



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:36 AM UTC

PDB ID : 6RQF / pdb_00006rqf
EMDB ID : EMD-4981
Title : 3.6 Angstrom cryo-EM structure of the dimeric cytochrome b6f complex from *Spinacia oleracea* with natively bound thylakoid lipids and plastoquinone molecules
Authors : Malone, L.A.; Qian, P.; Mayneord, G.E.; Hitchcock, A.; Farmer, D.; Thompson, R.; Swainsbury, D.J.K.; Ranson, N.; Hunter, C.N.; Johnson, M.P.
Deposited on : 2019-05-15
Resolution : 3.58 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

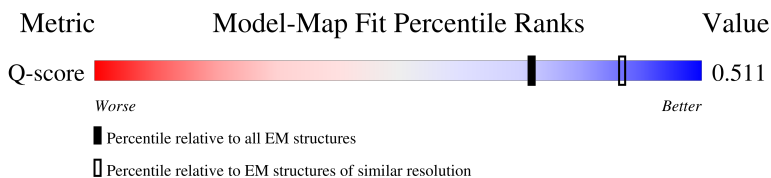
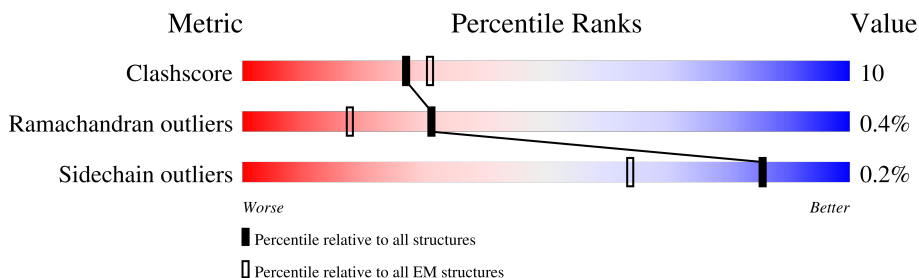
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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.



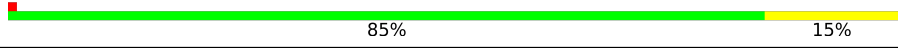
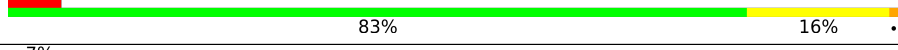
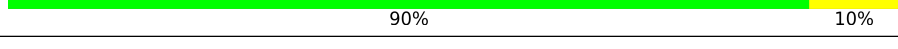
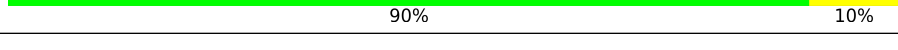
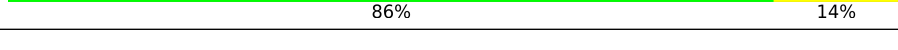
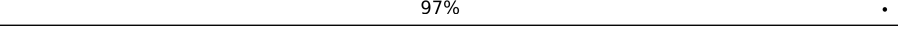
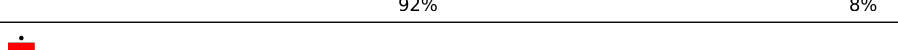
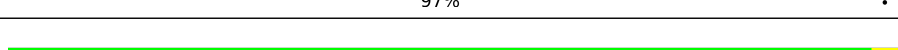
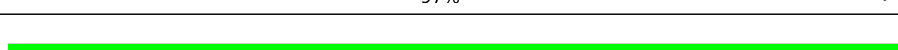
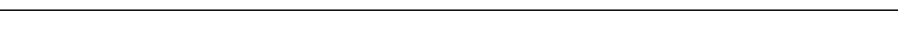
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12629 (3.08 - 4.08)

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	215	
1	I	215	
2	B	160	

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Mol	Chain	Length	Quality of chain
2	J	160	
3	C	285	
3	K	285	
4	D	179	
4	L	179	
5	E	31	
5	M	31	
6	F	36	
6	N	36	
7	G	37	
7	O	37	
8	H	29	
8	P	29	

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
10	HEC	C	301	-	-	X	-
11	CLA	A	304	X	-	-	-
11	CLA	I	304	X	-	-	-
13	PL9	A	306	-	-	X	-
13	PL9	I	306	-	-	X	-
17	FES	D	201	-	-	X	-
17	FES	L	201	-	-	X	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 16359 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 Cytochrome b6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	215	Total	C	N	O	S	0	0
			1705	1131	272	290	12		
1	A	215	Total	C	N	O	S	0	0
			1705	1131	272	290	12		

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	160	Total	C	N	O	S	0	0
			1234	825	194	210	5		
2	B	160	Total	C	N	O	S	0	0
			1234	825	194	210	5		

- Molecule 3 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	285	Total	C	N	O	S	0	0
			2209	1418	375	410	6		
3	C	285	Total	C	N	O	S	0	0
			2209	1418	375	410	6		

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	179	Total	C	N	O	S	0	0
			1333	850	225	251	7		
4	D	179	Total	C	N	O	S	0	0
			1333	850	225	251	7		

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	31	Total	C	N	O	S	0	0
			243	167	36	39	1		
5	E	31	Total	C	N	O	S	0	0
			243	167	36	39	1		

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	36	Total	C	N	O	S	0	0
			264	171	44	48	1		
6	F	36	Total	C	N	O	S	0	0
			264	171	44	48	1		

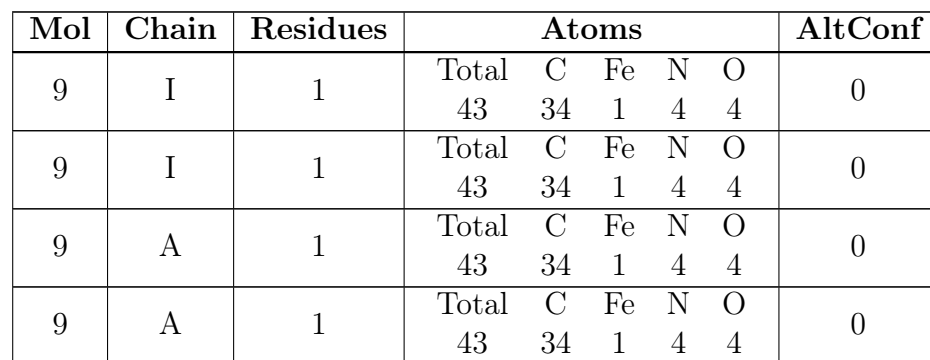
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	37	Total	C	N	O	S	0	0
			294	199	45	49	1		
7	G	37	Total	C	N	O	S	0	0
			294	199	45	49	1		

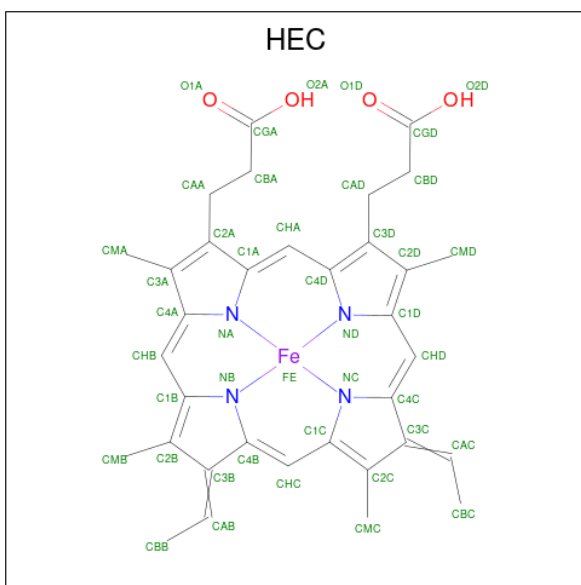
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	29	Total	C	N	O	S	0	0
			223	150	34	37	2		
8	H	29	Total	C	N	O	S	0	0
			223	150	34	37	2		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

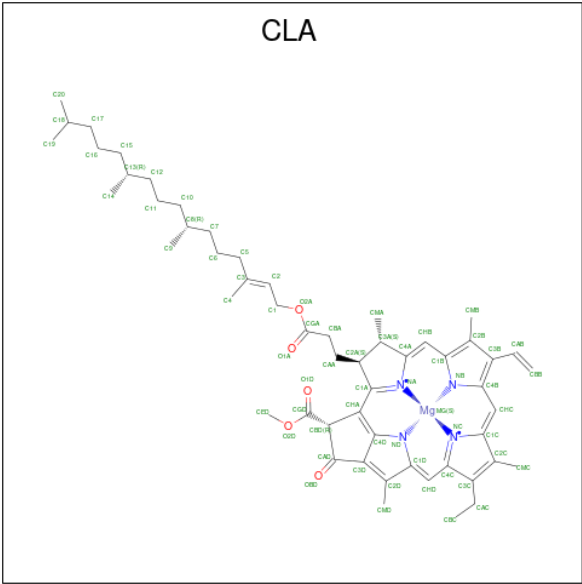


- Molecule 10 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



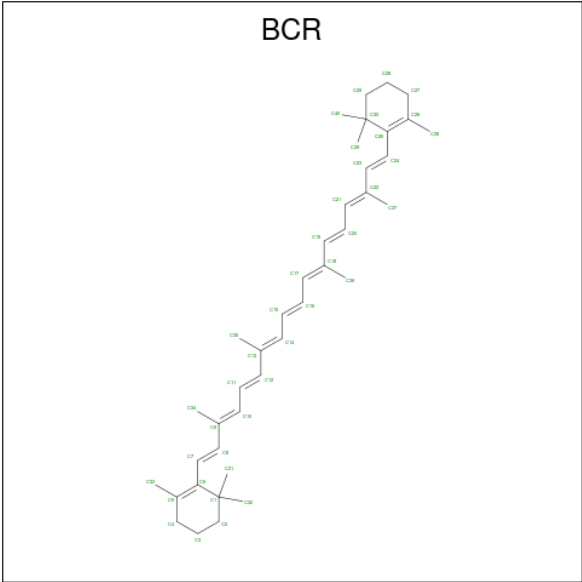
Mol	Chain	Residues	Atoms					AltConf
10	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



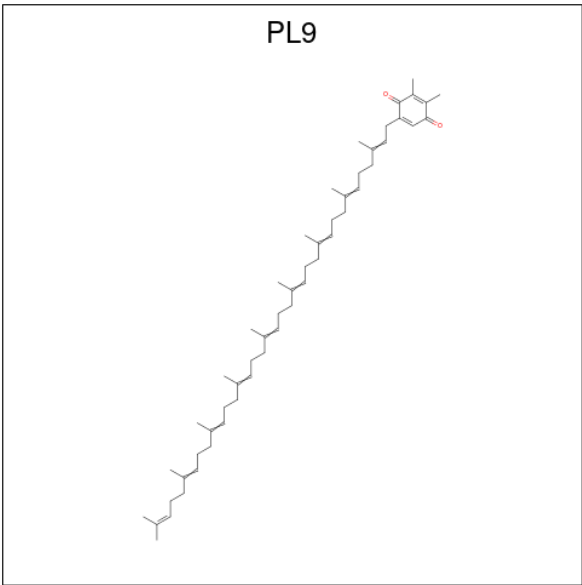
Mol	Chain	Residues	Atoms					AltConf
11	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 12 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
12	I	1	Total	C	0
			40	40	
12	H	1	Total	C	0
			40	40	

- Molecule 13 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: C₅₃H₈₀O₂).



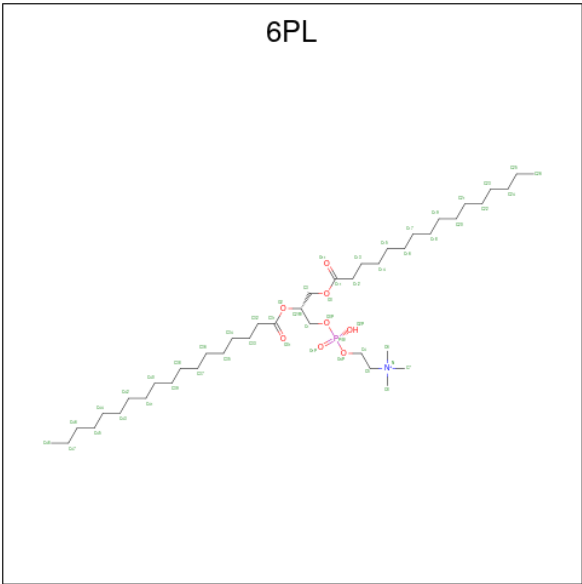
Mol	Chain	Residues	Atoms			AltConf
13	I	1	Total	C	O	0
			55	53	2	

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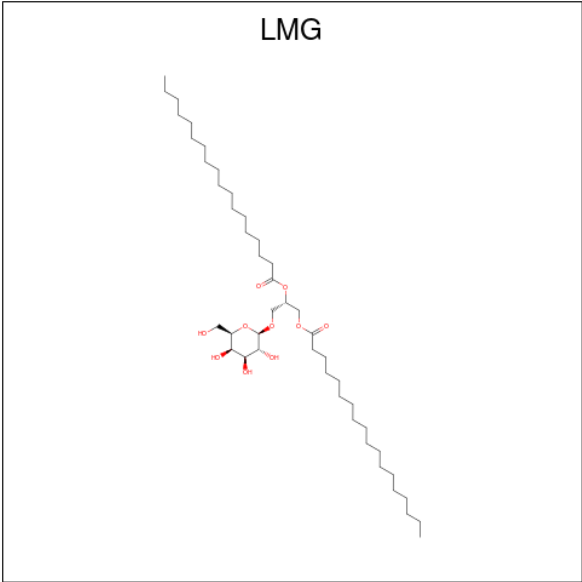
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			55	53	2	
13	A	1	Total	C	O	0
			55	53	2	

- Molecule 14 is (4S,7R)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: 6PL) (formula: C₄₂H₈₅NO₈P).



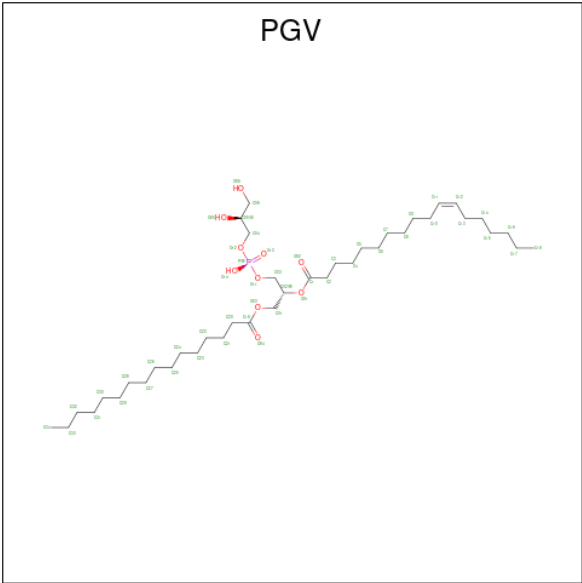
Mol	Chain	Residues	Atoms					AltConf
14	I	1	Total	C	N	O	P	0
			52	42	1	8	1	
14	N	1	Total	C	N	O	P	0
			52	42	1	8	1	
14	E	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 15 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
15	J	1	Total	C	O	0
			55	45	10	
15	F	1	Total	C	O	0
			55	45	10	

- Molecule 16 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



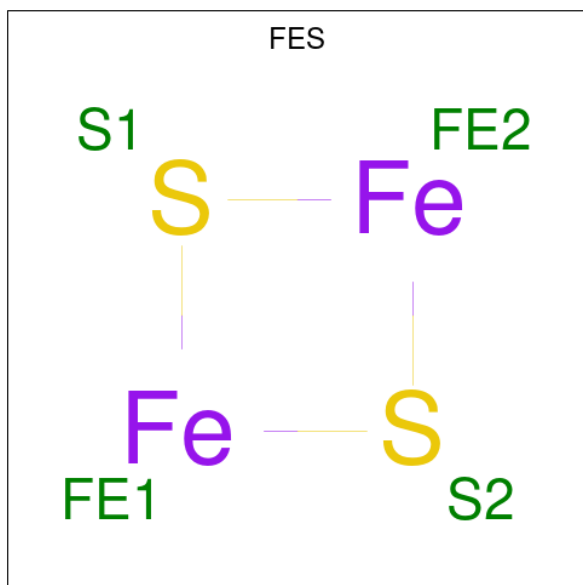
Mol	Chain	Residues	Atoms				AltConf
16	J	1	Total	C	O	P	0
			51	40	10	1	

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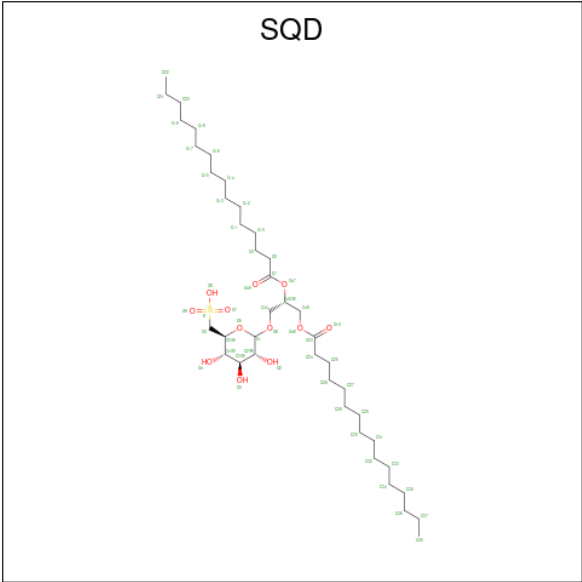
Mol	Chain	Residues	Atoms				AltConf
16	K	1	Total	C	O	P	0
			51	40	10	1	
16	A	1	Total	C	O	P	0
			45	34	10	1	
16	B	1	Total	C	O	P	0
			48	37	10	1	

- Molecule 17 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
17	L	1	Total	Fe	S	0
			4	2	2	
17	D	1	Total	Fe	S	0
			4	2	2	

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$).

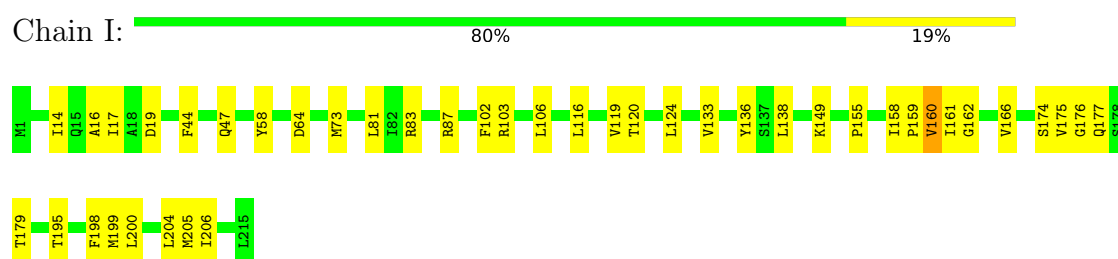


Mol	Chain	Residues	Atoms				AltConf
18	L	1	Total	C	O	S	0
			54	41	12	1	
18	A	1	Total	C	O	S	0
			54	41	12	1	
18	C	1	Total	C	O	S	0
			54	41	12	1	

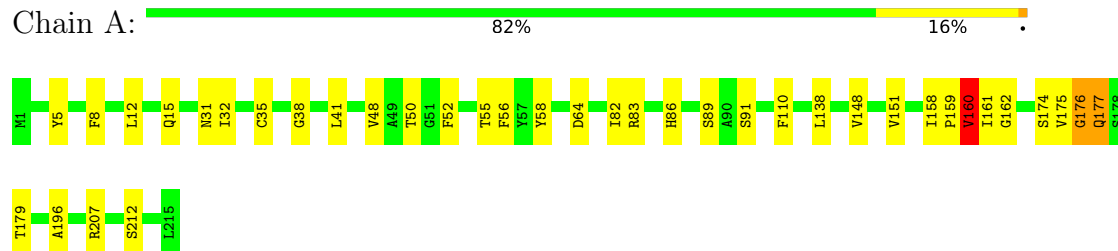
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

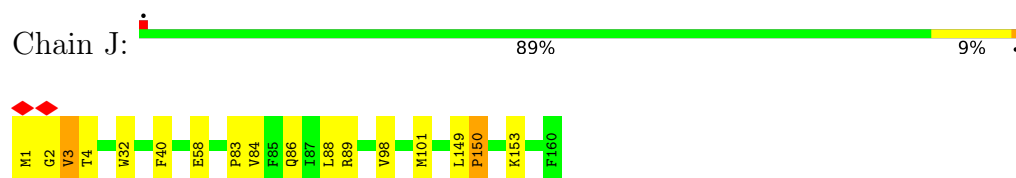
- Molecule 1: Cytochrome b6



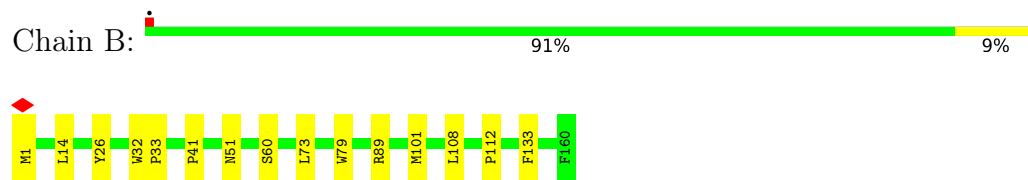
- Molecule 1: Cytochrome b6



- Molecule 2: Cytochrome b6-f complex subunit 4

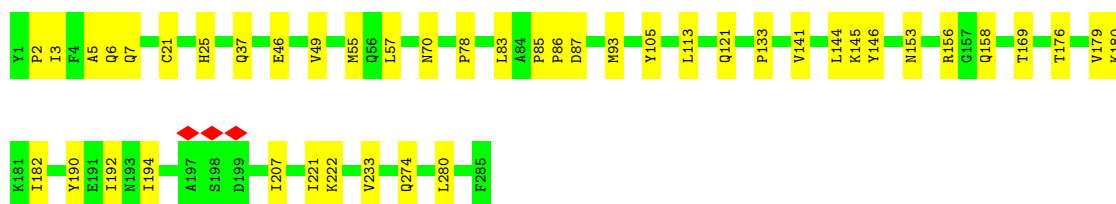


- Molecule 2: Cytochrome b6-f complex subunit 4



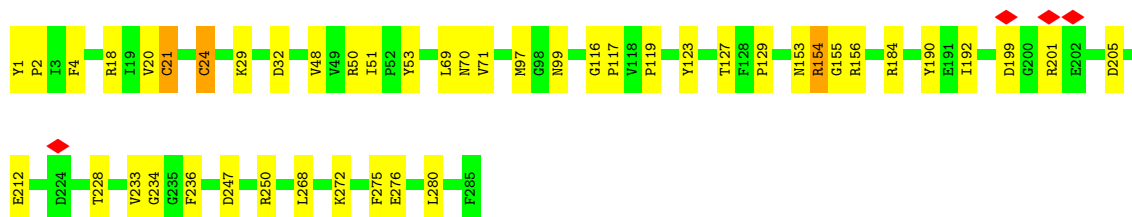
- Molecule 3: Cytochrome f

Chain K:  85% 15%



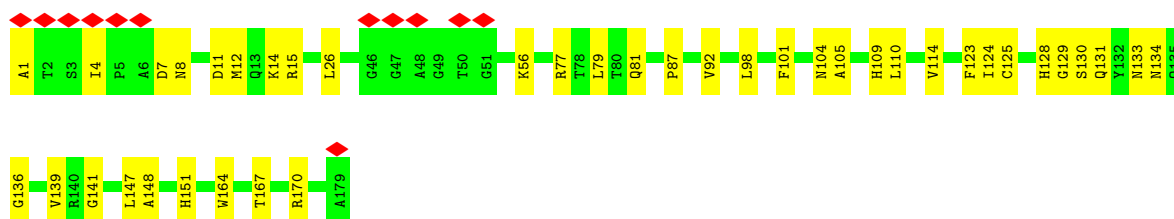
- Molecule 3: Cytochrome f

Chain C:  84% 15%



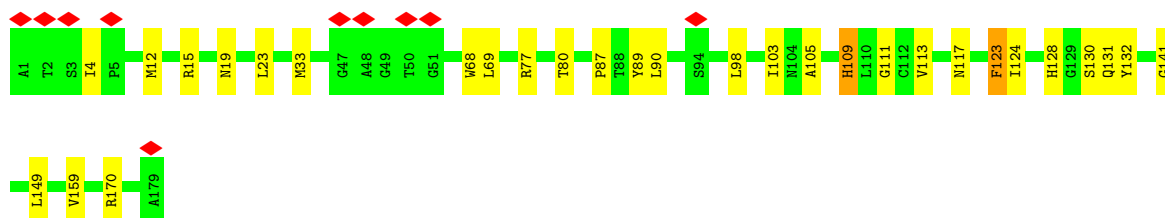
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain L:  7% 78% 22%



- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain D:  6% 83% 16%



- Molecule 5: Cytochrome b6-f complex subunit 6

Chain M:  90% 10%

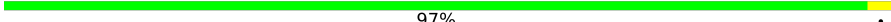


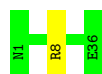
- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:  90% 10%



- Molecule 6: Cytochrome b6-f complex subunit 7

Chain N:  97% .

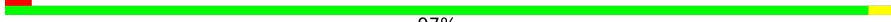


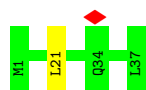
- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:  86% 14%



- Molecule 7: Cytochrome b6-f complex subunit 5

Chain O:  97% .



