



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 11:44 AM UTC

PDB ID : 7QRM / pdb_00007qrm
EMDB ID : EMD-14123
Title : Cryo-EM structure of catalytically active *Spinacia oleracea* cytochrome b6f in complex with endogenous plastoquinones at 2.7 Å resolution
Authors : Sarewicz, M.; Szwalec, M.; Indyka, P.; Rawski, M.; Pintscher, S.; Pietras, R.; Mielecki, B.; Jaciuk, M.; Glatt, S.; Osyczka, A.
Deposited on : 2022-01-11
Resolution : 2.70 Å (reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

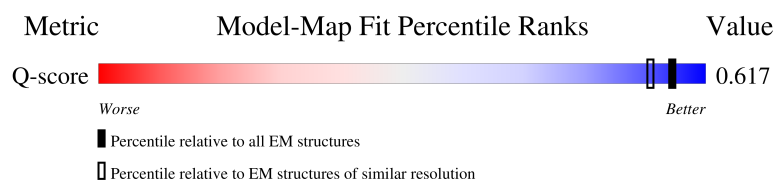
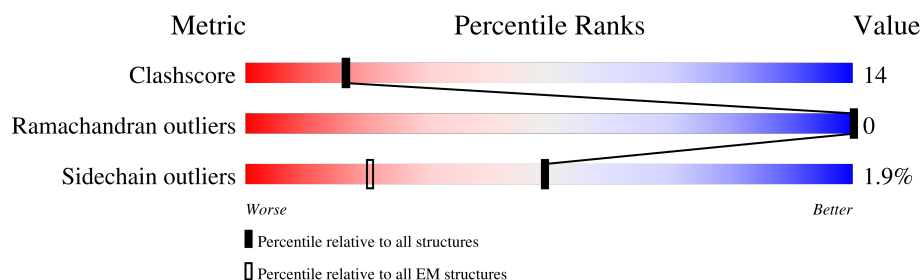
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	
2	J	160	

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Mol	Chain	Length	Quality of chain
3	C	320	
3	K	320	
4	D	230	
4	L	230	
5	E	31	
5	M	31	
6	F	36	
6	N	36	
7	G	37	
7	O	37	
8	H	29	
8	P	29	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	304	X	-	-	-
11	CLA	J	201	X	-	-	-
12	PL9	J	202	-	-	X	-

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 17012 atoms, of which 676 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	167	Total	C	N	O	S	0	0
			1263	809	213	234	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	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		

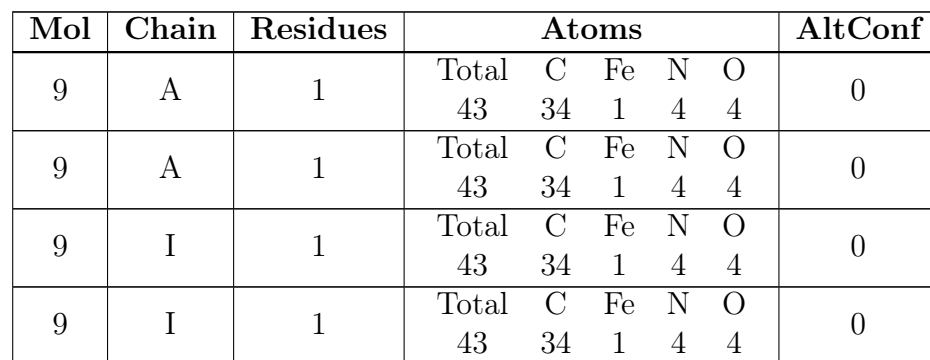
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

