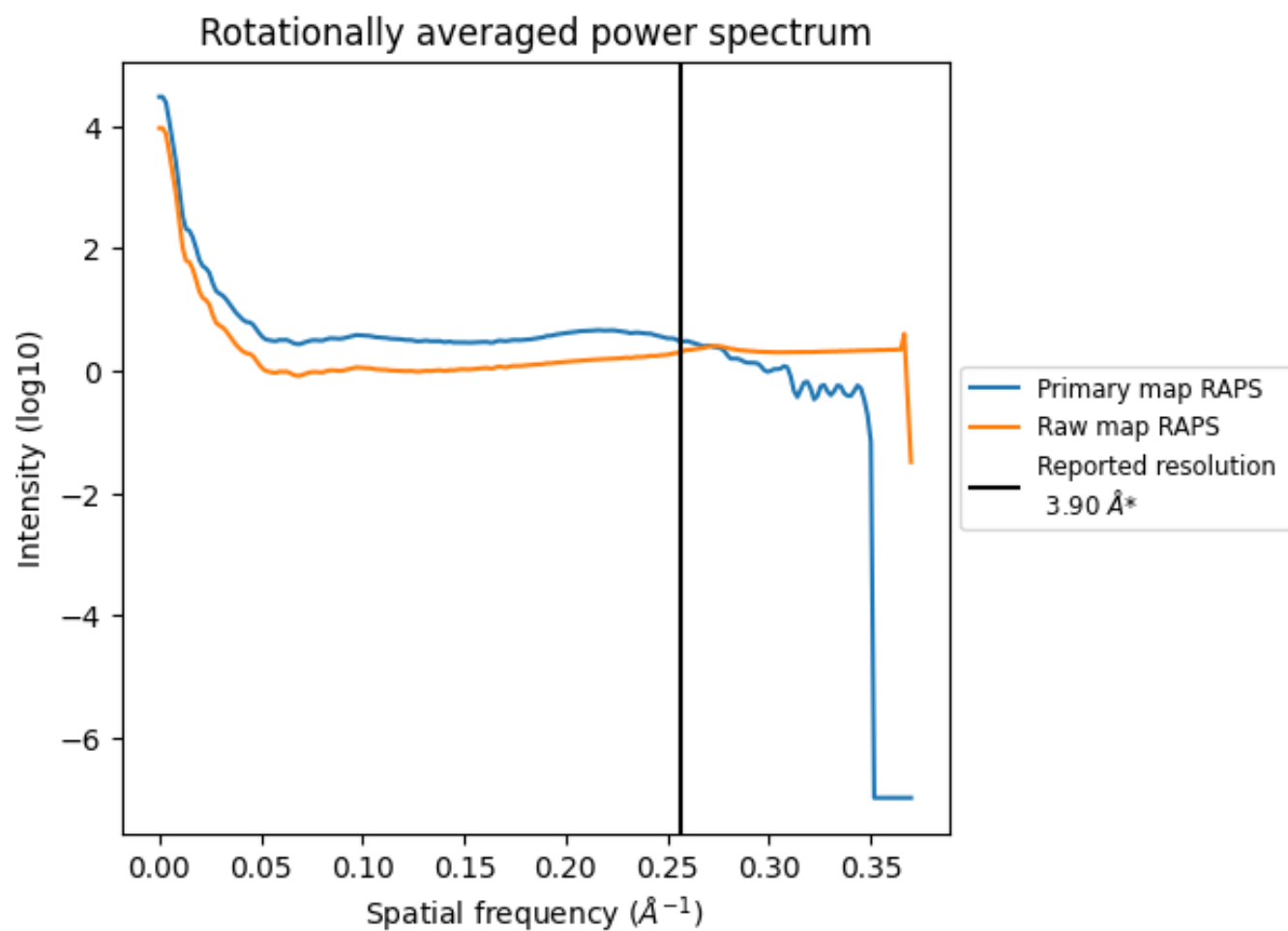
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 324 nm^3 ; this corresponds to an approximate mass of 292 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