- Molecule 7: Cytochrome b6-f complex subunit 5

Chain G:  92% 8%

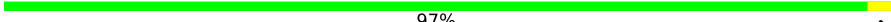


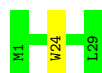
- Molecule 8: Cytochrome b6-f complex subunit 8

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 8: Cytochrome b6-f complex subunit 8

Chain H:  97% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108560	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 ($e^-/\text{\AA}^2$)	1.15	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0144	Depositor
Map size (Å)	330.15002, 330.15002, 330.15002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, BCR, HEC, LMG, CLA, FES, HEM, PGV, 6PL, PL9

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	0.36	0/1755	0.71	4/2392 (0.2%)
1	I	0.42	1/1755 (0.1%)	0.66	2/2392 (0.1%)
2	B	0.29	0/1271	0.56	0/1743
2	J	0.34	0/1271	0.62	0/1743
3	C	0.36	2/2256 (0.1%)	0.60	2/3058 (0.1%)
3	K	0.36	1/2256 (0.0%)	0.55	1/3058 (0.0%)
4	D	0.49	5/1369 (0.4%)	0.70	7/1875 (0.4%)
4	L	0.42	2/1369 (0.1%)	0.67	3/1875 (0.2%)
5	E	0.24	0/247	0.58	0/333
5	M	0.21	0/247	0.59	0/333
6	F	0.28	0/265	0.45	0/359
6	N	0.27	0/265	0.51	0/359
7	G	0.26	0/299	0.56	0/405
7	O	0.28	0/299	0.56	0/405
8	H	0.28	0/228	0.49	0/309
8	P	0.29	0/228	0.51	0/309
All	All	0.37	11/15380 (0.1%)	0.62	19/20948 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	21	CYS	C-N	9.09	1.47	1.33
1	I	206	ILE	C-N	8.91	1.45	1.33
4	L	123	PHE	C-N	8.46	1.44	1.33
3	C	20	VAL	C-N	8.40	1.46	1.33
4	D	123	PHE	C-N	7.65	1.43	1.33
4	D	131	GLN	C-N	-6.77	1.23	1.33
3	C	24	CYS	C-N	-6.29	1.25	1.33
4	D	105	ALA	C-N	-5.95	1.24	1.33
4	D	113	VAL	C-N	5.71	1.38	1.33
4	L	124	ILE	C-N	-5.44	1.20	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	109	HIS	C-N	5.37	1.41	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLY	N-CA-C	-10.75	91.12	111.66
1	A	177	GLN	N-CA-C	10.38	132.92	110.80
1	I	177	GLN	N-CA-C	8.42	121.52	111.33
4	L	124	ILE	O-C-N	6.63	130.07	123.18
3	C	4	PHE	O-C-N	6.61	128.87	122.07
4	D	113	VAL	CA-C-N	6.38	127.18	122.59
4	D	113	VAL	C-N-CA	6.38	127.18	122.59
1	A	177	GLN	N-CA-CB	-6.20	100.02	110.49
1	I	174	SER	N-CA-C	6.05	118.82	110.35
4	D	123	PHE	CA-C-N	5.77	130.62	123.12
4	D	123	PHE	C-N-CA	5.77	130.62	123.12
3	C	21	CYS	O-C-N	5.73	130.80	122.43
4	D	123	PHE	O-C-N	-5.27	115.65	122.77
1	A	160	VAL	N-CA-C	5.19	120.13	109.34
3	K	87	ASP	N-CA-C	-5.13	107.68	114.04
4	L	124	ILE	CA-C-N	-5.07	111.30	120.94
4	L	124	ILE	C-N-CA	-5.07	111.30	120.94
4	D	109	HIS	CA-C-N	5.01	131.11	121.54
4	D	109	HIS	C-N-CA	5.01	131.11	121.54

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	A	1705	0	1736	42	0
1	I	1705	0	1736	46	0
2	B	1234	0	1288	14	0
2	J	1234	0	1288	26	0
3	C	2209	0	2254	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2209	0	2252	30	0
4	D	1333	0	1304	20	0
4	L	1333	0	1304	41	0
5	E	243	0	268	9	0
5	M	243	0	268	3	0
6	F	264	0	282	4	0
6	N	264	0	282	3	0
7	G	294	0	314	2	0
7	O	294	0	314	1	0
8	H	223	0	234	2	0
8	P	223	0	234	0	0
9	A	86	0	60	3	0
9	I	86	0	60	1	0
10	A	43	0	31	7	0
10	C	43	0	32	21	0
10	I	43	0	32	5	0
10	K	43	0	29	2	0
11	A	65	0	72	2	0
11	I	65	0	72	3	0
12	H	40	0	56	1	0
12	I	40	0	56	0	0
13	A	110	0	160	41	0
13	I	55	0	80	26	0
14	E	51	0	79	11	0
14	I	52	0	84	1	0
14	N	52	0	84	3	0
15	F	55	0	86	0	0
15	J	55	0	86	1	0
16	A	45	0	62	1	0
16	B	48	0	67	0	0
16	J	51	0	76	0	0
16	K	51	0	76	1	0
17	D	4	0	0	2	0
17	L	4	0	0	3	0
18	A	54	0	78	8	0
18	C	54	0	78	10	0
18	L	54	0	77	5	0
All	All	16359	0	17031	332	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 10.

All (332) 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)
3:C:21:CYS:SG	10:C:301:HEC:CAB	2.11	1.37
3:C:24:CYS:SG	10:C:301:HEC:CAC	2.19	1.31
13:A:305:PL9:H252	13:A:306:PL9:C20	1.62	1.28
3:C:24:CYS:CB	10:C:301:HEC:HBC3	1.63	1.26
1:A:175:VAL:HG23	1:A:179:THR:CG2	1.65	1.25
3:C:275:PHE:CE2	18:C:302:SQD:H62	1.71	1.24
13:A:305:PL9:C25	13:A:306:PL9:H201	1.67	1.23
1:A:175:VAL:CG2	1:A:179:THR:HG21	1.68	1.22
4:L:128:HIS:HB2	17:L:201:FES:S1	1.83	1.18
1:I:200:LEU:O	1:I:204:LEU:HD23	1.44	1.17
13:A:305:PL9:C25	13:A:306:PL9:C20	2.21	1.12
13:A:305:PL9:H252	13:A:306:PL9:H201	1.10	1.05
3:K:3:ILE:HG22	3:K:7:GLN:HE22	1.18	1.04
4:L:109:HIS:CE1	4:L:128:HIS:CE1	2.45	1.02
4:L:109:HIS:HE1	4:L:128:HIS:CE1	1.77	1.02
1:I:133:VAL:HG11	11:I:304:CLA:H143	1.39	1.02
3:C:24:CYS:SG	10:C:301:HEC:CBC	0.92	1.01
1:A:41:LEU:HD23	10:A:303:HEC:HBC3	1.41	1.01
13:I:306:PL9:C23	13:I:306:PL9:H302	1.93	0.99
4:L:114:VAL:HG12	4:L:125:CYS:HB2	1.44	0.97
1:A:158:ILE:HG23	1:A:159:PRO:HD2	1.46	0.97
4:L:131:GLN:O	4:L:139:VAL:HG12	1.66	0.96
13:I:306:PL9:HC2	1:A:12:LEU:HD22	1.45	0.96
3:C:24:CYS:SG	10:C:301:HEC:HBC3	0.69	0.96
4:L:109:HIS:HE1	4:L:128:HIS:NE2	1.64	0.95
3:C:275:PHE:CE2	18:C:302:SQD:C6	2.50	0.95
10:I:303:HEC:O2D	13:A:306:PL9:H533	1.67	0.94
3:C:21:CYS:SG	10:C:301:HEC:CBB	0.82	0.92
13:A:305:PL9:H262	13:A:305:PL9:C30	2.04	0.88
5:E:1:MET:HE1	14:E:101:6PL:C6	2.03	0.88
13:A:306:PL9:C18	13:A:306:PL9:H151	2.04	0.86
5:E:1:MET:CE	14:E:101:6PL:H63	2.05	0.85
4:L:15:ARG:HD3	18:L:202:SQD:O9	1.77	0.85
3:C:21:CYS:SG	10:C:301:HEC:HBB3	0.85	0.85
2:J:40:PHE:HE2	13:A:306:PL9:C52	1.90	0.83
3:K:3:ILE:HG22	3:K:7:GLN:NE2	1.93	0.83
1:I:158:ILE:HG23	1:I:159:PRO:HD2	1.61	0.82
1:I:200:LEU:O	1:I:204:LEU:CD2	2.27	0.82
13:A:305:PL9:H251	13:A:306:PL9:C20	2.09	0.82
5:E:1:MET:SD	14:E:101:6PL:H63	2.20	0.81
2:J:1:MET:HE3	4:L:1:ALA:N	1.96	0.81
4:L:131:GLN:O	4:L:139:VAL:CG1	2.29	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:MET:CE	13:I:306:PL9:HC72	2.10	0.81
3:C:275:PHE:HE2	18:C:302:SQD:H62	1.46	0.80
13:A:305:PL9:H251	13:A:306:PL9:H203	1.62	0.80
2:J:2:GLY:O	2:J:4:THR:HG23	1.83	0.79
10:I:303:HEC:O2D	13:A:306:PL9:C53	2.30	0.79
1:A:176:GLY:O	1:A:179:THR:HG22	1.83	0.79
13:A:305:PL9:H262	13:A:305:PL9:H302	1.65	0.78
1:I:44:PHE:HE2	13:A:306:PL9:H212	1.47	0.77
1:I:158:ILE:CG2	1:I:159:PRO:HD2	2.15	0.77
1:I:205:MET:HE3	13:I:306:PL9:HC72	1.67	0.76
1:A:158:ILE:CG2	1:A:159:PRO:HD2	2.17	0.75
3:C:21:CYS:CB	10:C:301:HEC:HBB3	2.13	0.75
18:A:307:SQD:O2	18:A:307:SQD:O48	2.05	0.74
3:C:21:CYS:SG	10:C:301:HEC:HBB2	0.98	0.74
2:J:40:PHE:HE2	13:A:306:PL9:H522	1.53	0.73
1:I:133:VAL:HG11	11:I:304:CLA:C14	2.16	0.73
3:C:24:CYS:CB	10:C:301:HEC:CBC	2.43	0.73
13:I:306:PL9:C25	13:I:306:PL9:H48	2.19	0.73
1:A:91:SER:HB2	2:B:79:TRP:HE1	1.53	0.72
3:C:24:CYS:SG	10:C:301:HEC:HBC1	1.30	0.71
3:C:21:CYS:SG	10:C:301:HEC:HBB1	1.29	0.71
1:I:200:LEU:CD1	1:I:204:LEU:HD21	2.21	0.70
1:I:116:LEU:HD12	13:I:306:PL9:H13	1.74	0.70
10:I:303:HEC:CGD	13:A:306:PL9:H533	2.23	0.69
13:I:306:PL9:C2	1:A:12:LEU:HD22	2.22	0.69
4:L:128:HIS:CB	17:L:201:FES:S1	2.75	0.68
4:L:128:HIS:HE2	2:B:89:ARG:HB2	1.59	0.67
3:C:212:GLU:O	3:C:228:THR:HB	1.95	0.67
4:L:109:HIS:CE1	4:L:128:HIS:NE2	2.55	0.66
3:C:71:VAL:HG12	3:C:154:ARG:HG3	1.76	0.66
1:A:48:VAL:HG11	13:A:306:PL9:C35	2.27	0.65
3:C:24:CYS:HG	10:C:301:HEC:CBC	1.00	0.65
2:J:40:PHE:HE2	13:A:306:PL9:H523	1.62	0.64
2:J:3:VAL:O	2:J:3:VAL:HG13	1.98	0.64
1:A:56:PHE:HZ	18:A:307:SQD:HO4	1.44	0.64
1:I:176:GLY:O	1:I:179:THR:HG22	1.98	0.64
3:C:199:ASP:OD1	3:C:201:ARG:HG3	1.98	0.64
2:J:1:MET:HE3	4:L:1:ALA:H3	1.62	0.63
1:I:158:ILE:CG2	1:I:159:PRO:CD	2.77	0.63
4:L:92:VAL:HA	4:L:98:LEU:HA	1.79	0.63
4:L:164:TRP:NE1	4:L:167:THR:O	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ILE:HG23	1:A:159:PRO:CD	2.26	0.62
13:A:305:PL9:H252	13:A:306:PL9:H202	1.73	0.62
1:I:200:LEU:HD12	1:I:204:LEU:CD2	2.29	0.62
3:C:51:ILE:HG22	3:C:154:ARG:HD3	1.81	0.62
18:C:302:SQD:C23	4:D:19:ASN:OD1	2.48	0.62
18:A:307:SQD:HO2	18:A:307:SQD:H441	1.64	0.61
1:A:35:CYS:HA	10:A:303:HEC:C3B	2.30	0.61
1:A:160:VAL:HG23	1:A:161:ILE:H	1.64	0.61
13:I:306:PL9:C36	13:I:306:PL9:H402	2.31	0.61
3:C:192:ILE:HB	3:C:205:ASP:HB2	1.82	0.60
3:C:154:ARG:O	3:C:234:GLY:HA3	2.01	0.60
3:C:53:TYR:HB3	3:C:154:ARG:HE	1.64	0.60
1:I:149:LYS:NZ	4:D:111:GLY:O	2.35	0.60
4:L:26:LEU:HD21	18:L:202:SQD:H282	1.83	0.60
2:B:33:PRO:HG3	18:C:302:SQD:H4	1.81	0.60
1:A:196:ALA:HB2	13:A:306:PL9:H361	1.84	0.60
1:I:158:ILE:HG23	1:I:159:PRO:CD	2.32	0.59
13:I:306:PL9:H402	13:I:306:PL9:H361	1.84	0.59
1:A:177:GLN:O	1:A:177:GLN:NE2	2.35	0.59
13:I:306:PL9:H48	13:I:306:PL9:H253	1.84	0.58
4:L:133:ASN:OD1	4:L:136:GLY:N	2.31	0.58
18:A:307:SQD:H62	18:A:307:SQD:H2	1.84	0.58
4:L:109:HIS:CE1	4:L:128:HIS:CD2	2.91	0.58
2:J:1:MET:HE3	4:L:1:ALA:H1	1.68	0.58
9:A:302:HEM:HAA2	10:A:303:HEC:CHA	2.33	0.58
4:D:149:LEU:HD11	4:D:170:ARG:HE	1.68	0.58
10:I:303:HEC:CGD	13:A:306:PL9:C53	2.82	0.58
1:A:158:ILE:CG2	1:A:159:PRO:CD	2.82	0.58
14:I:307:6PL:H432	13:A:305:PL9:O1	2.03	0.57
18:A:307:SQD:H1	18:A:307:SQD:H462	1.85	0.57
4:D:130:SER:HA	4:D:141:GLY:HA3	1.85	0.57
13:A:306:PL9:H111	13:A:306:PL9:H152	1.85	0.56
3:C:21:CYS:CB	10:C:301:HEC:HBB2	2.24	0.56
4:L:114:VAL:CG1	4:L:125:CYS:HB2	2.29	0.56
4:L:109:HIS:CE1	4:L:128:HIS:ND1	2.74	0.56
3:C:48:VAL:HG12	3:C:127:THR:HG22	1.88	0.55
4:L:109:HIS:HE1	4:L:128:HIS:CD2	2.24	0.55
1:A:83:ARG:NH1	2:B:60:SER:OG	2.40	0.55
1:I:200:LEU:HD12	1:I:204:LEU:HD21	1.87	0.55
1:I:103:ARG:NH2	9:I:302:HEM:O1A	2.40	0.55
3:C:24:CYS:SG	10:C:301:HEC:HBC2	1.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:VAL:HG12	3:C:154:ARG:CG	2.36	0.55
5:E:4:LEU:CD1	14:E:101:6PL:H132	2.36	0.55
4:L:11:ASP:OD1	4:L:14:LYS:NZ	2.38	0.55
1:A:35:CYS:HA	10:A:303:HEC:C4B	2.37	0.55
2:J:150:PRO:HD2	2:J:153:LYS:HD3	1.89	0.55
1:A:48:VAL:HG11	13:A:306:PL9:H353	1.88	0.55
4:L:104:ASN:HD22	4:L:148:ALA:HB3	1.71	0.55
3:C:69:LEU:O	3:C:70:ASN:OD1	2.24	0.55
3:C:155:GLY:O	10:C:301:HEC:HBA1	2.07	0.55
2:J:40:PHE:CE2	13:A:306:PL9:H522	2.40	0.54
3:K:156:ARG:HA	10:K:301:HEC:HHA	1.89	0.54
13:A:306:PL9:H111	13:A:306:PL9:C15	2.37	0.54
1:I:195:THR:O	1:I:199:MET:HB2	2.06	0.54
13:I:306:PL9:HC2	1:A:12:LEU:CD2	2.29	0.54
1:A:56:PHE:HZ	18:A:307:SQD:O4	1.89	0.54
6:F:31:GLU:OE1	8:H:24:TRP:NE1	2.41	0.54
1:I:200:LEU:HD11	1:I:204:LEU:HD21	1.90	0.54
13:A:306:PL9:C15	13:A:306:PL9:C11	2.86	0.53
1:A:160:VAL:HG23	1:A:161:ILE:N	2.23	0.53
13:I:306:PL9:H253	13:I:306:PL9:C48	2.38	0.53
13:I:306:PL9:C25	13:I:306:PL9:C48	2.86	0.53
2:J:58:GLU:OE1	3:K:37:GLN:NE2	2.41	0.53
2:B:1:MET:SD	2:B:1:MET:N	2.79	0.53
4:D:123:PHE:HB2	4:D:132:TYR:HB2	1.90	0.53
1:I:58:TYR:OH	1:I:138:LEU:O	2.26	0.53
1:A:38:GLY:HA3	10:A:303:HEC:C1C	2.39	0.52
5:E:1:MET:CE	14:E:101:6PL:C6	2.70	0.52
1:I:200:LEU:CD1	1:I:204:LEU:CD2	2.87	0.52
2:J:1:MET:HB3	3:K:280:LEU:HD22	1.91	0.52
2:J:1:MET:HG3	2:J:1:MET:O	2.09	0.52
3:C:153:ASN:HB3	3:C:236:PHE:HD1	1.75	0.52
3:K:3:ILE:CG2	3:K:7:GLN:HE22	2.07	0.52
3:K:182:ILE:HD11	3:K:190:TYR:HB3	1.91	0.52
3:C:70:ASN:OD1	3:C:119:PRO:HA	2.10	0.52
1:I:87:ARG:HH12	1:I:136:TYR:HE1	1.58	0.51
3:K:194:ILE:HD13	3:K:221:ILE:HD11	1.93	0.51
3:K:70:ASN:HB2	10:K:301:HEC:HAA2	1.93	0.51
3:K:190:TYR:HB2	3:K:207:ILE:HB	1.93	0.51
1:A:207:ARG:HB2	10:A:303:HEC:O2D	2.11	0.51
1:I:158:ILE:HD11	2:J:98:VAL:HG11	1.92	0.51
2:J:40:PHE:CE2	13:A:306:PL9:H523	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:12:MET:SD	4:L:15:ARG:NH1	2.83	0.50
16:A:308:PGV:H302	4:D:33:MET:HA	1.92	0.50
3:C:275:PHE:CD2	18:C:302:SQD:C6	2.93	0.50
13:I:306:PL9:H302	13:I:306:PL9:H23	1.88	0.50
4:L:11:ASP:OD1	4:L:11:ASP:N	2.44	0.50
1:I:155:PRO:HG2	1:I:166:VAL:HG22	1.94	0.50
3:C:275:PHE:CD2	18:C:302:SQD:O9	2.65	0.50
13:I:306:PL9:C36	13:I:306:PL9:C40	2.89	0.50
2:J:89:ARG:HD2	4:D:128:HIS:HE2	1.76	0.50
4:L:79:LEU:HD22	4:L:87:PRO:HB2	1.93	0.50
1:A:207:ARG:HB2	10:A:303:HEC:CGD	2.41	0.50
7:G:34:GLN:HB2	7:G:37:LEU:HB2	1.94	0.50
1:A:64:ASP:OD1	1:A:64:ASP:N	2.45	0.49
1:A:212:SER:OG	9:A:302:HEM:O2D	2.27	0.49
1:I:176:GLY:O	1:I:179:THR:CG2	2.60	0.49
1:A:5:TYR:OH	1:A:15:GLN:NE2	2.46	0.49
3:C:272:LYS:NZ	3:C:276:GLU:OE2	2.44	0.49
3:C:99:ASN:OD1	3:C:123:TYR:OH	2.31	0.49
4:D:68:TRP:HD1	4:D:69:LEU:HD22	1.78	0.49
5:E:1:MET:SD	14:E:101:6PL:C6	2.99	0.49
4:L:4:ILE:HG22	4:L:7:ASP:H	1.77	0.49
4:D:12:MET:SD	4:D:15:ARG:NH2	2.86	0.49
2:J:40:PHE:CE2	13:A:306:PL9:C52	2.82	0.49
13:A:305:PL9:H262	13:A:305:PL9:H303	1.90	0.48
5:E:1:MET:HE1	14:E:101:6PL:H62	1.91	0.48
4:D:128:HIS:HB2	17:D:201:FES:S1	2.54	0.48
9:A:301:HEM:HHC	9:A:301:HEM:HBB2	1.94	0.48
3:K:5:ALA:O	3:K:105:TYR:OH	2.31	0.48
1:I:103:ARG:HG2	7:O:21:LEU:HD21	1.95	0.48
6:N:8:ARG:NH2	14:N:101:6PL:H52	2.28	0.48
3:C:29:LYS:NZ	3:C:233:VAL:O	2.33	0.48
6:N:8:ARG:HH21	14:N:101:6PL:H12	1.78	0.48
1:A:89:SER:OG	2:B:51:ASN:ND2	2.46	0.48
4:D:117:ASN:HD22	4:D:124:ILE:HD12	1.79	0.48
13:I:306:PL9:H422	13:I:306:PL9:H38	1.50	0.48
4:L:109:HIS:CE1	4:L:128:HIS:CG	3.02	0.48
3:C:247:ASP:HB3	3:C:250:ARG:HG3	1.95	0.48
1:A:50:THR:HG23	1:A:86:HIS:HD1	1.79	0.47
11:A:304:CLA:HBB1	2:B:133:PHE:HA	1.95	0.47
3:C:21:CYS:HG	10:C:301:HEC:CBB	1.12	0.47
2:J:58:GLU:OE2	3:K:145:LYS:NZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:176:THR:HG23	3:K:222:LYS:HA	1.96	0.47
4:L:147:LEU:O	4:L:170:ARG:NH1	2.47	0.47
6:F:28:LEU:HD22	8:H:24:TRP:HD1	1.79	0.47
3:C:1:TYR:CD1	3:C:117:PRO:HG3	2.50	0.47
1:A:8:PHE:O	1:A:12:LEU:HB2	2.15	0.47
13:A:306:PL9:H251	13:A:306:PL9:H272	1.64	0.47
3:C:2:PRO:HG2	3:C:116:GLY:HA2	1.96	0.47
13:A:305:PL9:H503	13:A:305:PL9:HC8	1.95	0.47
3:C:117:PRO:HB3	10:C:301:HEC:HMA1	1.97	0.47
13:A:306:PL9:C20	13:A:306:PL9:H151	2.45	0.46
3:K:57:LEU:HD21	3:K:233:VAL:HB	1.97	0.46
4:L:101:PHE:HA	4:L:151:HIS:HA	1.97	0.46
1:A:31:ASN:OD1	1:A:31:ASN:N	2.49	0.46
18:C:302:SQD:O10	4:D:23:LEU:HD11	2.15	0.46
13:I:306:PL9:H28	13:I:306:PL9:H322	1.47	0.46
4:L:15:ARG:HD3	18:L:202:SQD:S	2.54	0.46
1:I:64:ASP:N	1:I:64:ASP:OD1	2.46	0.46
3:K:25:HIS:CG	3:K:153:ASN:HD21	2.33	0.46
1:I:204:LEU:HG	13:I:306:PL9:H521	1.98	0.46
1:A:175:VAL:HG23	1:A:179:THR:HG21	0.72	0.46
1:A:52:PHE:O	1:A:55:THR:OG1	2.33	0.46
1:I:205:MET:HE2	13:I:306:PL9:HC72	1.96	0.45
13:I:306:PL9:H422	13:I:306:PL9:H461	1.64	0.45
13:A:305:PL9:C25	13:A:306:PL9:H222	2.47	0.45
2:B:73:LEU:HD11	3:C:18:ARG:HB3	1.97	0.45
3:C:280:LEU:HD22	4:D:4:ILE:HG13	1.97	0.45
1:I:73:MET:HE2	1:I:83:ARG:HD3	1.99	0.45
3:K:55:MET:HE1	3:K:121:GLN:HA	1.98	0.45
3:K:78:PRO:HG2	3:K:146:TYR:HB3	1.99	0.45
3:C:156:ARG:NE	10:C:301:HEC:O1D	2.47	0.45
13:A:306:PL9:H472	13:A:306:PL9:H451	1.88	0.45
3:C:21:CYS:SG	10:C:301:HEC:C3B	2.97	0.45
1:I:119:VAL:CG1	13:I:306:PL9:C15	2.95	0.45
11:I:304:CLA:H152	11:I:304:CLA:H18	1.74	0.45
3:C:1:TYR:HD1	3:C:117:PRO:HG3	1.82	0.45
1:I:160:VAL:C	1:I:162:GLY:H	2.24	0.44
4:L:87:PRO:HG2	4:L:105:ALA:HB3	1.98	0.44
4:L:110:LEU:HD23	4:L:110:LEU:HA	1.80	0.44
4:L:130:SER:HA	4:L:141:GLY:HA3	1.98	0.44
13:I:306:PL9:H151	13:I:306:PL9:H172	1.73	0.44
3:K:180:LYS:HD2	3:K:180:LYS:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:304:CLA:HAA1	2:B:108:LEU:HD11	1.99	0.44
13:A:305:PL9:H351	13:A:305:PL9:H372	1.43	0.44
3:K:133:PRO:HG2	3:K:141:VAL:HG11	2.00	0.44
4:L:77:ARG:NH2	4:L:134:ASN:O	2.42	0.44
4:L:110:LEU:HB2	17:L:201:FES:S2	2.58	0.44
13:I:306:PL9:H221	13:I:306:PL9:H201	1.51	0.44
18:A:307:SQD:HO2	18:A:307:SQD:C46	2.30	0.44
1:I:158:ILE:HG22	1:I:159:PRO:HD2	1.95	0.44
13:A:306:PL9:H122	13:A:306:PL9:HC8	1.71	0.44
13:I:306:PL9:H38	13:I:306:PL9:H461	2.00	0.44
13:A:305:PL9:C25	13:A:306:PL9:H203	2.16	0.44
3:C:184:ARG:HD3	3:C:190:TYR:HE1	1.83	0.44
13:I:306:PL9:H48	13:I:306:PL9:H252	1.97	0.43
2:J:3:VAL:O	2:J:3:VAL:CG1	2.66	0.43
3:K:274:GLN:HB2	5:M:31:ILE:HG13	2.00	0.43
4:D:109:HIS:HB3	17:D:201:FES:S2	2.57	0.43
5:E:3:THR:HG21	14:E:101:6PL:H12	2.00	0.43
3:K:83:LEU:HD12	3:K:113:LEU:HD13	2.01	0.43
1:A:148:VAL:HA	1:A:151:VAL:HG12	2.00	0.43
3:K:2:PRO:O	3:K:6:GLN:HG3	2.18	0.43
4:L:131:GLN:O	4:L:139:VAL:HG13	2.16	0.43
1:I:120:THR:HG23	1:I:198:PHE:HD2	1.83	0.43
6:N:8:ARG:NH2	14:N:101:6PL:H12	2.34	0.43
3:K:55:MET:HE3	3:K:55:MET:HB3	1.91	0.43
2:B:32:TRP:HA	2:B:33:PRO:HA	1.80	0.43
3:C:51:ILE:CG2	3:C:154:ARG:HD3	2.47	0.43
3:C:275:PHE:CZ	18:C:302:SQD:H62	2.41	0.43
4:D:77:ARG:HA	4:D:90:LEU:O	2.18	0.43
1:I:175:VAL:HG13	1:I:179:THR:HG21	1.99	0.43
3:C:32:ASP:OD1	3:C:50:ARG:NH1	2.51	0.43
1:I:81:LEU:HD21	16:K:302:PGV:H92	2.01	0.43
3:K:144:LEU:HD23	3:K:144:LEU:HA	1.85	0.43
3:K:46:GLU:HB3	3:K:93:MET:HE3	1.99	0.43
4:L:15:ARG:CD	18:L:202:SQD:O9	2.58	0.43
2:J:32:TRP:NE1	18:L:202:SQD:O3	2.48	0.43
1:I:158:ILE:HG22	1:I:159:PRO:CD	2.49	0.42
3:K:179:VAL:HA	3:K:194:ILE:HG22	2.00	0.42
4:D:123:PHE:N	4:D:132:TYR:O	2.53	0.42
14:E:101:6PL:H361	6:F:13:MET:HE1	2.01	0.42
18:A:307:SQD:H62	18:A:307:SQD:C2	2.48	0.42
3:C:51:ILE:HG22	3:C:154:ARG:CD	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:89:ARG:NH2	2:J:149:LEU:O	2.52	0.42
2:J:1:MET:HB3	3:K:280:LEU:CD2	2.48	0.42
10:I:303:HEC:O1D	13:A:306:PL9:C53	2.68	0.42
1:A:32:ILE:O	1:A:35:CYS:HB2	2.19	0.42
3:C:275:PHE:HD2	18:C:302:SQD:O9	2.02	0.42
1:A:160:VAL:C	1:A:162:GLY:H	2.28	0.42
4:D:69:LEU:HD21	4:D:98:LEU:HD22	2.02	0.42
13:A:306:PL9:H201	13:A:306:PL9:H222	1.39	0.41
2:J:88:LEU:HD13	2:J:101:MET:HE1	2.02	0.41
3:K:179:VAL:HG23	3:K:192:ILE:HD11	2.02	0.41
4:L:56:LYS:HB2	4:L:81:GLN:HB3	2.02	0.41
1:A:110:PHE:HD2	2:B:112:PRO:HB3	1.84	0.41
2:B:41:PRO:HB2	3:C:268:LEU:HD21	2.01	0.41
1:I:16:ALA:HA	1:I:19:ASP:HB2	2.02	0.41
3:C:97:MET:HE2	3:C:129:PRO:HG3	2.02	0.41
5:E:4:LEU:HD13	14:E:101:6PL:H132	2.02	0.41
1:I:47:GLN:H	1:I:47:GLN:HG2	1.71	0.41
1:I:102:PHE:HZ	15:J:201:LMG:H242	1.86	0.41
3:K:158:GLN:HB3	3:K:169:THR:HB	2.03	0.41
13:A:305:PL9:C30	13:A:305:PL9:C26	2.86	0.41
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.94	0.41
2:J:83:PRO:O	2:J:86:GLN:HB3	2.21	0.41
1:I:106:LEU:HD23	1:I:106:LEU:HA	1.88	0.40
2:J:84:VAL:HG13	2:J:101:MET:HG2	2.03	0.40
1:A:160:VAL:C	1:A:162:GLY:N	2.77	0.40
4:D:80:THR:O	4:D:87:PRO:HA	2.21	0.40
4:D:89:TYR:N	4:D:103:ILE:O	2.40	0.40
12:H:101:BCR:H20C	12:H:101:BCR:H361	1.84	0.40
1:I:158:ILE:HG22	1:I:159:PRO:N	2.36	0.40
3:K:85:PRO:HA	3:K:86:PRO:HD3	1.90	0.40
3:C:21:CYS:HG	10:C:301:HEC:CAB	1.98	0.40
1:I:119:VAL:HG12	13:I:306:PL9:C15	2.51	0.40
5:M:23:ILE:HD13	5:M:23:ILE:HA	1.93	0.40
1:A:82:ILE:HD13	1:A:82:ILE:HA	1.94	0.40
2:B:14:LEU:HD13	2:B:26:TYR:HD2	1.86	0.40
2:B:101:MET:HE3	2:B:101:MET:HB2	1.89	0.40
14:E:101:6PL:H402	14:E:101:6PL:H371	1.89	0.40
1:I:124:LEU:HD23	1:I:124:LEU:HA	1.91	0.40
2:J:89:ARG:HD2	4:D:128:HIS:NE2	2.37	0.40
1:A:58:TYR:OH	1:A:138:LEU:O	2.28	0.40
1:I:14:ILE:O	1:I:17:ILE:HB	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:8:ASN:OD1	5:M:29:ARG:NH1	2.48	0.40
13:A:306:PL9:H151	13:A:306:PL9:C19	2.51	0.40
6:F:5:GLU:OE1	6:F:8:ARG:NH2	2.54	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	213/215 (99%)	203 (95%)	8 (4%)	2 (1%)	14	46
1	I	213/215 (99%)	204 (96%)	7 (3%)	2 (1%)	14	46
2	B	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
2	J	158/160 (99%)	149 (94%)	7 (4%)	2 (1%)	9	39
3	C	283/285 (99%)	271 (96%)	12 (4%)	0	100	100
3	K	283/285 (99%)	273 (96%)	10 (4%)	0	100	100
4	D	177/179 (99%)	164 (93%)	13 (7%)	0	100	100
4	L	177/179 (99%)	163 (92%)	13 (7%)	1 (1%)	21	54
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
5	M	29/31 (94%)	29 (100%)	0	0	100	100
6	F	34/36 (94%)	34 (100%)	0	0	100	100
6	N	34/36 (94%)	34 (100%)	0	0	100	100
7	G	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
7	O	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	27 (100%)	0	0	100	100
All	All	1912/1944 (98%)	1824 (95%)	81 (4%)	7 (0%)	31	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	160	VAL
1	A	160	VAL
4	L	129	GLY
2	J	150	PRO
1	A	174	SER
1	I	161	ILE
2	J	3	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/186 (100%)	186 (100%)	0	100	100
1	I	186/186 (100%)	186 (100%)	0	100	100
2	B	135/135 (100%)	135 (100%)	0	100	100
2	J	135/135 (100%)	135 (100%)	0	100	100
3	C	242/242 (100%)	241 (100%)	1 (0%)	84	81
3	K	242/242 (100%)	241 (100%)	1 (0%)	84	81
4	D	141/141 (100%)	140 (99%)	1 (1%)	76	78
4	L	141/141 (100%)	141 (100%)	0	100	100
5	E	26/26 (100%)	26 (100%)	0	100	100
5	M	26/26 (100%)	26 (100%)	0	100	100
6	F	26/26 (100%)	26 (100%)	0	100	100
6	N	26/26 (100%)	26 (100%)	0	100	100
7	G	31/31 (100%)	31 (100%)	0	100	100
7	O	31/31 (100%)	31 (100%)	0	100	100
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	24 (100%)	0	100	100
All	All	1622/1622 (100%)	1619 (100%)	3 (0%)	85	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	49	VAL
3	C	154	ARG
4	D	159	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	86	GLN
3	K	7	GLN
3	K	99	ASN
3	K	111	ASN
3	K	142	HIS
4	L	104	ASN
4	L	135	GLN
1	A	15	GLN
1	A	142	GLN
1	A	177	GLN
1	A	209	GLN
2	B	51	ASN
3	C	6	GLN
3	C	103	GLN
4	D	8	ASN
4	D	61	ASN
4	D	117	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

