



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 02:15 AM JST

PDB ID : 6KHJ / pdb_00006khj
EMDB ID : EMD-9990
Title : Supercomplex for electron transfer
Authors : Pan, X.; Cao, D.; Xie, F.; Zhang, X.; Li, M.
Deposited on : 2019-07-15
Resolution : 3.00 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:

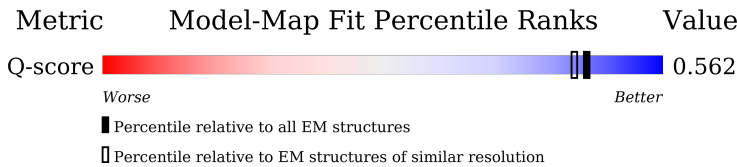
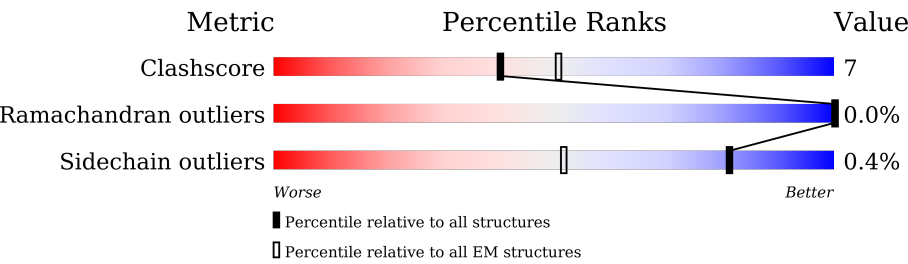
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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.



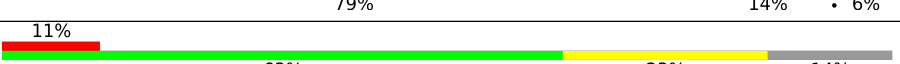
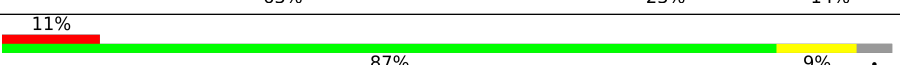
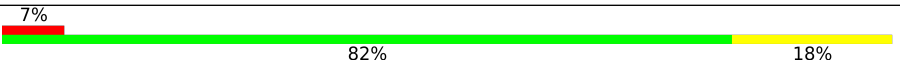
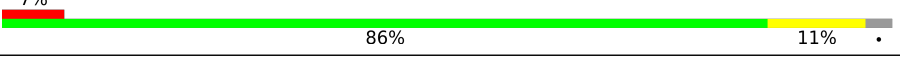
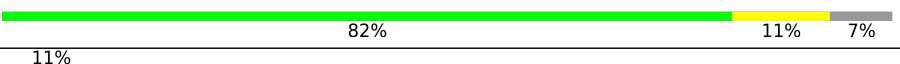
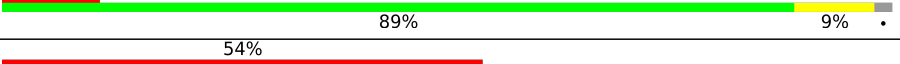
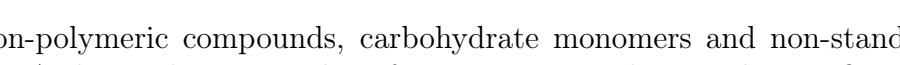
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	A	372	6% 84% 15% ..
2	B	515	80% 14% 5%
3	C	132	8% 71% 20% 9%
4	D	529	78% 17% 5%

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Mol	Chain	Length	Quality of chain
5	E	101	
6	F	656	
7	G	200	
8	H	394	
9	I	196	
10	J	168	
11	K	237	
12	L	76	
13	M	111	
14	N	150	
15	O	70	
16	P	44	
17	Q	45	
18	S	110	

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
23	BCR	D	602	-	X	-	-
23	BCR	F	701	-	X	-	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 31027 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	369	Total	C	N	O	S	0	0
			2843	1908	441	483	11		

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	488	Total	C	N	O	S	0	0
			3697	2454	574	653	16		

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	120	Total	C	N	O	S	0	0
			971	665	149	153	4		

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	504	Total	C	N	O	S	0	0
			3896	2614	605	655	22		

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	101	Total	C	N	O	S	0	0
			783	517	128	134	4		

- Molecule 6 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	639	Total	C	N	O	S	0	0
			4933	3278	778	840	37		

- Molecule 7 is a protein called NADH-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	170	Total	C	N	O	S	0	0
			1286	860	201	220	5		

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	393	Total	C	N	O	S	0	0
			3177	2048	545	565	19		

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	189	Total	C	N	O	S	0	0
			1516	967	260	276	13		

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	158	Total	C	N	O	S	0	0
			1292	825	220	242	5		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	204	Total	C	N	O	S	0	0
			1584	1016	274	281	13		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	73	Total	C	N	O	S	0	0
			590	406	90	93	1		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	111	Total	C	N	O	S	0	0
			885	551	161	171	2		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1148	747	198	202	1		

- Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	68	Total	C	N	O	0	0
			538	349	91	98		

- Molecule 16 is a protein called proton-translocating NADH-quinone dehydrogenase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	41	Total	C	N	O	S	0	0
			321	212	52	55	2		

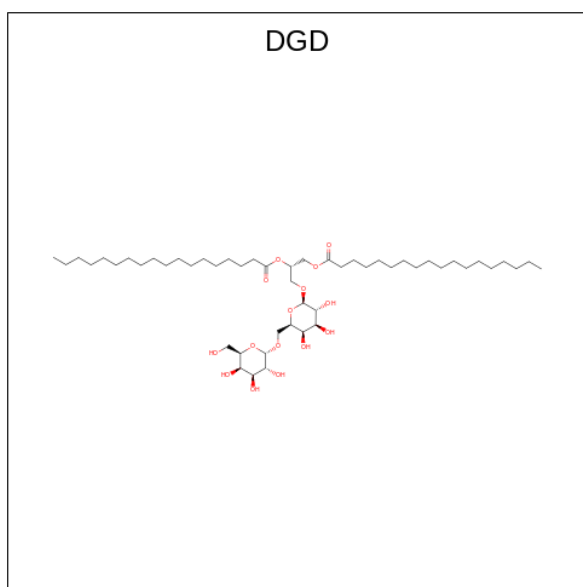
- Molecule 17 is a protein called proton-translocating NADH-quinone dehydrogenase subunit Q.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	44	Total	C	N	O	S	0	0
			333	222	53	56	2		

- Molecule 18 is a protein called Tlr0636 protein.

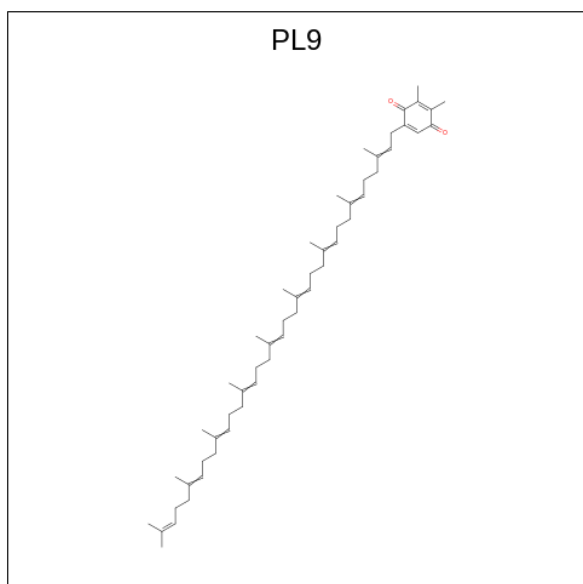
Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	60	Total	C	N	O	S	0	0
			469	304	74	89	2		

- Molecule 19 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



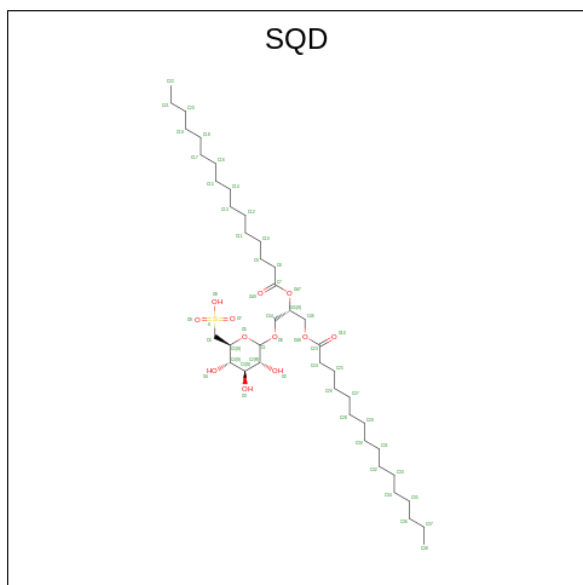
Mol	Chain	Residues	Atoms			AltConf
19	A	1	Total	C	O	0
			55	40	15	
19	A	1	Total	C	O	0
			62	47	15	

- Molecule 20 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



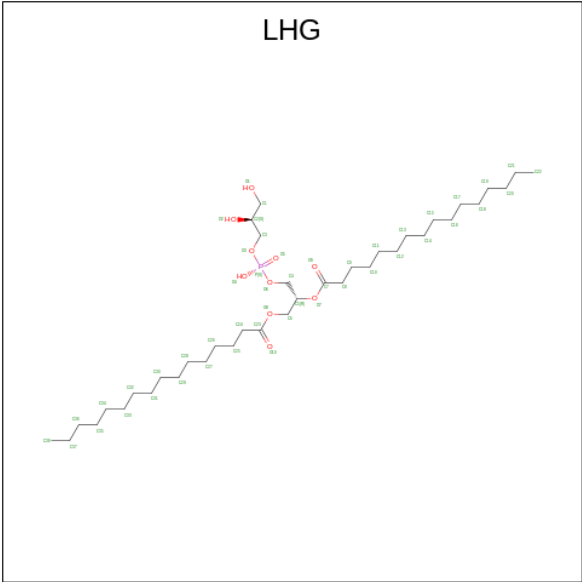
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			19	17	2	

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



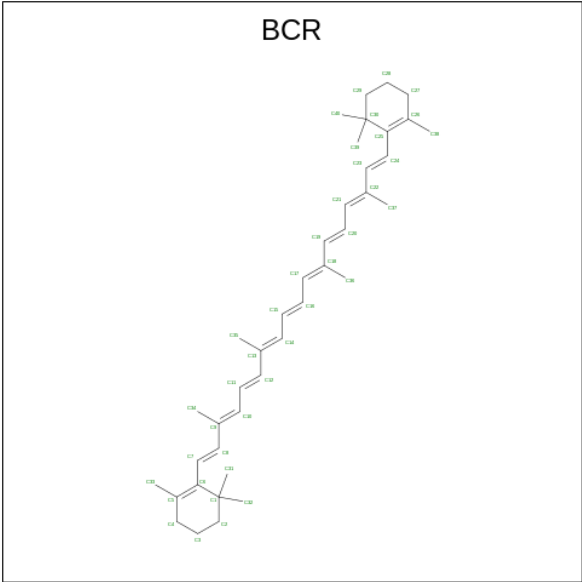
Mol	Chain	Residues	Atoms				AltConf
21	B	1	Total	C	O	S	0
			54	41	12	1	
21	C	1	Total	C	O	S	0
			40	27	12	1	
21	N	1	Total	C	O	S	0
			38	25	12	1	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



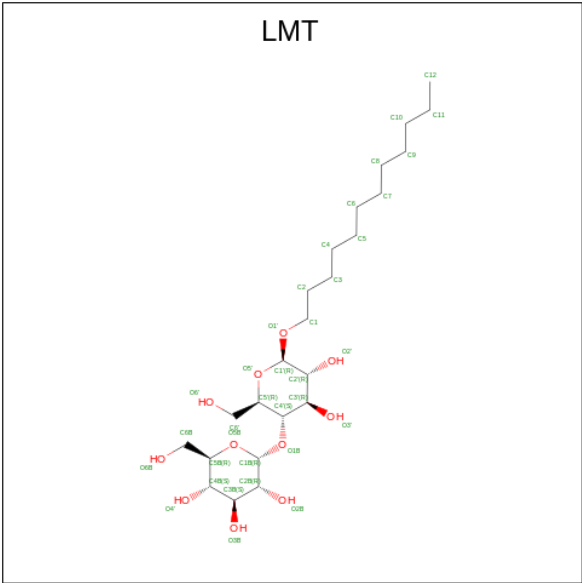
Mol	Chain	Residues	Atoms				AltConf
22	C	1	Total	C	O	P	0
			43	32	10	1	
22	D	1	Total	C	O	P	0
			46	35	10	1	
22	F	1	Total	C	O	P	0
			49	38	10	1	
22	F	1	Total	C	O	P	0
			45	34	10	1	
22	F	1	Total	C	O	P	0
			44	33	10	1	
22	I	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
23	D	1	Total	C	0
			40	40	
23	F	1	Total	C	0
			40	40	

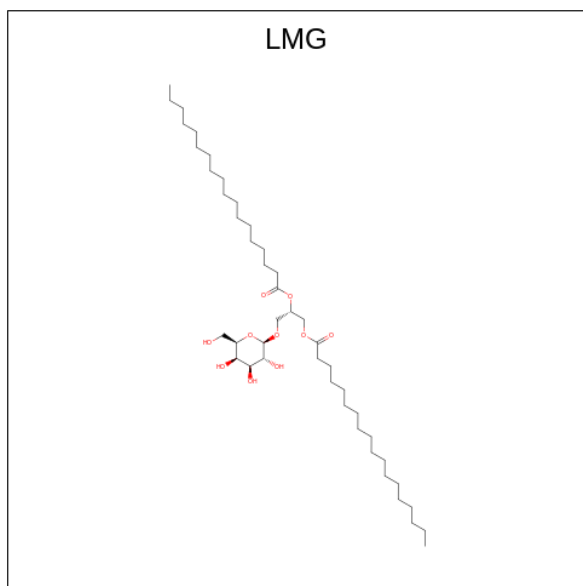
- Molecule 24 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

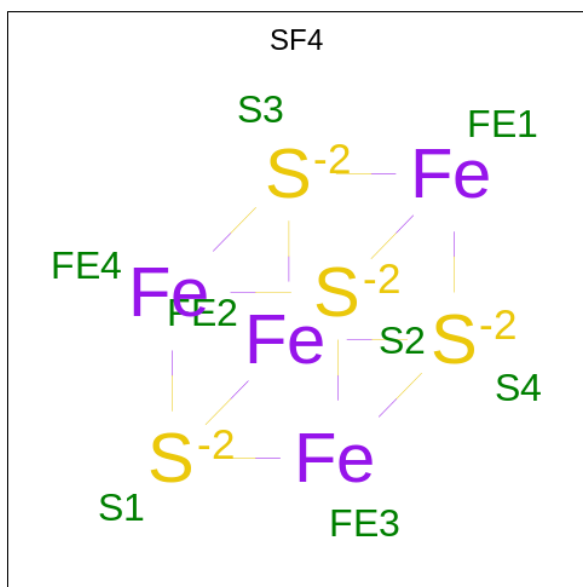
- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID:

LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

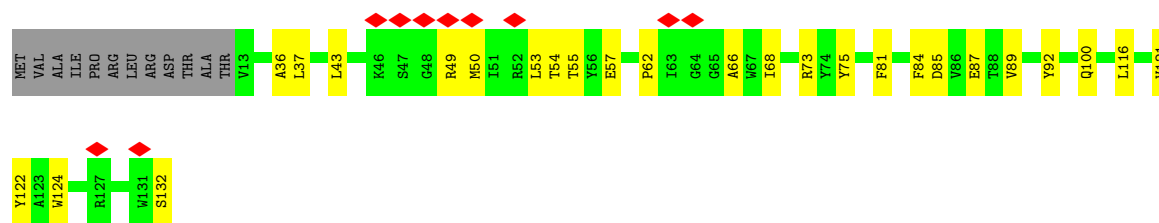


Mol	Chain	Residues	Atoms			AltConf
25	F	1	Total	C	O	0
			47	37	10	
25	F	1	Total	C	O	0
			40	30	10	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

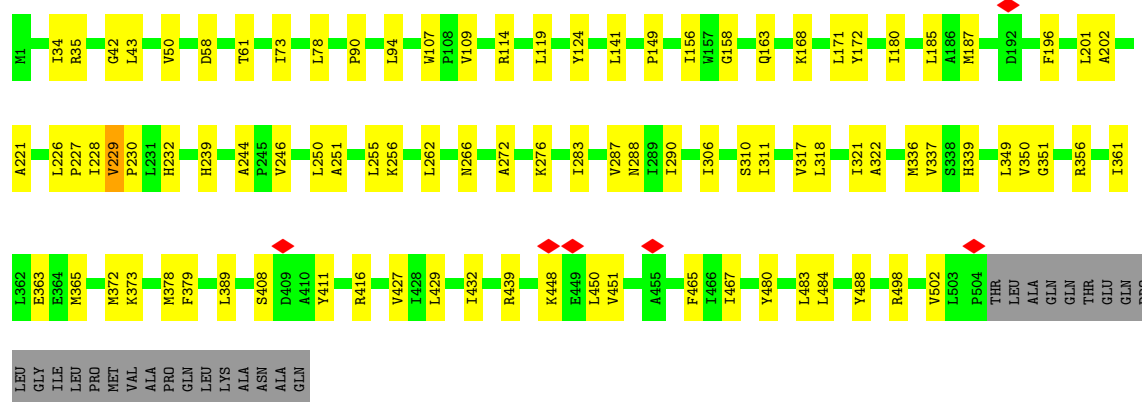


Mol	Chain	Residues	Atoms			AltConf
26	I	1	Total 8	Fe 4	S 4	0
26	I	1	Total 8	Fe 4	S 4	0
26	K	1	Total 8	Fe 4	S 4	0



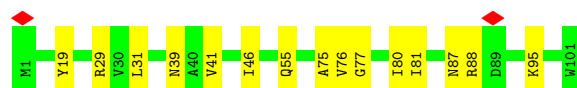
- Molecule 4: NAD(P)H-quinone oxidoreductase chain 4 1

Chain D: 78% 17% 5%



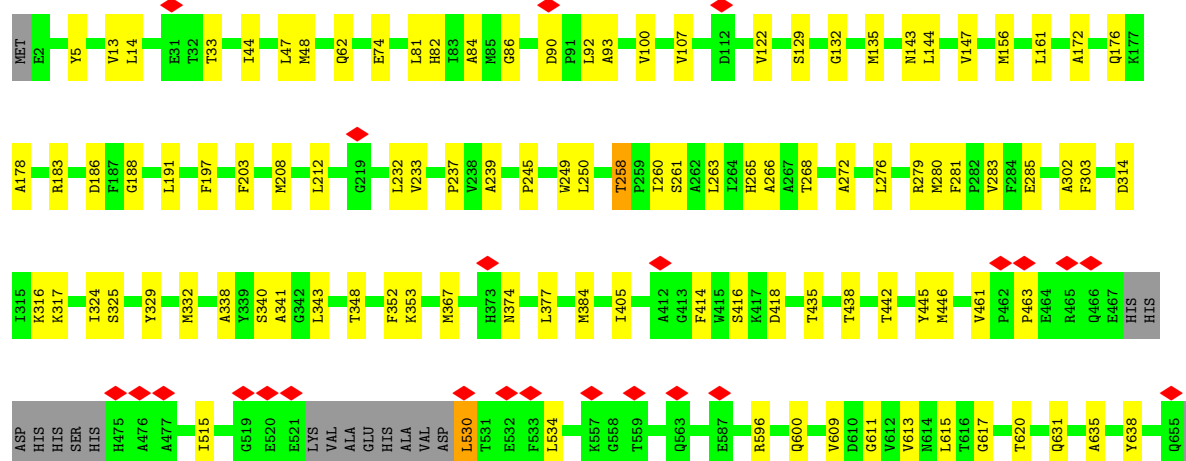
- Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L

Chain E: 85% 15%

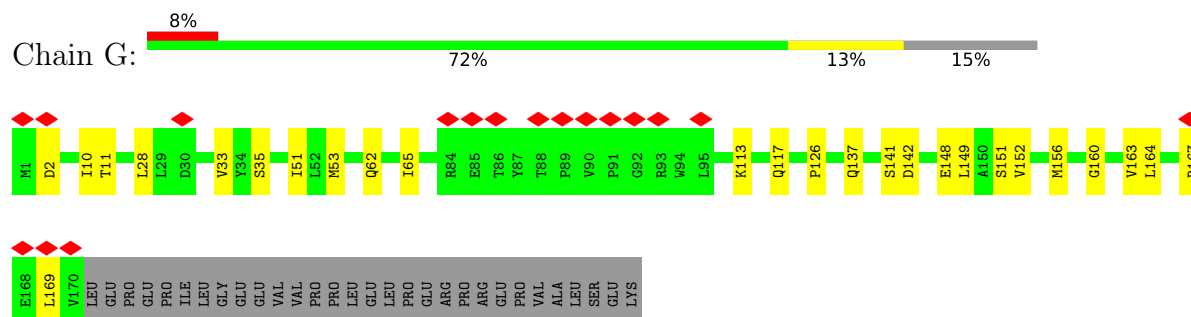


- Molecule 6: NADH dehydrogenase subunit 5

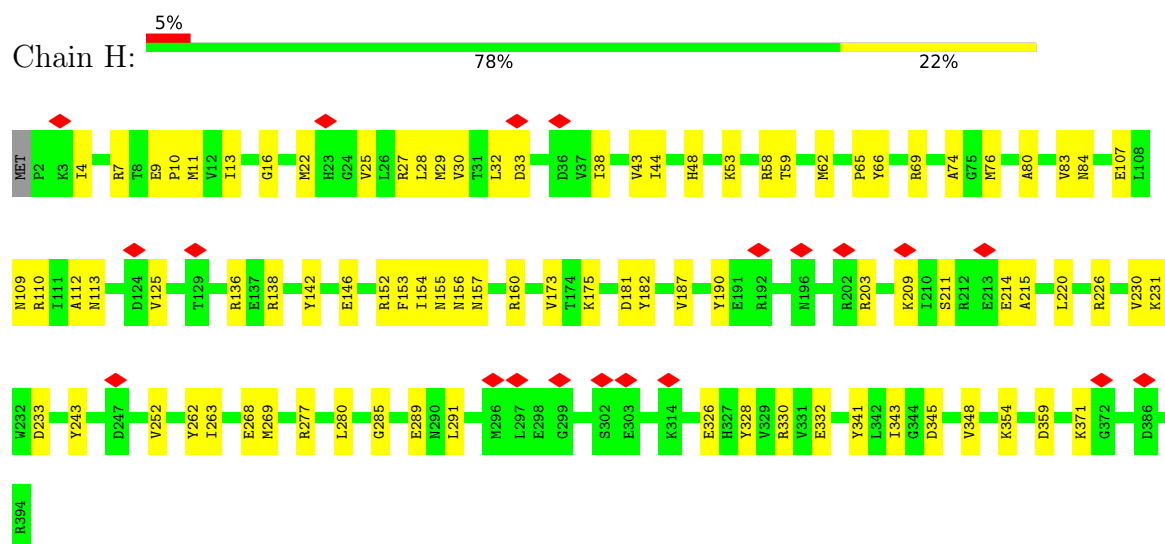
Chain F: 82% 16%



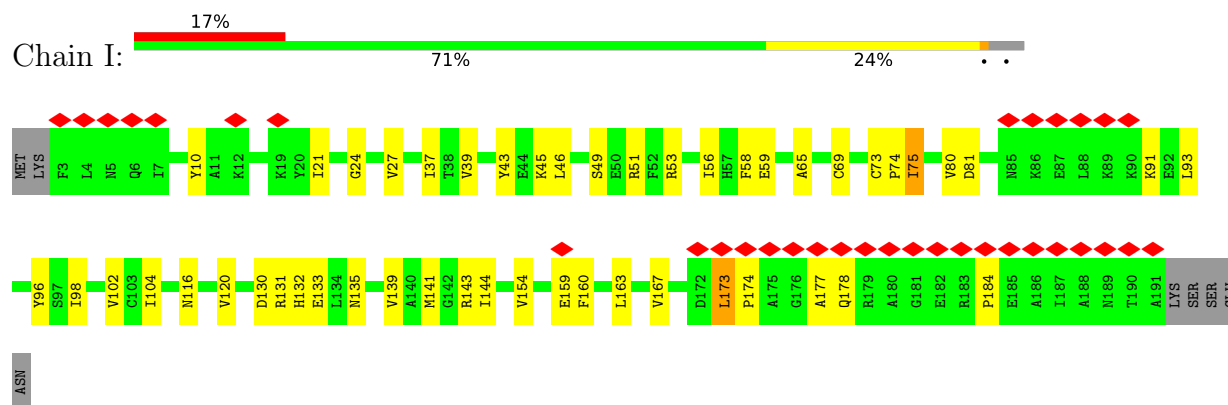
- Molecule 7: NADH-quinone oxidoreductase subunit J