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		

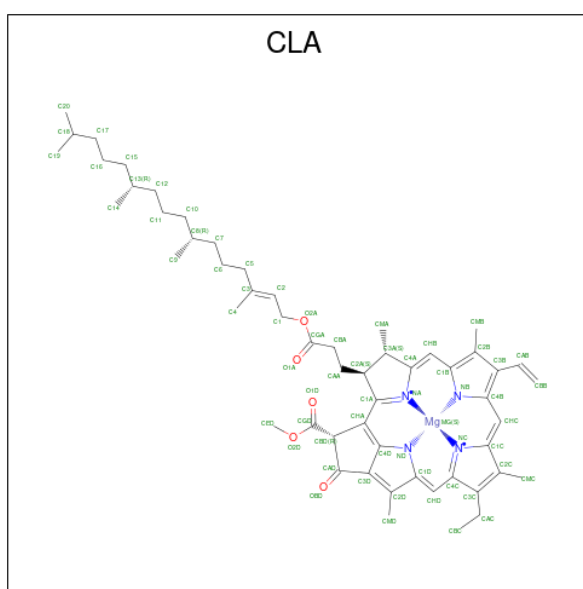
- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



- # HEC

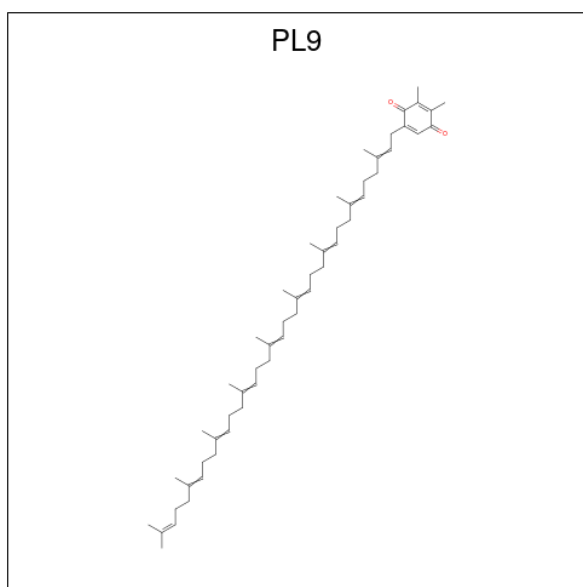
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	I	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
10	K	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



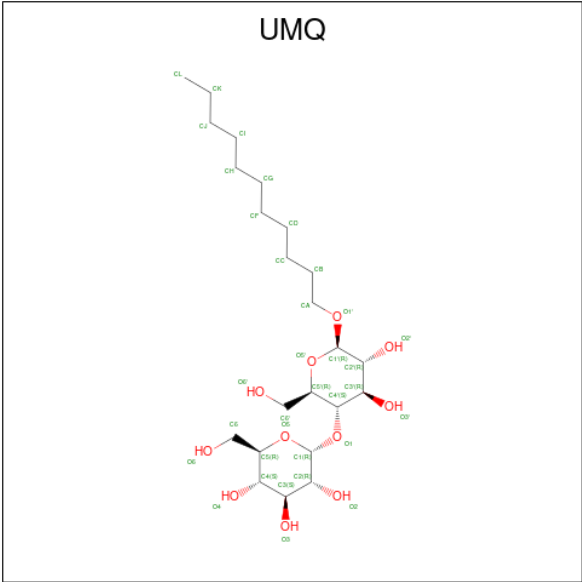
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 12 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).



