



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:24 PM UTC

PDB ID : 9TGG / pdb\_00009tgg  
EMDB ID : EMD-55898  
Title : Cryo-EM structure of Spinacia oleracea cytochrome b6f complex with bound plastocyanin  
Authors : Pietras, R.; Sarewicz, M.; Szwalec, M.; Indyka, P.; Rawski, M.; Pintscher, S.; Mielecki, B.; Jaciuk, M.; Koziej, L.; Glatt, S.; Osyczka, A.  
Deposited on : 2025-12-01  
Resolution : 3.18 Å (reported)  
Based on initial models : 2PCF, 7QRM

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

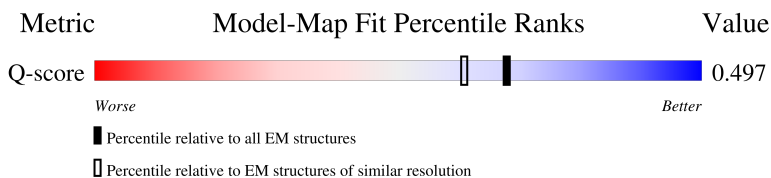
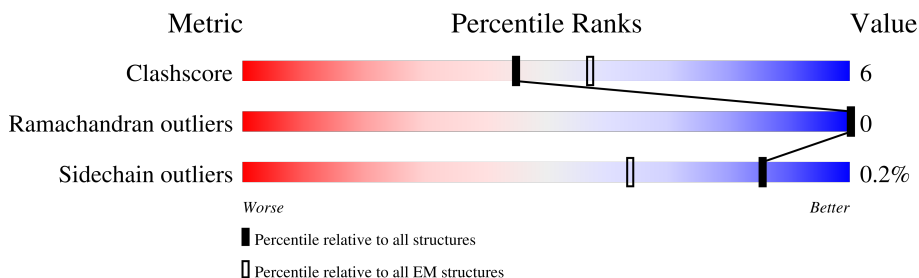
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.18 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	14470 ( 2.68 - 3.68 )

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  $\geq 3$ , 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	 92% 8%
3	C	285	 92% 8%
3	K	285	 88% 12%
4	D	179	 79% 14% 7%
4	L	179	 84% 8% 7%
5	E	31	 81% 19%
5	M	31	 87% 13%
6	F	36	 83% 17%
6	N	36	 92% 8%
7	G	37	 78% 5% 16%
7	O	37	 76% 8% 16%
8	H	29	 93% 7%
8	P	29	 97%
9	Q	99	 89% 78% 19%

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
14	CLA	A	307	X	-	-	-
14	CLA	J	201	X	-	-	-

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 16731 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	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	285	Total	C	N	O	S	0	0
			2209	1418	375	410	6		
3	K	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	D	166	Total	C	N	O	S	0	0
			1259	807	212	233	7		
4	L	166	Total	C	N	O	S	0	0
			1259	807	212	233	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	36	Total	C	N	O	S	0	0
			264	171	44	48	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	31	Total	C	N	O	S	0	0
			249	172	38	38	1		
7	O	31	Total	C	N	O	S	0	0
			249	172	38	38	1		

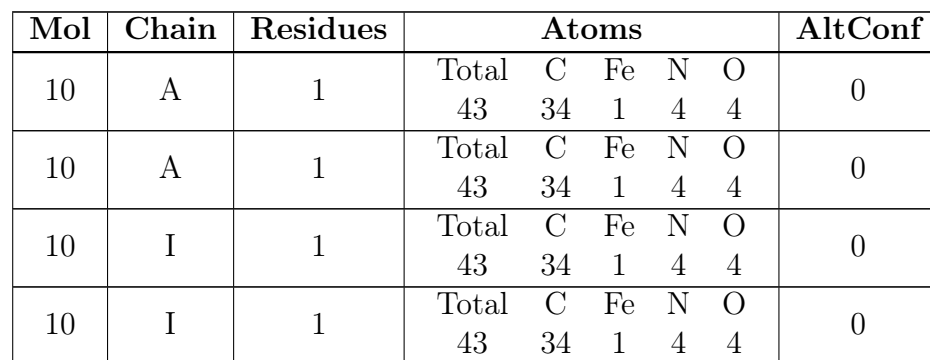
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

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 Plastocyanin, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	99	Total	C	N	O	S	0	0
			733	464	115	151	3		

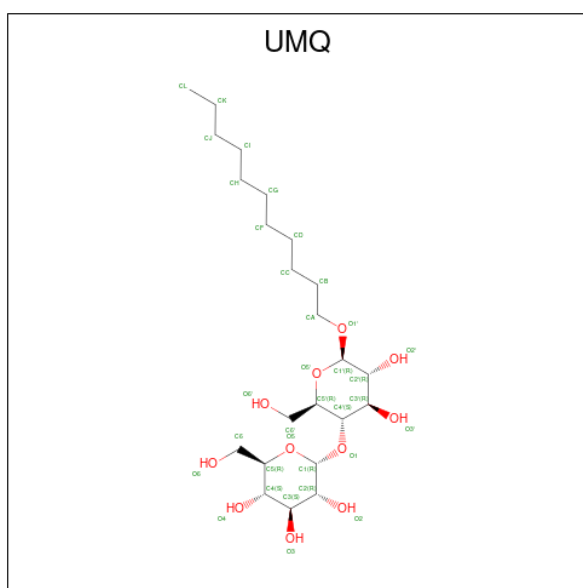
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



- [illegible]

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

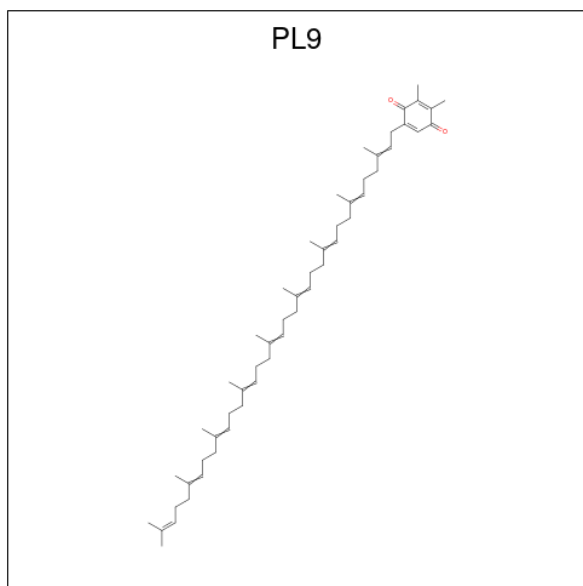
- Molecule 12 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula:  $C_{23}H_{44}O_{11}$ ).



Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			34	23	11	
12	A	1	Total	C	O	0
			34	23	11	
12	E	1	Total	C	O	0
			34	23	11	
12	I	1	Total	C	O	0
			34	23	11	
12	I	1	Total	C	O	0
			34	23	11	
12	P	1	Total	C	O	0
			34	23	11	

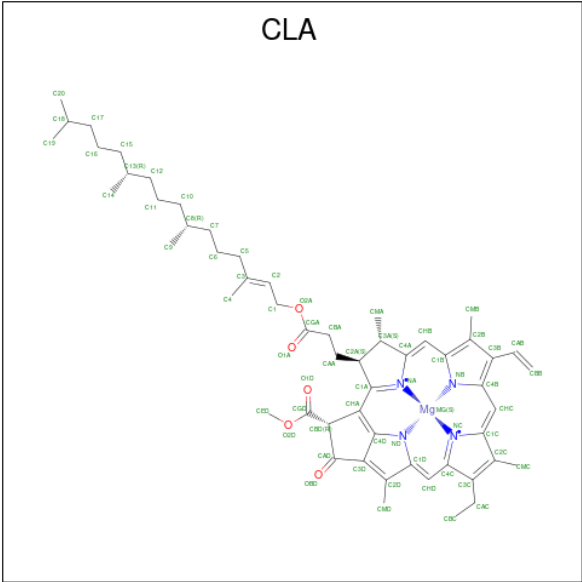
- Molecule 13 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula:  $C_{53}H_{80}O_2$ )

(labeled as "Ligand of Interest" by depositor).



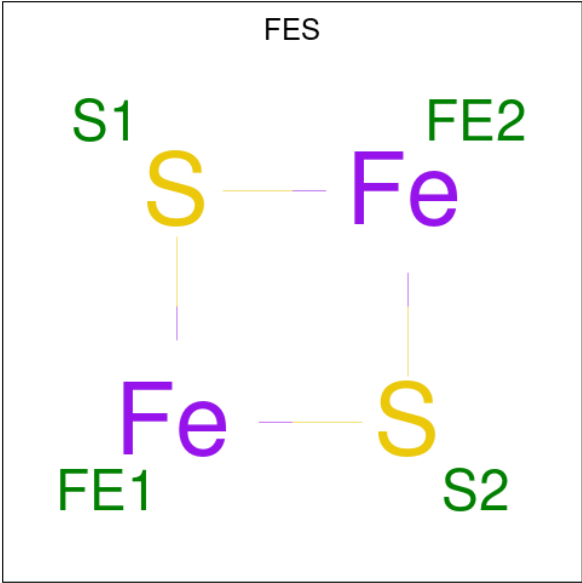
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			55	53	2	
13	A	1	Total	C	O	0
			55	53	2	
13	B	1	Total	C	O	0
			55	53	2	
13	I	1	Total	C	O	0
			55	53	2	
13	I	1	Total	C	O	0
			55	53	2	
13	I	1	Total	C	O	0
			55	53	2	
13	J	1	Total	C	O	0
			55	53	2	

- Molecule 14 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
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



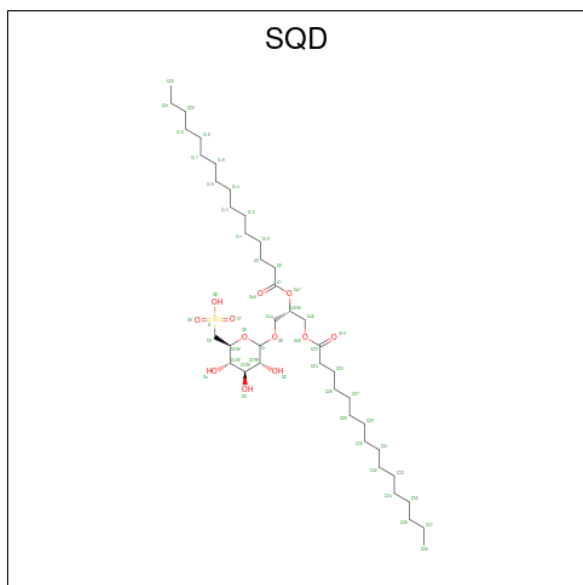
Mol	Chain	Residues	Atoms			AltConf
15	D	1	Total	Fe	S	0
			4	2	2	

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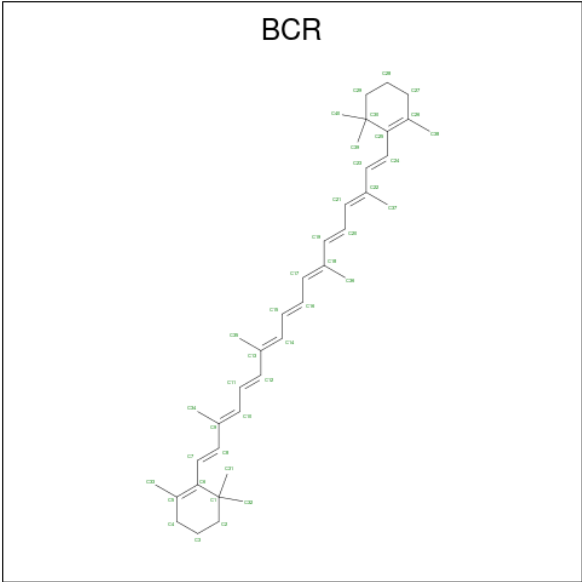
Mol	Chain	Residues	Atoms			AltConf
15	L	1	Total	Fe	S	0
			4	2	2	

- Molecule 16 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
16	D	1	Total	C	O	S	0
			54	41	12	1	
16	K	1	Total	C	O	S	0
			54	41	12	1	

- 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	H	1	Total	C	0
			40	40	
17	P	1	Total	C	0
			40	40	

- Molecule 18 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	Q	1	Total	Cu	0
			1	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

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: 




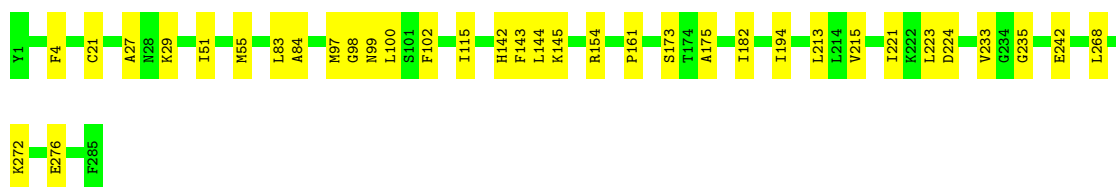
- Molecule 3: Cytochrome f

Chain C: 




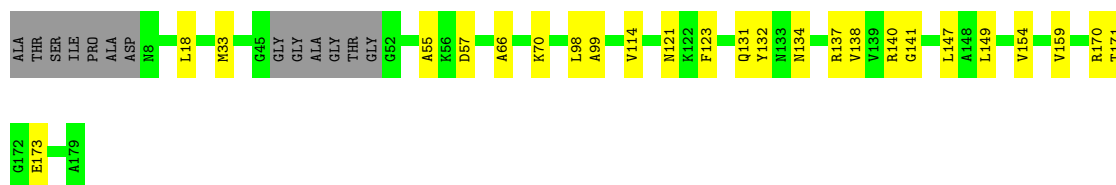
- Molecule 3: Cytochrome f

Chain K:  88% 12%




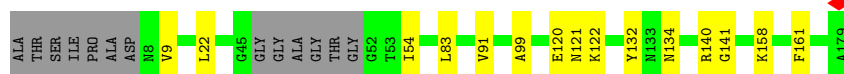
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain D:  79% 14% 7%




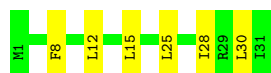
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic

Chain L:  84% 8% 7%




- Molecule 5: Cytochrome b6-f complex subunit 6

Chain E:  81% 19%




- Molecule 5: Cytochrome b6-f complex subunit 6

Chain M:  87% 13%



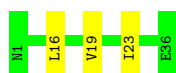
- Molecule 6: Cytochrome b6-f complex subunit 7

Chain F:  83% 17%

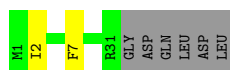
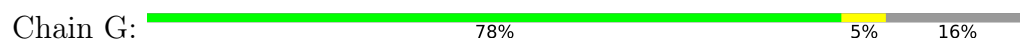


- Molecule 6: Cytochrome b6-f complex subunit 7

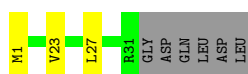
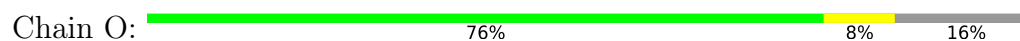
Chain N:  92% 8%



- Molecule 7: Cytochrome b6-f complex subunit 5



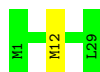
- Molecule 7: Cytochrome b6-f complex subunit 5



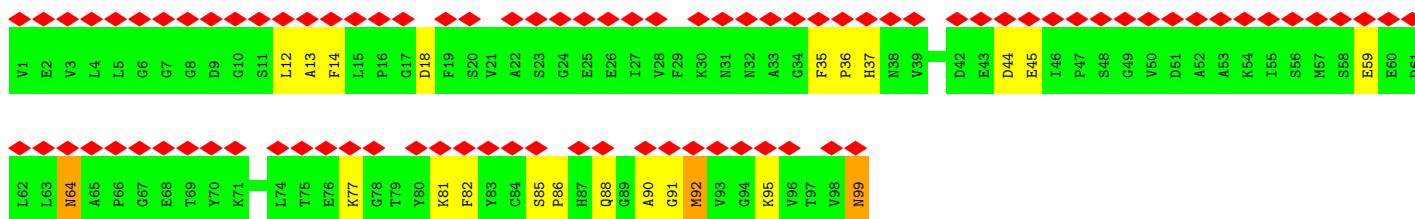
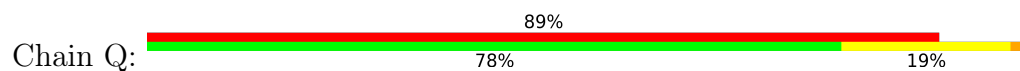
- Molecule 8: Cytochrome b6-f complex subunit 8



- Molecule 8: Cytochrome b6-f complex subunit 8



- Molecule 9: Plastocyanin, chloroplasic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87892	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	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	4.537	Depositor
Minimum map value	-2.549	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	344.0, 344.0, 344.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: HEC, HEM, UMQ, SQD, CLA, CU, FES, PL9, 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	0.18	0/1747	0.25	0/2382
1	I	0.19	0/1747	0.27	0/2382
2	B	0.15	0/1262	0.25	0/1733
2	J	0.16	0/1263	0.26	0/1733
3	C	0.12	0/2256	0.24	0/3058
3	K	0.14	0/2256	0.27	0/3058
4	D	0.14	0/1293	0.28	0/1769
4	L	0.12	0/1293	0.25	0/1769
5	E	0.17	0/247	0.26	0/333
5	M	0.15	0/247	0.20	0/333
6	F	0.17	0/265	0.25	0/359
6	N	0.15	0/265	0.20	0/359
7	G	0.18	0/254	0.21	0/344
7	O	0.16	0/254	0.20	0/344
8	H	0.18	0/227	0.19	0/309
8	P	0.18	0/228	0.20	0/309
9	Q	0.71	0/748	1.30	0/1012
All	All	0.22	0/15852	0.37	0/21586

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	11	0
1	I	1697	0	1724	17	0
2	B	1225	0	1276	9	0
2	J	1226	0	1276	11	0
3	C	2209	0	2253	19	0
3	K	2209	0	2253	29	0
4	D	1259	0	1232	16	0
4	L	1259	0	1232	11	0
5	E	243	0	268	5	0
5	M	243	0	268	2	0
6	F	264	0	282	6	0
6	N	264	0	282	2	0
7	G	249	0	273	2	0
7	O	249	0	273	2	0
8	H	222	0	234	2	0
8	P	223	0	234	2	0
9	Q	733	0	701	33	0
10	A	86	0	60	13	0
10	I	86	0	60	12	0
11	A	43	0	31	4	0
11	C	43	0	31	3	0
11	I	43	0	31	4	0
11	K	43	0	31	5	0
12	A	68	0	88	0	0
12	E	34	0	44	0	0
12	I	68	0	88	0	0
12	P	34	0	44	1	0
13	A	110	0	160	6	0
13	B	55	0	80	5	0
13	I	165	0	240	15	0
13	J	55	0	80	2	0
14	A	65	0	72	3	0
14	J	65	0	72	2	0
15	D	4	0	0	0	0
15	L	4	0	0	0	0
16	D	54	0	78	0	0
16	K	54	0	78	0	0
17	H	40	0	56	0	0
17	P	40	0	56	1	0
18	Q	1	0	0	0	0
All	All	16731	0	17265	214	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 6.