29 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
9	HEM	A	301	1	50,50,50	1.44	6 (12%)	67,82,82	1.22	9 (13%)
13	PL9	A	306	-	55,55,55	0.73	1 (1%)	68,69,69	0.60	1 (1%)
18	SQD	C	302	-	52,54,54	0.38	1 (1%)	62,65,65	0.41	0
14	6PL	E	101	-	50,50,51	1.62	4 (8%)	56,58,59	1.44	4 (7%)
9	HEM	A	302	1	50,50,50	1.31	7 (14%)	67,82,82	1.23	7 (10%)
17	FES	L	201	4	0,4,4	-	-	-	-	-
16	PGV	A	308	-	44,44,50	0.99	2 (4%)	47,50,56	1.07	3 (6%)
13	PL9	I	306	-	55,55,55	0.63	2 (3%)	68,69,69	1.78	21 (30%)
15	LMG	J	201	-	55,55,55	0.86	1 (1%)	63,63,63	1.41	8 (12%)
17	FES	D	201	4	0,4,4	-	-	-	-	-
14	6PL	I	307	-	51,51,51	1.61	4 (7%)	57,59,59	1.38	4 (7%)
18	SQD	A	307	-	52,54,54	0.38	1 (1%)	62,65,65	0.41	0
13	PL9	A	305	-	55,55,55	0.73	1 (1%)	68,69,69	0.59	2 (2%)
10	HEC	A	303	-	46,50,50	1.91	6 (13%)	58,82,82	1.13	4 (6%)
14	6PL	N	101	-	51,51,51	1.59	4 (7%)	57,59,59	1.54	5 (8%)
11	CLA	A	304	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	7 (8%)
16	PGV	K	302	-	50,50,50	0.92	2 (4%)	53,56,56	0.97	2 (3%)
9	HEM	I	302	1	50,50,50	1.35	6 (12%)	67,82,82	1.13	5 (7%)
16	PGV	B	201	-	47,47,50	0.94	2 (4%)	50,53,56	1.04	3 (6%)
10	HEC	C	301	3	46,50,50	1.74	11 (23%)	58,82,82	1.62	10 (17%)
10	HEC	K	301	3	46,50,50	1.92	7 (15%)	58,82,82	1.13	6 (10%)
16	PGV	J	202	-	50,50,50	0.93	2 (4%)	53,56,56	0.95	2 (3%)
18	SQD	L	202	-	52,54,54	0.97	6 (11%)	62,65,65	1.41	10 (16%)
10	HEC	I	303	1	46,50,50	1.90	6 (13%)	58,82,82	1.07	1 (1%)
15	LMG	F	101	-	55,55,55	0.79	2 (3%)	63,63,63	1.37	9 (14%)
11	CLA	I	304	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	BCR	H	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.21	7 (12%)
9	HEM	I	301	1	50,50,50	1.35	5 (10%)	67,82,82	1.06	2 (2%)
12	BCR	I	305	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	4 (7%)

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
9	HEM	A	301	1	-	5/14/54/54	-
13	PL9	A	306	-	-	32/53/73/73	0/1/1/1
18	SQD	C	302	-	-	20/49/69/69	0/1/1/1
14	6PL	E	101	-	-	21/54/54/55	-
9	HEM	A	302	1	-	1/14/54/54	-
17	FES	L	201	4	-	-	0/1/1/1
16	PGV	A	308	-	-	12/49/49/55	-
13	PL9	I	306	-	-	17/53/73/73	0/1/1/1
15	LMG	J	201	-	-	31/50/70/70	0/1/1/1
17	FES	D	201	4	-	-	0/1/1/1
14	6PL	I	307	-	-	14/55/55/55	-
18	SQD	A	307	-	-	21/49/69/69	0/1/1/1
13	PL9	A	305	-	-	34/53/73/73	0/1/1/1
10	HEC	A	303	-	-	5/14/54/54	-
14	6PL	N	101	-	-	17/55/55/55	-
11	CLA	A	304	-	1/1/15/20	14/39/115/115	-
16	PGV	K	302	-	-	12/55/55/55	-
9	HEM	I	302	1	-	2/14/54/54	-
16	PGV	B	201	-	-	13/52/52/55	-
10	HEC	C	301	3	-	6/14/54/54	-
10	HEC	K	301	3	-	4/14/54/54	-
16	PGV	J	202	-	-	15/55/55/55	-
18	SQD	L	202	-	-	21/49/69/69	0/1/1/1
10	HEC	I	303	1	-	5/14/54/54	-
15	LMG	F	101	-	-	21/50/70/70	0/1/1/1
11	CLA	I	304	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BCR	H	101	-	-	11/29/63/63	0/2/2/2
9	HEM	I	301	1	-	1/14/54/54	-
12	BCR	I	305	-	-	16/29/63/63	0/2/2/2

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	I	307	6PL	O11-C11	7.04	1.43	1.22
14	E	101	6PL	O31-C31	7.04	1.43	1.22
14	I	307	6PL	O31-C31	7.03	1.43	1.22
14	E	101	6PL	O11-C11	7.00	1.43	1.22
14	N	101	6PL	O11-C11	6.99	1.43	1.22
14	N	101	6PL	O31-C31	6.99	1.43	1.22
10	A	303	HEC	CAB-C3B	6.33	1.55	1.35
10	K	301	HEC	CAC-C3C	6.27	1.55	1.35
10	K	301	HEC	CAB-C3B	6.23	1.55	1.35
10	I	303	HEC	CAB-C3B	6.20	1.55	1.35
10	A	303	HEC	CAC-C3C	6.19	1.55	1.35
10	I	303	HEC	CAC-C3C	6.13	1.54	1.35
13	A	306	PL9	C3-C4	-4.79	1.42	1.49
13	A	305	PL9	C3-C4	-4.72	1.42	1.49
9	I	301	HEM	FE-ND	4.57	2.09	1.94
10	C	301	HEC	CBB-CAB	-4.39	1.33	1.49
10	C	301	HEC	CBC-CAC	-4.38	1.33	1.49
10	I	303	HEC	CBC-CAC	-4.28	1.33	1.49
10	K	301	HEC	CBB-CAB	-4.27	1.33	1.49
16	K	302	PGV	O01-C1	4.25	1.46	1.34
16	B	201	PGV	O01-C1	4.24	1.46	1.34
10	A	303	HEC	CBB-CAB	-4.23	1.33	1.49
16	A	308	PGV	O03-C19	4.22	1.45	1.33
10	A	303	HEC	CBC-CAC	-4.21	1.33	1.49
16	J	202	PGV	O03-C19	4.20	1.45	1.33
16	J	202	PGV	O01-C1	4.20	1.46	1.34
16	K	302	PGV	O03-C19	4.19	1.45	1.33
10	I	303	HEC	CBB-CAB	-4.18	1.34	1.49
10	K	301	HEC	CBC-CAC	-4.14	1.34	1.49
16	A	308	PGV	O01-C1	4.14	1.46	1.34
16	B	201	PGV	O03-C19	4.14	1.45	1.33
9	A	301	HEM	FE-NA	3.96	2.08	1.95
10	C	301	HEC	CAC-C3C	3.87	1.47	1.35
10	C	301	HEC	CAB-C3B	3.86	1.47	1.35
12	H	101	BCR	C1-C6	-3.73	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEM	FE-ND	3.64	2.06	1.94
14	E	101	6PL	O3-C11	3.35	1.43	1.33
9	I	302	HEM	FE-ND	3.32	2.05	1.94
14	I	307	6PL	O3-C11	3.25	1.42	1.33
12	H	101	BCR	C30-C25	-3.23	1.49	1.53
14	E	101	6PL	O2-C31	3.19	1.43	1.34
14	I	307	6PL	O2-C31	3.17	1.43	1.34
11	A	304	CLA	C1D-ND	3.15	1.42	1.37
14	N	101	6PL	O3-C11	3.14	1.42	1.33
9	A	302	HEM	FE-ND	3.13	2.04	1.94
11	I	304	CLA	C1D-ND	3.13	1.42	1.37
14	N	101	6PL	O2-C31	3.10	1.43	1.34
18	L	202	SQD	O48-C23	3.02	1.42	1.33
9	I	302	HEM	CAB-C3B	2.93	1.55	1.47
12	I	305	BCR	C1-C6	-2.90	1.50	1.53
9	I	301	HEM	CAC-C3C	2.87	1.55	1.47
15	J	201	LMG	O7-C8	-2.86	1.39	1.46
9	A	301	HEM	CAC-C3C	2.86	1.55	1.47
11	A	304	CLA	C4B-NB	2.83	1.41	1.37
9	I	301	HEM	CAB-C3B	2.82	1.54	1.47
9	A	302	HEM	CAC-C3C	2.80	1.54	1.47
12	I	305	BCR	C30-C25	-2.80	1.50	1.53
9	A	302	HEM	CAB-C3B	2.79	1.54	1.47
9	A	301	HEM	CAB-C3B	2.79	1.54	1.47
18	L	202	SQD	O47-C7	2.77	1.42	1.34
10	C	301	HEC	C1D-ND	-2.72	1.34	1.39
13	I	306	PL9	C6-C5	2.72	1.48	1.35
10	C	301	HEC	C1B-NB	-2.71	1.34	1.39
10	C	301	HEC	C4D-ND	-2.71	1.34	1.39
10	I	303	HEC	C3C-C2C	-2.66	1.32	1.41
10	C	301	HEC	C4B-NB	-2.57	1.34	1.39
9	I	302	HEM	CAC-C3C	2.57	1.54	1.47
11	I	304	CLA	C4B-NB	2.52	1.41	1.37
10	A	303	HEC	C3D-C2D	-2.52	1.32	1.38
9	I	302	HEM	FE-NA	2.51	2.03	1.95
11	A	304	CLA	CMB-C2B	-2.46	1.45	1.50
9	A	301	HEM	C2A-C3A	-2.44	1.32	1.38
10	A	303	HEC	C3C-C2C	-2.43	1.32	1.41
9	I	301	HEM	FE-NA	2.43	2.03	1.95
11	I	304	CLA	MG-NB	-2.43	2.01	2.05
9	I	301	HEM	C2A-C3A	-2.41	1.32	1.38
10	I	303	HEC	C3D-C2D	-2.38	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	304	CLA	CMB-C2B	-2.38	1.45	1.50
9	A	302	HEM	C2A-C3A	-2.37	1.32	1.38
11	A	304	CLA	MG-NB	-2.33	2.01	2.05
10	K	301	HEC	C3D-C2D	-2.32	1.32	1.38
10	C	301	HEC	C1A-C2A	-2.31	1.41	1.45
15	F	101	LMG	O7-C8	-2.31	1.41	1.46
9	A	301	HEM	C3B-C2B	-2.30	1.32	1.37
11	I	304	CLA	CMD-C2D	-2.25	1.46	1.50
11	I	304	CLA	C1B-C2B	2.25	1.48	1.43
18	L	202	SQD	O2-C2	-2.24	1.37	1.43
11	A	304	CLA	CMD-C2D	-2.24	1.46	1.50
9	I	302	HEM	C2A-C3A	-2.21	1.33	1.38
9	A	302	HEM	C3B-C2B	-2.20	1.32	1.37
10	C	301	HEC	C4A-C3A	-2.17	1.41	1.45
11	A	304	CLA	C1B-C2B	2.16	1.48	1.43
9	I	302	HEM	C3C-C2C	-2.15	1.32	1.37
11	A	304	CLA	CMC-C2C	-2.14	1.46	1.50
18	C	302	SQD	O8-S	2.14	1.55	1.47
11	I	304	CLA	C3B-C4B	2.14	1.49	1.42
9	A	302	HEM	C3D-C2D	-2.13	1.32	1.36
11	I	304	CLA	CMC-C2C	-2.13	1.46	1.50
18	A	307	SQD	O8-S	2.13	1.55	1.47
15	F	101	LMG	C4-C5	2.09	1.57	1.53
13	I	306	PL9	C2-C3	2.09	1.39	1.34
11	A	304	CLA	C3B-C4B	2.07	1.48	1.42
11	I	304	CLA	CHC-C1C	2.06	1.42	1.38
10	C	301	HEC	C3C-C4C	-2.05	1.42	1.46
18	L	202	SQD	O47-C45	-2.03	1.41	1.46
18	L	202	SQD	O3-C3	-2.03	1.37	1.43
9	A	302	HEM	FE-NA	2.03	2.01	1.95
10	K	301	HEC	CMB-C2B	2.02	1.54	1.50
10	K	301	HEC	CMC-C2C	2.02	1.54	1.50
11	A	304	CLA	CHC-C1C	2.02	1.42	1.38
18	L	202	SQD	O4-C4	-2.02	1.38	1.43

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	101	6PL	O2-C31-O31	-6.68	108.08	123.70
11	I	304	CLA	C4A-NA-C1A	6.30	109.55	106.68
11	A	304	CLA	C4A-NA-C1A	6.07	109.45	106.68
14	E	101	6PL	O2-C31-O31	-6.05	109.57	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	101	6PL	O3-C11-O11	-5.91	108.83	123.63
14	I	307	6PL	O3-C11-O11	-5.62	109.56	123.63
14	E	101	6PL	O3-C11-O11	-5.46	109.98	123.63
14	I	307	6PL	O2-C31-O31	-5.21	111.53	123.70
10	C	301	HEC	CHC-C4B-NB	4.92	129.81	124.45
16	A	308	PGV	O01-C1-C2	4.51	121.23	111.48
10	C	301	HEC	CBB-CAB-C3B	-4.08	119.27	127.43
10	C	301	HEC	CBC-CAC-C3C	-3.98	119.49	127.43
16	B	201	PGV	O01-C1-C2	3.93	119.99	111.48
14	N	101	6PL	O11-C11-C12	-3.92	108.43	123.78
16	J	202	PGV	O01-C1-C2	3.90	119.91	111.48
14	E	101	6PL	O31-C31-C32	-3.86	108.67	123.78
12	I	305	BCR	C2-C1-C6	3.85	116.03	110.44
14	E	101	6PL	O11-C11-C12	-3.82	108.85	123.78
14	I	307	6PL	O11-C11-C12	-3.74	109.16	123.78
16	K	302	PGV	O01-C1-C2	3.74	119.57	111.48
13	A	306	PL9	C7-C3-C4	3.64	119.91	116.91
14	I	307	6PL	O31-C31-C32	-3.64	109.56	123.78
18	L	202	SQD	O9-S-O7	-3.58	102.17	113.82
13	I	306	PL9	C7-C8-C9	-3.55	120.72	126.83
9	A	302	HEM	C3B-C2B-C1B	3.48	109.03	106.41
13	A	305	PL9	C7-C3-C4	3.48	119.77	116.91
18	L	202	SQD	O7-S-C6	3.44	111.89	106.76
12	I	305	BCR	C3-C4-C5	-3.43	107.94	114.06
14	N	101	6PL	O31-C31-C32	-3.40	110.48	123.78
13	I	306	PL9	C12-C13-C14	-3.23	120.22	127.62
16	B	201	PGV	O03-C19-C20	3.23	121.68	111.83
13	I	306	PL9	C32-C33-C34	-3.23	120.24	127.62
18	L	202	SQD	O6-C1-C2	3.19	113.12	108.27
9	A	301	HEM	C3B-C2B-C1B	3.15	108.78	106.41
13	I	306	PL9	C37-C38-C39	-3.07	120.59	127.62
13	I	306	PL9	C17-C18-C19	-3.07	120.60	127.62
11	A	304	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
13	I	306	PL9	C27-C28-C29	-3.03	120.69	127.62
10	A	303	HEC	CBD-CAD-C3D	-3.03	104.16	112.53
13	I	306	PL9	C42-C43-C44	-3.00	120.75	127.62
18	L	202	SQD	O47-C7-C8	3.00	117.98	111.48
11	I	304	CLA	C3B-C4B-NB	-3.00	107.85	110.53
15	J	201	LMG	O6-C1-O1	-2.99	102.97	110.04
13	I	306	PL9	C22-C23-C24	-2.96	120.84	127.62
9	I	301	HEM	CMB-C2B-C1B	-2.91	120.49	125.03
16	J	202	PGV	O03-C19-C20	2.91	120.70	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	I	306	PL9	C30-C29-C31	2.89	120.24	115.23
13	I	306	PL9	C20-C19-C21	2.88	120.23	115.23
11	I	304	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
13	I	306	PL9	C7-C3-C4	2.85	119.26	116.91
16	K	302	PGV	O03-C19-C20	2.83	120.47	111.83
13	I	306	PL9	C7-C3-C2	-2.81	120.08	123.39
13	I	306	PL9	C25-C24-C26	2.78	120.06	115.23
12	H	101	BCR	C24-C23-C22	-2.78	122.12	126.23
11	A	304	CLA	C3B-C4B-NB	-2.78	108.05	110.53
9	I	302	HEM	CHC-C1C-NC	2.76	127.46	124.45
10	C	301	HEC	CHD-C1D-ND	2.76	128.86	123.86
13	I	306	PL9	C40-C39-C41	2.75	120.00	115.23
13	I	306	PL9	C35-C34-C36	2.75	120.00	115.23
12	H	101	BCR	C27-C26-C25	2.74	126.41	122.70
16	A	308	PGV	O03-C19-C20	2.71	120.09	111.83
12	I	305	BCR	C27-C26-C25	2.70	126.36	122.70
10	C	301	HEC	CHA-C4D-ND	2.70	128.76	123.86
18	L	202	SQD	C4-C3-C2	2.70	115.56	110.83
13	I	306	PL9	C45-C44-C46	2.70	119.91	115.23
13	I	306	PL9	C10-C9-C11	2.68	119.88	115.23
12	I	305	BCR	C24-C23-C22	-2.67	122.28	126.23
15	F	101	LMG	O6-C1-O1	-2.66	103.75	110.04
11	I	304	CLA	CHB-C4A-NA	2.65	128.23	124.40
9	A	302	HEM	CMC-C2C-C1C	-2.65	120.06	124.73
13	I	306	PL9	C15-C14-C16	2.64	119.82	115.23
9	A	301	HEM	C3B-C4B-NB	-2.63	107.58	109.47
15	F	101	LMG	O1-C1-C2	-2.63	104.28	108.27
10	C	301	HEC	CHA-C1A-NA	2.62	127.31	124.45
18	L	202	SQD	O9-S-C6	2.61	110.65	106.76
15	J	201	LMG	O1-C7-C8	-2.60	104.50	110.82
18	L	202	SQD	O48-C23-C24	2.54	119.57	111.83
9	I	302	HEM	CAC-C3C-C4C	2.52	130.85	124.82
10	I	303	HEC	CMB-C2B-C1B	-2.52	121.58	125.42
15	J	201	LMG	C40-C39-C38	-2.50	101.71	114.37
13	I	306	PL9	C53-C6-C1	2.48	120.36	115.28
15	J	201	LMG	C38-C37-C36	-2.47	101.86	114.37
10	C	301	HEC	CHB-C1B-NB	2.45	128.31	123.86
15	F	101	LMG	C40-C39-C38	-2.45	101.97	114.37
10	A	303	HEC	CMB-C2B-C1B	-2.45	121.69	125.42
9	I	302	HEM	CMB-C2B-C1B	-2.43	121.24	125.03
9	A	301	HEM	CHB-C1B-NB	2.40	127.33	124.37
11	I	304	CLA	CAA-C2A-C3A	-2.36	106.61	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	304	CLA	CHB-C4A-NA	2.35	127.79	124.40
15	F	101	LMG	C38-C37-C36	-2.34	102.55	114.37
13	I	306	PL9	C51-C49-C50	2.30	119.89	114.59
15	J	201	LMG	O3-C3-C2	-2.29	104.98	110.38
15	F	101	LMG	O3-C3-C2	-2.29	104.99	110.38
9	A	302	HEM	CAB-C3B-C2B	-2.28	121.02	128.43
11	A	304	CLA	C1-C2-C3	-2.28	122.46	126.20
18	L	202	SQD	O47-C7-O49	-2.27	118.41	123.70
15	J	201	LMG	O2-C2-C1	-2.27	104.67	110.08
11	A	304	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
9	A	301	HEM	CAC-C3C-C4C	-2.26	119.43	124.82
14	N	101	6PL	C2-O2-C31	-2.26	112.39	117.80
10	K	301	HEC	CAA-CBA-CGA	-2.25	107.69	113.67
11	I	304	CLA	C1-C2-C3	-2.25	122.51	126.20
10	C	301	HEC	CHD-C4C-NC	2.24	126.89	124.45
10	K	301	HEC	CAA-C2A-C3A	-2.24	123.67	127.87
9	I	301	HEM	CAC-C3C-C4C	-2.22	119.51	124.82
9	I	302	HEM	CHD-C4C-C3C	2.22	128.95	125.21
9	A	301	HEM	CAB-C3B-C2B	-2.22	121.23	128.43
16	B	201	PGV	O03-C19-O04	-2.20	118.12	123.63
9	A	302	HEM	CHC-C4B-C3B	2.19	129.44	125.07
10	K	301	HEC	CMC-C2C-C1C	-2.18	122.09	125.42
15	J	201	LMG	C42-C41-C40	-2.18	103.34	114.37
15	F	101	LMG	O7-C10-O9	-2.18	118.61	123.70
9	A	301	HEM	CAA-CBA-CGA	-2.18	107.89	113.67
10	K	301	HEC	C2A-C1A-NA	-2.17	108.23	110.32
15	F	101	LMG	C42-C41-C40	-2.15	103.48	114.37
9	A	302	HEM	C1B-NB-C4B	2.13	107.73	105.21
9	I	302	HEM	CAC-C3C-C2C	-2.13	121.51	128.43
15	F	101	LMG	C1-C2-C3	-2.13	105.53	110.01
10	A	303	HEC	CHD-C4C-C3C	2.12	128.78	125.21
10	C	301	HEC	C4B-NB-C1B	2.12	109.27	105.82
12	H	101	BCR	C10-C11-C12	-2.11	117.08	123.20
11	I	304	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
9	A	302	HEM	C3B-C4B-NB	-2.10	107.96	109.47
18	L	202	SQD	C1-O5-C5	2.09	117.81	113.72
12	H	101	BCR	C7-C8-C9	-2.09	123.14	126.23
10	K	301	HEC	CHA-C1A-C2A	2.09	128.17	124.86
16	A	308	PGV	O01-C1-O02	-2.09	118.82	123.70
13	I	306	PL9	C47-C48-C49	-2.09	120.69	127.64
11	A	304	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
18	L	202	SQD	O8-S-C6	2.08	109.99	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	301	HEM	CMC-C2C-C1C	-2.08	121.07	124.73
10	C	301	HEC	CHD-C1D-C2D	-2.07	121.41	127.43
12	H	101	BCR	C15-C14-C13	-2.06	124.39	127.28
9	A	301	HEM	C1B-NB-C4B	2.06	107.64	105.21
12	H	101	BCR	C15-C16-C17	-2.05	119.31	123.52
9	A	301	HEM	CHC-C4B-C3B	2.05	129.16	125.07
12	H	101	BCR	C33-C5-C6	-2.05	122.25	124.48
15	J	201	LMG	C24-C23-C22	-2.04	104.04	114.37
15	F	101	LMG	O2-C2-C1	-2.04	105.21	110.08
13	A	305	PL9	C7-C3-C2	-2.02	121.00	123.39
9	A	302	HEM	CHC-C1C-NC	2.02	126.65	124.45
10	K	301	HEC	CMB-C2B-C1B	-2.02	122.34	125.42
10	A	303	HEC	CBA-CAA-C2A	-2.01	106.97	112.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	I	304	CLA	ND
11	A	304	CLA	ND