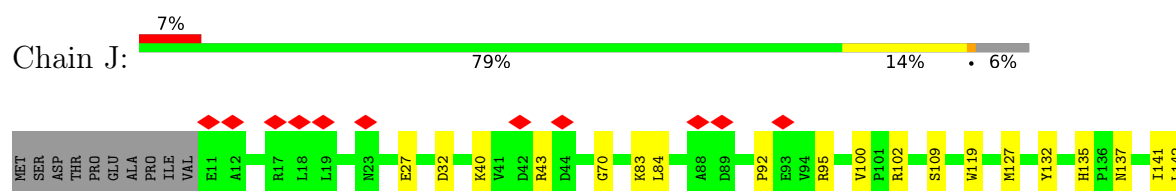
- Molecule 8: NAD(P)H-quinone oxidoreductase subunit H



- Molecule 9: NAD(P)H-quinone oxidoreductase subunit I

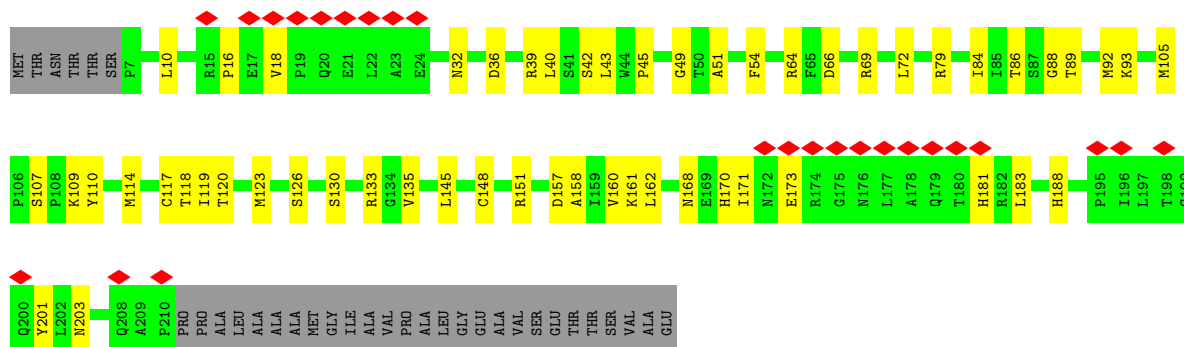


- Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

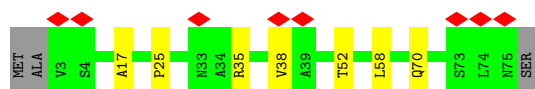
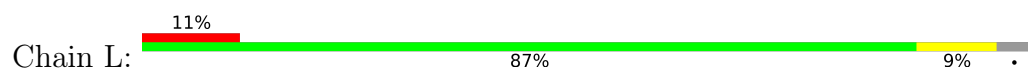




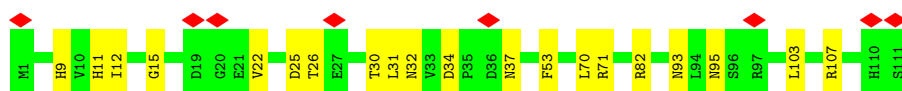
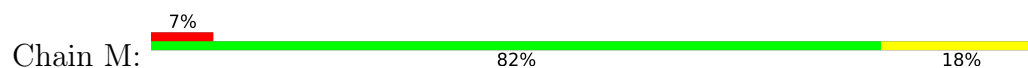
• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K



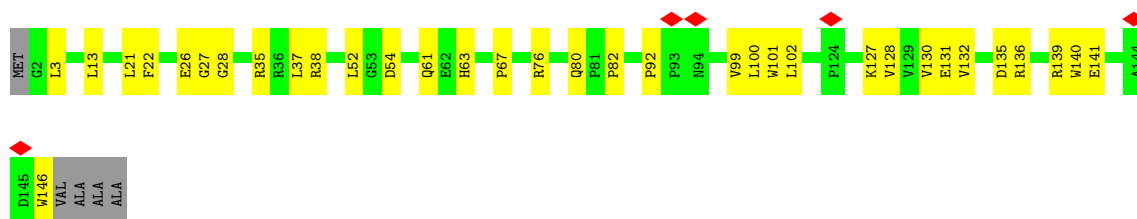
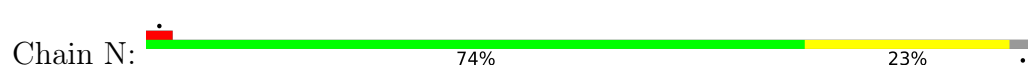
• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L



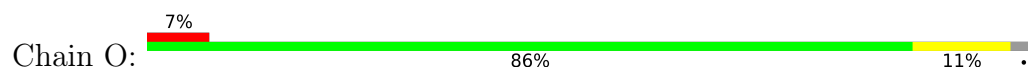
• Molecule 13: NAD(P)H-quinone oxidoreductase subunit M

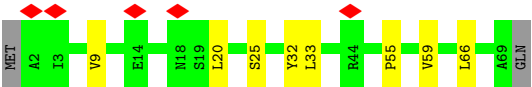


• Molecule 14: NAD(P)H-quinone oxidoreductase subunit N

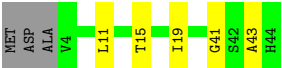
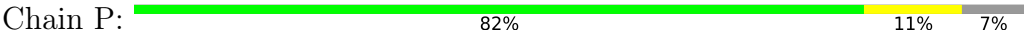


• Molecule 15: NAD(P)H-quinone oxidoreductase subunit O

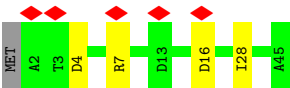
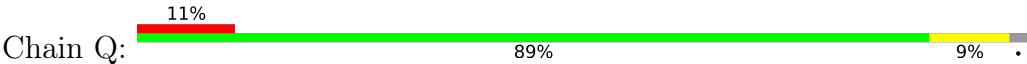




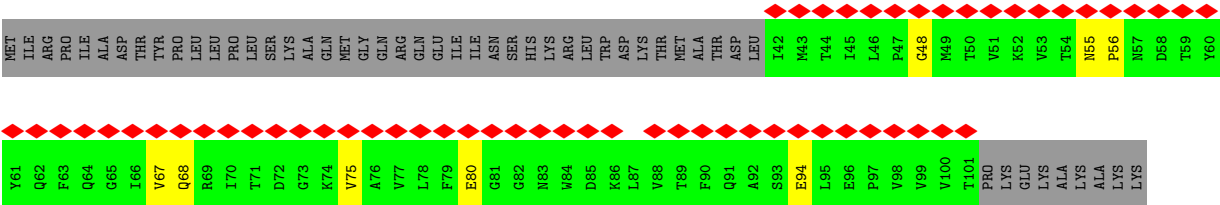
- Molecule 16: proton-translocating NADH-quinone dehydrogenase subunit P



- Molecule 17: proton-translocating NADH-quinone dehydrogenase subunit Q



- Molecule 18: Tlr0636 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	187788	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 ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.383	Depositor
Minimum map value	-0.138	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LMG, SQD, PL9, BCR, SF4, LMT, LHG

