



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 02:48 PM UTC

PDB ID : 7ZYV / pdb_00007zyv
EMDB ID : EMD-15027
Title : Cryo-EM structure of catalytically active *Spinacia oleracea* cytochrome b6f in complex with endogenous plastoquinones at 2.13 Å resolution
Authors : Sarewicz, M.; Szewalec, M.; Pintscher, S.; Indyka, P.; Rawski, M.; Pietras, R.; Mielecki, B.; Koziej, L.; Jaciuk, M.; Glatt, S.; Osyczka, A.
Deposited on : 2022-05-25
Resolution : 2.13 Å (reported)
Based on initial model : 7QRM

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

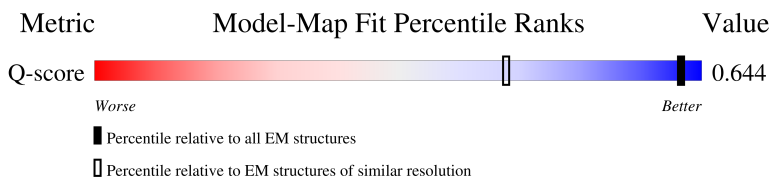
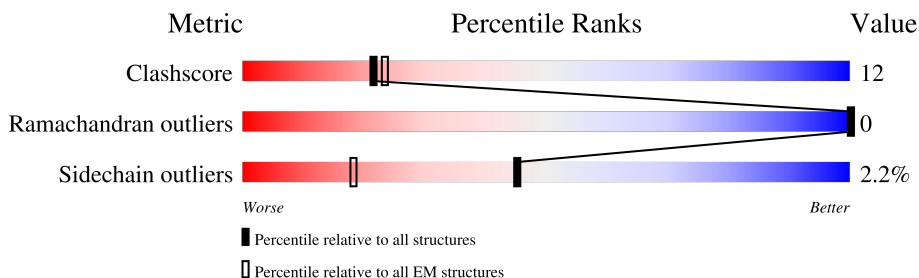
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.13 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.



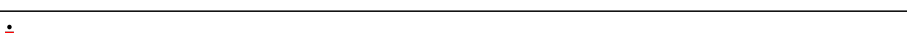
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2439 (1.64 - 2.63)

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	320	
3	K	320	
4	D	230	
4	L	230	
5	E	31	
5	M	31	
6	F	131	
6	N	131	
7	G	37	
7	O	37	
8	H	29	
8	P	29	
9	Q	103	
9	R	103	

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
12	CLA	A	304	X	-	-	-
12	CLA	I	304	X	-	-	-

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 16892 atoms, of which 440 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	A	214	Total	C	N	O	S	0	0
			1697	1126	271	289	11		
1	I	214	Total	C	N	O	S	0	0
			1697	1126	271	289	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	159	Total	C	N	O	S	0	0
			1225	820	193	208	4		
2	J	159	Total	C	N	O	S	0	0
			1226	820	193	209	4		

- Molecule 3 is a protein called Cytochrome f.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	278	Total	C	N	O	S	0	0
			2158	1391	365	396	6		
3	K	279	Total	C	N	O	S	0	0
			2167	1396	366	399	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	166	Total	C	N	O	S	0	0
			1259	807	212	233	7		
4	L	165	Total	C	N	O	S	0	0
			1254	804	211	232	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	31	Total	C	N	O	S	0	0
			243	167	36	39	1		
5	M	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	F	37	Total	C	N	O	S	0	0
			269	174	45	49	1		
6	N	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	G	34	Total	C	N	O	S	0	0
			266	181	41	43	1		
7	O	33	Total	C	N	O	S	0	0
			261	178	40	42	1		

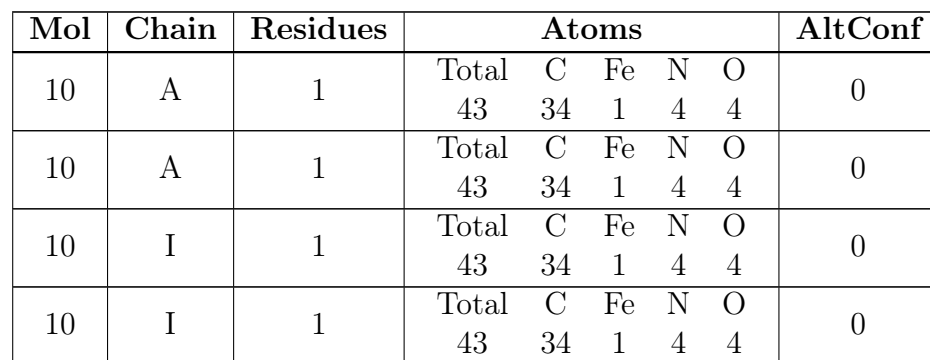
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	29	Total	C	N	O	S	0	0
			222	150	34	36	2		
8	P	29	Total	C	N	O	S	0	0
			223	150	34	37	2		

- Molecule 9 is a protein called Thylakoid soluble phosphoprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	26	Total	C	N	O	0	0
			219	144	34	41		
9	Q	26	Total	C	N	O	0	0
			219	144	34	41		

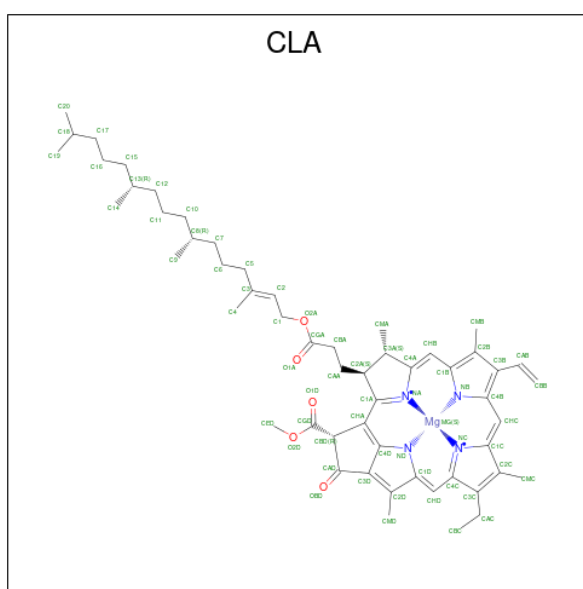
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



- # HEC

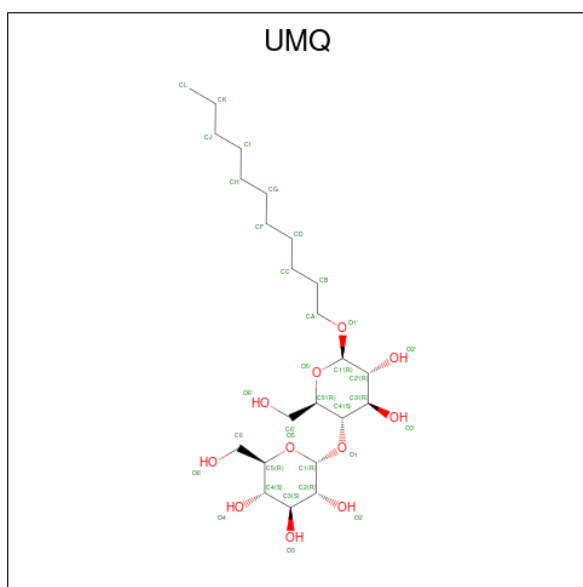
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
11	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



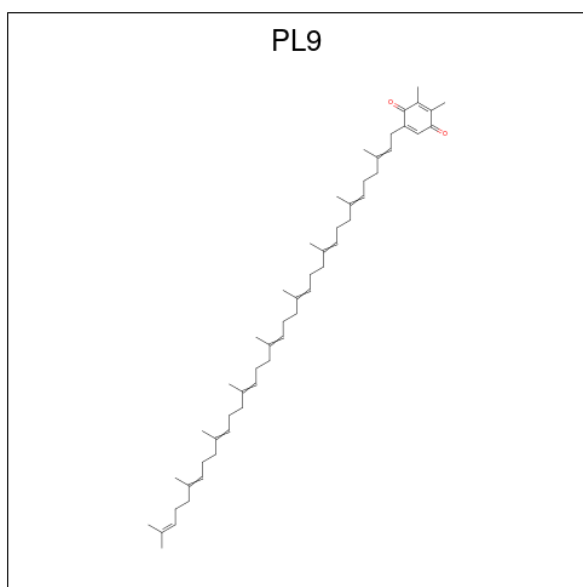
Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	I	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$) (labeled as "Ligand of Interest" by depositor).



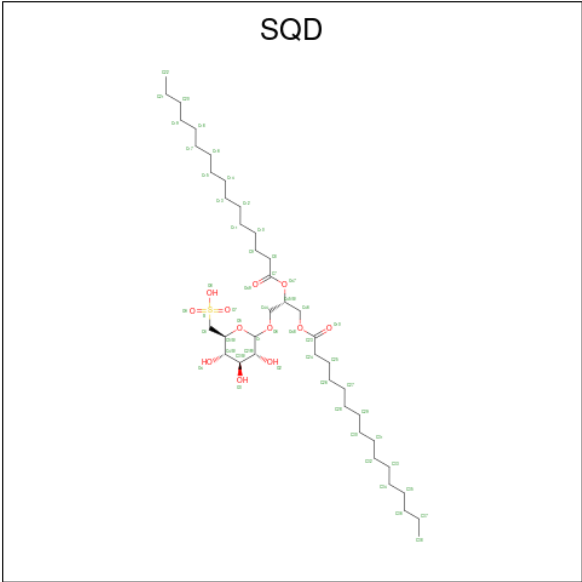
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	H	O	0
			78	23	44	11	
13	A	1	Total	C	H	O	0
			78	23	44	11	
13	B	1	Total	C	H	O	0
			78	23	44	11	
13	B	1	Total	C	H	O	0
			78	23	44	11	
13	H	1	Total	C	H	O	0
			78	23	44	11	
13	I	1	Total	C	H	O	0
			78	23	44	11	
13	I	1	Total	C	H	O	0
			78	23	44	11	
13	J	1	Total	C	H	O	0
			78	23	44	11	
13	J	1	Total	C	H	O	0
			78	23	44	11	
13	P	1	Total	C	H	O	0
			78	23	44	11	

- Molecule 14 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).



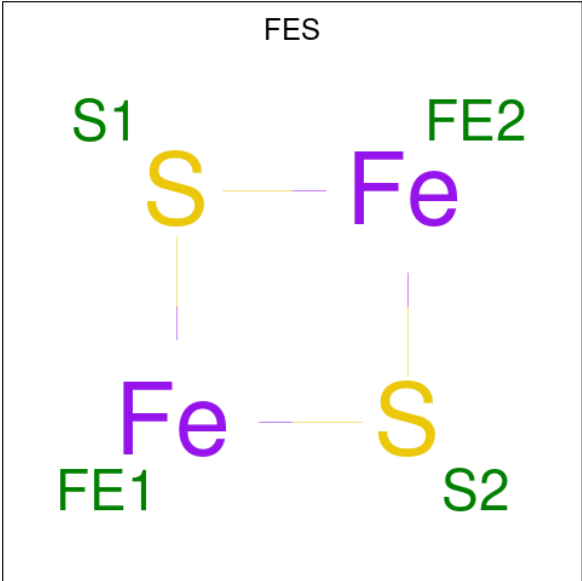
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			55	53	2	
14	B	1	Total	C	O	0
			55	53	2	
14	B	1	Total	C	O	0
			55	53	2	
14	J	1	Total	C	O	0
			55	53	2	
14	J	1	Total	C	O	0
			55	53	2	
14	K	1	Total	C	O	0
			55	53	2	

- Molecule 15 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
15	D	1	Total	C	O	S	0
			54	41	12	1	
15	L	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



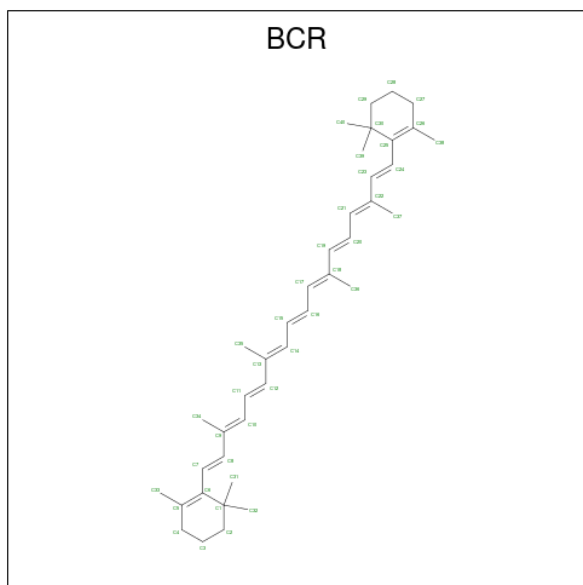
Mol	Chain	Residues	Atoms			AltConf
16	D	1	Total	Fe	S	0
			4	2	2	

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

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
17	F	1	Total	C	0
			40	40	
17	P	1	Total	C	0
			40	40	

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

Chain A: 



- Molecule 1: Cytochrome b6

Chain I: 



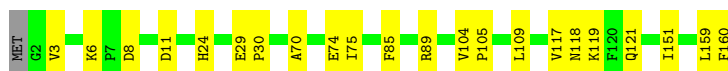
- Molecule 2: Cytochrome b6-f complex subunit 4

Chain B: 



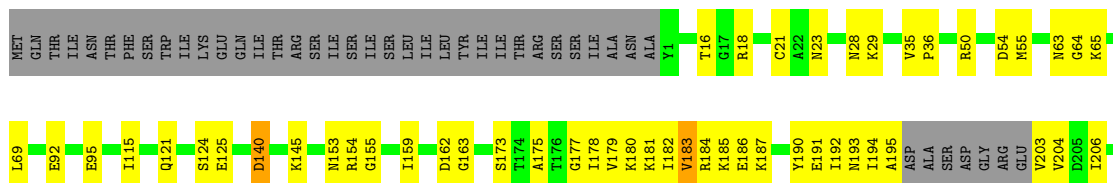
- Molecule 2: Cytochrome b6-f complex subunit 4

Chain J: 



- Molecule 3: Cytochrome f

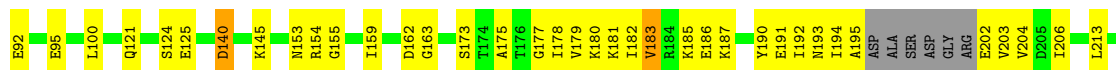
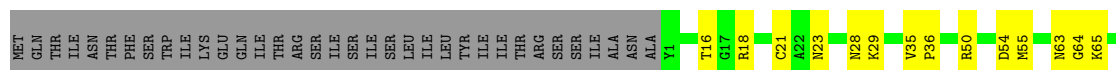
Chain C: 





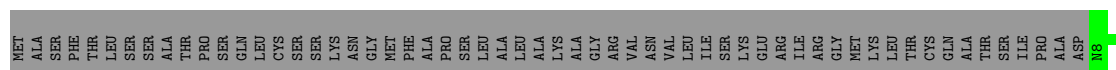
• Molecule 3: Cytochrome f

Chain K: 68% 19% 13%



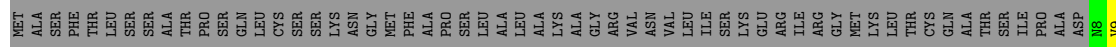
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain D: 59% 13% 28%



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

Chain L: 59% 13% 28%



• Molecule 5: Cytochrome b6-f complex subunit 6

Chain E: 90% 10%

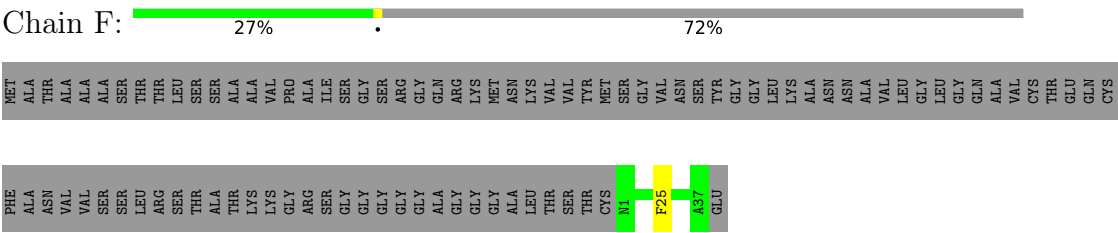


• Molecule 5: Cytochrome b6-f complex subunit 6

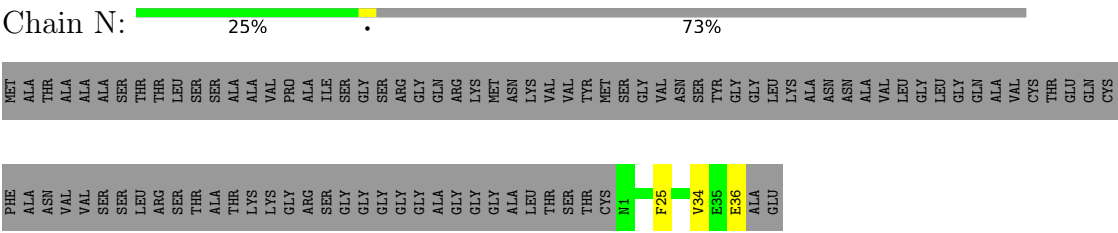
Chain M: 90% 10%



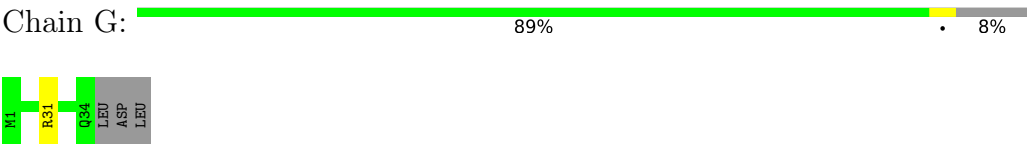
• Molecule 6: Cytochrome b6-f complex subunit 7



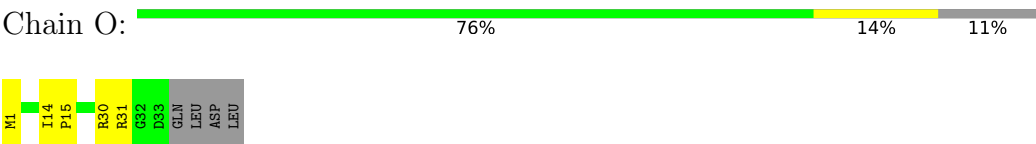
• Molecule 6: Cytochrome b6-f complex subunit 7



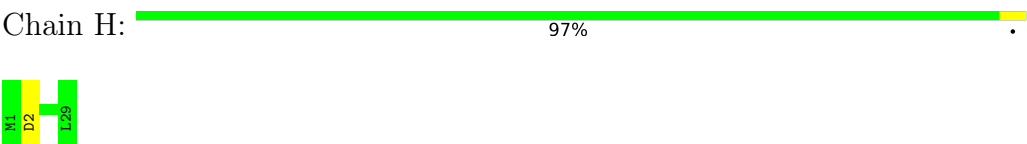
• Molecule 7: Cytochrome b6-f complex subunit 5



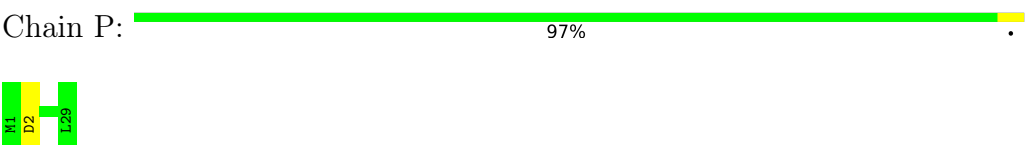
• Molecule 7: Cytochrome b6-f complex subunit 5



• Molecule 8: Cytochrome b6-f complex subunit 8

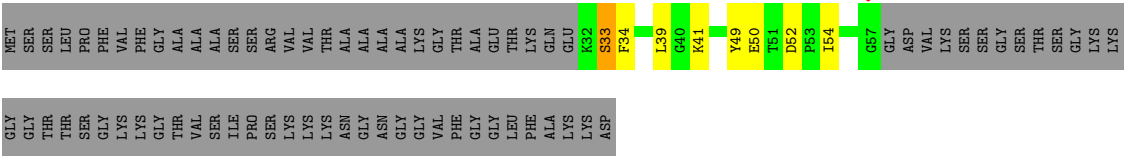


• Molecule 8: Cytochrome b6-f complex subunit 8

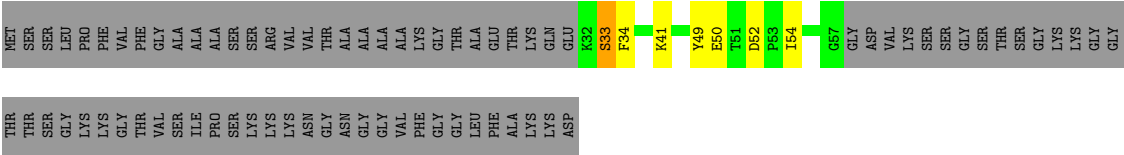


• Molecule 9: Thylakoid soluble phosphoprotein





● Molecule 9: Thylakoid soluble phosphoprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	685979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Non-uniform Refinement with iterative global CTF refinement and anisotropic magnification fitting	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.455	Depositor
Minimum map value	-0.577	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.208	Depositor
Map size ($\text{\AA}$)	319.92, 319.92, 319.92	wwPDB
Map dimensions	372, 372, 372	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	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: FES, SQD, HEM, CLA, UMQ, PL9, HEC, BCR

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	0.14	0/1747	0.33	0/2382
1	I	0.14	0/1747	0.33	0/2382
2	B	0.13	0/1262	0.32	0/1733
2	J	0.13	0/1263	0.31	0/1733
3	C	0.14	0/2204	0.33	0/2987
3	K	0.14	0/2213	0.33	0/2999
4	D	0.11	0/1293	0.30	0/1769
4	L	0.10	0/1288	0.28	0/1762
5	E	0.13	0/247	0.33	0/333
5	M	0.12	0/247	0.24	0/333
6	F	0.18	0/270	0.30	0/366
6	N	0.19	0/265	0.36	0/359
7	G	0.14	0/271	0.31	0/367
7	O	0.14	0/266	0.32	0/360
8	H	0.15	0/227	0.29	0/309
8	P	0.18	0/228	0.32	0/309
9	Q	0.10	0/224	0.22	0/301
9	R	0.10	0/224	0.22	0/301
All	All	0.13	0/15486	0.32	0/21085

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1724	21	0
1	I	1697	0	1724	23	0
2	B	1225	0	1276	29	0
2	J	1226	0	1276	25	0
3	C	2158	0	2212	84	0
3	K	2167	0	2218	78	0
4	D	1259	0	1232	23	0
4	L	1254	0	1227	24	0
5	E	243	0	268	1	0
5	M	243	0	268	4	0
6	F	269	0	287	2	0
6	N	264	0	282	2	0
7	G	266	0	282	1	0
7	O	261	0	280	4	0
8	H	222	0	234	1	0
8	P	223	0	234	1	0
9	Q	219	0	216	7	0
9	R	219	0	216	8	0
10	A	86	0	60	9	0
10	I	86	0	60	10	0
11	A	43	0	31	1	0
11	C	43	0	31	5	0
11	I	43	0	31	1	0
11	K	43	0	31	4	0
12	A	65	0	72	3	0
12	I	65	0	72	3	0
13	A	68	88	88	0	0
13	B	68	88	88	3	0
13	H	34	44	44	1	0
13	I	68	88	88	2	0
13	J	68	88	88	4	0
13	P	34	44	44	1	0
14	A	55	0	80	10	0
14	B	110	0	158	26	0
14	J	110	0	160	28	0
14	K	55	0	77	4	0
15	D	54	0	77	5	0
15	L	54	0	77	1	0
16	D	4	0	0	0	0
16	L	4	0	0	0	0
17	F	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	P	40	0	56	5	0
All	All	16452	440	17025	393	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 12.