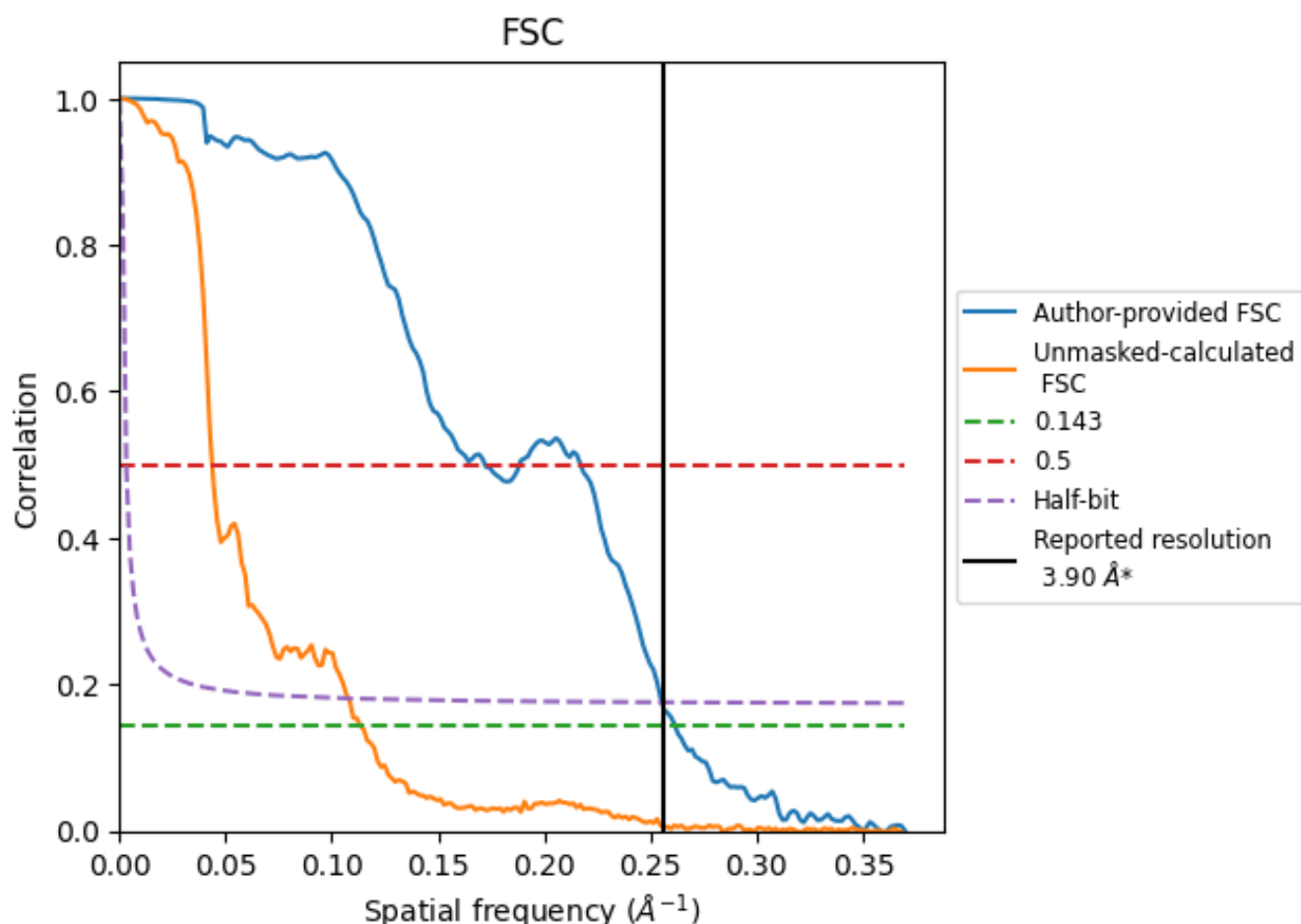


*Reported resolution corresponds to spatial frequency of 0.256 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

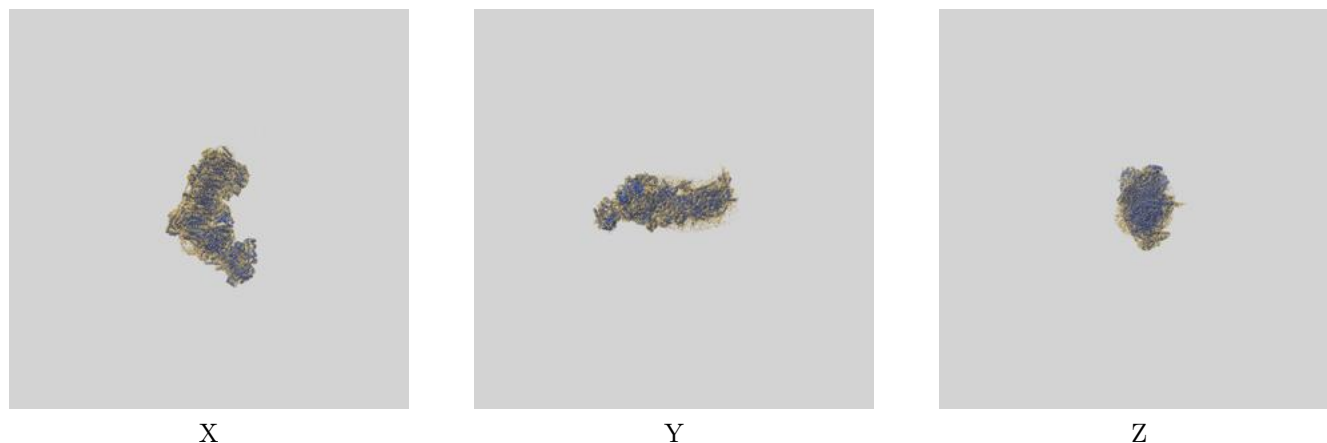
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.82	5.81	3.92
Unmasked-calculated*	8.82	22.88	9.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.82 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