All (382) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	301	HEM	C2A-CAA-CBA-CGA
10	I	303	HEC	C2B-C3B-CAB-CBB
10	I	303	HEC	C4B-C3B-CAB-CBB
10	K	301	HEC	C2B-C3B-CAB-CBB
10	K	301	HEC	C2C-C3C-CAC-CBC
10	K	301	HEC	C4C-C3C-CAC-CBC
10	C	301	HEC	C4B-C3B-CAB-CBB
11	I	304	CLA	C2B-C3B-CAB-CBB
11	I	304	CLA	C4B-C3B-CAB-CBB
11	A	304	CLA	C4B-C3B-CAB-CBB
12	I	305	BCR	C6-C7-C8-C9
12	I	305	BCR	C7-C8-C9-C34
12	I	305	BCR	C11-C10-C9-C34
12	I	305	BCR	C10-C11-C12-C13
12	I	305	BCR	C11-C12-C13-C35
12	I	305	BCR	C20-C21-C22-C37
12	H	101	BCR	C7-C8-C9-C10
12	H	101	BCR	C7-C8-C9-C34
12	H	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
12	H	101	BCR	C37-C22-C23-C24
12	H	101	BCR	C22-C23-C24-C25
13	I	306	PL9	C14-C16-C17-C18
13	I	306	PL9	C34-C36-C37-C38
13	A	305	PL9	C12-C13-C14-C15
13	A	305	PL9	C12-C13-C14-C16
13	A	305	PL9	C17-C18-C19-C20
13	A	305	PL9	C17-C18-C19-C21
13	A	305	PL9	C22-C23-C24-C25
13	A	305	PL9	C22-C23-C24-C26
13	A	305	PL9	C26-C27-C28-C29
13	A	305	PL9	C32-C33-C34-C35
13	A	305	PL9	C42-C43-C44-C45
13	A	305	PL9	C42-C43-C44-C46
13	A	305	PL9	C47-C48-C49-C51
13	A	306	PL9	C11-C12-C13-C14
13	A	306	PL9	C27-C28-C29-C30
13	A	306	PL9	C27-C28-C29-C31
13	A	306	PL9	C45-C44-C46-C47
14	I	307	6PL	C1-O3P-P-O1P
14	I	307	6PL	C1-O3P-P-O2P
14	I	307	6PL	C1-O3P-P-O4P
14	N	101	6PL	C1-O3P-P-O1P
14	N	101	6PL	O31-C31-O2-C2
14	N	101	6PL	C32-C31-O2-C2
14	E	101	6PL	C1-O3P-P-O2P
14	E	101	6PL	C1-O3P-P-O4P
14	E	101	6PL	C4-O4P-P-O3P
14	E	101	6PL	O31-C31-O2-C2
15	F	101	LMG	C11-C10-O7-C8
16	J	202	PGV	C03-O11-P-O12
16	J	202	PGV	C03-O11-P-O13
16	J	202	PGV	C04-O12-P-O13
16	J	202	PGV	O03-C01-C02-O01
16	K	302	PGV	C04-O12-P-O11
16	A	308	PGV	C04-O12-P-O11
16	A	308	PGV	C04-O12-P-O13
16	A	308	PGV	C04-O12-P-O14
16	A	308	PGV	O02-C1-O01-C02
16	A	308	PGV	C2-C1-O01-C02
16	B	201	PGV	C04-O12-P-O11
16	B	201	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
18	L	202	SQD	C5-C6-S-O7
18	L	202	SQD	C5-C6-S-O8
18	L	202	SQD	C5-C6-S-O9
18	A	307	SQD	C2-C1-O6-C44
18	A	307	SQD	O5-C1-O6-C44
18	A	307	SQD	O5-C5-C6-S
16	K	302	PGV	O04-C19-O03-C01
18	A	307	SQD	O10-C23-O48-C46
13	A	305	PL9	C47-C48-C49-C50
16	K	302	PGV	C20-C19-O03-C01
18	A	307	SQD	C24-C23-O48-C46
11	A	304	CLA	O1A-CGA-O2A-C1
14	N	101	6PL	O11-C11-O3-C3
15	J	201	LMG	O10-C28-O8-C9
16	J	202	PGV	O04-C19-O03-C01
15	F	101	LMG	O9-C10-O7-C8
15	J	201	LMG	C29-C28-O8-C9
16	J	202	PGV	C20-C19-O03-C01
16	B	201	PGV	C2-C1-O01-C02
13	I	306	PL9	C12-C11-C9-C10
13	I	306	PL9	C15-C14-C16-C17
13	I	306	PL9	C20-C19-C21-C22
13	A	305	PL9	C35-C34-C36-C37
13	A	305	PL9	C40-C39-C41-C42
13	A	306	PL9	C15-C14-C16-C17
13	A	306	PL9	C20-C19-C21-C22
13	A	306	PL9	C25-C24-C26-C27
13	A	306	PL9	C35-C34-C36-C37
13	I	306	PL9	C12-C11-C9-C8
13	I	306	PL9	C13-C14-C16-C17
13	I	306	PL9	C18-C19-C21-C22
13	A	305	PL9	C33-C34-C36-C37
13	A	306	PL9	C13-C14-C16-C17
13	A	306	PL9	C43-C44-C46-C47
14	I	307	6PL	O11-C11-O3-C3
11	A	304	CLA	CBA-CGA-O2A-C1
14	E	101	6PL	C12-C11-O3-C3
13	A	306	PL9	C17-C18-C19-C20
13	A	306	PL9	C37-C38-C39-C40
13	A	305	PL9	C32-C33-C34-C36
13	A	306	PL9	C17-C18-C19-C21
13	A	306	PL9	C37-C38-C39-C41

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Mol	Chain	Res	Type	Atoms
18	L	202	SQD	O49-C7-O47-C45
18	C	302	SQD	C11-C10-C9-C8
18	L	202	SQD	C8-C7-O47-C45
11	I	304	CLA	CBD-CGD-O2D-CED
18	A	307	SQD	C18-C19-C20-C21
13	A	305	PL9	C38-C39-C41-C42
13	A	306	PL9	C18-C19-C21-C22
13	A	306	PL9	C33-C34-C36-C37
15	F	101	LMG	O10-C28-O8-C9
13	I	306	PL9	C19-C21-C22-C23
13	I	306	PL9	C29-C31-C32-C33
13	I	306	PL9	C39-C41-C42-C43
13	I	306	PL9	C44-C46-C47-C48
13	A	305	PL9	C9-C11-C12-C13
13	A	305	PL9	C34-C36-C37-C38
13	A	306	PL9	C9-C11-C12-C13
13	A	306	PL9	C19-C21-C22-C23
13	A	306	PL9	C29-C31-C32-C33
13	A	306	PL9	C34-C36-C37-C38
9	A	301	HEM	C2A-CAA-CBA-CGA
15	J	201	LMG	O6-C1-O1-C7
13	A	305	PL9	C7-C8-C9-C10
13	A	305	PL9	C7-C8-C9-C11
13	A	306	PL9	C42-C43-C44-C46
12	I	305	BCR	C9-C10-C11-C12
15	F	101	LMG	C29-C28-O8-C9
13	A	306	PL9	C23-C24-C26-C27
14	N	101	6PL	C11-C12-C13-C14
13	A	305	PL9	C14-C16-C17-C18
13	A	306	PL9	C24-C26-C27-C28
15	F	101	LMG	C10-C11-C12-C13
18	C	302	SQD	C23-C24-C25-C26
11	A	304	CLA	C13-C15-C16-C17
10	I	303	HEC	C3D-CAD-CBD-CGD
11	I	304	CLA	C2A-CAA-CBA-CGA
11	A	304	CLA	C5-C6-C7-C8
18	L	202	SQD	C23-C24-C25-C26
16	A	308	PGV	O12-C04-C05-O05
16	K	302	PGV	C19-C20-C21-C22
13	A	306	PL9	C42-C43-C44-C45
18	A	307	SQD	C7-C8-C9-C10
16	A	308	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
18	C	302	SQD	C24-C23-O48-C46
11	A	304	CLA	C15-C16-C17-C18
13	A	306	PL9	C30-C29-C31-C32
13	A	306	PL9	C40-C39-C41-C42
14	E	101	6PL	C32-C31-O2-C2
11	I	304	CLA	O1D-CGD-O2D-CED
15	J	201	LMG	C2-C1-O1-C7
12	I	305	BCR	C7-C8-C9-C10
12	I	305	BCR	C21-C22-C23-C24
18	C	302	SQD	C16-C17-C18-C19
11	A	304	CLA	C16-C17-C18-C19
18	C	302	SQD	O10-C23-O48-C46
15	J	201	LMG	C23-C24-C25-C26
18	L	202	SQD	C12-C13-C14-C15
15	F	101	LMG	C29-C30-C31-C32
15	J	201	LMG	C29-C30-C31-C32
15	F	101	LMG	C12-C13-C14-C15
18	C	302	SQD	C18-C19-C20-C21
18	C	302	SQD	C29-C30-C31-C32
11	A	304	CLA	C10-C11-C12-C13
11	A	304	CLA	C16-C17-C18-C20
15	J	201	LMG	C32-C33-C34-C35
18	C	302	SQD	C9-C10-C11-C12
15	J	201	LMG	C11-C10-O7-C8
16	B	201	PGV	C2-C3-C4-C5
15	F	101	LMG	C31-C32-C33-C34
16	J	202	PGV	C28-C29-C30-C31
15	F	101	LMG	C16-C17-C18-C19
18	A	307	SQD	C14-C15-C16-C17
15	J	201	LMG	C28-C29-C30-C31
18	A	307	SQD	C23-C24-C25-C26
14	N	101	6PL	C36-C37-C38-C39
15	F	101	LMG	C30-C31-C32-C33
16	J	202	PGV	C24-C25-C26-C27
18	C	302	SQD	C32-C33-C34-C35
11	A	304	CLA	C2B-C3B-CAB-CBB
12	I	305	BCR	C23-C24-C25-C30
12	H	101	BCR	C23-C24-C25-C30
16	B	201	PGV	C7-C8-C9-C10
14	E	101	6PL	C17-C18-C19-C20
13	A	306	PL9	C28-C29-C31-C32
11	I	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	307	SQD	C13-C14-C15-C16
15	J	201	LMG	C30-C31-C32-C33
18	L	202	SQD	C11-C10-C9-C8
14	N	101	6PL	C12-C11-O3-C3
18	A	307	SQD	C24-C25-C26-C27
16	K	302	PGV	C11-C10-C9-C8
12	I	305	BCR	C37-C22-C23-C24
13	A	305	PL9	C37-C38-C39-C40
12	I	305	BCR	C11-C12-C13-C14
13	A	305	PL9	C15-C14-C16-C17
13	A	305	PL9	C13-C14-C16-C17
18	A	307	SQD	C31-C32-C33-C34
18	C	302	SQD	C33-C34-C35-C36
15	J	201	LMG	O7-C8-C9-O8
14	I	307	6PL	C36-C37-C38-C39
18	A	307	SQD	C11-C12-C13-C14
18	C	302	SQD	C11-C12-C13-C14
18	A	307	SQD	C28-C29-C30-C31
13	I	306	PL9	C36-C37-C38-C39
11	A	304	CLA	C4-C3-C5-C6
16	K	302	PGV	C4-C5-C6-C7
18	A	307	SQD	C33-C34-C35-C36
15	J	201	LMG	C15-C16-C17-C18
16	B	201	PGV	C01-C02-C03-O11
15	J	201	LMG	C19-C20-C21-C22
11	A	304	CLA	C6-C7-C8-C10
13	A	306	PL9	C38-C39-C41-C42
14	E	101	6PL	O11-C11-O3-C3
18	A	307	SQD	C15-C16-C17-C18
11	I	304	CLA	O1A-CGA-O2A-C1
13	A	306	PL9	C32-C33-C34-C35
16	J	202	PGV	O03-C01-C02-C03
15	J	201	LMG	C34-C35-C36-C37
14	I	307	6PL	C31-C32-C33-C34
14	N	101	6PL	C19-C20-C21-C22
15	J	201	LMG	C10-C11-C12-C13
11	A	304	CLA	C2-C3-C5-C6
15	J	201	LMG	C21-C22-C23-C24
15	F	101	LMG	C37-C38-C39-C40
16	B	201	PGV	C01-C02-O01-C1
18	L	202	SQD	C44-C45-O47-C7
18	A	307	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
12	I	305	BCR	C12-C13-C14-C15
18	L	202	SQD	C24-C25-C26-C27
15	F	101	LMG	C32-C33-C34-C35
18	C	302	SQD	C13-C14-C15-C16
15	F	101	LMG	C36-C37-C38-C39
14	N	101	6PL	C20-C21-C22-C23
18	C	302	SQD	C30-C31-C32-C33
11	A	304	CLA	C6-C7-C8-C9
14	I	307	6PL	C34-C35-C36-C37
16	B	201	PGV	O03-C01-C02-C03
11	I	304	CLA	C3-C5-C6-C7
18	C	302	SQD	C27-C28-C29-C30
12	I	305	BCR	C1-C6-C7-C8
12	H	101	BCR	C1-C6-C7-C8
18	L	202	SQD	C28-C29-C30-C31
16	K	302	PGV	O01-C1-C2-C3
18	L	202	SQD	O47-C45-C46-O48
13	A	305	PL9	C4-C3-C7-C8
13	A	306	PL9	C4-C3-C7-C8
16	A	308	PGV	C7-C8-C9-C10
15	F	101	LMG	C11-C12-C13-C14
13	A	306	PL9	C2-C3-C7-C8
15	J	201	LMG	C11-C12-C13-C14
18	L	202	SQD	C7-C8-C9-C10
15	J	201	LMG	C42-C43-C44-C45
13	A	305	PL9	C19-C21-C22-C23
18	C	302	SQD	C34-C35-C36-C37
14	I	307	6PL	C32-C31-O2-C2
14	I	307	6PL	C12-C11-O3-C3
15	J	201	LMG	C41-C42-C43-C44
11	I	304	CLA	C16-C17-C18-C19
14	I	307	6PL	O31-C31-O2-C2
16	B	201	PGV	O01-C02-C03-O11
9	A	301	HEM	C4B-C3B-CAB-CBB
9	A	302	HEM	C4B-C3B-CAB-CBB
15	F	101	LMG	C17-C18-C19-C20
18	A	307	SQD	C10-C11-C12-C13
14	I	307	6PL	O4P-C4-C5-N
14	N	101	6PL	O4P-C4-C5-N
15	J	201	LMG	C37-C38-C39-C40
15	J	201	LMG	O9-C10-O7-C8
18	L	202	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
10	K	301	HEC	C4B-C3B-CAB-CBB
16	J	202	PGV	C6-C7-C8-C9
15	J	201	LMG	C12-C13-C14-C15
14	E	101	6PL	O2-C2-C3-O3
15	F	101	LMG	O1-C7-C8-O7
15	F	101	LMG	O7-C8-C9-O8
16	B	201	PGV	O03-C01-C02-O01
16	J	202	PGV	C29-C30-C31-C32
15	J	201	LMG	C7-C8-C9-O8
15	F	101	LMG	C7-C8-C9-O8
16	B	201	PGV	C13-C14-C15-C16
14	E	101	6PL	C36-C37-C38-C39
10	C	301	HEC	C2B-C3B-CAB-CBB
10	C	301	HEC	C2C-C3C-CAC-CBC
14	I	307	6PL	C4-O4P-P-O1P
14	N	101	6PL	C1-O3P-P-O4P
14	N	101	6PL	C4-O4P-P-O3P
14	E	101	6PL	C4-O4P-P-O1P
16	B	201	PGV	C04-O12-P-O14
12	H	101	BCR	C23-C24-C25-C26
16	A	308	PGV	C05-C04-O12-P
18	L	202	SQD	C30-C31-C32-C33
16	K	302	PGV	C29-C30-C31-C32
12	H	101	BCR	C11-C10-C9-C8
11	I	304	CLA	C16-C17-C18-C20
18	C	302	SQD	C35-C36-C37-C38
18	C	302	SQD	O47-C45-C46-O48
15	F	101	LMG	O8-C28-C29-C30
18	L	202	SQD	O47-C7-C8-C9
15	J	201	LMG	C33-C34-C35-C36
13	A	305	PL9	C44-C46-C47-C48
15	J	201	LMG	C36-C37-C38-C39
16	K	302	PGV	C3-C4-C5-C6
13	I	306	PL9	C2-C3-C7-C8
16	A	308	PGV	C31-C32-C33-C34
13	I	306	PL9	C25-C24-C26-C27
18	A	307	SQD	C30-C31-C32-C33
15	F	101	LMG	C15-C16-C17-C18
18	A	307	SQD	C9-C10-C11-C12
14	I	307	6PL	C39-C40-C41-C42
12	H	101	BCR	C11-C10-C9-C34
18	L	202	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	E	101	6PL	C3-C2-O2-C31
18	C	302	SQD	C31-C32-C33-C34
10	C	301	HEC	CAA-CBA-CGA-O2A
16	K	302	PGV	O01-C02-C03-O11
9	I	302	HEM	C1A-C2A-CAA-CBA
12	I	305	BCR	C5-C6-C7-C8
12	I	305	BCR	C23-C24-C25-C26
12	H	101	BCR	C5-C6-C7-C8
10	C	301	HEC	CAA-CBA-CGA-O1A
10	A	303	HEC	C2A-CAA-CBA-CGA
14	E	101	6PL	C14-C15-C16-C17
13	I	306	PL9	C23-C24-C26-C27
14	N	101	6PL	C35-C36-C37-C38
13	A	305	PL9	C12-C11-C9-C10
13	A	305	PL9	C25-C24-C26-C27
13	A	305	PL9	C30-C29-C31-C32
13	A	305	PL9	C23-C24-C26-C27
13	A	305	PL9	C28-C29-C31-C32
18	C	302	SQD	C44-C45-C46-O48
16	J	202	PGV	O02-C1-O01-C02
14	E	101	6PL	C42-C43-C44-C45
14	N	101	6PL	C16-C17-C18-C19
15	F	101	LMG	C42-C43-C44-C45
16	B	201	PGV	O12-C04-C05-C06
13	I	306	PL9	C35-C34-C36-C37
10	I	303	HEC	CAD-CBD-CGD-O2D
13	A	306	PL9	C39-C41-C42-C43
16	K	302	PGV	O02-C1-C2-C3
18	L	202	SQD	C32-C33-C34-C35
16	J	202	PGV	C2-C1-O01-C02
10	I	303	HEC	CAD-CBD-CGD-O1D
16	A	308	PGV	O04-C19-O03-C01
14	E	101	6PL	O3-C11-C12-C13
16	K	302	PGV	C01-C02-C03-O11
13	A	305	PL9	C24-C26-C27-C28
15	J	201	LMG	C38-C39-C40-C41
14	E	101	6PL	O4P-C4-C5-N
15	J	201	LMG	C40-C41-C42-C43
16	A	308	PGV	C20-C19-O03-C01
14	N	101	6PL	C22-C23-C24-C25
18	L	202	SQD	C35-C36-C37-C38
18	L	202	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
14	E	101	6PL	C1-C2-C3-O3
16	J	202	PGV	O01-C1-C2-C3
14	I	307	6PL	C33-C34-C35-C36
10	A	303	HEC	CAA-CBA-CGA-O2A
15	J	201	LMG	C4-C5-C6-O5
10	C	301	HEC	C4C-C3C-CAC-CBC
16	J	202	PGV	O02-C1-C2-C3
14	E	101	6PL	C15-C16-C17-C18
18	C	302	SQD	O5-C5-C6-S
9	A	301	HEM	CAD-CBD-CGD-O2D
10	A	303	HEC	CAA-CBA-CGA-O1A
14	N	101	6PL	O11-C11-C12-C13
14	N	101	6PL	O31-C31-C32-C33
18	A	307	SQD	C45-C44-O6-C1
15	J	201	LMG	C22-C23-C24-C25
15	J	201	LMG	C14-C15-C16-C17
15	J	201	LMG	O1-C7-C8-C9
9	I	302	HEM	C2B-C3B-CAB-CBB
10	A	303	HEC	CAD-CBD-CGD-O2D
18	L	202	SQD	O48-C23-C24-C25
14	E	101	6PL	O31-C31-C32-C33
11	I	304	CLA	C15-C16-C17-C18
14	E	101	6PL	C22-C23-C24-C25
9	A	301	HEM	CAA-CBA-CGA-O1A
9	A	301	HEM	CAA-CBA-CGA-O2A
10	A	303	HEC	CAD-CBD-CGD-O1D
14	E	101	6PL	C35-C36-C37-C38

There are no ring outliers.