All (393) 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:K:180:LYS:HG2	3:K:194:ILE:HA	1.39	1.04
3:K:180:LYS:HE2	3:K:195:ALA:H	1.22	1.03
3:C:180:LYS:HE2	3:C:195:ALA:H	1.22	1.01
3:C:180:LYS:HG2	3:C:194:ILE:HA	1.39	1.00
3:C:179:VAL:HA	3:C:194:ILE:HG22	1.44	0.99
3:K:179:VAL:HA	3:K:194:ILE:HG22	1.44	0.99
3:C:178:ILE:HA	3:C:220:SER:HA	1.44	0.97
3:K:178:ILE:HA	3:K:220:SER:HA	1.44	0.97
3:K:21:CYS:HB2	11:K:301:HEC:HAB	1.47	0.97
3:C:222:LYS:HB3	3:C:222:LYS:HZ2	1.31	0.94
3:C:222:LYS:HB3	3:C:222:LYS:NZ	1.79	0.94
3:C:178:ILE:HG13	3:C:180:LYS:HZ3	1.33	0.94
3:C:21:CYS:HB2	11:C:301:HEC:HAB	1.47	0.94
3:C:29:LYS:HG3	3:C:235:GLY:HA3	1.50	0.92
3:K:29:LYS:HG3	3:K:235:GLY:HA3	1.50	0.91
3:C:182:ILE:HG12	3:C:192:ILE:HD12	1.54	0.90
3:K:182:ILE:HG12	3:K:192:ILE:HD12	1.54	0.89
13:J:404:UMQ:O3'	13:J:404:UMQ:O2	1.93	0.86
10:A:301:HEM:HBC2	10:A:301:HEM:HMC2	1.58	0.85
10:I:302:HEM:HBC2	10:I:302:HEM:HMC2	1.60	0.84
10:A:302:HEM:HBC2	10:A:302:HEM:HMC2	1.60	0.83
14:A:307:PL9:H453	15:D:201:SQD:H202	1.59	0.83
10:I:301:HEM:HBC2	10:I:301:HEM:HMC2	1.59	0.83
10:I:301:HEM:HMB1	10:I:301:HEM:HBB2	1.61	0.82
3:K:178:ILE:HG22	3:K:220:SER:HB2	1.61	0.82
3:C:178:ILE:HG22	3:C:220:SER:HB2	1.61	0.82
4:D:64:ILE:HG23	4:D:157:GLY:O	1.81	0.81
10:A:301:HEM:HMB1	10:A:301:HEM:HBB2	1.61	0.81
13:B:403:UMQ:O3'	13:B:403:UMQ:O2	1.93	0.80
3:C:177:GLY:O	3:C:220:SER:OG	2.00	0.79
3:K:180:LYS:HE2	3:K:195:ALA:N	1.98	0.79
10:A:302:HEM:HBB2	10:A:302:HEM:HMB1	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:178:ILE:HG13	3:K:180:LYS:NZ	1.99	0.78
10:I:302:HEM:HMB1	10:I:302:HEM:HBB2	1.63	0.78
3:C:178:ILE:HG13	3:C:180:LYS:NZ	1.99	0.78
3:C:180:LYS:HE2	3:C:195:ALA:N	1.98	0.77
3:C:179:VAL:HA	3:C:194:ILE:CG2	2.15	0.77
3:K:175:ALA:O	3:K:221:ILE:HD11	1.86	0.76
3:K:179:VAL:HA	3:K:194:ILE:CG2	2.15	0.76
3:K:177:GLY:O	3:K:220:SER:OG	2.00	0.76
3:C:175:ALA:O	3:C:221:ILE:HD11	1.86	0.75
3:K:195:ALA:HB2	3:K:202:GLU:HG3	1.68	0.74
2:J:121:GLN:N	9:R:50:GLU:OE2	2.21	0.74
4:L:122:LYS:HB2	4:L:132:TYR:O	1.87	0.74
3:C:179:VAL:HG13	3:C:218:GLY:H	1.53	0.74
3:C:173:SER:HB3	3:C:227:LEU:HD11	1.70	0.74
3:K:283:MET:HE3	3:K:283:MET:HA	1.69	0.73
3:C:283:MET:HE3	3:C:283:MET:HA	1.69	0.73
1:I:150:ILE:HG21	14:J:401:PL9:H502	1.70	0.73
3:K:179:VAL:HG13	3:K:218:GLY:H	1.53	0.72
3:K:173:SER:HB3	3:K:227:LEU:HD11	1.70	0.72
2:J:74:GLU:HB3	14:J:402:PL9:H121	1.70	0.72
14:B:402:PL9:HC72	14:B:402:PL9:H122	1.71	0.71
3:C:63:ASN:OD1	3:C:65:LYS:HG2	1.91	0.71
12:I:304:CLA:H151	14:J:401:PL9:H312	1.71	0.71
1:I:27:PRO:HG3	2:J:24:HIS:O	1.90	0.71
3:K:63:ASN:OD1	3:K:65:LYS:HG2	1.91	0.70
3:K:162:ASP:OD1	3:K:163:GLY:N	2.26	0.69
3:K:178:ILE:HG13	3:K:180:LYS:HZ3	1.56	0.69
3:C:181:LYS:HZ1	3:C:183:VAL:HG12	1.57	0.69
3:K:181:LYS:HZ1	3:K:183:VAL:HG12	1.56	0.69
4:D:28:LEU:HB2	4:D:29:PRO:HD3	1.74	0.68
3:C:162:ASP:OD1	3:C:163:GLY:N	2.26	0.68
2:B:121:GLN:N	9:Q:50:GLU:OE2	2.22	0.68
3:C:184:ARG:NH2	3:C:186:GLU:HA	2.08	0.68
1:A:27:PRO:HG3	2:B:24:HIS:O	1.93	0.68
8:P:2:ASP:OD2	13:P:102:UMQ:O4	2.07	0.68
1:A:150:ILE:HD13	14:B:401:PL9:H512	1.75	0.68
2:B:74:GLU:OE1	2:B:74:GLU:N	2.27	0.68
14:J:402:PL9:H252	14:J:402:PL9:H201	1.75	0.68
5:M:29:ARG:HG3	5:M:29:ARG:HH11	1.57	0.67
17:P:101:BCR:H401	9:R:39:LEU:HD21	1.76	0.67
2:J:74:GLU:N	2:J:74:GLU:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:GLN:OE1	3:C:121:GLN:HA	1.93	0.67
2:B:88:LEU:HB2	2:B:101:MET:CE	2.25	0.67
3:C:184:ARG:HH22	3:C:186:GLU:HA	1.59	0.67
4:L:93:GLU:OE2	4:L:93:GLU:HA	1.95	0.67
12:A:304:CLA:O1D	14:B:402:PL9:H502	1.95	0.67
3:C:182:ILE:HG12	3:C:192:ILE:CD1	2.24	0.67
7:G:31:ARG:HG2	9:Q:49:TYR:OH	1.95	0.67
3:K:182:ILE:HG12	3:K:192:ILE:CD1	2.24	0.66
4:L:137:ARG:HG2	4:L:137:ARG:HH21	1.60	0.66
3:K:121:GLN:HA	3:K:121:GLN:OE1	1.93	0.66
3:C:185:LYS:HD2	3:C:186:GLU:H	1.61	0.66
10:I:302:HEM:HBA1	10:I:302:HEM:HHA	1.78	0.66
4:L:67:GLU:O	4:L:71:THR:HG22	1.96	0.66
3:K:185:LYS:HD2	3:K:186:GLU:H	1.61	0.65
10:A:302:HEM:HHA	10:A:302:HEM:HBA1	1.78	0.65
3:C:63:ASN:OD1	3:C:64:GLY:N	2.30	0.65
3:C:185:LYS:HZ3	3:C:187:LYS:H	1.45	0.65
2:J:85:PHE:CE1	14:J:401:PL9:H503	2.33	0.64
3:K:185:LYS:HZ3	3:K:187:LYS:H	1.45	0.64
3:K:63:ASN:OD1	3:K:64:GLY:N	2.30	0.64
3:C:178:ILE:HG22	3:C:220:SER:CB	2.28	0.64
7:O:31:ARG:HG2	9:R:49:TYR:OH	1.97	0.64
4:L:64:ILE:HB	4:L:67:GLU:OE1	1.98	0.63
2:J:74:GLU:HA	14:J:402:PL9:O2	1.99	0.63
2:J:75:ILE:HG12	14:J:401:PL9:C51	2.29	0.63
2:B:75:ILE:HG12	14:B:401:PL9:H501	1.81	0.63
4:L:140:ARG:HD2	4:L:141:GLY:N	2.14	0.63
3:K:181:LYS:NZ	3:K:183:VAL:HG12	2.14	0.62
4:D:140:ARG:HD2	4:D:141:GLY:N	2.14	0.62
10:A:301:HEM:HBC2	10:A:301:HEM:CMC	2.30	0.62
3:C:181:LYS:NZ	3:C:183:VAL:HG12	2.14	0.62
14:J:402:PL9:H153	14:J:402:PL9:H101	1.81	0.62
3:K:178:ILE:HG22	3:K:220:SER:CB	2.28	0.62
11:C:301:HEC:HBC3	11:C:301:HEC:HHD	1.82	0.61
3:C:181:LYS:HG2	3:C:182:ILE:N	2.15	0.61
10:I:301:HEM:HBB2	10:I:301:HEM:CMB	2.31	0.61
1:I:145:TYR:O	1:I:148:VAL:HG12	2.00	0.61
10:I:301:HEM:HBC2	10:I:301:HEM:CMC	2.30	0.61
3:K:181:LYS:HG2	3:K:182:ILE:N	2.15	0.61
4:D:64:ILE:HB	4:D:67:GLU:OE1	2.01	0.61
10:I:302:HEM:HBC2	10:I:302:HEM:CMC	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	2.31	0.61
2:B:75:ILE:HG12	14:B:401:PL9:C50	2.31	0.61
1:A:145:TYR:O	1:A:148:VAL:HG12	2.01	0.60
3:C:191:GLU:O	3:C:192:ILE:HD13	2.01	0.60
17:P:101:BCR:H401	9:R:39:LEU:CD2	2.30	0.60
10:I:302:HEM:HBB2	10:I:302:HEM:CMB	2.31	0.60
3:K:194:ILE:O	3:K:203:VAL:HG22	2.01	0.60
11:K:301:HEC:HBC3	11:K:301:HEC:HHD	1.82	0.60
2:J:121:GLN:HB2	9:R:50:GLU:OE2	2.01	0.60
4:D:163:PRO:HB3	4:D:179:ALA:O	2.01	0.60
3:K:92:GLU:O	3:K:95:GLU:HG3	2.02	0.60
3:K:283:MET:HE3	3:K:283:MET:CA	2.32	0.60
2:B:74:GLU:HA	14:B:402:PL9:O2	2.01	0.60
3:C:194:ILE:O	3:C:203:VAL:HG22	2.01	0.60
3:K:173:SER:HG	3:K:224:ASP:H	1.50	0.60
10:A:302:HEM:HBC2	10:A:302:HEM:CMC	2.31	0.60
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.31	0.59
3:C:92:GLU:O	3:C:95:GLU:HG3	2.02	0.59
3:K:221:ILE:HD12	3:K:221:ILE:C	2.27	0.59
3:C:221:ILE:C	3:C:221:ILE:HD12	2.27	0.59
4:D:67:GLU:O	4:D:71:THR:HG22	2.01	0.59
4:L:64:ILE:HG23	4:L:157:GLY:O	2.02	0.59
3:K:191:GLU:O	3:K:192:ILE:HD13	2.01	0.59
4:D:64:ILE:HB	4:D:67:GLU:CD	2.28	0.59
14:A:307:PL9:H453	15:D:201:SQD:H223	1.86	0.58
8:H:2:ASP:OD2	13:H:201:UMQ:O4	2.19	0.58
3:K:185:LYS:NZ	3:K:186:GLU:HG3	2.18	0.58
3:K:202:GLU:OE1	3:K:202:GLU:N	2.36	0.58
3:C:185:LYS:NZ	3:C:186:GLU:HG3	2.18	0.58
4:D:64:ILE:HB	4:D:67:GLU:OE2	2.04	0.58
3:K:180:LYS:HG2	3:K:194:ILE:CA	2.26	0.57
3:K:193:ASN:OD1	3:K:204:VAL:HG22	2.05	0.57
4:L:64:ILE:HB	4:L:67:GLU:CD	2.29	0.57
4:L:70:LYS:HB2	4:L:70:LYS:NZ	2.20	0.57
3:C:193:ASN:OD1	3:C:204:VAL:HG22	2.04	0.57
3:K:195:ALA:HB2	3:K:202:GLU:CG	2.34	0.56
3:C:283:MET:HE3	3:C:283:MET:CA	2.32	0.56
3:K:173:SER:OG	3:K:224:ASP:N	2.39	0.56
2:B:88:LEU:HB2	2:B:101:MET:HE2	1.87	0.56
12:A:304:CLA:H151	14:B:401:PL9:H28	1.88	0.56
3:C:173:SER:OG	3:C:224:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:307:PL9:H453	15:D:201:SQD:C20	2.34	0.56
3:C:179:VAL:HG22	3:C:217:GLU:OE1	2.06	0.56
4:L:171:THR:HB	4:L:173:GLU:OE1	2.06	0.56
2:B:88:LEU:HB2	2:B:101:MET:HE1	1.88	0.55
14:J:402:PL9:H201	14:J:402:PL9:C25	2.36	0.55
1:A:113:PRO:HB2	1:I:11:ARG:HG2	1.88	0.55
3:C:180:LYS:HG2	3:C:194:ILE:CA	2.26	0.55
3:C:184:ARG:NH1	3:C:185:LYS:O	2.39	0.55
14:A:307:PL9:H451	14:A:307:PL9:C48	2.36	0.55
3:K:179:VAL:HG12	3:K:219:GLU:O	2.07	0.55
3:C:179:VAL:HG12	3:C:219:GLU:O	2.07	0.55
3:C:183:VAL:HG13	3:C:191:GLU:CB	2.38	0.54
4:L:74:PRO:HA	4:L:92:VAL:HG12	1.88	0.54
3:K:179:VAL:HG22	3:K:217:GLU:OE1	2.06	0.54
2:B:154:SER:OG	13:B:404:UMQ:O2'	2.25	0.54
4:L:137:ARG:HG2	4:L:137:ARG:NH2	2.20	0.54
3:C:179:VAL:HG12	3:C:219:GLU:H	1.73	0.54
2:J:74:GLU:HA	14:J:402:PL9:C1	2.38	0.54
3:K:183:VAL:HG13	3:K:191:GLU:CB	2.37	0.54
4:D:166:GLU:OE1	4:D:166:GLU:N	2.41	0.54
14:K:302:PL9:H301	14:K:302:PL9:H33	1.90	0.54
13:I:306:UMQ:O3'	13:I:306:UMQ:O2	2.21	0.53
3:K:179:VAL:HG12	3:K:219:GLU:H	1.73	0.53
14:B:402:PL9:C38	14:B:402:PL9:H351	2.38	0.53
3:K:179:VAL:CG1	3:K:219:GLU:H	2.21	0.53
5:M:29:ARG:HG3	5:M:29:ARG:NH1	2.23	0.53
2:J:70:ALA:HB1	3:K:16:THR:HG22	1.89	0.53
2:B:29:GLU:HG2	2:B:30:PRO:HD2	1.90	0.53
3:C:179:VAL:CG1	3:C:219:GLU:H	2.21	0.53
4:D:74:PRO:HA	4:D:92:VAL:HG12	1.90	0.53
3:K:155:GLY:O	11:K:301:HEC:HBA1	2.09	0.53
3:K:29:LYS:HB2	3:K:154:ARG:NH1	2.24	0.53
2:J:29:GLU:HG2	2:J:30:PRO:HD2	1.90	0.53
3:C:29:LYS:HE2	3:C:234:GLY:O	2.09	0.52
3:C:185:LYS:HD2	3:C:186:GLU:N	2.24	0.52
3:C:29:LYS:HB2	3:C:154:ARG:NH1	2.24	0.52
1:I:150:ILE:HD13	14:J:401:PL9:C50	2.39	0.52
3:C:155:GLY:O	11:C:301:HEC:HBA1	2.09	0.52
3:K:185:LYS:HD2	3:K:186:GLU:N	2.24	0.52
14:B:401:PL9:H101	14:B:401:PL9:H13	1.92	0.52
4:L:64:ILE:HB	4:L:67:GLU:OE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:SER:O	3:C:224:ASP:HA	2.10	0.52
3:K:183:VAL:HG13	3:K:191:GLU:HB3	1.92	0.52
3:C:179:VAL:CG1	3:C:218:GLY:H	2.23	0.51
4:D:29:PRO:O	4:D:33:MET:HG2	2.10	0.51
14:J:402:PL9:H252	14:J:402:PL9:C20	2.40	0.51
2:J:89:ARG:NH1	14:J:402:PL9:H523	2.25	0.51
3:K:140:ASP:OD1	3:K:140:ASP:N	2.43	0.51
3:K:173:SER:O	3:K:224:ASP:HA	2.10	0.51
13:I:305:UMQ:HJ2	15:L:401:SQD:H301	1.92	0.51
3:K:29:LYS:HE2	3:K:234:GLY:O	2.09	0.51
2:J:118:ASN:OD1	2:J:119:LYS:N	2.43	0.51
4:L:74:PRO:HA	4:L:92:VAL:CG1	2.41	0.51
3:C:183:VAL:HG13	3:C:191:GLU:HB3	1.92	0.51
3:K:190:TYR:CE2	3:K:213:LEU:HG	2.46	0.51
3:C:140:ASP:OD1	3:C:140:ASP:N	2.43	0.51
1:I:117:THR:HG22	1:I:202:HIS:CE1	2.46	0.51
3:K:178:ILE:HG13	3:K:180:LYS:HZ2	1.72	0.51
1:A:117:THR:HG22	1:A:202:HIS:CE1	2.46	0.50
2:B:85:PHE:CE1	14:B:401:PL9:H513	2.47	0.50
1:A:103:ARG:HD2	1:A:103:ARG:C	2.37	0.50
3:C:190:TYR:CE2	3:C:213:LEU:HG	2.46	0.50
3:C:185:LYS:HZ3	3:C:186:GLU:HG3	1.75	0.50
9:R:33:SER:O	9:R:34:PHE:HB3	2.12	0.50
3:K:179:VAL:CG1	3:K:218:GLY:H	2.23	0.49
1:I:103:ARG:C	1:I:103:ARG:HD2	2.37	0.49
14:A:307:PL9:H13	3:C:250:ARG:HA	1.94	0.49
6:F:25:PHE:HE1	9:Q:41:LYS:HB3	1.78	0.49
4:D:115:PRO:HD2	4:D:124:ILE:O	2.10	0.49
14:B:402:PL9:H251	14:B:402:PL9:H272	1.55	0.49
3:C:222:LYS:NZ	3:C:222:LYS:CB	2.66	0.49
2:J:70:ALA:HB1	3:K:16:THR:CG2	2.42	0.49
2:B:74:GLU:HG3	14:B:402:PL9:H152	1.94	0.49
1:I:81:LEU:HD21	14:K:302:PL9:H221	1.95	0.49
3:K:185:LYS:HZ3	3:K:186:GLU:HG3	1.78	0.49
2:B:74:GLU:HA	14:B:402:PL9:C1	2.43	0.48
2:B:144:GLY:HA3	14:B:402:PL9:H422	1.95	0.48
3:C:194:ILE:O	3:C:194:ILE:HD12	2.14	0.48
3:K:191:GLU:C	3:K:192:ILE:HD13	2.39	0.48
9:Q:33:SER:O	9:Q:34:PHE:HB3	2.12	0.48
3:C:191:GLU:C	3:C:192:ILE:HD13	2.39	0.48
2:B:89:ARG:NH1	14:B:402:PL9:H523	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:93:GLU:N	4:D:97:THR:O	2.43	0.48
2:J:159:LEU:O	2:J:160:PHE:C	2.57	0.48
2:B:159:LEU:O	2:B:160:PHE:C	2.57	0.47
14:B:402:PL9:H451	14:B:402:PL9:H471	1.56	0.47
6:N:25:PHE:HE1	9:R:41:LYS:HB3	1.79	0.47
4:L:166:GLU:OE1	4:L:166:GLU:N	2.47	0.47
2:J:8:ASP:O	2:J:8:ASP:CG	2.58	0.47
14:A:307:PL9:C45	15:D:201:SQD:H223	2.44	0.47
7:O:1:MET:HE2	7:O:1:MET:HB3	1.85	0.47
3:C:184:ARG:NH2	3:C:185:LYS:O	2.47	0.47
2:J:74:GLU:HB3	14:J:402:PL9:C12	2.42	0.47
14:B:402:PL9:H121	14:B:402:PL9:H172	1.96	0.47
3:K:194:ILE:O	3:K:194:ILE:HD12	2.14	0.47
1:A:150:ILE:HG21	14:B:401:PL9:H512	1.97	0.47
1:A:11:ARG:HG2	1:I:113:PRO:HB2	1.97	0.47
14:A:307:PL9:H322	14:A:307:PL9:H301	1.68	0.47
3:K:54:ASP:OD2	3:K:55:MET:N	2.49	0.46
4:L:67:GLU:OE1	4:L:67:GLU:N	2.38	0.46
2:B:125:ARG:NH1	9:Q:50:GLU:OE1	2.48	0.46
4:D:93:GLU:OE1	4:D:93:GLU:HA	2.16	0.46
2:B:85:PHE:CD1	14:B:401:PL9:H472	2.50	0.46
3:C:54:ASP:OD2	3:C:55:MET:N	2.49	0.46
17:F:101:BCR:C8	17:F:101:BCR:H331	2.45	0.46
1:A:150:ILE:HD13	14:B:401:PL9:C51	2.42	0.46
3:C:178:ILE:HB	3:C:219:GLU:O	2.16	0.46
14:B:401:PL9:H471	14:B:401:PL9:H451	1.70	0.46
3:C:180:LYS:CE	3:C:195:ALA:H	2.11	0.46
3:K:159:ILE:O	11:K:301:HEC:HBC3	2.16	0.46
3:K:178:ILE:HB	3:K:219:GLU:O	2.16	0.46
13:B:403:UMQ:O3'	13:B:403:UMQ:C2	2.64	0.46
1:I:207:ARG:HD2	11:I:303:HEC:O2D	2.15	0.46
3:K:145:LYS:HE3	3:K:242:GLU:HG3	1.98	0.46
1:A:207:ARG:HD2	11:A:303:HEC:O2D	2.15	0.45
2:B:8:ASP:O	2:B:8:ASP:CG	2.58	0.45
2:J:74:GLU:HA	14:J:402:PL9:C2	2.46	0.45
13:J:404:UMQ:O3'	13:J:404:UMQ:C2	2.64	0.45
3:C:145:LYS:HE3	3:C:242:GLU:HG3	1.98	0.45
3:C:159:ILE:O	11:C:301:HEC:HBC3	2.16	0.45
1:I:146:TRP:HB2	2:J:75:ILE:HD13	1.97	0.45
6:N:36:GLU:OE2	6:N:36:GLU:N	2.48	0.45
14:A:307:PL9:H151	14:A:307:PL9:H172	1.66	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:402:PL9:C38	14:J:402:PL9:H351	2.43	0.45
3:K:18:ARG:NH2	3:K:23:ASN:OD1	2.50	0.45
2:B:104:VAL:HB	2:B:105:PRO:CD	2.47	0.45
3:C:184:ARG:HH22	3:C:186:GLU:CA	2.28	0.45
2:J:104:VAL:HB	2:J:105:PRO:CD	2.47	0.45
3:K:206:ILE:H	3:K:206:ILE:HD12	1.82	0.45
1:A:92:MET:HA	1:A:92:MET:HE2	1.98	0.45
14:B:402:PL9:H212	14:B:402:PL9:H161	1.99	0.45
1:I:92:MET:HE2	1:I:92:MET:HA	1.98	0.45
5:E:27:LYS:CA	5:E:27:LYS:HE2	2.47	0.45
17:P:101:BCR:H20C	17:P:101:BCR:H361	1.84	0.45
3:C:206:ILE:HD12	3:C:206:ILE:H	1.82	0.45
3:K:180:LYS:CE	3:K:195:ALA:H	2.11	0.45
14:J:401:PL9:H23	14:J:401:PL9:C18	2.47	0.44
4:D:55:ALA:O	4:D:63:VAL:HG23	2.17	0.44
4:D:73:ALA:HB1	4:D:74:PRO:HD2	1.98	0.44
4:L:67:GLU:CD	4:L:67:GLU:H	2.19	0.44
1:A:211:ILE:HG13	1:A:212:SER:H	1.81	0.44
3:C:18:ARG:NH2	3:C:23:ASN:OD1	2.50	0.44
1:I:150:ILE:HD13	14:J:401:PL9:H502	1.98	0.44
17:P:101:BCR:H24C	17:P:101:BCR:H371	1.83	0.44
1:I:211:ILE:HG13	1:I:212:SER:H	1.81	0.44
3:C:223:LEU:O	3:C:224:ASP:HB2	2.18	0.44
1:I:63:THR:HG22	1:I:64:ASP:OD2	2.17	0.44
17:P:101:BCR:C8	17:P:101:BCR:H331	2.48	0.44
1:A:63:THR:HG22	1:A:64:ASP:OD2	2.18	0.44
9:R:54:ILE:HD12	9:R:54:ILE:H	1.83	0.44
1:I:163:SER:HB2	1:I:164:PRO:HD3	2.00	0.44
5:M:27:LYS:CA	5:M:27:LYS:HE2	2.47	0.44
1:A:163:SER:HB2	1:A:164:PRO:HD3	2.00	0.43
4:D:74:PRO:HA	4:D:92:VAL:CG1	2.48	0.43
1:I:138:LEU:N	1:I:139:PRO:CD	2.81	0.43
1:A:138:LEU:N	1:A:139:PRO:CD	2.81	0.43
3:K:35:VAL:HB	3:K:36:PRO:HD2	1.99	0.43
4:L:110:LEU:HD23	4:L:110:LEU:HA	1.85	0.43
14:J:401:PL9:H422	14:J:401:PL9:H401	1.58	0.43
3:K:223:LEU:O	3:K:224:ASP:HB2	2.18	0.43
1:A:165:LEU:HD12	1:A:165:LEU:HA	1.86	0.43
6:F:25:PHE:CE1	9:Q:41:LYS:HB3	2.54	0.43
4:L:95:ASP:OD1	4:L:97:THR:OG1	2.27	0.43
3:C:35:VAL:HB	3:C:36:PRO:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:LEU:HD21	4:D:98:LEU:HD13	2.01	0.43
7:O:30:ARG:HA	7:O:30:ARG:HD2	1.77	0.43
9:Q:54:ILE:H	9:Q:54:ILE:HD12	1.83	0.43
14:B:402:PL9:HC72	14:B:402:PL9:C12	2.39	0.43
3:K:178:ILE:O	3:K:180:LYS:HD3	2.19	0.43
14:J:402:PL9:H201	14:J:402:PL9:H221	1.64	0.43
3:K:283:MET:HA	3:K:283:MET:CE	2.45	0.43
4:L:69:LEU:HD21	4:L:98:LEU:HD23	2.01	0.43
1:A:47:GLN:O	1:A:48:VAL:C	2.61	0.43
1:A:154:VAL:N	1:A:155:PRO:HD2	2.34	0.42
15:D:201:SQD:H102	15:D:201:SQD:H132	1.87	0.42
1:I:154:VAL:N	1:I:155:PRO:HD2	2.34	0.42
10:I:302:HEM:HBA1	10:I:302:HEM:CHA	2.48	0.42
3:K:100:LEU:HD23	3:K:100:LEU:HA	1.93	0.42
4:D:139:VAL:O	4:D:140:ARG:HB2	2.20	0.42
3:C:178:ILE:O	3:C:180:LYS:HD3	2.19	0.42
4:D:97:THR:OG1	4:D:98:LEU:N	2.51	0.42
4:D:162:VAL:HG13	4:D:163:PRO:HD2	2.01	0.42
17:F:101:BCR:H24C	17:F:101:BCR:H371	1.82	0.42
1:I:45:LEU:HD12	14:K:302:PL9:H403	2.01	0.42
2:J:11:ASP:OD1	2:J:11:ASP:C	2.62	0.42
2:B:119:LYS:HB3	2:B:119:LYS:HE3	1.18	0.42
13:J:403:UMQ:O1	13:J:403:UMQ:O4	2.33	0.42
14:B:402:PL9:H351	14:B:402:PL9:H38	2.00	0.42
3:C:283:MET:HA	3:C:283:MET:CE	2.45	0.42
2:J:109:LEU:HD12	2:J:109:LEU:HA	1.86	0.42
5:M:29:ARG:HD2	5:M:29:ARG:N	2.34	0.42
3:C:50:ARG:NH2	3:C:125:GLU:OE1	2.53	0.42
14:J:401:PL9:H361	14:J:401:PL9:H321	1.67	0.42
4:L:78:THR:HG22	4:L:79:LEU:N	2.35	0.42
3:C:153:ASN:ND2	3:C:235:GLY:O	2.53	0.42
14:K:302:PL9:H422	14:K:302:PL9:H401	1.40	0.42
4:L:90:LEU:HD23	4:L:90:LEU:HA	1.83	0.42
2:B:70:ALA:HB1	3:C:16:THR:HG22	2.00	0.42
3:K:50:ARG:NH2	3:K:125:GLU:OE1	2.53	0.42
3:C:28:ASN:C	3:C:29:LYS:HG2	2.45	0.42
3:K:181:LYS:HE3	3:K:181:LYS:HB3	1.98	0.42
3:C:184:ARG:HG2	3:C:184:ARG:HH11	1.83	0.41
4:D:140:ARG:CD	4:D:141:GLY:N	2.83	0.41
2:J:29:GLU:HG2	2:J:30:PRO:CD	2.50	0.41
12:I:304:CLA:C20	14:J:401:PL9:H221	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:GLU:HG2	2:B:30:PRO:CD	2.50	0.41
1:I:150:ILE:HD13	14:J:401:PL9:H501	2.02	0.41
12:I:304:CLA:H61	12:I:304:CLA:H101	1.74	0.41
14:J:402:PL9:HC72	14:J:402:PL9:H112	1.70	0.41
1:I:47:GLN:O	1:I:48:VAL:C	2.61	0.41
2:B:144:GLY:HA3	14:B:402:PL9:C42	2.50	0.41
4:D:53:THR:O	4:D:160:VAL:HA	2.21	0.41
3:K:28:ASN:C	3:K:29:LYS:HG2	2.45	0.41
3:K:191:GLU:OE2	3:K:206:ILE:HG13	2.21	0.41
3:K:153:ASN:ND2	3:K:235:GLY:O	2.53	0.41
1:A:146:TRP:HB2	2:B:75:ILE:HD13	2.02	0.41
14:A:307:PL9:H112	3:C:250:ARG:HA	2.02	0.41
2:B:11:ASP:OD1	2:B:11:ASP:C	2.62	0.41
1:I:92:MET:O	1:I:96:MET:HG2	2.21	0.41
13:J:403:UMQ:O5	13:J:403:UMQ:O6'	2.30	0.41
2:B:119:LYS:H	2:B:119:LYS:HG2	1.69	0.41
1:I:46:VAL:O	1:I:47:GLN:C	2.63	0.41
2:B:74:GLU:HA	14:B:402:PL9:C2	2.51	0.40
3:C:191:GLU:OE2	3:C:206:ILE:HG13	2.21	0.40
2:J:6:LYS:HE3	2:J:6:LYS:HB3	1.74	0.40
14:J:402:PL9:H401	14:J:402:PL9:H422	1.74	0.40
4:L:56:LYS:O	4:L:80:THR:HB	2.21	0.40
12:A:304:CLA:H61	12:A:304:CLA:H101	1.74	0.40
14:A:307:PL9:C35	14:J:401:PL9:H532	2.51	0.40
3:C:21:CYS:HB2	11:C:301:HEC:CAB	2.35	0.40
2:J:85:PHE:HE1	14:J:401:PL9:H503	1.84	0.40
14:J:401:PL9:H301	14:J:401:PL9:H322	1.59	0.40
7:O:14:ILE:N	7:O:15:PRO:HD2	2.36	0.40
1:A:92:MET:O	1:A:96:MET:HG2	2.21	0.40
3:C:115:ILE:HG23	3:C:115:ILE:O	2.21	0.40
1:A:48:VAL:O	1:A:49:ALA:C	2.64	0.40
3:C:69:LEU:N	3:C:69:LEU:HD12	2.37	0.40
4:L:139:VAL:O	4:L:140:ARG:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
1	I	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
2	J	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
3	C	274/320 (86%)	263 (96%)	11 (4%)	0	100	100
3	K	275/320 (86%)	264 (96%)	11 (4%)	0	100	100
4	D	162/230 (70%)	151 (93%)	11 (7%)	0	100	100
4	L	161/230 (70%)	152 (94%)	9 (6%)	0	100	100
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
5	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	F	35/131 (27%)	35 (100%)	0	0	100	100
6	N	34/131 (26%)	34 (100%)	0	0	100	100
7	G	32/37 (86%)	31 (97%)	1 (3%)	0	100	100
7	O	31/37 (84%)	30 (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
9	Q	24/103 (23%)	23 (96%)	1 (4%)	0	100	100
9	R	24/103 (23%)	23 (96%)	1 (4%)	0	100	100
All	All	1902/2512 (76%)	1828 (96%)	74 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	185/186 (100%)	182 (98%)	3 (2%)	55	61
1	I	185/186 (100%)	182 (98%)	3 (2%)	55	61
2	B	134/135 (99%)	130 (97%)	4 (3%)	36	37
2	J	134/135 (99%)	131 (98%)	3 (2%)	45	49
3	C	237/275 (86%)	232 (98%)	5 (2%)	47	51
3	K	238/275 (86%)	234 (98%)	4 (2%)	53	58
4	D	135/183 (74%)	131 (97%)	4 (3%)	36	37
4	L	135/183 (74%)	133 (98%)	2 (2%)	57	63
5	E	26/26 (100%)	24 (92%)	2 (8%)	12	7
5	M	26/26 (100%)	25 (96%)	1 (4%)	29	28
6	F	26/90 (29%)	26 (100%)	0	100	100
6	N	26/90 (29%)	25 (96%)	1 (4%)	29	28
7	G	27/31 (87%)	27 (100%)	0	100	100
7	O	27/31 (87%)	27 (100%)	0	100	100
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	24 (100%)	0	100	100
9	Q	24/78 (31%)	22 (92%)	2 (8%)	10	6
9	R	24/78 (31%)	22 (92%)	2 (8%)	10	6
All	All	1637/2056 (80%)	1601 (98%)	36 (2%)	45	49