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	A	0.32	0/2914	0.61	0/3979
2	B	0.29	0/3783	0.57	1/5160 (0.0%)
3	C	0.27	0/1001	0.56	0/1365
4	D	0.30	0/4003	0.53	0/5462
5	E	0.26	0/793	0.50	0/1077
6	F	0.27	0/5076	0.55	2/6914 (0.0%)
7	G	0.25	0/1312	0.50	0/1796
8	H	0.29	0/3260	0.55	1/4417 (0.0%)
9	I	0.35	1/1554 (0.1%)	0.59	2/2108 (0.1%)
10	J	0.26	0/1328	0.50	0/1808
11	K	0.33	0/1624	0.66	2/2209 (0.1%)
12	L	0.25	0/610	0.61	0/835
13	M	0.26	0/901	0.57	0/1222
14	N	0.26	0/1180	0.59	0/1604
15	O	0.24	0/550	0.52	0/748
16	P	0.35	0/330	0.53	0/448
17	Q	0.23	0/342	0.44	0/466
18	S	0.17	0/478	0.48	0/652
All	All	0.29	1/31039 (0.0%)	0.56	8/42270 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	174	PRO	C-N	-8.12	1.23	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	530	LEU	CA-C-N	6.03	133.05	121.54
6	F	530	LEU	C-N-CA	6.03	133.05	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	49	GLY	CA-C-N	5.64	136.43	126.45
11	K	49	GLY	C-N-CA	5.64	136.43	126.45
2	B	387	PRO	N-CA-C	5.57	117.49	110.70
8	H	32	LEU	CA-CB-CG	5.28	134.79	116.30
9	I	173	LEU	CA-C-N	5.00	126.09	119.84
9	I	173	LEU	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	A	2843	0	2970	58	0
2	B	3697	0	3829	50	0
3	C	971	0	1001	24	0
4	D	3896	0	4042	65	0
5	E	783	0	837	13	0
6	F	4933	0	4981	65	0
7	G	1286	0	1372	22	0
8	H	3177	0	3157	64	0
9	I	1516	0	1482	38	0
10	J	1292	0	1244	19	0
11	K	1584	0	1617	48	0
12	L	590	0	603	5	0
13	M	885	0	865	14	0
14	N	1148	0	1157	26	0
15	O	538	0	549	7	0
16	P	321	0	317	5	0
17	Q	333	0	333	4	0
18	S	469	0	473	5	0
19	A	117	0	156	5	0
20	A	19	0	21	4	0
21	B	54	0	78	6	0
21	C	40	0	44	1	0
21	N	38	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	43	0	59	2	0
22	D	46	0	62	1	0
22	F	138	0	198	5	0
22	I	44	0	61	1	0
23	D	40	0	56	3	0
23	F	40	0	56	4	0
24	D	35	0	45	0	0
25	F	87	0	114	1	0
26	I	16	0	0	2	0
26	K	8	0	0	0	0
All	All	31027	0	31819	439	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (439) 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)
1:A:230:LEU:HB3	1:A:231:PRO:CD	1.61	1.30
1:A:230:LEU:CB	1:A:231:PRO:HD2	1.65	1.26
1:A:231:PRO:HD3	1:A:332:VAL:HG21	1.24	1.14
1:A:231:PRO:HD3	1:A:332:VAL:CG2	1.85	1.05
1:A:231:PRO:CD	1:A:332:VAL:HG21	1.99	0.92
8:H:22:MET:HG2	11:K:54:PHE:CE2	2.08	0.86
8:H:22:MET:HG2	11:K:54:PHE:HE2	1.43	0.81
1:A:230:LEU:HB3	1:A:231:PRO:HD2	0.83	0.79
1:A:237:ALA:HB3	20:A:403:PL9:C2	2.19	0.72
2:B:178:LEU:HB3	5:E:41:VAL:HG11	1.78	0.66
6:F:414:PHE:O	6:F:418:ASP:HB2	1.95	0.65
2:B:80:SER:HB3	2:B:261:ARG:HH21	1.62	0.65
13:M:11:HIS:HB2	13:M:32:ASN:HB3	1.79	0.64
18:S:55:ASN:HB2	18:S:94:GLU:HB2	1.79	0.64
9:I:73:CYS:HA	26:I:202:SF4:S1	2.38	0.64
1:A:52:GLU:CD	1:A:229:ARG:NH1	2.56	0.63
1:A:237:ALA:HB3	20:A:403:PL9:C1	2.29	0.63
2:B:35:GLN:HB2	2:B:39:ALA:HB2	1.81	0.62
2:B:69:SER:HB3	2:B:74:PHE:HB3	1.80	0.62
6:F:233:VAL:HG11	6:F:280:MET:HE2	1.81	0.61
10:J:127:MET:HB3	10:J:152:LEU:HB2	1.82	0.61
6:F:266:ALA:HB1	6:F:353:LYS:HG3	1.83	0.60
4:D:246:VAL:O	4:D:250:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:76:MET:HE3	8:H:109:ASN:HD21	1.66	0.60
8:H:125:VAL:O	8:H:203:ARG:NH2	2.34	0.60
14:N:101:TRP:NE1	14:N:131:GLU:OE2	2.35	0.60
3:C:81:PHE:O	3:C:85:ASP:HB2	2.02	0.59
8:H:65:PRO:O	8:H:69:ARG:NH1	2.36	0.59
8:H:69:ARG:NH2	11:K:148:CYS:SG	2.76	0.59
2:B:420:ILE:HG12	21:B:601:SQD:H272	1.83	0.59
21:B:601:SQD:H271	6:F:620:THR:HG21	1.85	0.58
11:K:45:PRO:HD3	11:K:72:LEU:HB2	1.86	0.58
2:B:77:ASP:OD1	2:B:261:ARG:NH2	2.37	0.58
7:G:113:LYS:O	7:G:117:GLN:HB2	2.04	0.58
22:F:703:LHG:H141	22:F:703:LHG:H281	1.85	0.58
8:H:27:ARG:NH2	8:H:29:MET:SD	2.77	0.57
4:D:244:ALA:HB2	4:D:351:GLY:HA3	1.86	0.57
1:A:53:ARG:NH1	1:A:79:ASP:OD2	2.38	0.57
6:F:100:VAL:HG22	6:F:268:THR:HG23	1.85	0.57
14:N:37:LEU:HD21	14:N:99:VAL:HG21	1.86	0.57
4:D:484:LEU:HD13	23:D:602:BCR:H391	1.86	0.57
4:D:272:ALA:HA	4:D:502:VAL:HG11	1.87	0.57
10:J:135:HIS:NE2	10:J:137:ASN:O	2.38	0.57
3:C:100:GLN:OE1	7:G:137:GLN:NE2	2.38	0.57
1:A:174:ILE:HD13	3:C:84:PHE:HB2	1.87	0.57
4:D:228:ILE:HG22	4:D:230:PRO:HD2	1.87	0.56
9:I:104:ILE:HG21	11:K:123:MET:HB3	1.87	0.56
6:F:84:ALA:O	6:F:143:ASN:ND2	2.38	0.56
8:H:136:ARG:NH2	8:H:182:TYR:OH	2.38	0.56
11:K:133:ARG:NH1	15:O:55:PRO:O	2.38	0.56
9:I:56:ILE:HD13	9:I:120:VAL:HG23	1.88	0.56
6:F:245:PRO:HG2	23:F:701:BCR:HC8	1.87	0.56
8:H:173:VAL:HG13	8:H:280:LEU:HD22	1.85	0.56
3:C:89:VAL:HG11	7:G:65:ILE:HD11	1.87	0.56
2:B:126:ILE:HD11	2:B:139:LEU:HA	1.88	0.56
9:I:46:LEU:HD21	9:I:159:GLU:HB3	1.88	0.56
2:B:150:THR:HG23	2:B:239:ALA:HB2	1.87	0.56
4:D:262:LEU:HD23	4:D:266:ASN:HD22	1.70	0.56
4:D:228:ILE:HA	4:D:288:ASN:HD21	1.70	0.55
8:H:138:ARG:NE	8:H:142:TYR:OH	2.38	0.55
1:A:52:GLU:OE1	1:A:326:ILE:HG12	2.06	0.55
1:A:332:VAL:HG12	9:I:21:ILE:HD12	1.88	0.55
4:D:109:VAL:HA	16:P:41:GLY:HA3	1.88	0.55
14:N:132:VAL:HG21	14:N:146:TRP:HH2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ASP:OD1	6:F:631:GLN:NE2	2.40	0.55
4:D:35:ARG:NH1	4:D:107:TRP:O	2.40	0.55
8:H:58:ARG:HH22	11:K:126:SER:HB3	1.72	0.55
4:D:306:ILE:HG13	4:D:350:VAL:HG21	1.88	0.55
1:A:208:ASN:HB2	1:A:276:TYR:HA	1.87	0.55
2:B:226:VAL:HG11	2:B:284:LEU:HB3	1.89	0.55
6:F:161:LEU:HD22	6:F:260:ILE:HG21	1.88	0.55
9:I:81:ASP:N	9:I:81:ASP:OD1	2.39	0.55
11:K:114:MET:HG3	11:K:145:LEU:HD23	1.89	0.55
4:D:256:LYS:HD2	4:D:336:MET:HB2	1.89	0.54
11:K:119:ILE:HG22	11:K:120:THR:HG23	1.88	0.54
2:B:68:ILE:HD11	2:B:72:GLY:HA2	1.90	0.54
9:I:130:ASP:HB3	9:I:133:GLU:HG3	1.87	0.54
1:A:121:GLN:NE2	1:A:197:GLU:OE2	2.40	0.54
4:D:229:VAL:HG21	4:D:287:VAL:HG12	1.89	0.54
3:C:75:TYR:OH	5:E:75:ALA:O	2.26	0.54
8:H:156:ASN:HA	9:I:53:ARG:HH22	1.72	0.54
14:N:100:LEU:HB3	14:N:128:VAL:HG12	1.89	0.54
11:K:157:ASP:OD2	11:K:161:LYS:NZ	2.41	0.54
10:J:43:ARG:HD3	10:J:100:VAL:HG12	1.89	0.54
2:B:237:GLU:OE1	2:B:301:ARG:NH1	2.41	0.54
6:F:135:MET:HE1	6:F:272:ALA:HB2	1.89	0.54
6:F:367:MET:HE3	6:F:384:MET:HG2	1.89	0.53
11:K:84:ILE:HB	11:K:105:MET:HE1	1.90	0.53
8:H:16:GLY:HA2	8:H:27:ARG:HG2	1.91	0.53
8:H:80:ALA:O	8:H:84:ASN:ND2	2.40	0.53
14:N:21:LEU:HD23	14:N:140:TRP:HB3	1.91	0.53
14:N:139:ARG:NH1	14:N:141:GLU:OE2	2.40	0.53
2:B:279:THR:HG23	2:B:410:LEU:HD11	1.89	0.53
5:E:55:GLN:NE2	7:G:126:PRO:O	2.42	0.53
8:H:285:GLY:HA3	8:H:291:LEU:HD13	1.90	0.53
14:N:13:LEU:HD22	14:N:37:LEU:HD11	1.91	0.53
6:F:144:LEU:HB2	6:F:208:MET:HE1	1.91	0.53
2:B:160:ASN:ND2	5:E:87:ASN:OD1	2.42	0.53
2:B:294:LEU:O	2:B:427:ARG:NH2	2.40	0.53
6:F:161:LEU:HB3	6:F:260:ILE:HD13	1.91	0.53
6:F:611:GLY:O	6:F:615:LEU:HB2	2.09	0.53
1:A:232:PHE:HA	1:A:340:LEU:HD22	1.91	0.53
2:B:194:LEU:HD22	2:B:266:ALA:HB2	1.90	0.52
4:D:373:LYS:HB3	25:F:702:LMG:HC8	1.91	0.52
1:A:87:GLU:HG2	11:K:107:SER:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:290:ILE:HB	23:F:701:BCR:H402	1.91	0.52
5:E:29:ARG:NH1	7:G:35:SER:OG	2.42	0.52
2:B:148:LEU:HD13	7:G:160:GLY:HA3	1.91	0.52
6:F:374:ASN:HD22	6:F:377:LEU:HD13	1.74	0.52
6:F:631:GLN:NE2	6:F:638:TYR:OH	2.43	0.52
9:I:135:ASN:HD21	14:N:67:PRO:HA	1.74	0.52
1:A:230:LEU:HD12	1:A:230:LEU:N	2.25	0.52
4:D:168:LYS:O	4:D:172:TYR:HB2	2.10	0.52
4:D:365:MET:HA	4:D:450:LEU:HD22	1.92	0.52
4:D:480:TYR:HD2	4:D:483:LEU:HG	1.75	0.52
1:A:5:ILE:O	19:A:402:DGD:O2D	2.27	0.52
4:D:119:LEU:HD22	4:D:149:PRO:HA	1.90	0.52
6:F:33:THR:HG22	6:F:122:VAL:HG11	1.92	0.52
10:J:83:LYS:HB2	10:J:92:PRO:HD2	1.91	0.52
11:K:170:HIS:HB3	11:K:173:GLU:HB2	1.91	0.52
13:M:37:ASN:O	13:M:93:ASN:ND2	2.43	0.51
18:S:48:GLY:H	18:S:67:VAL:HG13	1.73	0.51
6:F:281:PHE:O	6:F:285:GLU:HB2	2.11	0.51
6:F:596:ARG:NH1	6:F:600:GLN:OE1	2.43	0.51
8:H:146:GLU:OE2	11:K:151:ARG:NH2	2.42	0.51
7:G:2:ASP:N	7:G:2:ASP:OD1	2.39	0.51
4:D:202:ALA:O	4:D:498:ARG:NH1	2.43	0.51
4:D:378:MET:HB3	4:D:467:ILE:HG21	1.92	0.51
4:D:158:GLY:HA2	16:P:43:ALA:H	1.76	0.51
6:F:107:VAL:HG21	6:F:263:LEU:HB2	1.92	0.51
8:H:38:ILE:HG22	11:K:203:ASN:HD21	1.76	0.51
1:A:115:ILE:HG23	1:A:125:ILE:HB	1.92	0.51
21:B:601:SQD:H81	6:F:617:GLY:HA3	1.92	0.50
7:G:163:VAL:HG12	7:G:164:LEU:HD23	1.94	0.50
4:D:361:ILE:HG21	17:Q:7:ARG:HH12	1.76	0.50
9:I:116:ASN:ND2	18:S:80:GLU:OE2	2.44	0.50
1:A:62:ARG:NH2	11:K:66:ASP:OD1	2.41	0.50
1:A:231:PRO:HG2	1:A:232:PHE:CE1	2.47	0.50
8:H:27:ARG:HB2	8:H:43:VAL:HB	1.93	0.50
9:I:98:ILE:HD12	9:I:141:MET:HE1	1.93	0.50
4:D:227:PRO:HB2	4:D:311:ILE:HG23	1.93	0.50
9:I:49:SER:OG	9:I:51:ARG:O	2.30	0.50
11:K:168:ASN:O	14:N:38:ARG:NH1	2.44	0.50
23:F:701:BCR:H271	17:Q:28:ILE:HD12	1.92	0.50
6:F:178:ALA:HA	6:F:249:TRP:HB2	1.93	0.49
4:D:448:LYS:HA	4:D:451:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:176:GLN:NE2	22:F:705:LHG:O4	2.45	0.49
3:C:54:THR:O	11:K:79:ARG:NH2	2.45	0.49
4:D:42:GLY:HA2	4:D:124:TYR:HE2	1.78	0.49
6:F:5:TYR:OH	6:F:62:GLN:NE2	2.43	0.49
4:D:287:VAL:HG22	23:F:701:BCR:H401	1.94	0.49
2:B:236:TYR:HA	2:B:244:VAL:HG11	1.95	0.49
8:H:230:VAL:HG11	10:J:84:LEU:HD21	1.95	0.49
12:L:70:GLN:OE1	14:N:136:ARG:NH2	2.45	0.49
6:F:303:PHE:HA	6:F:438:THR:HG21	1.94	0.49
6:F:348:THR:HG22	6:F:352:PHE:HE2	1.77	0.49
9:I:58:PHE:HB3	9:I:141:MET:HG3	1.94	0.49
8:H:74:ALA:HB2	8:H:113:ASN:HB2	1.95	0.49
9:I:59:GLU:HB2	18:S:68:GLN:HE21	1.78	0.49
4:D:378:MET:HA	23:D:602:BCR:HC32	1.95	0.49
6:F:14:LEU:HD22	6:F:47:LEU:HD22	1.95	0.49
13:M:15:GLY:O	13:M:30:THR:OG1	2.29	0.49
1:A:52:GLU:OE1	1:A:326:ILE:HG23	2.12	0.48
11:K:43:LEU:HD21	11:K:162:LEU:HD23	1.93	0.48
11:K:51:ALA:HB3	11:K:88:GLY:HA3	1.95	0.48
1:A:286:LEU:HD21	1:A:309:LEU:HD22	1.96	0.48
11:K:39:ARG:NH1	11:K:110:TYR:OH	2.38	0.48
4:D:58:ASP:OD2	4:D:61:THR:OG1	2.30	0.48
4:D:356:ARG:HB3	4:D:372:MET:HE1	1.96	0.48
9:I:80:VAL:HG23	9:I:93:LEU:HD13	1.95	0.48
10:J:32:ASP:OD2	10:J:95:ARG:NH2	2.41	0.48
3:C:87:GLU:HB2	3:C:116:LEU:HD13	1.96	0.48
7:G:167:ARG:HH11	7:G:169:LEU:HD13	1.78	0.48
11:K:10:LEU:HB2	13:M:107:ARG:HG3	1.96	0.48
11:K:188:HIS:NE2	13:M:26:THR:O	2.41	0.48
9:I:93:LEU:HD11	9:I:96:TYR:HB2	1.96	0.48
10:J:70:GLY:O	10:J:102:ARG:NH2	2.47	0.48
11:K:32:ASN:HD21	11:K:171:ILE:H	1.60	0.48
14:N:3:LEU:HD13	21:N:201:SQD:H61	1.95	0.48
7:G:167:ARG:HE	7:G:169:LEU:HD22	1.79	0.48
8:H:181:ASP:OD1	8:H:277:ARG:NH2	2.38	0.48
14:N:22:PHE:HB2	14:N:139:ARG:O	2.14	0.48
4:D:484:LEU:HG	4:D:488:TYR:HE2	1.78	0.48
6:F:258:THR:HG23	6:F:316:LYS:HD3	1.95	0.48
2:B:387:PRO:HA	2:B:392:PHE:CG	2.49	0.47
6:F:86:GLY:HA2	22:F:706:LHG:H121	1.96	0.47
8:H:211:SER:HB2	8:H:214:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:105:MET:HB2	11:K:109:LYS:HD3	1.95	0.47
12:L:35:ARG:HG3	12:L:38:VAL:HB	1.96	0.47
4:D:94:LEU:HD13	4:D:337:VAL:HG13	1.96	0.47
4:D:50:VAL:HG21	16:P:15:THR:HG21	1.96	0.47
8:H:107:GLU:OE2	8:H:243:TYR:OH	2.27	0.47
11:K:42:SER:OG	11:K:43:LEU:N	2.43	0.47
6:F:530:LEU:HD13	6:F:534:LEU:HD13	1.95	0.47
11:K:110:TYR:HB3	11:K:162:LEU:HD11	1.96	0.47
1:A:199:GLN:HE21	1:A:208:ASN:H	1.63	0.47
2:B:305:TYR:HA	2:B:308:ILE:HD12	1.96	0.47
6:F:74:GLU:OE2	6:F:82:HIS:ND1	2.45	0.47
8:H:136:ARG:HD3	9:I:37:ILE:HD13	1.97	0.47
9:I:143:ARG:NH1	14:N:52:LEU:O	2.41	0.47
2:B:220:SER:HA	2:B:223:ILE:HB	1.97	0.47
4:D:439:ARG:HG2	6:F:172:ALA:HB1	1.97	0.47
8:H:142:TYR:HB3	8:H:152:ARG:HG2	1.97	0.47
2:B:241:THR:HA	2:B:244:VAL:HG22	1.97	0.46
3:C:73:ARG:HD2	3:C:132:SER:HA	1.97	0.46
4:D:349:LEU:HB3	4:D:379:PHE:HD1	1.80	0.46
1:A:283:PRO:HD3	1:A:313:MET:HE2	1.97	0.46
9:I:46:LEU:HD11	11:K:64:ARG:HH21	1.81	0.46
4:D:43:LEU:HD22	16:P:19:ILE:HA	1.97	0.46
7:G:156:MET:HE3	7:G:156:MET:HB3	1.86	0.46
8:H:328:TYR:O	8:H:330:ARG:NH1	2.49	0.46
8:H:345:ASP:N	8:H:345:ASP:OD1	2.48	0.46
9:I:65:ALA:HB3	9:I:91:LYS:HB3	1.97	0.46
9:I:163:LEU:HB3	9:I:167:VAL:HB	1.96	0.46
15:O:9:VAL:HG21	15:O:66:LEU:HD13	1.97	0.46
1:A:311:ILE:HG21	19:A:402:DGD:HB92	1.97	0.46
4:D:411:TYR:O	4:D:416:ARG:NH1	2.48	0.46
9:I:139:VAL:HG11	14:N:54:ASP:HB2	1.96	0.46
1:A:45:VAL:HG23	1:A:262:TYR:HB2	1.97	0.46
1:A:252:MET:HE2	3:C:36:ALA:HB1	1.96	0.46
2:B:144:ILE:HG23	5:E:76:VAL:HG21	1.96	0.46
2:B:212:LEU:HD21	2:B:274:TRP:HB3	1.97	0.46
2:B:458:ARG:NH2	2:B:461:GLN:OE1	2.48	0.46
4:D:90:PRO:HB3	4:D:484:LEU:HD11	1.97	0.46
8:H:7:ARG:NH2	8:H:9:GLU:OE2	2.45	0.46
14:N:63:HIS:NE2	14:N:80:GLN:OE1	2.39	0.46
1:A:336:ARG:HH12	8:H:203:ARG:HG2	1.81	0.46
3:C:57:GLU:HG2	3:C:62:PRO:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:359:ASP:OD1	8:H:359:ASP:N	2.47	0.46
2:B:226:VAL:HB	2:B:285:SER:HA	1.97	0.46
21:B:601:SQD:H212	6:F:609:VAL:HG13	1.96	0.46
4:D:232:HIS:HD2	4:D:311:ILE:HD13	1.81	0.46
6:F:338:ALA:HB1	6:F:341:ALA:HB3	1.98	0.46
6:F:348:THR:OG1	6:F:416:SER:OG	2.32	0.46
13:M:9:HIS:HA	13:M:34:ASP:HA	1.98	0.46
2:B:29:LEU:HB2	2:B:114:THR:HG21	1.98	0.46
3:C:121:VAL:HG22	22:C:202:LHG:H121	1.97	0.46
4:D:389:LEU:HD11	6:F:156:MET:HB2	1.97	0.46
6:F:405:ILE:HG21	6:F:446:MET:HE3	1.98	0.46
17:Q:4:ASP:N	17:Q:4:ASP:OD1	2.40	0.46
2:B:318:PHE:HD1	2:B:329:MET:HE1	1.80	0.45
4:D:187:MET:HG3	4:D:201:LEU:HD13	1.97	0.45
5:E:19:TYR:HE2	7:G:28:LEU:HD21	1.82	0.45
8:H:215:ALA:HA	8:H:220:LEU:HD12	1.98	0.45
7:G:137:GLN:O	7:G:141:SER:OG	2.31	0.45
8:H:341:TYR:HB3	8:H:354:LYS:HB3	1.98	0.45
9:I:178:GLN:NE2	18:S:56:PRO:O	2.46	0.45
4:D:408:SER:O	4:D:416:ARG:NH1	2.49	0.45
8:H:110:ARG:NH2	8:H:332:GLU:O	2.41	0.45
12:L:25:PRO:HB3	12:L:58:LEU:HD23	1.98	0.45
8:H:187:VAL:HG12	8:H:269:MET:HE2	1.98	0.45
14:N:99:VAL:HA	14:N:127:LYS:O	2.17	0.45
1:A:81:LEU:HD23	1:A:84:ILE:HD12	1.99	0.45
1:A:230:LEU:CB	1:A:231:PRO:CD	2.40	0.45
4:D:429:LEU:HD23	4:D:432:ILE:HD12	1.97	0.45
6:F:332:MET:HE2	6:F:332:MET:HB3	1.79	0.45
8:H:62:MET:HB2	9:I:74:PRO:HA	1.99	0.45
9:I:43:TYR:OH	14:N:26:GLU:OE1	2.30	0.45
9:I:69:CYS:HB3	26:I:203:SF4:S3	2.57	0.45
14:N:102:LEU:HD12	14:N:130:VAL:HG22	1.98	0.45
2:B:165:LYS:HB2	6:F:635:ALA:HB2	1.99	0.45
6:F:461:VAL:HG12	6:F:463:PRO:HD2	1.98	0.45
1:A:92:ALA:HB3	3:C:55:THR:HG23	1.99	0.45
4:D:349:LEU:HD13	4:D:379:PHE:HA	1.99	0.45
6:F:237:PRO:HD3	6:F:276:LEU:HD23	1.99	0.45
8:H:53:LYS:NZ	10:J:151:PRO:O	2.41	0.45
8:H:190:TYR:O	8:H:262:TYR:OH	2.29	0.45
11:K:160:VAL:HG13	14:N:27:GLY:HA2	1.97	0.45
4:D:239:HIS:CE1	4:D:251:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:HZ	3:C:89:VAL:HG23	1.80	0.44
3:C:68:ILE:HA	8:H:11:MET:HE3	1.99	0.44
3:C:121:VAL:HG21	22:C:202:LHG:H383	1.99	0.44
21:B:601:SQD:H161	6:F:613:VAL:HG22	1.98	0.44
4:D:251:ALA:HA	4:D:255:LEU:HG	2.00	0.44
10:J:109:SER:HB2	10:J:132:TYR:HB3	1.99	0.44
4:D:73:ILE:HB	4:D:78:LEU:HB3	1.99	0.44
6:F:90:ASP:H	6:F:93:ALA:HB3	1.81	0.44
6:F:261:SER:HA	6:F:265:HIS:HB2	1.99	0.44
11:K:170:HIS:HA	14:N:35:ARG:HD2	2.00	0.44
1:A:229:ARG:HG2	1:A:230:LEU:HD12	1.99	0.44
4:D:349:LEU:HD21	4:D:378:MET:HE3	1.98	0.44
8:H:33:ASP:OD1	8:H:33:ASP:N	2.48	0.44
8:H:157:ASN:HB3	8:H:160:ARG:HH21	1.83	0.44
8:H:326:GLU:HB3	8:H:343:ILE:HG23	1.98	0.44
1:A:52:GLU:CD	1:A:229:ARG:HH12	2.25	0.44
2:B:423:TYR:HB2	4:D:171:LEU:HD21	1.98	0.44
5:E:39:ASN:HD21	7:G:62:GLN:HE22	1.66	0.44
6:F:250:LEU:HD23	6:F:324:ILE:HG13	1.98	0.44
1:A:204:ILE:O	1:A:210:TRP:NE1	2.46	0.44
6:F:48:MET:HE1	6:F:132:GLY:HA3	2.00	0.44
1:A:203:GLY:O	1:A:207:TRP:NE1	2.50	0.44
8:H:44:ILE:O	11:K:93:LYS:NZ	2.50	0.44
11:K:36:ASP:O	11:K:40:LEU:HB2	2.18	0.44
11:K:92:MET:O	13:M:71:ARG:NH2	2.50	0.44
1:A:188:ASN:OD1	1:A:363:LYS:NZ	2.39	0.44
8:H:175:LYS:HA	8:H:175:LYS:HD2	1.76	0.44
10:J:27:GLU:HB2	10:J:40:LYS:HB3	2.00	0.44
4:D:246:VAL:O	4:D:250:LEU:CB	2.65	0.43
8:H:69:ARG:HD3	11:K:123:MET:HE1	2.00	0.43
14:N:135:ASP:OD2	14:N:139:ARG:NE	2.42	0.43
23:D:602:BCR:H24C	16:P:11:LEU:HD13	2.00	0.43
6:F:314:ASP:HB3	6:F:317:LYS:HB2	1.99	0.43
2:B:374:LEU:HB2	22:D:601:LHG:H252	2.01	0.43
1:A:33:PRO:HB3	19:A:401:DGD:HG2	2.00	0.43
2:B:434:VAL:HG11	4:D:163:GLN:HE22	1.83	0.43
11:K:86:THR:HG21	11:K:135:VAL:HG21	2.01	0.43
8:H:112:ALA:O	8:H:138:ARG:NH1	2.51	0.43
13:M:15:GLY:HA2	13:M:25:ASP:H	1.83	0.43
4:D:226:LEU:HD13	4:D:262:LEU:HD12	2.00	0.43
8:H:13:ILE:HB	8:H:30:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:39:VAL:HG11	9:I:46:LEU:HB2	2.01	0.43
2:B:118:THR:HG23	7:G:152:VAL:HG12	1.99	0.43
6:F:329:TYR:OH	6:F:435:THR:O	2.32	0.43
8:H:155:ASN:ND2	9:I:104:ILE:O	2.52	0.43
11:K:18:VAL:HG22	14:N:92:PRO:HB3	2.00	0.43
14:N:22:PHE:HB3	14:N:135:ASP:HB2	2.01	0.43
2:B:421:SER:HA	2:B:424:TYR:CE2	2.54	0.43
8:H:59:THR:HG23	8:H:348:VAL:HG22	2.01	0.43
9:I:53:ARG:HA	9:I:120:VAL:HG21	2.01	0.43
2:B:442:GLU:HG3	2:B:445:ARG:HH21	1.83	0.43
6:F:340:SER:OG	6:F:515:ILE:O	2.35	0.43
14:N:61:GLN:H	14:N:82:PRO:HB3	1.83	0.43
1:A:237:ALA:HB3	20:A:403:PL9:O2	2.18	0.42
1:A:252:MET:HB3	3:C:37:LEU:HD23	2.01	0.42
2:B:387:PRO:HB3	4:D:141:LEU:HG	2.01	0.42
4:D:427:VAL:HG12	6:F:183:ARG:HD2	2.01	0.42
2:B:86:LEU:HD11	2:B:334:LEU:HA	2.01	0.42
5:E:46:ILE:HG22	7:G:53:MET:HG3	2.00	0.42
11:K:145:LEU:HD13	11:K:158:ALA:HB2	2.01	0.42
2:B:167:LEU:HD13	5:E:80:ILE:HD12	1.99	0.42
2:B:346:CYS:HB2	2:B:376:LEU:HD13	2.02	0.42
4:D:185:LEU:HD23	4:D:196:PHE:HZ	1.84	0.42
4:D:465:PHE:HA	22:F:703:LHG:H122	2.00	0.42
5:E:31:LEU:HD13	5:E:81:ILE:HD11	2.01	0.42
8:H:153:PHE:CD2	8:H:154:ILE:HG23	2.54	0.42
9:I:173:LEU:HD11	9:I:177:ALA:HB3	2.00	0.42
1:A:230:LEU:N	1:A:230:LEU:CD1	2.82	0.42
4:D:34:ILE:HG12	4:D:114:ARG:HG2	2.01	0.42
4:D:361:ILE:HG22	4:D:363:GLU:H	1.84	0.42
6:F:92:LEU:HD13	6:F:343:LEU:HD13	2.01	0.42
8:H:58:ARG:NH2	8:H:66:TYR:OH	2.52	0.42
9:I:75:ILE:HD12	9:I:102:VAL:HG12	2.01	0.42
10:J:158:THR:O	15:O:32:TYR:OH	2.30	0.42
1:A:172:TYR:OH	1:A:340:LEU:O	2.35	0.42
2:B:33:LEU:HD13	3:C:121:VAL:HG12	2.00	0.42
2:B:242:PRO:HD3	2:B:348:ILE:HD11	2.01	0.42
3:C:49:ARG:HB3	11:K:181:HIS:HB3	2.01	0.42
4:D:228:ILE:HG12	4:D:318:LEU:HD11	2.01	0.42
4:D:317:VAL:O	4:D:321:ILE:HG12	2.19	0.42
6:F:188:GLY:HA2	6:F:191:LEU:HB2	2.02	0.42
2:B:336:TYR:HA	2:B:339:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:322:ALA:O	4:D:411:TYR:OH	2.28	0.42
6:F:81:LEU:HD22	6:F:197:PHE:HE2	1.83	0.42
6:F:93:ALA:HB2	6:F:279:ARG:HH12	1.84	0.42
6:F:183:ARG:HD3	6:F:186:ASP:HB2	2.02	0.42
9:I:24:GLY:HA2	9:I:27:VAL:HG22	2.01	0.42
10:J:102:ARG:HD2	15:O:20:LEU:HD13	2.01	0.42
1:A:231:PRO:HB2	1:A:335:VAL:HG22	2.02	0.42
8:H:231:LYS:HG2	8:H:252:VAL:HG11	2.01	0.42
10:J:141:ILE:HG23	10:J:142:LEU:HG	2.00	0.42
2:B:434:VAL:HA	4:D:156:ILE:HG12	2.02	0.42
11:K:114:MET:O	11:K:118:THR:OG1	2.36	0.42
1:A:199:GLN:O	1:A:206:SER:OG	2.31	0.42
9:I:131:ARG:HH21	9:I:132:HIS:CE1	2.38	0.42
1:A:185:MET:HB3	1:A:185:MET:HE2	1.82	0.41
6:F:302:ALA:HA	6:F:325:SER:HA	2.01	0.41
8:H:28:LEU:HD23	8:H:28:LEU:HA	1.78	0.41
9:I:131:ARG:NH2	10:J:167:ALA:O	2.53	0.41
2:B:21:LEU:HD12	2:B:21:LEU:HA	1.88	0.41
6:F:191:LEU:HB3	6:F:232:LEU:HD13	2.02	0.41
10:J:157:ILE:HG13	15:O:59:VAL:HG11	2.02	0.41
1:A:65:PRO:HA	11:K:69:ARG:HA	2.02	0.41
6:F:442:THR:HA	6:F:445:TYR:CE2	2.55	0.41
8:H:209:LYS:HA	8:H:209:LYS:HD2	1.80	0.41
21:N:201:SQD:H1	21:N:201:SQD:H45	1.83	0.41
1:A:335:VAL:HA	8:H:203:ARG:NH1	2.35	0.41
2:B:137:VAL:HG12	7:G:149:LEU:HD23	2.02	0.41
2:B:396:ILE:HD13	2:B:396:ILE:HA	1.94	0.41
8:H:289:GLU:HB2	9:I:184:PRO:HD3	2.03	0.41
9:I:45:LYS:HB2	9:I:154:VAL:HG11	2.03	0.41
20:A:403:PL9:HC71	20:A:403:PL9:H112	1.83	0.41
2:B:258:LEU:O	2:B:262:PHE:HB2	2.20	0.41
3:C:50:MET:HG2	13:M:32:ASN:ND2	2.35	0.41
10:J:157:ILE:HG21	15:O:33:LEU:HD11	2.02	0.41
6:F:13:VAL:HG22	22:F:706:LHG:H382	2.03	0.41
6:F:239:ALA:O	6:F:249:TRP:NE1	2.53	0.41
1:A:46:LEU:HD22	1:A:76:PRO:HB2	2.02	0.41
1:A:47:VAL:HG11	12:L:52:THR:HG23	2.01	0.41
2:B:334:LEU:HD21	2:B:481:LEU:HD22	2.02	0.41
4:D:283:ILE:HD13	4:D:283:ILE:HA	1.96	0.41
8:H:74:ALA:HB1	8:H:109:ASN:HB3	2.01	0.41
8:H:226:ARG:NH2	8:H:233:ASP:OD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:119:TRP:NE1	11:K:201:TYR:OH	2.45	0.41
1:A:92:ALA:HA	3:C:53:LEU:HB3	2.02	0.41
5:E:88:ARG:HH21	5:E:95:LYS:HB3	1.85	0.41
7:G:148:GLU:O	7:G:151:SER:OG	2.39	0.41
13:M:12:ILE:HG21	13:M:70:LEU:HD22	2.03	0.41
1:A:91:PRO:HB3	11:K:79:ARG:HH12	1.85	0.41
1:A:346:LYS:O	9:I:10:TYR:OH	2.38	0.41
2:B:263:LEU:HD12	2:B:318:PHE:HZ	1.86	0.41
21:B:601:SQD:H352	21:B:601:SQD:H131	2.02	0.41
4:D:310:SER:HA	4:D:339:HIS:HE2	1.86	0.41
5:E:31:LEU:HD21	5:E:77:GLY:HA3	2.03	0.41
8:H:48:HIS:O	11:K:130:SER:OG	2.31	0.41
8:H:226:ARG:NH1	8:H:268:GLU:OE2	2.54	0.41
8:H:263:ILE:HD13	8:H:263:ILE:HA	1.91	0.41
8:H:371:LYS:HD2	8:H:371:LYS:HA	1.80	0.41
10:J:166:GLU:OE2	14:N:76:ARG:NH1	2.47	0.41
6:F:44:ILE:HG23	6:F:129:SER:HB3	2.02	0.41
6:F:353:LYS:HD3	6:F:353:LYS:HA	1.91	0.41
9:I:159:GLU:HG2	9:I:160:PHE:H	1.86	0.41
11:K:40:LEU:HD11	14:N:28:GLY:HA3	2.02	0.41
11:K:89:THR:OG1	11:K:117:CYS:SG	2.65	0.41
1:A:151:TYR:CE2	7:G:33:VAL:HG21	2.56	0.40
4:D:276:LYS:HB3	4:D:276:LYS:HE3	1.85	0.40
13:M:31:LEU:HD22	13:M:53:PHE:CG	2.55	0.40
7:G:10:ILE:HD13	7:G:10:ILE:HA	1.95	0.40
8:H:76:MET:HG3	8:H:156:ASN:HD22	1.86	0.40
10:J:157:ILE:H	15:O:25:SER:HB3	1.86	0.40
11:K:16:PRO:HB3	13:M:95:ASN:HD21	1.86	0.40
17:Q:16:ASP:OD1	17:Q:16:ASP:N	2.52	0.40
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.91	0.40
4:D:180:ILE:HG12	4:D:221:ALA:HB1	2.03	0.40
6:F:212:LEU:HD22	6:F:283:VAL:HG13	2.03	0.40
11:K:10:LEU:HD23	11:K:10:LEU:HA	1.87	0.40
13:M:12:ILE:HD13	13:M:12:ILE:HA	1.89	0.40
3:C:66:ALA:HB1	8:H:4:ILE:HD13	2.02	0.40
3:C:124:TRP:HE1	22:I:201:LHG:HC61	1.86	0.40
21:C:201:SQD:H121	7:G:11:THR:HG21	2.03	0.40
6:F:147:VAL:HG11	6:F:276:LEU:HD13	2.02	0.40
11:K:183:LEU:HD23	11:K:183:LEU:HA	1.85	0.40
13:M:82:ARG:HG3	13:M:103:LEU:HB3	2.03	0.40
1:A:181:LEU:HD11	3:C:92:TYR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:GLN:HB3	19:A:402:DGD:HD5	2.04	0.40
19:A:402:DGD:HA72	12:L:17:ALA:HA	2.03	0.40
2:B:111:GLU:OE1	3:C:122:TYR:OH	2.32	0.40
6:F:203:PHE:HD1	6:F:203:PHE:HA	1.79	0.40
7:G:51:ILE:HD13	7:G:51:ILE:HA	1.85	0.40
8:H:10:PRO:HG3	8:H:33:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/372 (98%)	341 (93%)	23 (6%)	1 (0%)	36	70
2	B	486/515 (94%)	456 (94%)	30 (6%)	0	100	100
3	C	118/132 (89%)	110 (93%)	8 (7%)	0	100	100
4	D	502/529 (95%)	485 (97%)	17 (3%)	0	100	100
5	E	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
6	F	633/656 (96%)	580 (92%)	53 (8%)	0	100	100
7	G	168/200 (84%)	155 (92%)	13 (8%)	0	100	100
8	H	391/394 (99%)	347 (89%)	44 (11%)	0	100	100
9	I	187/196 (95%)	166 (89%)	21 (11%)	0	100	100
10	J	156/168 (93%)	141 (90%)	15 (10%)	0	100	100
11	K	202/237 (85%)	187 (93%)	15 (7%)	0	100	100
12	L	71/76 (93%)	61 (86%)	10 (14%)	0	100	100
13	M	109/111 (98%)	92 (84%)	17 (16%)	0	100	100
14	N	143/150 (95%)	126 (88%)	17 (12%)	0	100	100
15	O	66/70 (94%)	63 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	39/44 (89%)	36 (92%)	3 (8%)	0	100	100
17	Q	42/45 (93%)	41 (98%)	1 (2%)	0	100	100
18	S	58/110 (53%)	56 (97%)	2 (3%)	0	100	100
All	All	3835/4106 (93%)	3533 (92%)	301 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	LEU

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	A	298/302 (99%)	296 (99%)	2 (1%)	76	86
2	B	392/413 (95%)	392 (100%)	0	100	100
3	C	99/109 (91%)	98 (99%)	1 (1%)	68	84
4	D	403/424 (95%)	402 (100%)	1 (0%)	87	92
5	E	82/82 (100%)	82 (100%)	0	100	100
6	F	511/527 (97%)	510 (100%)	1 (0%)	87	92
7	G	138/166 (83%)	137 (99%)	1 (1%)	76	86
8	H	337/338 (100%)	335 (99%)	2 (1%)	78	88
9	I	165/172 (96%)	163 (99%)	2 (1%)	63	82
10	J	139/148 (94%)	138 (99%)	1 (1%)	76	86
11	K	173/196 (88%)	173 (100%)	0	100	100
12	L	61/63 (97%)	61 (100%)	0	100	100
13	M	96/96 (100%)	95 (99%)	1 (1%)	68	84
14	N	118/120 (98%)	118 (100%)	0	100	100
15	O	57/59 (97%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	35/37 (95%)	35 (100%)	0	100	100
17	Q	31/32 (97%)	31 (100%)	0	100	100
18	S	53/97 (55%)	52 (98%)	1 (2%)	50	76
All	All	3188/3381 (94%)	3175 (100%)	13 (0%)	81	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	PHE
1	A	233	ASP
3	C	43	LEU
4	D	229	VAL
6	F	258	THR
7	G	142	ASP
8	H	25	VAL
8	H	83	VAL
9	I	75	ILE
9	I	144	ILE
10	J	158	THR
13	M	22	VAL
18	S	75	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	155	ASN
1	A	199	GLN
1	A	299	ASN
3	C	71	ASN
4	D	55	ASN
4	D	134	GLN
4	D	163	GLN
4	D	266	ASN
4	D	274	HIS
4	D	288	ASN
4	D	335	GLN
5	E	39	ASN
5	E	97	ASN
6	F	66	HIS