All (214) 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)
9:Q:12:LEU:CD1	9:Q:90:ALA:HB1	1.80	1.11
9:Q:12:LEU:HD12	9:Q:90:ALA:HB1	1.06	1.05
9:Q:12:LEU:HD12	9:Q:90:ALA:CB	1.91	1.00
9:Q:12:LEU:CD1	9:Q:90:ALA:CB	2.43	0.96
13:I:307:PL9:H501	2:J:75:ILE:HD12	1.52	0.90
10:I:303:HEM:HBC2	10:I:303:HEM:HMC2	1.56	0.86
10:I:302:HEM:HMB1	10:I:302:HEM:HBB2	1.59	0.85
10:I:302:HEM:HBC2	10:I:302:HEM:HMC2	1.58	0.84
10:I:303:HEM:HBB2	10:I:303:HEM:HMB2	1.59	0.84
10:A:302:HEM:HBC2	10:A:302:HEM:HMC2	1.57	0.84
9:Q:14:PHE:CD2	9:Q:82:PHE:HE1	1.97	0.82
10:A:302:HEM:HBB2	10:A:302:HEM:HMB2	1.59	0.82
10:A:301:HEM:HBC2	10:A:301:HEM:HMC2	1.60	0.80
10:A:301:HEM:HMB1	10:A:301:HEM:HBB2	1.63	0.79
9:Q:14:PHE:CD2	9:Q:82:PHE:CE1	2.71	0.79
9:Q:12:LEU:HD13	9:Q:90:ALA:CB	2.15	0.77
3:K:21:CYS:HB3	11:K:301:HEC:HAB	1.67	0.76
10:A:302:HEM:HHA	10:A:302:HEM:HBA1	1.67	0.75
9:Q:14:PHE:CE2	9:Q:82:PHE:CE1	2.75	0.74
1:I:151:VAL:HG12	13:I:307:PL9:H43	1.70	0.73
2:J:90:THR:HG22	2:J:151:ILE:HD11	1.71	0.72
9:Q:12:LEU:HB2	9:Q:90:ALA:O	1.91	0.71
10:I:303:HEM:HHA	10:I:303:HEM:HBA1	1.74	0.69
9:Q:64:ASN:H	9:Q:64:ASN:HD22	1.40	0.69
3:C:62:ALA:HB3	9:Q:88:GLN:OE1	1.94	0.67
11:A:303:HEC:HBB3	11:A:303:HEC:HHC	1.78	0.65
9:Q:77:LYS:HE3	9:Q:99:ASN:HA	1.79	0.65
1:A:54:MET:HE3	10:A:301:HEM:HBA1	1.78	0.64
9:Q:14:PHE:CE2	9:Q:82:PHE:CD1	2.85	0.64
1:I:170:ARG:HG2	1:I:175:VAL:HG12	1.79	0.63
10:I:302:HEM:HBC2	10:I:302:HEM:CMC	2.28	0.63
3:K:21:CYS:CB	11:K:301:HEC:HAB	2.27	0.63
10:I:302:HEM:HBB2	10:I:302:HEM:CMB	2.28	0.62
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.30	0.62
10:A:301:HEM:HBC2	10:A:301:HEM:CMC	2.30	0.61
10:I:303:HEM:HBC2	10:I:303:HEM:CMC	2.30	0.61
3:K:98:GLY:O	3:K:99:ASN:OD1	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:195:THR:CG2	1:I:199:MET:HE3	2.30	0.61
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	2.30	0.61
3:K:97:MET:O	3:K:100:LEU:HD13	2.01	0.61
13:B:201:PL9:H252	7:G:2:ILE:HD13	1.83	0.60
10:I:302:HEM:HBA1	10:I:302:HEM:CHA	2.31	0.60
3:C:213:LEU:HD21	3:C:215:VAL:O	2.01	0.60
10:I:303:HEM:HBB2	10:I:303:HEM:CMB	2.29	0.60
13:I:307:PL9:H351	2:J:101:MET:HE3	1.84	0.60
9:Q:35:PHE:HB2	9:Q:36:PRO:HA	1.84	0.60
10:I:302:HEM:HBA1	10:I:302:HEM:HHA	1.84	0.60
11:I:304:HEC:HHC	11:I:304:HEC:HBB3	1.83	0.60
1:I:150:ILE:HD13	13:I:307:PL9:H502	1.84	0.59
1:I:152:THR:HG21	1:I:170:ARG:HG3	1.85	0.59
9:Q:14:PHE:CE2	9:Q:92:MET:O	2.56	0.59
9:Q:12:LEU:HD13	9:Q:90:ALA:HB3	1.83	0.59
3:C:21:CYS:HB2	11:C:301:HEC:HAB	1.84	0.58
1:I:192:PRO:HB2	13:I:301:PL9:H252	1.84	0.58
1:I:151:VAL:HG13	13:I:307:PL9:H453	1.84	0.58
5:E:15:LEU:CD1	6:F:27:LEU:HD21	2.33	0.58
1:I:150:ILE:CD1	13:I:307:PL9:H502	2.33	0.58
10:A:302:HEM:HBC2	10:A:302:HEM:CMC	2.30	0.57
3:C:190:TYR:HD2	3:C:213:LEU:HD12	1.69	0.57
1:I:5:TYR:OH	1:I:15:GLN:OE1	2.21	0.57
9:Q:13:ALA:N	9:Q:92:MET:HE3	2.20	0.56
10:A:301:HEM:HBD2	10:A:301:HEM:HHA	1.88	0.56
9:Q:99:ASN:C	9:Q:99:ASN:HD22	2.14	0.56
4:D:98:LEU:HD23	4:D:99:ALA:O	2.06	0.55
5:E:28:ILE:O	5:E:28:ILE:HG22	2.05	0.55
9:Q:14:PHE:CE1	9:Q:92:MET:HG2	2.41	0.55
9:Q:12:LEU:O	9:Q:91:GLY:C	2.50	0.55
10:I:303:HEM:HBA1	10:I:303:HEM:CHA	2.33	0.55
4:D:66:ALA:O	4:D:70:LYS:HG2	2.07	0.54
3:K:143:PHE:C	3:K:144:LEU:HD12	2.33	0.54
1:A:128:THR:HA	1:A:131:PHE:HD2	1.73	0.53
3:K:98:GLY:O	3:K:100:LEU:HD12	2.07	0.53
1:I:151:VAL:CG1	13:I:307:PL9:H43	2.38	0.53
3:K:268:LEU:HD23	4:L:22:LEU:HD11	1.90	0.53
4:L:54:ILE:HD11	4:L:158:LYS:HD3	1.91	0.53
3:K:145:LYS:CE	3:K:242:GLU:HG3	2.39	0.53
9:Q:14:PHE:CZ	9:Q:92:MET:O	2.62	0.53
2:J:61:MET:SD	7:O:1:MET:HE1	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:173:GLU:N	4:D:173:GLU:OE1	2.42	0.52
9:Q:14:PHE:CE2	9:Q:82:PHE:HE1	2.21	0.52
9:Q:37:HIS:CE1	9:Q:92:MET:HE1	2.45	0.52
3:K:142:HIS:HB2	3:K:144:LEU:HD13	1.93	0.51
13:A:306:PL9:H422	2:B:81:PHE:CD1	2.46	0.51
13:I:307:PL9:H501	2:J:75:ILE:CD1	2.32	0.50
9:Q:14:PHE:HE2	9:Q:82:PHE:CD1	2.26	0.50
13:A:306:PL9:H33	14:A:307:CLA:H162	1.94	0.50
1:I:24:LYS:HZ3	1:I:207:ARG:NH2	2.09	0.50
14:J:201:CLA:O1D	13:J:202:PL9:H48	2.11	0.50
3:K:175:ALA:O	3:K:221:ILE:HD12	2.11	0.50
5:M:19:SER:O	5:M:23:ILE:HD12	2.10	0.50
10:A:302:HEM:HBA1	10:A:302:HEM:CHA	2.33	0.50
3:K:145:LYS:HE3	3:K:242:GLU:HG3	1.92	0.50
11:A:303:HEC:HBC3	11:A:303:HEC:HHD	1.94	0.50
4:D:55:ALA:HB3	4:D:159:VAL:HG23	1.93	0.50
6:F:16:LEU:HD12	8:H:16:THR:OG1	2.12	0.50
3:K:272:LYS:O	3:K:276:GLU:HG3	2.11	0.49
3:K:102:PHE:CE1	3:K:115:ILE:HD13	2.47	0.49
1:I:195:THR:HG22	1:I:199:MET:HE3	1.94	0.49
3:K:223:LEU:O	3:K:224:ASP:HB2	2.13	0.49
2:B:48:ILE:HG21	4:D:33:MET:HE1	1.95	0.49
6:F:36:GLU:N	6:F:36:GLU:OE1	2.46	0.49
7:O:23:VAL:O	7:O:27:LEU:HD23	2.13	0.49
9:Q:45:GLU:HB2	9:Q:81:LYS:HB3	1.95	0.48
3:K:102:PHE:CD1	3:K:115:ILE:HD13	2.48	0.48
1:I:160:VAL:HG13	1:I:161:ILE:HG23	1.95	0.48
14:A:307:CLA:O1D	13:B:201:PL9:H502	2.14	0.48
3:C:187:LYS:HE2	9:Q:44:ASP:CG	2.38	0.48
3:C:20:VAL:HG23	3:C:20:VAL:O	2.14	0.47
4:D:132:TYR:CE1	4:D:138:VAL:HG22	2.49	0.47
3:K:27:ALA:HB3	3:K:235:GLY:HA2	1.95	0.47
4:L:9:VAL:O	4:L:9:VAL:HG12	2.14	0.47
1:A:81:LEU:HG	13:A:308:PL9:H253	1.97	0.47
1:A:123:VAL:O	1:A:126:VAL:HG22	2.14	0.47
1:A:131:PHE:CE1	1:A:191:LEU:HB3	2.50	0.47
4:L:83:LEU:HD21	4:L:161:PHE:CB	2.44	0.47
1:A:54:MET:CE	10:A:301:HEM:HBA1	2.45	0.47
11:I:304:HEC:HBB3	11:I:304:HEC:CHC	2.45	0.47
2:B:115:GLU:O	2:B:115:GLU:HG2	2.15	0.46
1:I:136:TYR:OH	1:I:143:ILE:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:303:HEC:HHD	11:A:303:HEC:CBC	2.45	0.46
9:Q:64:ASN:HD22	9:Q:64:ASN:N	2.02	0.46
9:Q:85:SER:HB3	9:Q:86:PRO:HD3	1.98	0.46
4:D:137:ARG:HH11	4:D:171:THR:HG22	1.81	0.46
11:K:301:HEC:CMC	11:K:301:HEC:HBC3	2.46	0.46
2:B:73:LEU:O	13:B:201:PL9:HC2	2.15	0.46
5:E:8:PHE:O	5:E:12:LEU:HD23	2.15	0.46
5:M:8:PHE:O	5:M:12:LEU:HD23	2.15	0.46
13:A:306:PL9:H33	14:A:307:CLA:C16	2.44	0.46
6:F:12:VAL:O	6:F:16:LEU:HD23	2.16	0.46
4:L:91:VAL:HG13	4:L:99:ALA:HB3	1.98	0.45
4:L:121:ASN:OD1	4:L:134:ASN:HB3	2.16	0.45
1:I:81:LEU:HG	13:I:308:PL9:H252	1.98	0.45
9:Q:35:PHE:HA	9:Q:36:PRO:C	2.41	0.45
1:A:41:LEU:O	1:A:45:LEU:HD13	2.16	0.45
11:C:301:HEC:CMC	11:C:301:HEC:HBC3	2.47	0.45
1:A:138:LEU:N	1:A:139:PRO:CD	2.80	0.45
3:K:233:VAL:HG22	3:K:233:VAL:O	2.16	0.45
4:D:131:GLN:CD	4:D:140:ARG:HH21	2.25	0.45
3:C:211:PRO:HB2	3:C:228:THR:CG2	2.47	0.45
11:C:301:HEC:HBC3	11:C:301:HEC:HMC1	1.97	0.45
11:I:304:HEC:CBC	11:I:304:HEC:HHD	2.46	0.45
3:K:55:MET:O	3:K:55:MET:HG3	2.17	0.45
2:J:95:LEU:O	2:J:98:VAL:HG12	2.17	0.45
6:F:28:LEU:HD23	8:H:24:TRP:HD1	1.80	0.45
6:N:16:LEU:HD11	8:P:12:MET:HE2	1.99	0.45
3:C:170:VAL:CG1	3:C:230:ASN:OD1	2.65	0.44
3:C:74:VAL:HG23	3:C:114:VAL:HG12	2.00	0.44
5:E:25:LEU:HD12	5:E:30:LEU:HD22	1.98	0.44
2:B:145:ILE:HA	13:B:201:PL9:H352	1.99	0.44
2:J:145:ILE:HD12	13:J:202:PL9:C35	2.48	0.44
3:K:29:LYS:HB2	3:K:154:ARG:NH1	2.33	0.44
4:D:132:TYR:CE2	4:D:147:LEU:HG	2.52	0.44
5:E:25:LEU:CD1	5:E:30:LEU:HD13	2.48	0.44
11:K:301:HEC:CMB	11:K:301:HEC:HBB3	2.48	0.44
8:P:12:MET:HE3	12:P:102:UMQ:HB1	1.98	0.44
2:B:71:THR:O	2:B:71:THR:HG23	2.17	0.44
13:I:307:PL9:H351	13:I:307:PL9:H371	1.69	0.44
11:K:301:HEC:HBC3	11:K:301:HEC:HMC1	1.99	0.44
2:B:96:LEU:O	2:B:100:LEU:HD13	2.18	0.44
13:I:308:PL9:H151	13:I:308:PL9:H202	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:115:GLU:CG	2:J:115:GLU:O	2.65	0.44
4:L:91:VAL:HG13	4:L:99:ALA:CB	2.48	0.44
4:L:122:LYS:HB2	4:L:132:TYR:O	2.17	0.44
1:A:127:LEU:O	1:A:131:PHE:CD2	2.70	0.44
3:C:62:ALA:CB	9:Q:88:GLN:OE1	2.65	0.43
3:C:27:ALA:HB3	3:C:235:GLY:HA2	2.00	0.43
3:C:190:TYR:CD2	3:C:213:LEU:HD12	2.52	0.43
3:K:4:PHE:HE2	3:K:161:PRO:CG	2.31	0.43
3:C:25:HIS:CE1	3:C:153:ASN:HD21	2.37	0.43
4:D:114:VAL:CG1	4:D:123:PHE:HB3	2.48	0.43
3:K:194:ILE:HG21	3:K:221:ILE:HD11	2.01	0.43
4:D:57:ASP:OD1	4:D:57:ASP:C	2.62	0.43
13:B:201:PL9:H33	7:G:7:PHE:CD2	2.53	0.43
4:D:149:LEU:HD11	4:D:170:ARG:CZ	2.49	0.43
1:A:128:THR:HA	1:A:131:PHE:CD2	2.53	0.42
13:I:307:PL9:H353	14:J:201:CLA:H18	1.99	0.42
3:C:274:GLN:OE1	4:D:18:LEU:HD22	2.19	0.42
2:J:134:LEU:O	2:J:138:VAL:HG23	2.18	0.42
4:L:83:LEU:HD21	4:L:161:PHE:HB3	2.01	0.42
3:K:154:ARG:HG2	3:K:154:ARG:HH11	1.84	0.42
3:C:10:GLU:OE1	3:C:106:ARG:NH1	2.52	0.42
11:I:304:HEC:HHD	11:I:304:HEC:HBC3	2.02	0.42
1:A:81:LEU:CD2	13:A:308:PL9:H253	2.49	0.42
2:B:98:VAL:O	2:B:101:MET:HG2	2.19	0.42
9:Q:13:ALA:H	9:Q:92:MET:HE3	1.83	0.42
4:L:120:GLU:OE1	4:L:122:LYS:HE2	2.20	0.42
2:B:137:THR:O	2:B:141:LEU:HD13	2.19	0.42
6:F:34:VAL:HG22	6:F:34:VAL:O	2.19	0.42
3:K:173:SER:O	3:K:224:ASP:OD1	2.38	0.42
9:Q:18:ASP:OD1	9:Q:95:LYS:HB3	2.20	0.42
3:C:213:LEU:HD23	3:C:214:LEU:N	2.34	0.42
3:K:142:HIS:HB2	3:K:144:LEU:CD1	2.50	0.42
9:Q:85:SER:HB3	9:Q:86:PRO:CD	2.49	0.42
17:P:101:BCR:H24C	17:P:101:BCR:H371	1.93	0.42
13:A:306:PL9:H401	13:A:306:PL9:H421	1.87	0.42
4:D:121:ASN:OD1	4:D:134:ASN:HB3	2.19	0.41
4:D:140:ARG:HG2	4:D:141:GLY:N	2.35	0.41
3:K:51:ILE:HG23	3:K:154:ARG:NH2	2.36	0.41
11:A:303:HEC:HBB3	11:A:303:HEC:CHC	2.45	0.41
4:D:154:VAL:O	4:D:154:VAL:HG23	2.21	0.41
3:K:213:LEU:HD21	3:K:215:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:34:TYR:CE2	1:I:211:ILE:HD11	2.56	0.41
3:K:182:ILE:HD11	3:K:213:LEU:HD11	2.02	0.41
4:L:140:ARG:HG2	4:L:141:GLY:N	2.36	0.41
3:C:186:GLU:OE1	3:C:186:GLU:N	2.54	0.41
3:C:202:GLU:N	3:C:202:GLU:OE1	2.54	0.41
3:C:211:PRO:HB2	3:C:228:THR:HG21	2.03	0.41
3:K:51:ILE:HG23	3:K:154:ARG:HH21	1.86	0.41
13:I:308:PL9:H122	13:I:308:PL9:H101	1.97	0.40
3:K:83:LEU:HD23	3:K:84:ALA:O	2.21	0.40
1:I:116:LEU:HB3	1:I:205:MET:HE1	2.03	0.40
6:N:19:VAL:O	6:N:23:ILE:HG12	2.22	0.40
2:J:71:THR:HG23	2:J:71:THR:O	2.20	0.40
13:I:307:PL9:H351	2:J:101:MET:CE	2.49	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%)	207 (98%)	5 (2%)	0	100	100
1	I	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
2	B	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
2	J	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
3	C	283/285 (99%)	272 (96%)	11 (4%)	0	100	100
3	K	283/285 (99%)	277 (98%)	6 (2%)	0	100	100
4	D	162/179 (90%)	153 (94%)	9 (6%)	0	100	100
4	L	162/179 (90%)	151 (93%)	11 (7%)	0	100	100
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
5	M	29/31 (94%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	34/36 (94%)	34 (100%)	0	0	100	100
6	N	34/36 (94%)	34 (100%)	0	0	100	100
7	G	29/37 (78%)	29 (100%)	0	0	100	100
7	O	29/37 (78%)	28 (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	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
All	All	1963/2043 (96%)	1902 (97%)	61 (3%)	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%)	185 (100%)	0	100	100
1	I	185/186 (100%)	185 (100%)	0	100	100
2	B	134/135 (99%)	134 (100%)	0	100	100
2	J	134/135 (99%)	134 (100%)	0	100	100
3	C	242/242 (100%)	242 (100%)	0	100	100
3	K	242/242 (100%)	242 (100%)	0	100	100
4	D	135/141 (96%)	135 (100%)	0	100	100
4	L	135/141 (96%)	135 (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	26/31 (84%)	26 (100%)	0	100	100
7	O	26/31 (84%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	24 (100%)	0	100	100
9	Q	79/79 (100%)	75 (95%)	4 (5%)	21	51
All	All	1675/1701 (98%)	1671 (100%)	4 (0%)	85	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Q	59	GLU
9	Q	64	ASN
9	Q	92	MET
9	Q	99	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
3	C	238	GLN
1	I	29	HIS
1	I	77	ASN
2	J	121	GLN
3	K	25	HIS
3	K	142	HIS
3	K	225	GLN
4	L	72	HIS
4	L	131	GLN
4	L	135	GLN
9	Q	64	ASN
9	Q	99	ASN

### 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
16	SQD	D	202	-	52,54,54	1.56	7 (13%)	62,65,65	1.34	6 (9%)
12	UMQ	I	305	-	35,35,35	0.53	0	46,46,46	0.60	0
10	HEM	A	301	1	50,50,50	1.41	7 (14%)	67,82,82	1.16	7 (10%)
11	HEC	I	304	1	46,50,50	1.84	6 (13%)	58,82,82	1.55	4 (6%)
13	PL9	I	307	-	55,55,55	1.12	5 (9%)	68,69,69	1.64	14 (20%)
10	HEM	A	302	1	50,50,50	1.41	8 (16%)	67,82,82	1.06	4 (5%)
11	HEC	C	301	3	46,50,50	1.84	7 (15%)	58,82,82	1.87	4 (6%)
17	BCR	P	101	-	41,41,41	0.30	0	56,56,56	0.50	0
13	PL9	I	301	-	55,55,55	0.82	2 (3%)	68,69,69	1.66	11 (16%)
10	HEM	I	302	1	50,50,50	1.40	7 (14%)	67,82,82	1.11	3 (4%)
17	BCR	H	101	-	41,41,41	0.30	0	56,56,56	0.47	0
12	UMQ	E	101	-	35,35,35	0.54	0	46,46,46	0.59	0
16	SQD	K	302	-	52,54,54	1.56	8 (15%)	62,65,65	1.37	5 (8%)
12	UMQ	A	304	-	35,35,35	0.54	0	46,46,46	0.61	0
10	HEM	I	303	1	50,50,50	1.41	7 (14%)	67,82,82	1.07	5 (7%)
12	UMQ	A	305	-	35,35,35	0.52	0	46,46,46	0.61	0
11	HEC	K	301	3	46,50,50	1.84	8 (17%)	58,82,82	1.84	4 (6%)
12	UMQ	I	306	-	35,35,35	0.52	0	46,46,46	0.62	0
14	CLA	A	307	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
13	PL9	A	306	-	55,55,55	0.94	3 (5%)	68,69,69	1.85	14 (20%)
15	FES	L	201	4	0,4,4	-	-	-	-	-
14	CLA	J	201	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
13	PL9	A	308	-	55,55,55	1.13	4 (7%)	68,69,69	1.55	12 (17%)
15	FES	D	201	4	0,4,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	UMQ	P	102	-	35,35,35	0.54	0	46,46,46	0.58	0
13	PL9	J	202	-	55,55,55	1.01	3 (5%)	68,69,69	1.58	15 (22%)
13	PL9	B	201	-	55,55,55	1.45	5 (9%)	68,69,69	1.50	11 (16%)
13	PL9	I	308	-	55,55,55	1.16	6 (10%)	68,69,69	1.54	9 (13%)
11	HEC	A	303	1	46,50,50	1.82	7 (15%)	58,82,82	1.56	5 (8%)

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
16	SQD	D	202	-	-	21/49/69/69	0/1/1/1
12	UMQ	I	305	-	-	2/20/60/60	0/2/2/2
10	HEM	A	301	1	-	4/14/54/54	-
11	HEC	I	304	1	-	5/14/54/54	-
13	PL9	I	307	-	-	26/53/73/73	0/1/1/1
10	HEM	A	302	1	-	5/14/54/54	-
11	HEC	C	301	3	-	8/14/54/54	-
17	BCR	P	101	-	-	4/29/63/63	0/2/2/2
13	PL9	I	301	-	-	28/53/73/73	0/1/1/1
10	HEM	I	302	1	-	4/14/54/54	-
17	BCR	H	101	-	-	4/29/63/63	0/2/2/2
12	UMQ	E	101	-	-	2/20/60/60	0/2/2/2
16	SQD	K	302	-	-	17/49/69/69	0/1/1/1
12	UMQ	A	304	-	-	2/20/60/60	0/2/2/2
10	HEM	I	303	1	-	3/14/54/54	-
12	UMQ	A	305	-	-	8/20/60/60	0/2/2/2
11	HEC	K	301	3	-	10/14/54/54	-
12	UMQ	I	306	-	-	8/20/60/60	0/2/2/2
14	CLA	A	307	-	1/1/15/20	15/39/115/115	-
13	PL9	A	306	-	-	29/53/73/73	0/1/1/1
15	FES	L	201	4	-	-	0/1/1/1
14	CLA	J	201	-	1/1/15/20	18/39/115/115	-
13	PL9	A	308	-	-	15/53/73/73	0/1/1/1
15	FES	D	201	4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	UMQ	P	102	-	-	2/20/60/60	0/2/2/2
13	PL9	J	202	-	-	23/53/73/73	0/1/1/1
13	PL9	B	201	-	-	29/53/73/73	0/1/1/1
13	PL9	I	308	-	-	21/53/73/73	0/1/1/1
11	HEC	A	303	1	-	6/14/54/54	-