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	A	133	VAL
1	A	151	VAL
2	B	3	VAL
2	B	117	VAL
2	B	119	LYS
2	B	151	ILE
3	C	124	SER
3	C	140	ASP
3	C	183	VAL
3	C	222	LYS

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Mol	Chain	Res	Type
3	C	242	GLU
4	D	13	GLN
4	D	71	THR
4	D	137	ARG
4	D	165	THR
5	E	26	ASN
5	E	29	ARG
1	I	89	SER
1	I	133	VAL
1	I	151	VAL
2	J	3	VAL
2	J	117	VAL
2	J	151	ILE
3	K	124	SER
3	K	140	ASP
3	K	183	VAL
3	K	242	GLU
4	L	9	VAL
4	L	165	THR
5	M	26	ASN
6	N	34	VAL
9	R	33	SER
9	R	52	ASP
9	Q	33	SER
9	Q	52	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	GLN
3	C	25	HIS
3	C	153	ASN
4	D	121	ASN
6	F	14	ASN
3	K	6	GLN
3	K	25	HIS
3	K	153	ASN
3	K	193	ASN
9	R	47	GLN
9	Q	47	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 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$
10	HEM	I	301	1	50,50,50	1.39	7 (14%)	67,82,82	1.10	3 (4%)
14	PL9	A	307	-	55,55,55	1.01	4 (7%)	68,69,69	1.51	11 (16%)
16	FES	L	402	4	0,4,4	-	-	-		
15	SQD	L	401	-	52,54,54	0.98	5 (9%)	62,65,65	1.40	8 (12%)
13	UMQ	I	306	-	35,35,35	1.13	1 (2%)	46,46,46	0.99	1 (2%)
11	HEC	C	301	3	46,50,50	1.82	5 (10%)	58,82,82	2.03	4 (6%)
13	UMQ	J	403	-	35,35,35	1.17	3 (8%)	46,46,46	0.94	2 (4%)
13	UMQ	A	305	-	35,35,35	1.14	1 (2%)	46,46,46	0.86	0
10	HEM	I	302	1	50,50,50	1.40	6 (12%)	67,82,82	1.08	5 (7%)
13	UMQ	B	403	-	35,35,35	1.22	3 (8%)	46,46,46	1.42	7 (15%)
14	PL9	K	302	14	55,55,55	1.01	4 (7%)	68,69,69	1.50	11 (16%)
13	UMQ	H	201	-	35,35,35	1.12	1 (2%)	46,46,46	0.94	3 (6%)
13	UMQ	P	102	-	35,35,35	1.11	1 (2%)	46,46,46	1.08	3 (6%)
14	PL9	B	402	-	55,55,55	1.07	4 (7%)	68,69,69	1.51	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	304	-	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
12	CLA	I	304	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
14	PL9	B	401	14	55,55,55	1.01	4 (7%)	68,69,69	1.52	13 (19%)
11	HEC	A	303	1	46,50,50	1.82	5 (10%)	58,82,82	2.03	4 (6%)
11	HEC	I	303	1	46,50,50	1.82	5 (10%)	58,82,82	2.03	4 (6%)
10	HEM	A	301	1	50,50,50	1.40	8 (16%)	67,82,82	1.11	3 (4%)
11	HEC	K	301	3	46,50,50	1.83	5 (10%)	58,82,82	2.03	4 (6%)
14	PL9	J	402	-	55,55,55	1.04	4 (7%)	68,69,69	1.50	11 (16%)
13	UMQ	A	306	-	35,35,35	1.14	1 (2%)	46,46,46	0.97	3 (6%)
13	UMQ	J	404	-	35,35,35	1.22	3 (8%)	46,46,46	1.42	7 (15%)
10	HEM	A	302	1	50,50,50	1.40	6 (12%)	67,82,82	1.08	5 (7%)
13	UMQ	I	305	-	35,35,35	1.15	1 (2%)	46,46,46	0.97	3 (6%)
13	UMQ	B	404	-	35,35,35	1.13	1 (2%)	46,46,46	1.07	5 (10%)
16	FES	D	202	4	0,4,4	-	-	-	-	-
14	PL9	J	401	-	55,55,55	1.02	4 (7%)	68,69,69	1.52	12 (17%)
17	BCR	P	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.26	9 (16%)
17	BCR	F	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	7 (12%)
15	SQD	D	201	-	52,54,54	0.97	4 (7%)	62,65,65	1.48	8 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	I	301	1	-	3/14/54/54	-
14	PL9	A	307	-	-	18/53/73/73	0/1/1/1
16	FES	L	402	4	-	-	0/1/1/1
15	SQD	L	401	-	-	20/49/69/69	0/1/1/1
13	UMQ	I	306	-	-	12/20/60/60	0/2/2/2
11	HEC	C	301	3	-	6/14/54/54	-
13	UMQ	J	403	-	-	12/20/60/60	0/2/2/2
13	UMQ	A	305	-	-	7/20/60/60	0/2/2/2
10	HEM	I	302	1	-	2/14/54/54	-
13	UMQ	B	403	-	-	8/20/60/60	0/2/2/2
14	PL9	K	302	14	-	21/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	UMQ	H	201	-	-	5/20/60/60	0/2/2/2
13	UMQ	P	102	-	-	8/20/60/60	0/2/2/2
14	PL9	B	402	-	-	24/53/73/73	0/1/1/1
12	CLA	A	304	-	1/1/15/20	15/39/115/115	-
12	CLA	I	304	-	1/1/15/20	15/39/115/115	-
14	PL9	B	401	14	-	19/53/73/73	0/1/1/1
11	HEC	A	303	1	-	7/14/54/54	-
11	HEC	I	303	1	-	7/14/54/54	-
10	HEM	A	301	1	-	3/14/54/54	-
11	HEC	K	301	3	-	6/14/54/54	-
14	PL9	J	402	-	-	21/53/73/73	0/1/1/1
13	UMQ	A	306	-	-	9/20/60/60	0/2/2/2
13	UMQ	J	404	-	-	8/20/60/60	0/2/2/2
10	HEM	A	302	1	-	2/14/54/54	-
13	UMQ	I	305	-	-	9/20/60/60	0/2/2/2
13	UMQ	B	404	-	-	11/20/60/60	0/2/2/2
16	FES	D	202	4	-	-	0/1/1/1
14	PL9	J	401	-	-	20/53/73/73	0/1/1/1
17	BCR	P	101	-	-	2/29/63/63	0/2/2/2
17	BCR	F	101	-	-	4/29/63/63	0/2/2/2
15	SQD	D	201	-	-	15/49/69/69	0/1/1/1

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	303	HEC	CAC-C3C	6.10	1.54	1.35
11	K	301	HEC	CAB-C3B	6.10	1.54	1.35
11	C	301	HEC	CAB-C3B	6.10	1.54	1.35
11	I	303	HEC	CAB-C3B	6.08	1.54	1.35
11	A	303	HEC	CAC-C3C	6.08	1.54	1.35
11	C	301	HEC	CAC-C3C	6.07	1.54	1.35
11	K	301	HEC	CAC-C3C	6.06	1.54	1.35
11	A	303	HEC	CAB-C3B	6.05	1.54	1.35
11	K	301	HEC	C3D-C2D	5.67	1.53	1.38
11	C	301	HEC	C3D-C2D	5.64	1.53	1.38
11	I	303	HEC	C3D-C2D	5.64	1.53	1.38
11	A	303	HEC	C3D-C2D	5.63	1.53	1.38
17	F	101	BCR	C1-C6	-3.91	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	101	BCR	C30-C25	-3.66	1.49	1.53
17	F	101	BCR	C30-C25	-3.54	1.49	1.53
17	P	101	BCR	C1-C6	-3.51	1.49	1.53
12	A	304	CLA	C1D-ND	3.50	1.42	1.37
12	I	304	CLA	C1D-ND	3.50	1.42	1.37
10	A	302	HEM	FE-ND	3.30	2.05	1.94
10	I	302	HEM	FE-ND	3.30	2.05	1.94
10	A	301	HEM	FE-NB	3.22	2.04	1.94
10	I	301	HEM	FE-NB	3.21	2.04	1.94
10	A	302	HEM	FE-NB	3.19	2.04	1.94
10	I	302	HEM	FE-NB	3.18	2.04	1.94
10	A	301	HEM	FE-ND	3.16	2.04	1.94
10	I	301	HEM	FE-ND	3.13	2.04	1.94
15	D	201	SQD	O48-C23	3.10	1.42	1.33
15	L	401	SQD	O48-C23	3.09	1.42	1.33
10	A	302	HEM	FE-NA	3.00	2.05	1.95
10	I	302	HEM	FE-NA	3.00	2.05	1.95
10	A	302	HEM	FE-NC	3.00	2.05	1.95
12	A	304	CLA	C4B-NB	3.00	1.41	1.37
10	I	302	HEM	FE-NC	2.99	2.05	1.95
10	A	301	HEM	FE-NA	2.97	2.05	1.95
10	I	301	HEM	FE-NA	2.97	2.05	1.95
12	I	304	CLA	C4B-NB	2.97	1.41	1.37
14	B	402	PL9	C3-C4	-2.94	1.45	1.49
10	I	301	HEM	CAB-C3B	2.89	1.55	1.47
10	A	302	HEM	CAB-C3B	2.89	1.55	1.47
10	A	301	HEM	FE-NC	2.89	2.04	1.95
14	J	402	PL9	C3-C4	-2.89	1.45	1.49
10	A	301	HEM	CAB-C3B	2.89	1.55	1.47
10	I	301	HEM	FE-NC	2.88	2.04	1.95
10	I	302	HEM	CAB-C3B	2.87	1.55	1.47
10	A	302	HEM	CAC-C3C	2.87	1.55	1.47
10	A	301	HEM	CAC-C3C	2.87	1.55	1.47
10	I	301	HEM	CAC-C3C	2.85	1.55	1.47
10	I	302	HEM	CAC-C3C	2.85	1.55	1.47
15	D	201	SQD	O47-C7	2.83	1.42	1.34
15	L	401	SQD	O47-C7	2.81	1.42	1.34
14	B	401	PL9	C7-C3	-2.81	1.47	1.51
14	K	302	PL9	C3-C4	-2.77	1.45	1.49
14	A	307	PL9	C7-C3	-2.73	1.47	1.51
12	A	304	CLA	C1B-C2B	2.72	1.49	1.43
12	I	304	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	402	PL9	C7-C3	-2.68	1.47	1.51
13	B	403	UMQ	O5'-C5'	2.65	1.50	1.44
13	J	404	UMQ	O5'-C5'	2.65	1.50	1.44
14	A	307	PL9	C3-C4	-2.64	1.45	1.49
14	J	402	PL9	C7-C3	-2.63	1.47	1.51
14	J	401	PL9	C3-C4	-2.61	1.45	1.49
14	B	401	PL9	C3-C4	-2.61	1.45	1.49
14	K	302	PL9	C7-C3	-2.59	1.47	1.51
14	J	401	PL9	C7-C3	-2.56	1.47	1.51
13	B	403	UMQ	O5'-C1'	2.55	1.48	1.41
14	J	402	PL9	C6-C1	-2.53	1.44	1.48
13	J	404	UMQ	O5'-C1'	2.53	1.48	1.41
14	B	402	PL9	C6-C1	-2.29	1.44	1.48
13	I	305	UMQ	C3-C4	-2.28	1.46	1.52
14	J	401	PL9	C53-C6	-2.28	1.46	1.50
14	A	307	PL9	C6-C1	-2.27	1.44	1.48
11	I	303	HEC	C3B-C2B	-2.27	1.33	1.41
13	A	306	UMQ	C3-C4	-2.26	1.46	1.52
11	A	303	HEC	C3B-C2B	-2.25	1.33	1.41
12	A	304	CLA	CHC-C1C	2.23	1.43	1.38
12	A	304	CLA	C3B-C4B	2.22	1.49	1.42
11	I	303	HEC	C3C-C2C	-2.21	1.33	1.41
14	J	401	PL9	C6-C1	-2.21	1.44	1.48
12	I	304	CLA	C3B-C4B	2.21	1.49	1.42
11	K	301	HEC	C3B-C2B	-2.21	1.33	1.41
11	K	301	HEC	C3C-C2C	-2.20	1.33	1.41
13	A	305	UMQ	C3-C4	-2.20	1.46	1.52
11	A	303	HEC	C3C-C2C	-2.20	1.33	1.41
11	C	301	HEC	C3C-C2C	-2.20	1.33	1.41
11	C	301	HEC	C3B-C2B	-2.19	1.33	1.41
12	I	304	CLA	CHC-C1C	2.18	1.42	1.38
14	B	401	PL9	C6-C1	-2.17	1.45	1.48
15	D	201	SQD	O2-C2	-2.17	1.37	1.43
15	L	401	SQD	O2-C2	-2.16	1.37	1.43
14	J	402	PL9	C53-C6	-2.15	1.46	1.50
14	K	302	PL9	C6-C1	-2.15	1.45	1.48
14	K	302	PL9	C53-C6	-2.14	1.46	1.50
14	A	307	PL9	C53-C6	-2.13	1.46	1.50
13	J	403	UMQ	C3-C4	-2.12	1.46	1.52
13	J	403	UMQ	O5'-C1'	2.12	1.47	1.41
14	B	401	PL9	C53-C6	-2.10	1.46	1.50
13	H	201	UMQ	C3-C4	-2.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	304	CLA	CMD-C2D	-2.09	1.46	1.50
13	I	306	UMQ	C3-C4	-2.08	1.46	1.52
14	B	402	PL9	C53-C6	-2.07	1.46	1.50
12	I	304	CLA	MG-NB	-2.07	2.01	2.05
13	B	404	UMQ	O5'-C5'	2.07	1.49	1.44
12	I	304	CLA	CMD-C2D	-2.07	1.46	1.50
12	A	304	CLA	MG-NB	-2.05	2.01	2.05
13	J	404	UMQ	C3'-C4'	-2.05	1.46	1.52
13	B	403	UMQ	C3'-C4'	-2.05	1.46	1.52
12	I	304	CLA	CMB-C2B	-2.04	1.46	1.50
13	P	102	UMQ	C3-C4	-2.04	1.47	1.52
12	A	304	CLA	CMB-C2B	-2.03	1.46	1.50
13	J	403	UMQ	O5'-C5'	2.03	1.49	1.44
15	L	401	SQD	O4-C4	-2.03	1.37	1.43
15	D	201	SQD	O3-C3	-2.02	1.37	1.43
10	I	301	HEM	CMC-C2C	2.02	1.54	1.50
10	A	301	HEM	CMB-C2B	2.01	1.54	1.50
15	L	401	SQD	O3-C3	-2.01	1.38	1.43
10	A	301	HEM	CMC-C2C	2.00	1.54	1.50

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	301	HEC	CBC-CAC-C3C	-9.44	108.56	127.43
11	C	301	HEC	CBC-CAC-C3C	-9.43	108.58	127.43
11	A	303	HEC	CBB-CAB-C3B	-9.23	108.99	127.43
11	I	303	HEC	CBB-CAB-C3B	-9.22	109.00	127.43
11	C	301	HEC	CBB-CAB-C3B	-9.13	109.19	127.43
11	K	301	HEC	CBB-CAB-C3B	-9.11	109.23	127.43
11	I	303	HEC	CBC-CAC-C3C	-8.75	109.94	127.43
11	A	303	HEC	CBC-CAC-C3C	-8.74	109.96	127.43
12	A	304	CLA	C4A-NA-C1A	6.33	109.56	106.68
12	I	304	CLA	C4A-NA-C1A	6.27	109.54	106.68
14	J	401	PL9	C7-C3-C4	5.49	121.43	116.91
14	A	307	PL9	C7-C3-C4	5.44	121.39	116.91
14	B	401	PL9	C7-C3-C4	5.28	121.25	116.91
14	K	302	PL9	C7-C3-C4	5.20	121.19	116.91
14	J	402	PL9	C7-C3-C4	5.16	121.16	116.91
14	B	402	PL9	C7-C3-C4	4.92	120.96	116.91
15	D	201	SQD	O6-C1-C2	4.38	114.92	108.27
14	J	401	PL9	C7-C3-C2	-4.25	118.38	123.39
14	A	307	PL9	C7-C3-C2	-4.22	118.41	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	401	PL9	C7-C3-C2	-4.14	118.51	123.39
14	K	302	PL9	C7-C3-C2	-4.03	118.64	123.39
14	J	402	PL9	C7-C3-C2	-3.95	118.73	123.39
15	L	401	SQD	O9-S-O7	-3.91	101.09	113.82
13	P	102	UMQ	CA-O1'-C1'	-3.90	107.01	113.68
15	D	201	SQD	O9-S-O7	-3.90	101.16	113.82
14	B	402	PL9	C7-C3-C2	-3.82	118.89	123.39
15	D	201	SQD	O47-C7-C8	3.75	119.59	111.48
13	J	404	UMQ	O1-C1-C2	3.68	117.14	108.09
13	B	403	UMQ	O1-C1-C2	3.67	117.12	108.09
11	A	303	HEC	C4D-ND-C1D	3.53	111.58	105.82
11	I	303	HEC	C4D-ND-C1D	3.51	111.55	105.82
11	K	301	HEC	C4D-ND-C1D	3.50	111.52	105.82
11	C	301	HEC	C4D-ND-C1D	3.49	111.51	105.82
15	L	401	SQD	O6-C1-C2	3.47	113.55	108.27
15	D	201	SQD	O9-S-C6	3.37	111.78	106.76
15	L	401	SQD	O9-S-C6	3.35	111.75	106.76
13	J	403	UMQ	O1-C4'-C5'	3.30	118.13	109.48
15	L	401	SQD	O47-C7-C8	3.26	118.54	111.48
15	L	401	SQD	O7-S-C6	3.14	111.45	106.76
15	D	201	SQD	O7-S-C6	3.14	111.45	106.76
13	J	404	UMQ	C1'-O5'-C5'	3.13	119.83	113.72
13	B	403	UMQ	C1'-O5'-C5'	3.12	119.81	113.72
13	I	305	UMQ	C1-O1-C4'	-3.09	110.66	117.98
13	A	306	UMQ	C1-O1-C4'	-3.05	110.74	117.98
13	B	403	UMQ	O5-C1-C2	3.04	116.61	110.37
13	J	404	UMQ	O5-C1-C2	3.02	116.58	110.37
14	A	307	PL9	C40-C39-C41	2.98	120.40	115.23
12	A	304	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
12	I	304	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	K	302	PL9	C40-C39-C41	2.93	120.31	115.23
13	B	403	UMQ	C1-C2-C3	2.86	116.04	110.01
13	J	404	UMQ	C1-C2-C3	2.86	116.03	110.01
14	B	402	PL9	C27-C28-C29	-2.85	121.09	127.62
12	I	304	CLA	C3B-C4B-NB	-2.84	108.00	110.53
14	B	402	PL9	C22-C23-C24	-2.83	121.15	127.62
12	A	304	CLA	C3B-C4B-NB	-2.82	108.02	110.53
14	J	402	PL9	C22-C23-C24	-2.80	121.22	127.62
14	J	402	PL9	C40-C39-C41	2.80	120.08	115.23
14	J	402	PL9	C27-C28-C29	-2.79	121.25	127.62
15	D	201	SQD	O5-C5-C4	2.78	114.72	109.70
17	P	101	BCR	C2-C1-C6	2.78	114.47	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	401	PL9	C27-C28-C29	-2.76	121.30	127.62
13	P	102	UMQ	O1'-C1'-C2'	2.76	112.46	108.27
17	F	101	BCR	C33-C5-C6	-2.76	121.48	124.48
14	B	401	PL9	C22-C23-C24	-2.73	121.37	127.62
17	P	101	BCR	C27-C26-C25	2.72	126.39	122.70
13	B	404	UMQ	C1-O1-C4'	-2.72	111.54	117.98
17	F	101	BCR	C27-C26-C25	2.70	126.36	122.70
17	P	101	BCR	C15-C16-C17	-2.69	118.02	123.52
14	B	401	PL9	C7-C8-C9	-2.68	122.21	126.83
15	L	401	SQD	O5-C5-C4	2.68	114.53	109.70
13	B	403	UMQ	C4-C3-C2	2.67	115.51	110.83
13	J	404	UMQ	C4-C3-C2	2.66	115.50	110.83
13	P	102	UMQ	C1'-O5'-C5'	-2.66	108.53	113.72
13	H	201	UMQ	CA-O1'-C1'	-2.65	109.14	113.68
14	K	302	PL9	C22-C23-C24	-2.65	121.56	127.62
17	F	101	BCR	C15-C16-C17	-2.64	118.11	123.52
14	B	401	PL9	C27-C28-C29	-2.63	121.60	127.62
14	J	401	PL9	C40-C39-C41	2.58	119.71	115.23
14	K	302	PL9	C7-C8-C9	-2.54	122.46	126.83
14	K	302	PL9	C27-C28-C29	-2.52	121.85	127.62
14	A	307	PL9	C27-C28-C29	-2.52	121.86	127.62
11	A	303	HEC	C2A-C1A-NA	-2.51	107.90	110.32
14	A	307	PL9	C22-C23-C24	-2.51	121.88	127.62
14	J	401	PL9	C22-C23-C24	-2.50	121.90	127.62
11	I	303	HEC	C2A-C1A-NA	-2.49	107.92	110.32
14	J	402	PL9	C20-C19-C21	2.46	119.50	115.23
14	J	402	PL9	C7-C8-C9	-2.45	122.62	126.83
14	B	402	PL9	C7-C8-C9	-2.44	122.62	126.83
15	D	201	SQD	O48-C23-C24	2.44	119.28	111.83
14	A	307	PL9	C7-C8-C9	-2.43	122.65	126.83
14	J	401	PL9	C20-C19-C21	2.42	119.43	115.23
17	P	101	BCR	C33-C5-C6	-2.40	121.87	124.48
13	H	201	UMQ	O1'-C1'-C2'	2.40	111.91	108.27
10	I	302	HEM	C4D-ND-C1D	2.39	108.04	105.21
14	J	401	PL9	C7-C8-C9	-2.39	122.71	126.83
14	K	302	PL9	O2-C1-C6	2.39	124.28	120.48
14	B	401	PL9	O2-C1-C6	2.38	124.27	120.48
10	A	301	HEM	C4D-ND-C1D	2.38	108.02	105.21
14	J	401	PL9	O2-C1-C6	2.36	124.24	120.48
14	A	307	PL9	O2-C1-C6	2.36	124.23	120.48
10	A	302	HEM	C4D-ND-C1D	2.35	107.99	105.21
14	B	402	PL9	O2-C1-C6	2.35	124.21	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	402	PL9	C32-C33-C34	-2.34	122.27	127.62
10	I	301	HEM	C4D-ND-C1D	2.34	107.97	105.21
12	A	304	CLA	C1-C2-C3	-2.33	122.38	126.20
10	A	301	HEM	C1B-NB-C4B	2.32	107.95	105.21
17	P	101	BCR	C15-C14-C13	-2.31	124.03	127.28
17	P	101	BCR	C7-C8-C9	-2.31	122.81	126.23
10	I	301	HEM	C1B-NB-C4B	2.31	107.94	105.21
12	I	304	CLA	C1-C2-C3	-2.30	122.42	126.20
17	F	101	BCR	C15-C14-C13	-2.30	124.05	127.28
14	B	401	PL9	C40-C39-C41	2.29	119.20	115.23
14	B	402	PL9	C37-C38-C39	-2.29	122.39	127.62
12	I	304	CLA	CHB-C4A-NA	2.29	127.70	124.40
12	A	304	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	J	402	PL9	O2-C1-C6	2.28	124.11	120.48
13	J	404	UMQ	C3-C4-C5	2.28	114.36	110.23
17	F	101	BCR	C38-C26-C25	-2.28	122.00	124.48
10	A	301	HEM	C3B-C2B-C1B	2.28	108.12	106.41
14	B	402	PL9	O1-C4-C3	-2.27	118.33	120.73
15	L	401	SQD	O8-S-C6	2.26	110.34	105.97
14	B	401	PL9	C20-C19-C21	2.26	119.16	115.23
13	B	404	UMQ	O5'-C5'-C4'	2.26	114.40	109.72
14	K	302	PL9	C37-C38-C39	-2.26	122.45	127.62
17	P	101	BCR	C24-C23-C22	-2.26	122.89	126.23
10	A	302	HEM	C1B-NB-C4B	2.26	107.88	105.21
10	I	302	HEM	C1B-NB-C4B	2.25	107.88	105.21
14	B	401	PL9	C37-C38-C39	-2.25	122.46	127.62
15	L	401	SQD	O48-C23-C24	2.25	118.69	111.83
13	B	404	UMQ	C3'-C4'-C5'	2.25	115.91	110.93
14	A	307	PL9	C37-C38-C39	-2.25	122.48	127.62
13	B	403	UMQ	C3-C4-C5	2.25	114.30	110.23
11	K	301	HEC	C2A-C1A-NA	-2.24	108.16	110.32
15	D	201	SQD	O8-S-C6	2.24	110.30	105.97
11	C	301	HEC	C2A-C1A-NA	-2.24	108.17	110.32
17	P	101	BCR	C3-C4-C5	-2.24	110.07	114.06
14	K	302	PL9	O1-C4-C3	-2.22	118.39	120.73
17	F	101	BCR	C7-C8-C9	-2.22	122.95	126.23
10	I	301	HEM	C3B-C2B-C1B	2.21	108.07	106.41
14	J	402	PL9	O1-C4-C3	-2.21	118.40	120.73
14	J	402	PL9	C32-C33-C34	-2.20	122.59	127.62
17	P	101	BCR	C38-C26-C25	-2.19	122.09	124.48
13	A	306	UMQ	CA-O1'-C1'	-2.19	109.94	113.68
13	I	305	UMQ	CA-O1'-C1'	-2.19	109.94	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	I	302	HEM	C2A-C1A-NA	-2.18	107.73	110.15
13	B	403	UMQ	O5'-C5'-C4'	2.18	114.24	109.72
13	J	404	UMQ	O5'-C5'-C4'	2.18	114.24	109.72
14	J	401	PL9	C12-C13-C14	-2.18	122.63	127.62
14	B	401	PL9	O1-C4-C3	-2.17	118.44	120.73
14	B	402	PL9	C40-C39-C41	2.15	118.97	115.23
10	A	302	HEM	C2A-C1A-NA	-2.15	107.77	110.15
14	A	307	PL9	O2-C1-C2	-2.15	116.94	121.83
14	B	401	PL9	O2-C1-C2	-2.15	116.94	121.83
12	I	304	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
10	I	302	HEM	C3D-C4D-ND	-2.15	107.82	110.17
13	I	305	UMQ	O1'-C1'-C2'	2.14	111.53	108.27
12	A	304	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
10	I	302	HEM	C3B-C2B-C1B	2.14	108.02	106.41
13	A	306	UMQ	O1'-C1'-C2'	2.14	111.52	108.27
17	F	101	BCR	C24-C23-C22	-2.14	123.08	126.23
13	J	403	UMQ	O5'-C1'-C2'	2.13	114.74	110.37
14	B	402	PL9	C20-C19-C21	2.13	118.92	115.23
14	K	302	PL9	O2-C1-C2	-2.13	117.00	121.83
14	B	402	PL9	C42-C43-C44	-2.12	122.78	127.62
14	J	401	PL9	C37-C38-C39	-2.11	122.79	127.62
10	A	302	HEM	C3D-C4D-ND	-2.10	107.87	110.17
14	A	307	PL9	O1-C4-C3	-2.10	118.52	120.73
14	B	402	PL9	O2-C1-C2	-2.10	117.06	121.83
14	J	401	PL9	O2-C1-C2	-2.09	117.08	121.83
10	A	302	HEM	C3B-C2B-C1B	2.09	107.98	106.41
13	B	404	UMQ	O5-C5-C4	2.08	113.45	109.70
13	H	201	UMQ	C1'-O5'-C5'	-2.08	109.66	113.72
14	A	307	PL9	C32-C33-C34	-2.06	122.91	127.62
14	B	401	PL9	C42-C43-C44	-2.05	122.92	127.62
14	J	402	PL9	O2-C1-C2	-2.05	117.16	121.83
14	K	302	PL9	C12-C13-C14	-2.05	122.93	127.62
13	I	306	UMQ	C2'-C3'-C4'	2.05	114.33	109.68
14	B	401	PL9	C12-C13-C14	-2.04	122.95	127.62
14	B	402	PL9	C12-C13-C14	-2.03	122.97	127.62
13	B	404	UMQ	C6'-C5'-C4'	-2.02	107.69	113.38
14	J	401	PL9	O1-C4-C3	-2.01	118.61	120.73