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Mol	Chain	Res	Type
6	F	117	HIS
6	F	217	ASN
6	F	374	ASN
6	F	574	GLN
6	F	607	ASN
7	G	138	HIS
8	H	60	ASN
8	H	157	ASN
8	H	217	ASN
8	H	290	ASN
8	H	310	GLN
9	I	135	ASN
10	J	64	GLN
10	J	73	GLN
10	J	120	GLN
11	K	32	ASN
11	K	200	GLN
11	K	203	ASN
12	L	70	GLN
13	M	32	ASN
13	M	59	ASN
13	M	95	ASN
18	S	55	ASN
18	S	64	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
21	SQD	N	201	-	37,38,54	2.20	11 (29%)	46,49,65	6.41	7 (15%)
19	DGD	A	402	-	63,63,67	1.22	7 (11%)	77,77,81	1.10	4 (5%)
26	SF4	K	301	11	0,12,12	-	-	-	-	-
23	BCR	D	602	-	41,41,41	5.44	17 (41%)	56,56,56	5.57	32 (57%)
25	LMG	F	702	-	47,47,55	0.85	2 (4%)	55,55,63	1.43	9 (16%)
21	SQD	C	201	-	39,40,54	2.16	11 (28%)	48,51,65	6.13	7 (14%)
22	LHG	F	705	-	44,44,48	0.93	4 (9%)	47,50,54	1.09	2 (4%)
22	LHG	F	706	-	43,43,48	0.94	4 (9%)	46,49,54	1.05	2 (4%)
20	PL9	A	403	-	19,19,55	1.74	5 (26%)	24,25,69	1.70	7 (29%)
21	SQD	B	601	-	53,54,54	1.90	11 (20%)	62,65,65	5.64	6 (9%)
19	DGD	A	401	-	56,56,67	1.29	7 (12%)	70,70,81	1.13	3 (4%)
22	LHG	D	601	-	45,45,48	0.92	4 (8%)	48,51,54	1.08	2 (4%)
22	LHG	C	202	-	42,42,48	0.97	4 (9%)	45,48,54	1.07	2 (4%)
25	LMG	F	704	-	40,40,55	0.86	1 (2%)	48,48,63	1.27	6 (12%)
22	LHG	I	201	-	43,43,48	0.93	3 (6%)	46,49,54	1.14	2 (4%)
24	LMT	D	603	-	36,36,36	1.16	5 (13%)	47,47,47	1.06	4 (8%)
23	BCR	F	701	-	41,41,41	5.46	17 (41%)	56,56,56	5.49	35 (62%)
26	SF4	I	202	9	0,12,12	-	-	-	-	-
26	SF4	I	203	9	0,12,12	-	-	-	-	-
22	LHG	F	703	-	48,48,48	0.91	4 (8%)	51,54,54	1.06	2 (3%)

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
21	SQD	N	201	-	-	19/33/53/69	0/1/1/1
19	DGD	A	402	-	-	18/51/91/95	0/2/2/2
26	SF4	K	301	11	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	D	602	-	-	16/29/63/63	0/2/2/2
25	LMG	F	702	-	-	13/42/62/70	0/1/1/1
21	SQD	C	201	-	-	24/35/55/69	0/1/1/1
22	LHG	F	705	-	-	21/49/49/53	-
22	LHG	F	706	-	-	26/48/48/53	-
20	PL9	A	403	-	-	6/10/30/73	0/1/1/1
21	SQD	B	601	-	-	23/49/69/69	0/1/1/1
19	DGD	A	401	-	-	15/44/84/95	0/2/2/2
22	LHG	D	601	-	-	15/50/50/53	-
22	LHG	C	202	-	-	19/47/47/53	-
25	LMG	F	704	-	-	14/35/55/70	0/1/1/1
22	LHG	I	201	-	-	26/48/48/53	-
24	LMT	D	603	-	-	9/21/61/61	0/2/2/2
23	BCR	F	701	-	-	14/29/63/63	0/2/2/2
26	SF4	I	202	9	-	-	0/6/5/5
26	SF4	I	203	9	-	-	0/6/5/5
22	LHG	F	703	-	-	21/53/53/53	-

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	701	BCR	C10-C9	14.86	1.55	1.35
23	D	602	BCR	C10-C9	14.81	1.55	1.35
23	F	701	BCR	C17-C18	14.30	1.54	1.35
23	F	701	BCR	C14-C13	14.27	1.54	1.35
23	D	602	BCR	C17-C18	13.75	1.54	1.35
23	D	602	BCR	C21-C22	13.68	1.53	1.35
23	D	602	BCR	C14-C13	13.60	1.53	1.35
23	F	701	BCR	C21-C22	13.39	1.53	1.35
23	F	701	BCR	C26-C25	12.50	1.56	1.34
23	D	602	BCR	C26-C25	12.40	1.55	1.34
23	D	602	BCR	C5-C6	11.97	1.55	1.34
23	F	701	BCR	C5-C6	11.31	1.54	1.34
21	C	201	SQD	O9-S	7.27	1.66	1.45
21	B	601	SQD	O9-S	7.26	1.66	1.45
21	N	201	SQD	O9-S	7.15	1.66	1.45
21	B	601	SQD	O8-S	5.37	1.66	1.47
21	C	201	SQD	O8-S	5.34	1.66	1.47
21	N	201	SQD	O8-S	5.26	1.66	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	403	PL9	C7-C3	-5.03	1.46	1.51
21	B	601	SQD	O5-C5	4.33	1.54	1.44
21	N	201	SQD	C6-S	-4.19	1.62	1.77
23	D	602	BCR	C23-C22	4.17	1.54	1.45
21	N	201	SQD	O5-C5	4.14	1.54	1.44
21	C	201	SQD	O5-C5	4.12	1.54	1.44
21	B	601	SQD	C6-S	-4.07	1.62	1.77
21	C	201	SQD	C6-S	-3.96	1.62	1.77
23	F	701	BCR	C23-C22	3.89	1.54	1.45
23	F	701	BCR	C11-C10	3.83	1.55	1.43
23	D	602	BCR	C11-C10	3.80	1.55	1.43
23	F	701	BCR	C15-C14	3.74	1.55	1.43
23	D	602	BCR	C15-C14	3.62	1.54	1.43
19	A	401	DGD	O6E-C1E	3.59	1.51	1.41
19	A	402	DGD	O6E-C1E	3.54	1.50	1.41
23	F	701	BCR	C16-C17	3.39	1.54	1.43
23	D	602	BCR	C16-C17	3.36	1.53	1.43
20	A	403	PL9	C3-C4	-3.36	1.44	1.49
19	A	402	DGD	O6D-C1D	3.36	1.50	1.41
19	A	401	DGD	O2G-C1B	3.36	1.43	1.34
23	D	602	BCR	C24-C25	3.32	1.56	1.45
19	A	401	DGD	O6D-C1D	3.30	1.50	1.41
23	D	602	BCR	C7-C6	3.29	1.56	1.45
23	D	602	BCR	C20-C21	3.24	1.53	1.43
21	C	201	SQD	O48-C23	3.21	1.42	1.33
19	A	402	DGD	O2G-C1B	3.16	1.43	1.34
23	F	701	BCR	C20-C21	3.16	1.53	1.43
23	F	701	BCR	C7-C6	3.13	1.56	1.45
23	F	701	BCR	C12-C13	3.09	1.52	1.45
23	F	701	BCR	C19-C18	3.06	1.52	1.45
21	N	201	SQD	O48-C23	3.04	1.42	1.33
21	B	601	SQD	O48-C23	3.04	1.42	1.33
23	D	602	BCR	C12-C13	2.99	1.52	1.45
23	F	701	BCR	C24-C25	2.89	1.55	1.45
23	D	602	BCR	C19-C18	2.88	1.52	1.45
21	C	201	SQD	O47-C45	-2.81	1.39	1.46
21	B	601	SQD	O47-C45	-2.73	1.39	1.46
24	D	603	LMT	O3'-C3'	-2.72	1.36	1.43
22	F	703	LHG	O7-C5	-2.63	1.40	1.46
22	F	705	LHG	O7-C5	-2.62	1.40	1.46
19	A	401	DGD	O1G-C1G	-2.61	1.39	1.45
20	A	403	PL9	C6-C1	-2.59	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	402	DGD	O1G-C1A	2.58	1.40	1.33
22	I	201	LHG	O7-C7	2.53	1.41	1.34
21	C	201	SQD	O47-C7	2.52	1.41	1.34
22	C	202	LHG	O7-C5	-2.51	1.40	1.46
22	F	706	LHG	O7-C5	-2.49	1.40	1.46
22	C	202	LHG	O8-C23	2.49	1.40	1.33
23	D	602	BCR	C8-C9	2.47	1.51	1.45
21	N	201	SQD	O47-C7	2.47	1.41	1.34
21	B	601	SQD	O47-C7	2.46	1.41	1.34
22	D	601	LHG	O8-C23	2.44	1.40	1.33
22	I	201	LHG	O8-C23	2.44	1.40	1.33
22	D	601	LHG	O7-C5	-2.42	1.40	1.46
21	B	601	SQD	O5-C1	2.42	1.48	1.41
19	A	402	DGD	O1G-C1G	-2.42	1.39	1.45
23	F	701	BCR	C8-C9	2.42	1.51	1.45
22	F	703	LHG	O8-C23	2.41	1.40	1.33
23	F	701	BCR	C38-C26	2.41	1.54	1.50
21	B	601	SQD	O2-C2	2.40	1.48	1.43
21	B	601	SQD	C3-C2	-2.40	1.46	1.52
19	A	401	DGD	O1G-C1A	2.39	1.40	1.33
21	C	201	SQD	O5-C1	2.39	1.47	1.41
21	C	201	SQD	O2-C2	2.39	1.48	1.43
22	F	706	LHG	O8-C23	2.37	1.40	1.33
24	D	603	LMT	O2B-C2B	-2.37	1.37	1.43
25	F	702	LMG	O6-C1	2.35	1.47	1.41
21	N	201	SQD	O47-C45	-2.35	1.40	1.46
22	F	705	LHG	O8-C23	2.35	1.40	1.33
19	A	401	DGD	O5D-C1E	-2.33	1.36	1.40
25	F	704	LMG	O7-C8	-2.31	1.40	1.46
24	D	603	LMT	O2'-C2'	-2.26	1.37	1.43
21	B	601	SQD	O3-C3	2.26	1.48	1.43
21	C	201	SQD	O3-C3	2.26	1.48	1.43
21	N	201	SQD	O5-C1	2.25	1.47	1.41
21	N	201	SQD	O2-C2	2.25	1.48	1.43
24	D	603	LMT	O3B-C3B	-2.24	1.37	1.43
21	N	201	SQD	O3-C3	2.24	1.48	1.43
22	D	601	LHG	O7-C7	2.23	1.40	1.34
22	C	202	LHG	O7-C7	2.23	1.40	1.34
21	N	201	SQD	C3-C2	-2.22	1.46	1.52
22	F	706	LHG	O7-C7	2.21	1.40	1.34
24	D	603	LMT	O4'-C4B	-2.19	1.37	1.43
22	F	705	LHG	O8-C6	-2.17	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	F	702	LMG	C4-C5	2.17	1.57	1.53
22	C	202	LHG	O8-C6	-2.17	1.40	1.45
22	D	601	LHG	O8-C6	-2.17	1.40	1.45
22	F	703	LHG	O8-C6	-2.16	1.40	1.45
22	F	706	LHG	O8-C6	-2.14	1.40	1.45
19	A	402	DGD	O2G-C2G	-2.14	1.41	1.46
23	D	602	BCR	C38-C26	2.11	1.54	1.50
19	A	402	DGD	O5D-C1E	-2.10	1.36	1.40
21	C	201	SQD	C3-C2	-2.10	1.47	1.52
22	I	201	LHG	O8-C6	-2.10	1.40	1.45
20	A	403	PL9	C53-C6	-2.08	1.46	1.50
22	F	703	LHG	O7-C7	2.07	1.40	1.34
20	A	403	PL9	C52-C5	-2.07	1.46	1.50
22	F	705	LHG	O7-C7	2.07	1.40	1.34
19	A	401	DGD	O3G-C1D	-2.02	1.36	1.40

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	601	SQD	O9-S-C6	29.43	141.92	106.94
21	C	201	SQD	O9-S-C6	29.31	141.77	106.94
21	N	201	SQD	O9-S-C6	29.18	141.61	106.94
21	B	601	SQD	O7-S-C6	-28.40	73.19	106.94
21	N	201	SQD	O7-S-C6	-27.41	74.36	106.94
21	C	201	SQD	O7-S-C6	-25.38	76.77	106.94
23	F	701	BCR	C33-C5-C6	-14.12	108.67	124.53
23	F	701	BCR	C11-C10-C9	-13.44	108.12	127.31
23	D	602	BCR	C33-C5-C6	-12.93	110.01	124.53
23	D	602	BCR	C15-C14-C13	-11.86	110.39	127.31
23	D	602	BCR	C16-C17-C18	-11.65	110.68	127.31
21	B	601	SQD	O8-S-O7	11.51	139.40	111.27
23	D	602	BCR	C11-C10-C9	-11.41	111.03	127.31
21	C	201	SQD	O8-S-O7	11.38	139.09	111.27
23	F	701	BCR	C16-C17-C18	-11.24	111.27	127.31
23	D	602	BCR	C38-C26-C25	-11.19	111.96	124.53
21	N	201	SQD	O8-S-O7	11.15	138.52	111.27
21	B	601	SQD	O9-S-O7	-10.73	76.81	113.95
23	D	602	BCR	C36-C18-C17	-10.66	107.98	122.92
21	N	201	SQD	O9-S-O7	-10.66	77.04	113.95
23	D	602	BCR	C35-C13-C14	-10.59	108.09	122.92
21	C	201	SQD	O9-S-O7	-10.57	77.37	113.95
23	F	701	BCR	C34-C9-C10	-10.24	108.58	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	602	BCR	C34-C9-C10	-10.14	108.72	122.92
23	F	701	BCR	C38-C26-C25	-10.10	113.19	124.53
23	F	701	BCR	C23-C22-C21	-9.37	104.56	118.94
23	F	701	BCR	C36-C18-C17	-9.19	110.05	122.92
23	F	701	BCR	C37-C22-C21	-9.03	110.27	122.92
23	F	701	BCR	C15-C14-C13	-8.81	114.73	127.31
23	D	602	BCR	C37-C22-C21	-8.38	111.19	122.92
23	D	602	BCR	C20-C21-C22	-8.12	115.72	127.31
23	F	701	BCR	C35-C13-C14	-8.01	111.70	122.92
23	F	701	BCR	C20-C21-C22	-7.55	116.54	127.31
23	F	701	BCR	C19-C18-C17	-7.39	107.60	118.94
23	D	602	BCR	C19-C18-C17	-7.18	107.92	118.94
23	D	602	BCR	C30-C25-C26	-7.03	112.72	122.61
23	D	602	BCR	C23-C22-C21	-6.87	108.39	118.94
23	D	602	BCR	C8-C9-C10	-6.86	108.42	118.94
23	F	701	BCR	C12-C13-C14	-6.66	108.72	118.94
23	F	701	BCR	C4-C5-C6	-6.36	113.50	122.73
23	F	701	BCR	C35-C13-C12	-6.32	108.12	118.08
23	D	602	BCR	C12-C13-C14	-6.27	109.31	118.94
23	D	602	BCR	C27-C26-C25	-6.08	113.91	122.73
23	D	602	BCR	C37-C22-C23	-5.83	108.89	118.08
23	F	701	BCR	C27-C26-C25	-5.74	114.40	122.73
23	F	701	BCR	C1-C6-C5	-5.65	114.66	122.61
23	F	701	BCR	C34-C9-C8	-5.51	109.40	118.08
23	D	602	BCR	C35-C13-C12	-5.46	109.47	118.08
23	D	602	BCR	C33-C5-C4	-5.17	103.69	113.62
23	D	602	BCR	C24-C23-C22	-5.13	118.49	126.23
23	D	602	BCR	C4-C5-C6	-5.11	115.31	122.73
23	F	701	BCR	C37-C22-C23	-4.92	110.33	118.08
23	F	701	BCR	C7-C6-C5	-4.82	109.78	121.46
23	D	602	BCR	C34-C9-C8	-4.77	110.57	118.08
20	A	403	PL9	C7-C3-C4	4.73	120.72	116.88
23	D	602	BCR	C36-C18-C19	-4.68	110.71	118.08
23	D	602	BCR	C1-C6-C5	-4.64	116.08	122.61
23	F	701	BCR	C24-C25-C26	-4.58	110.36	121.46
23	F	701	BCR	C8-C9-C10	-4.56	111.94	118.94
23	F	701	BCR	C30-C25-C26	-4.45	116.34	122.61
22	I	201	LHG	O7-C7-C8	4.37	120.92	111.50
23	F	701	BCR	C36-C18-C19	-4.34	111.24	118.08
23	F	701	BCR	C23-C24-C25	-4.21	115.39	127.20
22	D	601	LHG	O7-C7-C8	4.20	120.56	111.50
23	F	701	BCR	C7-C8-C9	-4.18	119.92	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	202	LHG	O7-C7-C8	4.03	120.19	111.50
19	A	402	DGD	O2G-C1B-C2B	4.01	120.13	111.50
22	F	705	LHG	O7-C7-C8	4.00	120.13	111.50
21	C	201	SQD	O47-C7-C8	3.99	120.10	111.50
21	B	601	SQD	O47-C7-C8	3.96	120.05	111.50
22	F	703	LHG	O7-C7-C8	3.89	119.88	111.50
23	D	602	BCR	C7-C8-C9	-3.87	120.39	126.23
21	N	201	SQD	O47-C7-C8	3.85	119.80	111.50
22	F	706	LHG	O7-C7-C8	3.85	119.79	111.50
19	A	401	DGD	O2G-C1B-C2B	3.72	119.51	111.50
23	F	701	BCR	C29-C30-C25	3.70	116.17	110.48
23	D	602	BCR	C7-C6-C5	-3.62	112.69	121.46
23	F	701	BCR	C33-C5-C4	-3.41	107.07	113.62
20	A	403	PL9	C7-C3-C2	-3.39	118.84	123.30
24	D	603	LMT	O5'-C5'-C4'	2.99	116.06	109.75
23	D	602	BCR	C24-C25-C26	-2.97	114.27	121.46
20	A	403	PL9	C11-C12-C13	-2.89	106.34	112.59
25	F	702	LMG	O6-C5-C4	2.88	114.93	109.69
23	F	701	BCR	C11-C12-C13	-2.87	118.35	126.42
23	F	701	BCR	C38-C26-C27	-2.86	108.13	113.62
21	C	201	SQD	O48-C23-C24	2.83	120.79	111.91
23	D	602	BCR	C1-C6-C7	-2.82	107.81	115.78
22	F	705	LHG	O8-C23-C24	2.77	120.61	111.91
22	F	703	LHG	O8-C23-C24	2.72	120.45	111.91
19	A	402	DGD	O1G-C1A-C2A	2.72	120.44	111.91
22	D	601	LHG	O8-C23-C24	2.70	120.37	111.91
22	C	202	LHG	O8-C23-C24	2.68	120.31	111.91
21	B	601	SQD	O48-C23-C24	2.66	120.27	111.91
23	D	602	BCR	C11-C12-C13	-2.65	118.98	126.42
19	A	401	DGD	C4D-C3D-C2D	2.64	115.43	110.82
19	A	401	DGD	O1G-C1A-C2A	2.62	120.14	111.91
23	F	701	BCR	C16-C15-C14	-2.62	118.11	123.47
22	I	201	LHG	O8-C23-C24	2.59	120.04	111.91
25	F	702	LMG	C1-O6-C5	2.57	118.73	113.69
22	F	706	LHG	O8-C23-C24	2.53	119.86	111.91
25	F	704	LMG	O6-C1-O1	-2.50	104.06	109.97
21	N	201	SQD	O6-C1-C2	2.45	112.12	108.30
23	F	701	BCR	C21-C20-C19	-2.45	115.58	123.22
23	F	701	BCR	C1-C6-C7	-2.43	108.90	115.78
21	N	201	SQD	O48-C23-C24	2.43	119.53	111.91
25	F	702	LMG	O3-C3-C2	-2.42	104.75	110.35
25	F	704	LMG	O1-C1-C2	-2.41	104.54	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	F	702	LMG	O1-C7-C8	-2.40	105.11	110.90
24	D	603	LMT	O5'-C5'-C6'	2.36	112.31	106.44
25	F	704	LMG	O3-C3-C2	-2.36	104.90	110.35
23	F	701	BCR	C8-C7-C6	-2.34	120.64	127.20
20	A	403	PL9	C7-C8-C9	-2.32	122.93	126.79
24	D	603	LMT	O5B-C5B-C4B	2.32	113.91	109.69
25	F	702	LMG	O6-C1-C2	2.31	115.23	110.35
25	F	704	LMG	O7-C10-O9	-2.24	118.28	123.70
25	F	702	LMG	C38-C37-C36	-2.19	103.31	114.42
25	F	704	LMG	O2-C2-C1	-2.19	104.73	110.05
19	A	402	DGD	C4E-C3E-C2E	2.12	114.53	110.82
25	F	702	LMG	C4-C3-C2	-2.11	107.14	110.82
21	C	201	SQD	C4-C3-C2	2.09	114.47	110.82
23	D	602	BCR	C38-C26-C27	-2.09	109.60	113.62
25	F	702	LMG	C1-C2-C3	-2.08	105.66	110.00
20	A	403	PL9	O1-C4-C3	-2.07	118.44	120.72
20	A	403	PL9	O2-C1-C6	2.05	124.14	120.59
23	D	602	BCR	C28-C27-C26	-2.04	110.43	114.08
23	F	701	BCR	C24-C23-C22	-2.03	123.16	126.23
20	A	403	PL9	O2-C1-C2	-2.03	117.13	121.78
23	D	602	BCR	C20-C19-C18	-2.03	120.73	126.42
25	F	702	LMG	O6-C1-O1	-2.02	105.19	109.97
19	A	402	DGD	C2G-O2G-C1B	-2.02	112.82	117.79
24	D	603	LMT	C1'-O5'-C5'	2.02	117.65	113.69
25	F	704	LMG	O1-C7-C8	-2.01	106.04	110.90

There are no chirality outliers.