24 monomers are involved in 151 short contacts:

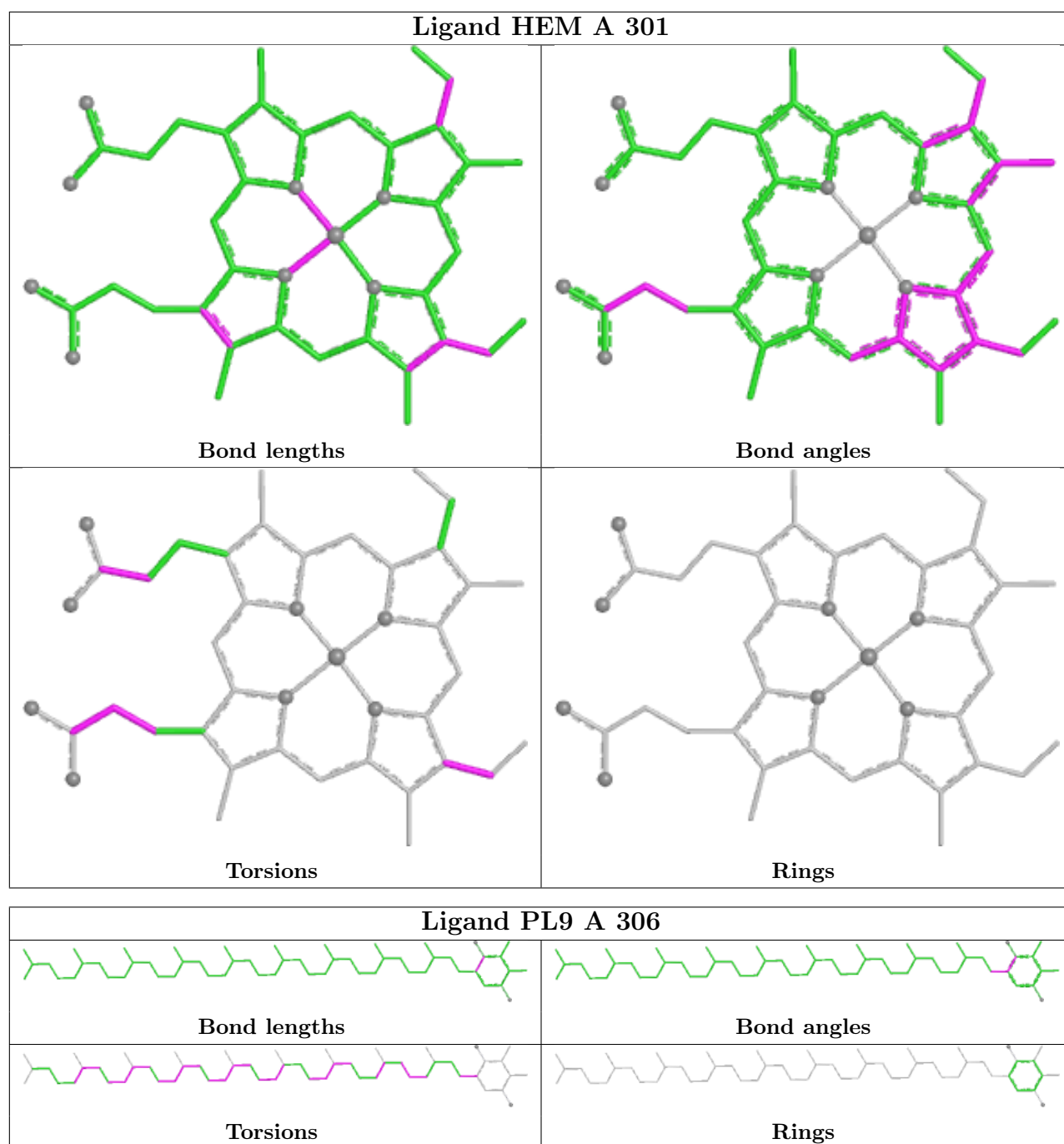
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	301	HEM	1	0
13	A	306	PL9	34	0
18	C	302	SQD	10	0
14	E	101	6PL	11	0
9	A	302	HEM	2	0
17	L	201	FES	3	0
16	A	308	PGV	1	0
13	I	306	PL9	26	0
15	J	201	LMG	1	0
17	D	201	FES	2	0

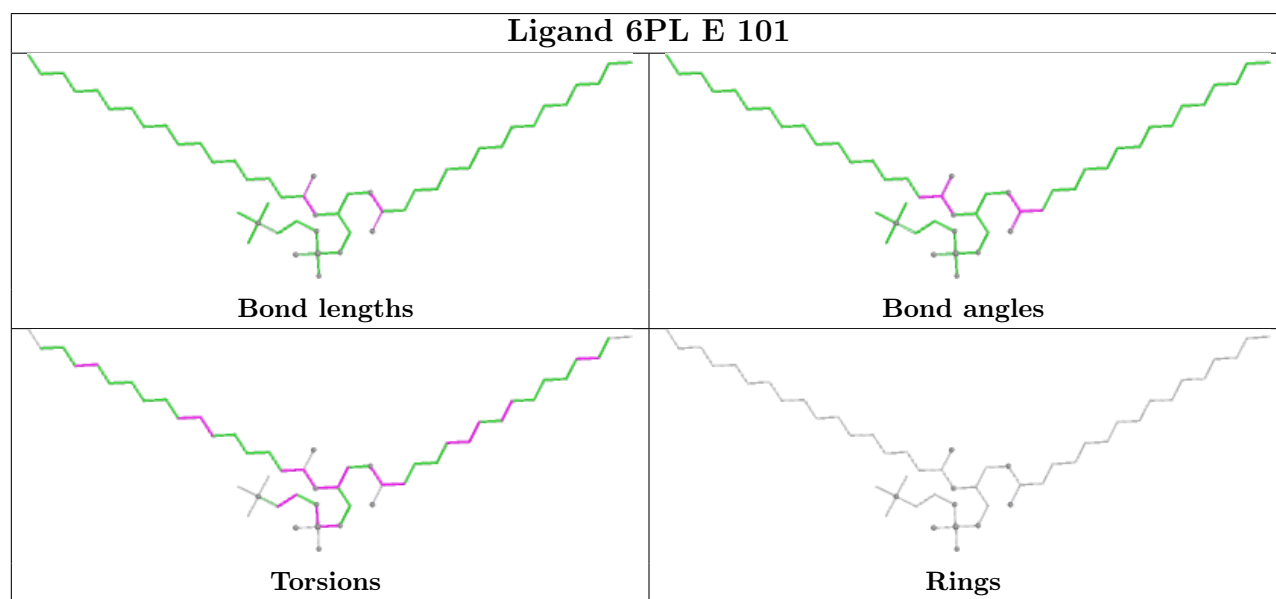
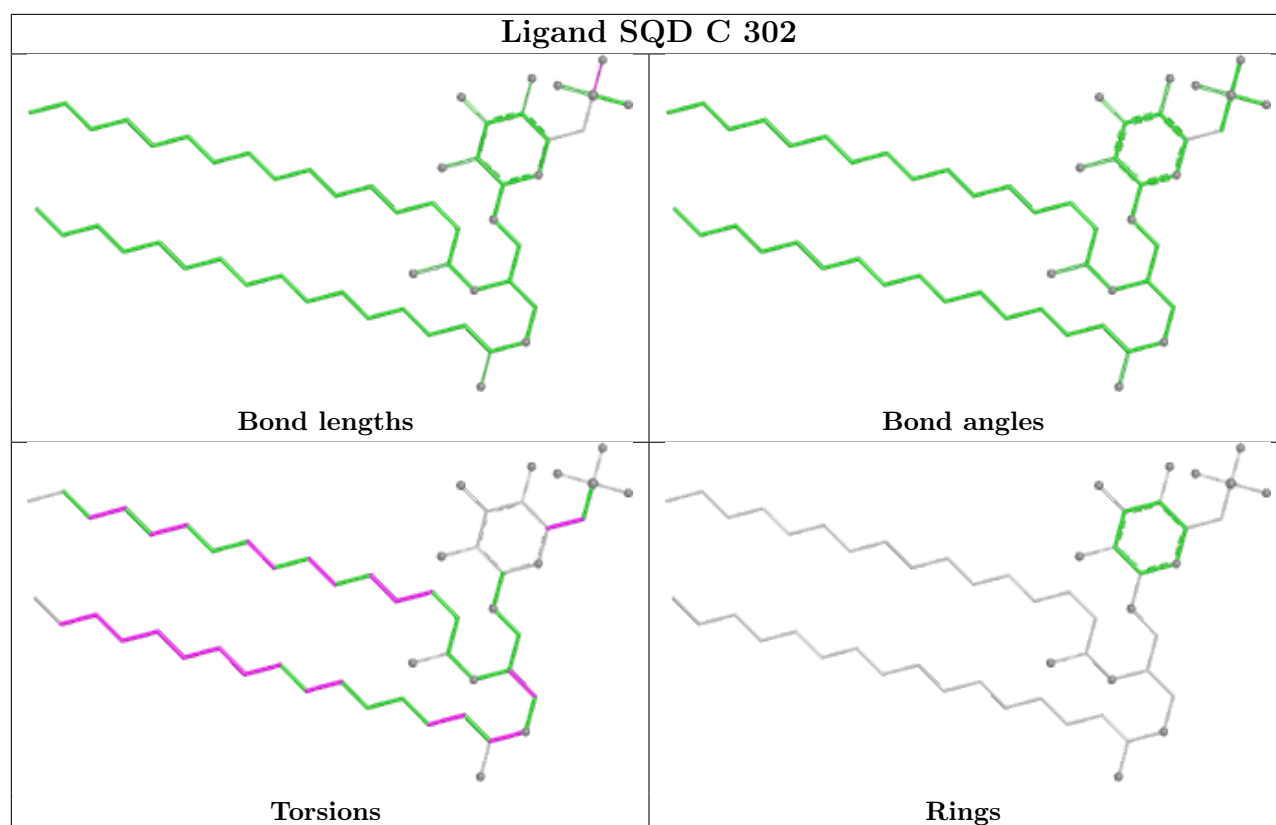
Continued on next page...

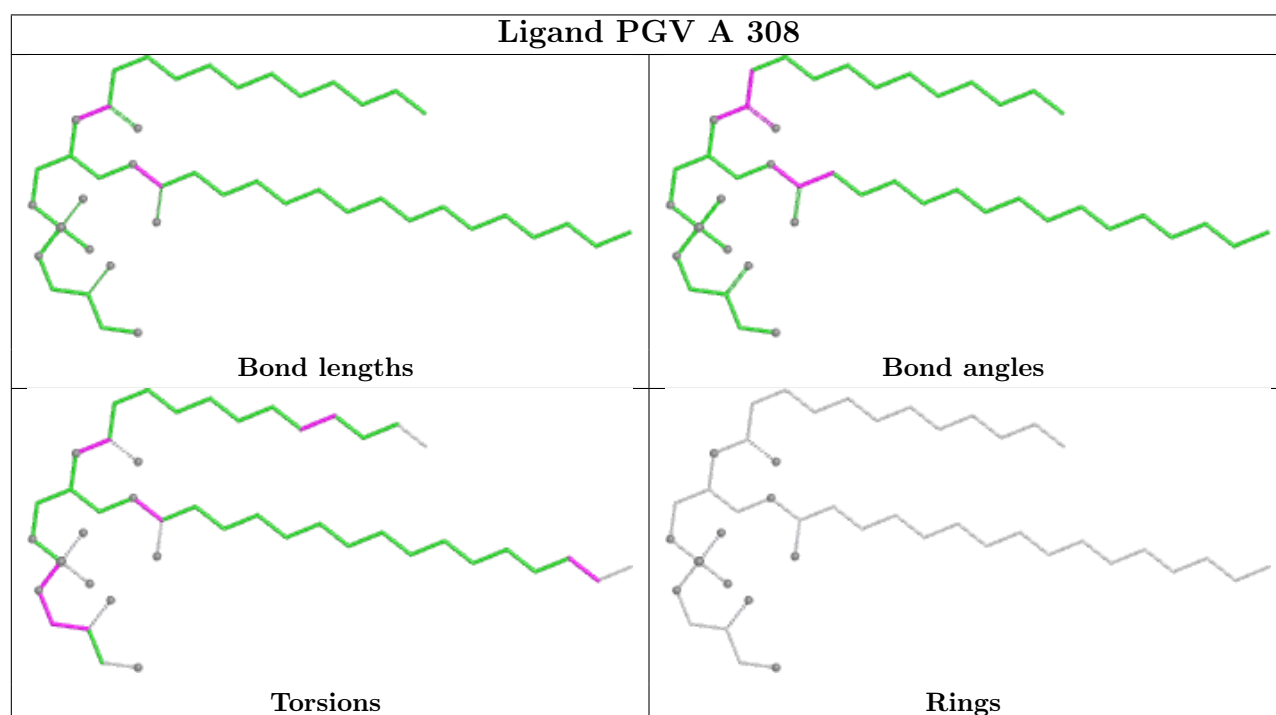
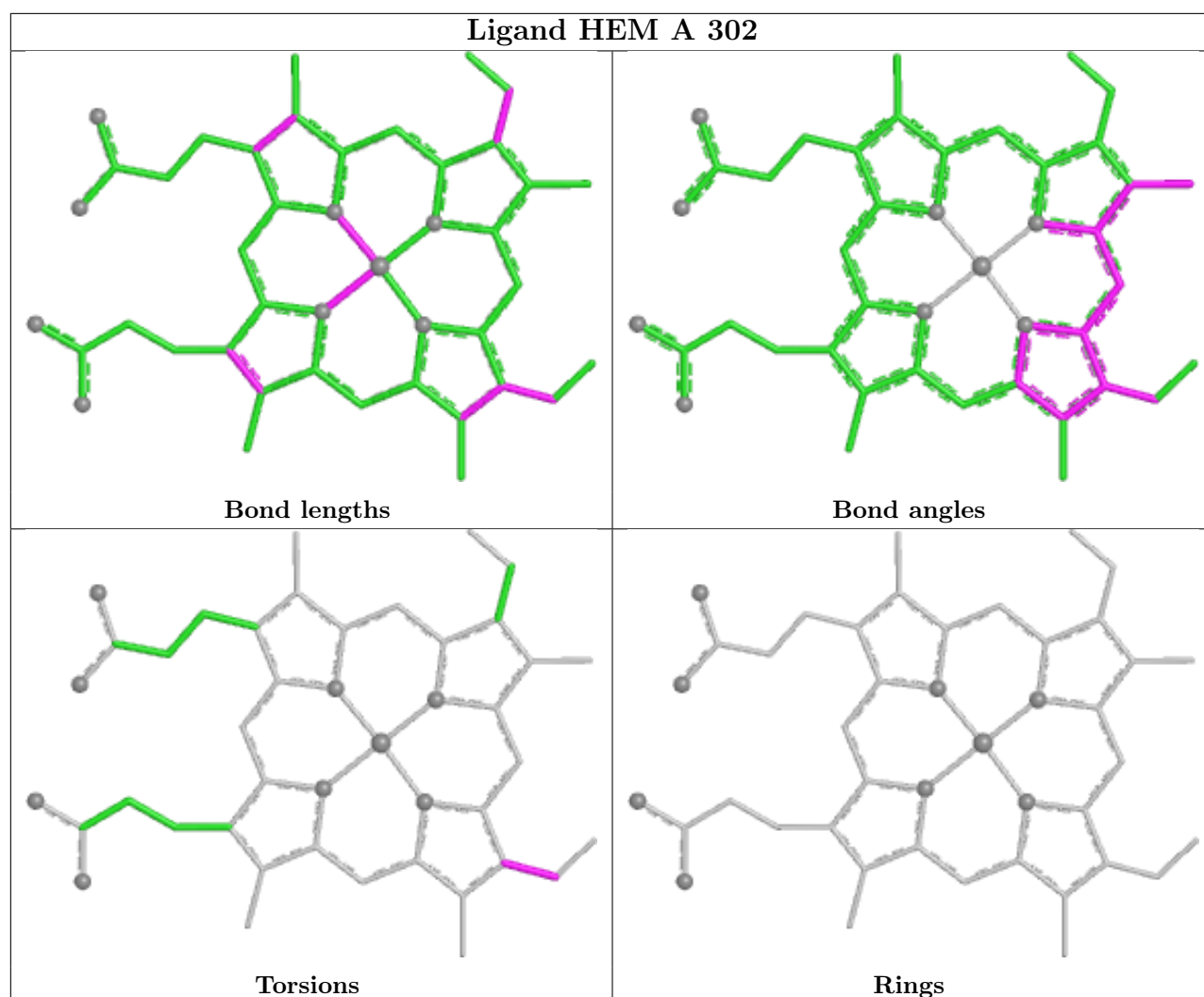
Continued from previous page...

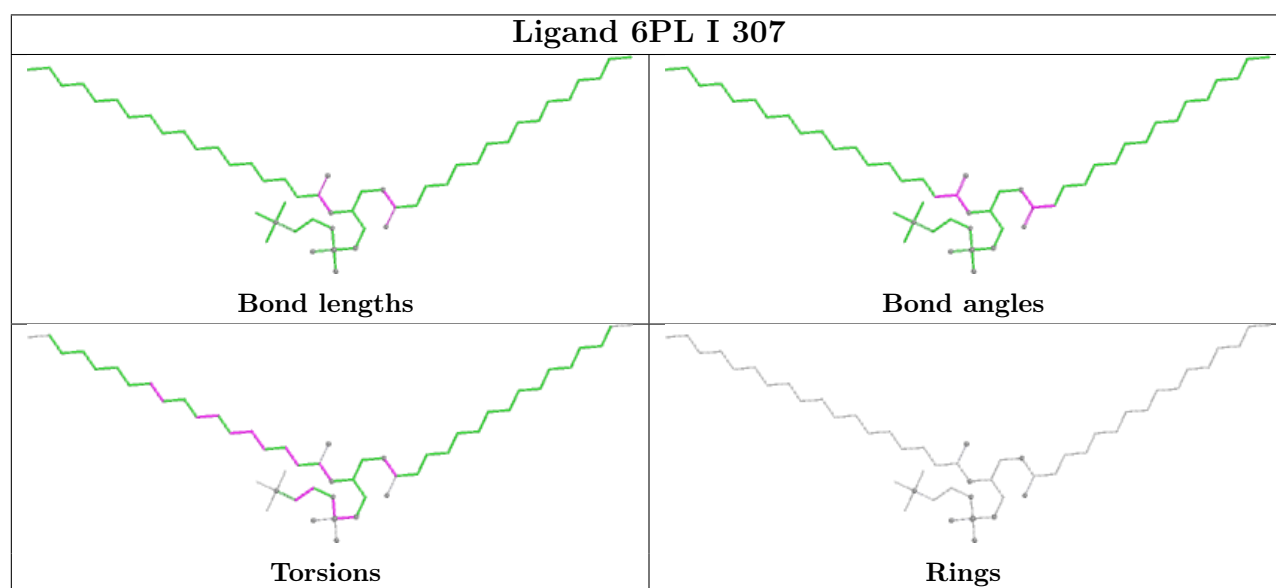
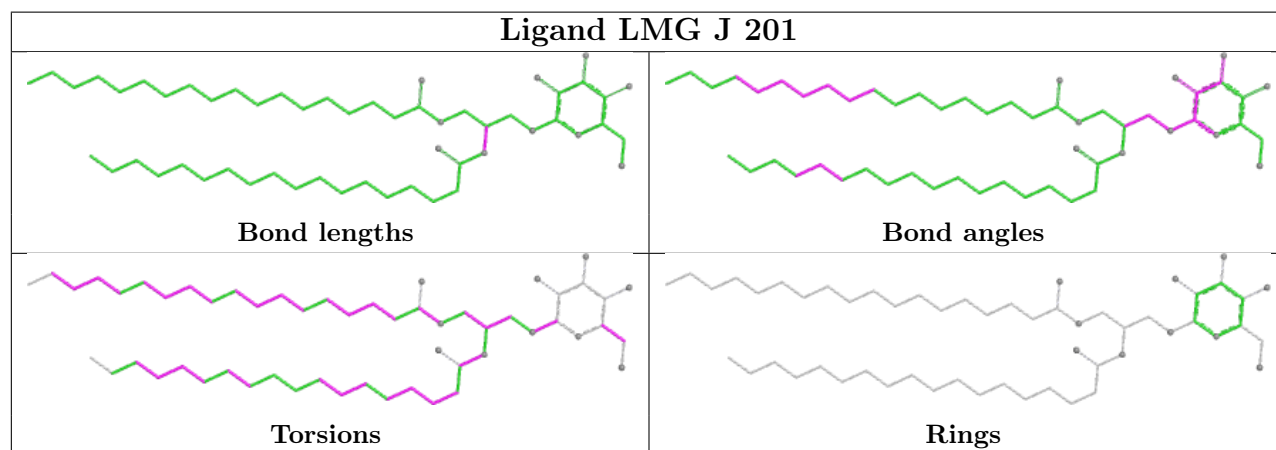
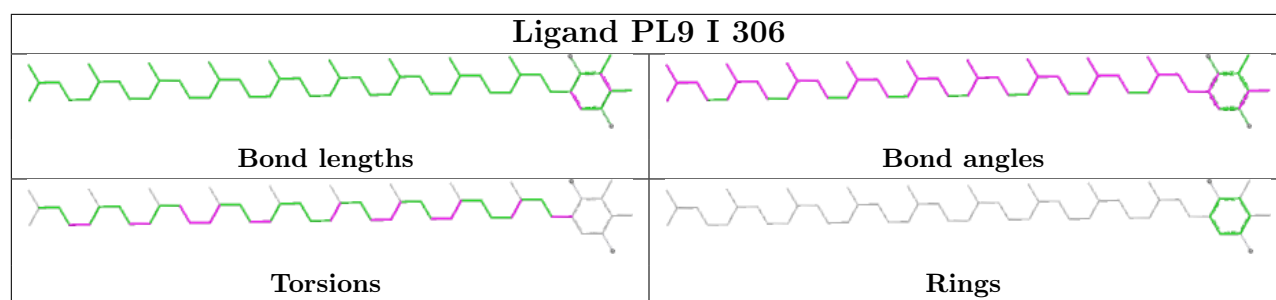
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	I	307	6PL	1	0
18	A	307	SQD	8	0
13	A	305	PL9	16	0
10	A	303	HEC	7	0
14	N	101	6PL	3	0
11	A	304	CLA	2	0
16	K	302	PGV	1	0
9	I	302	HEM	1	0
10	C	301	HEC	21	0
10	K	301	HEC	2	0
18	L	202	SQD	5	0
10	I	303	HEC	5	0
11	I	304	CLA	3	0
12	H	101	BCR	1	0

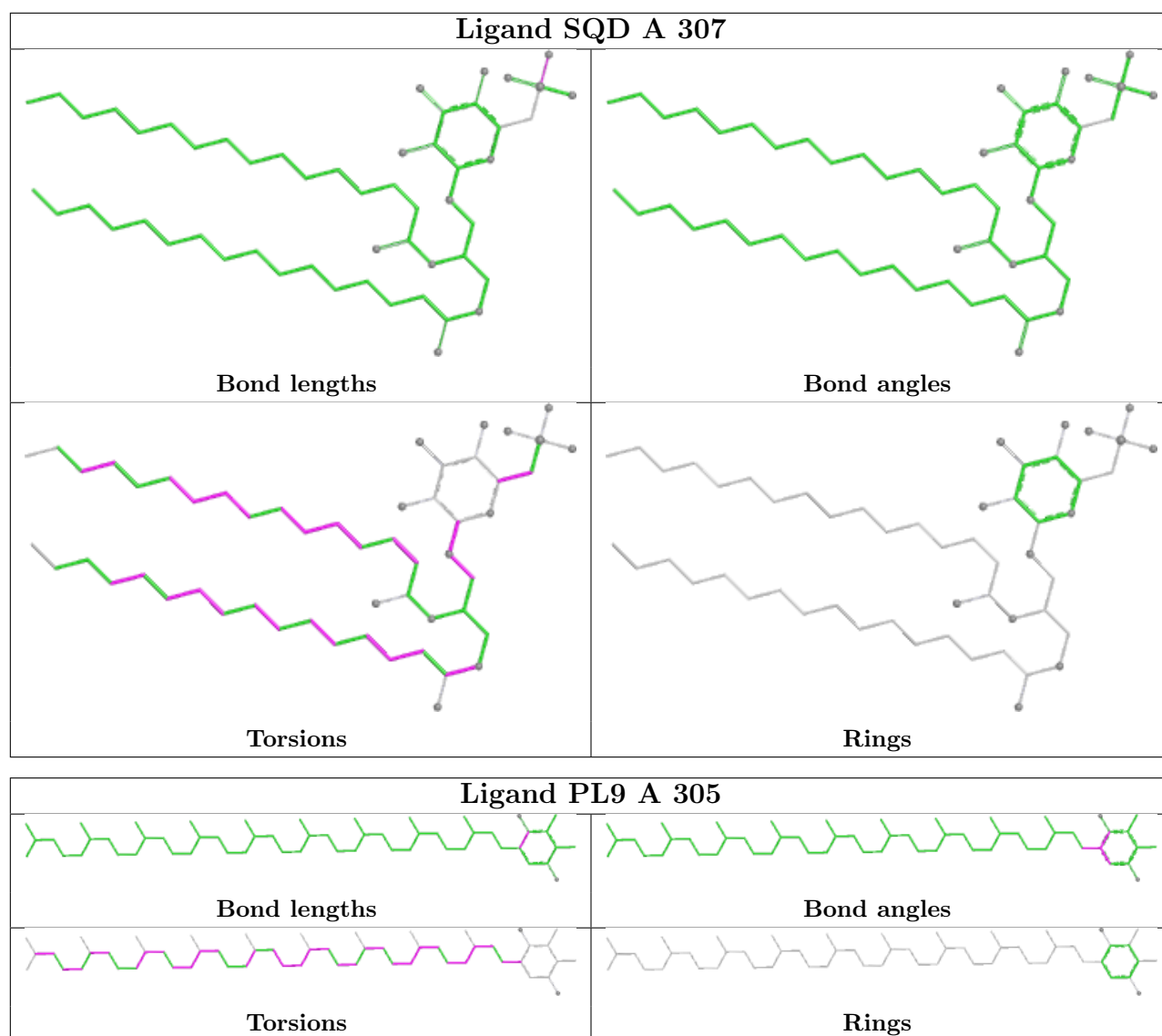
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