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	304	CLA	ND

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Mol	Chain	Res	Type	Atom
12	I	304	CLA	ND

All (319) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	302	HEM	C1A-C2A-CAA-CBA
10	I	302	HEM	C1A-C2A-CAA-CBA
11	A	303	HEC	C2B-C3B-CAB-CBB
11	A	303	HEC	C4B-C3B-CAB-CBB
11	A	303	HEC	C2C-C3C-CAC-CBC
11	A	303	HEC	C4C-C3C-CAC-CBC
11	C	301	HEC	C2B-C3B-CAB-CBB
11	C	301	HEC	C4B-C3B-CAB-CBB
11	C	301	HEC	C2C-C3C-CAC-CBC
11	C	301	HEC	C4C-C3C-CAC-CBC
11	I	303	HEC	C2B-C3B-CAB-CBB
11	I	303	HEC	C4B-C3B-CAB-CBB
11	I	303	HEC	C2C-C3C-CAC-CBC
11	I	303	HEC	C4C-C3C-CAC-CBC
11	K	301	HEC	C2B-C3B-CAB-CBB
11	K	301	HEC	C4B-C3B-CAB-CBB
11	K	301	HEC	C2C-C3C-CAC-CBC
11	K	301	HEC	C4C-C3C-CAC-CBC
12	A	304	CLA	C1A-C2A-CAA-CBA
12	A	304	CLA	C3A-C2A-CAA-CBA
12	I	304	CLA	C1A-C2A-CAA-CBA
12	I	304	CLA	C3A-C2A-CAA-CBA
13	B	403	UMQ	O5'-C1'-O1'-CA
13	J	403	UMQ	C5'-C4'-O1-C1
13	J	404	UMQ	O5'-C1'-O1'-CA
14	A	307	PL9	C12-C13-C14-C16
14	A	307	PL9	C13-C14-C16-C17
14	A	307	PL9	C27-C28-C29-C30
14	A	307	PL9	C27-C28-C29-C31
14	A	307	PL9	C47-C48-C49-C51
14	B	401	PL9	C22-C23-C24-C26
14	B	401	PL9	C37-C38-C39-C41
14	B	401	PL9	C40-C39-C41-C42
14	B	401	PL9	C45-C44-C46-C47
14	B	402	PL9	C7-C8-C9-C11
14	B	402	PL9	C25-C24-C26-C27
14	B	402	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
14	B	402	PL9	C37-C38-C39-C41
14	B	402	PL9	C42-C43-C44-C46
14	J	401	PL9	C4-C3-C7-C8
14	J	401	PL9	C14-C16-C17-C18
14	J	401	PL9	C22-C23-C24-C25
14	J	401	PL9	C22-C23-C24-C26
14	J	402	PL9	C22-C23-C24-C26
14	J	402	PL9	C27-C28-C29-C31
14	J	402	PL9	C38-C39-C41-C42
14	K	302	PL9	C32-C33-C34-C35
14	K	302	PL9	C32-C33-C34-C36
14	K	302	PL9	C42-C43-C44-C45
14	K	302	PL9	C42-C43-C44-C46
15	D	201	SQD	O6-C44-C45-O47
15	L	401	SQD	O49-C7-O47-C45
15	L	401	SQD	C8-C7-O47-C45
13	B	403	UMQ	C2-C1-O1-C4'
13	J	404	UMQ	C2-C1-O1-C4'
13	B	403	UMQ	O5-C1-O1-C4'
13	J	404	UMQ	O5-C1-O1-C4'
14	A	307	PL9	C47-C48-C49-C50
12	A	304	CLA	O1A-CGA-O2A-C1
12	I	304	CLA	O1A-CGA-O2A-C1
12	A	304	CLA	CBA-CGA-O2A-C1
12	I	304	CLA	CBA-CGA-O2A-C1
14	A	307	PL9	C30-C29-C31-C32
14	B	402	PL9	C45-C44-C46-C47
14	J	401	PL9	C15-C14-C16-C17
14	J	401	PL9	C40-C39-C41-C42
14	K	302	PL9	C12-C11-C9-C10
14	B	401	PL9	C43-C44-C46-C47
14	J	402	PL9	C33-C34-C36-C37
14	B	402	PL9	C42-C43-C44-C45
14	K	302	PL9	C27-C28-C29-C30
14	B	402	PL9	C12-C13-C14-C16
14	K	302	PL9	C27-C28-C29-C31
13	J	403	UMQ	O5-C5-C6-O6
14	J	402	PL9	C20-C19-C21-C22
14	J	402	PL9	C35-C34-C36-C37
14	K	302	PL9	C40-C39-C41-C42
14	J	401	PL9	C28-C29-C31-C32
14	J	401	PL9	C38-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
14	J	402	PL9	C18-C19-C21-C22
14	K	302	PL9	C38-C39-C41-C42
13	A	306	UMQ	O5-C5-C6-O6
13	I	305	UMQ	O5-C5-C6-O6
14	A	307	PL9	C14-C16-C17-C18
14	A	307	PL9	C34-C36-C37-C38
14	B	401	PL9	C24-C26-C27-C28
14	B	401	PL9	C34-C36-C37-C38
14	B	402	PL9	C19-C21-C22-C23
14	B	402	PL9	C24-C26-C27-C28
14	B	402	PL9	C29-C31-C32-C33
14	J	401	PL9	C24-C26-C27-C28
14	J	401	PL9	C39-C41-C42-C43
14	J	402	PL9	C9-C11-C12-C13
14	J	402	PL9	C24-C26-C27-C28
14	K	302	PL9	C44-C46-C47-C48
13	J	403	UMQ	C4-C5-C6-O6
14	A	307	PL9	C12-C13-C14-C15
13	J	403	UMQ	O5'-C5'-C6'-O6'
14	B	402	PL9	C17-C18-C19-C21
14	J	401	PL9	C7-C8-C9-C11
14	J	401	PL9	C47-C48-C49-C51
15	D	201	SQD	C10-C11-C12-C13
14	A	307	PL9	C15-C14-C16-C17
14	J	401	PL9	C30-C29-C31-C32
14	B	402	PL9	C43-C44-C46-C47
14	K	302	PL9	C12-C11-C9-C8
14	J	401	PL9	C2-C3-C7-C8
13	J	403	UMQ	C4'-C5'-C6'-O6'
15	D	201	SQD	O10-C23-O48-C46
15	D	201	SQD	O47-C45-C46-O48
15	D	201	SQD	C24-C23-O48-C46
13	A	306	UMQ	C4-C5-C6-O6
13	I	305	UMQ	C4-C5-C6-O6
14	J	401	PL9	C27-C28-C29-C30
12	A	304	CLA	C13-C15-C16-C17
12	I	304	CLA	C13-C15-C16-C17
14	B	401	PL9	C29-C31-C32-C33
14	J	401	PL9	C9-C11-C12-C13
14	J	401	PL9	C34-C36-C37-C38
14	J	402	PL9	C44-C46-C47-C48
14	K	302	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
15	D	201	SQD	C23-C24-C25-C26
13	I	306	UMQ	O1'-CA-CB-CC
13	A	306	UMQ	O5'-C1'-O1'-CA
13	I	305	UMQ	O5'-C1'-O1'-CA
15	D	201	SQD	C11-C10-C9-C8
14	K	302	PL9	C20-C19-C21-C22
14	B	401	PL9	C37-C38-C39-C40
14	A	307	PL9	C44-C46-C47-C48
10	A	301	HEM	C2A-CAA-CBA-CGA
10	I	301	HEM	C2A-CAA-CBA-CGA
10	A	302	HEM	C3A-C2A-CAA-CBA
10	I	302	HEM	C3A-C2A-CAA-CBA
13	B	403	UMQ	CB-CC-CD-CF
13	I	306	UMQ	CC-CD-CF-CG
13	J	404	UMQ	CB-CC-CD-CF
13	I	306	UMQ	CD-CF-CG-CH
13	P	102	UMQ	CB-CC-CD-CF
13	B	403	UMQ	CB-CA-O1'-C1'
13	J	404	UMQ	CB-CA-O1'-C1'
15	L	401	SQD	C28-C29-C30-C31
13	B	404	UMQ	CH-CI-CJ-CK
12	A	304	CLA	C15-C16-C17-C18
12	I	304	CLA	C15-C16-C17-C18
15	L	401	SQD	C27-C28-C29-C30
14	B	402	PL9	C4-C3-C7-C8
14	K	302	PL9	C15-C14-C16-C17
14	K	302	PL9	C12-C13-C14-C16
14	A	307	PL9	C28-C29-C31-C32
15	L	401	SQD	C31-C32-C33-C34
13	A	306	UMQ	CC-CD-CF-CG
13	I	305	UMQ	CC-CD-CF-CG
13	I	306	UMQ	O5-C5-C6-O6
15	D	201	SQD	C24-C25-C26-C27
11	A	303	HEC	C1A-C2A-CAA-CBA
11	I	303	HEC	C1A-C2A-CAA-CBA
12	A	304	CLA	C2A-CAA-CBA-CGA
12	I	304	CLA	C2A-CAA-CBA-CGA
15	L	401	SQD	C10-C11-C12-C13
14	B	402	PL9	C34-C36-C37-C38
14	K	302	PL9	C47-C48-C49-C50
13	B	404	UMQ	O5'-C5'-C6'-O6'
13	P	102	UMQ	CC-CD-CF-CG

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Mol	Chain	Res	Type	Atoms
13	A	305	UMQ	O5-C5-C6-O6
13	P	102	UMQ	CA-CB-CC-CD
13	I	306	UMQ	CH-CI-CJ-CK
13	H	201	UMQ	CA-CB-CC-CD
13	J	403	UMQ	CH-CI-CJ-CK
13	B	403	UMQ	CC-CD-CF-CG
13	J	404	UMQ	CC-CD-CF-CG
14	B	401	PL9	C42-C43-C44-C46
14	J	402	PL9	C47-C48-C49-C51
13	I	306	UMQ	O5'-C5'-C6'-O6'
14	B	402	PL9	C7-C8-C9-C10
14	B	402	PL9	C12-C13-C14-C15
13	B	403	UMQ	C2'-C1'-O1'-CA
13	J	404	UMQ	C2'-C1'-O1'-CA
13	B	404	UMQ	CD-CF-CG-CH
13	H	201	UMQ	CF-CG-CH-CI
13	I	306	UMQ	CF-CG-CH-CI
13	B	403	UMQ	O5'-C5'-C6'-O6'
13	J	404	UMQ	O5'-C5'-C6'-O6'
13	A	305	UMQ	O1'-CA-CB-CC
13	P	102	UMQ	C4-C5-C6-O6
15	D	201	SQD	C11-C12-C13-C14
14	J	402	PL9	C25-C24-C26-C27
15	L	401	SQD	C24-C25-C26-C27
14	J	402	PL9	C42-C43-C44-C45
15	D	201	SQD	C12-C13-C14-C15
13	I	306	UMQ	CB-CA-O1'-C1'
13	P	102	UMQ	CG-CH-CI-CJ
11	A	303	HEC	C3A-C2A-CAA-CBA
11	I	303	HEC	C3A-C2A-CAA-CBA
13	A	305	UMQ	CF-CG-CH-CI
13	A	306	UMQ	CH-CI-CJ-CK
13	I	305	UMQ	CH-CI-CJ-CK
14	A	307	PL9	C24-C26-C27-C28
14	K	302	PL9	C29-C31-C32-C33
15	D	201	SQD	O6-C44-C45-C46
15	D	201	SQD	C44-C45-C46-O48
15	L	401	SQD	C44-C45-C46-O48
13	H	201	UMQ	CH-CI-CJ-CK
13	I	305	UMQ	CB-CC-CD-CF
13	A	306	UMQ	CB-CC-CD-CF
13	I	306	UMQ	C2-C1-O1-C4'

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Mol	Chain	Res	Type	Atoms
14	J	402	PL9	C12-C13-C14-C15
17	F	101	BCR	C23-C24-C25-C30
15	L	401	SQD	C29-C30-C31-C32
13	I	305	UMQ	CG-CH-CI-CJ
13	A	306	UMQ	CG-CH-CI-CJ
14	J	402	PL9	C4-C3-C7-C8
15	L	401	SQD	C19-C20-C21-C22
13	I	306	UMQ	O5-C1-O1-C4'
13	I	306	UMQ	CB-CC-CD-CF
15	D	201	SQD	C13-C14-C15-C16
14	A	307	PL9	C9-C11-C12-C13
14	B	402	PL9	C32-C33-C34-C36
12	A	304	CLA	C11-C12-C13-C15
12	I	304	CLA	C11-C12-C13-C15
13	J	403	UMQ	CD-CF-CG-CH
14	A	307	PL9	C43-C44-C46-C47
13	J	403	UMQ	O1'-CA-CB-CC
12	A	304	CLA	C4-C3-C5-C6
12	I	304	CLA	C4-C3-C5-C6
14	B	401	PL9	C47-C48-C49-C50
13	H	201	UMQ	C4-C5-C6-O6
15	L	401	SQD	O47-C45-C46-O48
13	A	305	UMQ	CH-CI-CJ-CK
11	A	303	HEC	C3D-CAD-CBD-CGD
11	I	303	HEC	C3D-CAD-CBD-CGD
13	B	404	UMQ	CF-CG-CH-CI
13	B	404	UMQ	C3'-C4'-O1-C1
13	A	305	UMQ	CB-CC-CD-CF
13	I	306	UMQ	CG-CH-CI-CJ
14	A	307	PL9	C25-C24-C26-C27
13	P	102	UMQ	CD-CF-CG-CH
12	A	304	CLA	C11-C12-C13-C14
12	I	304	CLA	C11-C12-C13-C14
13	P	102	UMQ	O5-C5-C6-O6
13	J	403	UMQ	CC-CD-CF-CG
12	A	304	CLA	C2-C3-C5-C6
12	I	304	CLA	C2-C3-C5-C6
14	J	401	PL9	C13-C14-C16-C17
14	J	401	PL9	C43-C44-C46-C47
15	L	401	SQD	C14-C15-C16-C17
14	J	401	PL9	C37-C38-C39-C41
14	B	402	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
15	D	201	SQD	C33-C34-C35-C36
14	B	401	PL9	C15-C14-C16-C17
14	J	402	PL9	C12-C11-C9-C10
14	K	302	PL9	C25-C24-C26-C27
13	A	305	UMQ	CB-CA-O1'-C1'
12	A	304	CLA	C11-C10-C8-C9
12	I	304	CLA	C11-C10-C8-C9
14	B	402	PL9	C12-C11-C9-C10
17	F	101	BCR	C11-C10-C9-C34
17	P	101	BCR	C11-C10-C9-C34
14	J	402	PL9	C2-C3-C7-C8
14	K	302	PL9	C24-C26-C27-C28
14	B	401	PL9	C47-C48-C49-C51
15	L	401	SQD	C18-C19-C20-C21
13	I	305	UMQ	CD-CF-CG-CH
13	A	306	UMQ	CD-CF-CG-CH
17	F	101	BCR	C11-C10-C9-C8
17	P	101	BCR	C11-C10-C9-C8
17	F	101	BCR	C23-C24-C25-C26
13	J	403	UMQ	CG-CH-CI-CJ
14	J	402	PL9	C19-C21-C22-C23
14	J	402	PL9	C34-C36-C37-C38
13	B	404	UMQ	C5'-C4'-O1-C1
14	A	307	PL9	C4-C3-C7-C8
14	B	401	PL9	C12-C13-C14-C15
13	A	305	UMQ	CC-CD-CF-CG
14	B	402	PL9	C40-C39-C41-C42
14	J	402	PL9	C7-C8-C9-C11
14	B	402	PL9	C23-C24-C26-C27
12	A	304	CLA	C2-C1-O2A-CGA
12	I	304	CLA	C2-C1-O2A-CGA
14	B	401	PL9	C30-C29-C31-C32
13	P	102	UMQ	CF-CG-CH-CI
15	L	401	SQD	C2-C1-O6-C44
14	B	401	PL9	C20-C19-C21-C22
14	J	402	PL9	C40-C39-C41-C42
13	I	305	UMQ	CI-CJ-CK-CL
14	K	302	PL9	C7-C8-C9-C11
13	A	306	UMQ	CI-CJ-CK-CL
15	L	401	SQD	C33-C34-C35-C36
14	B	401	PL9	C13-C14-C16-C17
14	B	402	PL9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
13	H	201	UMQ	O5-C5-C6-O6
13	B	404	UMQ	O5-C1-O1-C4'
15	L	401	SQD	C11-C12-C13-C14
11	C	301	HEC	CAA-CBA-CGA-O2A
15	L	401	SQD	O6-C44-C45-O47
11	K	301	HEC	CAA-CBA-CGA-O2A
15	L	401	SQD	C34-C35-C36-C37
14	B	401	PL9	C39-C41-C42-C43
13	B	404	UMQ	C2-C1-O1-C4'
14	B	401	PL9	C4-C3-C7-C8
12	A	304	CLA	CAA-CBA-CGA-O2A
12	I	304	CLA	CAA-CBA-CGA-O2A
15	D	201	SQD	C9-C10-C11-C12
14	B	402	PL9	C28-C29-C31-C32
15	L	401	SQD	C11-C10-C9-C8
10	A	301	HEM	CAD-CBD-CGD-O2D
10	I	301	HEM	CAD-CBD-CGD-O2D
11	C	301	HEC	CAA-CBA-CGA-O1A
11	K	301	HEC	CAA-CBA-CGA-O1A
13	B	404	UMQ	CG-CH-CI-CJ
13	J	403	UMQ	CA-CB-CC-CD
13	B	404	UMQ	O5-C5-C6-O6
14	K	302	PL9	C35-C34-C36-C37
12	A	304	CLA	CAA-CBA-CGA-O1A
12	I	304	CLA	CAA-CBA-CGA-O1A
10	I	301	HEM	CAD-CBD-CGD-O1D
10	A	301	HEM	CAD-CBD-CGD-O1D
15	L	401	SQD	C32-C33-C34-C35
13	J	403	UMQ	O5-C1-O1-C4'
13	B	404	UMQ	CB-CC-CD-CF

There are no ring outliers.

28 monomers are involved in 118 short contacts:

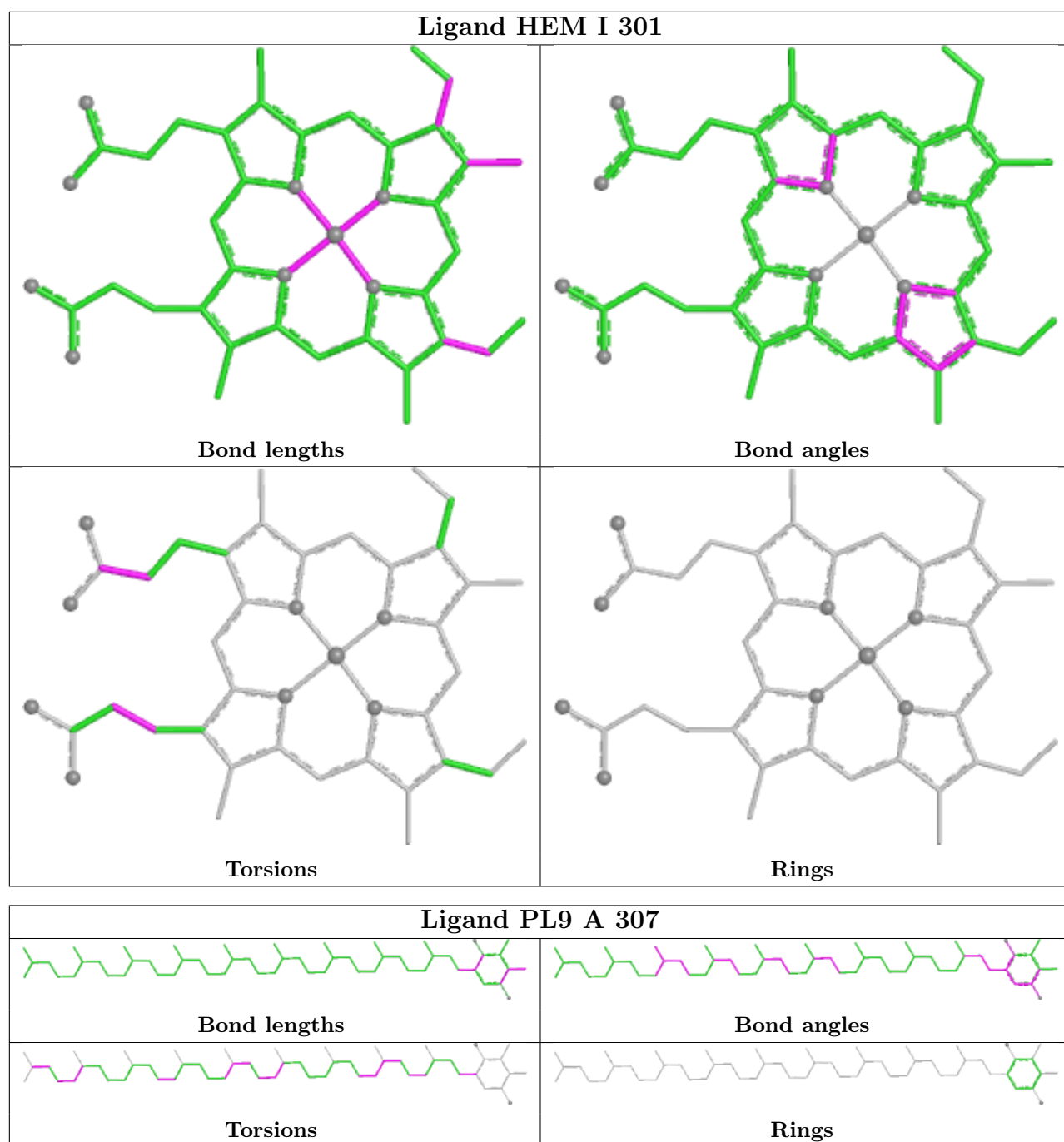
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	301	HEM	4	0
14	A	307	PL9	10	0
15	L	401	SQD	1	0
13	I	306	UMQ	1	0
11	C	301	HEC	5	0
13	J	403	UMQ	2	0
10	I	302	HEM	6	0