All (299) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	402	DGD	C2D-C1D-O3G-C3G
19	A	402	DGD	O6D-C1D-O3G-C3G
20	A	403	PL9	C7-C8-C9-C10
21	B	601	SQD	C2-C1-O6-C44
21	B	601	SQD	O5-C1-O6-C44
21	B	601	SQD	O5-C5-C6-S
21	B	601	SQD	C5-C6-S-O9
21	C	201	SQD	C2-C1-O6-C44
21	C	201	SQD	O6-C44-C45-O47
21	C	201	SQD	O10-C23-O48-C46
21	C	201	SQD	C24-C23-O48-C46
21	C	201	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
21	N	201	SQD	C45-C44-O6-C1
21	N	201	SQD	C2-C1-O6-C44
21	N	201	SQD	O49-C7-O47-C45
21	N	201	SQD	C4-C5-C6-S
21	N	201	SQD	C5-C6-S-O7
21	N	201	SQD	C5-C6-S-O8
22	C	202	LHG	O1-C1-C2-C3
22	C	202	LHG	C4-O6-P-O4
22	C	202	LHG	C4-O6-P-O5
22	C	202	LHG	O9-C7-O7-C5
22	D	601	LHG	O1-C1-C2-C3
22	F	703	LHG	O1-C1-C2-C3
22	F	705	LHG	O1-C1-C2-O2
22	F	705	LHG	O1-C1-C2-C3
22	F	705	LHG	C4-O6-P-O3
22	F	705	LHG	C4-O6-P-O4
22	F	706	LHG	C3-O3-P-O4
22	F	706	LHG	C3-O3-P-O5
22	I	201	LHG	O1-C1-C2-C3
22	I	201	LHG	C4-O6-P-O3
22	I	201	LHG	C4-O6-P-O4
22	I	201	LHG	C4-O6-P-O5
22	I	201	LHG	C8-C7-O7-C5
22	I	201	LHG	O10-C23-O8-C6
23	D	602	BCR	C5-C6-C7-C8
23	D	602	BCR	C7-C8-C9-C34
23	D	602	BCR	C11-C10-C9-C8
23	D	602	BCR	C11-C10-C9-C34
23	D	602	BCR	C35-C13-C14-C15
23	D	602	BCR	C16-C17-C18-C36
23	D	602	BCR	C20-C21-C22-C23
23	D	602	BCR	C23-C24-C25-C30
23	F	701	BCR	C5-C6-C7-C8
23	F	701	BCR	C7-C8-C9-C10
23	F	701	BCR	C11-C10-C9-C34
23	F	701	BCR	C11-C12-C13-C35
23	F	701	BCR	C35-C13-C14-C15
23	F	701	BCR	C16-C17-C18-C36
23	F	701	BCR	C20-C21-C22-C37
23	F	701	BCR	C37-C22-C23-C24
24	D	603	LMT	C2'-C1'-O1'-C1
25	F	702	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
25	F	702	LMG	O6-C1-O1-C7
25	F	704	LMG	C11-C10-O7-C8
21	N	201	SQD	O10-C23-O48-C46
22	D	601	LHG	O10-C23-O8-C6
22	F	703	LHG	O10-C23-O8-C6
21	B	601	SQD	O49-C7-O47-C45
22	I	201	LHG	O9-C7-O7-C5
21	N	201	SQD	C24-C23-O48-C46
22	I	201	LHG	C24-C23-O8-C6
21	B	601	SQD	C8-C7-O47-C45
21	N	201	SQD	C8-C7-O47-C45
22	C	202	LHG	C8-C7-O7-C5
21	B	601	SQD	C24-C23-O48-C46
22	D	601	LHG	C24-C23-O8-C6
22	F	703	LHG	C24-C23-O8-C6
25	F	702	LMG	C29-C28-O8-C9
20	A	403	PL9	C7-C8-C9-C11
19	A	401	DGD	O1A-C1A-O1G-C1G
21	B	601	SQD	O10-C23-O48-C46
25	F	702	LMG	O10-C28-O8-C9
24	D	603	LMT	C4'-C5'-C6'-O6'
21	N	201	SQD	C9-C10-C11-C12
19	A	401	DGD	C2A-C1A-O1G-C1G
21	C	201	SQD	O5-C1-O6-C44
21	N	201	SQD	O5-C1-O6-C44
20	A	403	PL9	C9-C11-C12-C13
19	A	401	DGD	C2B-C1B-O2G-C2G
22	F	706	LHG	C1-C2-C3-O3
22	F	705	LHG	C24-C23-O8-C6
22	F	706	LHG	O2-C2-C3-O3
23	D	602	BCR	C11-C12-C13-C35
23	F	701	BCR	C11-C12-C13-C14
23	F	701	BCR	C17-C18-C19-C20
19	A	401	DGD	O1B-C1B-O2G-C2G
22	D	601	LHG	C23-C24-C25-C26
22	F	705	LHG	O10-C23-O8-C6
19	A	402	DGD	C1A-C2A-C3A-C4A
22	D	601	LHG	C7-C8-C9-C10
24	D	603	LMT	O5'-C1'-O1'-C1
24	D	603	LMT	O5'-C5'-C6'-O6'
22	C	202	LHG	C4-O6-P-O3
22	F	703	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
22	F	706	LHG	C3-O3-P-O6
25	F	704	LMG	O9-C10-O7-C8
19	A	402	DGD	C5A-C6A-C7A-C8A
23	D	602	BCR	C20-C21-C22-C37
21	B	601	SQD	C25-C26-C27-C28
22	D	601	LHG	C24-C25-C26-C27
25	F	702	LMG	C30-C31-C32-C33
21	B	601	SQD	C18-C19-C20-C21
22	F	706	LHG	C24-C25-C26-C27
19	A	402	DGD	CEB-CFB-CGB-CHB
21	C	201	SQD	C10-C11-C12-C13
21	B	601	SQD	C26-C27-C28-C29
22	C	202	LHG	C31-C32-C33-C34
22	D	601	LHG	C14-C15-C16-C17
22	F	703	LHG	C27-C28-C29-C30
21	B	601	SQD	C23-C24-C25-C26
22	F	705	LHG	C23-C24-C25-C26
23	D	602	BCR	C16-C17-C18-C19
23	F	701	BCR	C12-C13-C14-C15
21	B	601	SQD	C27-C28-C29-C30
22	F	703	LHG	C26-C27-C28-C29
22	F	706	LHG	C29-C30-C31-C32
22	D	601	LHG	C9-C10-C11-C12
22	I	201	LHG	C12-C13-C14-C15
25	F	704	LMG	C30-C31-C32-C33
23	D	602	BCR	C36-C18-C19-C20
23	D	602	BCR	C37-C22-C23-C24
23	F	701	BCR	C7-C8-C9-C34
22	F	706	LHG	O1-C1-C2-C3
19	A	402	DGD	C6B-C7B-C8B-C9B
21	C	201	SQD	C23-C24-C25-C26
21	C	201	SQD	C11-C10-C9-C8
21	N	201	SQD	C11-C10-C9-C8
22	I	201	LHG	C25-C26-C27-C28
19	A	401	DGD	C3A-C4A-C5A-C6A
19	A	401	DGD	CAB-CBB-CCB-CDB
22	F	703	LHG	C13-C14-C15-C16
22	I	201	LHG	C17-C18-C19-C20
22	D	601	LHG	C31-C32-C33-C34
22	I	201	LHG	C23-C24-C25-C26
22	F	703	LHG	C8-C7-O7-C5
22	F	705	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
22	C	202	LHG	O1-C1-C2-O2
22	D	601	LHG	O1-C1-C2-O2
22	F	703	LHG	O1-C1-C2-O2
22	I	201	LHG	O1-C1-C2-O2
22	D	601	LHG	C10-C11-C12-C13
22	D	601	LHG	C25-C26-C27-C28
22	F	703	LHG	C11-C12-C13-C14
21	B	601	SQD	C11-C10-C9-C8
22	F	705	LHG	C16-C17-C18-C19
22	F	703	LHG	O9-C7-O7-C5
22	F	705	LHG	O9-C7-O7-C5
22	F	705	LHG	C9-C10-C11-C12
24	D	603	LMT	C6-C7-C8-C9
25	F	702	LMG	C31-C32-C33-C34
21	C	201	SQD	C25-C26-C27-C28
19	A	401	DGD	C1B-C2B-C3B-C4B
22	F	706	LHG	C23-C24-C25-C26
23	F	701	BCR	C23-C24-C25-C26
22	F	703	LHG	C10-C11-C12-C13
21	B	601	SQD	C17-C18-C19-C20
21	B	601	SQD	C34-C35-C36-C37
22	F	703	LHG	C23-C24-C25-C26
25	F	702	LMG	C28-C29-C30-C31
19	A	402	DGD	CAA-CBA-CCA-CDA
25	F	702	LMG	C17-C18-C19-C20
22	D	601	LHG	C15-C16-C17-C18
25	F	704	LMG	C28-C29-C30-C31
19	A	402	DGD	C2A-C1A-O1G-C1G
22	I	201	LHG	C18-C19-C20-C21
19	A	401	DGD	C4D-C5D-C6D-O5D
19	A	402	DGD	C2A-C3A-C4A-C5A
22	C	202	LHG	C27-C28-C29-C30
25	F	704	LMG	C14-C15-C16-C17
22	I	201	LHG	C29-C30-C31-C32
22	F	705	LHG	C17-C18-C19-C20
22	I	201	LHG	C14-C15-C16-C17
19	A	401	DGD	C1A-C2A-C3A-C4A
19	A	402	DGD	C2B-C1B-O2G-C2G
19	A	402	DGD	O1B-C1B-O2G-C2G
25	F	704	LMG	C10-C11-C12-C13
21	B	601	SQD	C31-C32-C33-C34
19	A	402	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
25	F	702	LMG	O6-C5-C6-O5
25	F	702	LMG	C18-C19-C20-C21
23	D	602	BCR	C19-C20-C21-C22
25	F	702	LMG	C29-C30-C31-C32
25	F	704	LMG	C33-C34-C35-C36
22	I	201	LHG	C5-C4-O6-P
22	C	202	LHG	C23-C24-C25-C26
19	A	401	DGD	C2A-C3A-C4A-C5A
25	F	702	LMG	C19-C20-C21-C22
22	C	202	LHG	C28-C29-C30-C31
21	N	201	SQD	C44-C45-C46-O48
19	A	402	DGD	O1A-C1A-O1G-C1G
21	B	601	SQD	C45-C44-O6-C1
22	F	706	LHG	O1-C1-C2-O2
22	F	706	LHG	C8-C7-O7-C5
22	F	705	LHG	C31-C32-C33-C34
22	F	705	LHG	C7-C8-C9-C10
19	A	401	DGD	C1G-C2G-O2G-C1B
21	N	201	SQD	C46-C45-O47-C7
22	I	201	LHG	C4-C5-O7-C7
19	A	402	DGD	CBB-CCB-CDB-CEB
22	F	706	LHG	C24-C23-O8-C6
23	D	602	BCR	C7-C8-C9-C10
22	F	703	LHG	C1-C2-C3-O3
25	F	702	LMG	C16-C17-C18-C19
22	F	703	LHG	O2-C2-C3-O3
21	C	201	SQD	C27-C28-C29-C30
22	C	202	LHG	C2-C3-O3-P
22	F	703	LHG	C5-C4-O6-P
21	C	201	SQD	C28-C29-C30-C31
22	C	202	LHG	C24-C23-O8-C6
19	A	402	DGD	O1G-C1G-C2G-C3G
22	F	705	LHG	C4-C5-C6-O8
21	C	201	SQD	C7-C8-C9-C10
21	C	201	SQD	C9-C10-C11-C12
22	F	705	LHG	C14-C15-C16-C17
19	A	401	DGD	C3B-C4B-C5B-C6B
19	A	401	DGD	C4B-C5B-C6B-C7B
25	F	704	LMG	C15-C16-C17-C18
21	C	201	SQD	O47-C45-C46-O48
22	F	705	LHG	O7-C5-C6-O8
22	F	706	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
22	F	706	LHG	O10-C23-O8-C6
22	F	703	LHG	C33-C34-C35-C36
20	A	403	PL9	C12-C13-C14-C15
22	F	706	LHG	C10-C11-C12-C13
19	A	401	DGD	O6D-C5D-C6D-O5D
25	F	704	LMG	C34-C35-C36-C37
21	C	201	SQD	O6-C44-C45-C46
22	C	202	LHG	C4-C5-C6-O8
22	F	706	LHG	C2-C3-O3-P
22	F	706	LHG	C25-C26-C27-C28
22	D	601	LHG	C11-C10-C9-C8
22	C	202	LHG	O10-C23-O8-C6
19	A	402	DGD	CAB-CBB-CCB-CDB
22	C	202	LHG	O7-C5-C6-O8
21	C	201	SQD	C5-C6-S-O8
24	D	603	LMT	C4-C5-C6-C7
22	I	201	LHG	C3-O3-P-O6
22	F	706	LHG	C12-C13-C14-C15
22	F	703	LHG	C2-C3-O3-P
22	F	705	LHG	C2-C3-O3-P
22	I	201	LHG	C2-C3-O3-P
20	A	403	PL9	C3-C7-C8-C9
22	F	703	LHG	C3-O3-P-O4
22	F	705	LHG	C4-O6-P-O5
19	A	401	DGD	C8B-C9B-CAB-CBB
22	I	201	LHG	C26-C27-C28-C29
24	D	603	LMT	C1-C2-C3-C4
21	N	201	SQD	C28-C29-C30-C31
21	C	201	SQD	C44-C45-C46-O48
21	N	201	SQD	O6-C44-C45-O47
21	N	201	SQD	O47-C45-C46-O48
21	B	601	SQD	C24-C25-C26-C27
21	B	601	SQD	C35-C36-C37-C38
22	F	703	LHG	C35-C36-C37-C38
21	N	201	SQD	C26-C27-C28-C29
19	A	402	DGD	CBA-CCA-CDA-CEA
21	N	201	SQD	C10-C11-C12-C13
19	A	402	DGD	C7B-C8B-C9B-CAB
21	B	601	SQD	C28-C29-C30-C31
25	F	704	LMG	O7-C8-C9-O8
22	D	601	LHG	C3-O3-P-O6
22	I	201	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
21	C	201	SQD	C24-C25-C26-C27
22	I	201	LHG	C9-C10-C11-C12
25	F	704	LMG	C29-C28-O8-C9
21	B	601	SQD	C30-C31-C32-C33
22	F	706	LHG	C27-C28-C29-C30
25	F	704	LMG	C7-C8-C9-O8
22	F	705	LHG	C29-C30-C31-C32
25	F	704	LMG	C32-C33-C34-C35
20	A	403	PL9	C12-C11-C9-C10
22	C	202	LHG	C34-C35-C36-C37
22	F	706	LHG	C11-C10-C9-C8
22	F	706	LHG	O7-C7-C8-C9
22	F	705	LHG	C26-C27-C28-C29
22	F	706	LHG	C4-C5-C6-O8
22	F	706	LHG	C14-C15-C16-C17
22	I	201	LHG	O7-C7-C8-C9
23	F	701	BCR	C9-C10-C11-C12
24	D	603	LMT	O5B-C5B-C6B-O6B
22	F	706	LHG	O7-C5-C6-O8
22	I	201	LHG	O7-C5-C6-O8
21	B	601	SQD	C4-C5-C6-S
21	C	201	SQD	C4-C5-C6-S
21	C	201	SQD	C11-C12-C13-C14
22	I	201	LHG	O9-C7-C8-C9
22	F	703	LHG	C9-C10-C11-C12
22	F	706	LHG	O9-C7-C8-C9
23	D	602	BCR	C15-C16-C17-C18
21	C	201	SQD	O5-C5-C6-S
21	C	201	SQD	O48-C23-C24-C25
22	C	202	LHG	C32-C33-C34-C35
25	F	704	LMG	C36-C37-C38-C39
22	C	202	LHG	C1-C2-C3-O3
21	C	201	SQD	O10-C23-C24-C25
24	D	603	LMT	O1'-C1-C2-C3
22	F	706	LHG	O8-C23-C24-C25

There are no ring outliers.

17 monomers are involved in 37 short contacts:

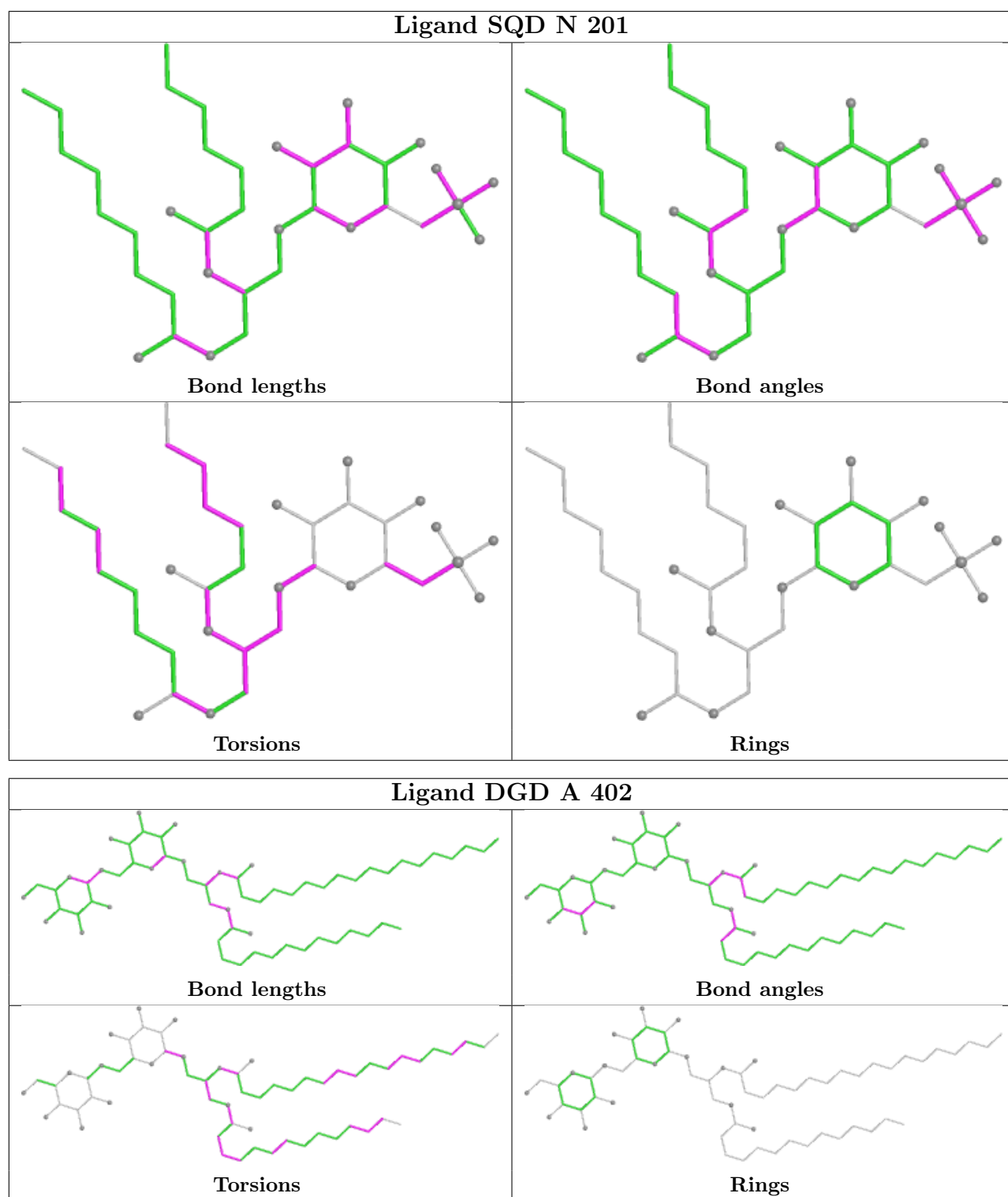
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	N	201	SQD	2	0
19	A	402	DGD	4	0