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	301	HEC	CAC-C3C	6.23	1.55	1.35
11	I	304	HEC	CAB-C3B	6.17	1.55	1.35
11	A	303	HEC	CAB-C3B	6.16	1.55	1.35
11	K	301	HEC	CAC-C3C	6.15	1.55	1.35
11	I	304	HEC	CAC-C3C	6.12	1.54	1.35
11	A	303	HEC	CAC-C3C	6.11	1.54	1.35
11	K	301	HEC	CAB-C3B	6.07	1.54	1.35
11	C	301	HEC	CAB-C3B	6.06	1.54	1.35
11	C	301	HEC	C3D-C2D	5.68	1.53	1.38
11	K	301	HEC	C3D-C2D	5.66	1.53	1.38
11	I	304	HEC	C3D-C2D	5.62	1.53	1.38
13	B	201	PL9	C3-C4	-5.57	1.40	1.49
11	A	303	HEC	C3D-C2D	5.44	1.53	1.38
16	D	202	SQD	O48-C23	4.71	1.47	1.33
16	K	302	SQD	O48-C23	4.66	1.46	1.33
13	B	201	PL9	C52-C5	-4.62	1.41	1.50
10	I	302	HEM	FE-NB	3.81	2.06	1.94
16	D	202	SQD	O47-C45	-3.74	1.37	1.46
10	I	303	HEM	FE-NB	3.69	2.06	1.94
13	I	307	PL9	C35-C34	-3.68	1.41	1.50
13	B	201	PL9	C7-C3	-3.66	1.46	1.51
13	A	306	PL9	C6-C1	-3.65	1.42	1.48
13	B	201	PL9	C6-C1	-3.63	1.42	1.48
10	A	302	HEM	FE-ND	3.57	2.05	1.94
16	K	302	SQD	O47-C45	-3.56	1.38	1.46
10	A	301	HEM	FE-NC	3.55	2.06	1.95
14	A	307	CLA	C1D-ND	3.51	1.42	1.37
13	A	308	PL9	C3-C4	-3.44	1.44	1.49
16	K	302	SQD	O47-C7	3.42	1.43	1.34
14	J	201	CLA	C1D-ND	3.42	1.42	1.37
10	I	303	HEM	FE-ND	3.32	2.05	1.94
10	I	302	HEM	FE-NC	3.29	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	308	PL9	C7-C3	-3.28	1.46	1.51
10	A	301	HEM	FE-NB	3.27	2.05	1.94
16	D	202	SQD	O47-C7	3.26	1.43	1.34
10	A	301	HEM	FE-ND	3.26	2.04	1.94
10	A	302	HEM	FE-NB	3.25	2.04	1.94
16	K	302	SQD	O5-C1	3.15	1.49	1.41
13	I	308	PL9	C3-C4	-3.14	1.44	1.49
13	J	202	PL9	C3-C4	-3.12	1.44	1.49
16	K	302	SQD	C24-C23	3.12	1.59	1.50
16	D	202	SQD	O5-C1	3.09	1.49	1.41
16	D	202	SQD	C24-C23	3.06	1.59	1.50
13	A	308	PL9	C7-C3	-3.06	1.47	1.51
10	I	303	HEM	FE-NA	3.00	2.05	1.95
14	J	201	CLA	C4B-NB	2.95	1.41	1.37
13	I	307	PL9	C3-C4	-2.95	1.44	1.49
14	A	307	CLA	C4B-NB	2.92	1.41	1.37
10	A	302	HEM	FE-NA	2.89	2.04	1.95
10	A	302	HEM	CAC-C3C	2.88	1.55	1.47
10	I	302	HEM	CAC-C3C	2.88	1.55	1.47
10	A	302	HEM	CAB-C3B	2.87	1.55	1.47
10	I	303	HEM	CAB-C3B	2.86	1.55	1.47
10	A	301	HEM	CAB-C3B	2.85	1.55	1.47
10	A	301	HEM	CAC-C3C	2.85	1.55	1.47
10	I	303	HEM	CAC-C3C	2.83	1.54	1.47
10	I	302	HEM	CAB-C3B	2.82	1.54	1.47
10	I	302	HEM	FE-NA	2.73	2.04	1.95
14	J	201	CLA	C1B-C2B	2.71	1.49	1.43
14	A	307	CLA	C1B-C2B	2.66	1.49	1.43
13	I	307	PL9	C46-C44	-2.64	1.45	1.51
10	A	301	HEM	FE-NA	2.57	2.03	1.95
13	I	308	PL9	C6-C1	-2.54	1.44	1.48
13	J	202	PL9	C6-C1	-2.53	1.44	1.48
10	I	303	HEM	FE-NC	2.50	2.03	1.95
10	A	302	HEM	FE-NC	2.48	2.03	1.95
13	I	307	PL9	C7-C3	-2.46	1.48	1.51
10	I	302	HEM	FE-ND	2.45	2.02	1.94
13	A	308	PL9	C6-C1	-2.40	1.44	1.48
13	I	308	PL9	C25-C24	-2.39	1.44	1.50
13	J	202	PL9	C7-C3	-2.38	1.48	1.51
13	I	307	PL9	C6-C1	-2.38	1.44	1.48
13	A	306	PL9	C3-C4	-2.35	1.45	1.49
13	I	301	PL9	C6-C1	-2.35	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	I	308	PL9	C52-C5	-2.31	1.46	1.50
14	J	201	CLA	CHC-C1C	2.30	1.43	1.38
14	J	201	CLA	C3B-C4B	2.27	1.49	1.42
11	A	303	HEC	C3C-C2C	-2.26	1.33	1.41
11	I	304	HEC	C3C-C2C	-2.25	1.33	1.41
11	K	301	HEC	C3B-C2B	-2.19	1.33	1.41
11	C	301	HEC	C3B-C2B	-2.18	1.33	1.41
16	K	302	SQD	O9-S	2.18	1.51	1.45
13	A	308	PL9	C53-C6	-2.17	1.46	1.50
14	A	307	CLA	C3B-C4B	2.16	1.49	1.42
14	A	307	CLA	CHC-C1C	2.16	1.42	1.38
11	A	303	HEC	C3B-C2B	-2.16	1.33	1.41
16	D	202	SQD	O9-S	2.15	1.51	1.45
11	I	304	HEC	C3B-C2B	-2.15	1.33	1.41
13	A	306	PL9	C53-C6	-2.13	1.46	1.50
13	B	201	PL9	C53-C6	-2.11	1.46	1.50
14	J	201	CLA	CMD-C2D	-2.10	1.46	1.50
16	K	302	SQD	O7-S	2.09	1.51	1.45
10	A	302	HEM	C2A-C3A	-2.09	1.33	1.38
10	I	302	HEM	C2A-C3A	-2.07	1.33	1.38
16	D	202	SQD	O7-S	2.07	1.51	1.45
14	A	307	CLA	CMD-C2D	-2.07	1.46	1.50
11	K	301	HEC	CMD-C2D	2.06	1.55	1.50
10	I	303	HEM	C2A-C3A	-2.06	1.33	1.38
13	I	301	PL9	C53-C6	-2.06	1.46	1.50
11	A	303	HEC	CMA-C3A	2.05	1.55	1.50
14	A	307	CLA	CMB-C2B	-2.05	1.46	1.50
11	K	301	HEC	CMC-C2C	2.05	1.55	1.50
11	K	301	HEC	C3C-C2C	-2.04	1.34	1.41
14	A	307	CLA	MG-NB	-2.04	2.01	2.05
11	C	301	HEC	CMC-C2C	2.04	1.55	1.50
14	J	201	CLA	CMB-C2B	-2.04	1.46	1.50
16	K	302	SQD	C8-C7	2.03	1.56	1.50
10	A	301	HEM	C2A-C3A	-2.03	1.33	1.38
11	I	304	HEC	CMB-C2B	2.02	1.54	1.50
11	K	301	HEC	CMA-C3A	2.01	1.54	1.50
11	C	301	HEC	CMA-C3A	2.01	1.54	1.50
11	C	301	HEC	CMB-C2B	2.01	1.54	1.50
14	J	201	CLA	MG-NB	-2.01	2.01	2.05
10	A	302	HEM	CMC-C2C	2.00	1.54	1.50
11	A	303	HEC	CMB-C2B	2.00	1.54	1.50
13	I	308	PL9	C53-C6	-2.00	1.46	1.50

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	301	HEC	CBB-CAB-C3B	-8.89	109.66	127.43
11	K	301	HEC	CBB-CAB-C3B	-8.49	110.46	127.43
11	C	301	HEC	CBC-CAC-C3C	-7.99	111.47	127.43
11	K	301	HEC	CBC-CAC-C3C	-7.98	111.49	127.43
11	I	304	HEC	CBB-CAB-C3B	-7.97	111.51	127.43
11	A	303	HEC	CBB-CAB-C3B	-7.93	111.59	127.43
13	I	301	PL9	C7-C3-C4	7.45	123.04	116.91
13	A	306	PL9	C40-C39-C41	6.50	126.50	115.23
14	A	307	CLA	C4A-NA-C1A	6.48	109.64	106.68
14	J	201	CLA	C4A-NA-C1A	6.29	109.55	106.68
13	A	306	PL9	C7-C3-C4	6.25	122.05	116.91
13	I	308	PL9	C7-C3-C4	5.66	121.57	116.91
13	I	301	PL9	C7-C3-C2	-5.22	117.24	123.39
13	J	202	PL9	C7-C3-C4	5.12	121.13	116.91
13	I	307	PL9	C7-C3-C4	4.91	120.95	116.91
16	K	302	SQD	O47-C7-C8	4.70	121.66	111.48
13	I	308	PL9	C7-C3-C2	-4.44	118.16	123.39
13	A	308	PL9	C7-C3-C4	4.42	120.55	116.91
13	A	306	PL9	C7-C3-C2	-4.32	118.29	123.39
16	D	202	SQD	O9-S-O7	-4.07	100.58	113.82
13	B	201	PL9	C7-C3-C4	4.06	120.25	116.91
13	I	307	PL9	C42-C43-C44	-4.03	118.39	127.62
13	A	306	PL9	C20-C19-C21	3.96	122.10	115.23
13	I	307	PL9	C40-C39-C41	3.91	122.02	115.23
13	J	202	PL9	C7-C3-C2	-3.86	118.84	123.39
16	D	202	SQD	O47-C7-C8	3.85	119.81	111.48
16	K	302	SQD	O9-S-O7	-3.84	101.33	113.82
13	I	307	PL9	C7-C3-C2	-3.73	119.00	123.39
11	I	304	HEC	C4D-ND-C1D	3.66	111.79	105.82
13	I	308	PL9	C27-C28-C29	-3.61	119.36	127.62
11	A	303	HEC	C4D-ND-C1D	3.54	111.59	105.82
13	A	308	PL9	C7-C3-C2	-3.52	119.24	123.39
16	D	202	SQD	O7-S-C6	3.40	111.84	106.76
13	J	202	PL9	C40-C39-C41	3.39	121.12	115.23
11	C	301	HEC	C4D-ND-C1D	3.25	111.12	105.82
13	B	201	PL9	C22-C23-C24	-3.24	120.21	127.62
16	K	302	SQD	O9-S-C6	3.22	111.57	106.76
16	K	302	SQD	O7-S-C6	3.22	111.57	106.76
13	B	201	PL9	C27-C28-C29	-3.19	120.33	127.62
11	K	301	HEC	C4D-ND-C1D	3.17	110.99	105.82
14	A	307	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
13	A	308	PL9	C22-C23-C24	-3.10	120.53	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	201	PL9	C7-C3-C2	-3.04	119.81	123.39
13	B	201	PL9	C40-C39-C41	3.02	120.47	115.23
14	J	201	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
16	D	202	SQD	O9-S-C6	3.00	111.24	106.76
13	A	306	PL9	C27-C28-C29	-3.00	120.77	127.62
14	J	201	CLA	C3B-C4B-NB	-2.97	107.88	110.53
13	J	202	PL9	C22-C23-C24	-2.88	121.03	127.62
13	A	308	PL9	C20-C19-C21	2.88	120.22	115.23
13	A	308	PL9	C40-C39-C41	2.85	120.17	115.23
16	D	202	SQD	O48-C23-C24	2.84	120.50	111.83
14	J	201	CLA	O2D-CGD-CBD	2.82	116.15	111.23
11	A	303	HEC	CBC-CAC-C3C	-2.72	122.00	127.43
13	I	307	PL9	C20-C19-C21	2.70	119.92	115.23
14	A	307	CLA	C3B-C4B-NB	-2.69	108.13	110.53
13	B	201	PL9	C12-C13-C14	-2.69	121.46	127.62
16	K	302	SQD	O48-C23-C24	2.69	120.02	111.83
13	I	307	PL9	C7-C8-C9	-2.66	122.24	126.83
11	I	304	HEC	CBC-CAC-C3C	-2.64	122.15	127.43
13	I	301	PL9	C22-C23-C24	-2.64	121.59	127.62
13	A	306	PL9	C37-C38-C39	-2.62	121.63	127.62
13	J	202	PL9	C7-C8-C9	-2.60	122.36	126.83
13	I	301	PL9	C40-C39-C41	2.59	119.72	115.23
13	J	202	PL9	C35-C34-C36	2.56	119.68	115.23
13	I	308	PL9	C40-C39-C41	2.55	119.65	115.23
13	A	306	PL9	C41-C39-C38	-2.54	115.47	121.17
13	A	306	PL9	C40-C39-C38	-2.52	117.17	123.63
13	I	307	PL9	C35-C34-C33	-2.51	117.19	123.63
13	A	306	PL9	C25-C24-C26	2.51	119.58	115.23
13	A	306	PL9	C26-C24-C23	-2.48	115.59	121.17
13	A	306	PL9	C22-C23-C24	-2.48	121.94	127.62
13	I	308	PL9	C10-C9-C11	2.47	119.52	115.23
13	I	301	PL9	C36-C34-C33	-2.47	115.61	121.17
13	I	308	PL9	O2-C1-C6	2.47	124.41	120.48
13	J	202	PL9	C32-C33-C34	-2.47	121.98	127.62
13	I	301	PL9	C7-C8-C9	-2.46	122.59	126.83
13	B	201	PL9	O1-C4-C3	-2.46	118.14	120.73
11	I	304	HEC	C2A-C1A-NA	-2.45	107.96	110.32
13	I	308	PL9	C22-C23-C24	-2.44	122.03	127.62
11	A	303	HEC	C2A-C1A-NA	-2.43	107.98	110.32
13	A	306	PL9	C7-C8-C9	-2.43	122.65	126.83
14	A	307	CLA	CHB-C4A-NA	2.43	127.90	124.40
14	J	201	CLA	CHB-C4A-NA	2.43	127.90	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	308	PL9	O2-C1-C6	2.43	124.34	120.48
13	A	308	PL9	C37-C38-C39	-2.40	122.13	127.62
13	I	307	PL9	C12-C13-C14	-2.39	122.15	127.62
10	A	302	HEM	C3B-C2B-C1B	2.38	108.20	106.41
10	A	301	HEM	C4D-ND-C1D	2.37	108.01	105.21
10	A	301	HEM	C3B-C2B-C1B	2.35	108.17	106.41
13	A	306	PL9	C12-C13-C14	-2.34	122.26	127.62
13	I	301	PL9	O2-C1-C6	2.34	124.20	120.48
10	A	301	HEM	C1B-NB-C4B	2.34	107.98	105.21
13	I	307	PL9	O2-C1-C6	2.34	124.20	120.48
13	I	307	PL9	C41-C39-C38	-2.33	115.93	121.17
13	I	308	PL9	C12-C13-C14	-2.32	122.31	127.62
13	A	308	PL9	O1-C4-C3	-2.31	118.29	120.73
13	J	202	PL9	C12-C13-C14	-2.31	122.34	127.62
13	I	307	PL9	C30-C29-C28	-2.30	117.72	123.63
16	D	202	SQD	O8-S-C6	2.29	110.39	105.97
13	J	202	PL9	C27-C28-C29	-2.28	122.41	127.62
13	J	202	PL9	C20-C19-C21	2.28	119.18	115.23
13	I	307	PL9	O1-C4-C3	-2.27	118.34	120.73
10	I	302	HEM	C1B-NB-C4B	2.26	107.88	105.21
13	I	301	PL9	C8-C7-C3	2.24	117.82	112.03
14	J	201	CLA	O2A-CGA-O1A	-2.24	118.04	123.63
10	I	302	HEM	C4D-ND-C1D	2.21	107.83	105.21
13	I	301	PL9	C27-C28-C29	-2.21	122.56	127.62
13	J	202	PL9	C21-C19-C18	-2.21	116.21	121.17
10	A	301	HEM	C3D-C4D-ND	-2.20	107.75	110.17
13	B	201	PL9	O2-C1-C6	2.20	123.98	120.48
10	I	303	HEM	C4D-ND-C1D	2.20	107.81	105.21
14	A	307	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	J	202	PL9	C36-C34-C33	-2.19	116.26	121.17
13	J	202	PL9	O2-C1-C6	2.18	123.96	120.48
13	A	308	PL9	C32-C33-C34	-2.18	122.64	127.62
10	I	302	HEM	C3B-C2B-C1B	2.18	108.05	106.41
13	I	301	PL9	O2-C1-C2	-2.17	116.90	121.83
13	A	306	PL9	C35-C34-C36	2.15	118.96	115.23
13	A	308	PL9	O2-C1-C2	-2.15	116.95	121.83
10	A	302	HEM	C4D-ND-C1D	2.14	107.74	105.21
10	I	303	HEM	C1B-NB-C4B	2.14	107.74	105.21
13	J	202	PL9	O1-C4-C3	-2.14	118.48	120.73
13	I	308	PL9	O2-C1-C2	-2.12	117.00	121.83
10	I	303	HEM	C3B-C2B-C1B	2.12	108.00	106.41
13	A	308	PL9	C36-C34-C33	-2.12	116.41	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	201	PL9	C26-C24-C23	-2.11	116.42	121.17
14	J	201	CLA	C14-C13-C12	-2.11	103.76	111.27
13	I	307	PL9	O2-C1-C2	-2.09	117.09	121.83
11	K	301	HEC	C2A-C1A-NA	-2.07	108.33	110.32
13	I	307	PL9	C22-C23-C24	-2.07	122.89	127.62
13	B	201	PL9	C42-C43-C44	-2.06	122.90	127.62
13	I	301	PL9	C37-C38-C39	-2.05	122.93	127.62
13	J	202	PL9	O2-C1-C2	-2.05	117.17	121.83
10	A	302	HEM	C1B-NB-C4B	2.04	107.63	105.21
11	C	301	HEC	C2A-C1A-NA	-2.04	108.35	110.32
10	I	303	HEM	C2A-C1A-NA	-2.03	107.90	110.15
13	A	308	PL9	C11-C9-C8	-2.03	116.62	121.17
10	A	301	HEM	C3B-C4B-NB	-2.02	108.02	109.47
10	A	301	HEM	C2A-C1A-NA	-2.01	107.92	110.15
11	A	303	HEC	CAD-C3D-C4D	2.01	128.87	124.94
10	A	302	HEM	C2A-C1A-NA	-2.01	107.92	110.15
13	B	201	PL9	C7-C8-C9	-2.01	123.38	126.83
10	A	301	HEM	CAA-CBA-CGA	-2.01	108.35	113.67
10	I	303	HEM	C3D-C4D-ND	-2.00	107.97	110.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	307	CLA	ND
14	J	201	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
10	I	303	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	C4D-C3D-CAD-CBD
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	C	301	HEC	C2D-C3D-CAD-CBD
11	C	301	HEC	C4D-C3D-CAD-CBD
11	I	304	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	I	304	HEC	C4B-C3B-CAB-CBB
11	I	304	HEC	C4D-C3D-CAD-CBD
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
11	K	301	HEC	C2D-C3D-CAD-CBD
11	K	301	HEC	C4D-C3D-CAD-CBD
13	A	306	PL9	C2-C3-C7-C8
13	A	306	PL9	C4-C3-C7-C8
13	A	306	PL9	C7-C8-C9-C10
13	A	306	PL9	C7-C8-C9-C11
13	A	306	PL9	C12-C13-C14-C16
13	A	306	PL9	C17-C18-C19-C21
13	A	306	PL9	C22-C23-C24-C26
13	A	306	PL9	C27-C28-C29-C31
13	A	306	PL9	C37-C38-C39-C41
13	A	308	PL9	C7-C8-C9-C11
13	A	308	PL9	C22-C23-C24-C25
13	A	308	PL9	C22-C23-C24-C26
13	A	308	PL9	C32-C33-C34-C36
13	B	201	PL9	C7-C8-C9-C11
13	B	201	PL9	C12-C13-C14-C15
13	B	201	PL9	C12-C13-C14-C16
13	B	201	PL9	C17-C18-C19-C21
13	B	201	PL9	C23-C24-C26-C27
13	B	201	PL9	C27-C28-C29-C30
13	B	201	PL9	C27-C28-C29-C31
13	B	201	PL9	C42-C43-C44-C46
13	I	301	PL9	C2-C3-C7-C8
13	I	301	PL9	C4-C3-C7-C8
13	I	301	PL9	C7-C8-C9-C11
13	I	301	PL9	C17-C18-C19-C20
13	I	301	PL9	C17-C18-C19-C21
13	I	301	PL9	C22-C23-C24-C26
13	I	301	PL9	C27-C28-C29-C31
13	I	301	PL9	C32-C33-C34-C35
13	I	301	PL9	C32-C33-C34-C36
13	I	301	PL9	C37-C38-C39-C41
13	I	301	PL9	C39-C41-C42-C43
13	I	301	PL9	C42-C43-C44-C46
13	I	307	PL9	C3-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	I	307	PL9	C7-C8-C9-C10
13	I	307	PL9	C7-C8-C9-C11
13	I	307	PL9	C30-C29-C31-C32
13	I	307	PL9	C42-C43-C44-C45
13	I	307	PL9	C42-C43-C44-C46
13	I	308	PL9	C7-C8-C9-C11
13	I	308	PL9	C12-C13-C14-C16
13	I	308	PL9	C13-C14-C16-C17
13	I	308	PL9	C27-C28-C29-C30
13	I	308	PL9	C27-C28-C29-C31
13	I	308	PL9	C30-C29-C31-C32
13	I	308	PL9	C42-C43-C44-C46
13	J	202	PL9	C7-C8-C9-C10
13	J	202	PL9	C7-C8-C9-C11
13	J	202	PL9	C12-C13-C14-C15
13	J	202	PL9	C22-C23-C24-C25
13	J	202	PL9	C22-C23-C24-C26
13	J	202	PL9	C27-C28-C29-C31
13	J	202	PL9	C35-C34-C36-C37
16	K	302	SQD	O49-C7-O47-C45
16	K	302	SQD	C8-C7-O47-C45
17	H	101	BCR	C7-C8-C9-C10
17	P	101	BCR	C7-C8-C9-C10
13	I	301	PL9	C47-C48-C49-C50
13	I	301	PL9	C47-C48-C49-C51
13	I	307	PL9	C47-C48-C49-C51
14	J	201	CLA	O1A-CGA-O2A-C1
16	D	202	SQD	O10-C23-O48-C46
14	A	307	CLA	O1A-CGA-O2A-C1
14	J	201	CLA	CBA-CGA-O2A-C1
16	D	202	SQD	C24-C23-O48-C46
16	K	302	SQD	C24-C23-O48-C46
13	A	306	PL9	C15-C14-C16-C17
13	A	308	PL9	C15-C14-C16-C17
13	I	301	PL9	C25-C24-C26-C27
13	I	301	PL9	C35-C34-C36-C37
13	I	308	PL9	C12-C11-C9-C10
13	I	308	PL9	C15-C14-C16-C17
13	J	202	PL9	C30-C29-C31-C32
13	A	306	PL9	C23-C24-C26-C27
13	A	306	PL9	C38-C39-C41-C42
13	I	308	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
14	J	201	CLA	C2A-CAA-CBA-CGA
14	A	307	CLA	CBA-CGA-O2A-C1
13	A	308	PL9	C37-C38-C39-C40
13	B	201	PL9	C17-C18-C19-C20
13	I	301	PL9	C37-C38-C39-C40
13	I	301	PL9	C42-C43-C44-C45
13	I	308	PL9	C7-C8-C9-C10
13	A	306	PL9	C32-C33-C34-C36
13	A	308	PL9	C37-C38-C39-C41
13	I	308	PL9	C32-C33-C34-C36
16	K	302	SQD	O10-C23-O48-C46
13	B	201	PL9	C47-C48-C49-C51
13	A	306	PL9	C40-C39-C41-C42
13	J	202	PL9	C12-C11-C9-C10
13	A	306	PL9	C13-C14-C16-C17
13	A	306	PL9	C18-C19-C21-C22
13	I	301	PL9	C23-C24-C26-C27
13	I	307	PL9	C28-C29-C31-C32
13	J	202	PL9	C28-C29-C31-C32
13	A	306	PL9	C39-C41-C42-C43
13	A	308	PL9	C14-C16-C17-C18
13	B	201	PL9	C34-C36-C37-C38
13	B	201	PL9	C39-C41-C42-C43
13	I	301	PL9	C9-C11-C12-C13
13	I	301	PL9	C14-C16-C17-C18
13	I	301	PL9	C44-C46-C47-C48
13	I	307	PL9	C14-C16-C17-C18
13	I	307	PL9	C44-C46-C47-C48
13	I	308	PL9	C29-C31-C32-C33
13	J	202	PL9	C24-C26-C27-C28
13	J	202	PL9	C34-C36-C37-C38
13	J	202	PL9	C44-C46-C47-C48
10	A	301	HEM	C2A-CAA-CBA-CGA
13	B	201	PL9	C31-C32-C33-C34
13	A	306	PL9	C17-C18-C19-C20
13	A	306	PL9	C22-C23-C24-C25
13	I	307	PL9	C32-C33-C34-C35
13	A	308	PL9	C12-C13-C14-C16
13	A	308	PL9	C27-C28-C29-C31
13	I	307	PL9	C22-C23-C24-C26
13	I	307	PL9	C47-C48-C49-C50
13	A	306	PL9	C20-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
13	B	201	PL9	C25-C24-C26-C27
13	I	301	PL9	C33-C34-C36-C37
13	I	307	PL9	C33-C34-C36-C37
17	H	101	BCR	C7-C8-C9-C34
17	P	101	BCR	C7-C8-C9-C34
11	A	303	HEC	C2D-C3D-CAD-CBD
13	A	306	PL9	C37-C38-C39-C40
10	A	301	HEM	C4D-C3D-CAD-CBD
13	B	201	PL9	C29-C31-C32-C33
13	I	301	PL9	C29-C31-C32-C33
13	I	307	PL9	C19-C21-C22-C23
13	J	202	PL9	C39-C41-C42-C43
14	A	307	CLA	C2A-CAA-CBA-CGA
12	I	306	UMQ	O1'-CA-CB-CC
13	A	306	PL9	C32-C33-C34-C35
13	I	301	PL9	C7-C8-C9-C10
14	A	307	CLA	C15-C16-C17-C18
12	A	305	UMQ	O1'-CA-CB-CC
10	A	302	HEM	C3A-C2A-CAA-CBA
10	I	303	HEM	C3A-C2A-CAA-CBA
13	A	306	PL9	C25-C24-C26-C27
13	A	306	PL9	C47-C48-C49-C51
13	B	201	PL9	C42-C43-C44-C45
13	I	308	PL9	C12-C13-C14-C15
13	A	306	PL9	C14-C16-C17-C18
13	I	307	PL9	C24-C26-C27-C28
13	I	308	PL9	C39-C41-C42-C43
10	A	301	HEM	C2D-C3D-CAD-CBD
12	I	305	UMQ	O5'-C1'-O1'-CA
13	A	306	PL9	C28-C29-C31-C32
12	P	102	UMQ	CC-CD-CF-CG
12	A	305	UMQ	CG-CH-CI-CJ
12	I	306	UMQ	CG-CH-CI-CJ
12	I	306	UMQ	CB-CA-O1'-C1'
13	J	202	PL9	C17-C18-C19-C21
16	D	202	SQD	C9-C10-C11-C12
14	A	307	CLA	C3A-C2A-CAA-CBA
14	J	201	CLA	C3A-C2A-CAA-CBA
13	I	308	PL9	C12-C11-C9-C8
16	D	202	SQD	C32-C33-C34-C35
12	I	306	UMQ	CD-CF-CG-CH
13	I	301	PL9	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
12	A	305	UMQ	CD-CF-CG-CH
13	B	201	PL9	C4-C3-C7-C8
13	A	308	PL9	C20-C19-C21-C22
13	I	307	PL9	C15-C14-C16-C17
13	J	202	PL9	C12-C13-C14-C16
10	I	302	HEM	C3A-C2A-CAA-CBA
16	D	202	SQD	C8-C7-O47-C45
16	D	202	SQD	O49-C7-O47-C45
13	B	201	PL9	C47-C48-C49-C50
13	I	308	PL9	C47-C48-C49-C51
11	I	304	HEC	C2D-C3D-CAD-CBD
12	A	305	UMQ	O5'-C5'-C6'-O6'
12	I	306	UMQ	O5'-C5'-C6'-O6'
13	J	202	PL9	C19-C21-C22-C23
16	D	202	SQD	C25-C26-C27-C28
16	K	302	SQD	C16-C17-C18-C19
13	I	307	PL9	C13-C14-C16-C17
13	B	201	PL9	C7-C8-C9-C10
16	D	202	SQD	C11-C12-C13-C14
14	A	307	CLA	C1A-C2A-CAA-CBA
14	J	201	CLA	C1A-C2A-CAA-CBA
14	J	201	CLA	C13-C15-C16-C17
13	B	201	PL9	C15-C14-C16-C17
16	K	302	SQD	C26-C27-C28-C29
13	B	201	PL9	C32-C33-C34-C35
13	J	202	PL9	C27-C28-C29-C30
16	K	302	SQD	C11-C10-C9-C8
16	D	202	SQD	C44-C45-C46-O48
14	A	307	CLA	C2-C3-C5-C6
16	K	302	SQD	C12-C13-C14-C15
14	A	307	CLA	C4-C3-C5-C6
12	A	305	UMQ	CI-CJ-CK-CL
12	I	306	UMQ	CI-CJ-CK-CL
16	K	302	SQD	O47-C45-C46-O48
14	A	307	CLA	C13-C15-C16-C17
13	J	202	PL9	C37-C38-C39-C40
12	P	102	UMQ	CB-CC-CD-CF
14	J	201	CLA	C11-C10-C8-C9
14	J	201	CLA	C14-C13-C15-C16
16	D	202	SQD	C29-C30-C31-C32
14	A	307	CLA	C11-C12-C13-C15
14	J	201	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
14	J	201	CLA	C12-C13-C15-C16
13	B	201	PL9	C30-C29-C31-C32
12	E	101	UMQ	CA-CB-CC-CD
14	J	201	CLA	C16-C17-C18-C20
12	E	101	UMQ	CF-CG-CH-CI
16	D	202	SQD	O47-C45-C46-O48
13	I	301	PL9	C19-C21-C22-C23
12	I	306	UMQ	C5'-C4'-O1-C1
13	I	308	PL9	C14-C16-C17-C18
14	J	201	CLA	C10-C11-C12-C13
12	I	306	UMQ	C3'-C4'-O1-C1
16	D	202	SQD	C16-C17-C18-C19
14	A	307	CLA	C11-C12-C13-C14
16	D	202	SQD	C26-C27-C28-C29
14	J	201	CLA	C16-C17-C18-C19
12	A	305	UMQ	CB-CA-O1'-C1'
13	A	308	PL9	C34-C36-C37-C38
10	A	302	HEM	C2D-C3D-CAD-CBD
13	I	307	PL9	C45-C44-C46-C47
13	I	308	PL9	C40-C39-C41-C42
16	K	302	SQD	O5-C5-C6-S
14	J	201	CLA	C4-C3-C5-C6
13	J	202	PL9	C47-C48-C49-C50
16	D	202	SQD	C30-C31-C32-C33
13	I	307	PL9	C12-C13-C14-C16
13	A	306	PL9	C34-C36-C37-C38
10	A	302	HEM	C4D-C3D-CAD-CBD
16	K	302	SQD	C44-C45-C46-O48
13	J	202	PL9	C32-C33-C34-C36
16	K	302	SQD	C9-C10-C11-C12
12	A	305	UMQ	C5'-C4'-O1-C1
14	A	307	CLA	C14-C13-C15-C16
13	J	202	PL9	C11-C12-C13-C14
13	A	306	PL9	C12-C13-C14-C15
13	B	201	PL9	C13-C14-C16-C17
14	J	201	CLA	C2-C3-C5-C6
16	D	202	SQD	C34-C35-C36-C37
17	H	101	BCR	C11-C10-C9-C34
17	P	101	BCR	C11-C10-C9-C34
12	A	305	UMQ	C3'-C4'-O1-C1
13	A	308	PL9	C9-C11-C12-C13
11	C	301	HEC	C3A-C2A-CAA-CBA