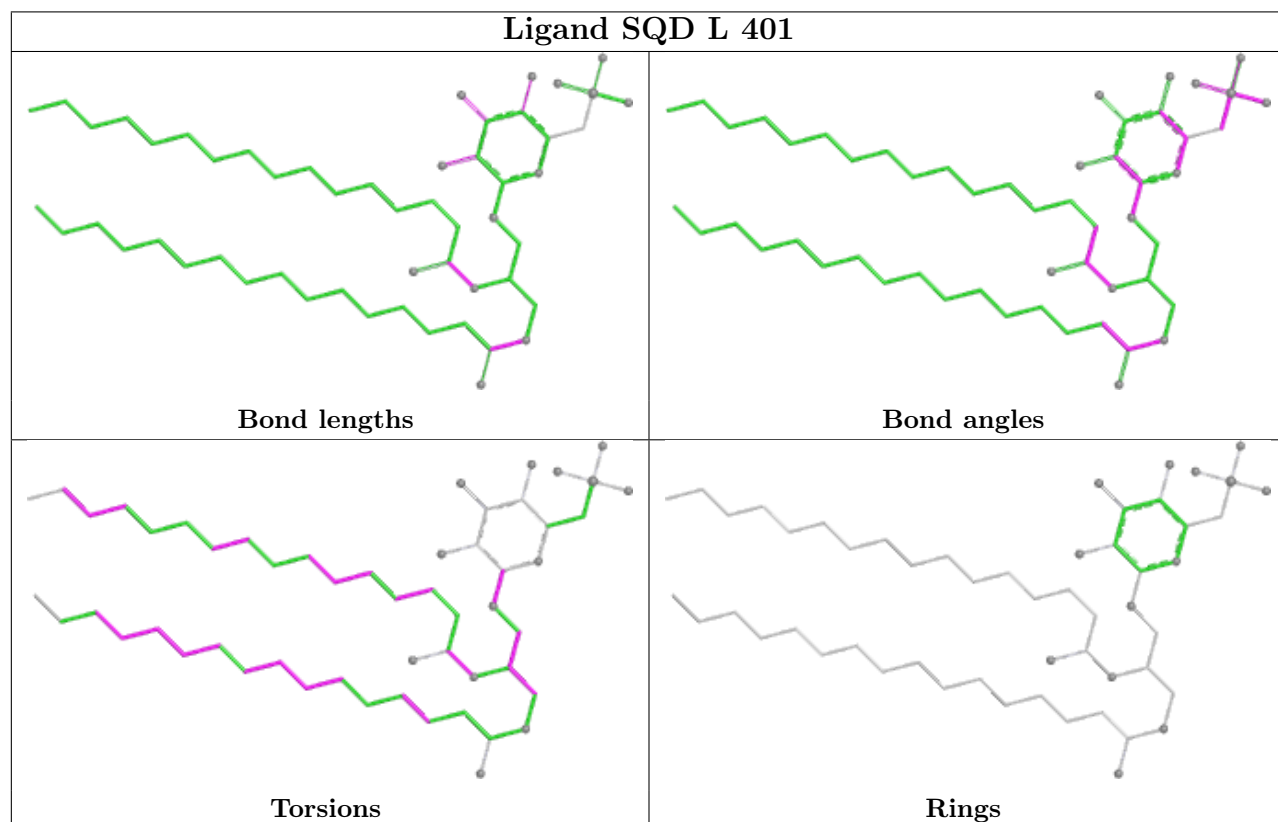
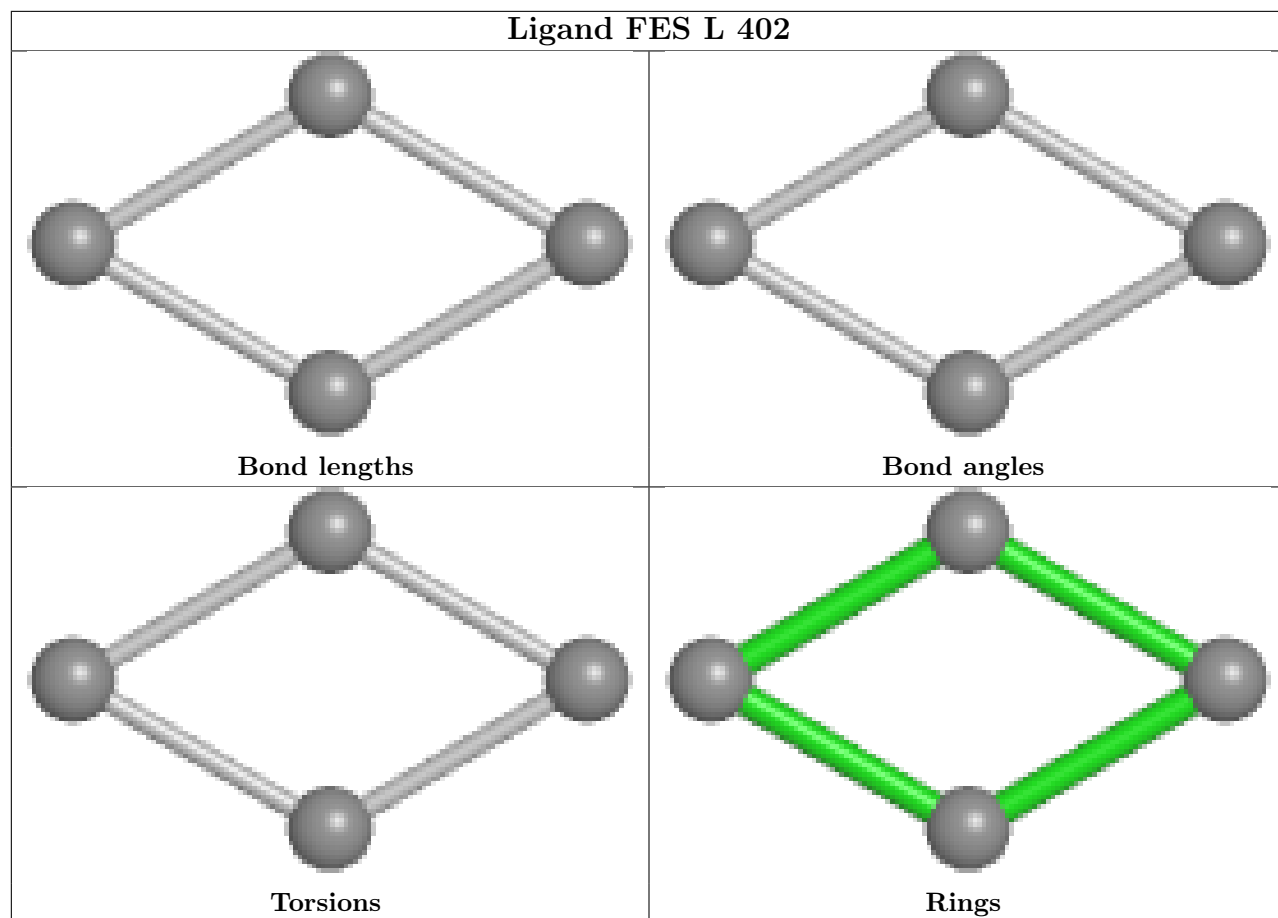
Continued on next page...

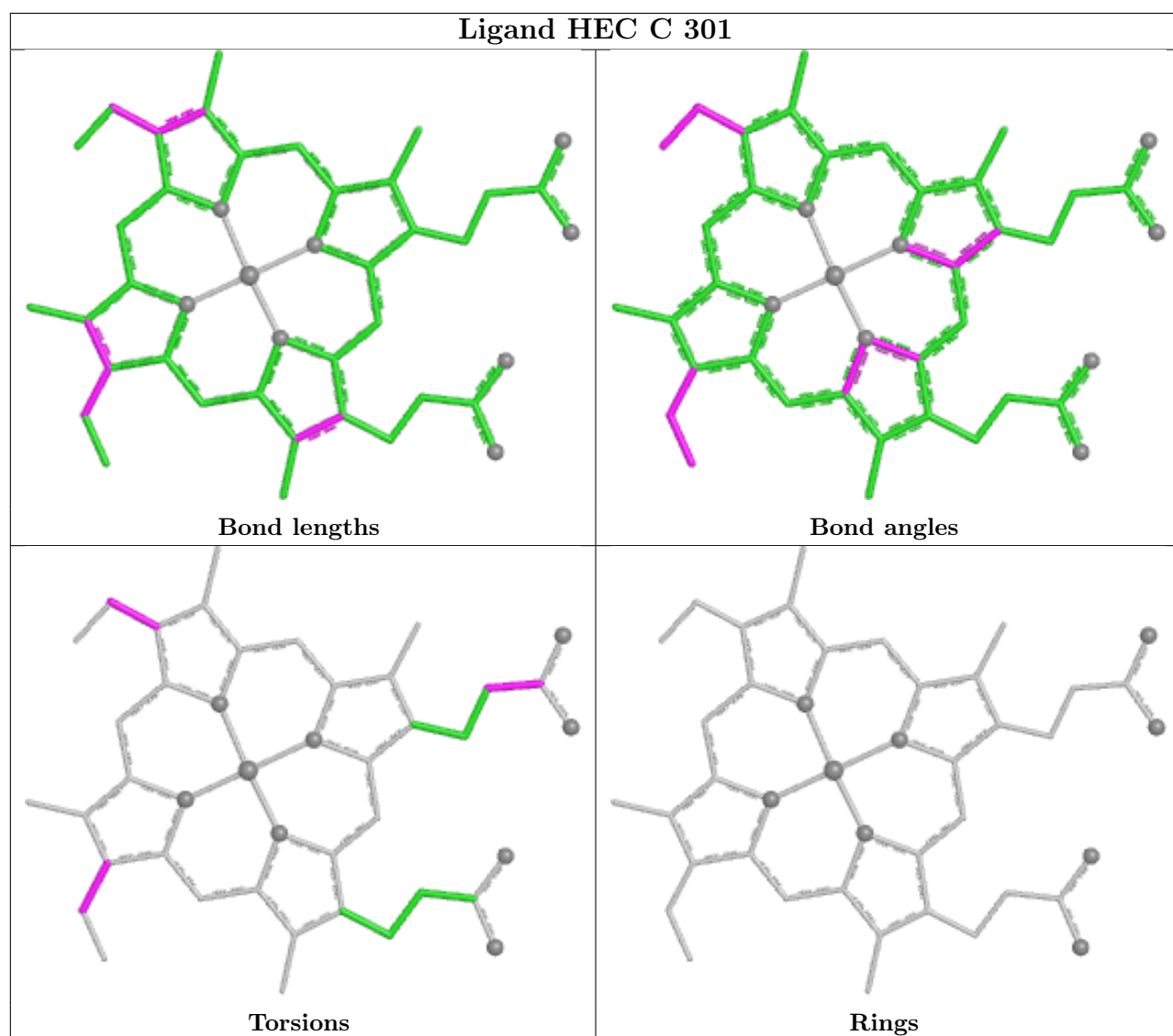
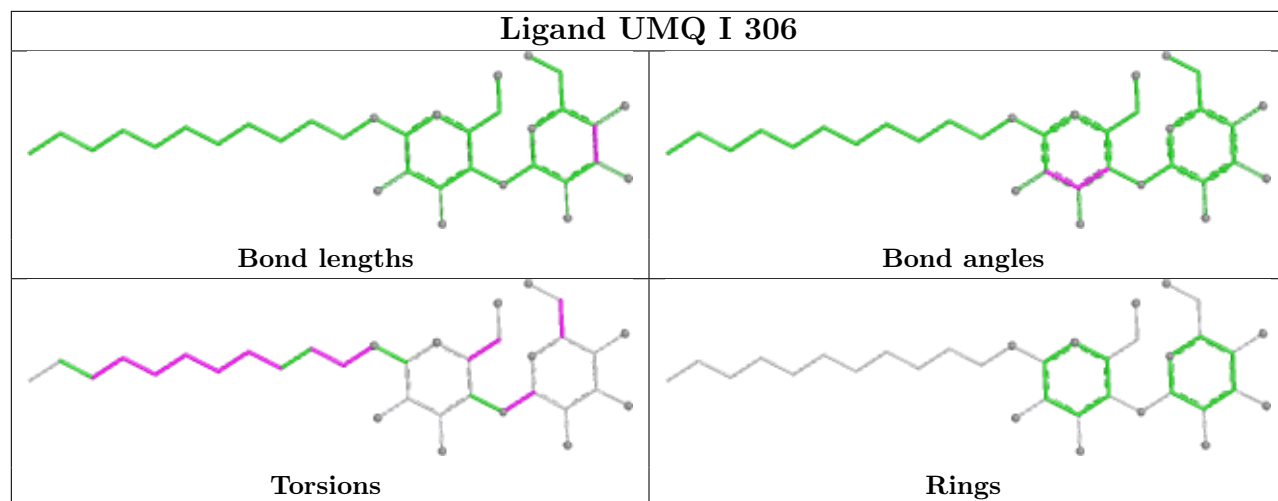
Continued from previous page...

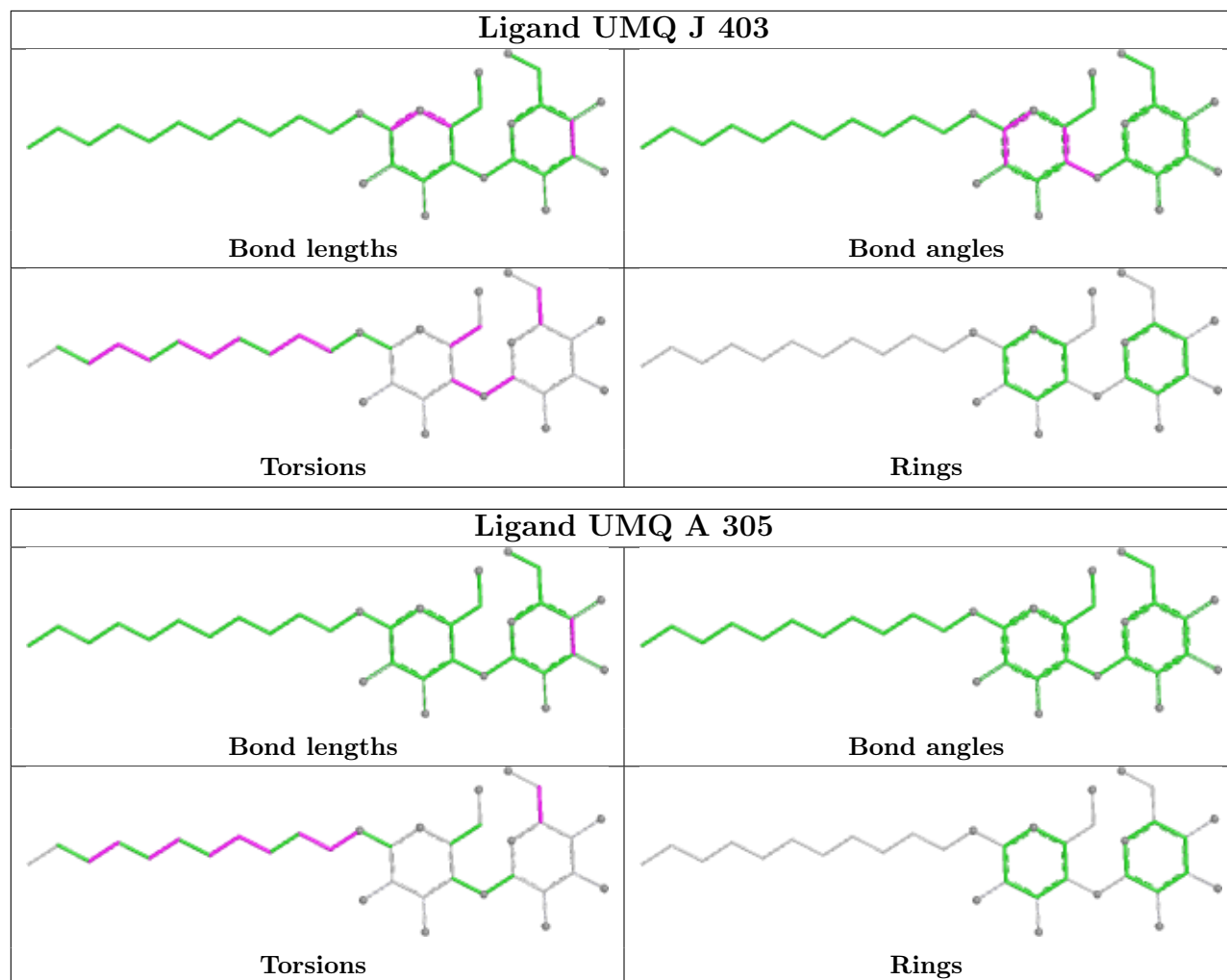
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	403	UMQ	2	0
14	K	302	PL9	4	0
13	H	201	UMQ	1	0
13	P	102	UMQ	1	0
14	B	402	PL9	16	0
12	A	304	CLA	3	0
12	I	304	CLA	3	0
14	B	401	PL9	10	0
11	A	303	HEC	1	0
11	I	303	HEC	1	0
10	A	301	HEM	4	0
11	K	301	HEC	4	0
14	J	402	PL9	14	0
13	J	404	UMQ	2	0
10	A	302	HEM	5	0
13	I	305	UMQ	1	0
13	B	404	UMQ	1	0
14	J	401	PL9	14	0
17	P	101	BCR	5	0
17	F	101	BCR	2	0
15	D	201	SQD	5	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.

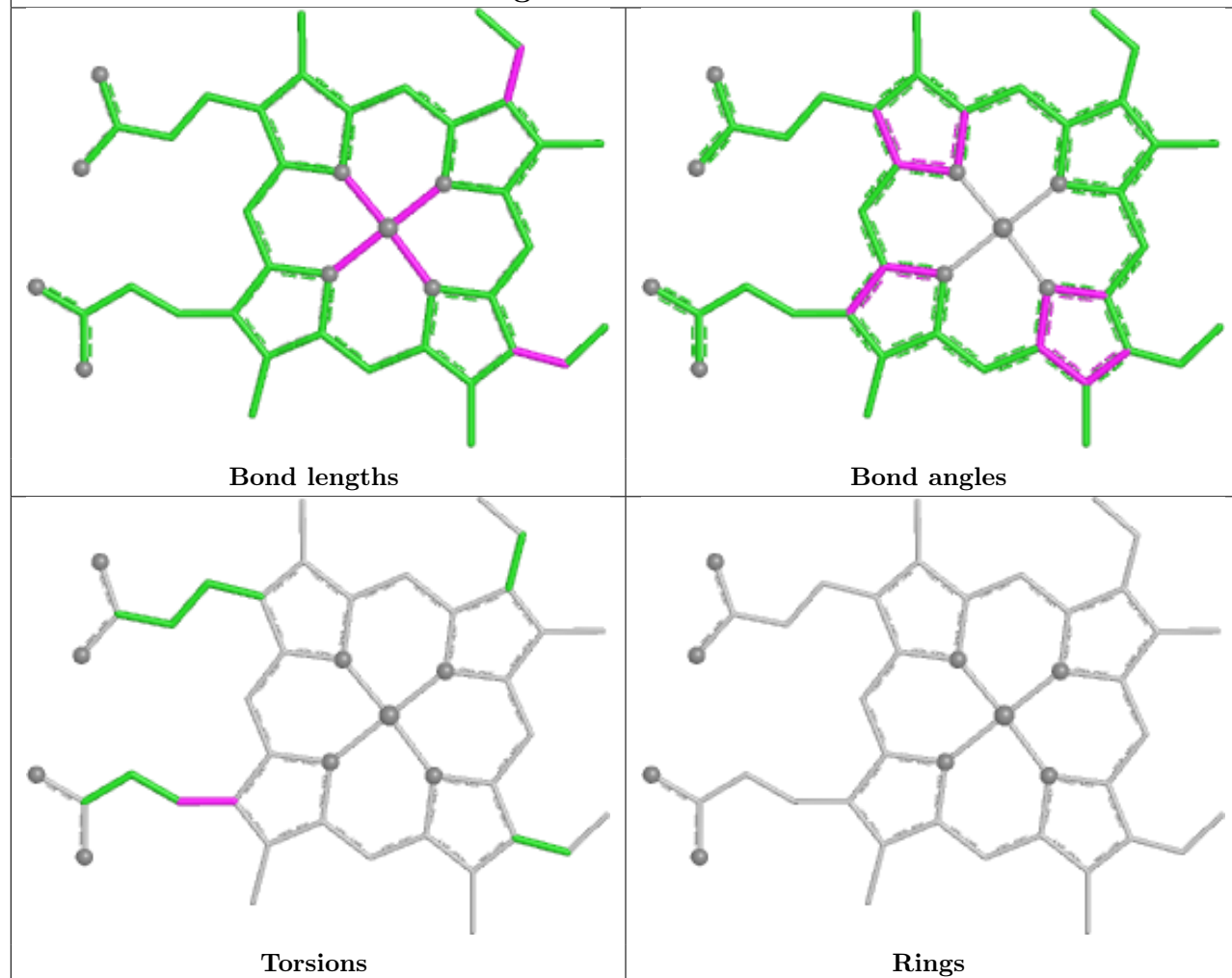




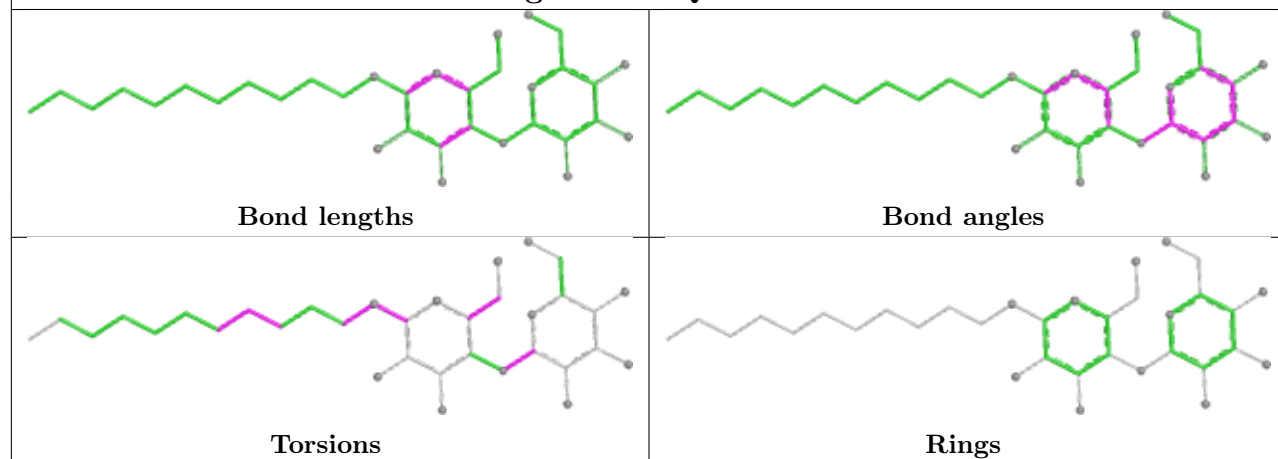


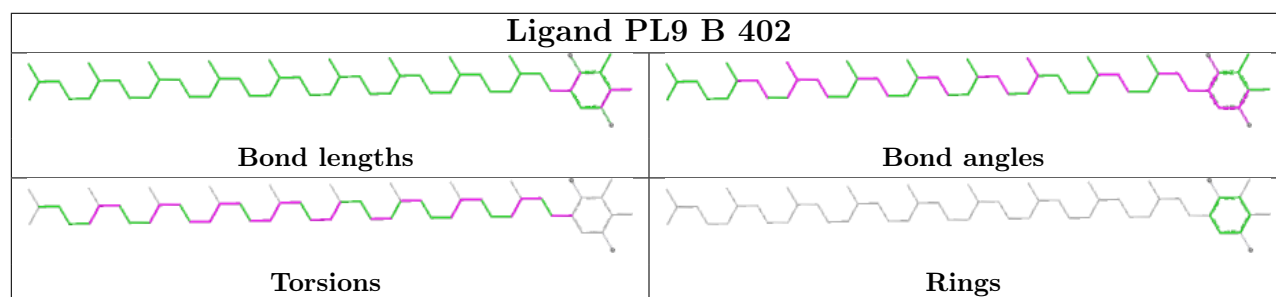
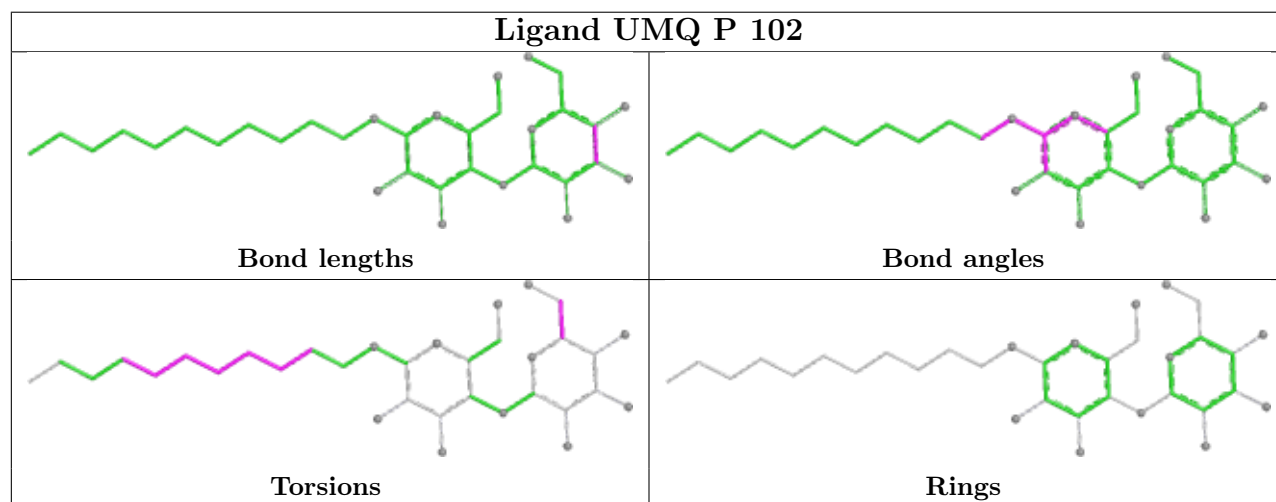
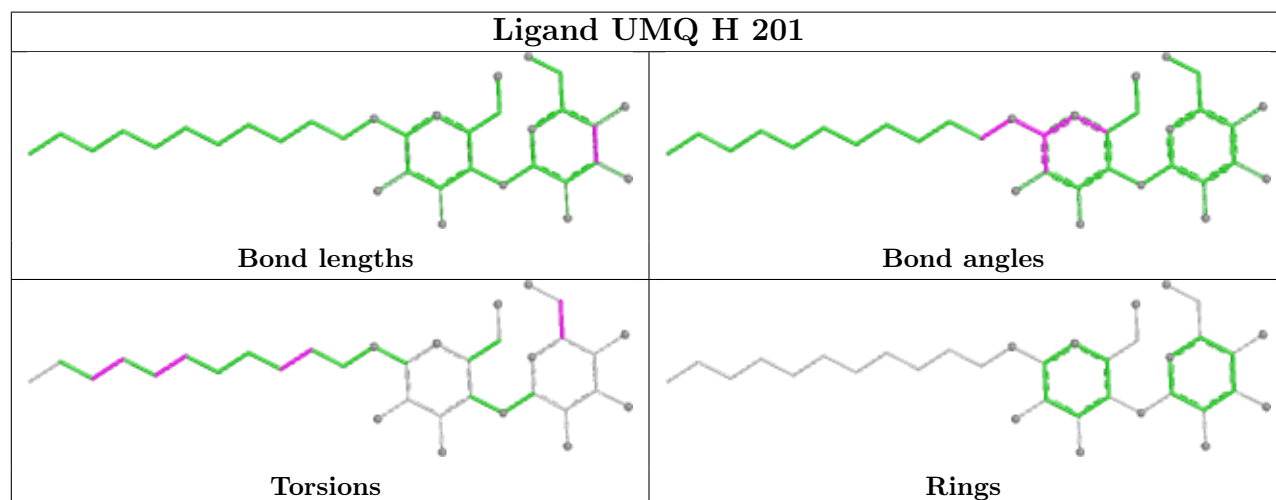
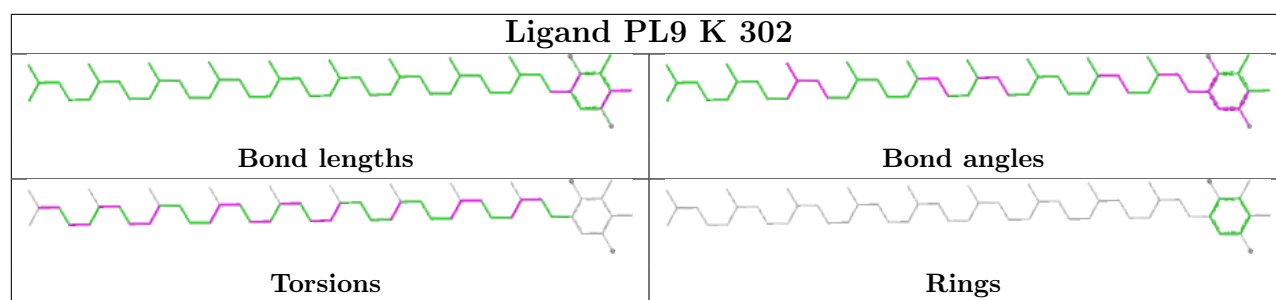