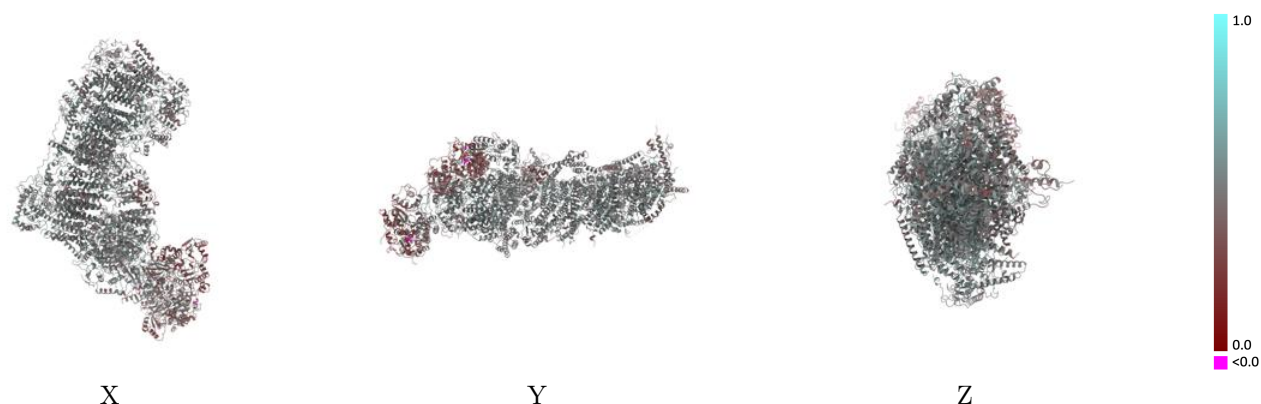
This section contains information regarding the fit between EMDB map EMD-16518 and PDB model 8CA5. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



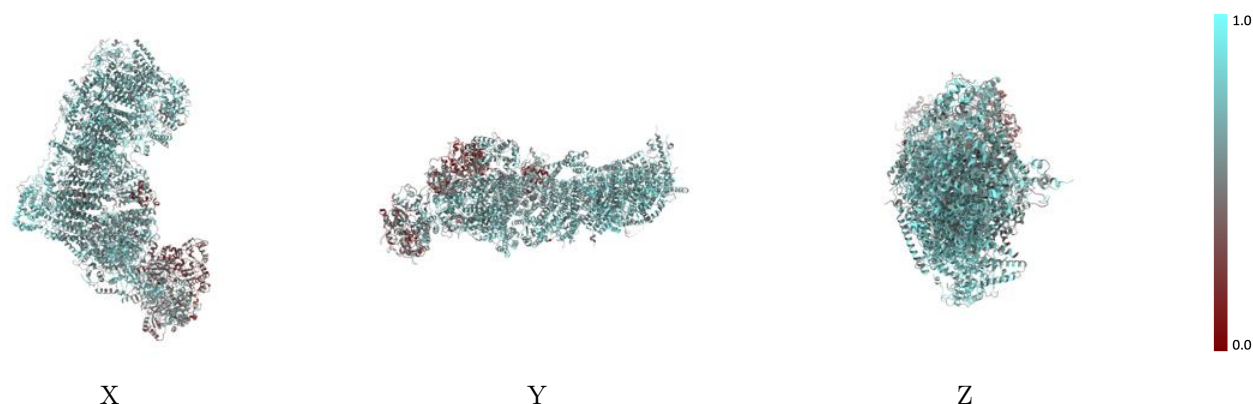
The images above show the 3D surface view of the map at the recommended contour level 1.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