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
17	H	101	BCR	C11-C10-C9-C8
17	P	101	BCR	C11-C10-C9-C8
13	I	307	PL9	C20-C19-C21-C22
13	I	307	PL9	C35-C34-C36-C37
13	I	307	PL9	C38-C39-C41-C42
11	A	303	HEC	C3D-CAD-CBD-CGD
14	A	307	CLA	C12-C13-C15-C16
16	D	202	SQD	O6-C44-C45-O47
11	C	301	HEC	C1A-C2A-CAA-CBA
13	A	308	PL9	C25-C24-C26-C27
13	J	202	PL9	C15-C14-C16-C17
13	I	308	PL9	C23-C24-C26-C27
16	D	202	SQD	C24-C25-C26-C27
16	K	302	SQD	C30-C31-C32-C33
13	I	301	PL9	C22-C23-C24-C25
13	B	201	PL9	C12-C11-C9-C10
10	A	302	HEM	C3D-CAD-CBD-CGD
13	B	201	PL9	C19-C21-C22-C23
11	K	301	HEC	CAA-CBA-CGA-O2A
12	A	304	UMQ	CB-CC-CD-CF
13	B	201	PL9	C28-C29-C31-C32
10	I	302	HEM	CAA-CBA-CGA-O2A
11	K	301	HEC	CAA-CBA-CGA-O1A
12	A	304	UMQ	CF-CG-CH-CI
11	K	301	HEC	CAD-CBD-CGD-O2D
13	I	307	PL9	C12-C13-C14-C15
16	D	202	SQD	C33-C34-C35-C36
16	D	202	SQD	C13-C14-C15-C16
16	D	202	SQD	C14-C15-C16-C17
10	I	302	HEM	CAA-CBA-CGA-O1A
11	K	301	HEC	CAD-CBD-CGD-O1D
13	A	308	PL9	C4-C3-C7-C8
16	D	202	SQD	C19-C20-C21-C22
13	I	307	PL9	C40-C39-C41-C42
13	A	306	PL9	C42-C43-C44-C46
14	J	201	CLA	CAA-CBA-CGA-O2A
13	I	307	PL9	C23-C24-C26-C27
16	K	302	SQD	C34-C35-C36-C37
14	J	201	CLA	C4B-C3B-CAB-CBB
14	A	307	CLA	CAA-CBA-CGA-O2A
16	K	302	SQD	C19-C20-C21-C22
13	B	201	PL9	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
13	B	201	PL9	C37-C38-C39-C41
13	I	308	PL9	C20-C19-C21-C22
16	K	302	SQD	C15-C16-C17-C18
14	A	307	CLA	CAA-CBA-CGA-O1A
16	K	302	SQD	C45-C44-O6-C1
11	A	303	HEC	CAA-CBA-CGA-O2A
14	J	201	CLA	CAA-CBA-CGA-O1A
10	A	301	HEM	C2C-C3C-CAC-CBC
10	I	303	HEM	C2B-C3B-CAB-CBB
12	I	305	UMQ	CF-CG-CH-CI
11	I	304	HEC	CAA-CBA-CGA-O2A
13	B	201	PL9	C2-C3-C7-C8

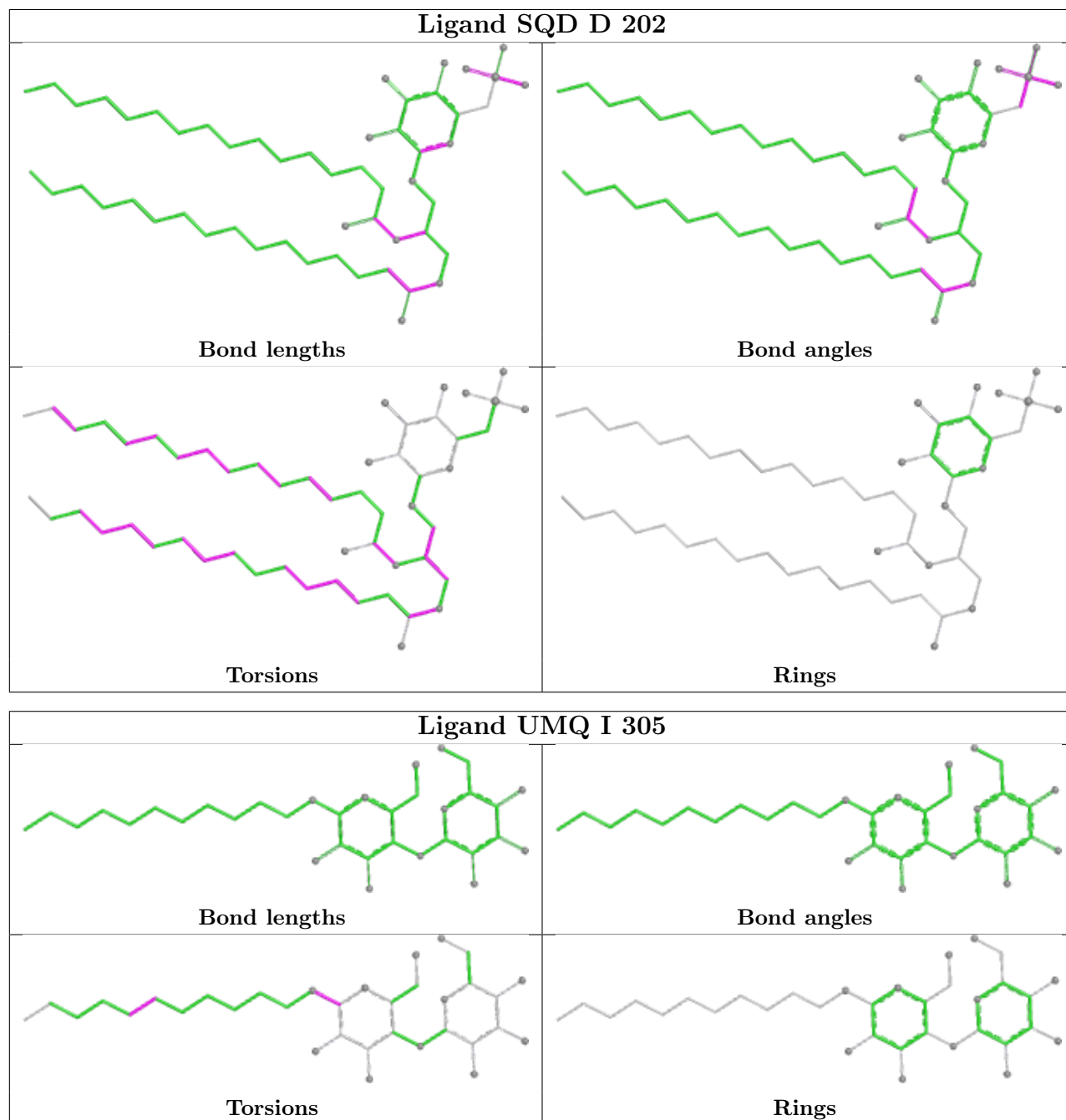
There are no ring outliers.

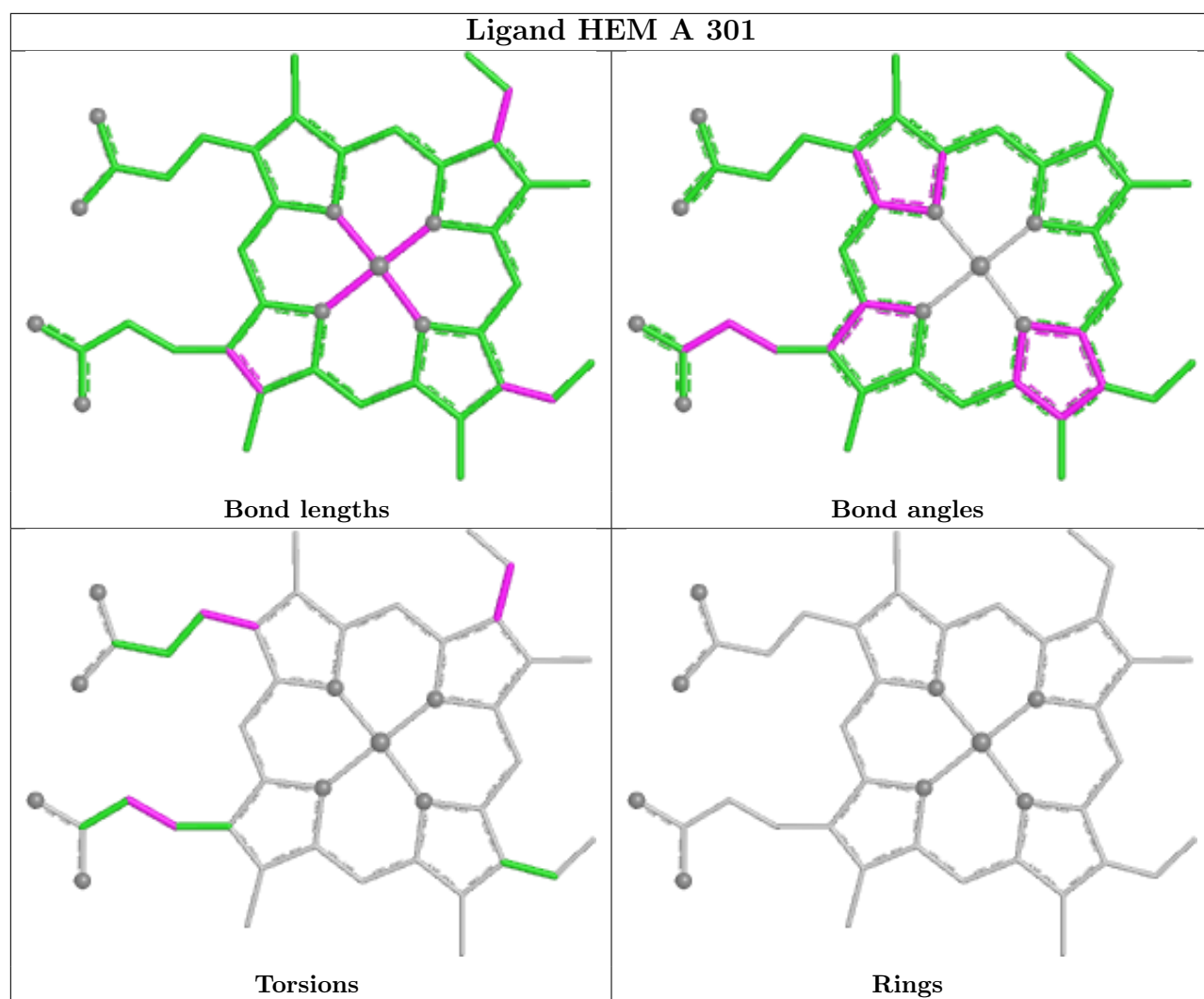
19 monomers are involved in 71 short contacts:

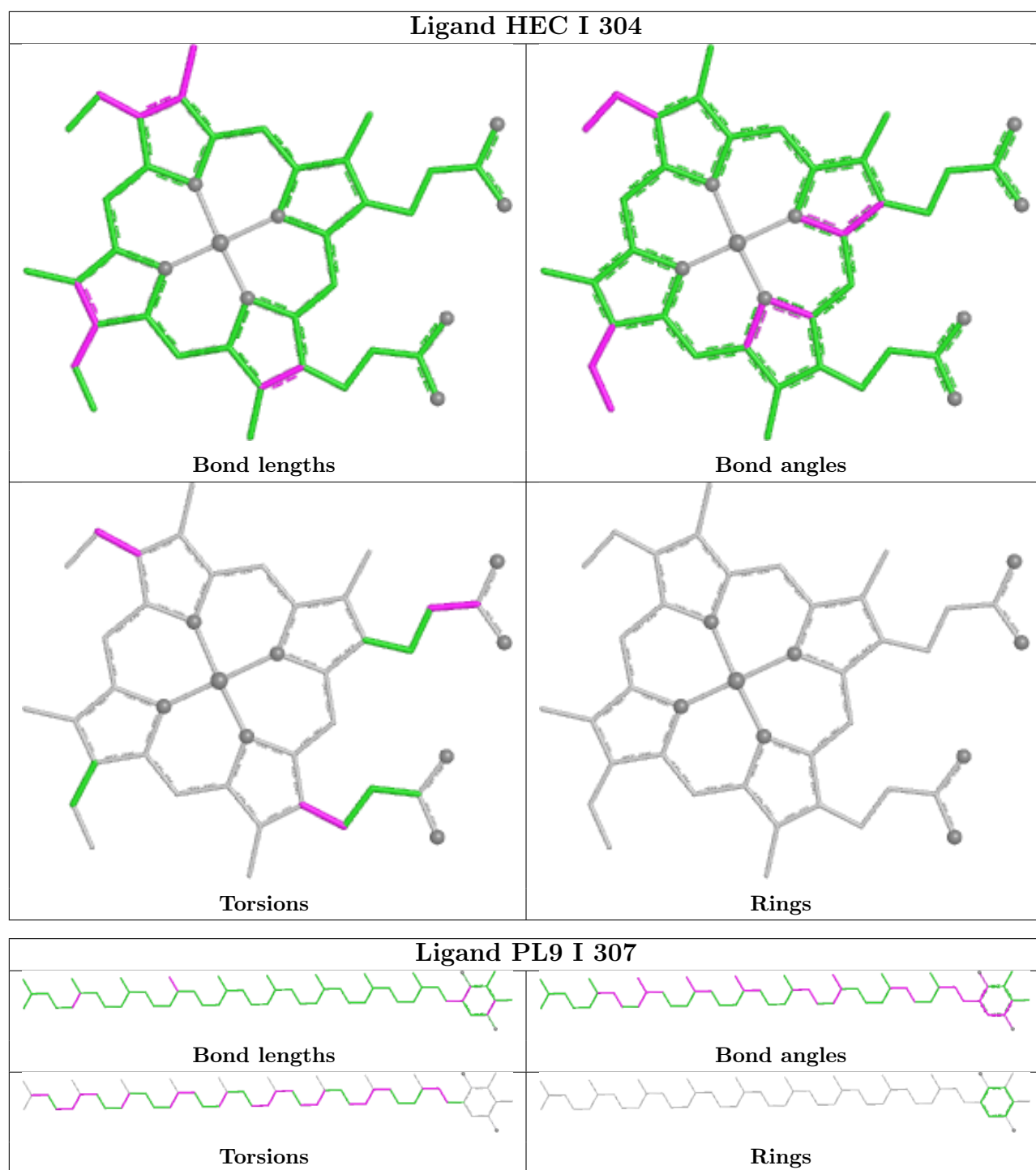
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	301	HEM	7	0
11	I	304	HEC	4	0
13	I	307	PL9	11	0
10	A	302	HEM	6	0
11	C	301	HEC	3	0
17	P	101	BCR	1	0
13	I	301	PL9	1	0
10	I	302	HEM	6	0
10	I	303	HEM	6	0
11	K	301	HEC	5	0
14	A	307	CLA	3	0
13	A	306	PL9	4	0
14	J	201	CLA	2	0
13	A	308	PL9	2	0
12	P	102	UMQ	1	0
13	J	202	PL9	2	0
13	B	201	PL9	5	0
13	I	308	PL9	3	0
11	A	303	HEC	4	0

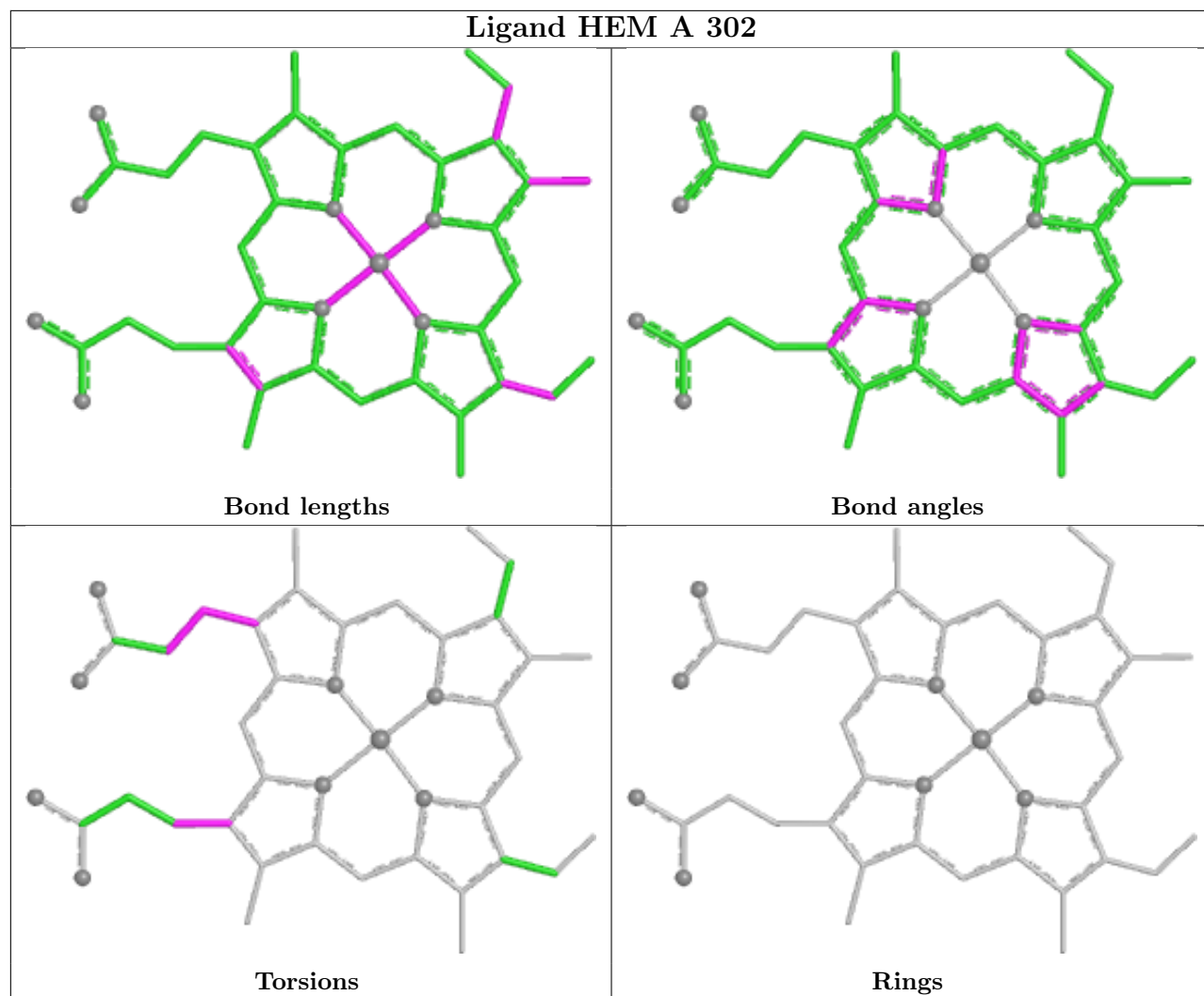
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