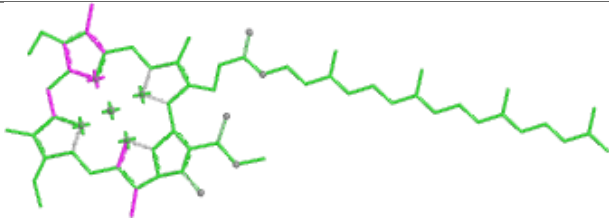
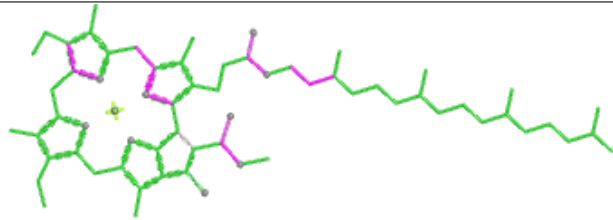
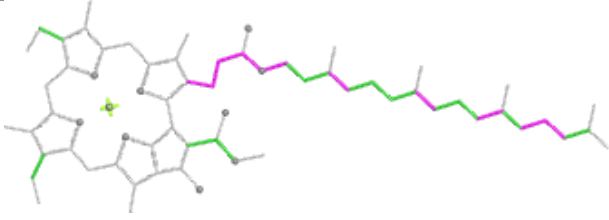
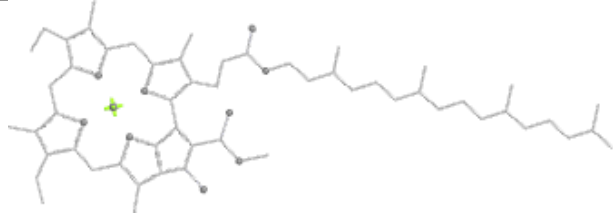
Ligand HEM I 302

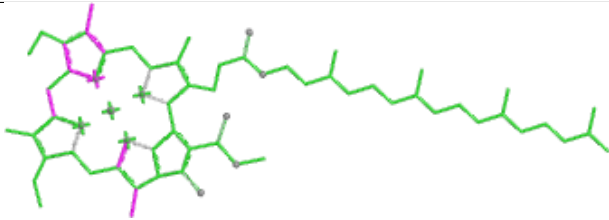
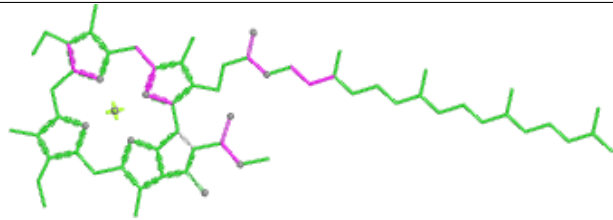
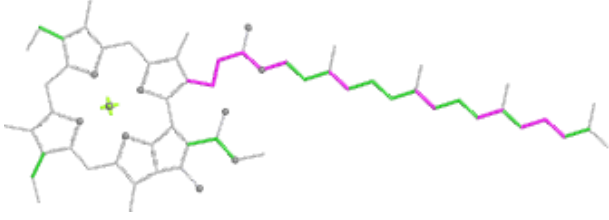
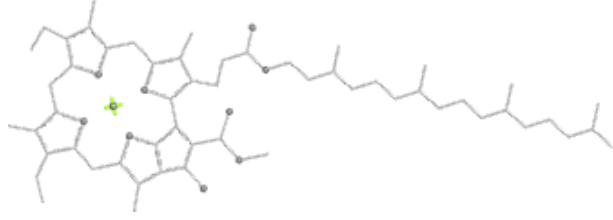


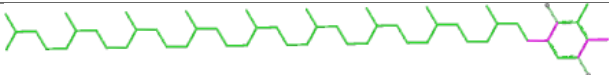
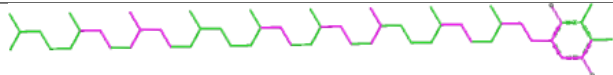
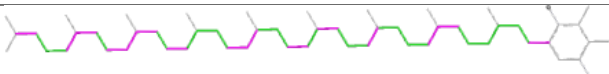
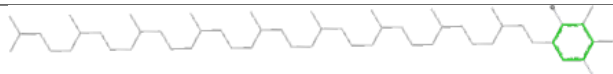
Ligand UMQ B 403

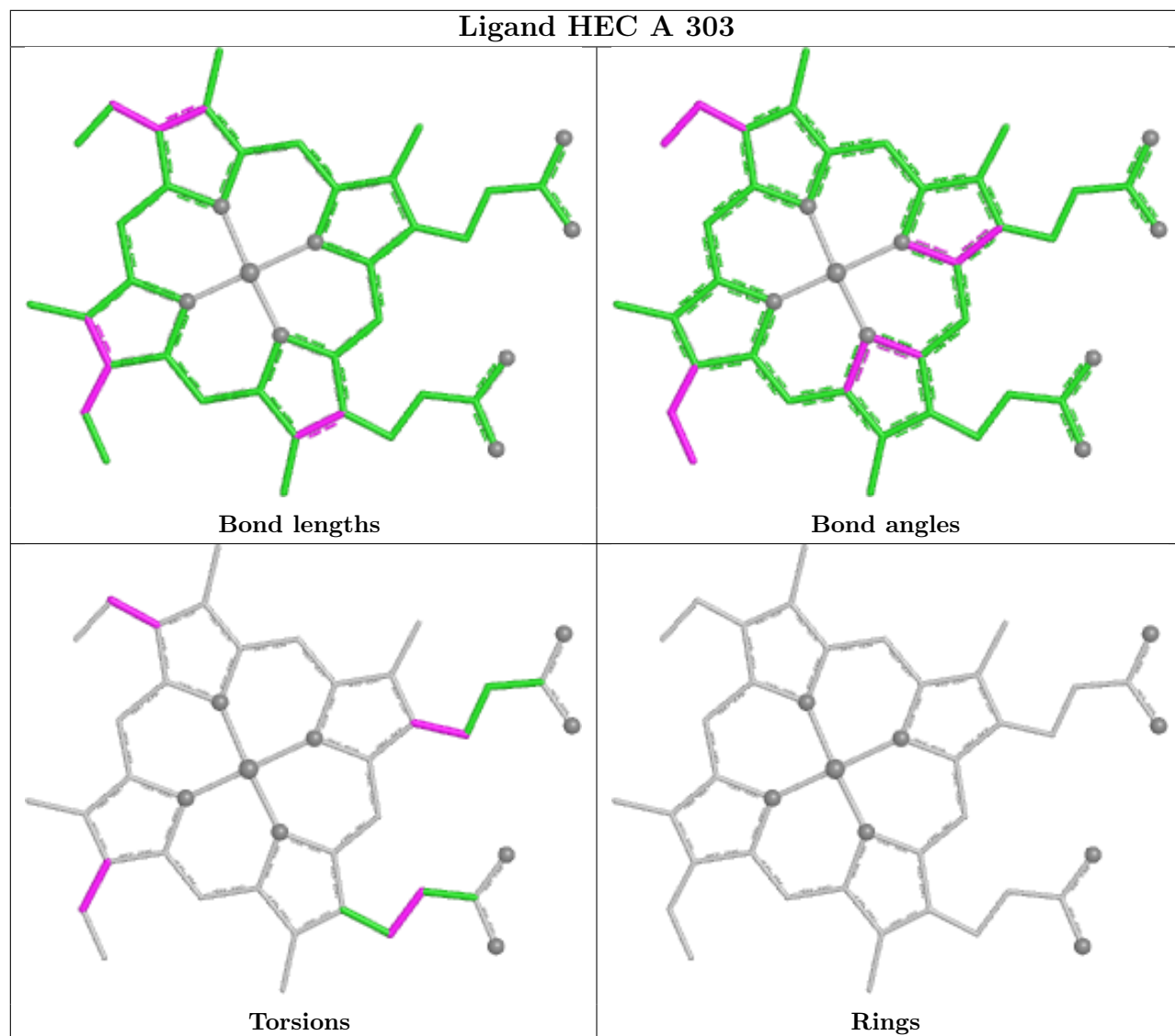




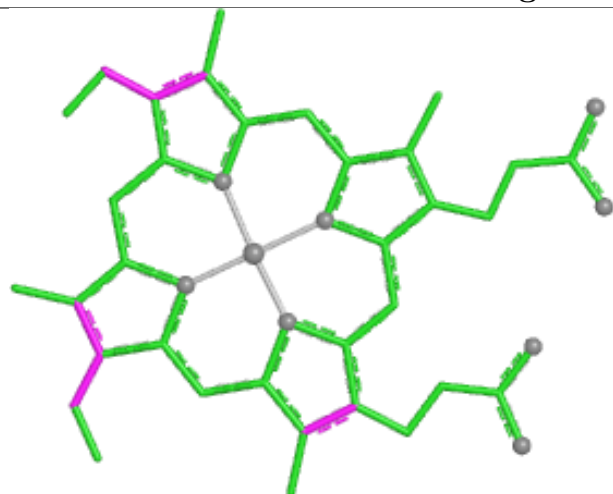
Ligand CLA A 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA I 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

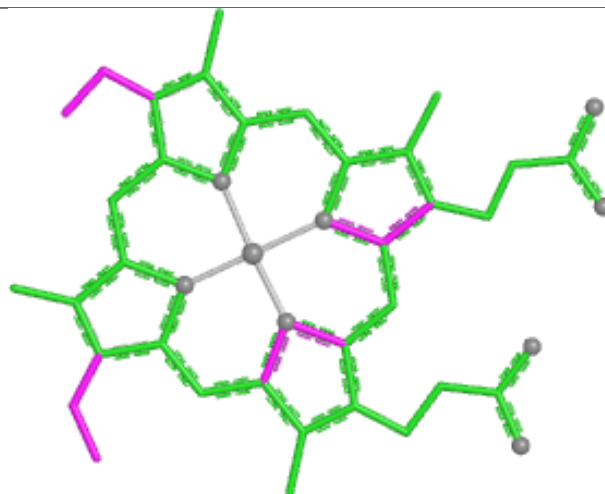
Ligand PL9 B 401	
	
Bond lengths	Bond angles
	
Torsions	Rings



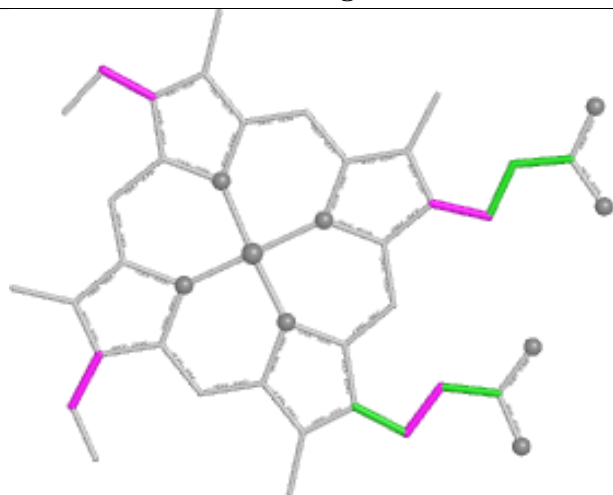
Ligand HEC I 303



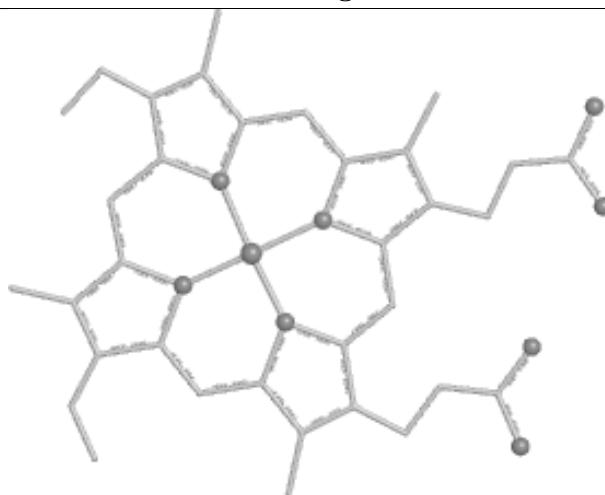
Bond lengths



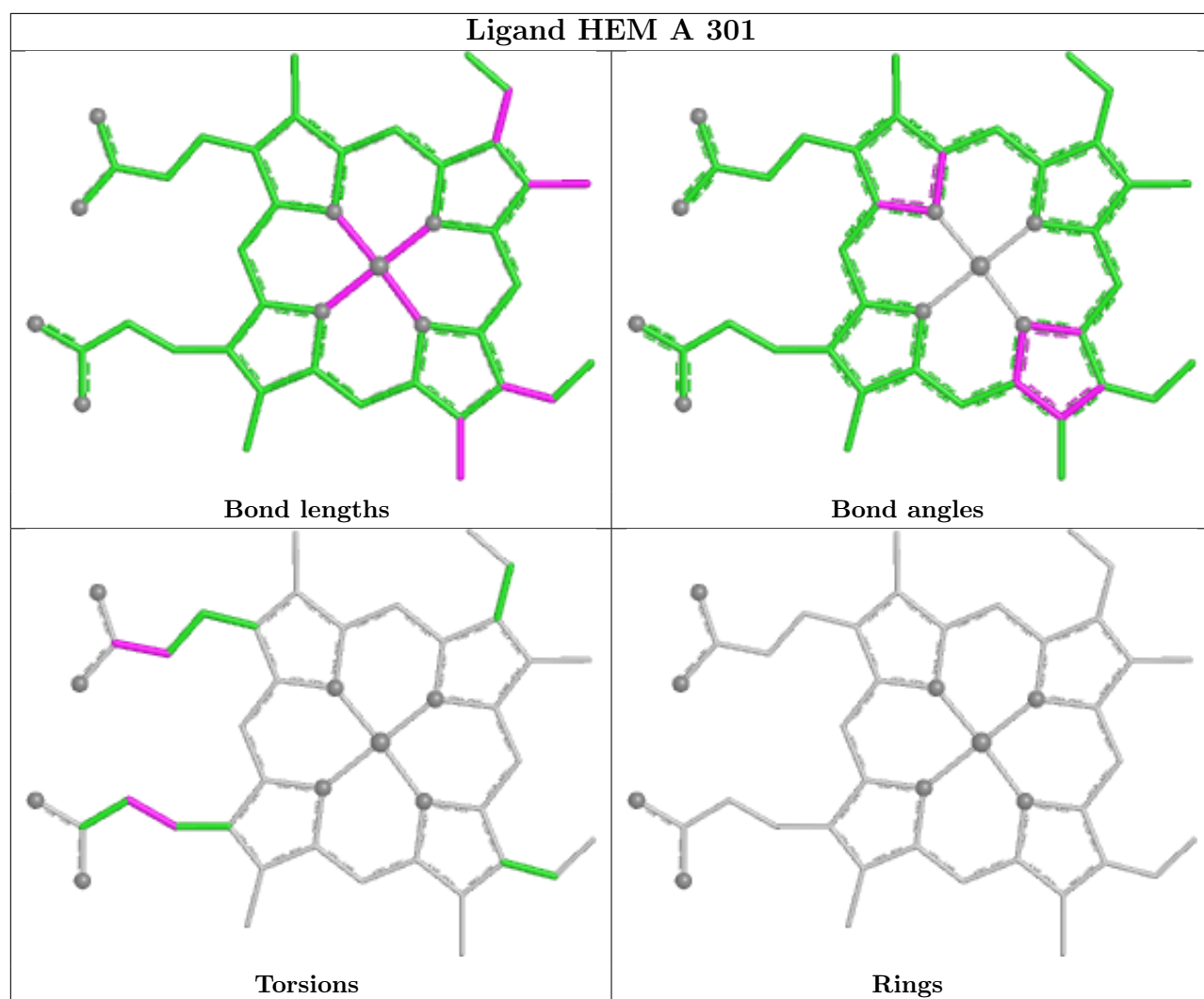
Bond angles

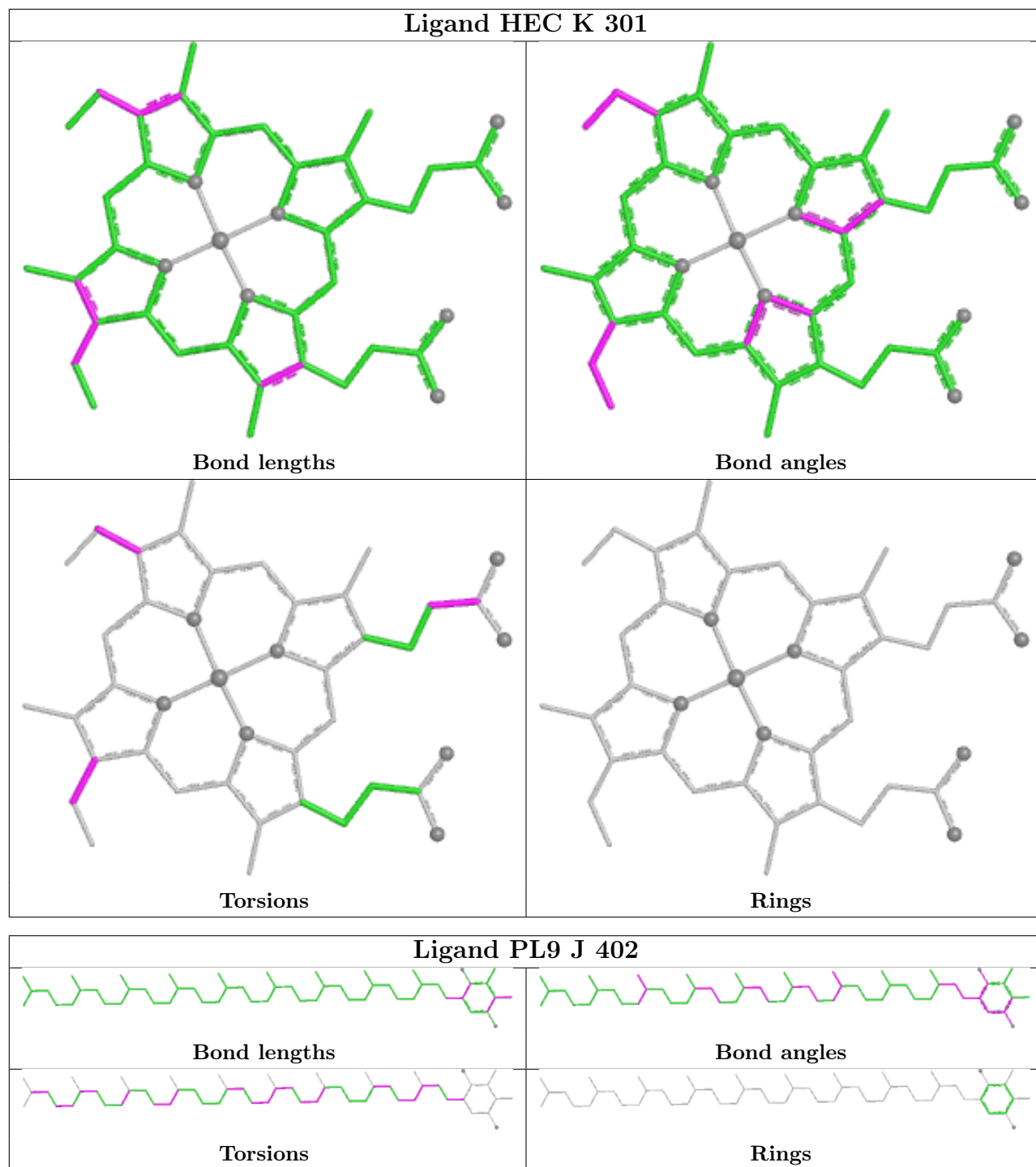


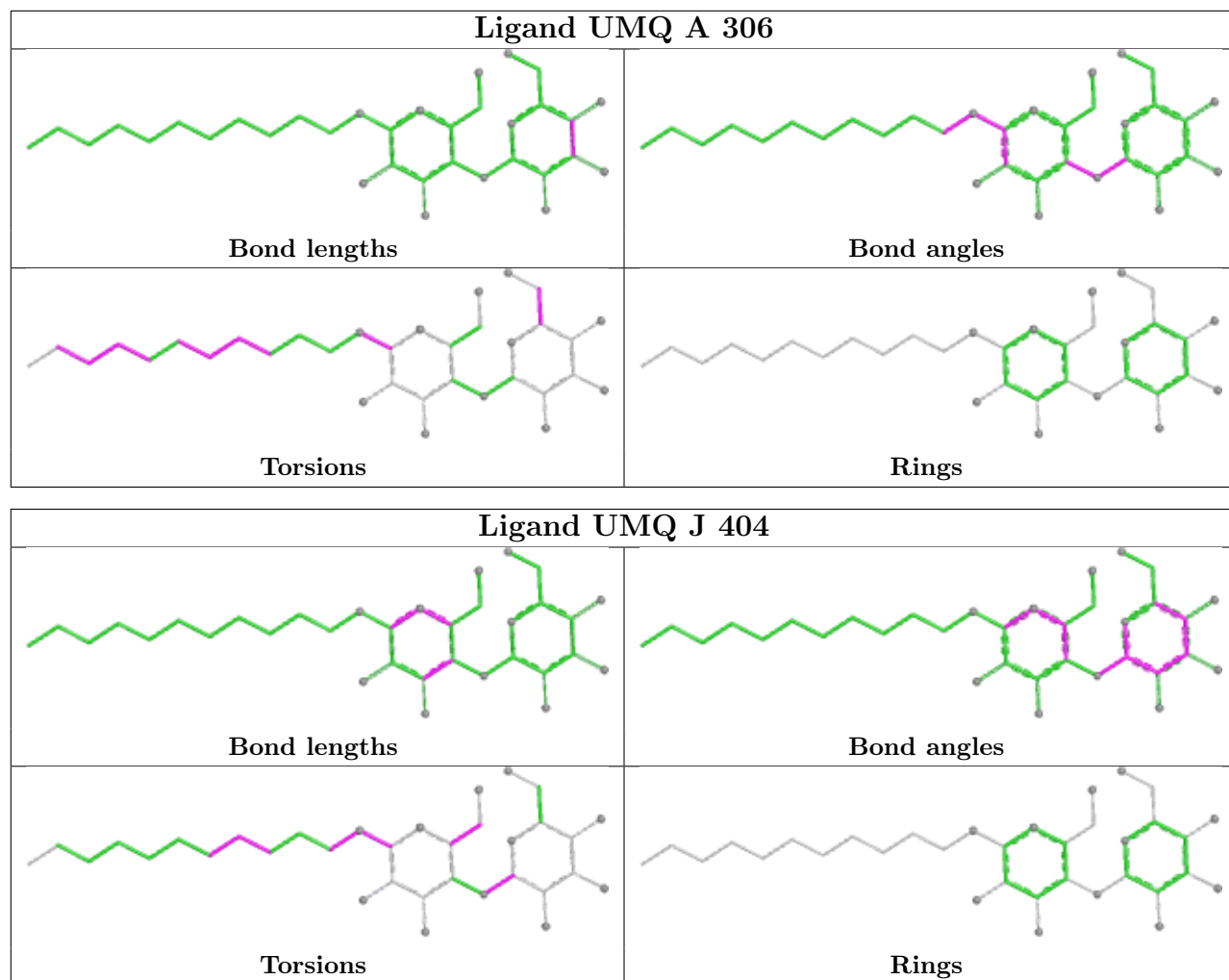
Torsions

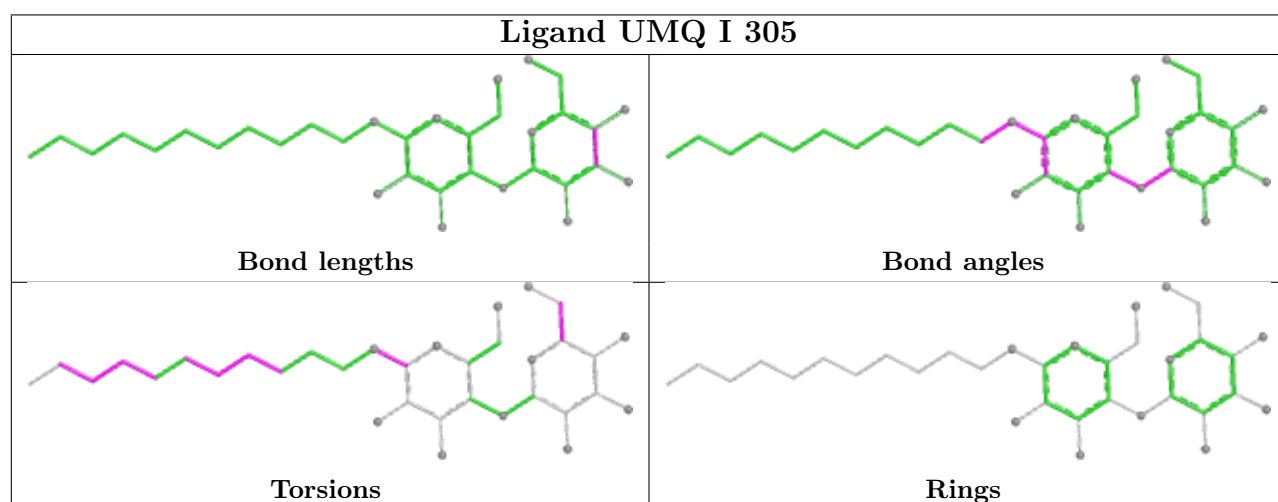
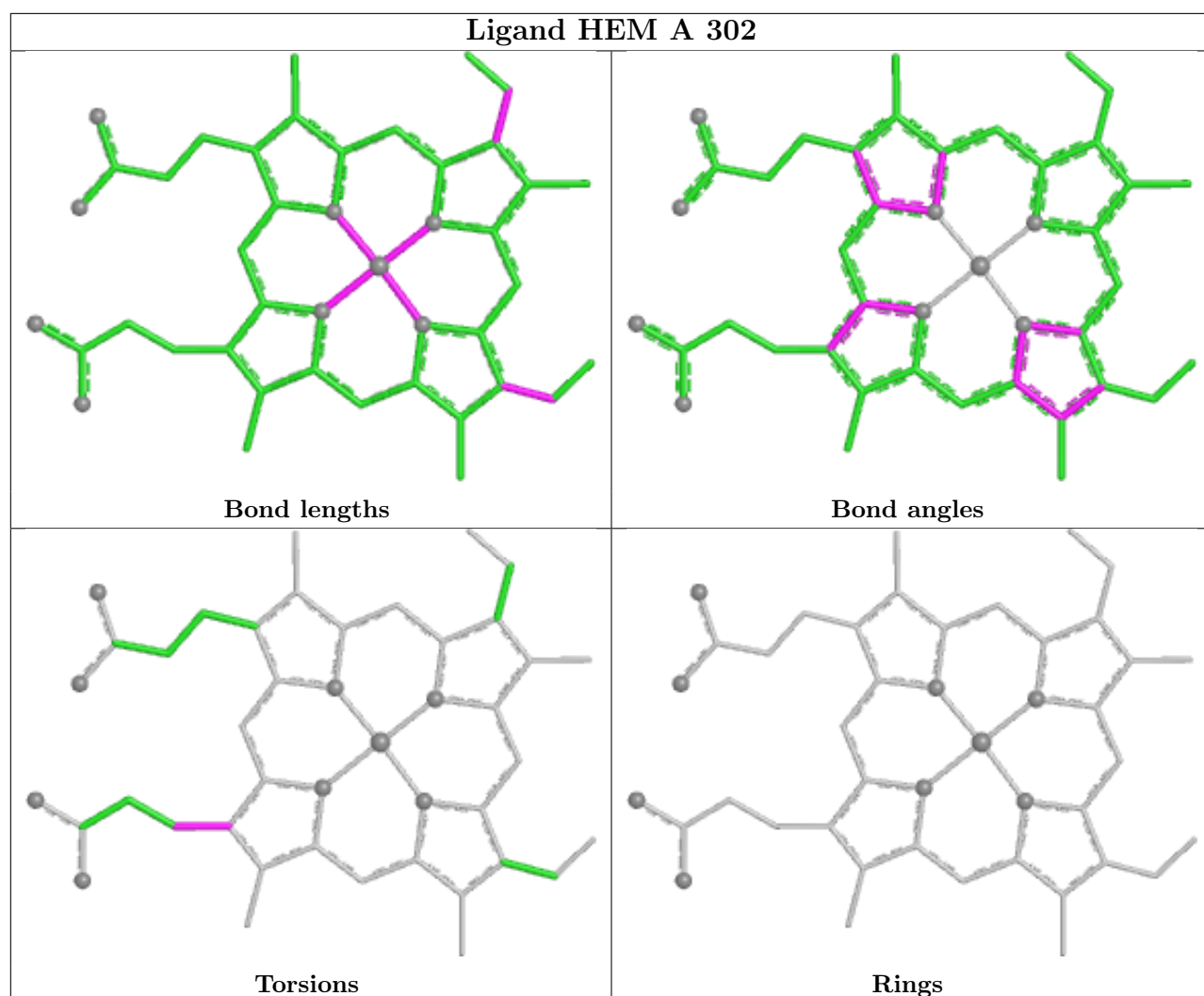