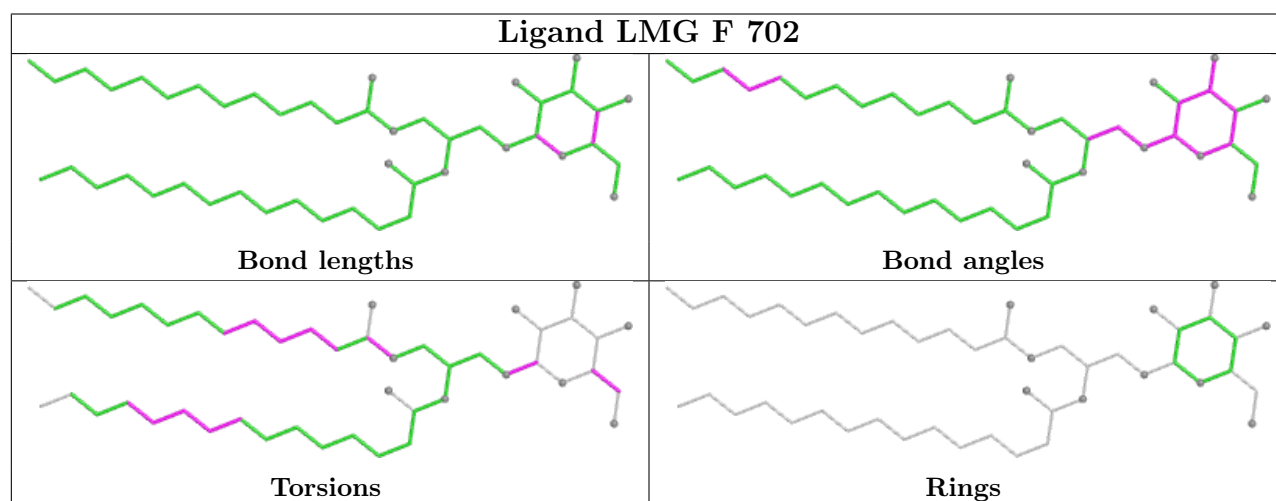
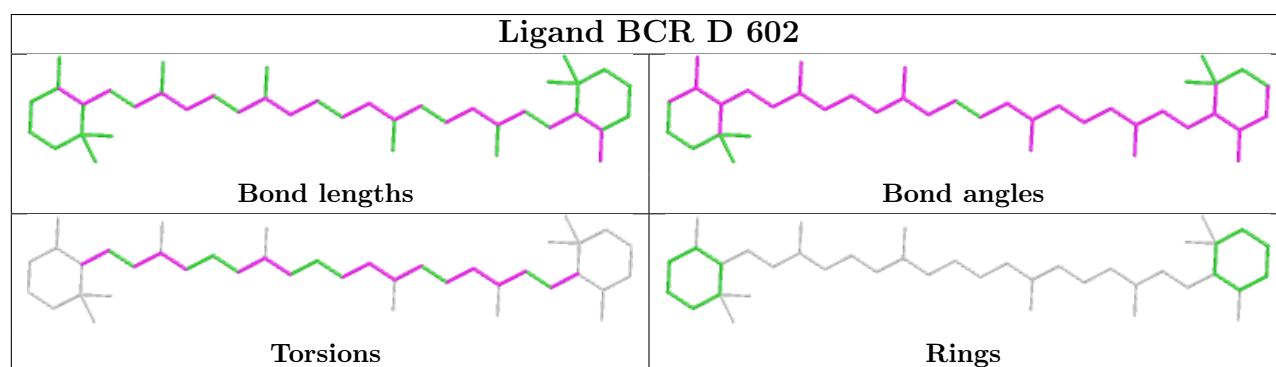
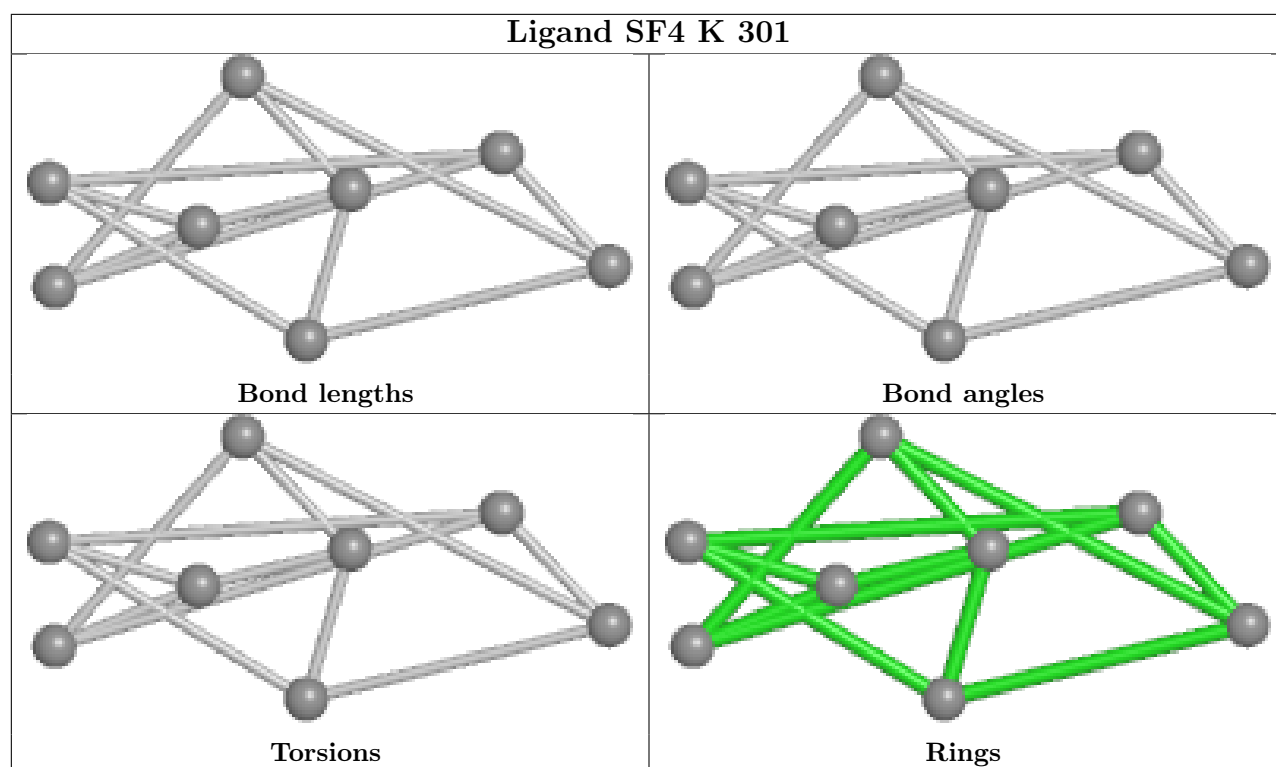
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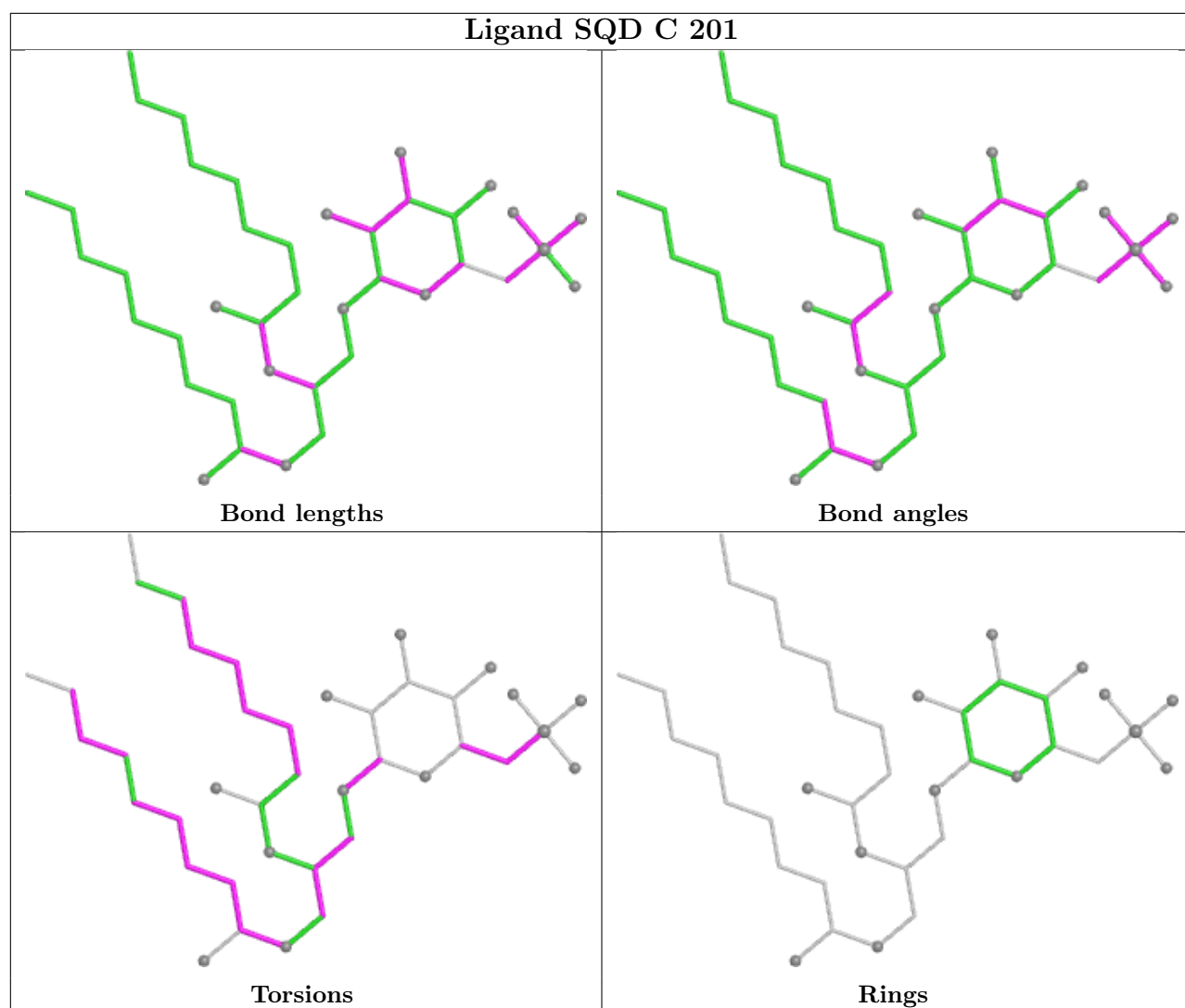
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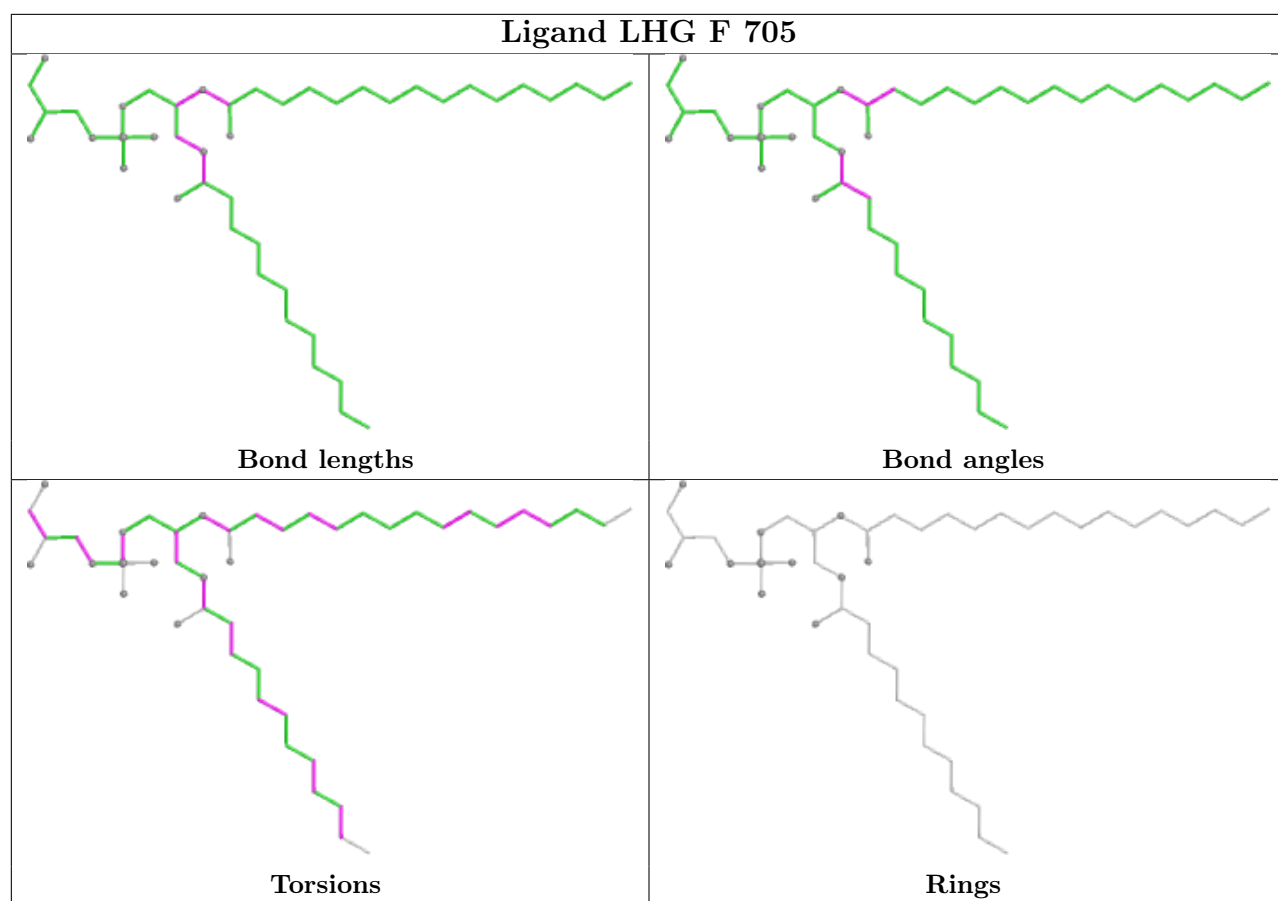
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	602	BCR	3	0
25	F	702	LMG	1	0
21	C	201	SQD	1	0
22	F	705	LHG	1	0
22	F	706	LHG	2	0
20	A	403	PL9	4	0
21	B	601	SQD	6	0
19	A	401	DGD	1	0
22	D	601	LHG	1	0
22	C	202	LHG	2	0
22	I	201	LHG	1	0
23	F	701	BCR	4	0
26	I	202	SF4	1	0
26	I	203	SF4	1	0
22	F	703	LHG	2	0

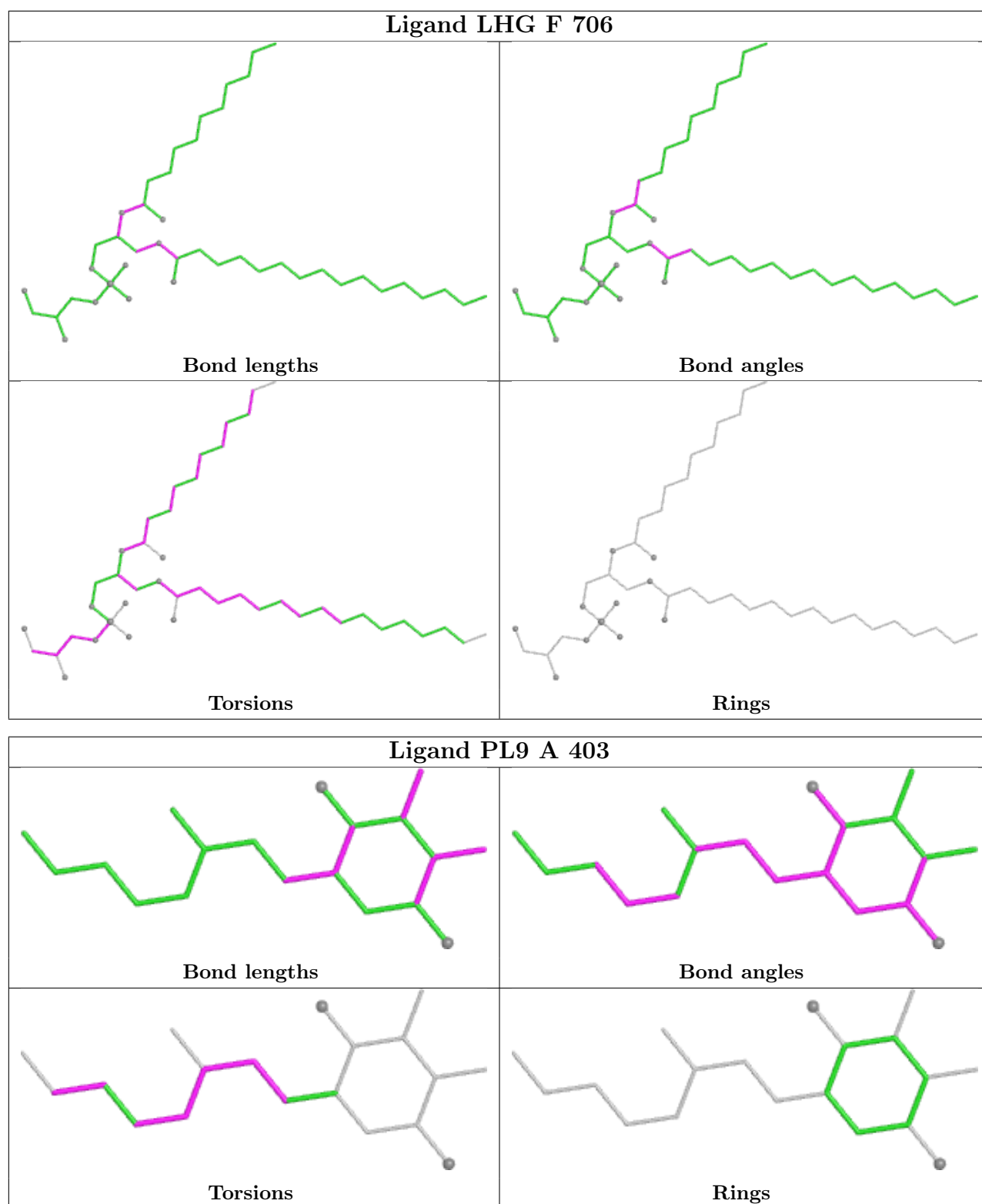
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

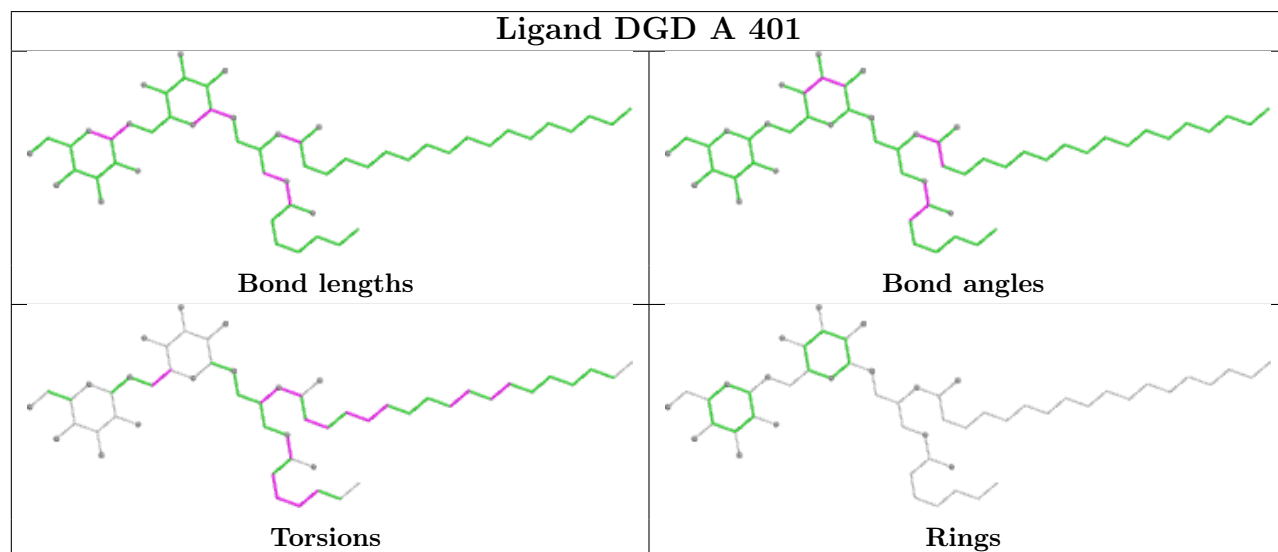
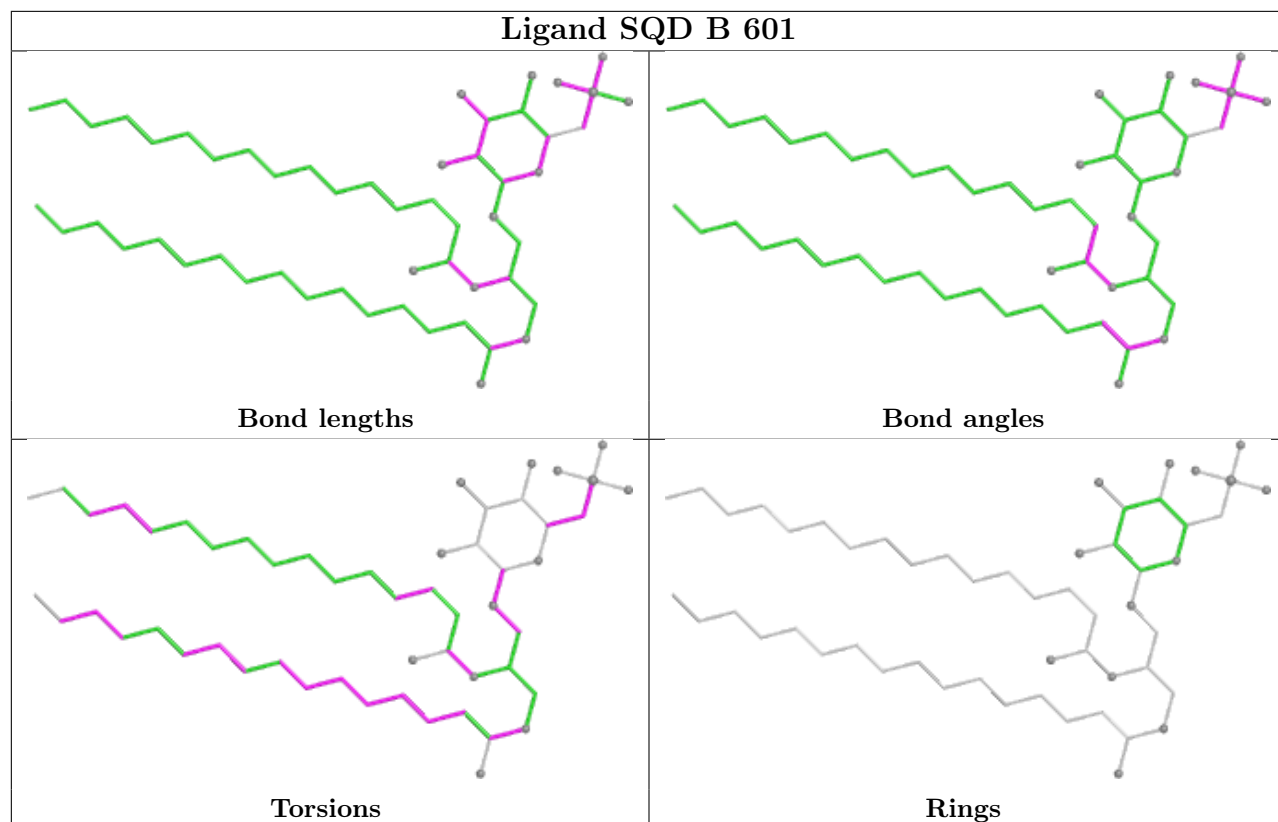


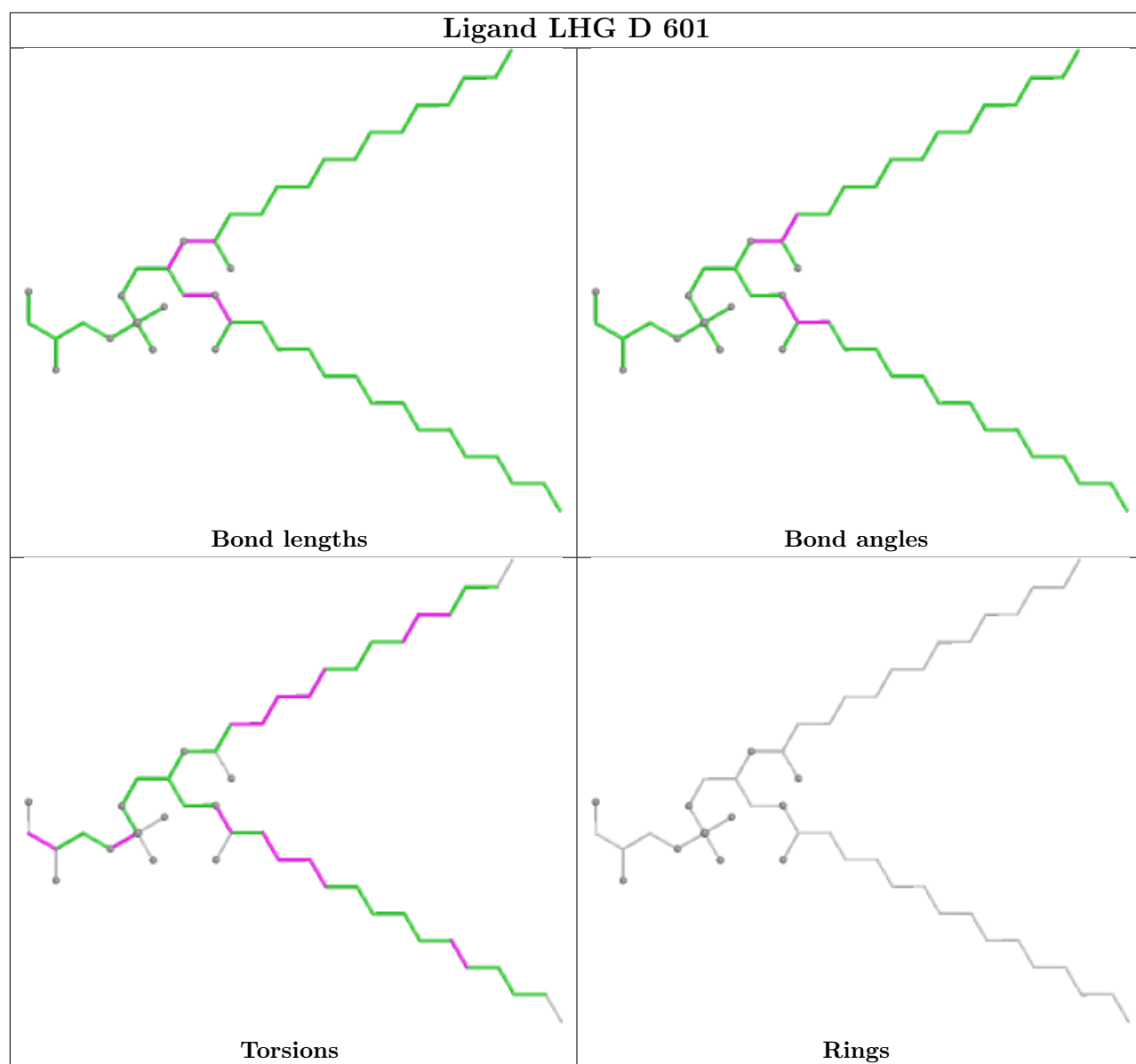


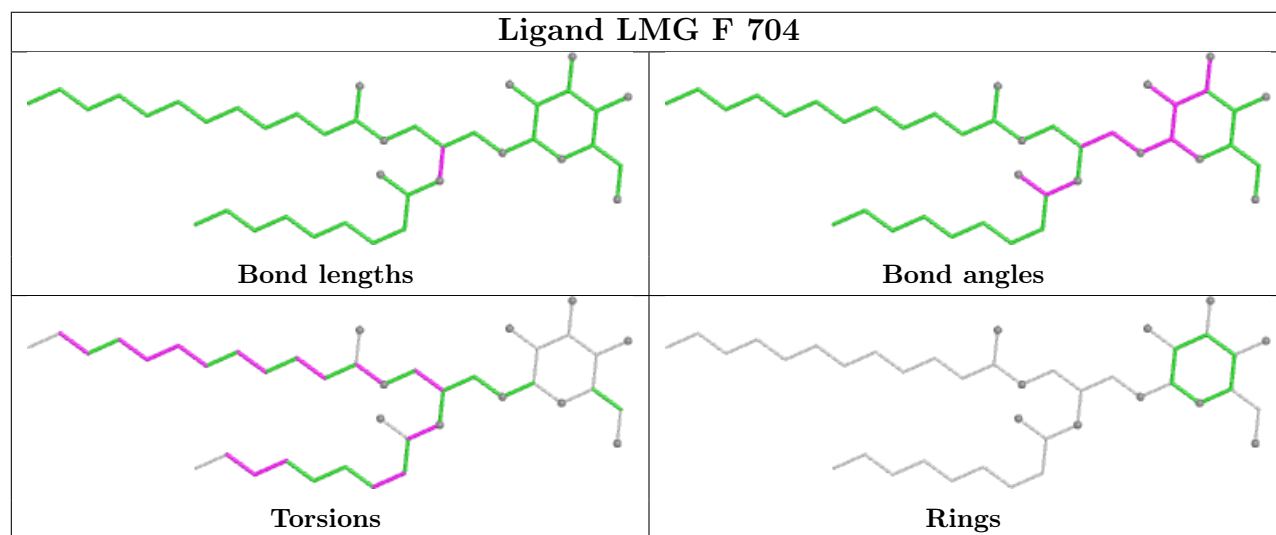
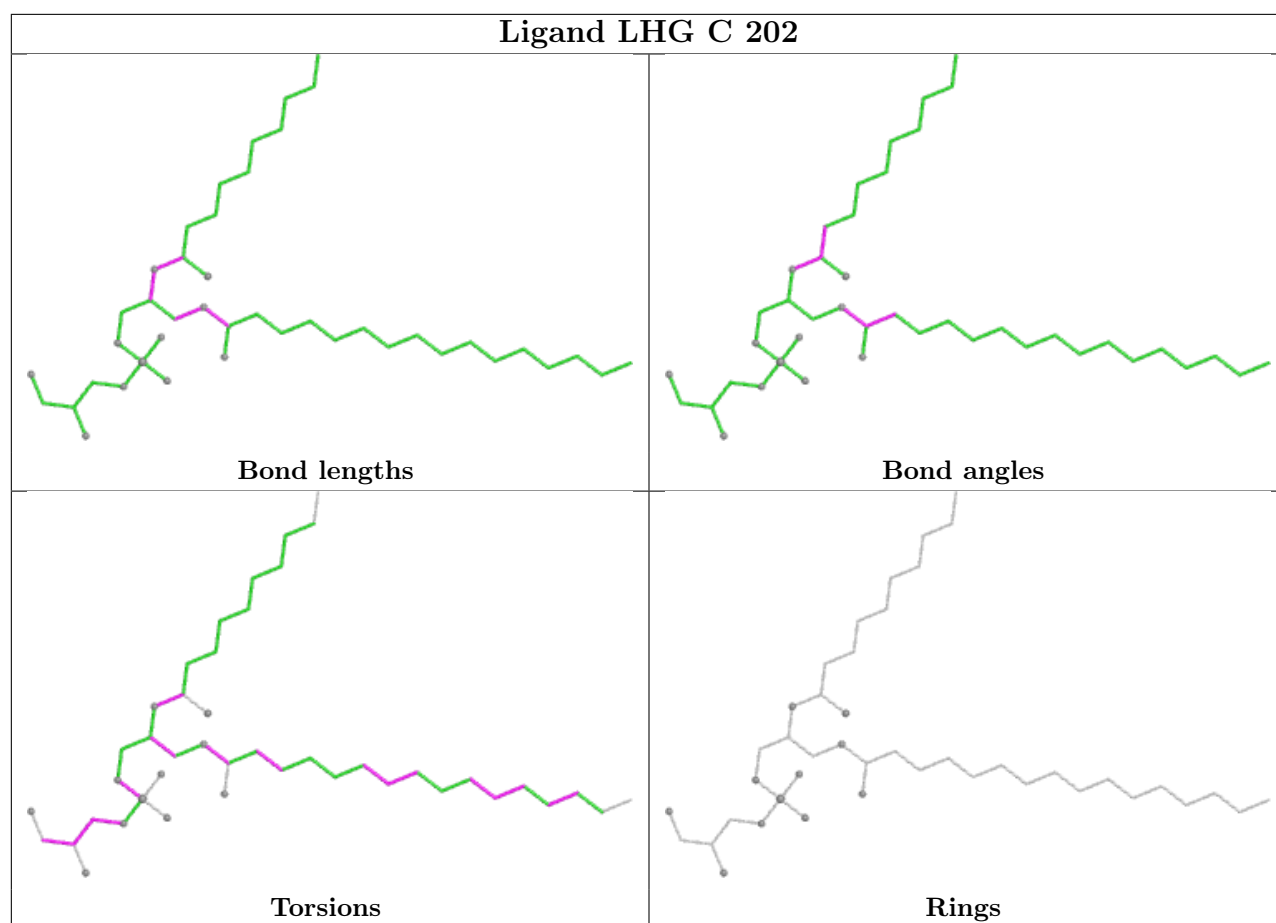