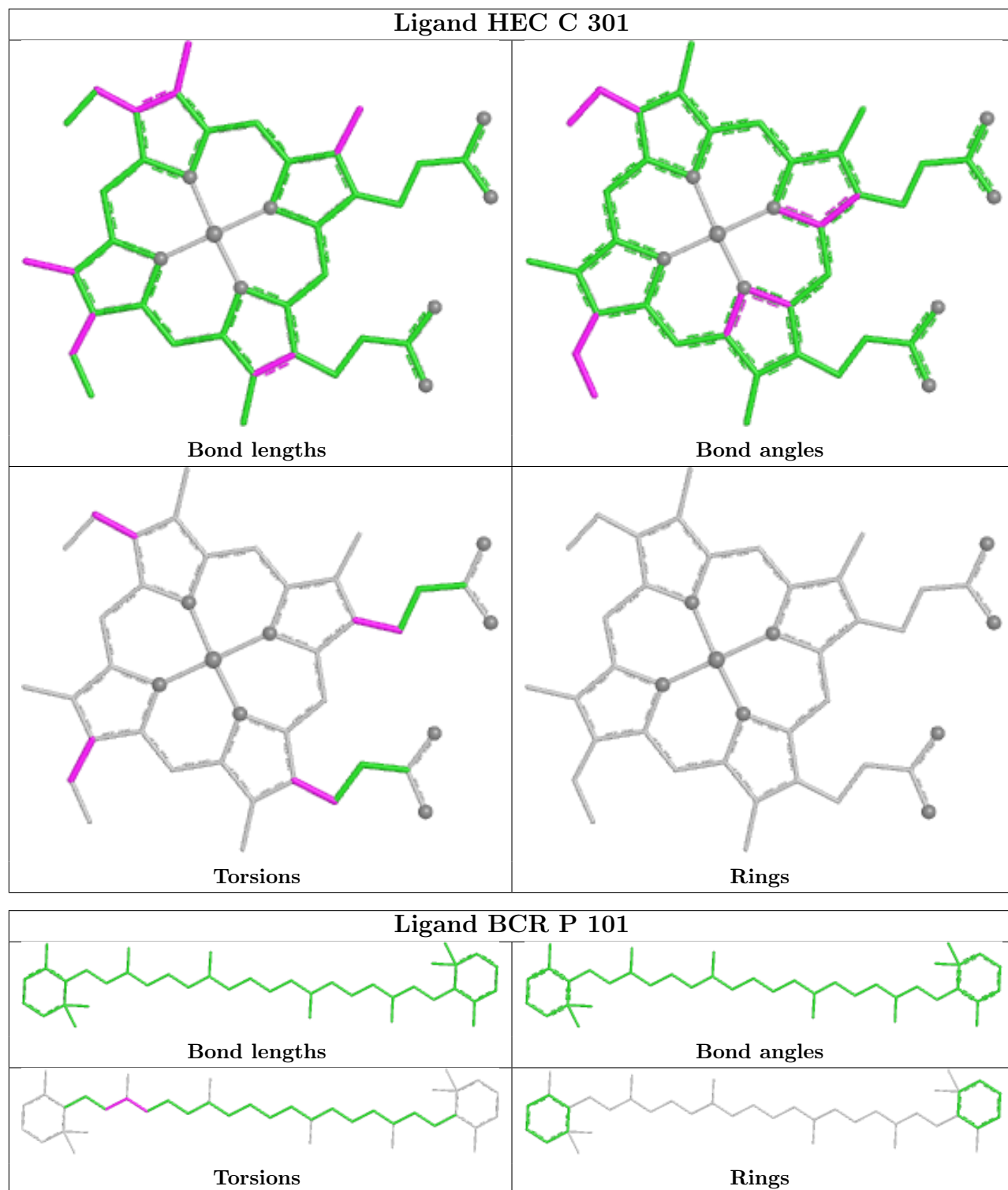
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

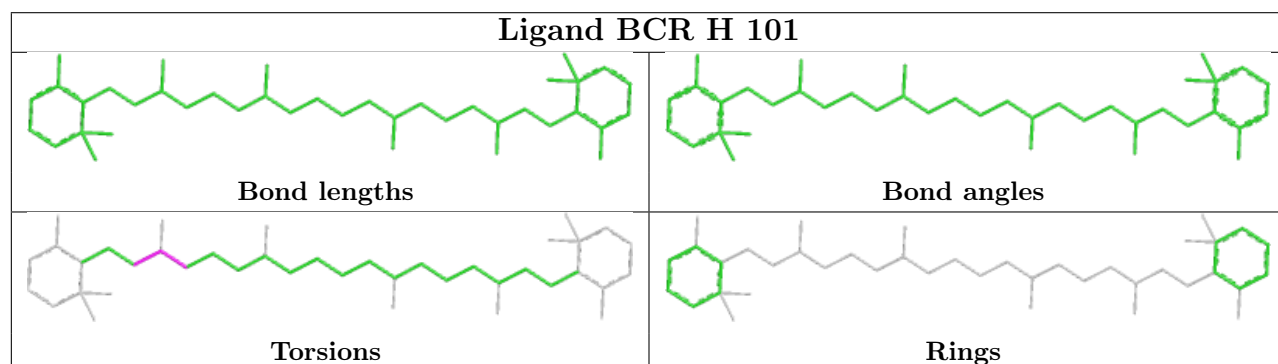
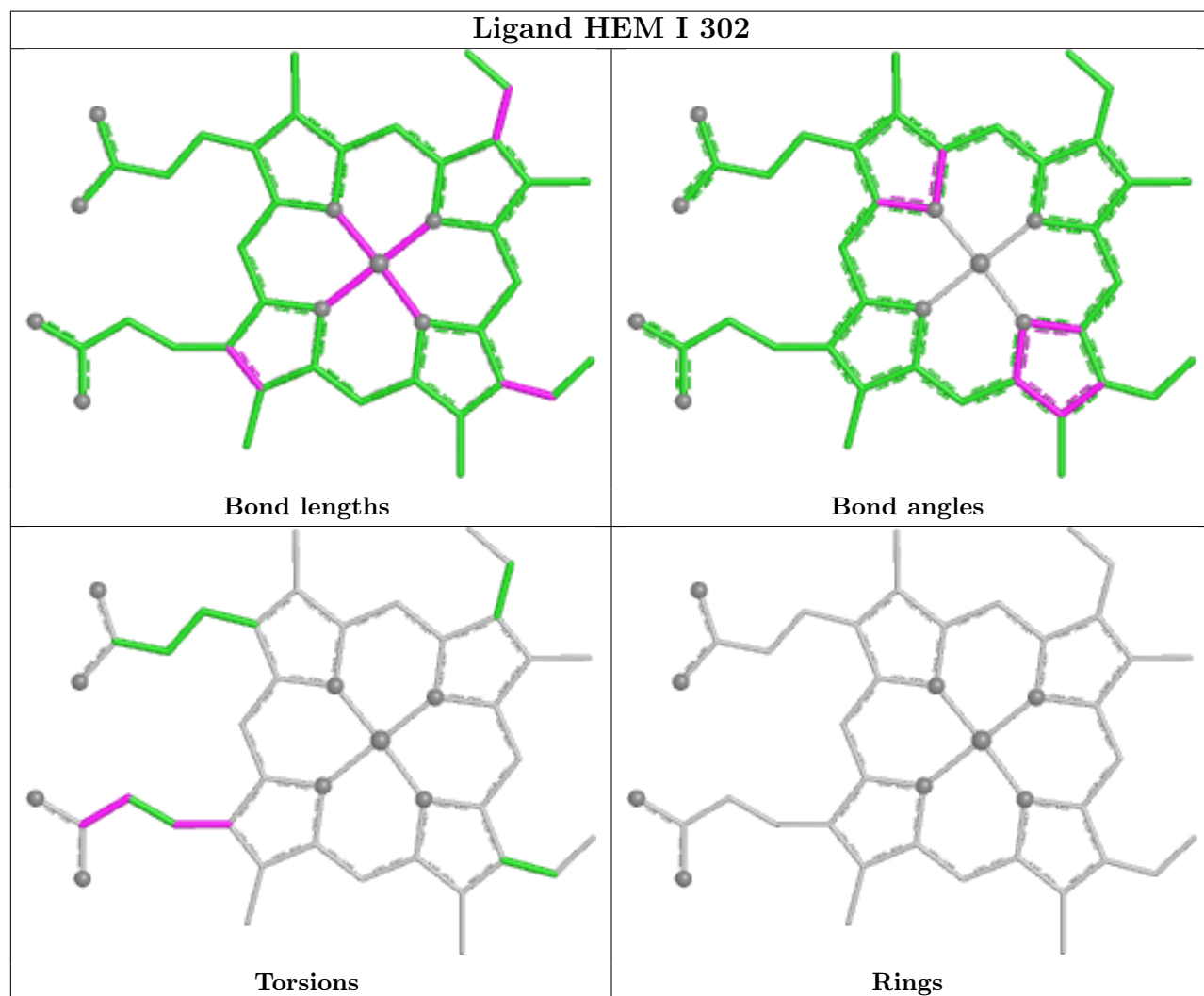
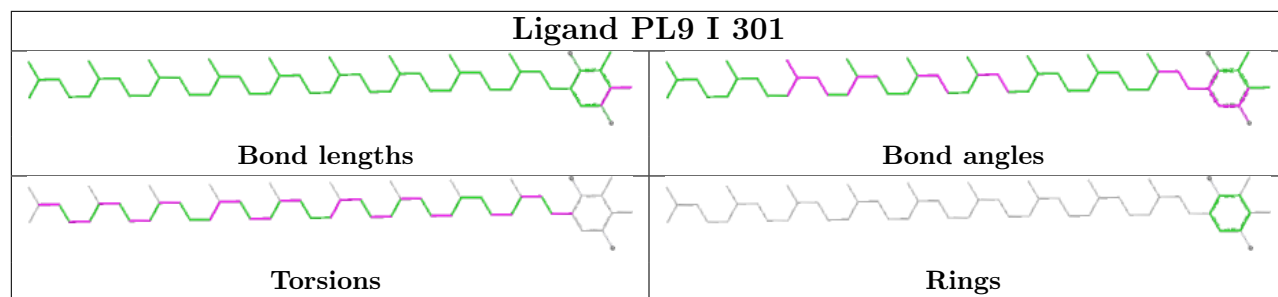


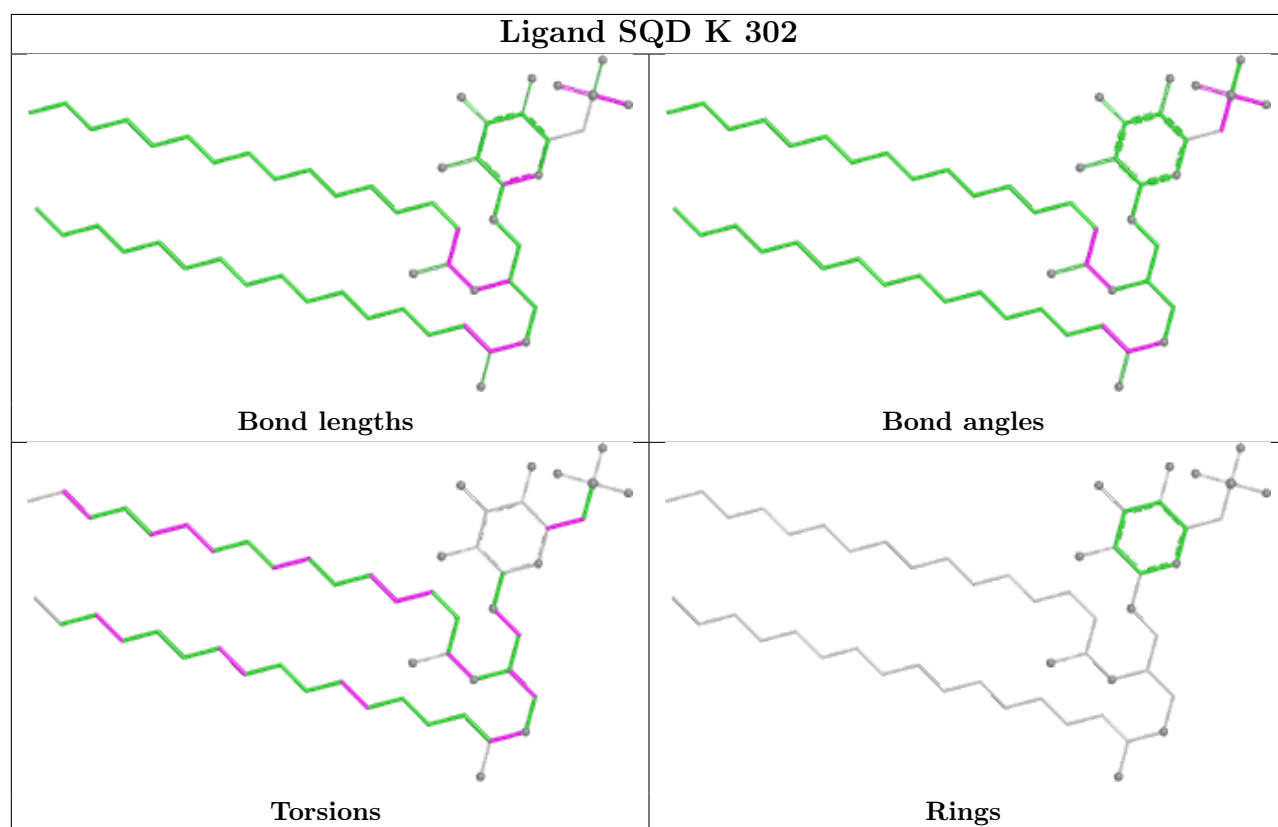
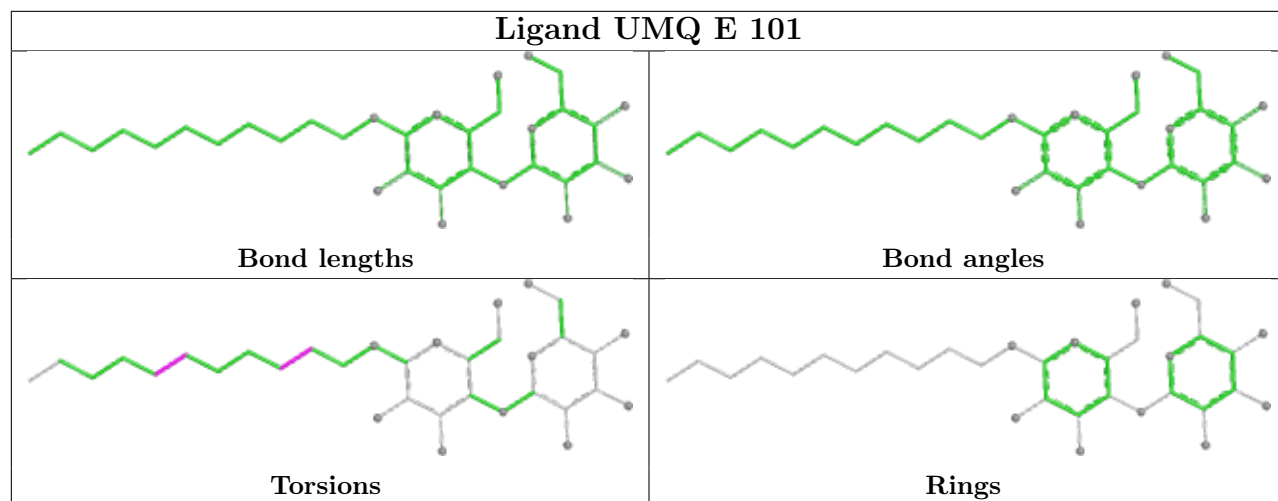


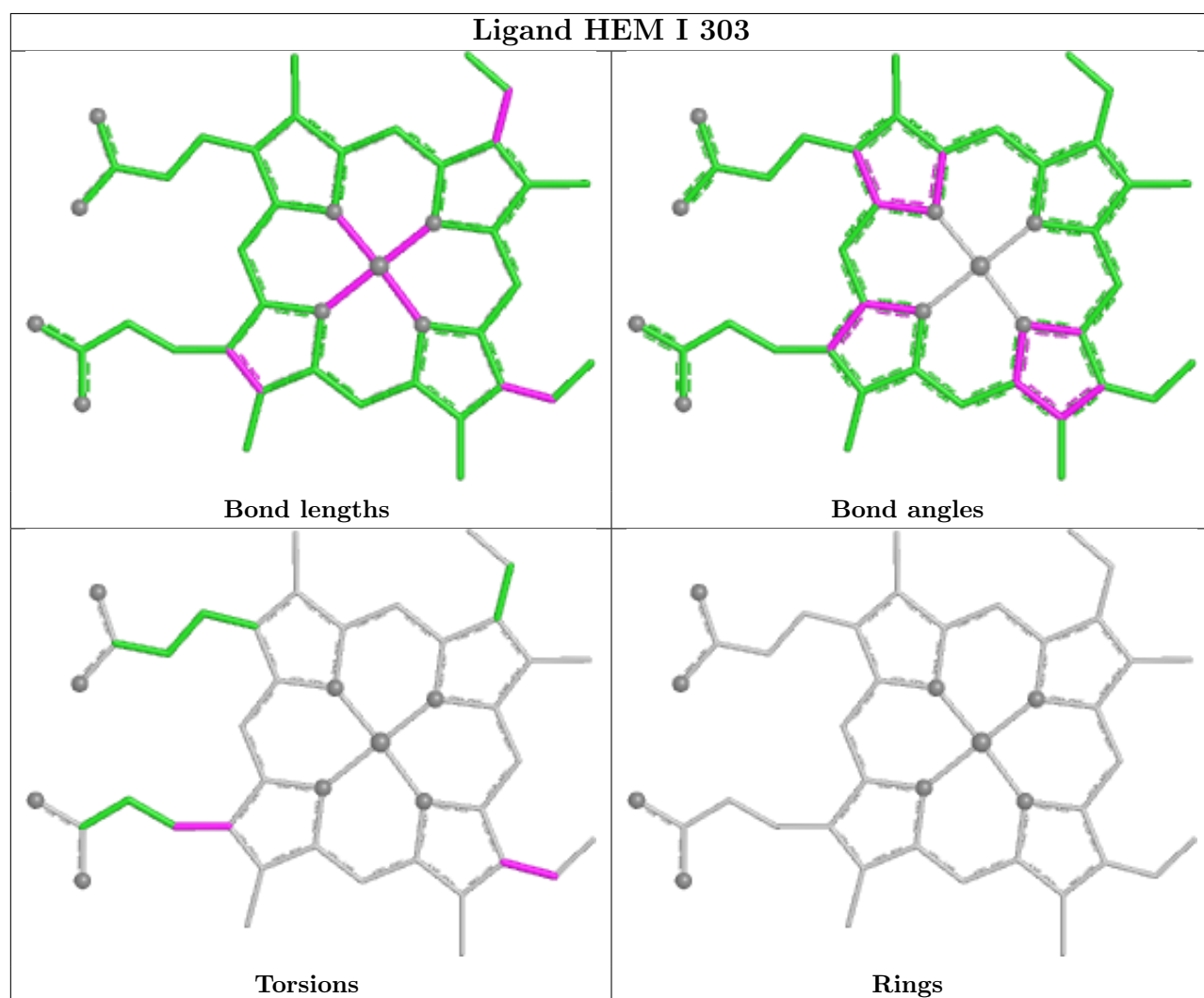
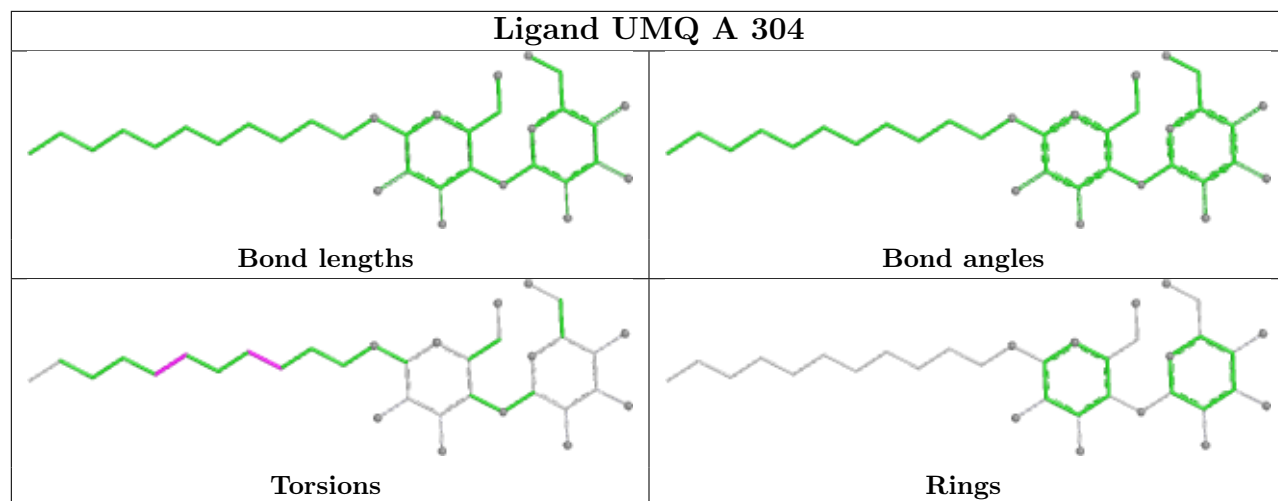