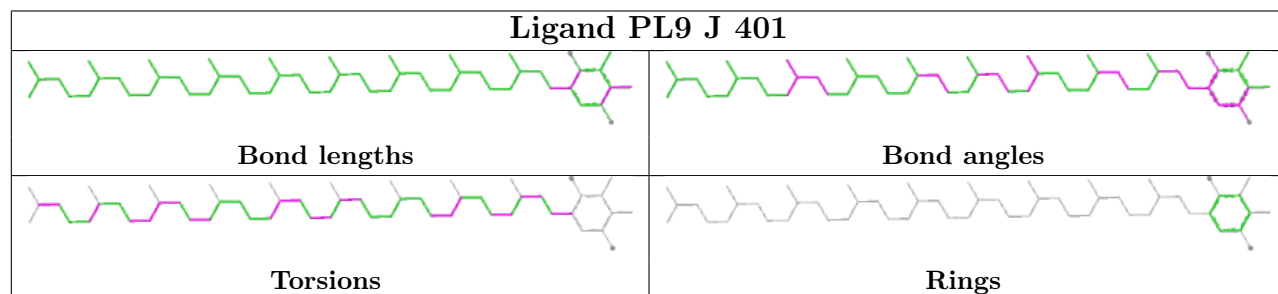
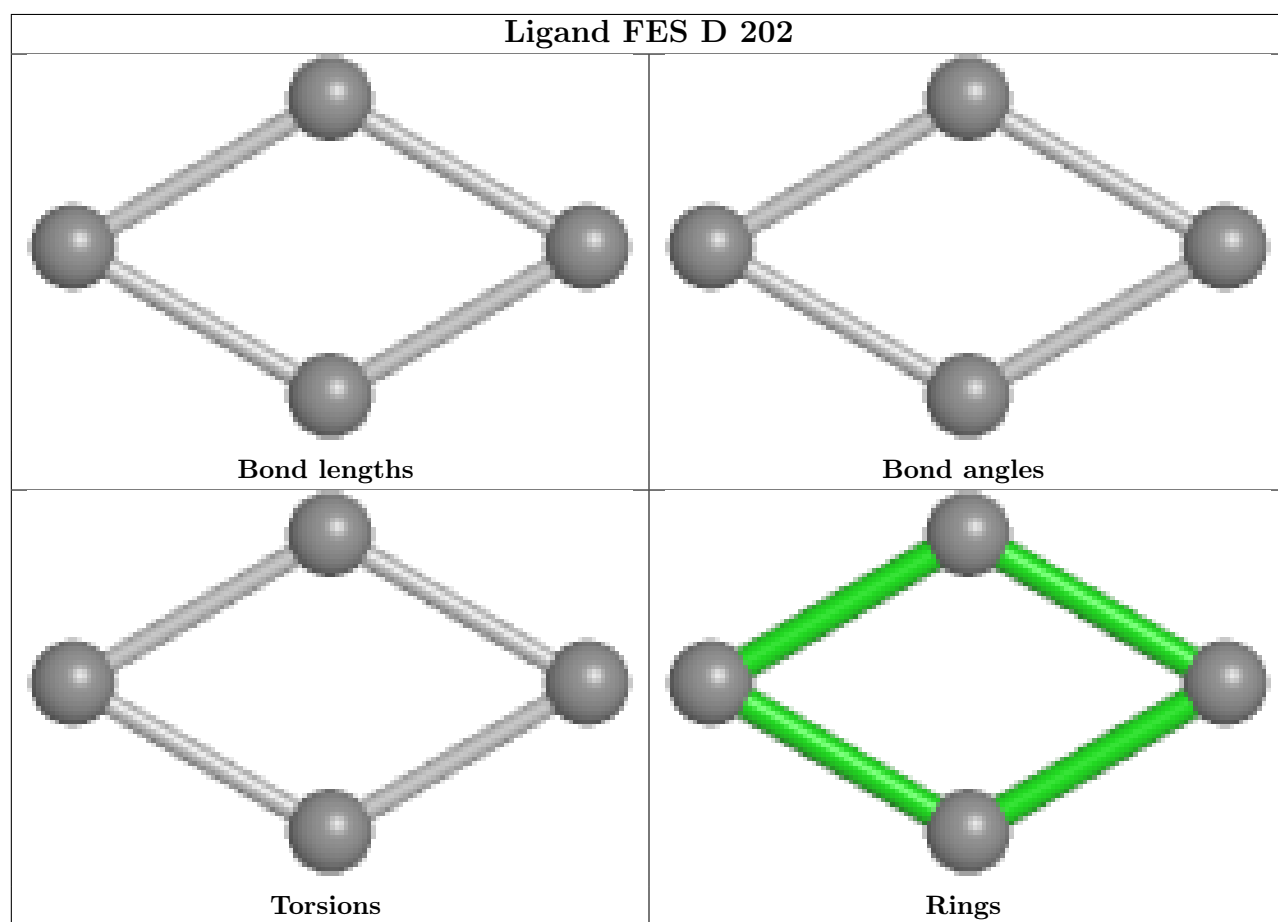
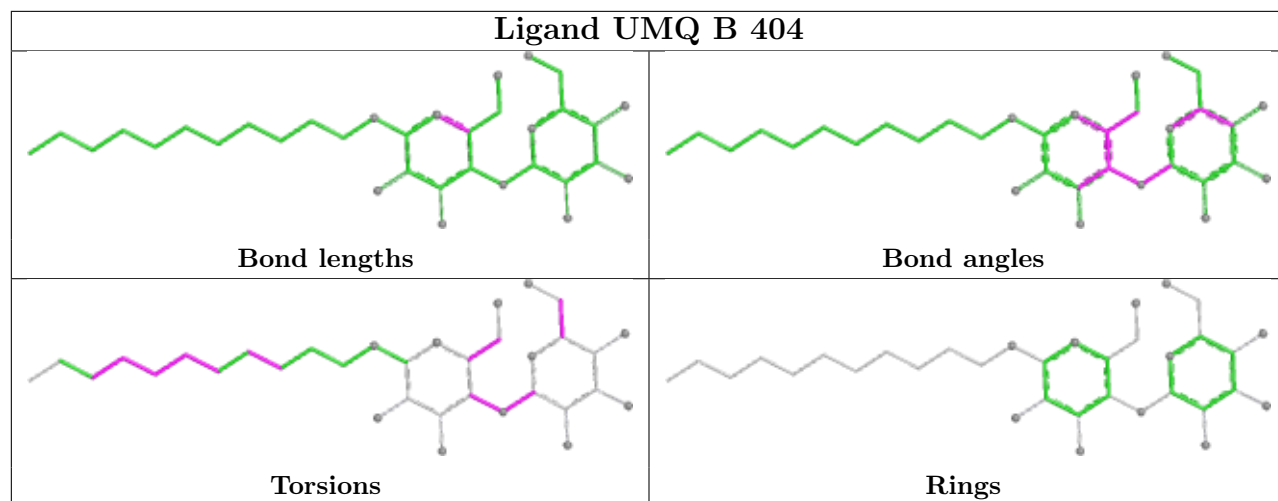
Rings

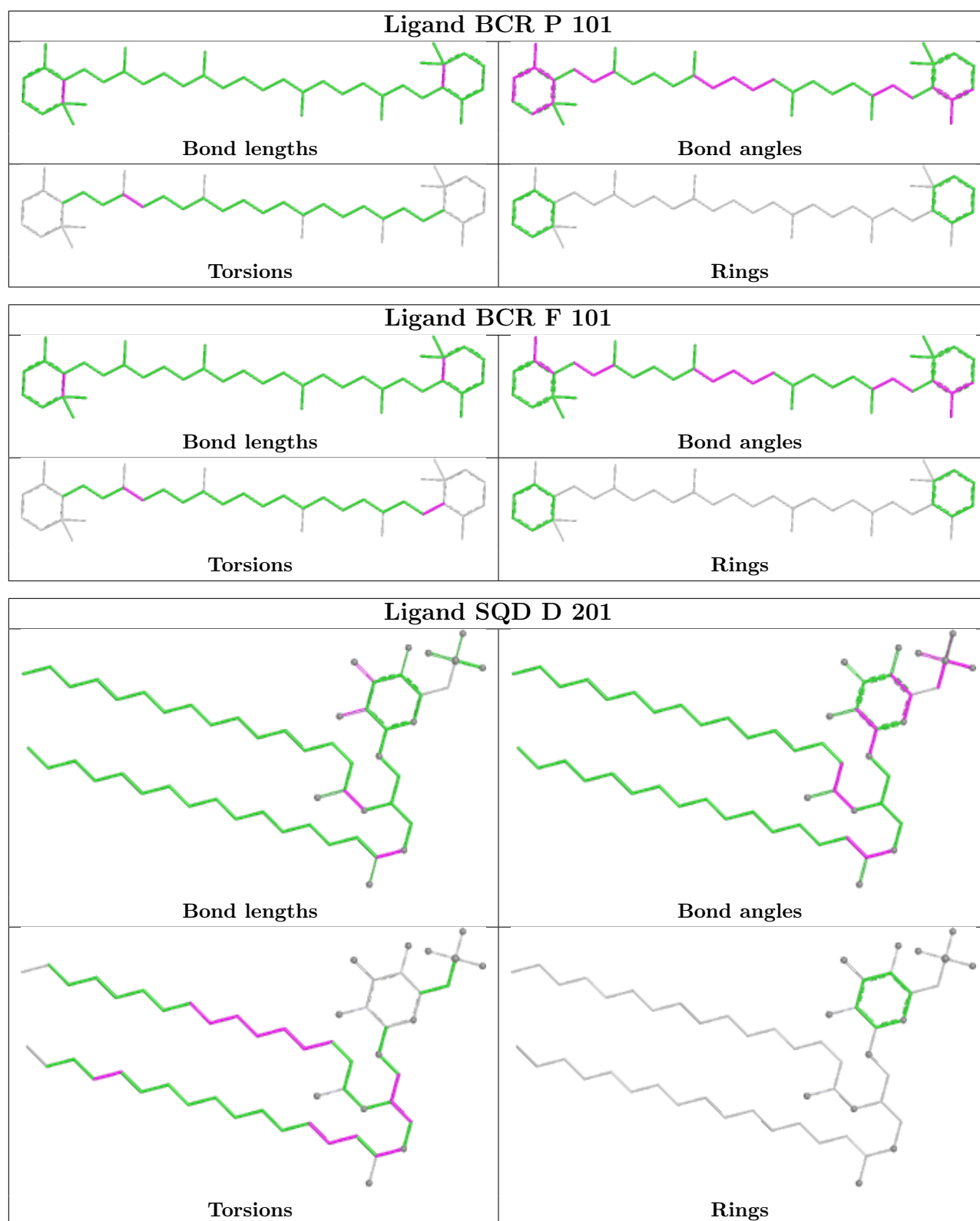












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

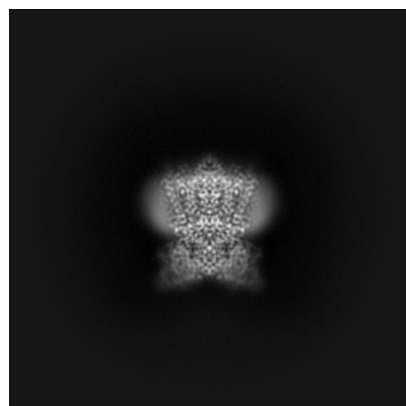
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15027. These allow visual inspection of the internal detail of the map and identification of artifacts.

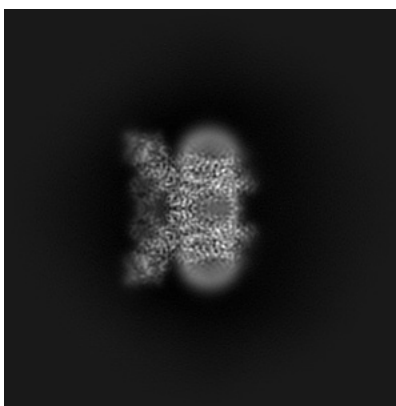
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

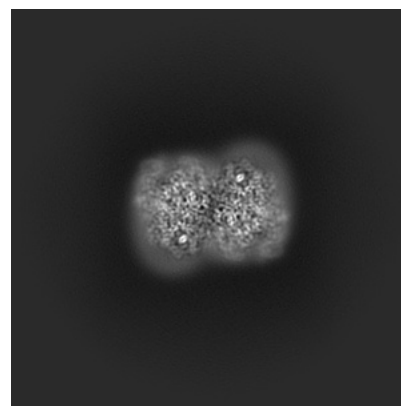
6.1.1 Primary map



X

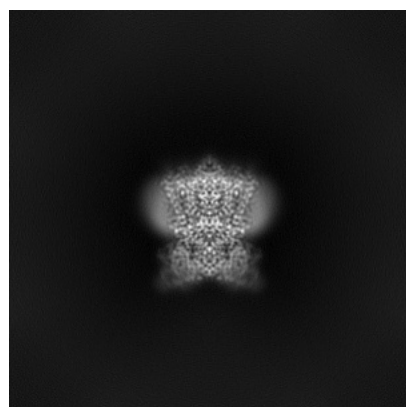


Y

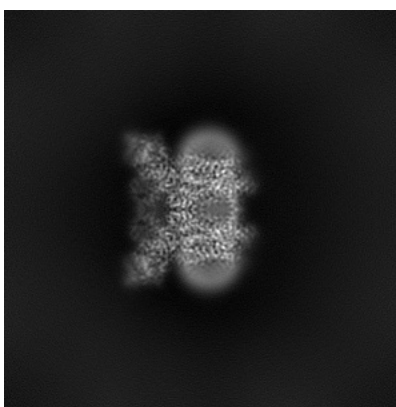


Z

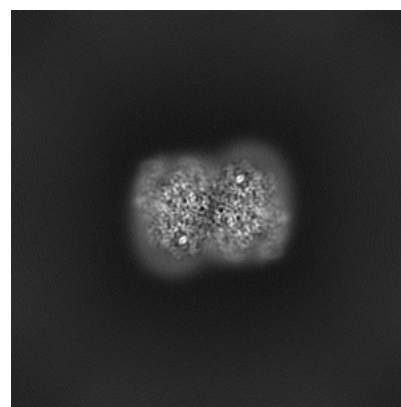
6.1.2 Raw map



X



Y

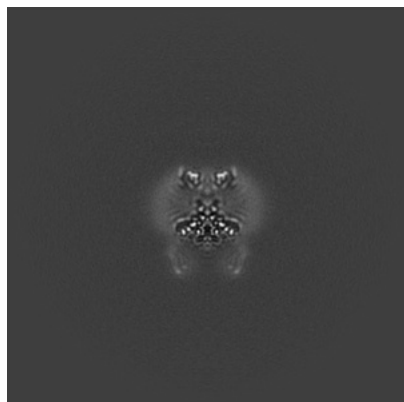


Z

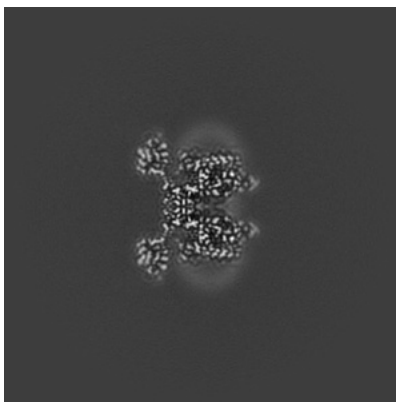
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

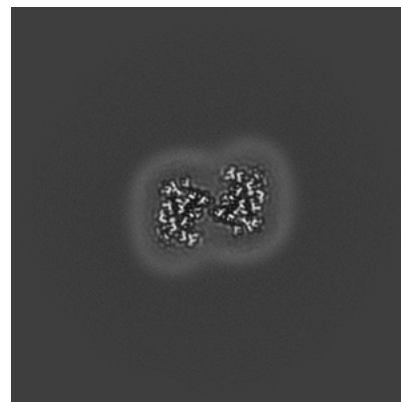
6.2.1 Primary map



X Index: 186

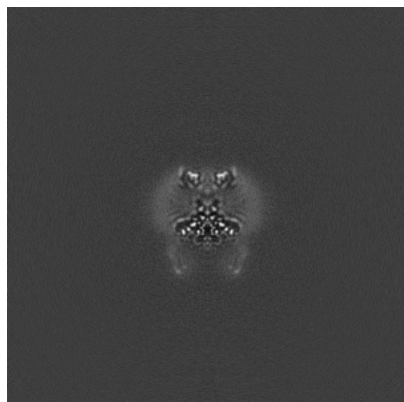


Y Index: 186

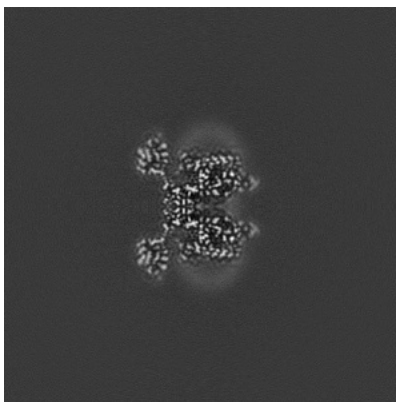


Z Index: 186

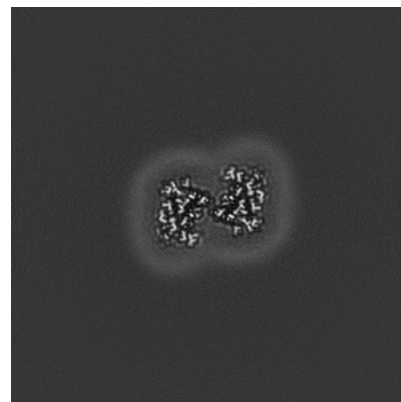
6.2.2 Raw map



X Index: 186



Y Index: 186

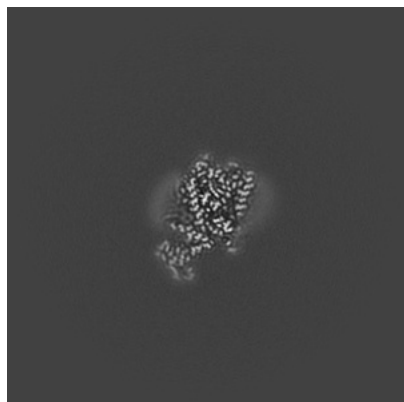


Z Index: 186

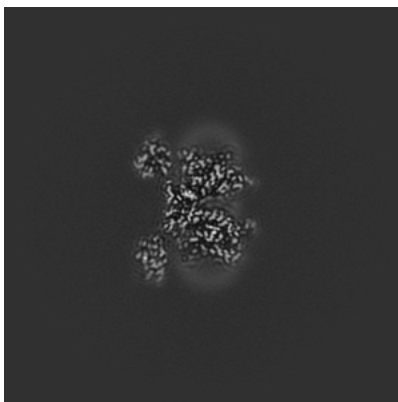
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

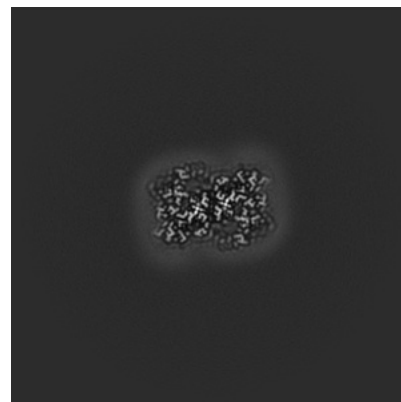
6.3.1 Primary map



X Index: 205

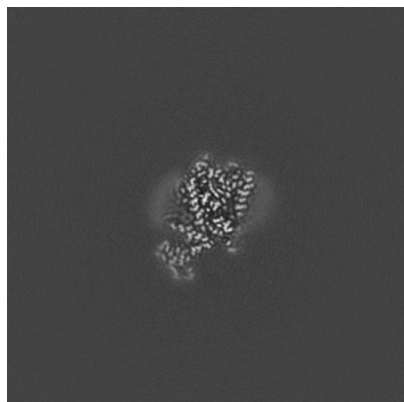


Y Index: 189

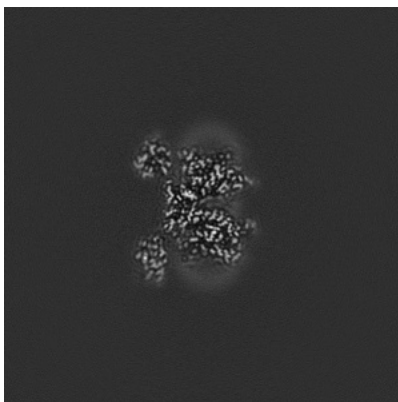


Z Index: 173

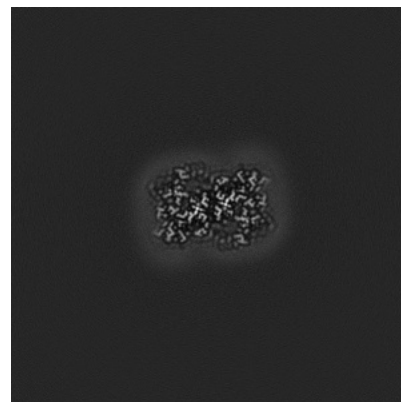
6.3.2 Raw map



X Index: 205



Y Index: 189

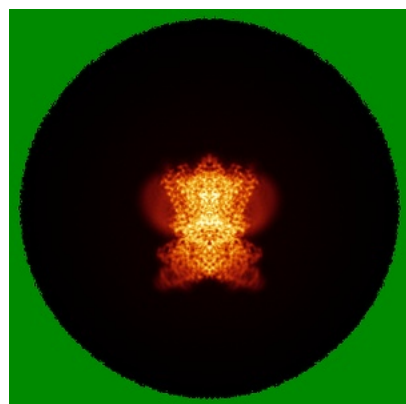


Z Index: 173

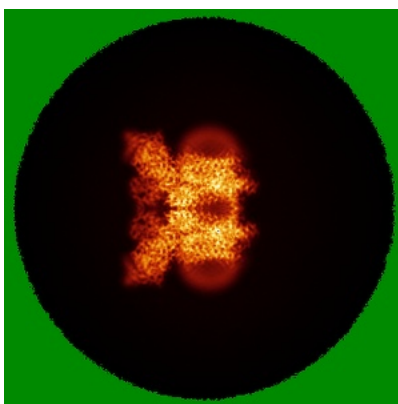
The images above show the largest variance slices of the map in three orthogonal directions.

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

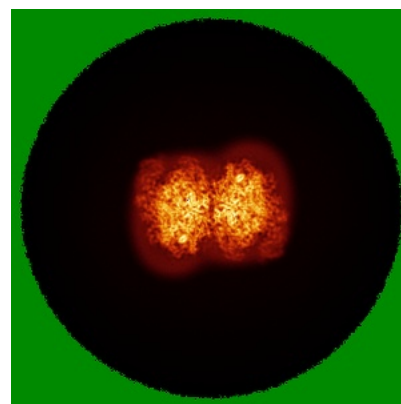
6.4.1 Primary map



X

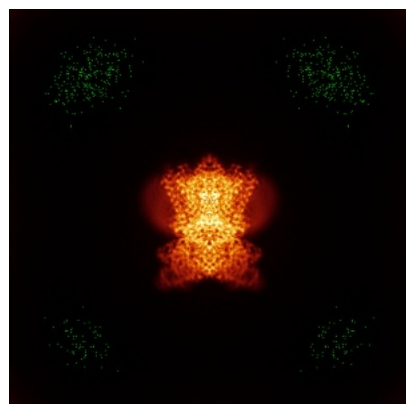


Y

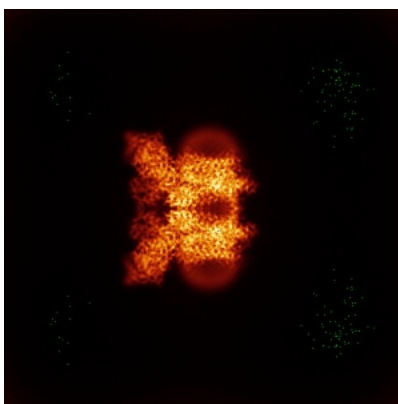


Z

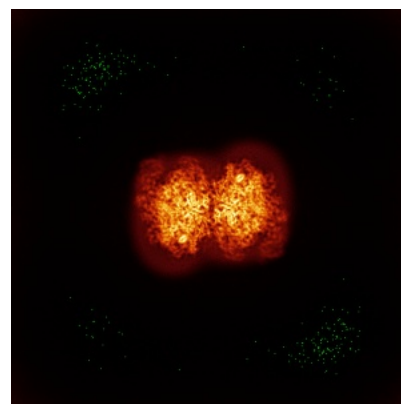
6.4.2 Raw map



X



Y

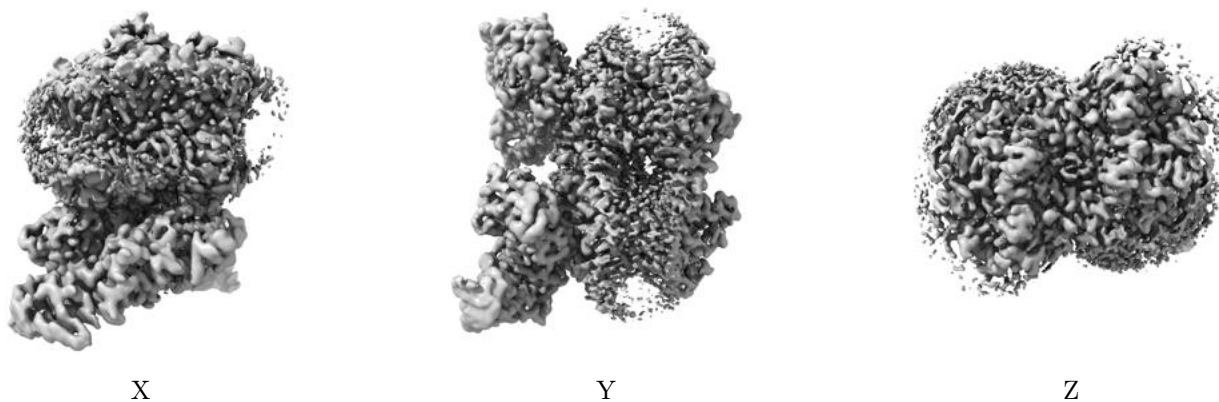


Z

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.