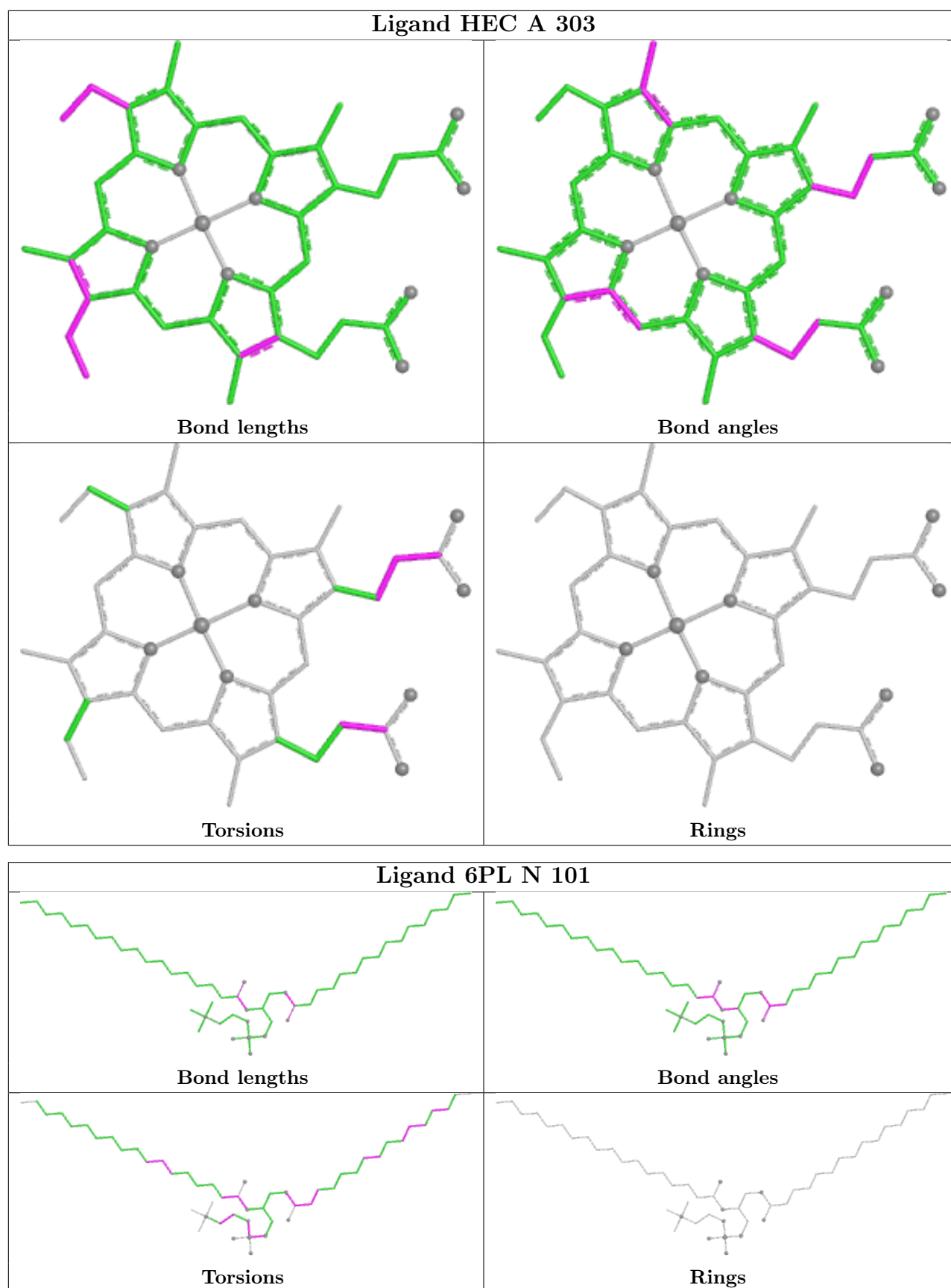


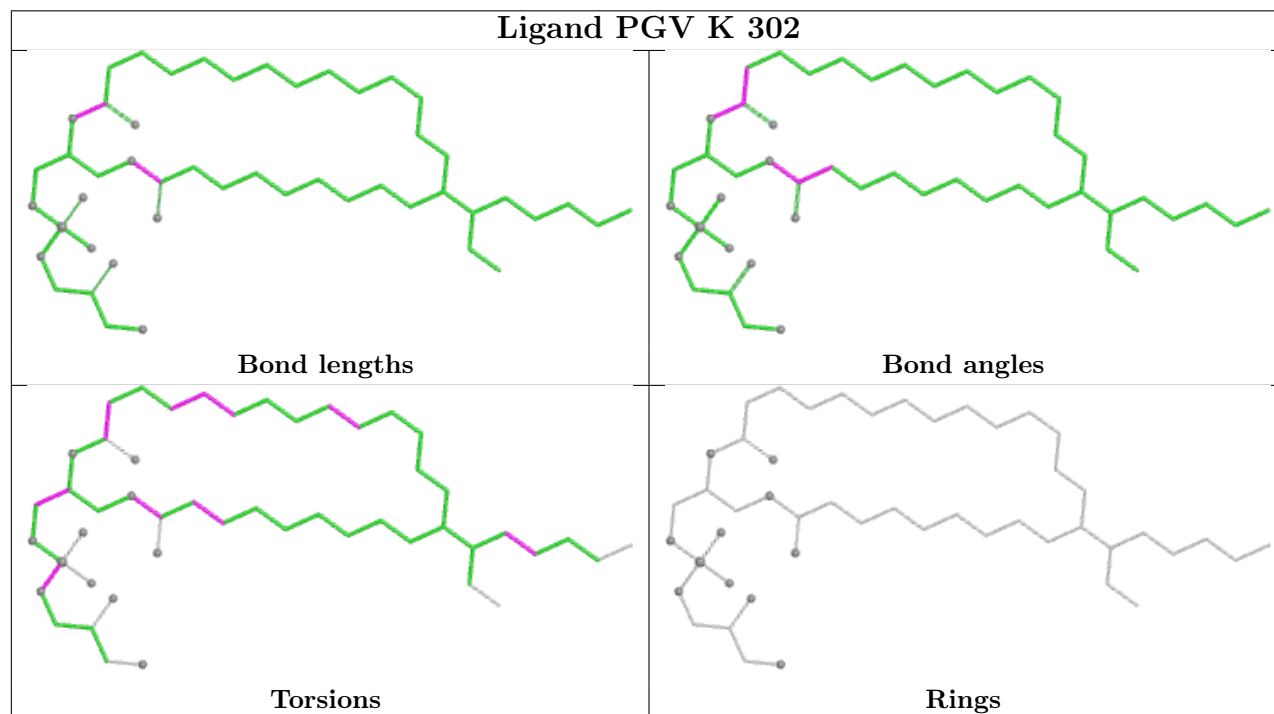
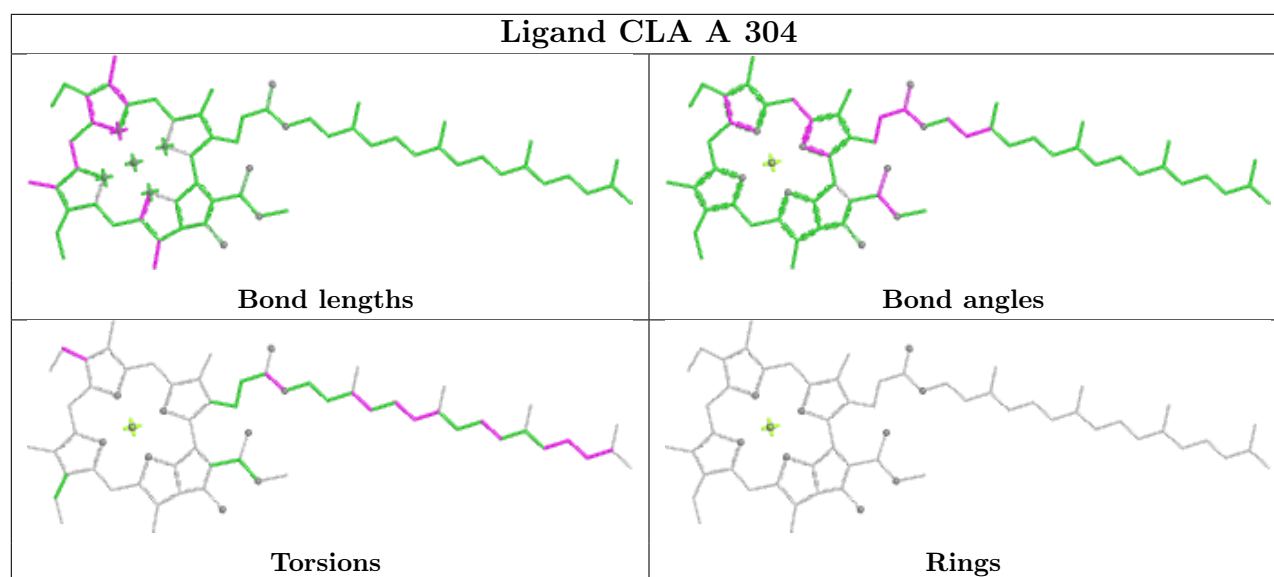


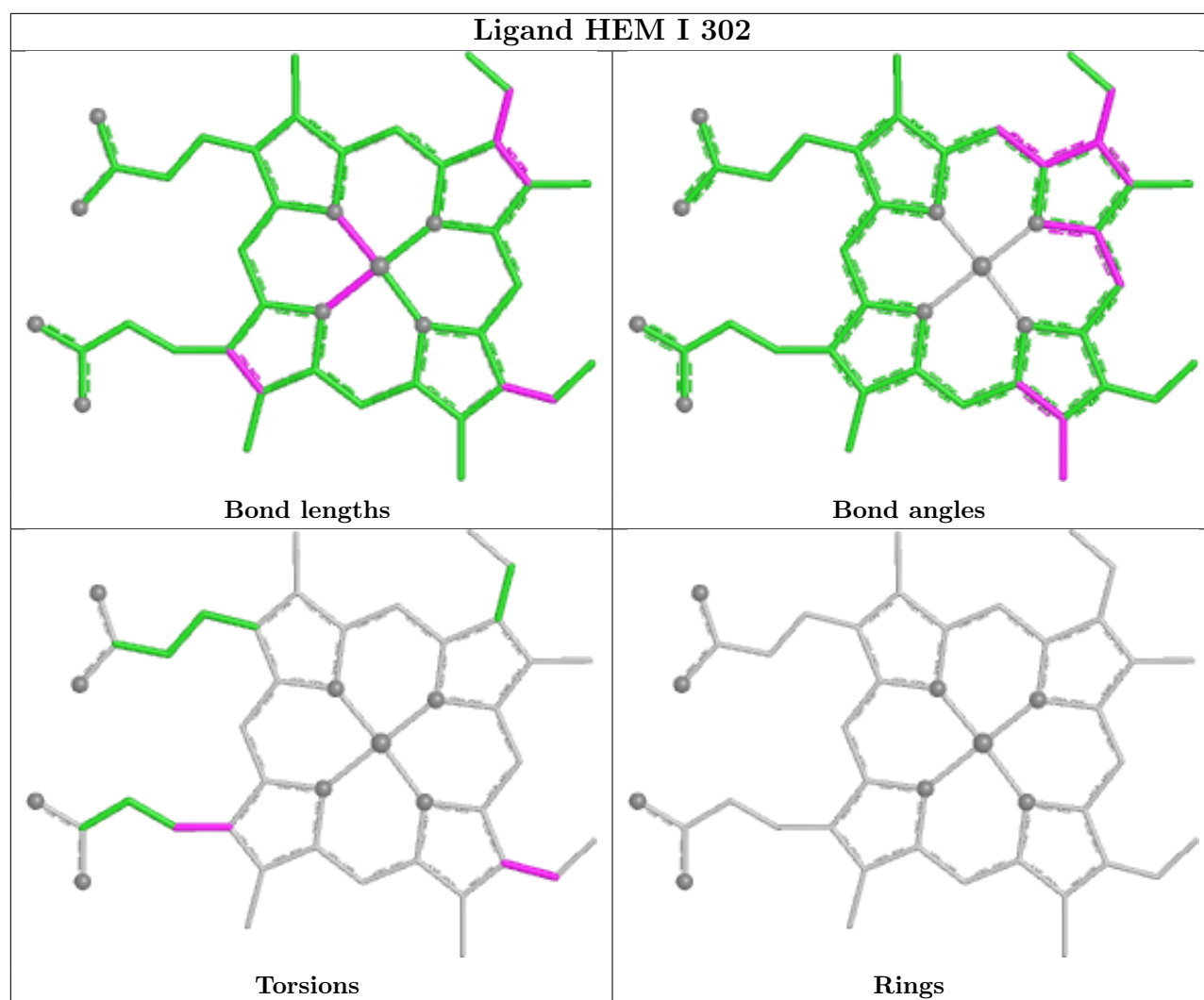


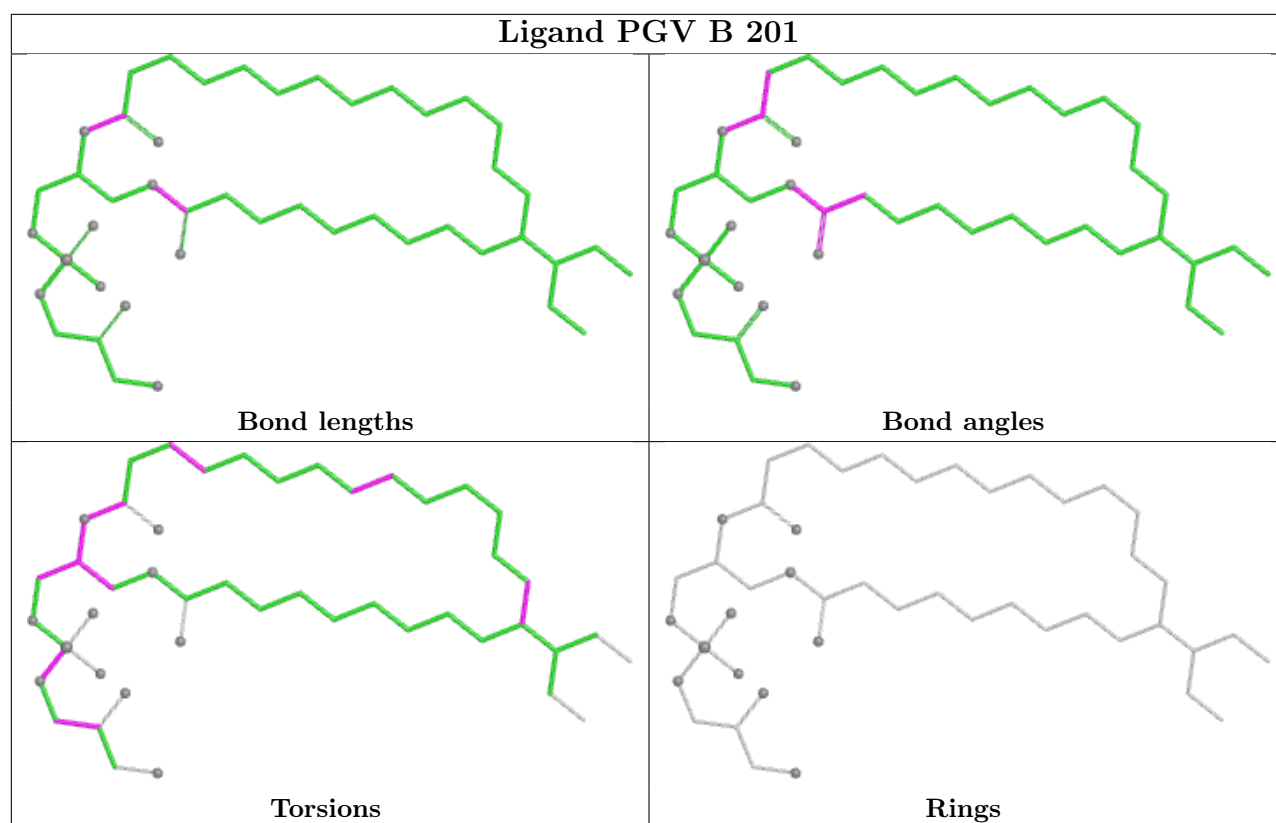


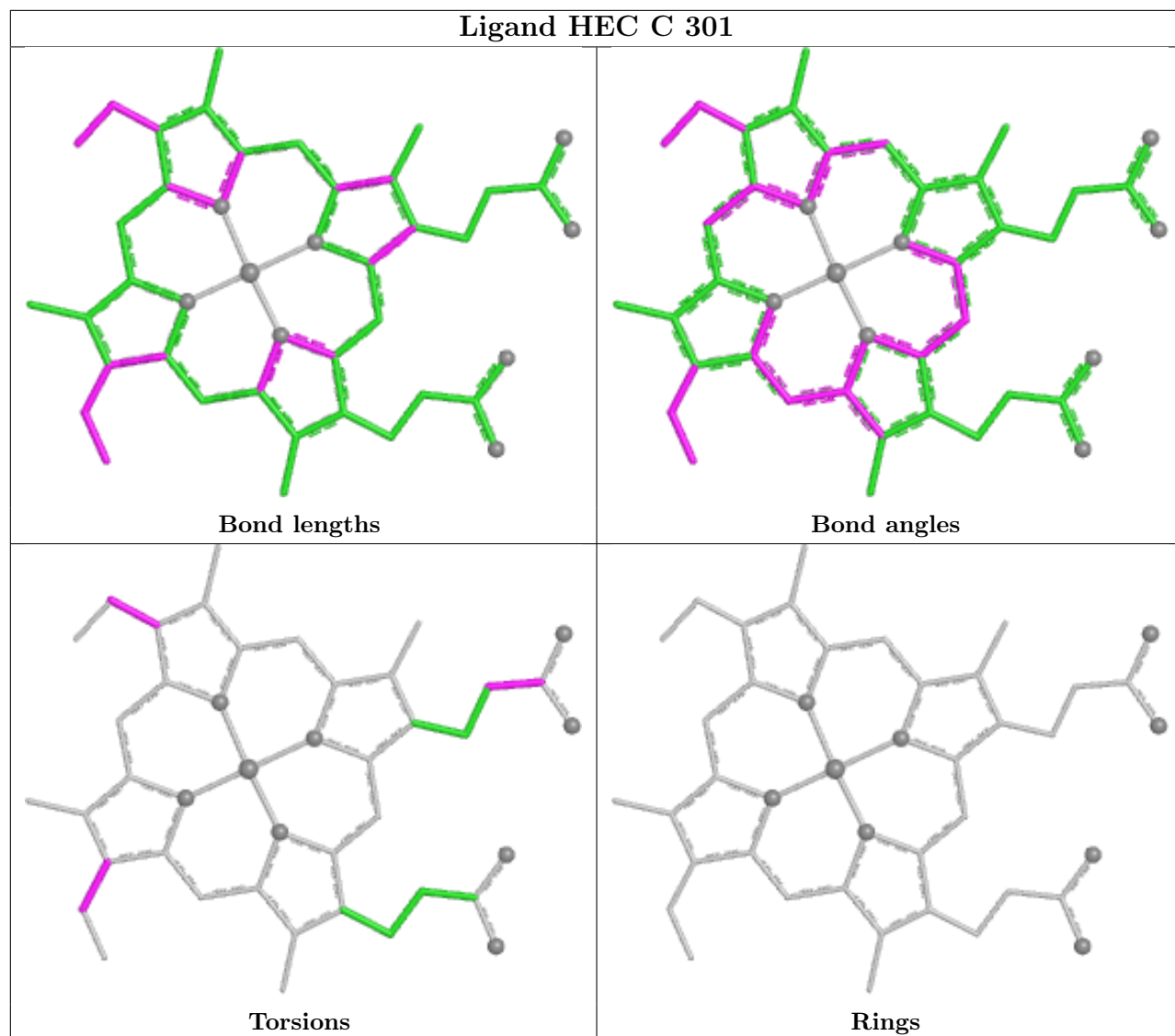


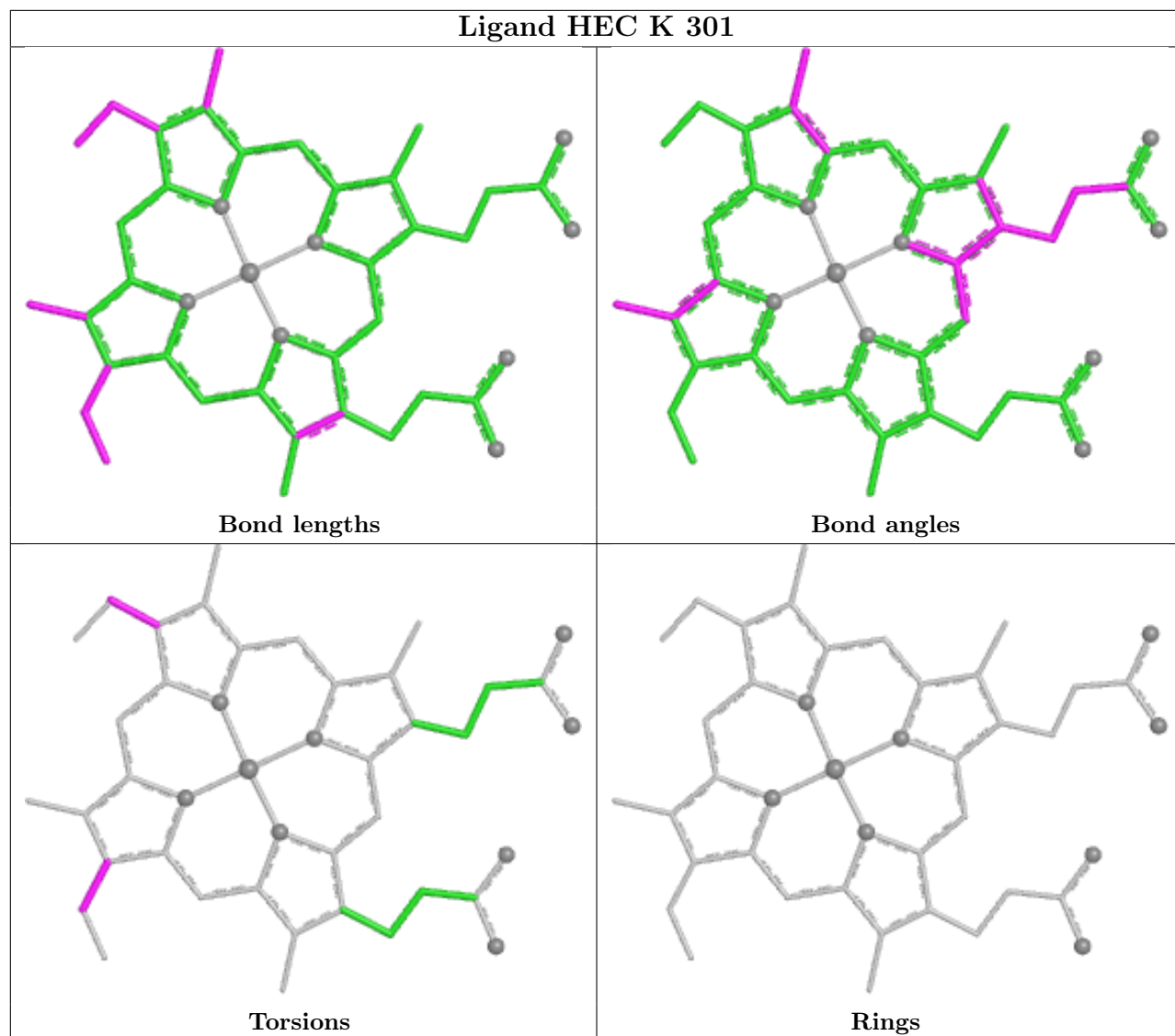


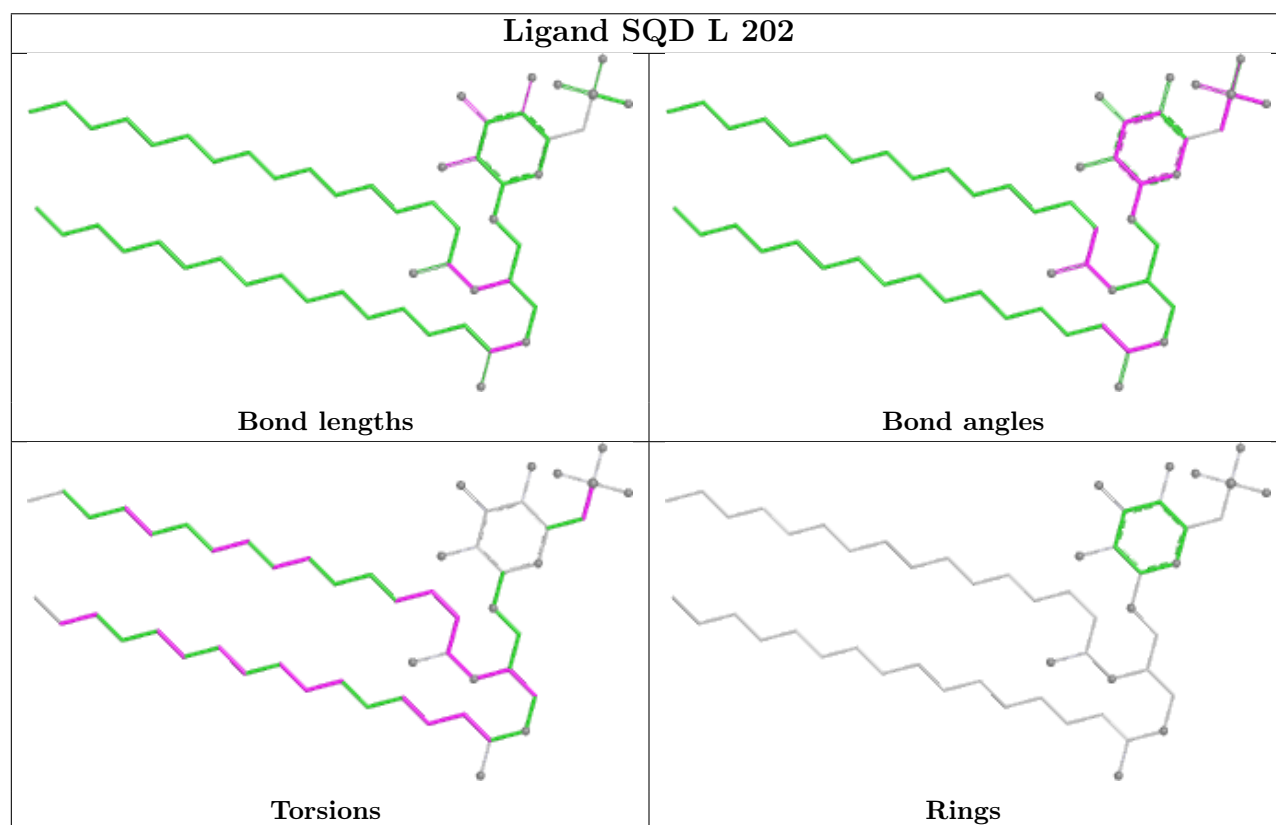
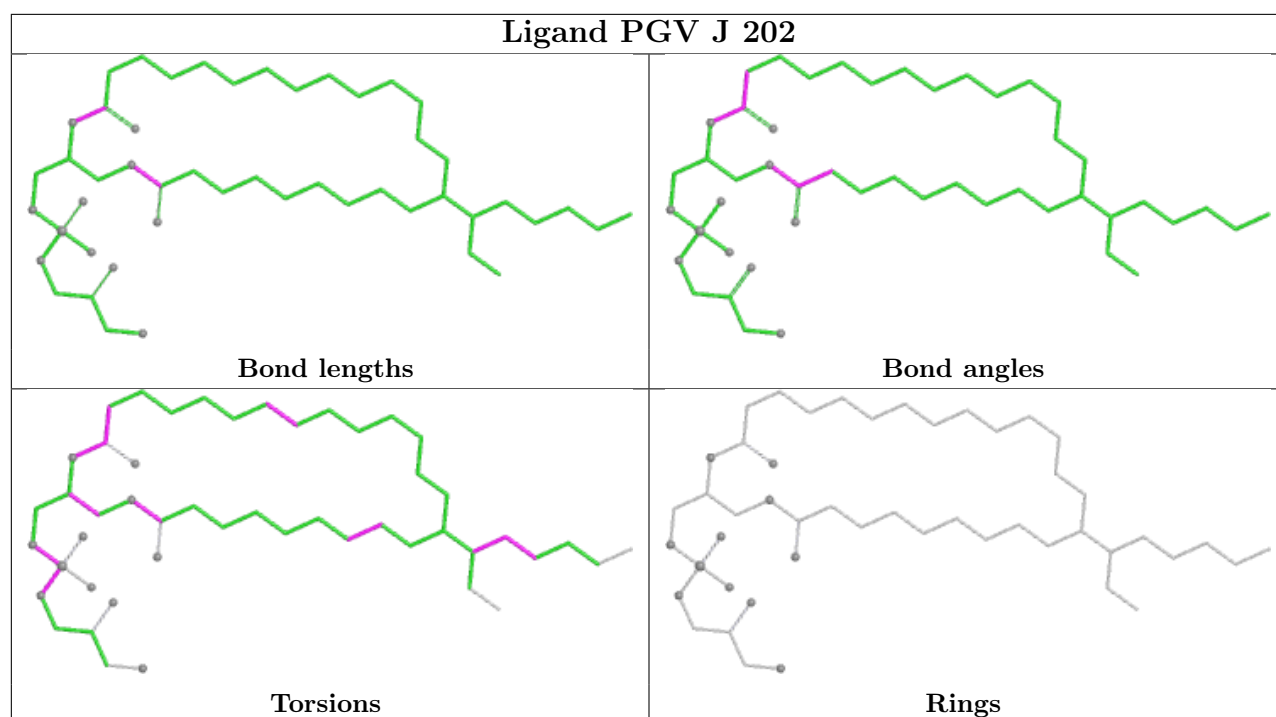