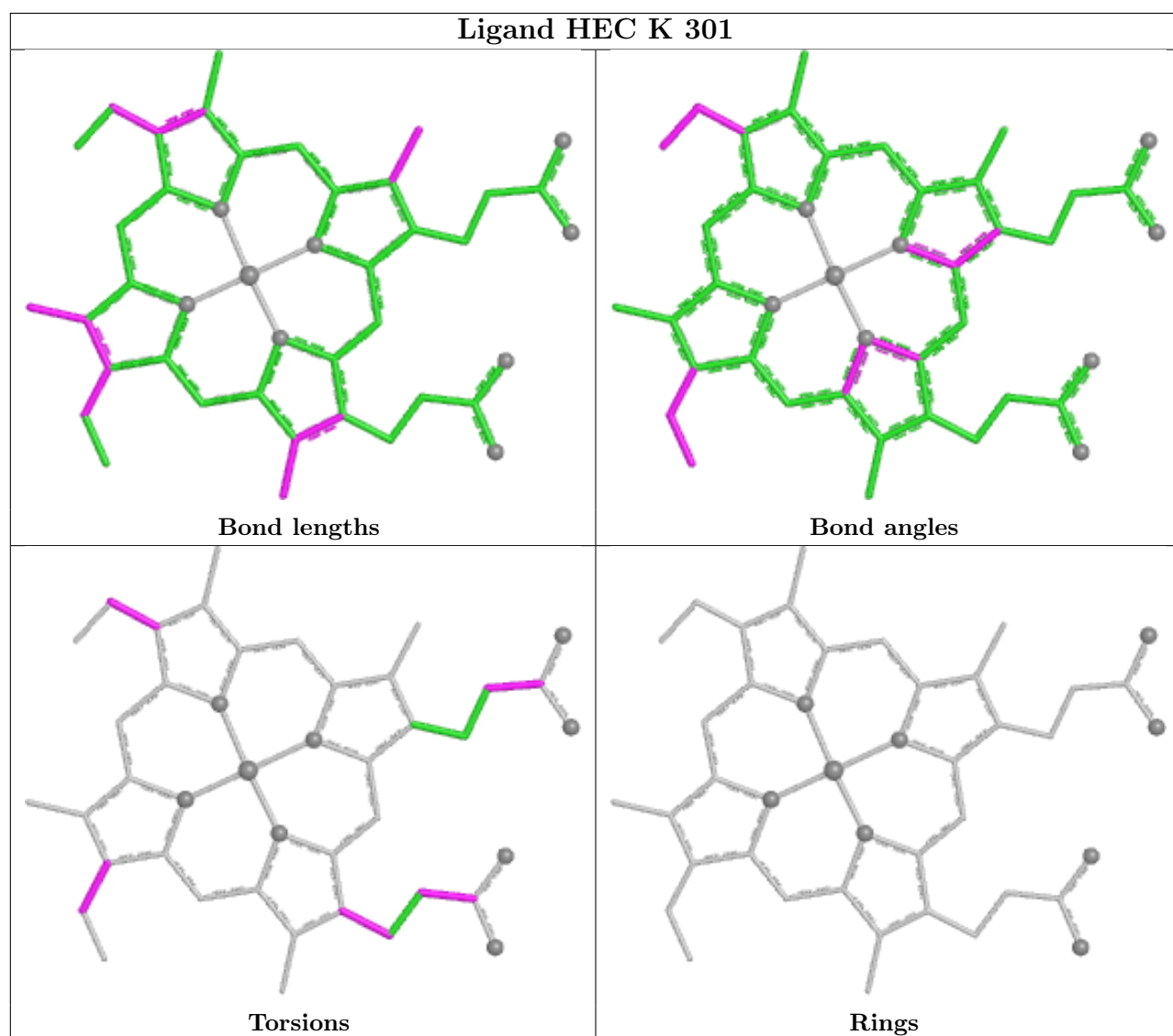
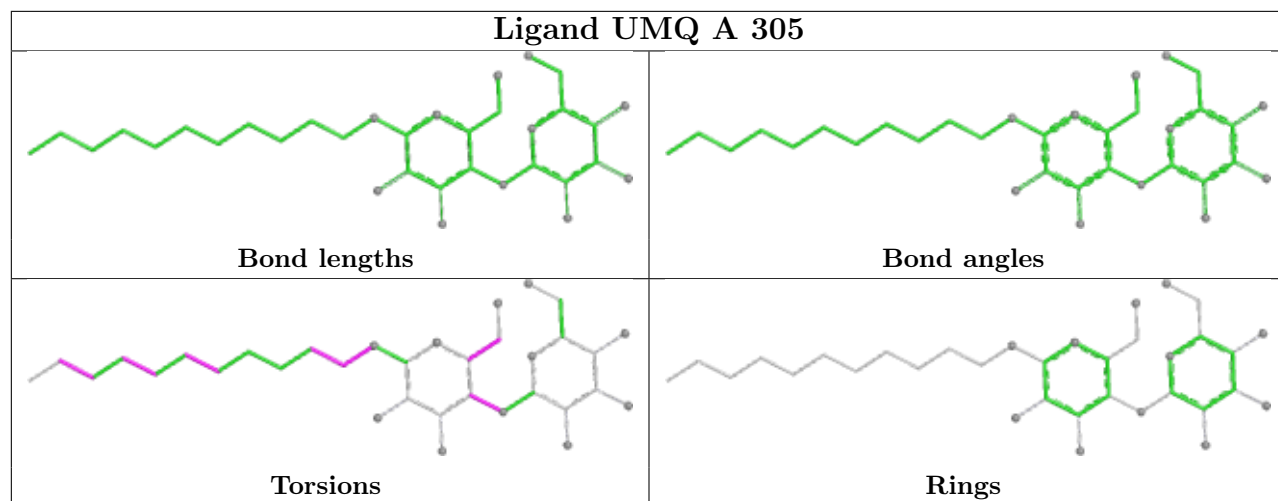


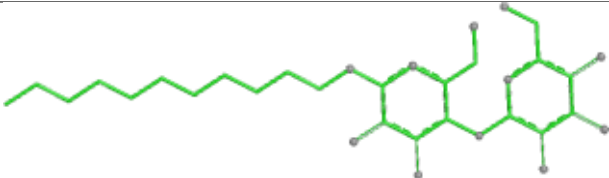
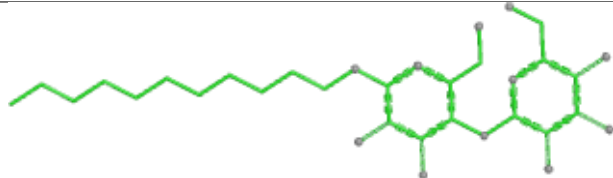
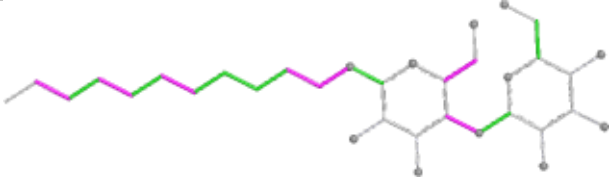
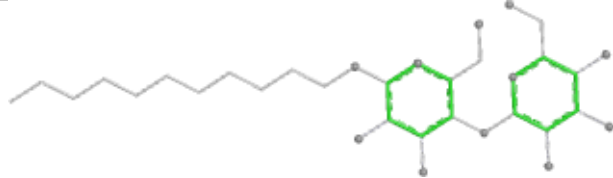


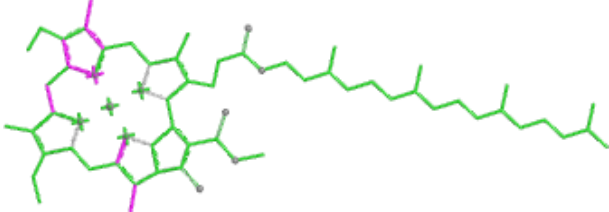
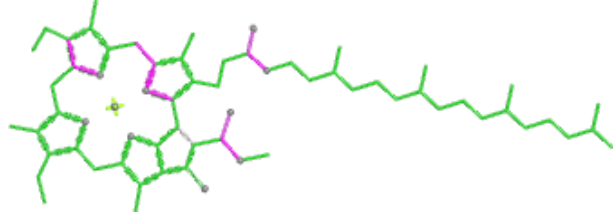
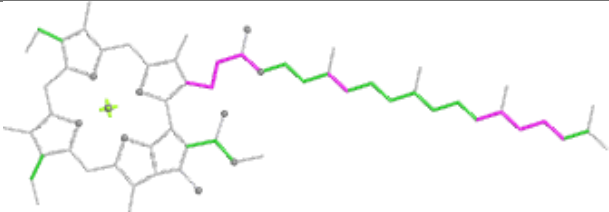
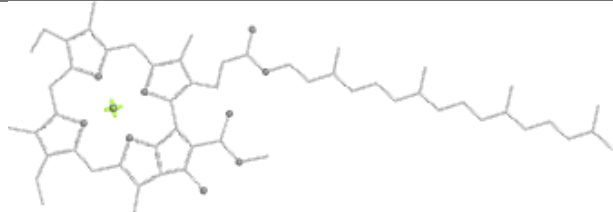


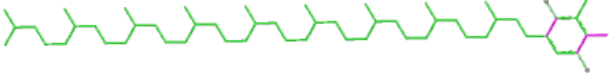
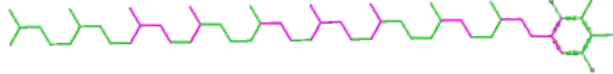
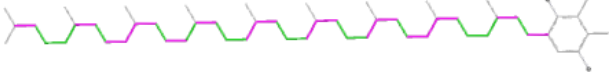
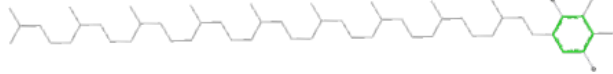


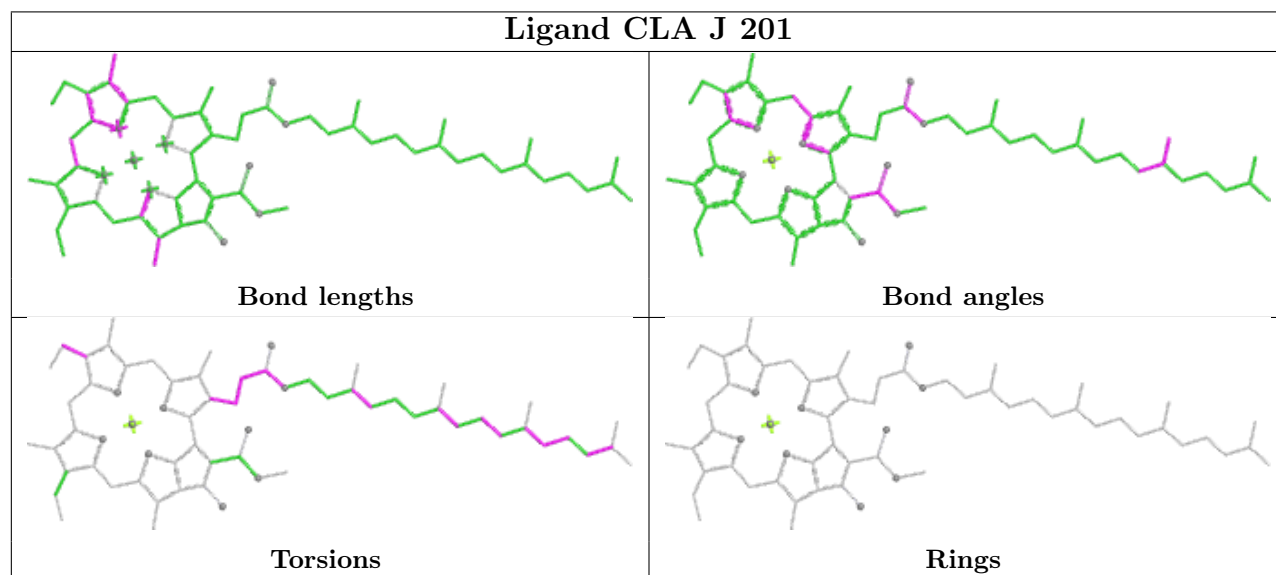
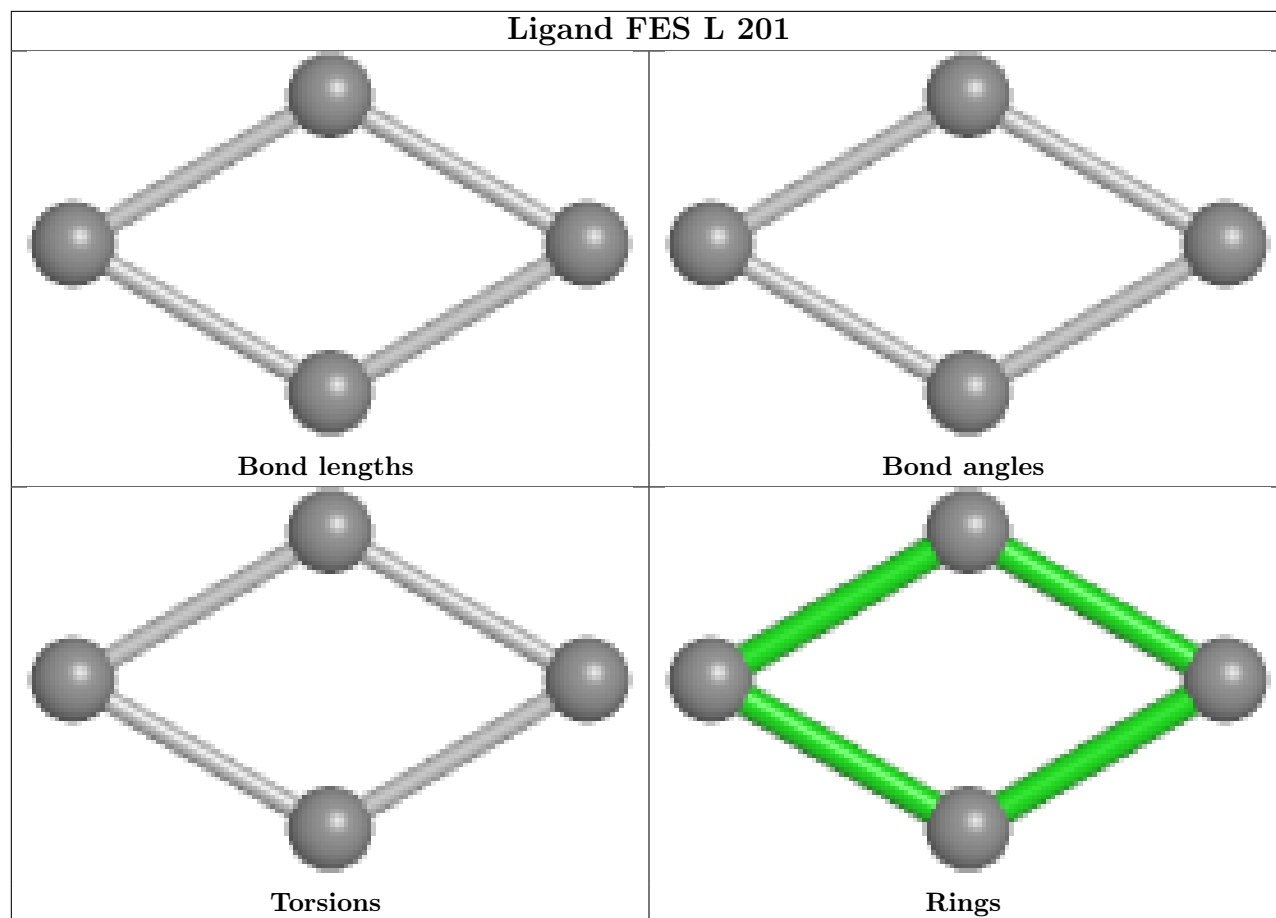


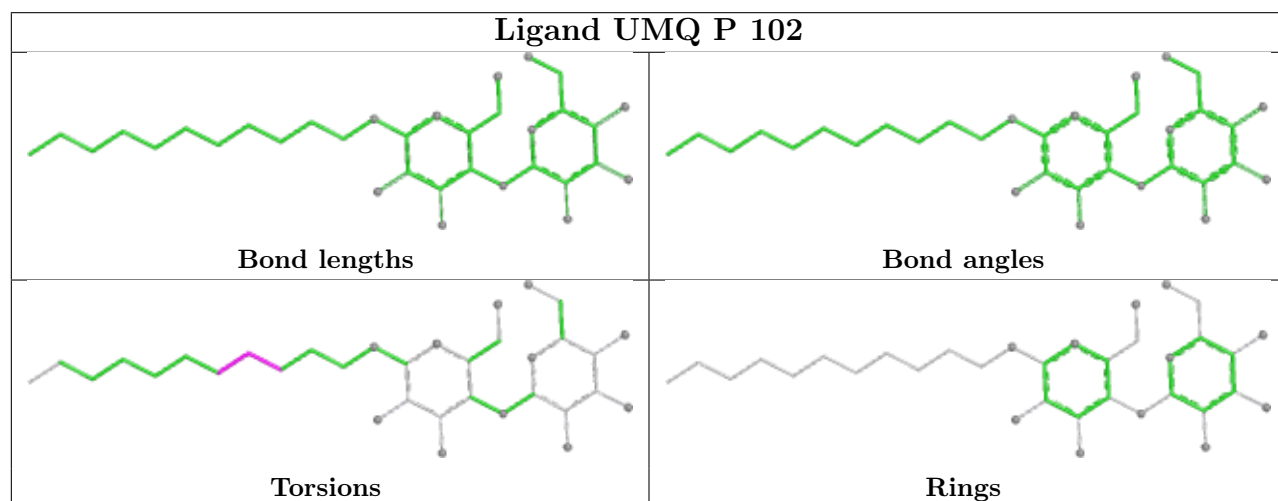
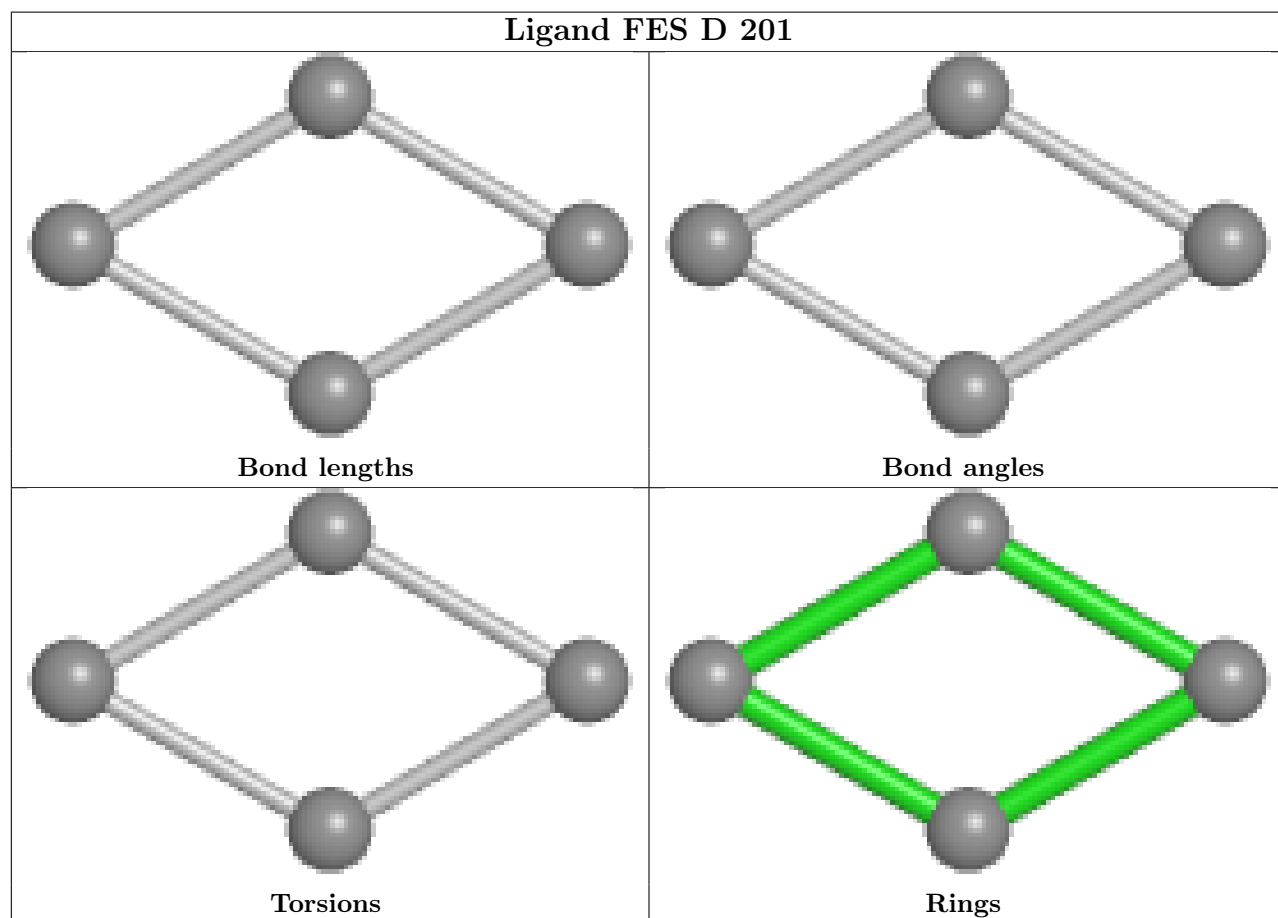
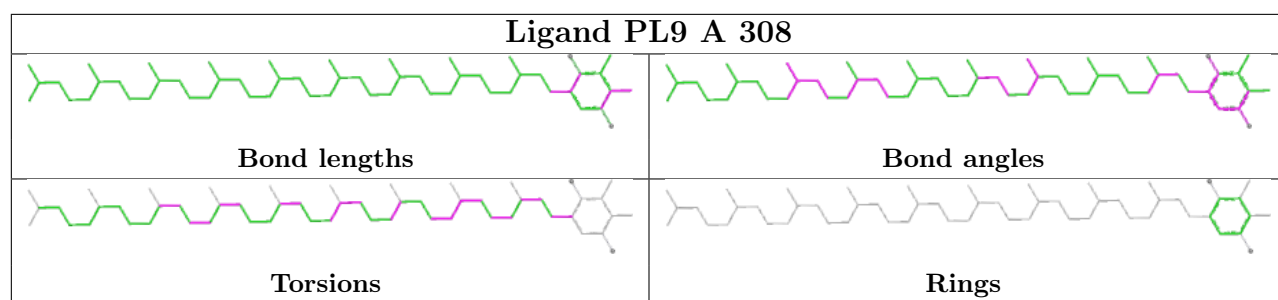


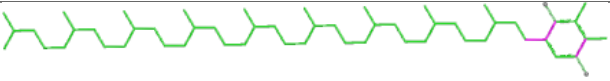
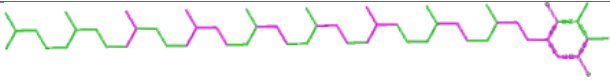
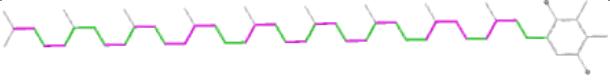
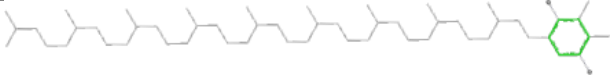
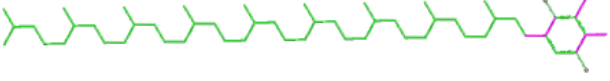
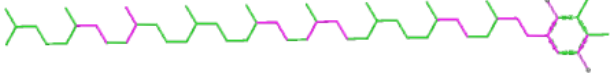
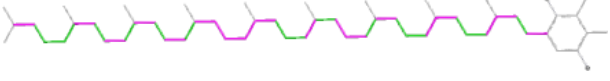
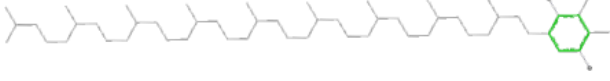
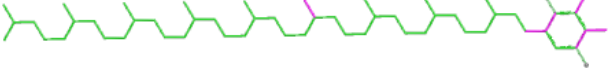
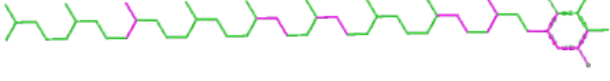
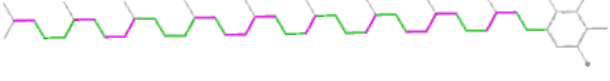
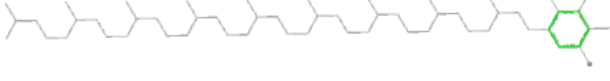
Ligand UMQ I 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

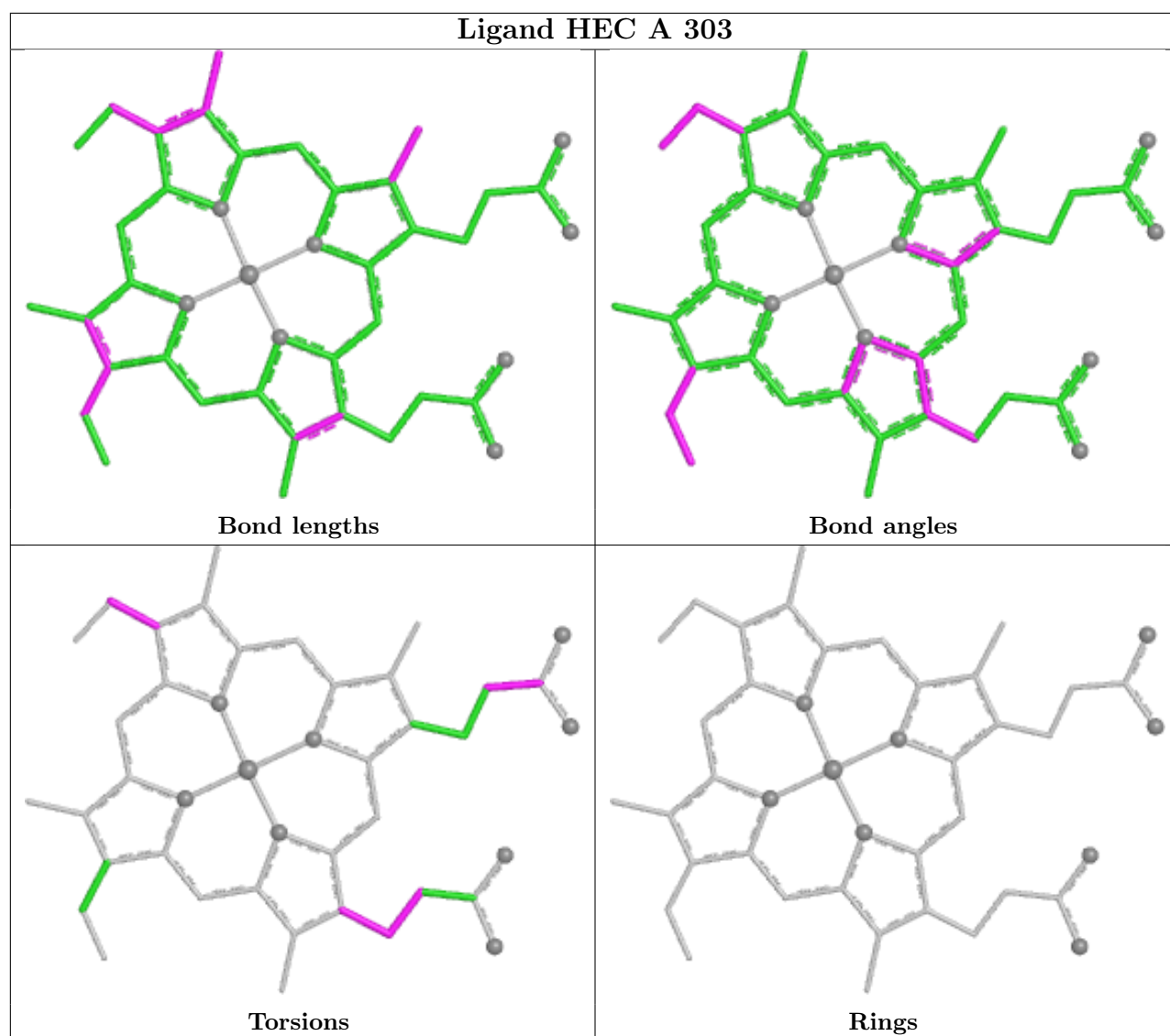
Ligand CLA A 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 A 306	
	
Bond lengths	Bond angles
	
Torsions	Rings





Ligand PL9 J 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 B 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 I 308	
 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.