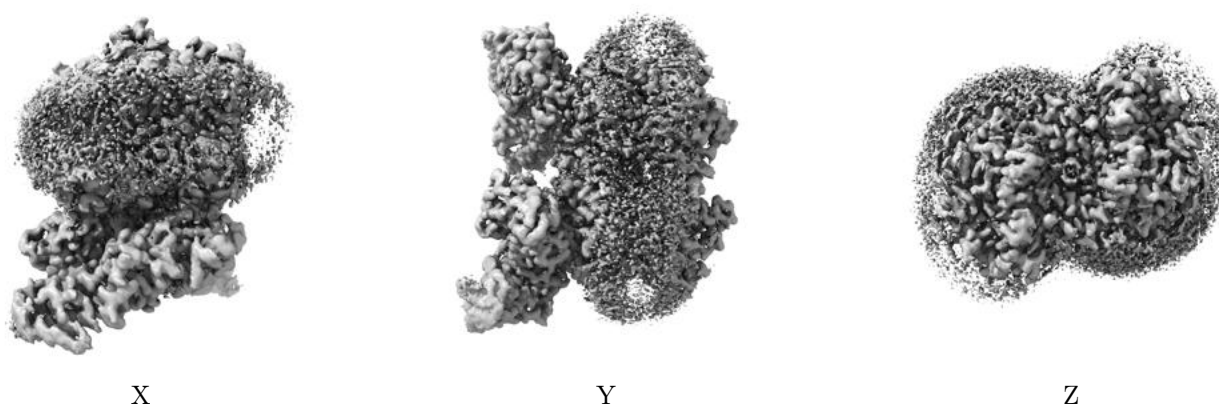
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.208. 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



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

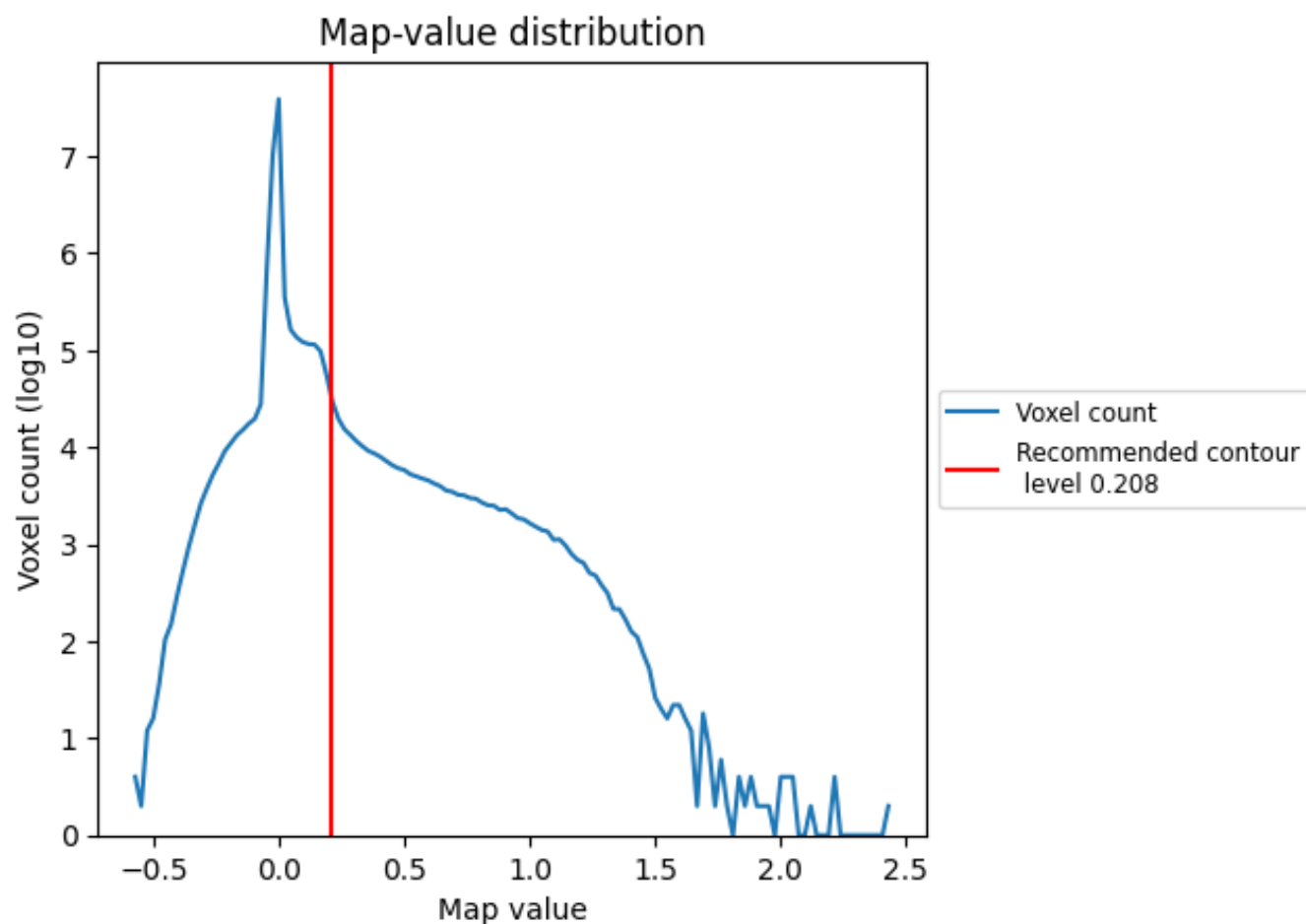
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

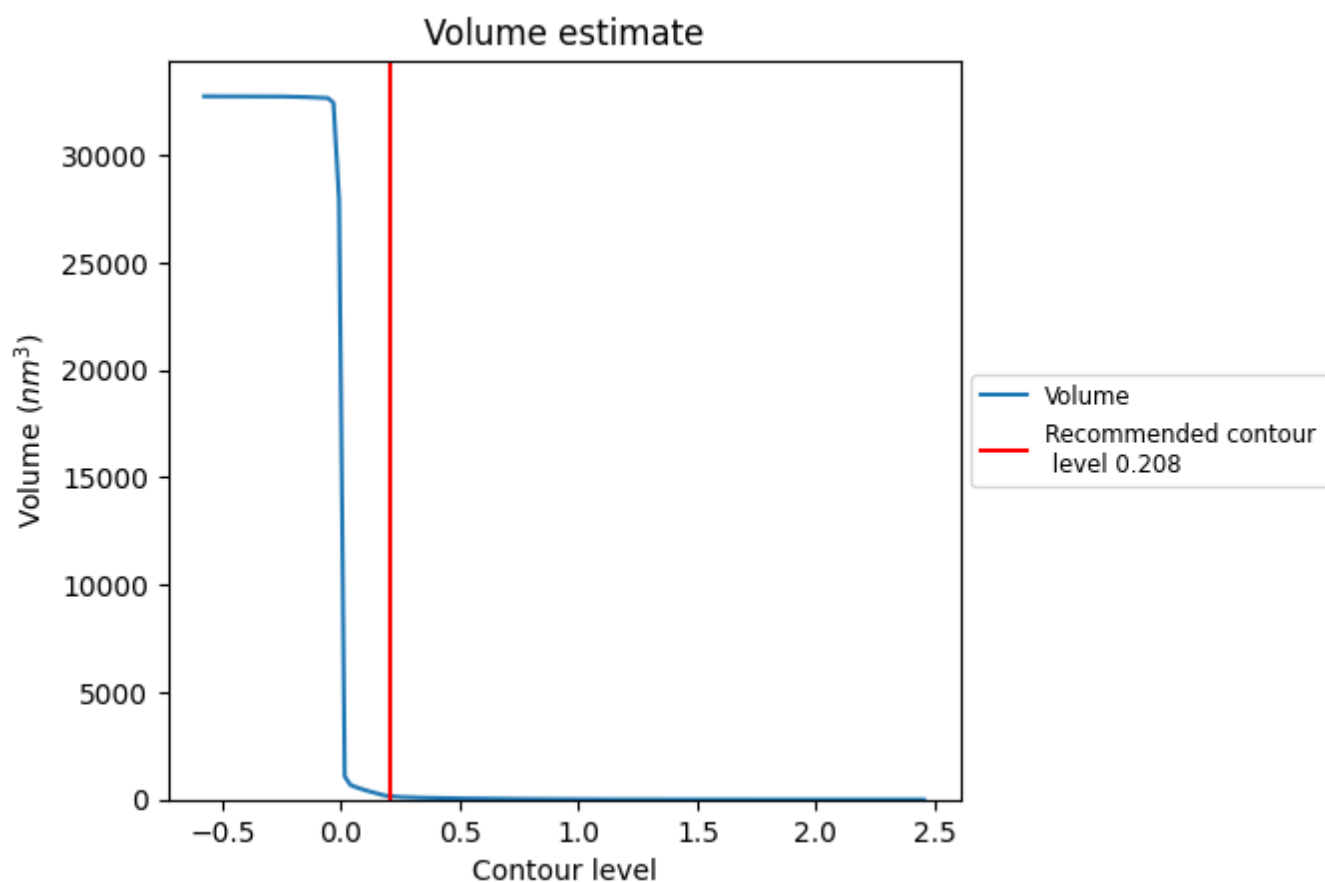
This section contains the results of statistical analysis of the map.

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.

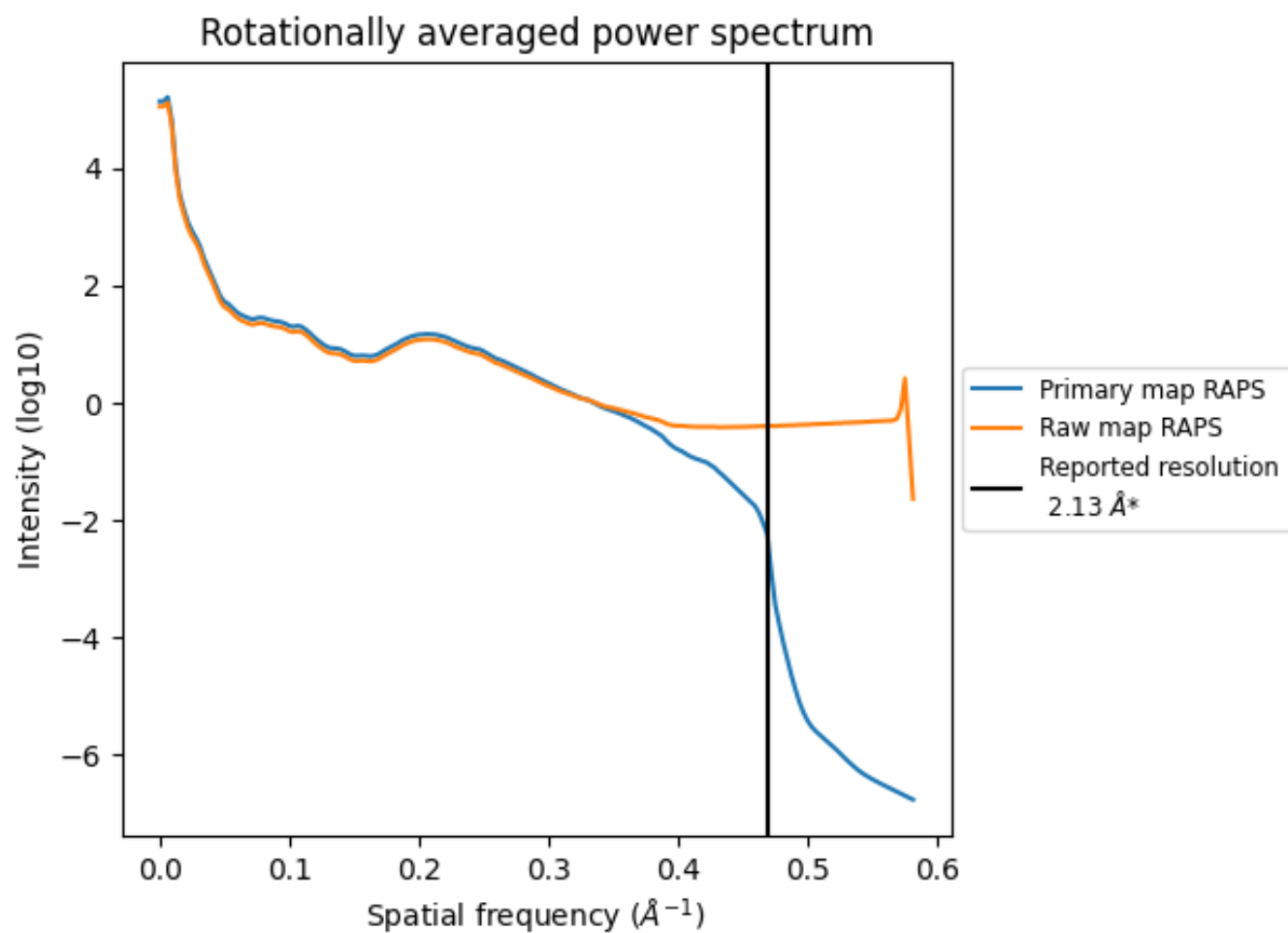
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 150 nm³; this corresponds to an approximate mass of 136 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 ⓘ

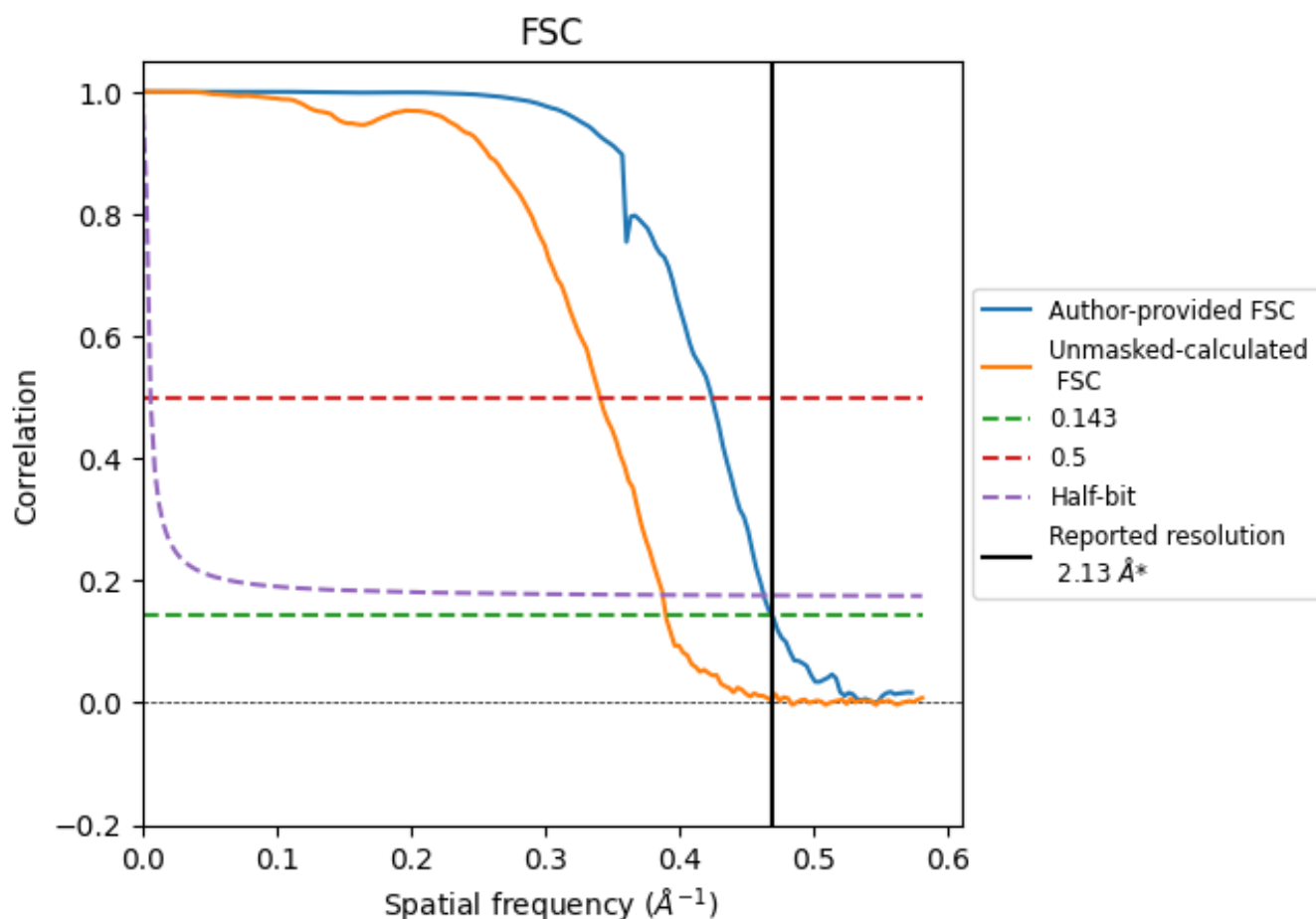


*Reported resolution corresponds to spatial frequency of 0.469 Å⁻¹

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 0.469 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

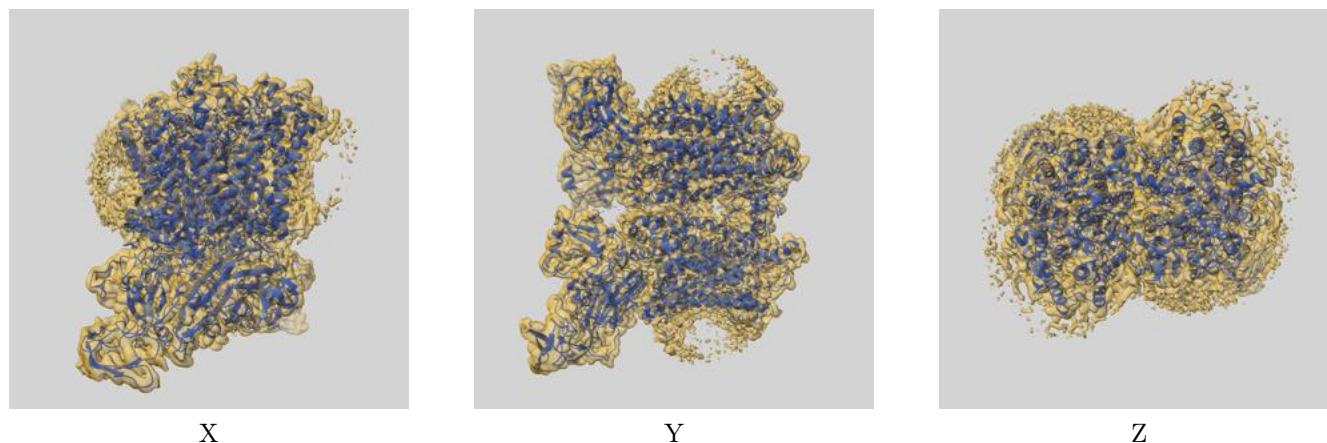
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	2.13	2.36	2.16
Unmasked-calculated*	2.56	2.93	2.58

*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 2.56 differs from the reported value 2.13 by more than 10 %

9 Map-model fit [i](#)

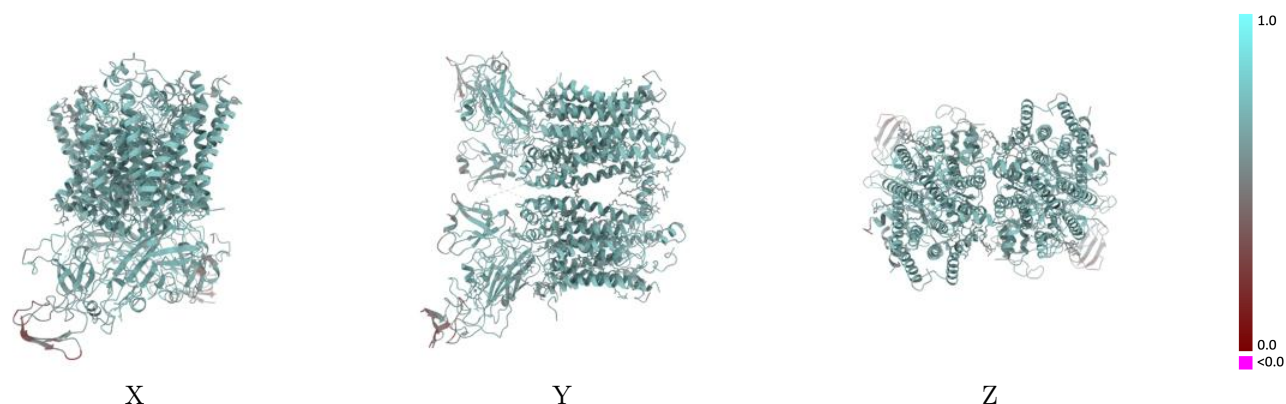
This section contains information regarding the fit between EMDB map EMD-15027 and PDB model 7ZYV. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



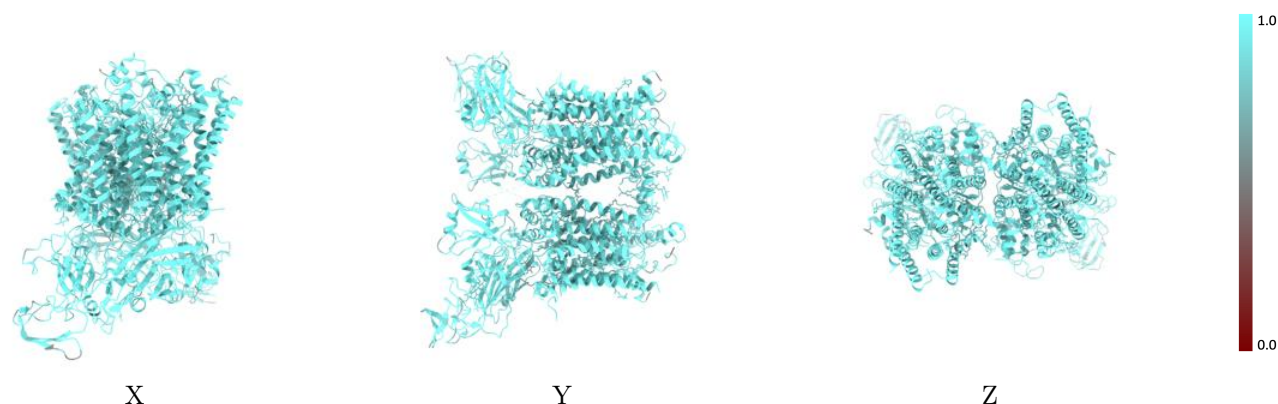
The images above show the 3D surface view of the map at the recommended contour level 0.208 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



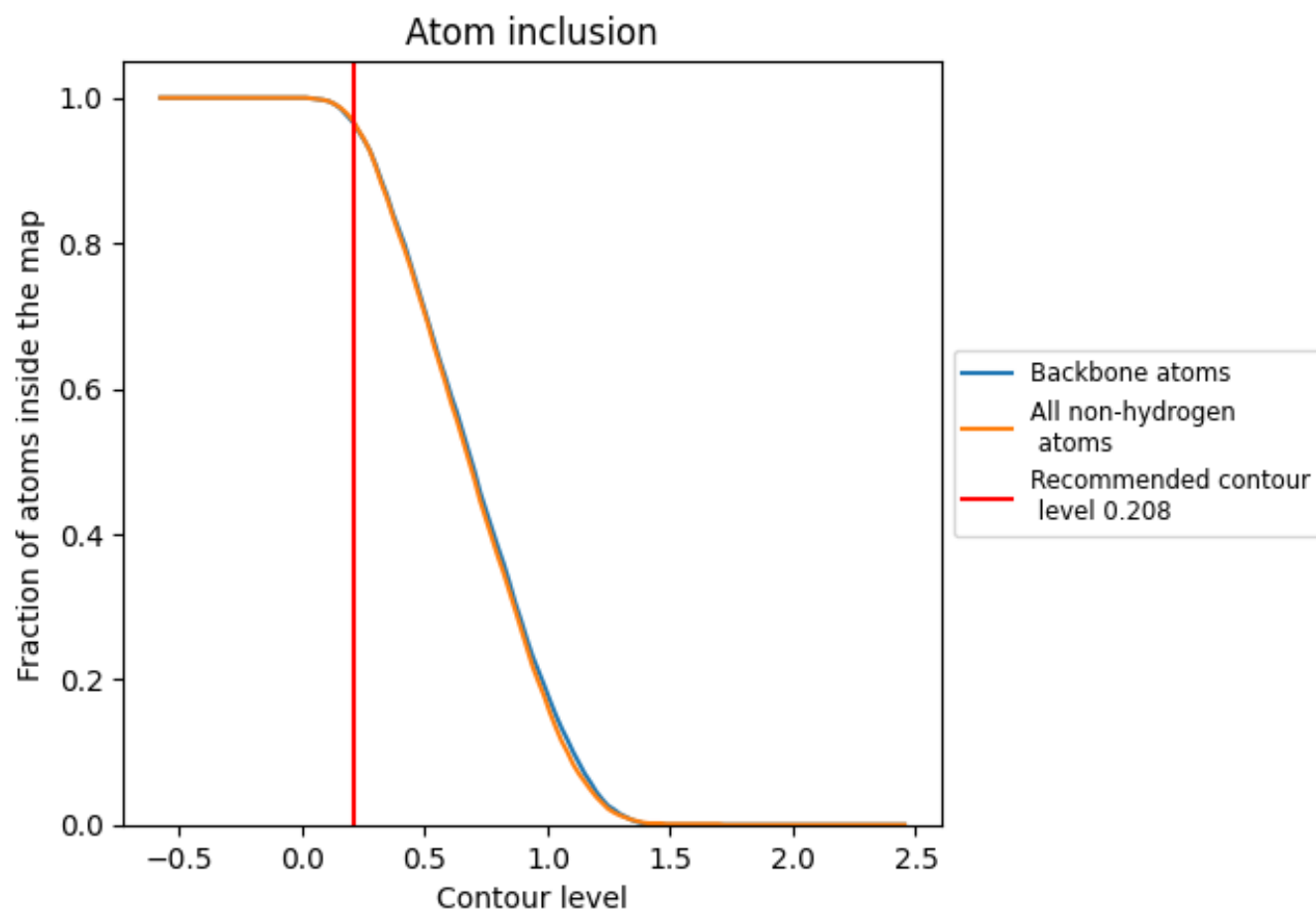
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.208).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 97% 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 (0.208) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9680	0.6440
A	0.9870	0.6780
B	0.9650	0.6510
C	0.9570	0.6120
D	0.9650	0.6270
E	0.9920	0.6400
F	0.9640	0.6470
G	0.9890	0.6670
H	0.9920	0.6740
I	0.9890	0.6820
J	0.9640	0.6510
K	0.9540	0.6110
L	0.9610	0.6300
M	0.9960	0.6480
N	0.9810	0.6500
O	0.9960	0.6730
P	0.9830	0.6700
Q	0.8930	0.6110
R	0.8880	0.5990

1.0

0.0

<0.0