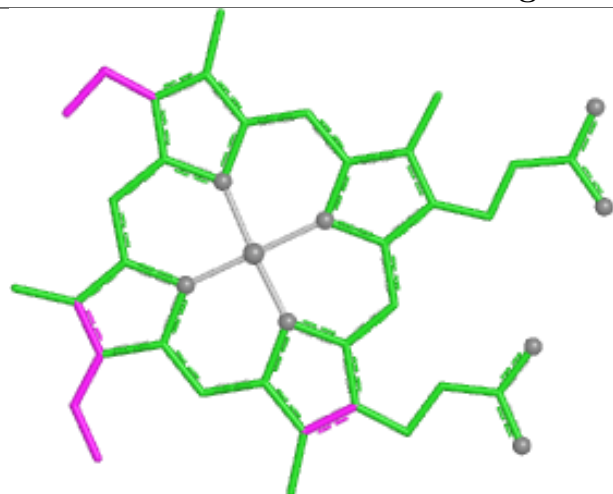




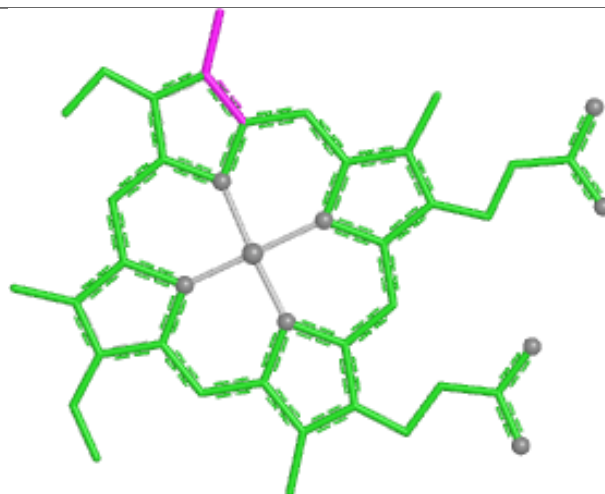




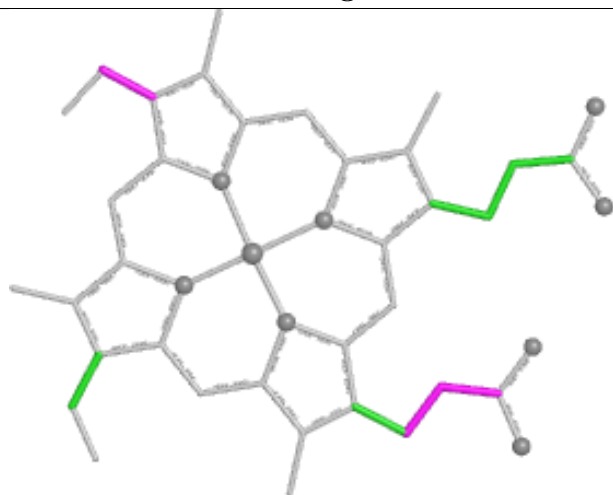
Ligand HEC I 303



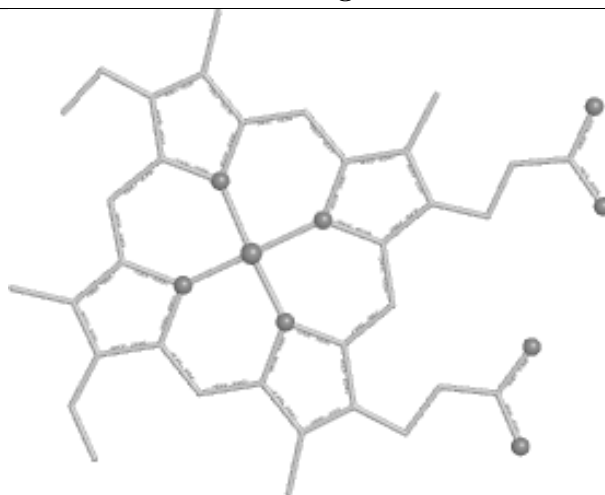
Bond lengths



Bond angles

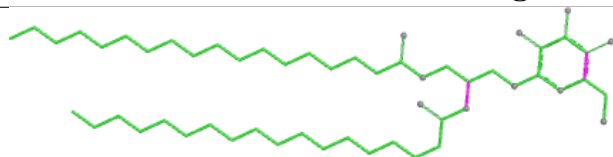


Torsions

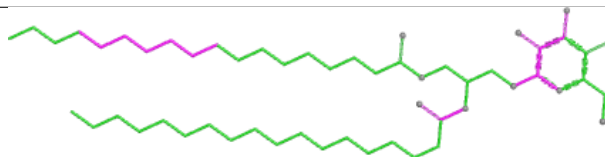


Rings

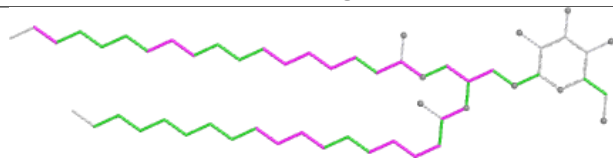
Ligand LMG F 101



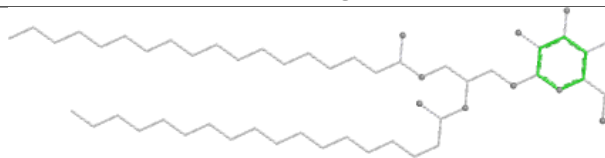
Bond lengths



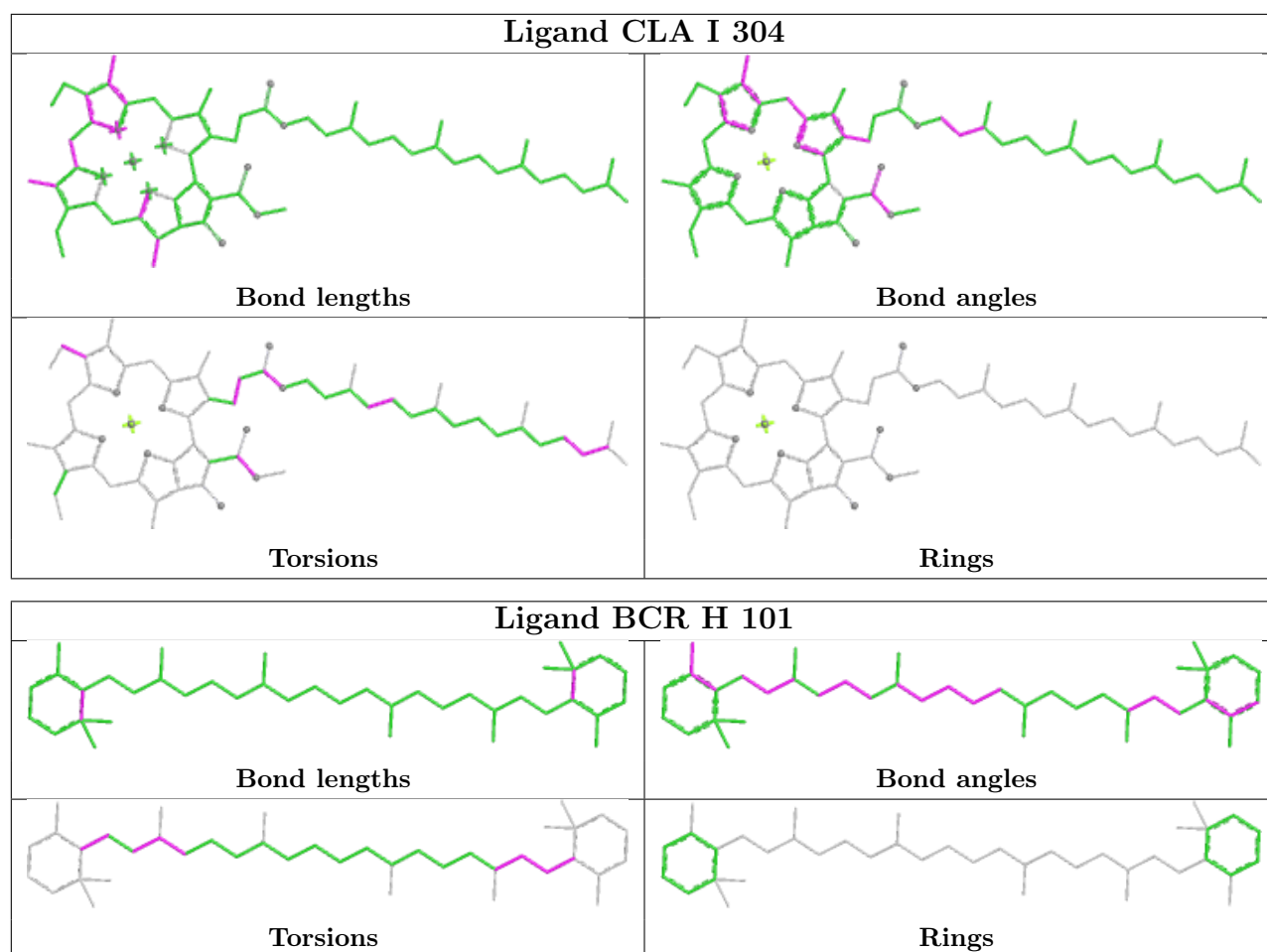
Bond angles

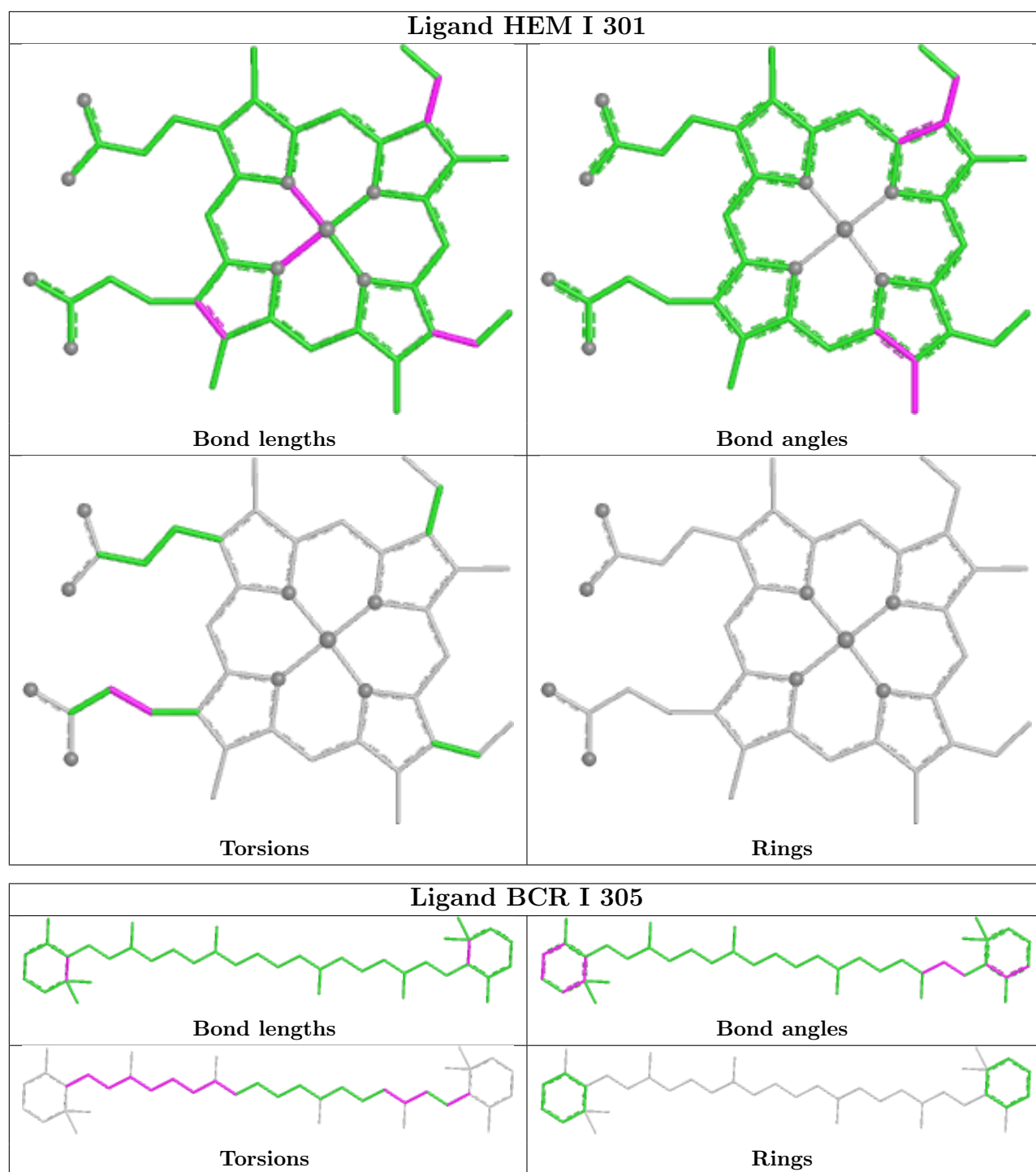


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

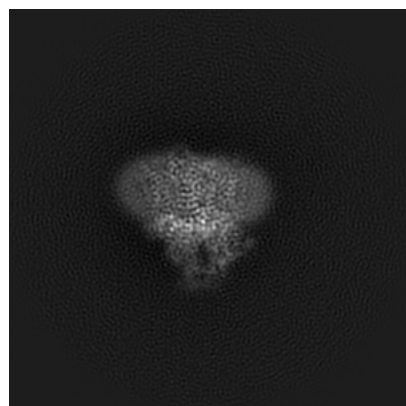
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4981. These allow visual inspection of the internal detail of the map and identification of artifacts.

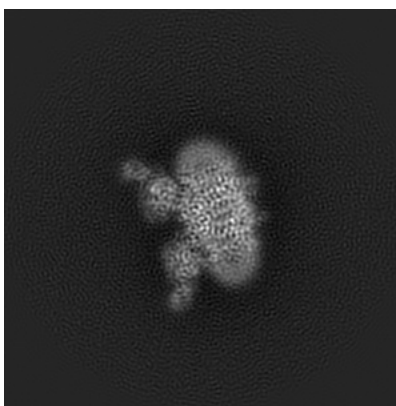
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

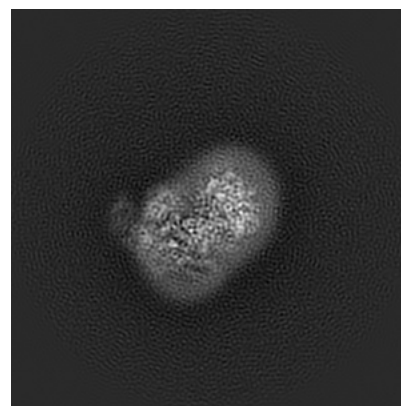
6.1.1 Primary map



X

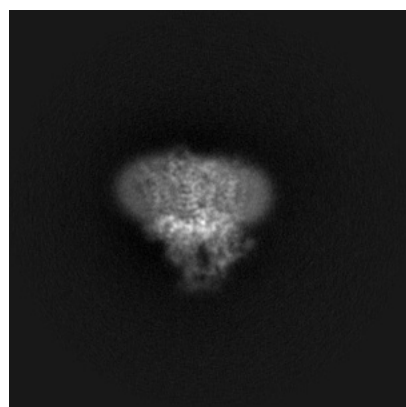


Y

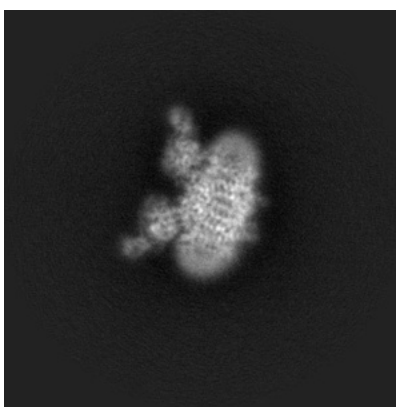


Z

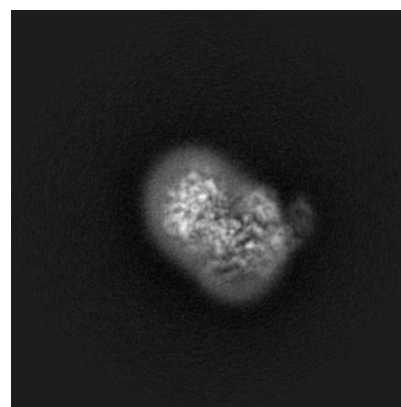
6.1.2 Raw map



X



Y

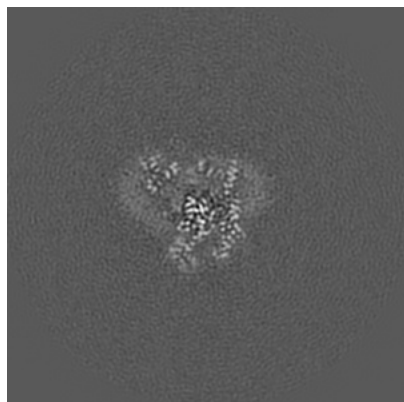


Z

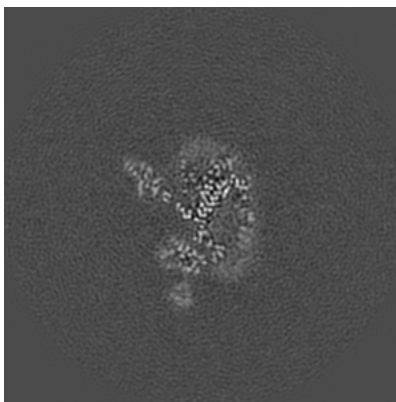
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

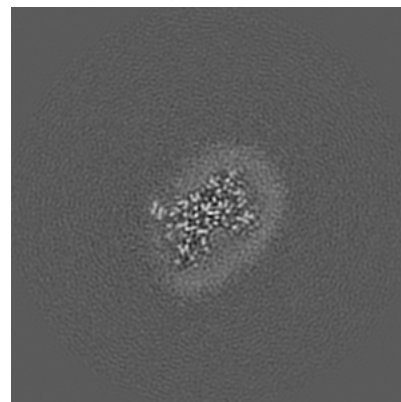
6.2.1 Primary map



X Index: 155

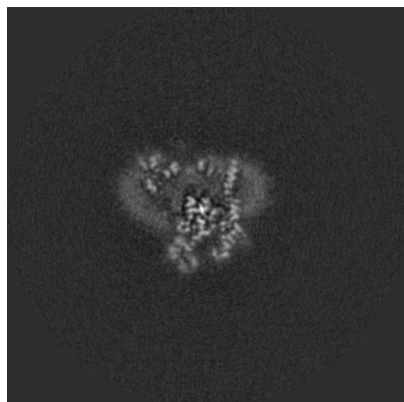


Y Index: 155

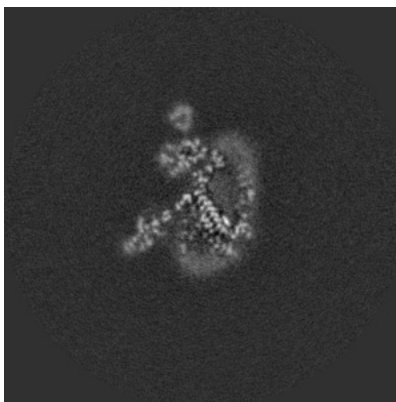


Z Index: 155

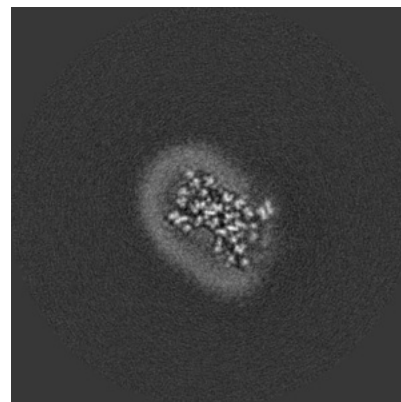
6.2.2 Raw map



X Index: 155



Y Index: 155

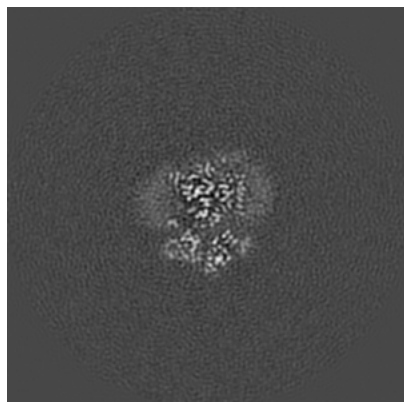


Z Index: 155

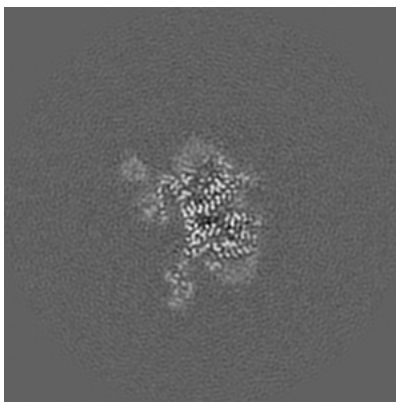
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

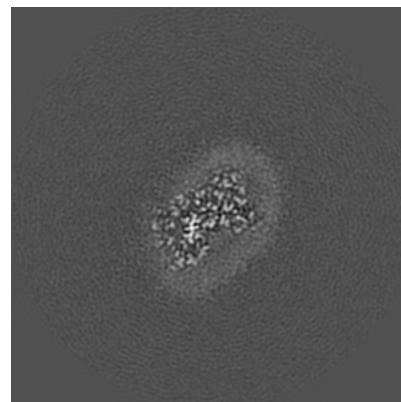
6.3.1 Primary map



X Index: 170

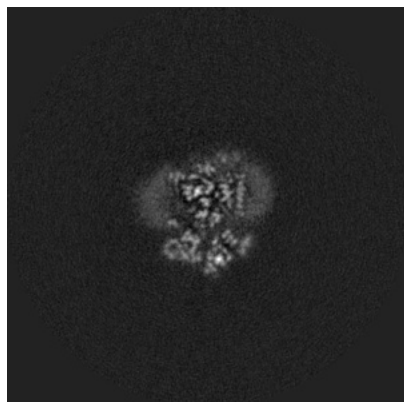


Y Index: 141

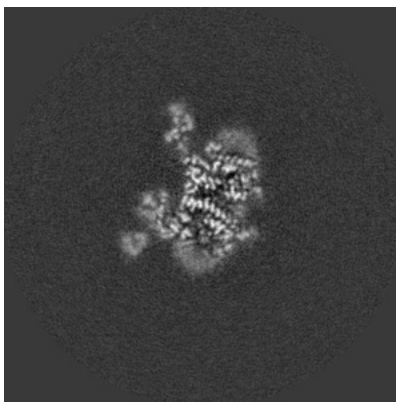


Z Index: 157

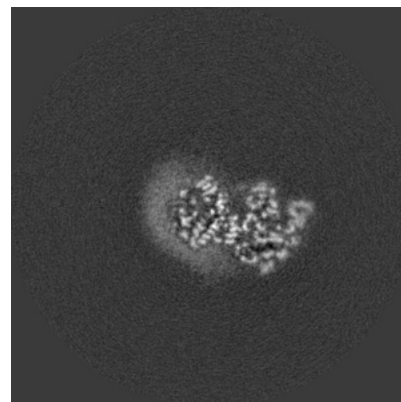
6.3.2 Raw map



X Index: 140



Y Index: 141

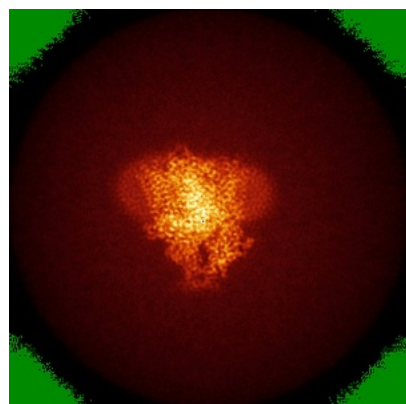


Z Index: 142

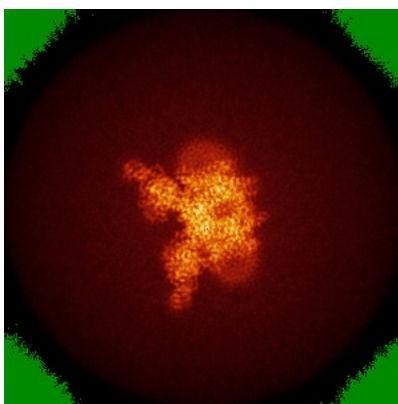
The images above show the largest variance slices of the map in three orthogonal directions.

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

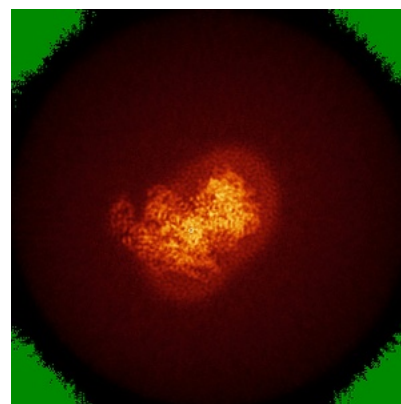
6.4.1 Primary map



X



Y

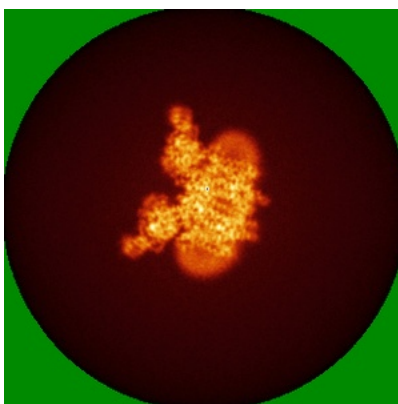


Z

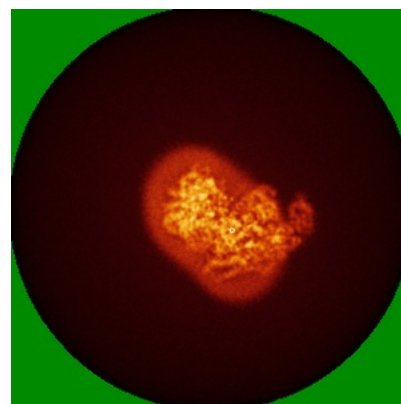
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



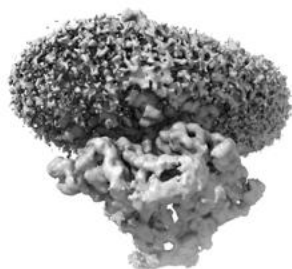
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0144. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

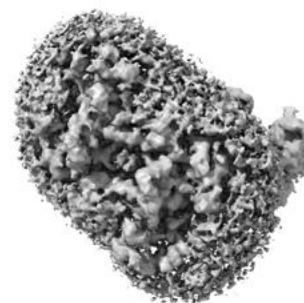
6.5.2 Raw map



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.