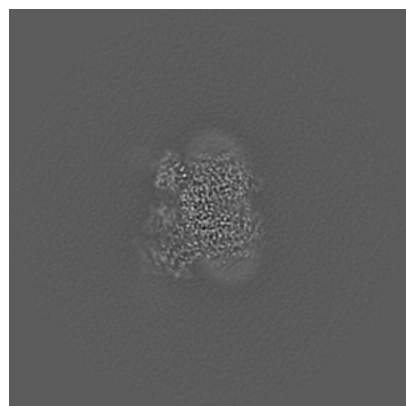
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55898. These allow visual inspection of the internal detail of the map and identification of artifacts.

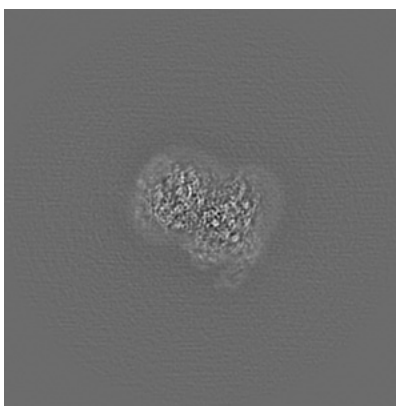
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

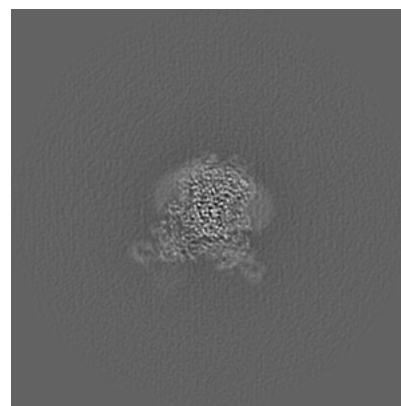
#### 6.1.1 Primary map



X

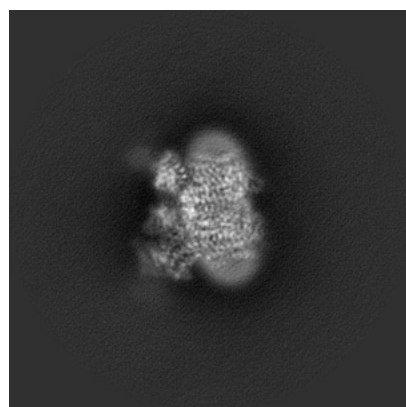


Y

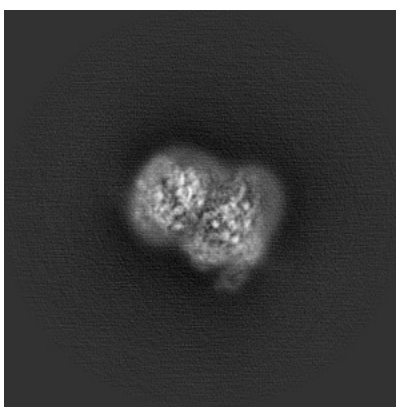


Z

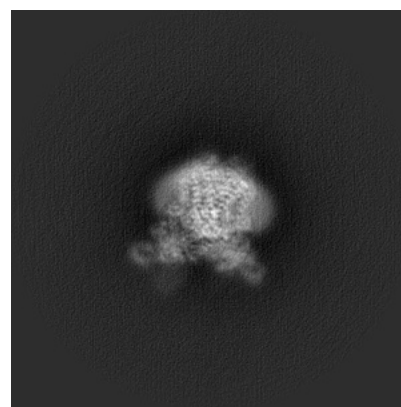
#### 6.1.2 Raw map



X



Y

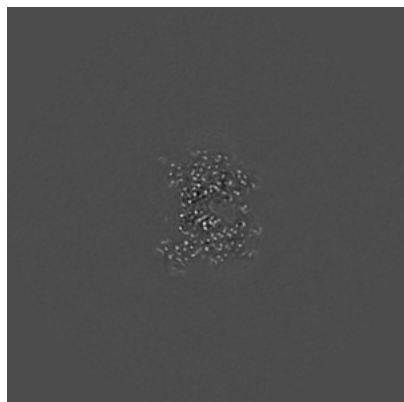


Z

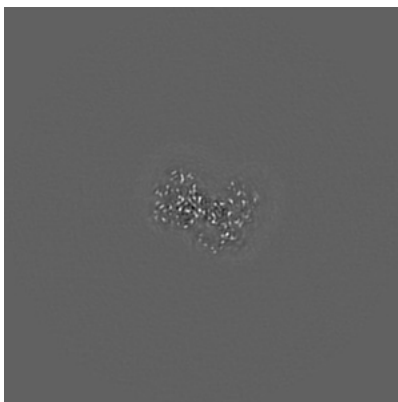
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

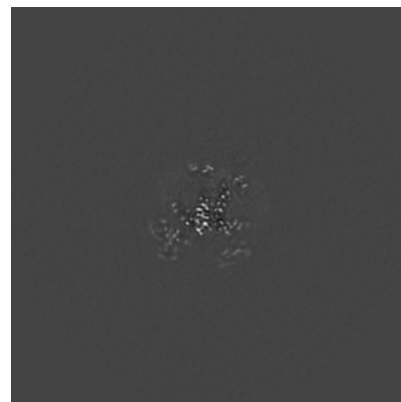
### 6.2.1 Primary map



X Index: 200

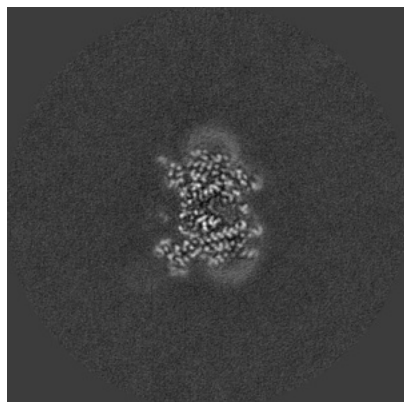


Y Index: 200

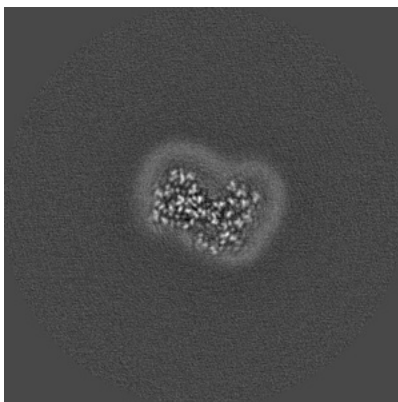


Z Index: 200

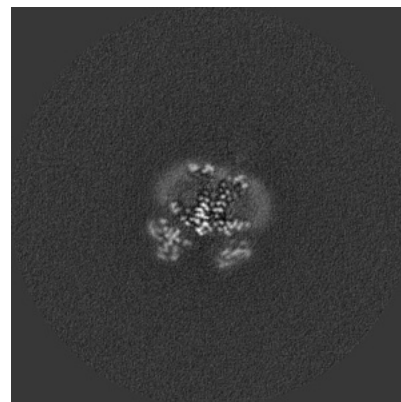
### 6.2.2 Raw map



X Index: 200



Y Index: 200

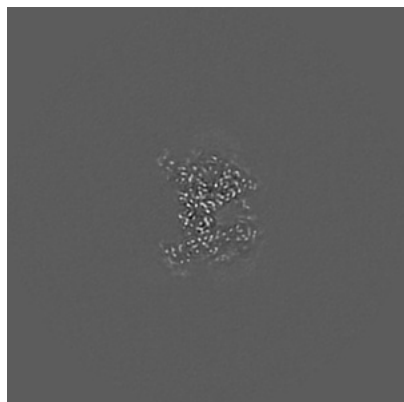


Z Index: 200

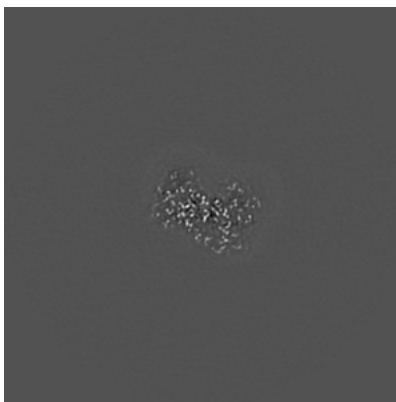
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

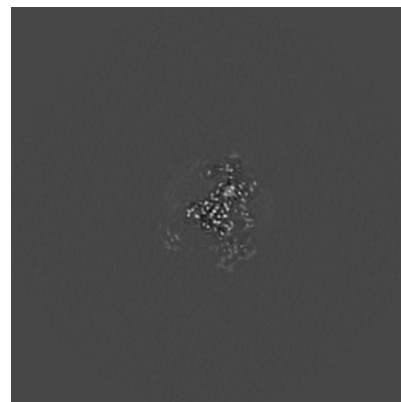
### 6.3.1 Primary map



X Index: 196

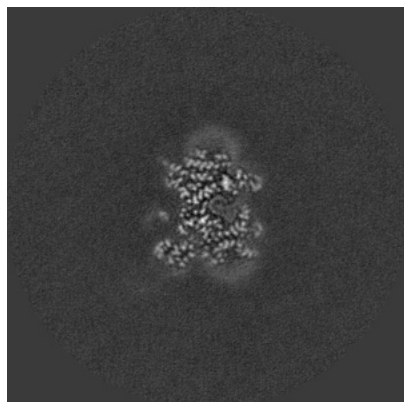


Y Index: 197

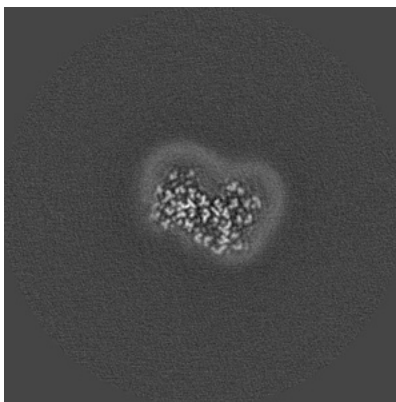


Z Index: 186

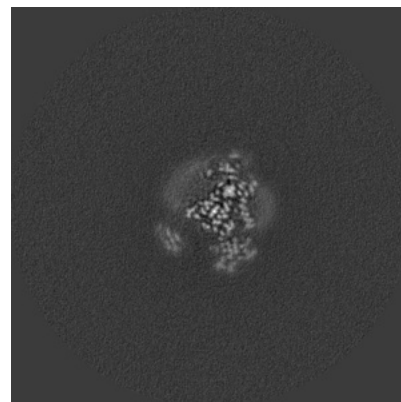
### 6.3.2 Raw map



X Index: 202



Y Index: 197

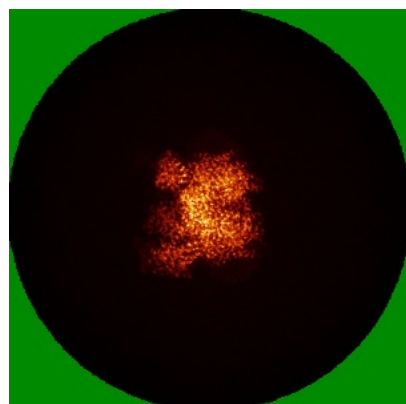


Z Index: 186

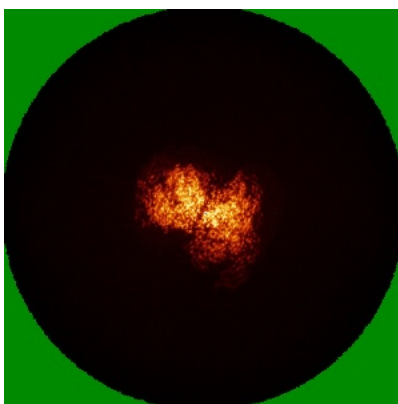
The images above show the largest variance slices of the map in three orthogonal directions.

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

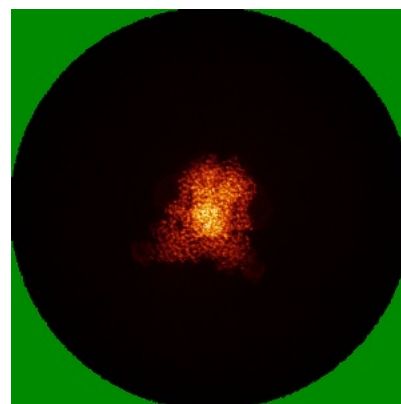
### 6.4.1 Primary map



X

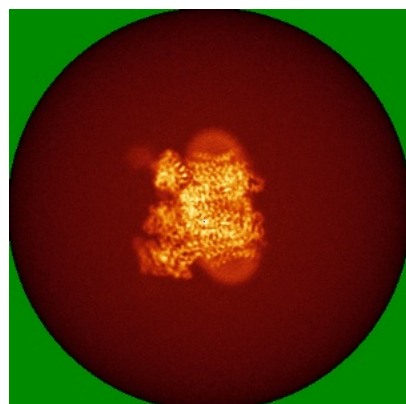


Y

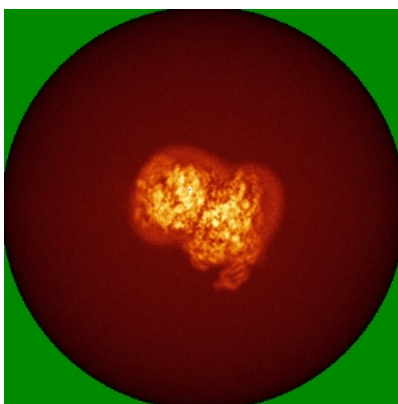


Z

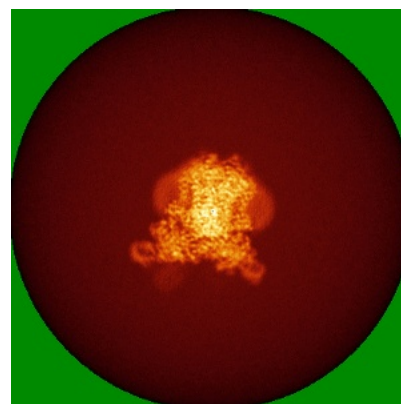
### 6.4.2 Raw map



X



Y

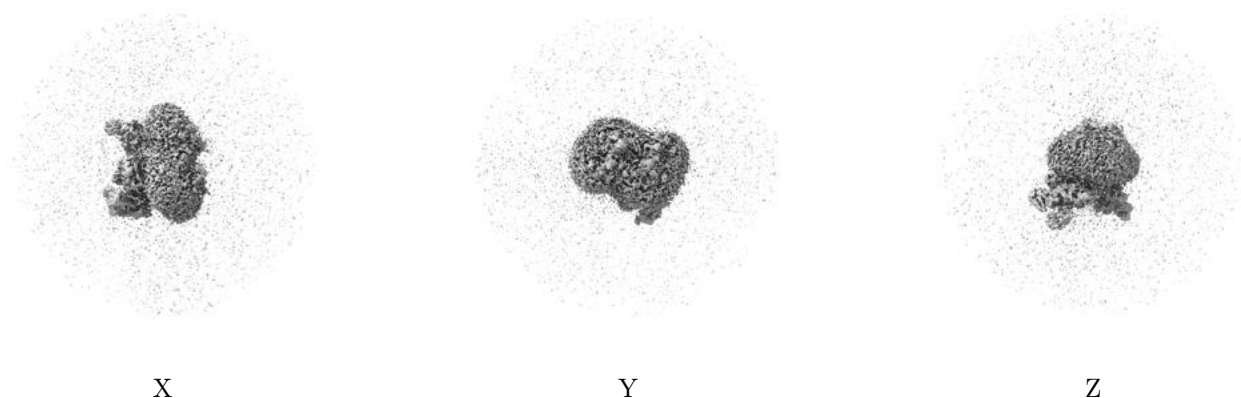


Z

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.

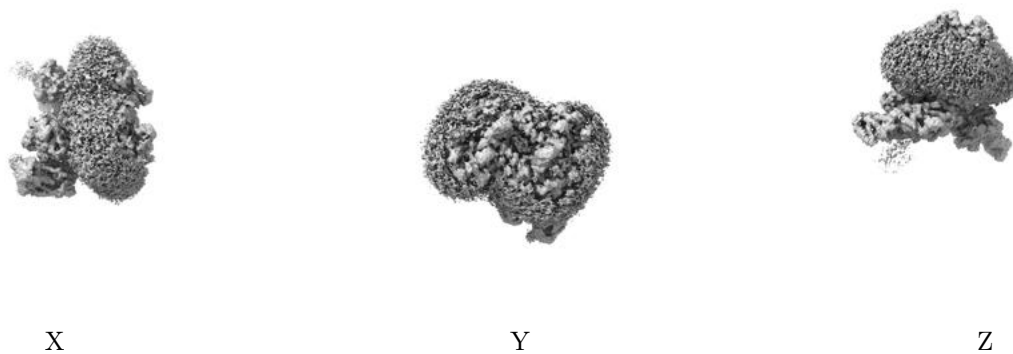
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

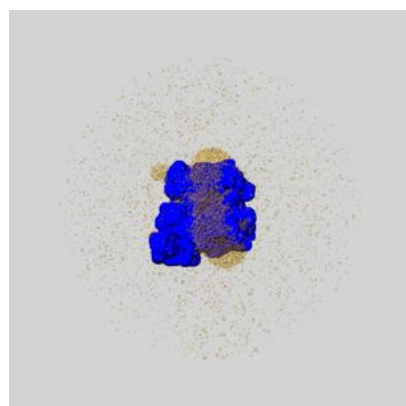
## 6.6 Mask visualisation [i](#)

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

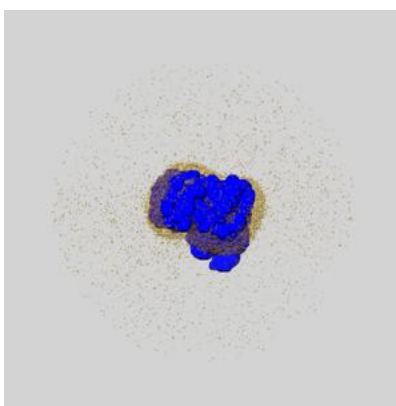
A mask typically either:

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

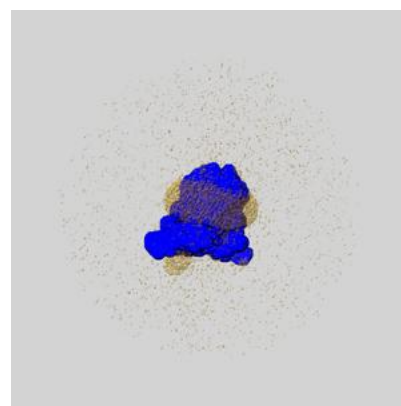
### 6.6.1 emd\_55898\_msk\_1.map [i](#)