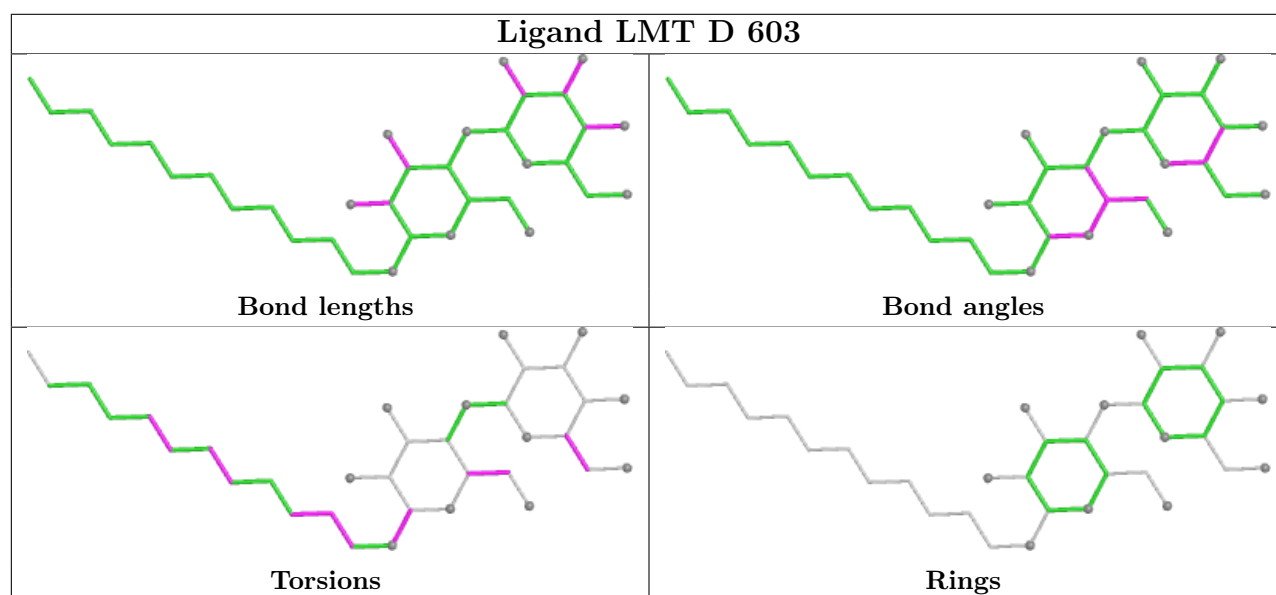
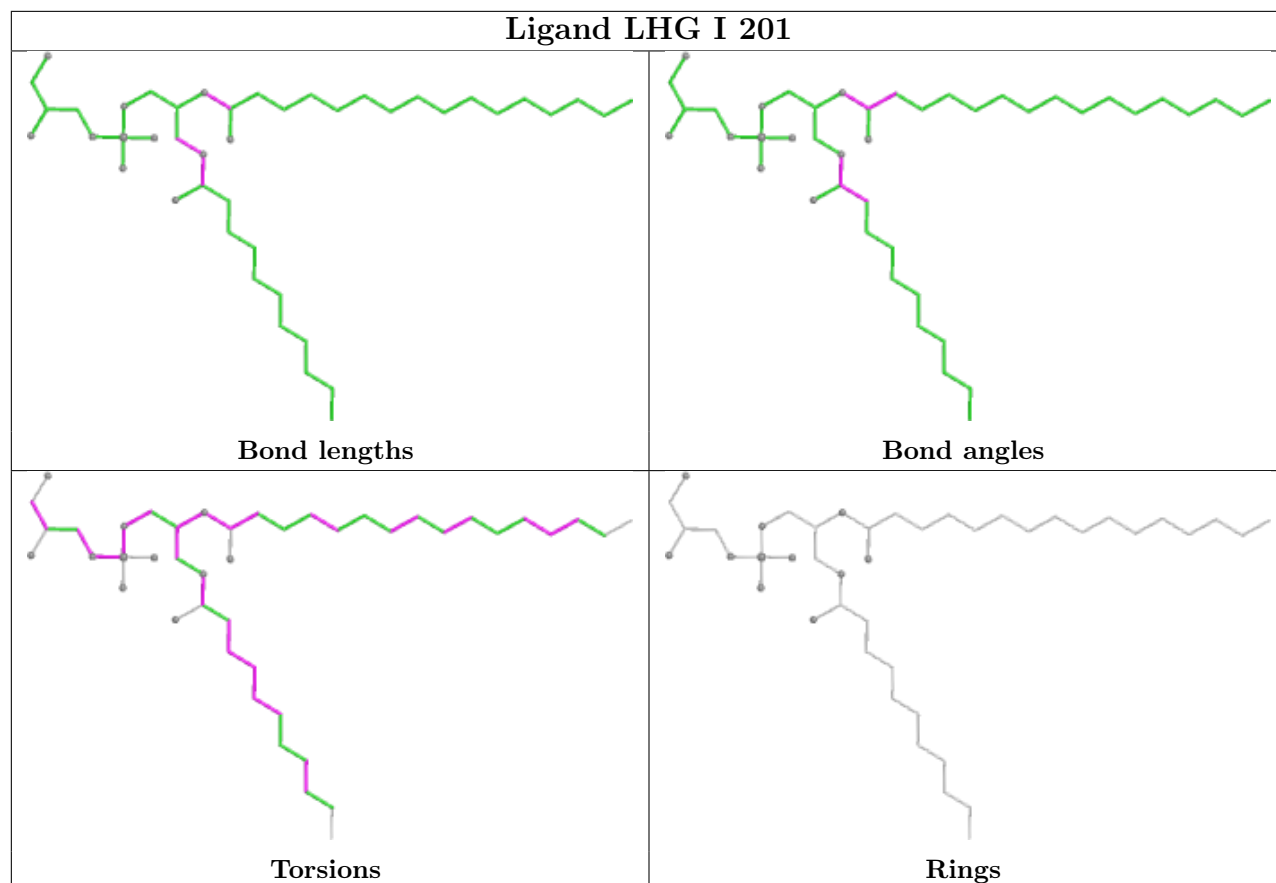


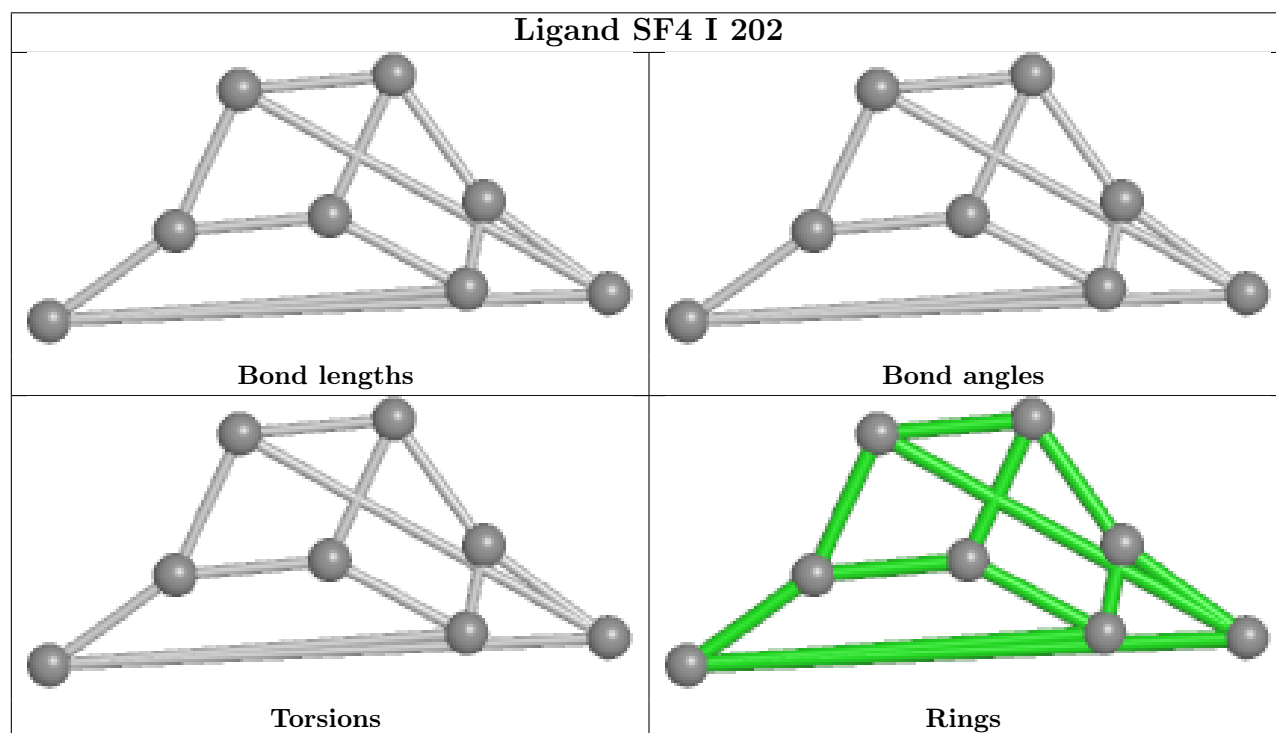
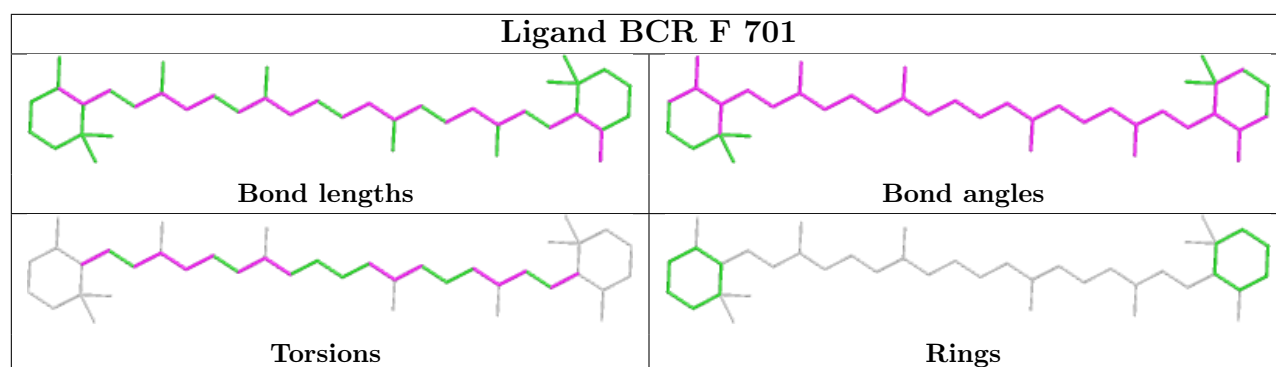


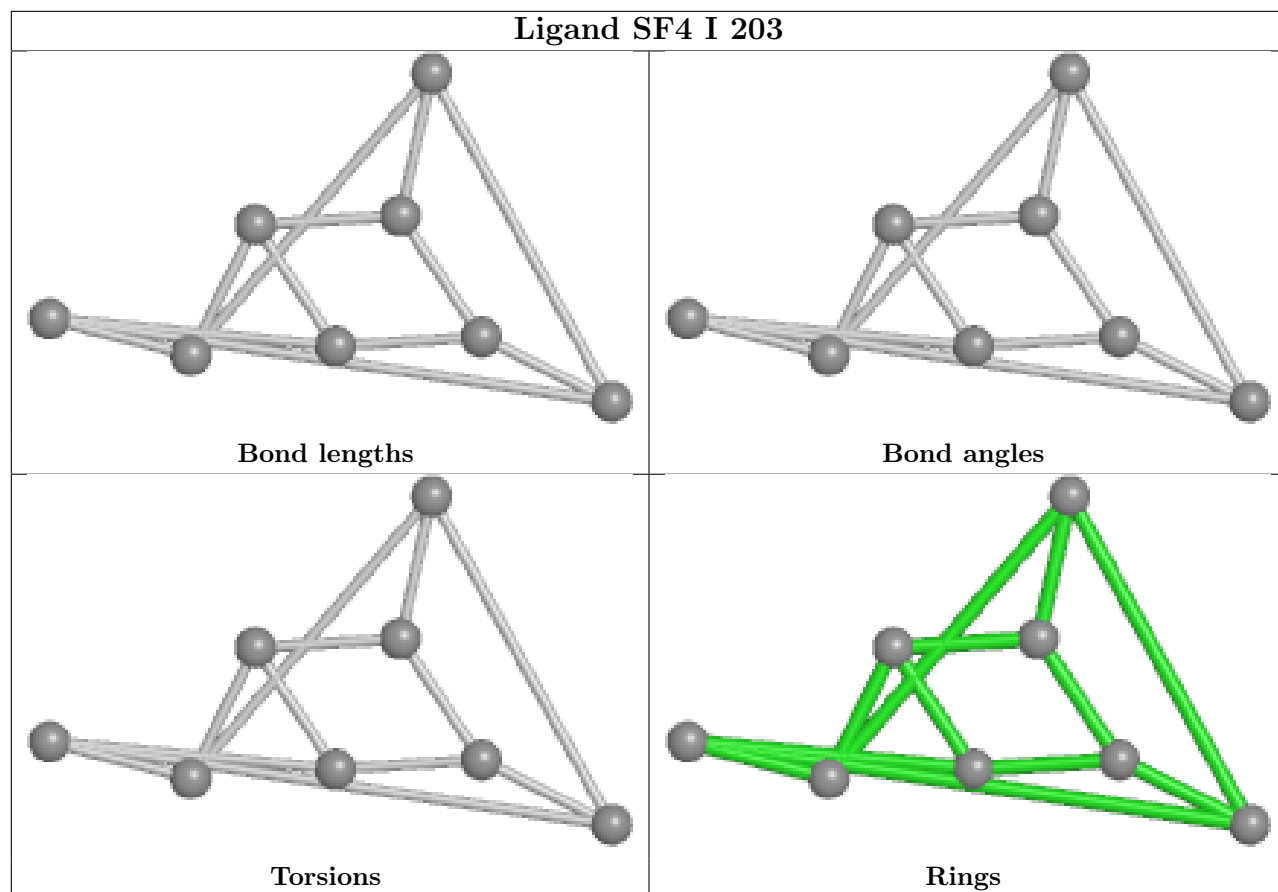


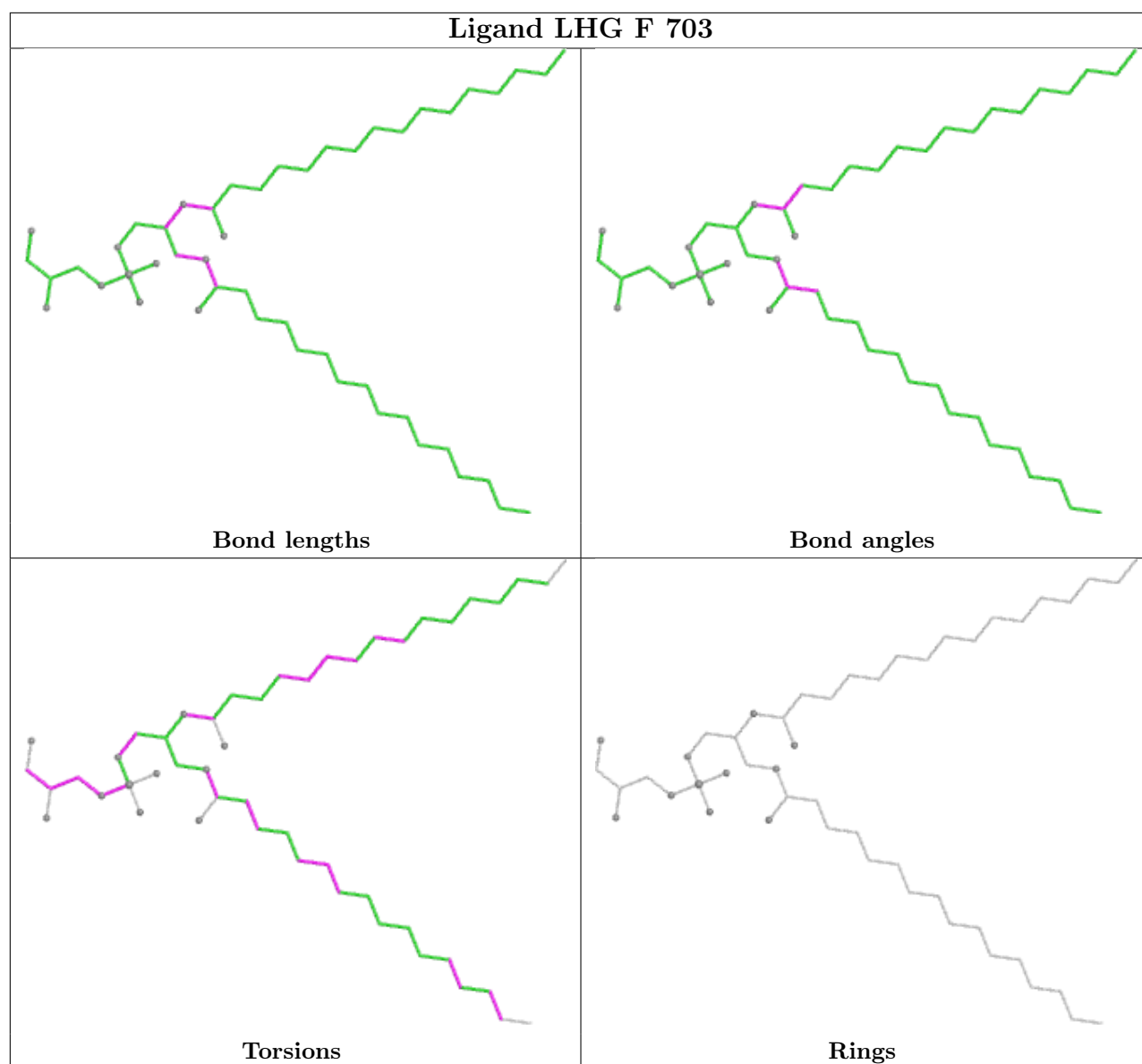












5.7 Other polymers [i](#)

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-9990. These allow visual inspection of the internal detail of the map and identification of artifacts.

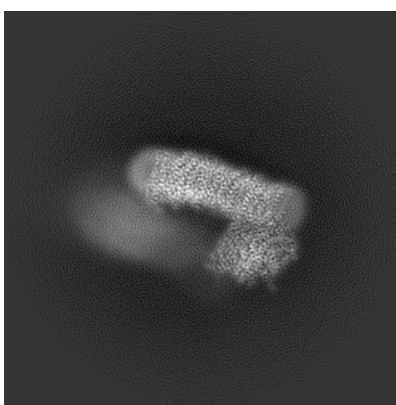
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

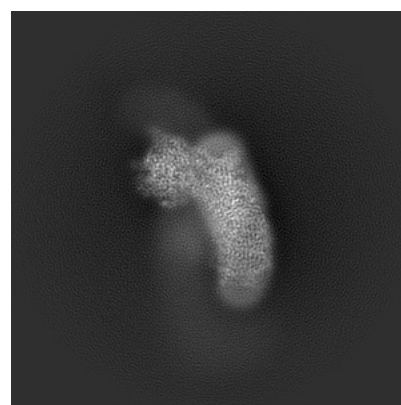
6.1.1 Primary map



X



Y

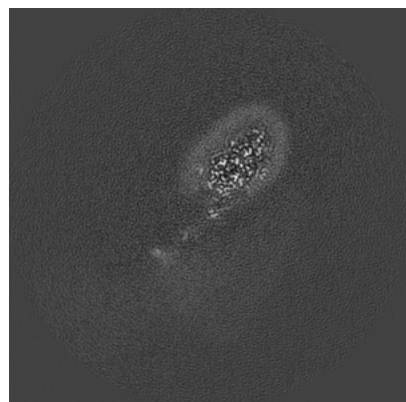


Z

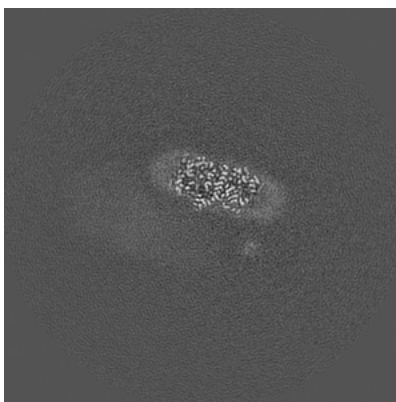
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

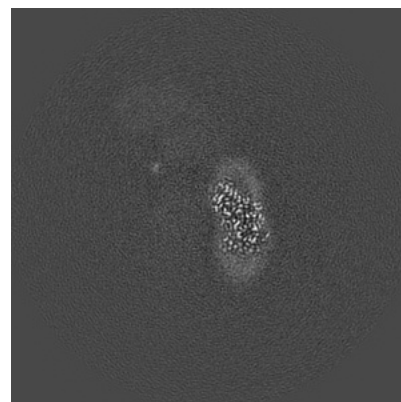
6.2.1 Primary map



X Index: 200



Y Index: 200

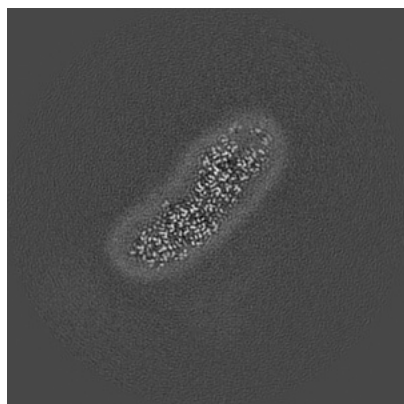


Z Index: 200

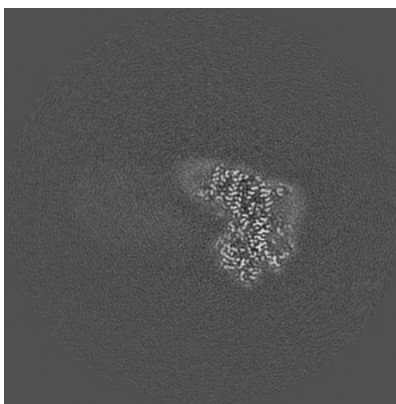
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

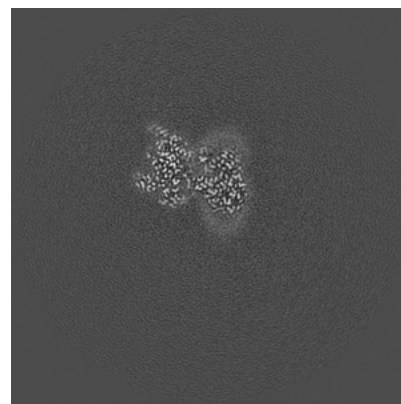
6.3.1 Primary map



X Index: 222



Y Index: 226

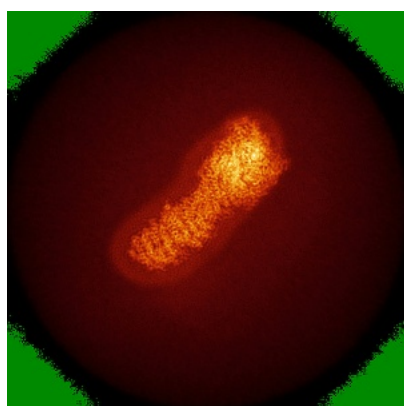


Z Index: 247

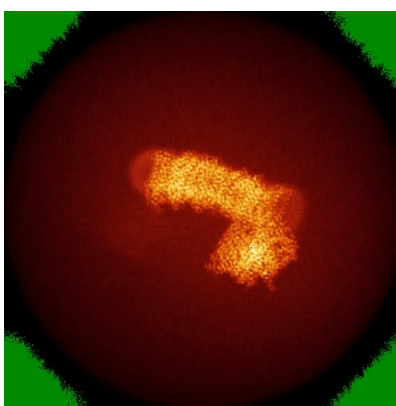
The images above show the largest variance slices of the map in three orthogonal directions.