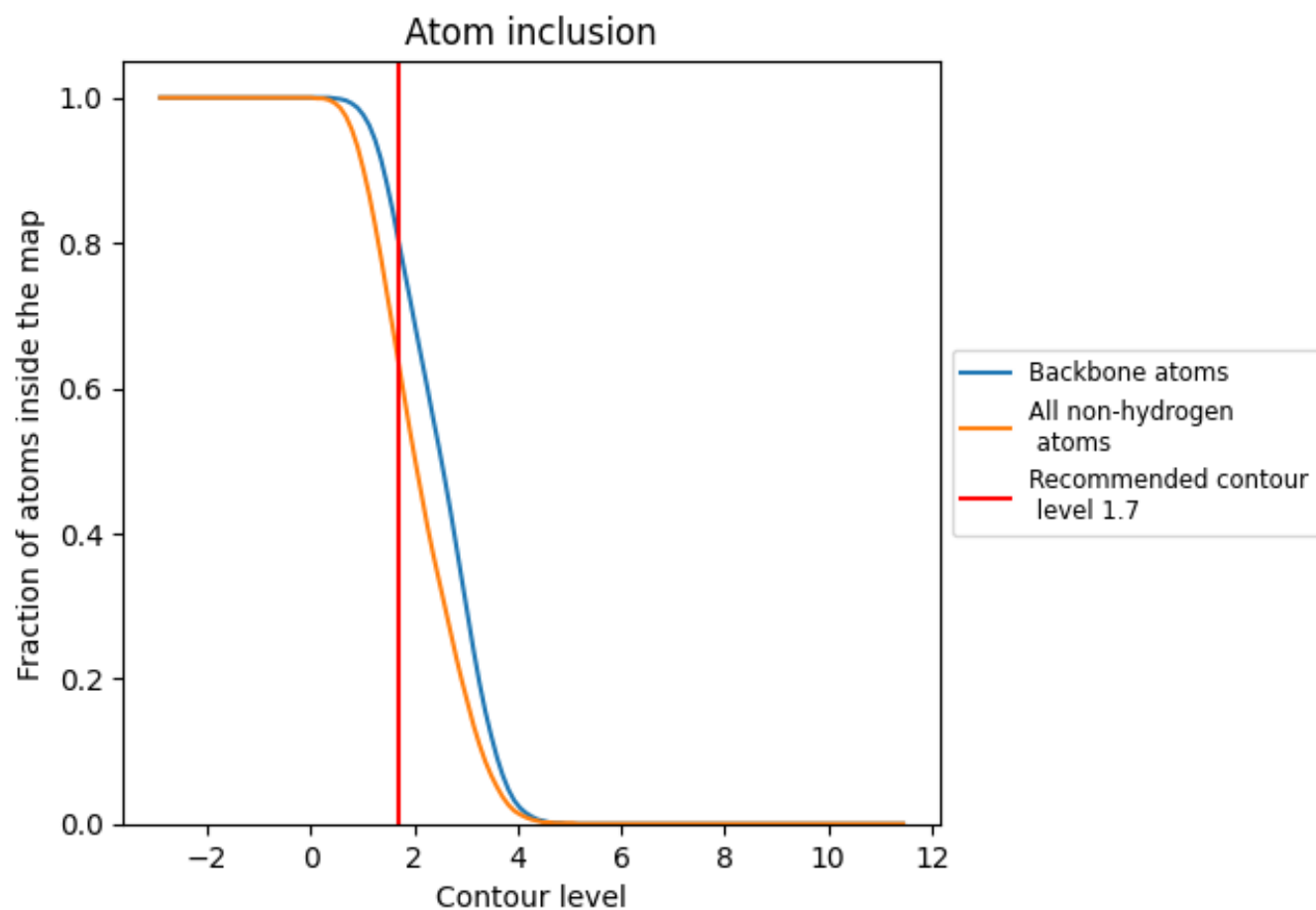
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.7).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



















The table lists the average atom inclusion at the recommended contour level (1.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6340	 0.4760
A	 0.6360	 0.5060
B	 0.7200	 0.5200
C	 0.6650	 0.5100
D	 0.6970	 0.5160
E	 0.4580	 0.3640
F	 0.4750	 0.3830
G	 0.4680	 0.4010
H	 0.6910	 0.5110
I	 0.7180	 0.4970
J	 0.5980	 0.4760
K	 0.6640	 0.5080
L	 0.6630	 0.5010
M	 0.7080	 0.5220
N	 0.6890	 0.5170
O	 0.6950	 0.4880
P	 0.6180	 0.4790
S	 0.3310	 0.2960
T	 0.3440	 0.3720
U	 0.6170	 0.4590
V	 0.6430	 0.4820
W	 0.5560	 0.4650
X	 0.7440	 0.4990
Y	 0.6240	 0.4710
Z	 0.7190	 0.4980
a	 0.7390	 0.5130
b	 0.7160	 0.4950
c	 0.6590	 0.4720
d	 0.6730	 0.5070
e	 0.7280	 0.5140
f	 0.6370	 0.4780
g	 0.6910	 0.5030
h	 0.7240	 0.5100
i	 0.6280	 0.4860
j	 0.6630	 0.4710



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Chain	Atom inclusion	Q-score
k	 0.6720	 0.4690
l	 0.7110	 0.5010
m	 0.6930	 0.4840
n	 0.7060	 0.4850
o	 0.6410	 0.4440
p	 0.6990	 0.4800
r	 0.5200	 0.4750
s	 0.4050	 0.3800
t	 0.5220	 0.4660