X



Y

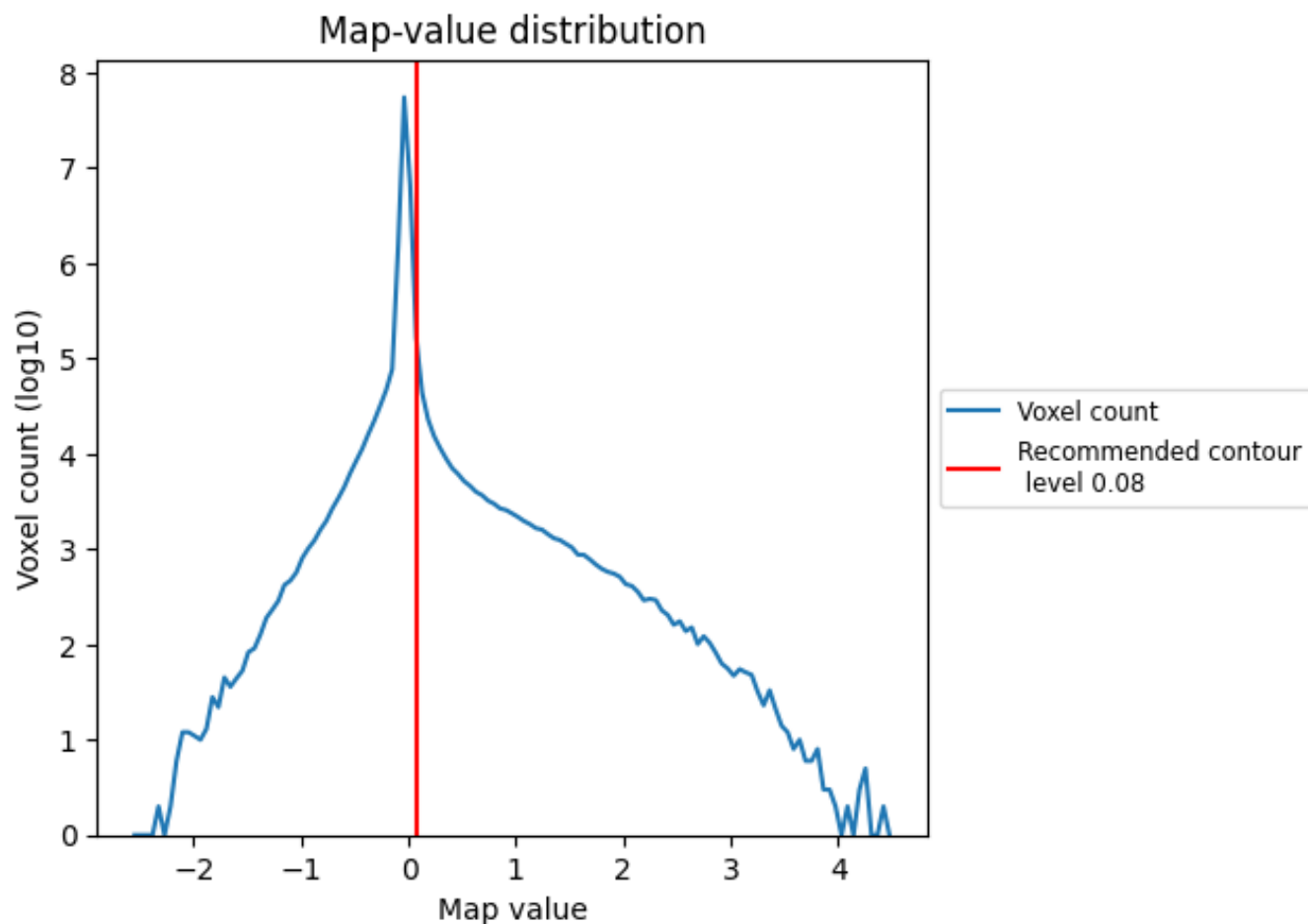


Z

## 7 Map analysis [i](#)

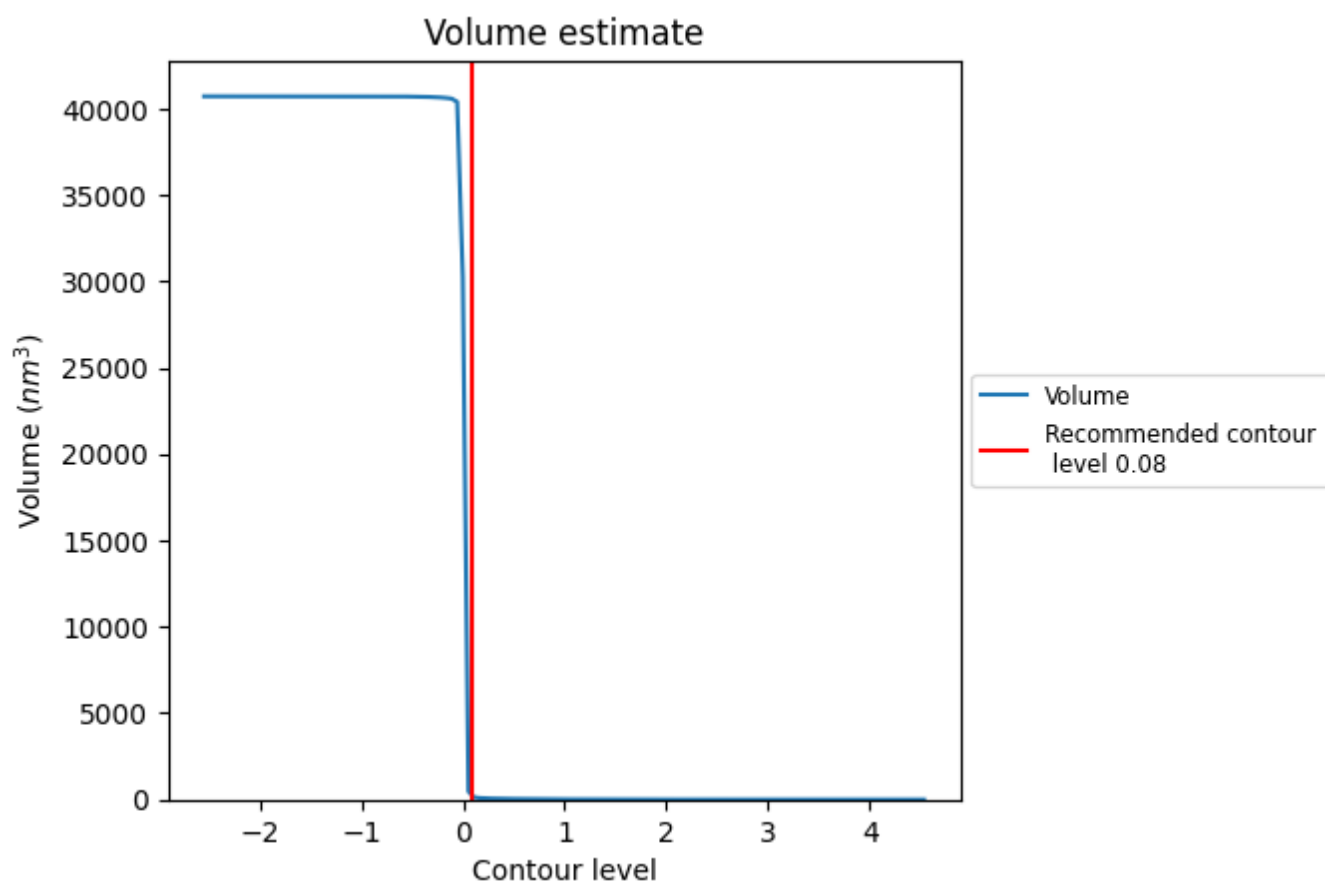
This section contains the results of statistical analysis of the map.

### 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.

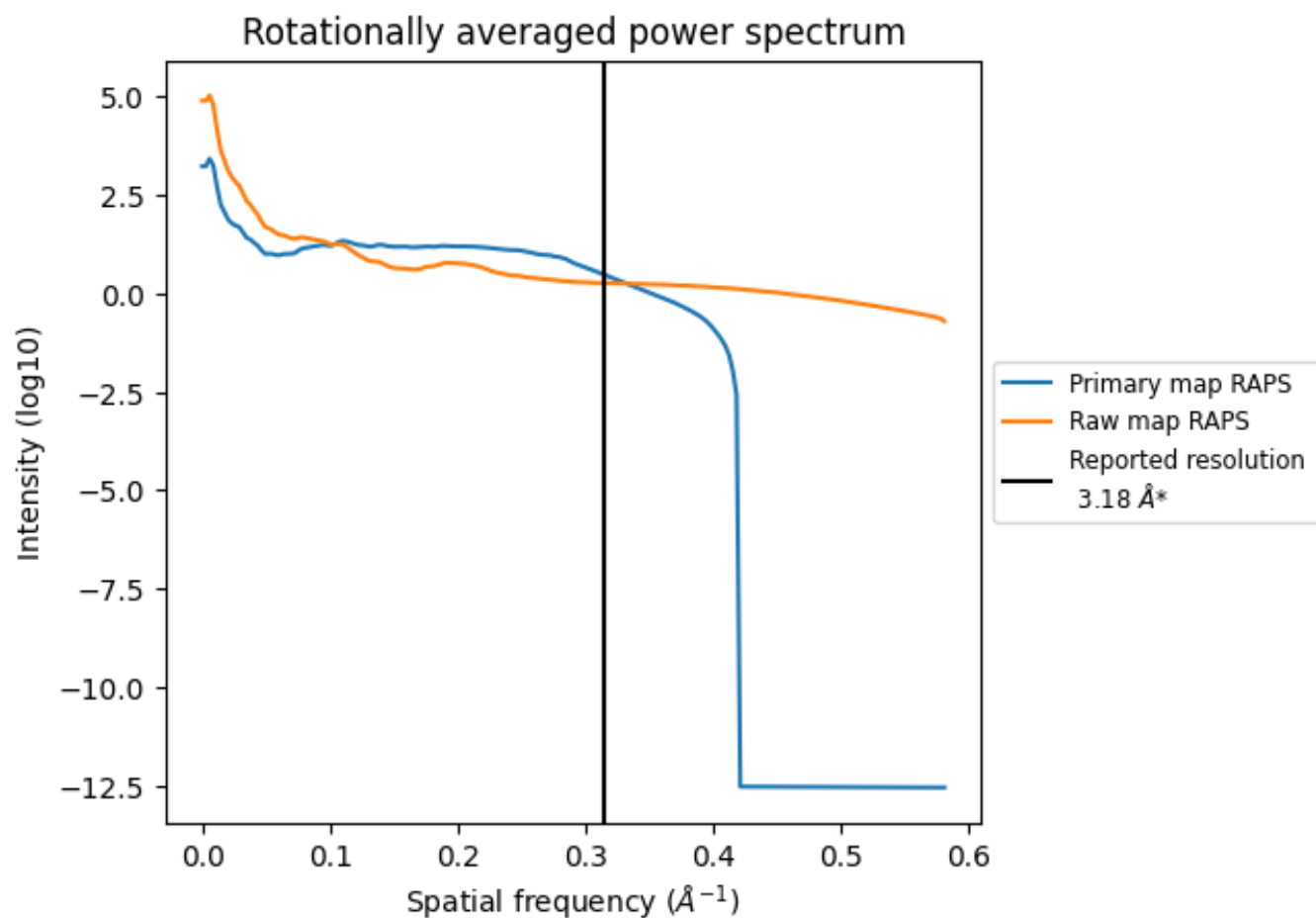
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 302 nm<sup>3</sup>; this corresponds to an approximate mass of 273 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 ⓘ

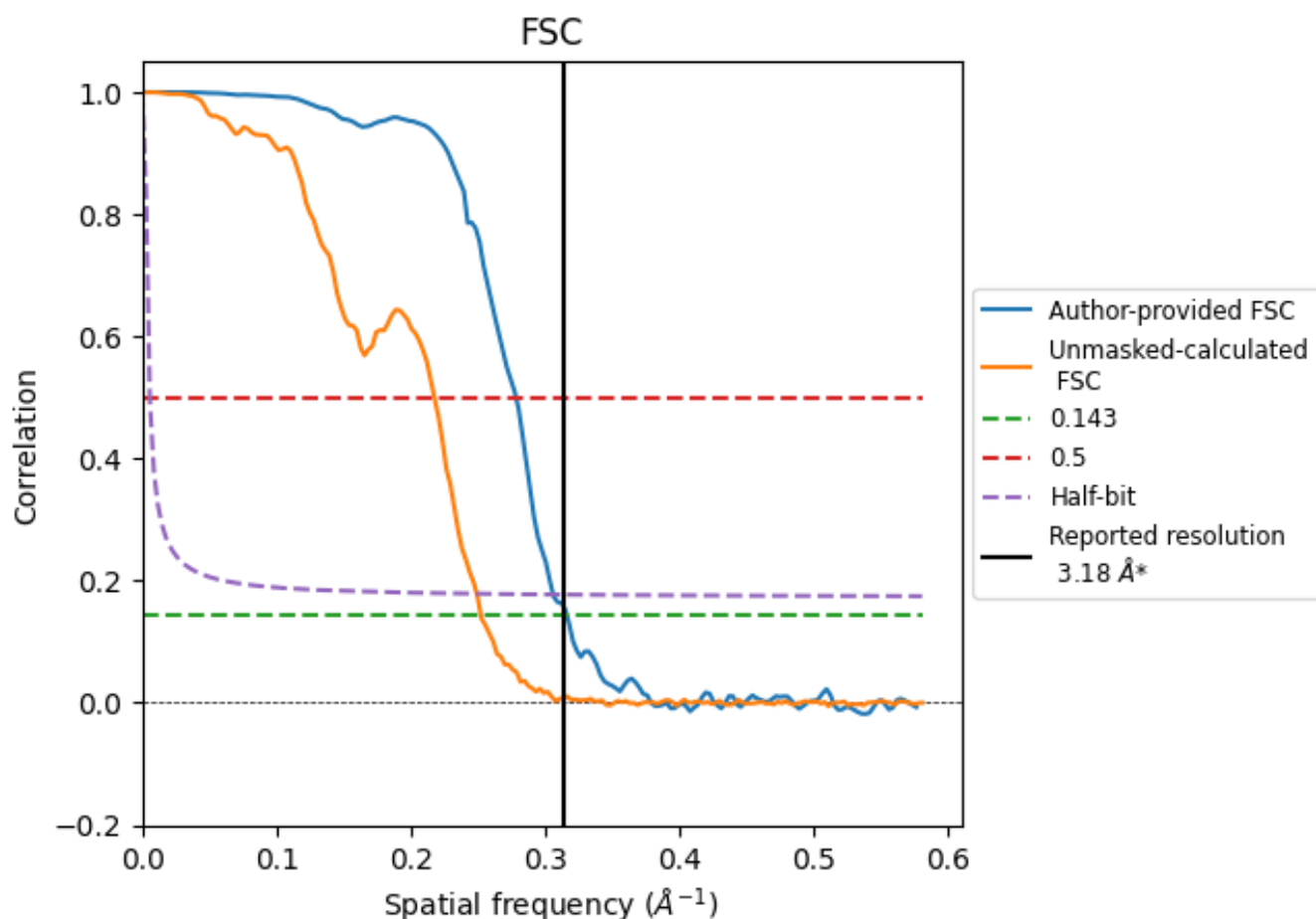


\*Reported resolution corresponds to spatial frequency of  $0.314 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.314  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

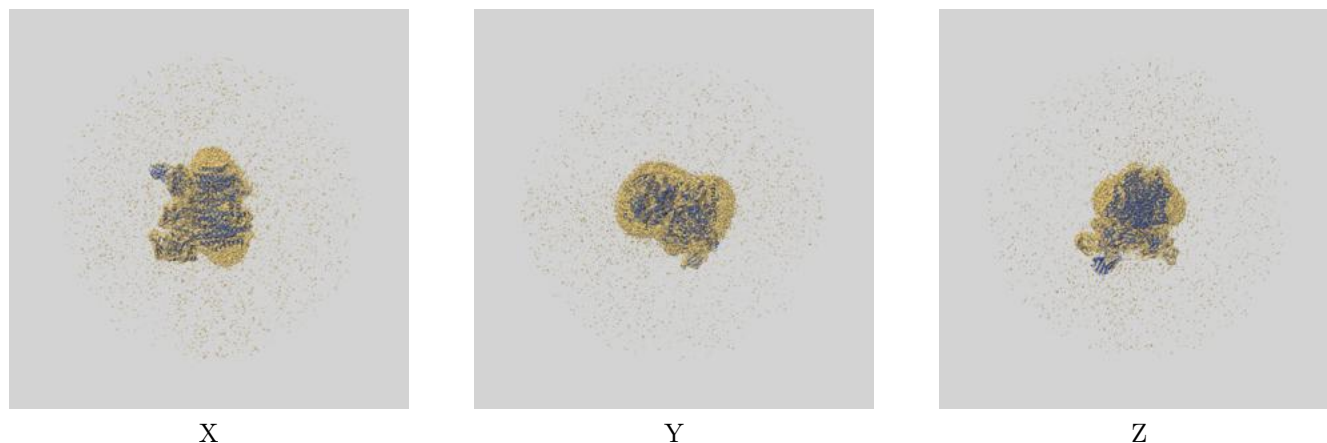
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.18	-	-
Author-provided FSC curve	3.16	3.59	3.26
Unmasked-calculated*	3.96	4.59	4.01

\*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 3.96 differs from the reported value 3.18 by more than 10 %

## 9 Map-model fit [i](#)

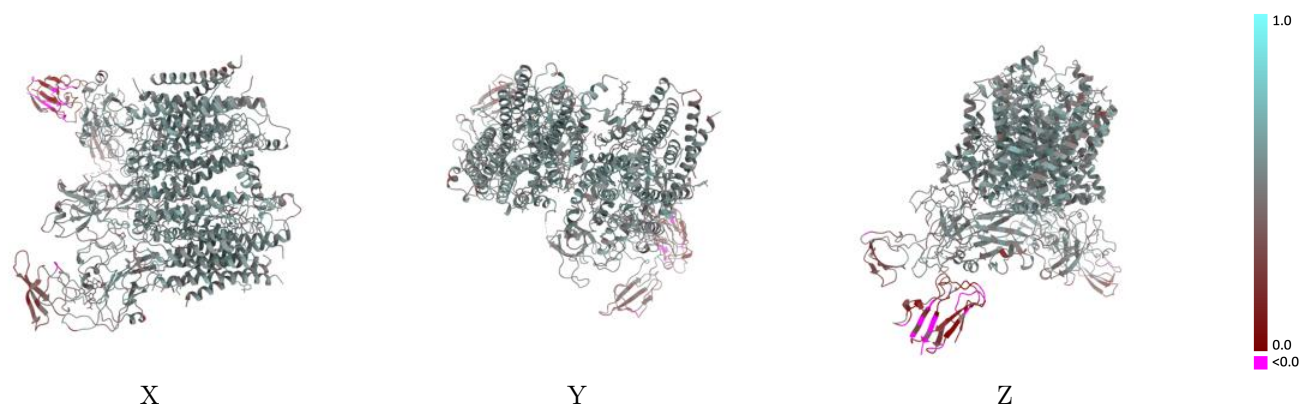
This section contains information regarding the fit between EMDB map EMD-55898 and PDB model 9TGG. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

### 9.1 Map-model overlay [i](#)



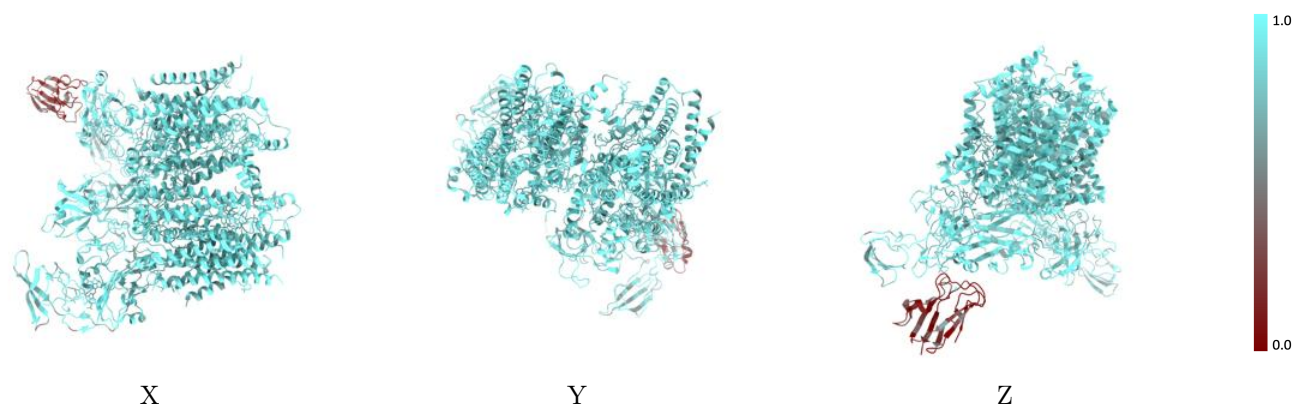
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



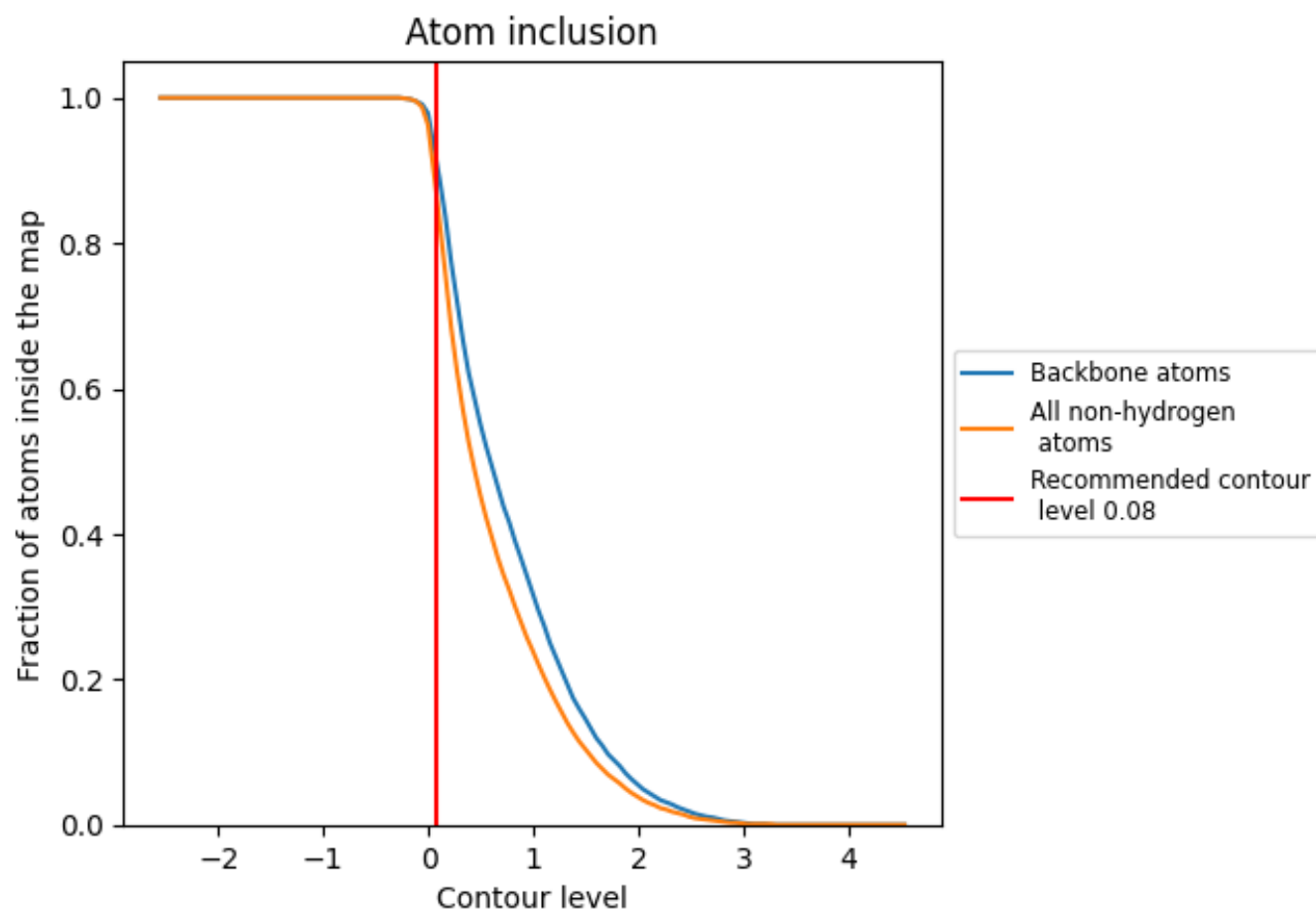
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8660	<div></div> 0.4970
A	<div></div> 0.9390	<div></div> 0.5680
B	<div></div> 0.9000	<div></div> 0.5210
C	<div></div> 0.8800	<div></div> 0.4750
D	<div></div> 0.9010	<div></div> 0.4950
E	<div></div> 0.8500	<div></div> 0.4900
F	<div></div> 0.8730	<div></div> 0.5080
G	<div></div> 0.9050	<div></div> 0.5250
H	<div></div> 0.8910	<div></div> 0.5310
I	<div></div> 0.9270	<div></div> 0.5550
J	<div></div> 0.8920	<div></div> 0.5240
K	<div></div> 0.8660	<div></div> 0.4760
L	<div></div> 0.8890	<div></div> 0.4950
M	<div></div> 0.8540	<div></div> 0.4970
N	<div></div> 0.9190	<div></div> 0.5290
O	<div></div> 0.9380	<div></div> 0.5360
P	<div></div> 0.8970	<div></div> 0.5390
Q	<div></div> 0.1660	<div></div> 0.1150