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

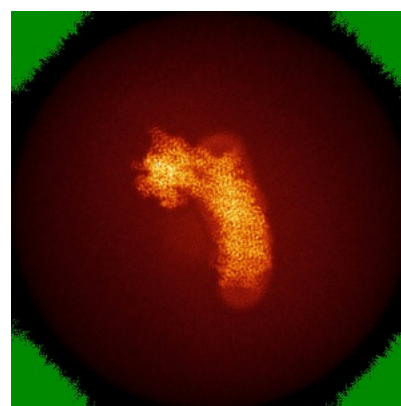
6.4.1 Primary map



X



Y

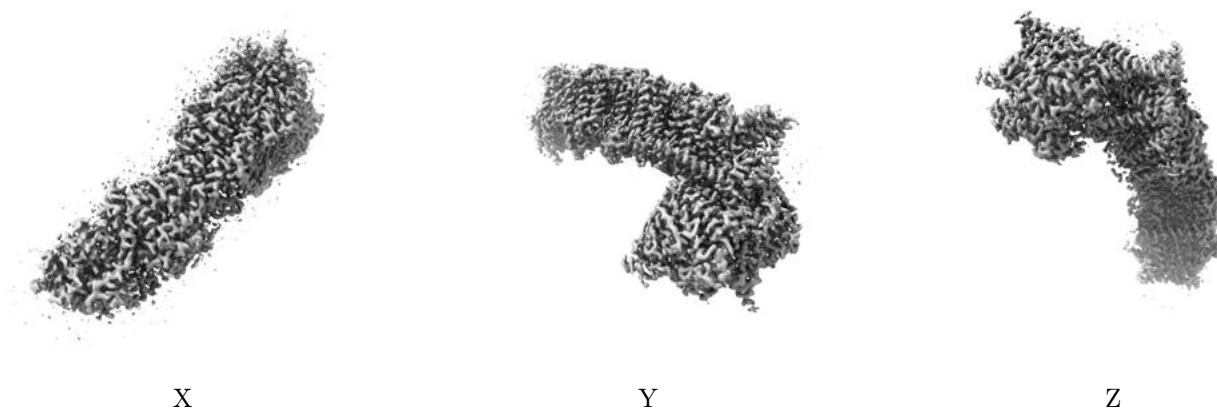


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

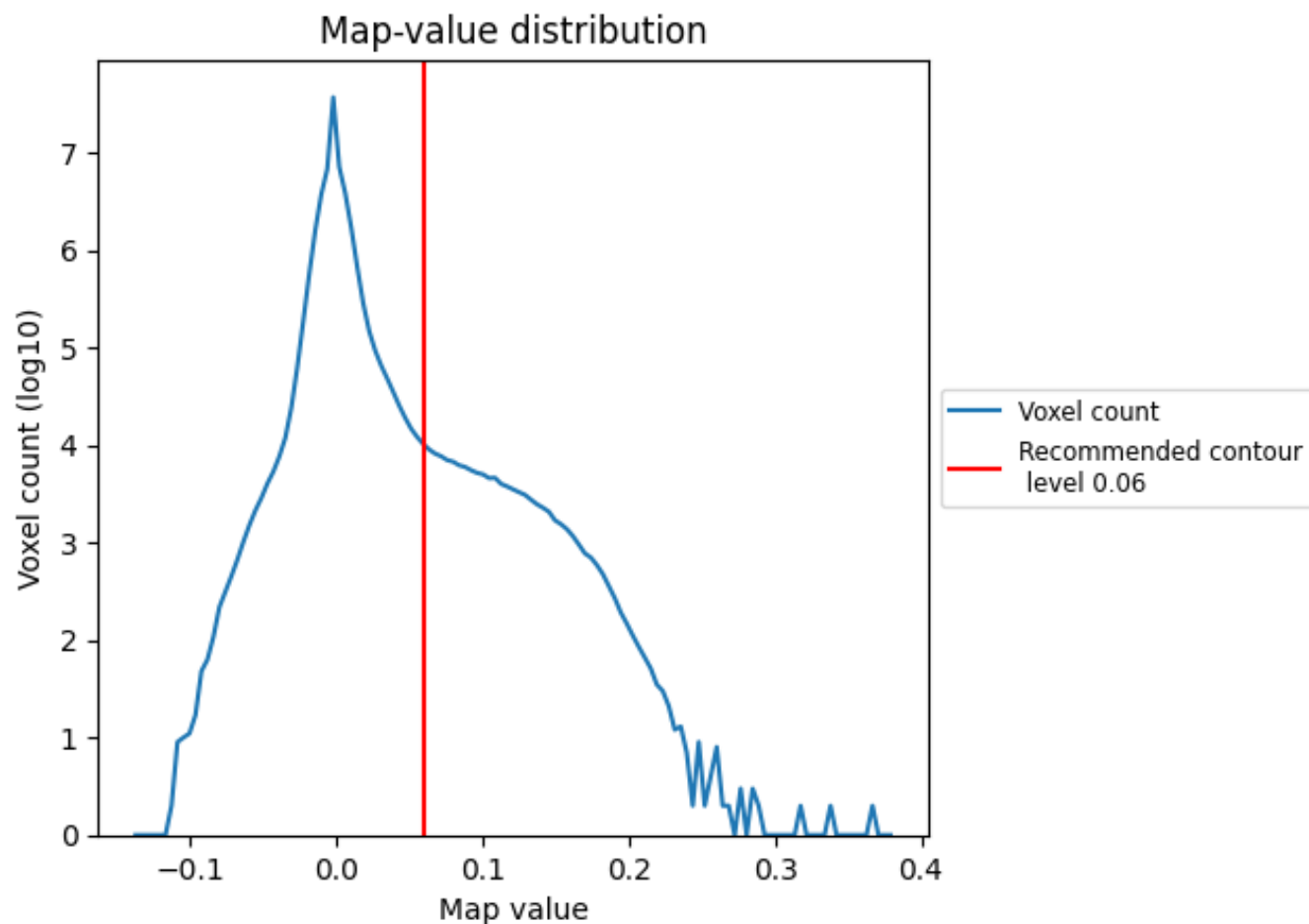
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

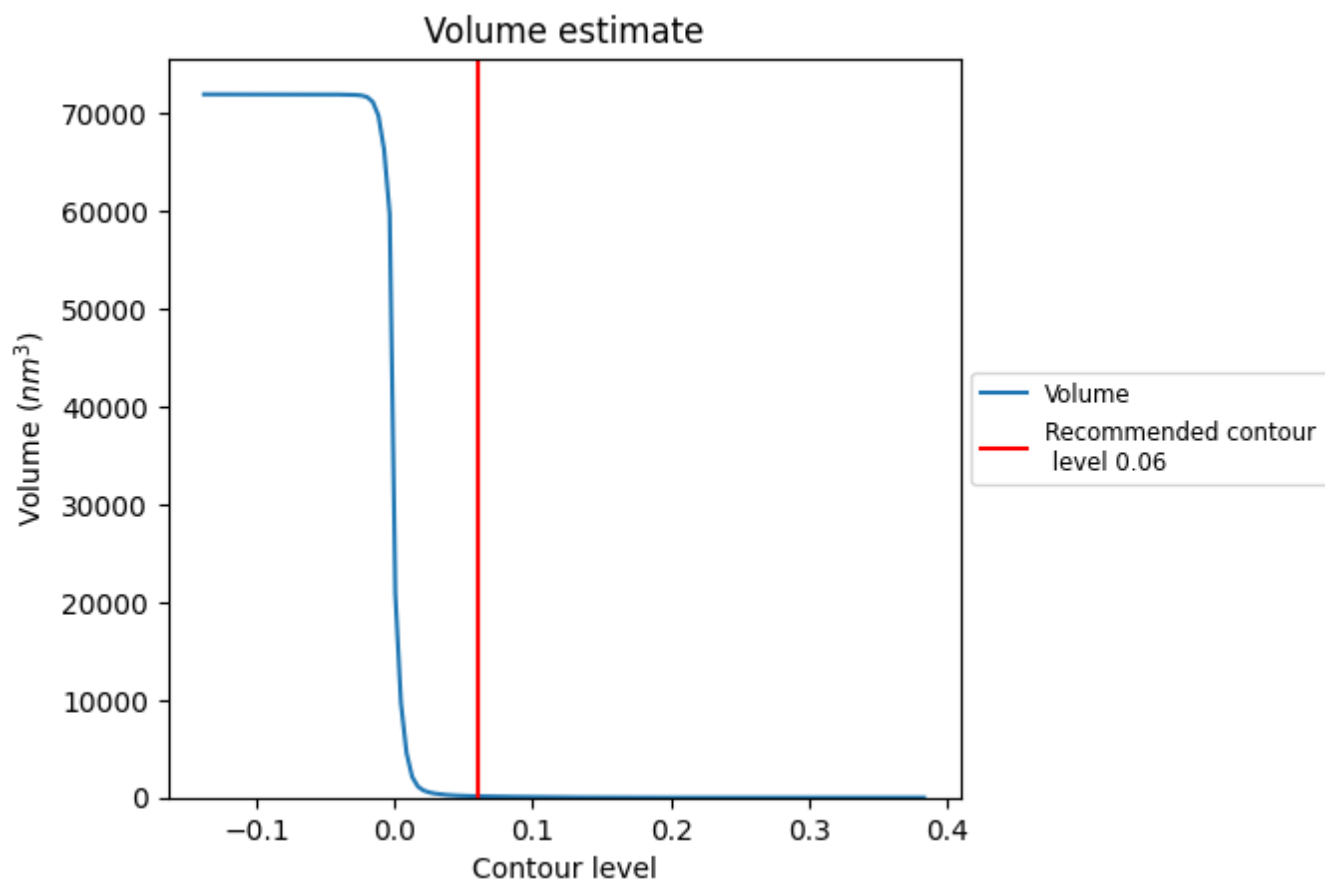
This section contains the results of statistical analysis of the map.

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.

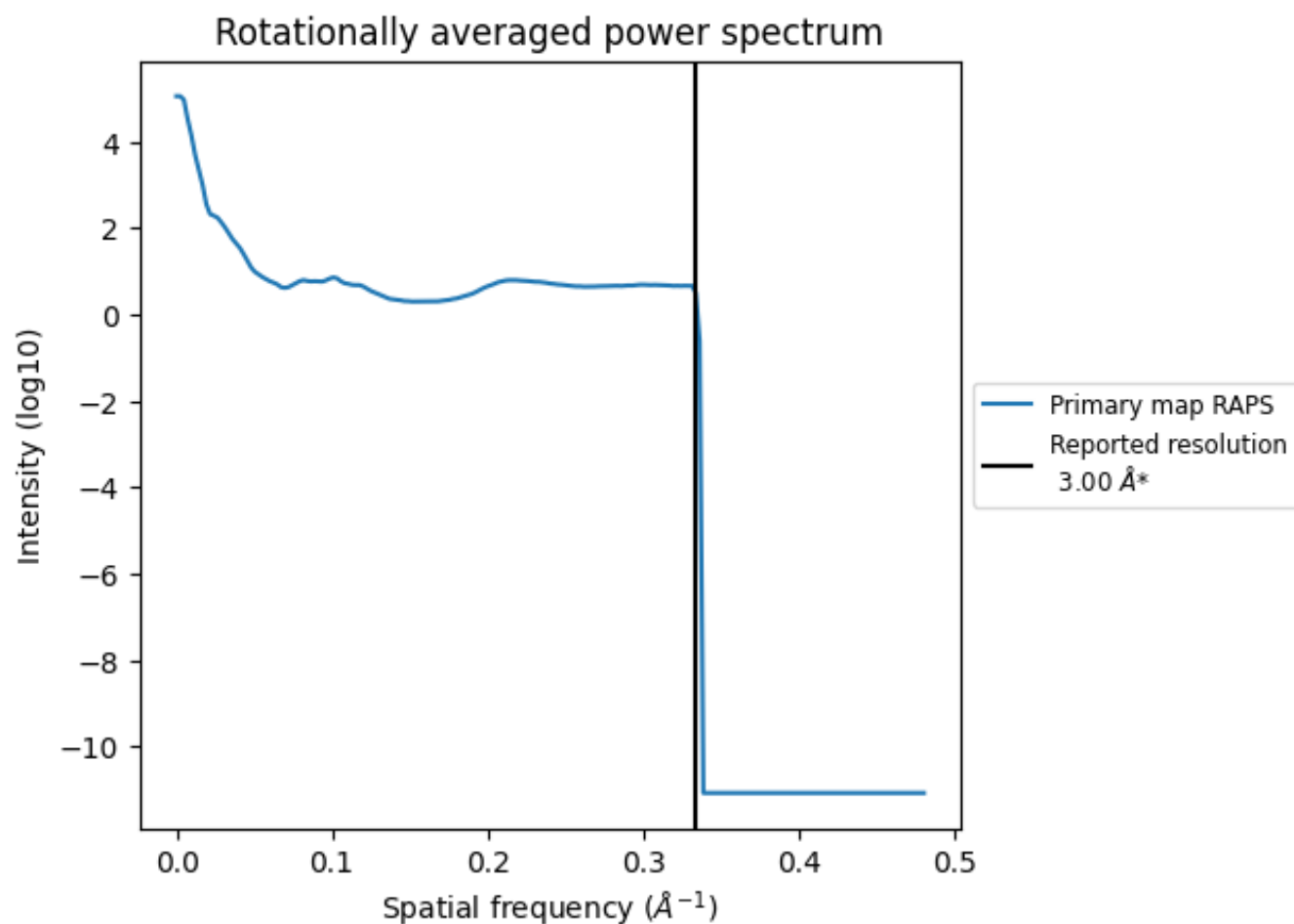
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 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 0.333 Å⁻¹

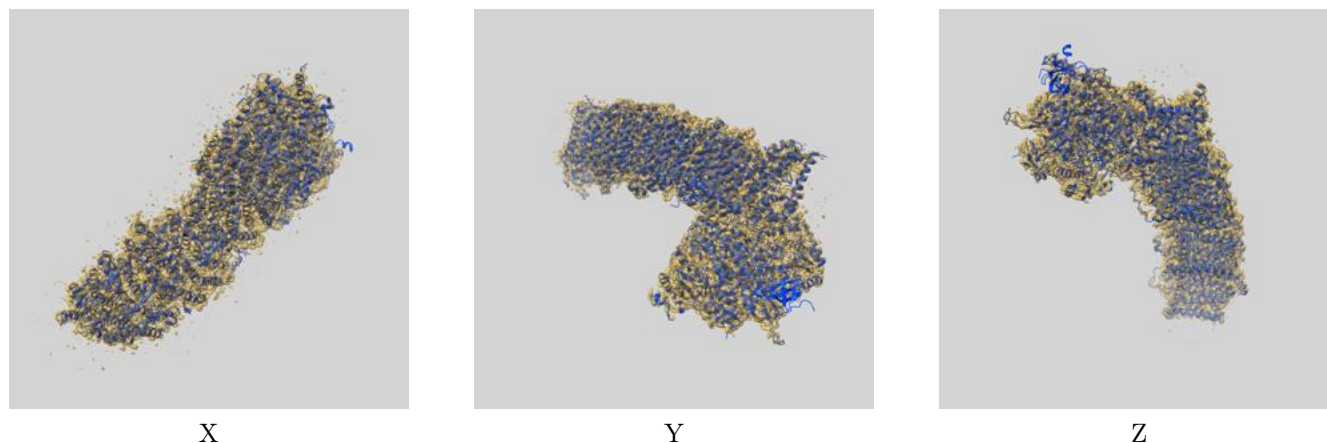
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

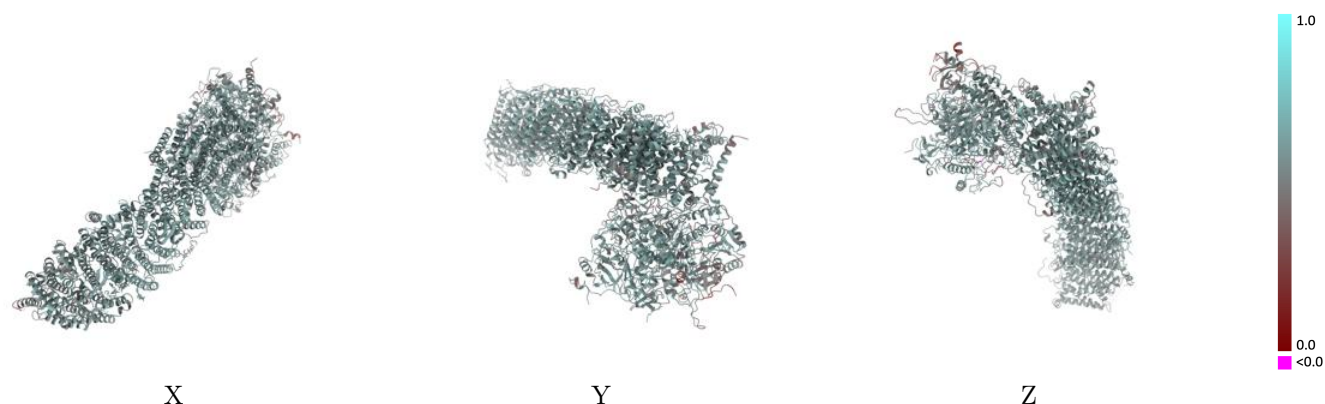
This section contains information regarding the fit between EMDB map EMD-9990 and PDB model 6KHJ. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



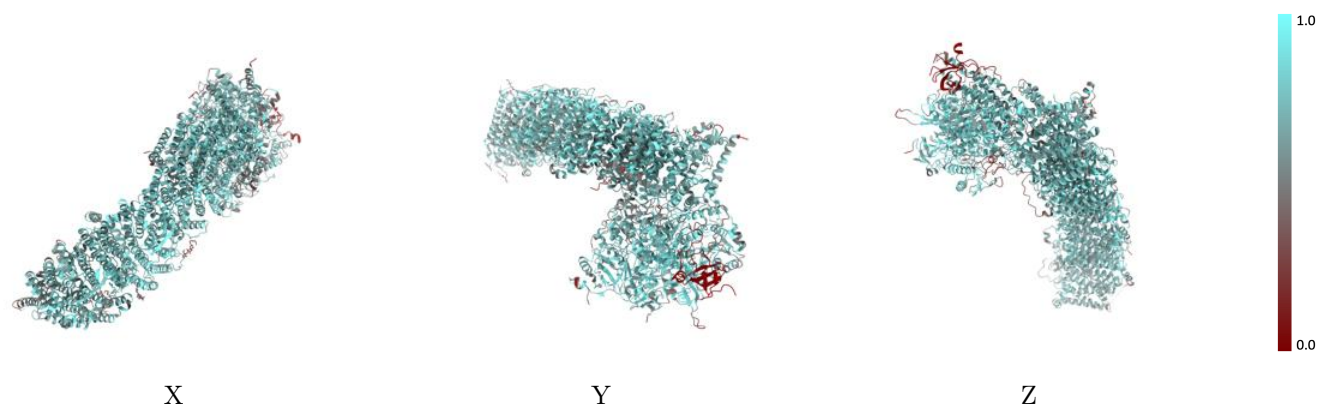
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



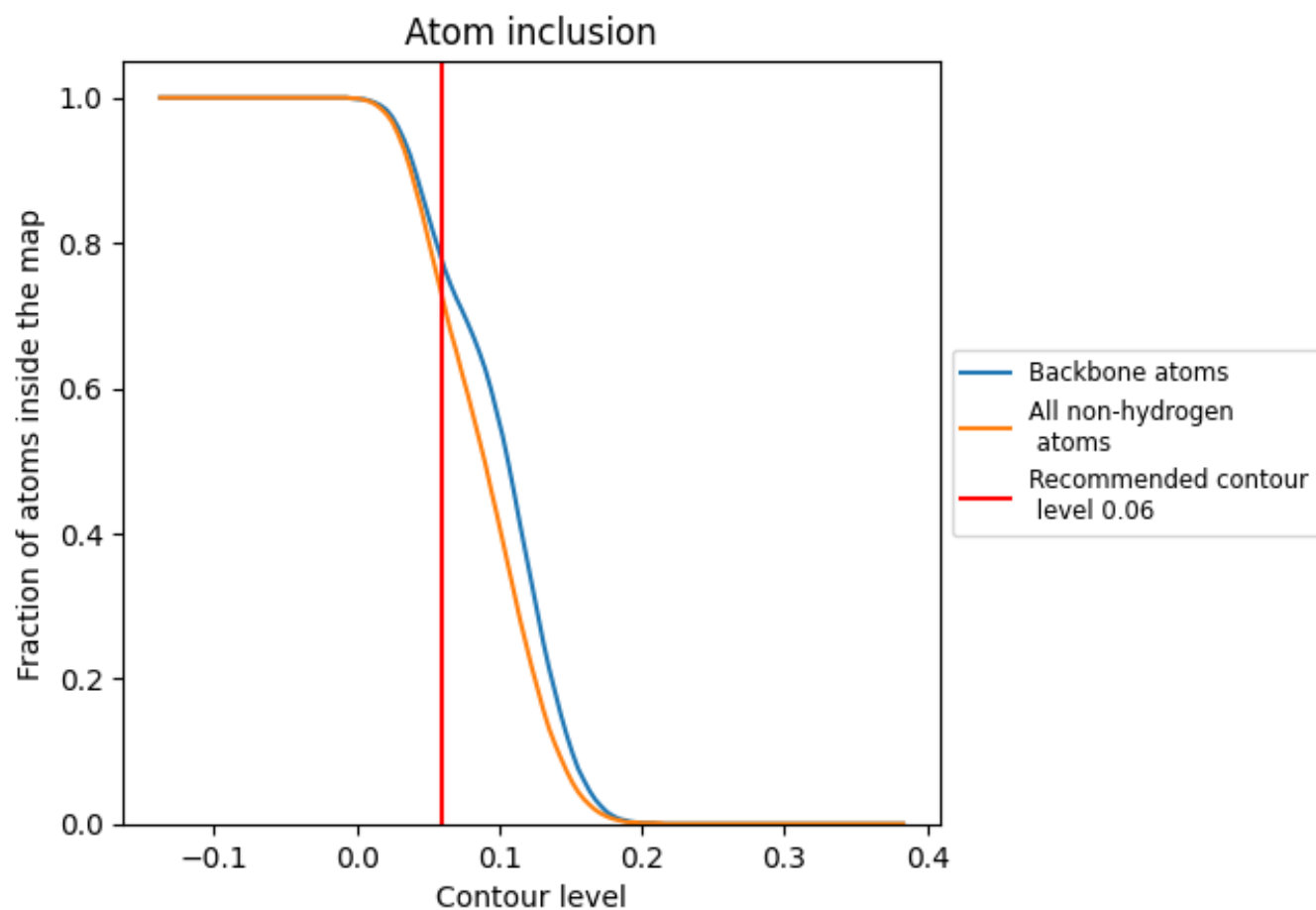
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.5620
A	0.7210	0.5630
B	0.7720	0.5820
C	0.7160	0.5540
D	0.7870	0.5850
E	0.7640	0.5800
F	0.7140	0.5560
G	0.7120	0.5670
H	0.7360	0.5620
I	0.6710	0.5370
J	0.7560	0.5650
K	0.7430	0.5550
L	0.6610	0.5260
M	0.7480	0.5590
N	0.7250	0.5490
O	0.7340	0.5710
P	0.7570	0.5730
Q	0.6310	0.5320
S	0.0260	0.4260