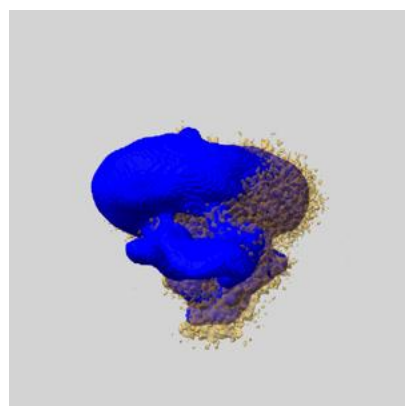
6.6 Mask visualisation [i](#)

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

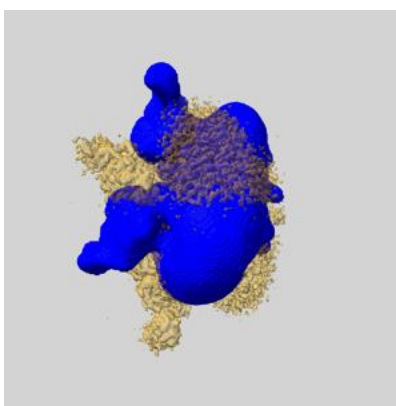
A mask typically either:

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

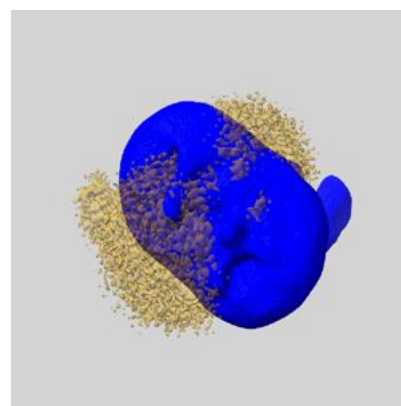
6.6.1 emd_4981_msk_1.map [i](#)



X



Y

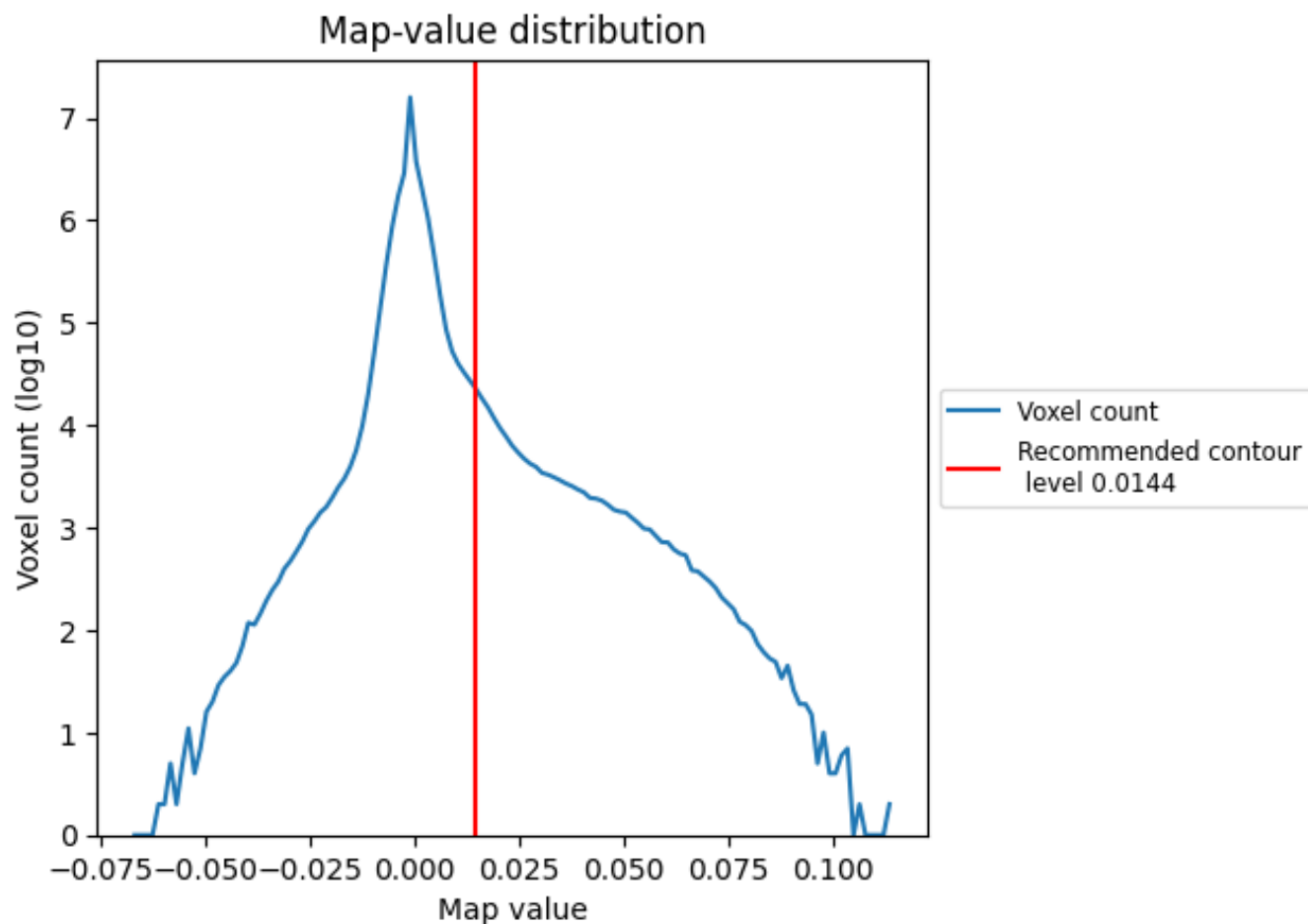


Z

7 Map analysis [i](#)

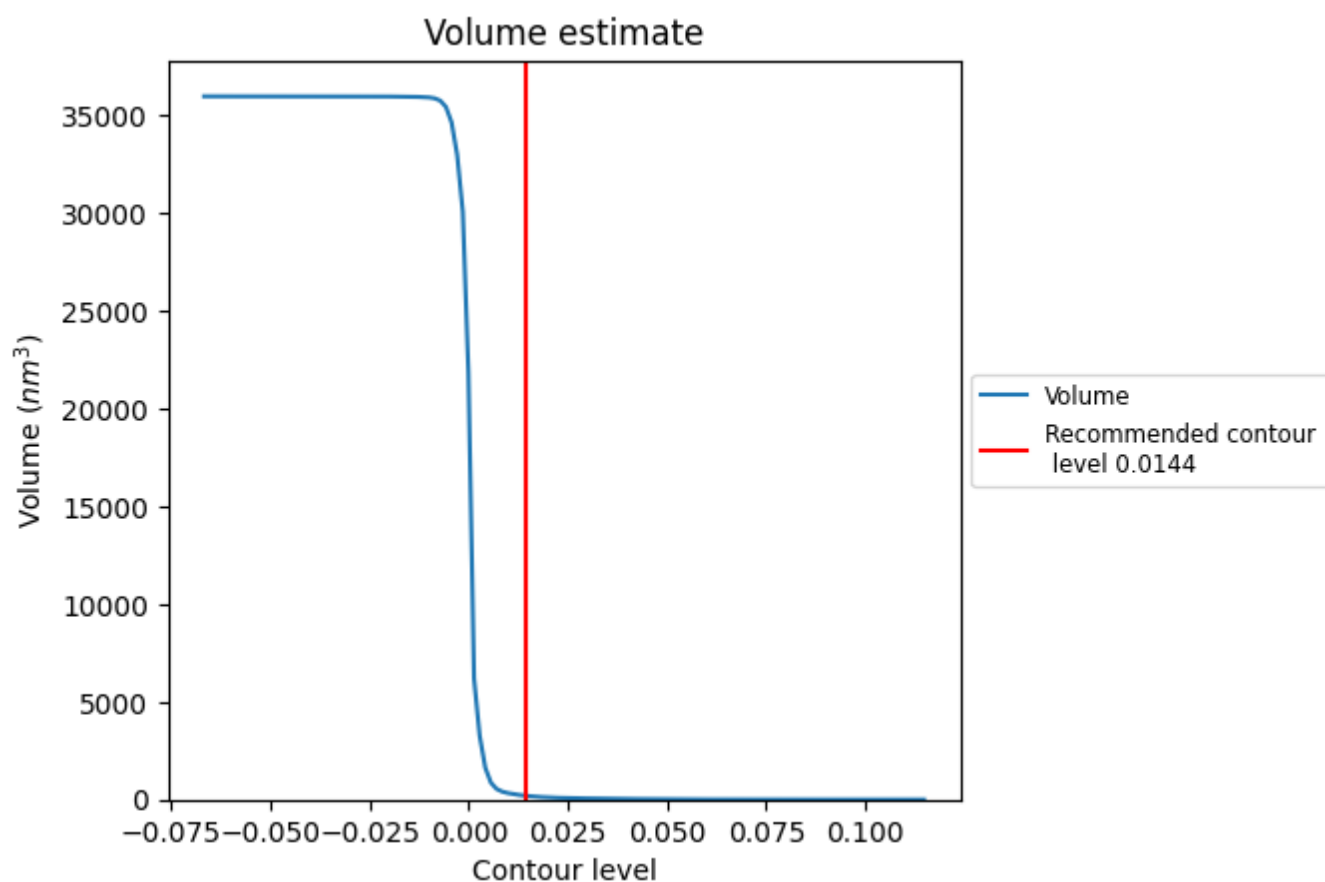
This section contains the results of statistical analysis of the map.

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.

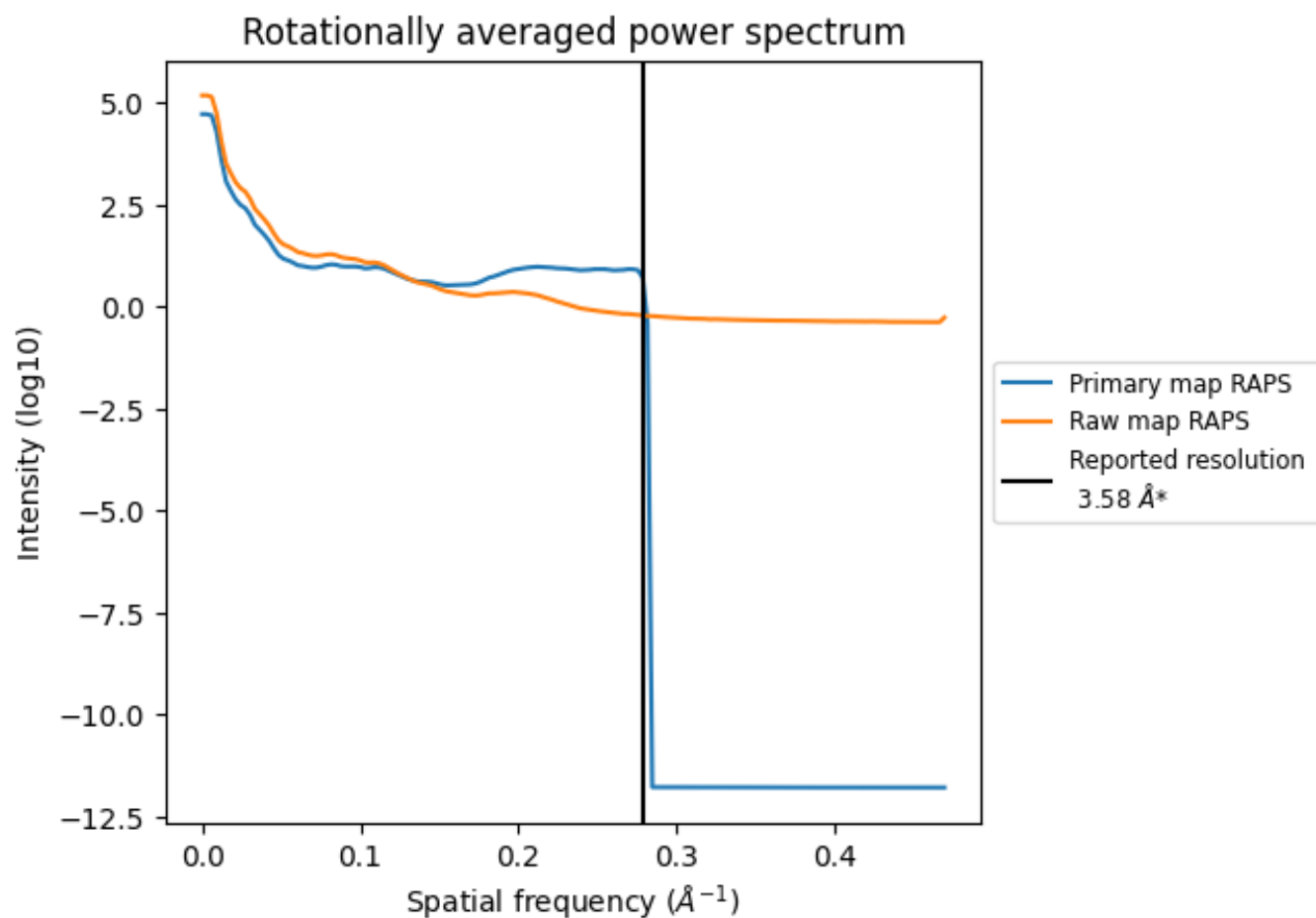
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm³; this corresponds to an approximate mass of 176 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 ⓘ

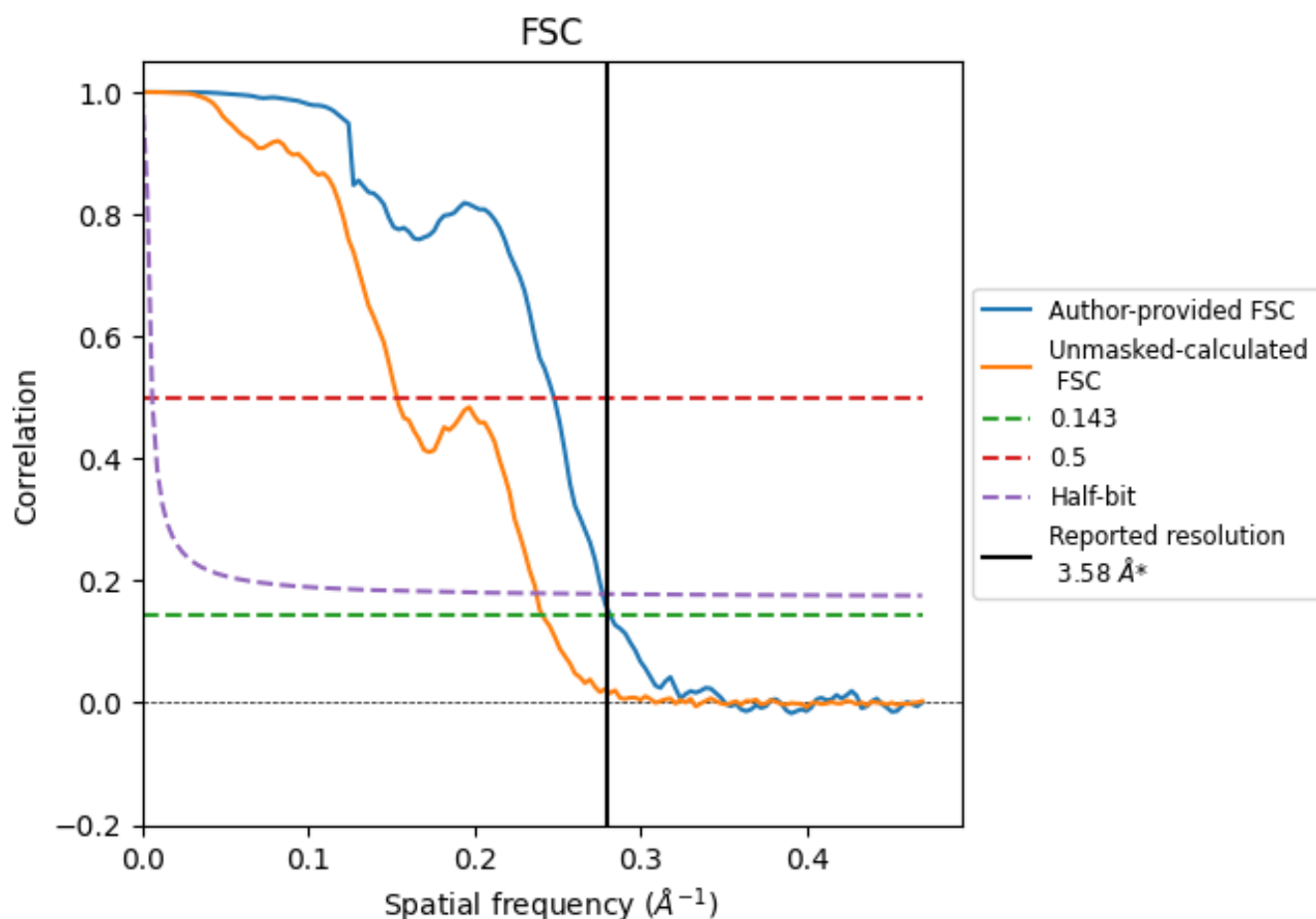


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

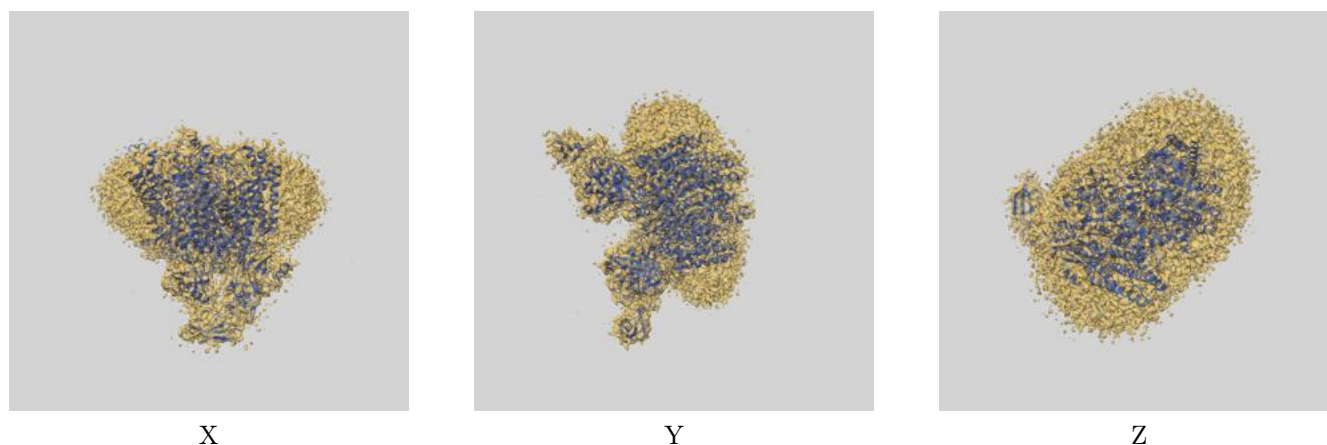
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.55	4.04	3.61
Unmasked-calculated*	4.15	6.52	4.22

*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 4.15 differs from the reported value 3.58 by more than 10 %

9 Map-model fit [i](#)

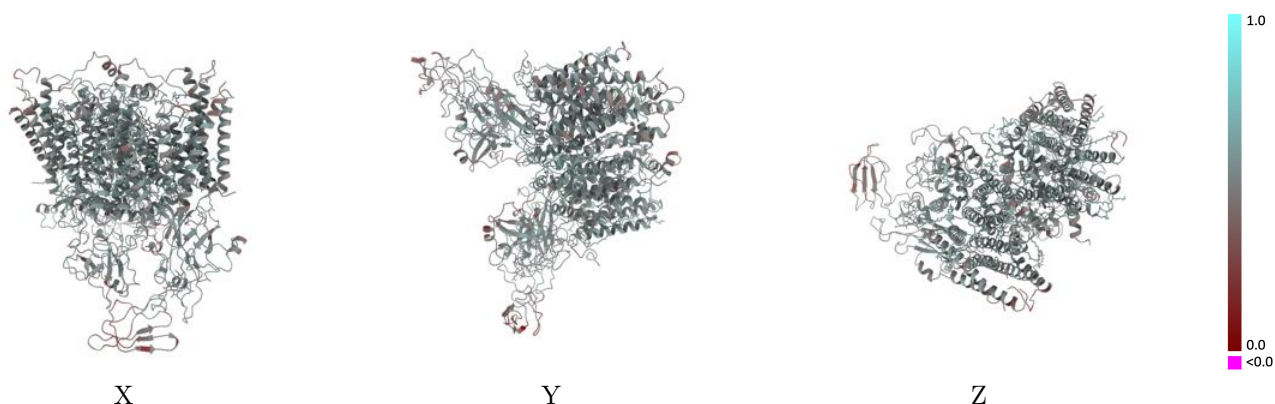
This section contains information regarding the fit between EMDB map EMD-4981 and PDB model 6RQF. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



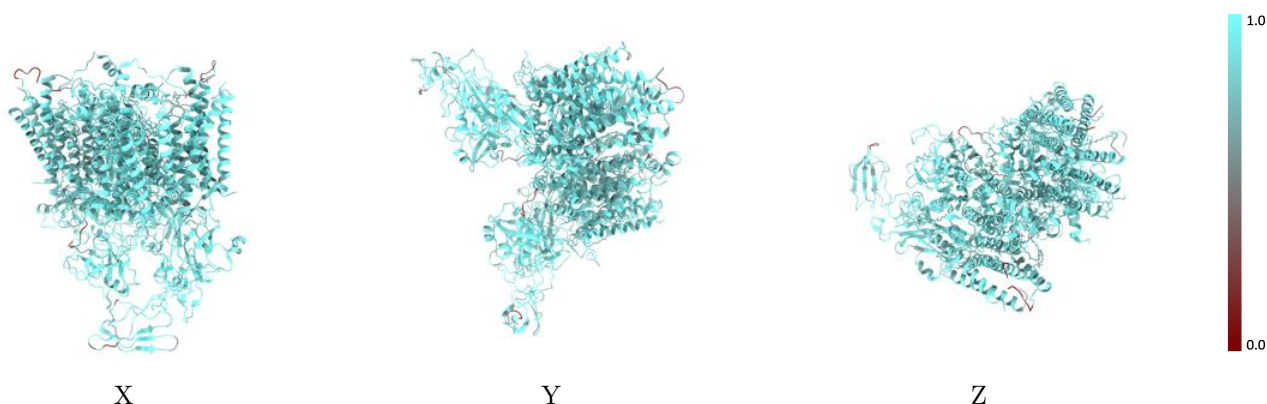
The images above show the 3D surface view of the map at the recommended contour level 0.0144 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



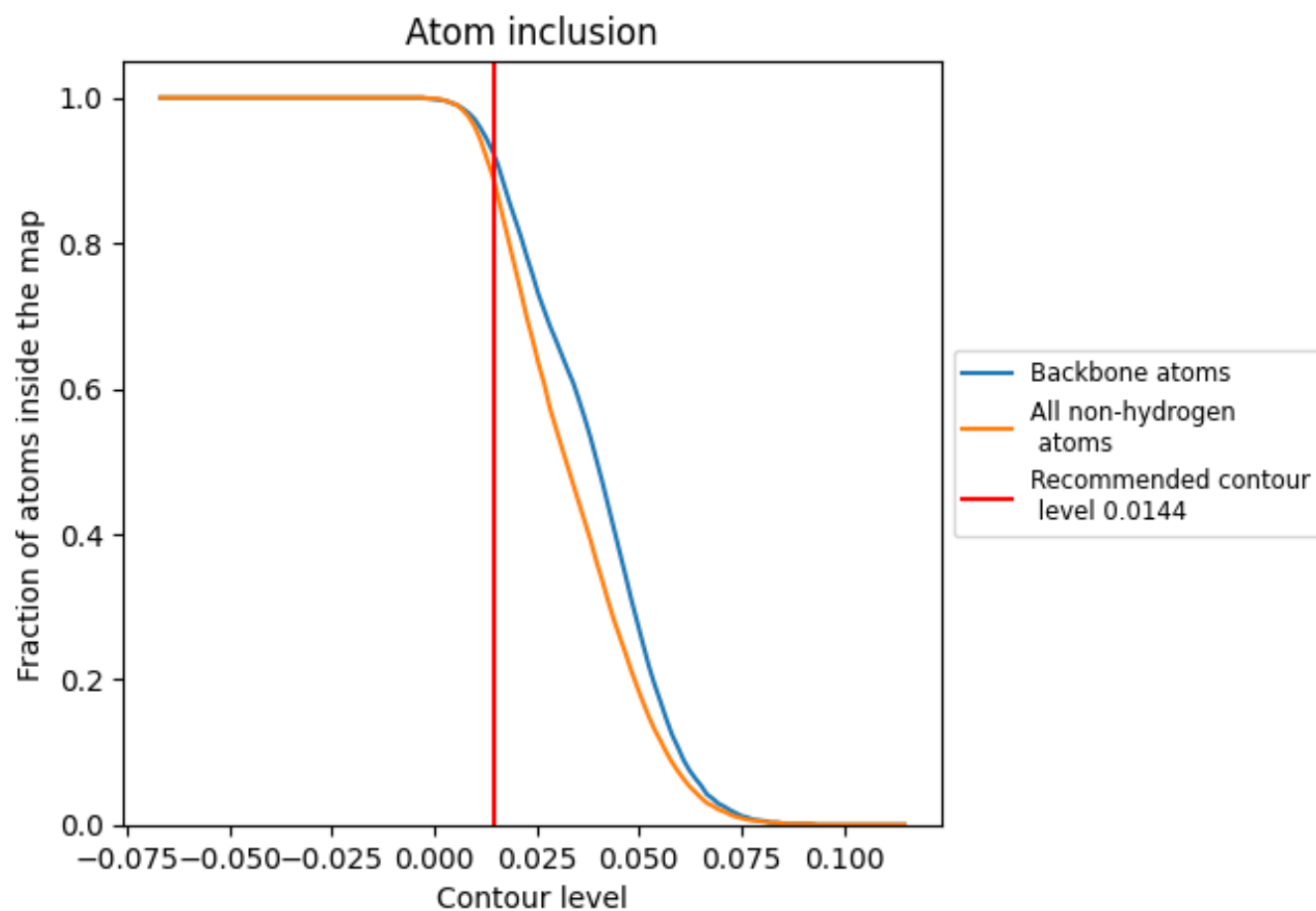
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0144).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (0.0144) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8910	 0.5110
A	 0.9220	 0.5400
B	 0.9070	 0.5240
C	 0.8890	 0.4920
D	 0.8690	 0.4830
E	 0.8730	 0.4910
F	 0.8730	 0.4990
G	 0.8820	 0.4900
H	 0.9150	 0.5330
I	 0.9170	 0.5360
J	 0.8870	 0.5290
K	 0.8810	 0.4980
L	 0.8570	 0.4920
M	 0.8420	 0.4810
N	 0.8490	 0.5030
O	 0.8610	 0.5050
P	 0.9180	 0.5210