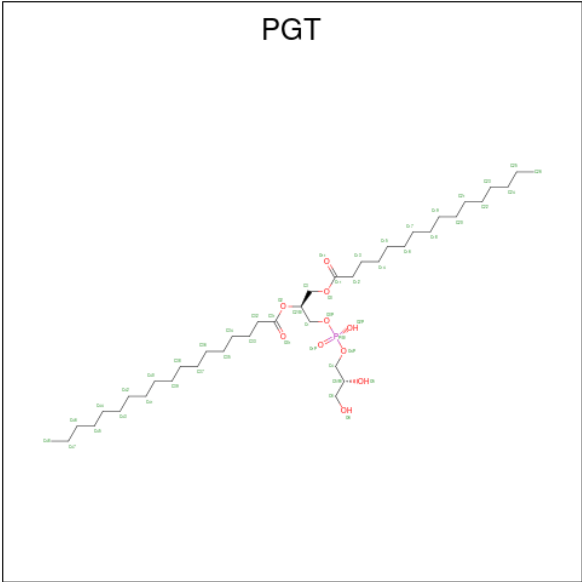
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O		0
			55	53	2		
12	B	1	Total	C	O		0
			55	53	2		
12	D	1	Total	C	O		0
			55	53	2		
12	I	1	Total	C	H	O	0
			135	53	80	2	
12	I	1	Total	C	O		0
			55	53	2		
12	J	1	Total	C	O		0
			55	53	2		
12	J	1	Total	C	O		0
			55	53	2		

- Molecule 13 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



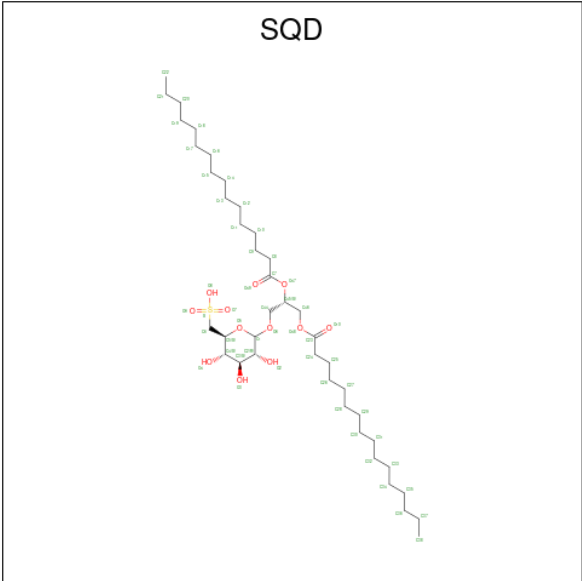
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	H	O	0
			78	23	44	11	
13	A	1	Total	C	H	O	0
			78	23	44	11	
13	B	1	Total	C	H	O	0
			78	23	44	11	
13	B	1	Total	C	H	O	0
			78	23	44	11	
13	H	1	Total	C	H	O	0
			78	23	44	11	
13	I	1	Total	C	H	O	0
			78	23	44	11	
13	I	1	Total	C	H	O	0
			78	23	44	11	
13	J	1	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 (1S)-2-{{{[(2R)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(palmitoyloxy)methyl]ethyl stearate (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



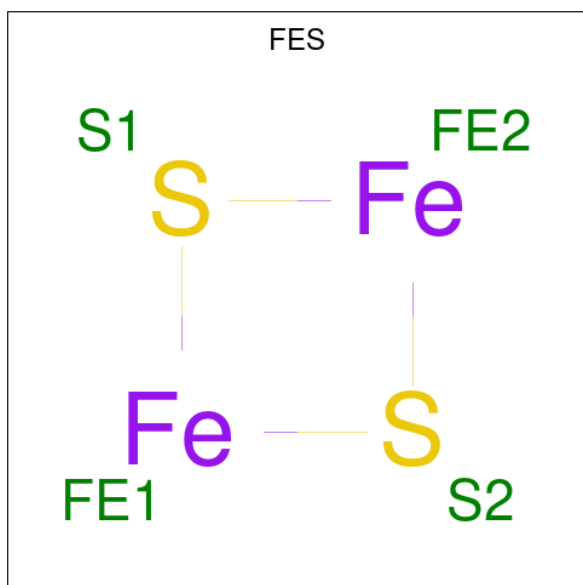
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	H	O	P	0
			129	40	78	10	1	
14	D	1	Total	C	O	P		0
			51	40	10	1		
14	I	1	Total	C	H	O	P	0
			129	40	78	10	1	
14	L	1	Total	C	O	P		0
			51	40	10	1		

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



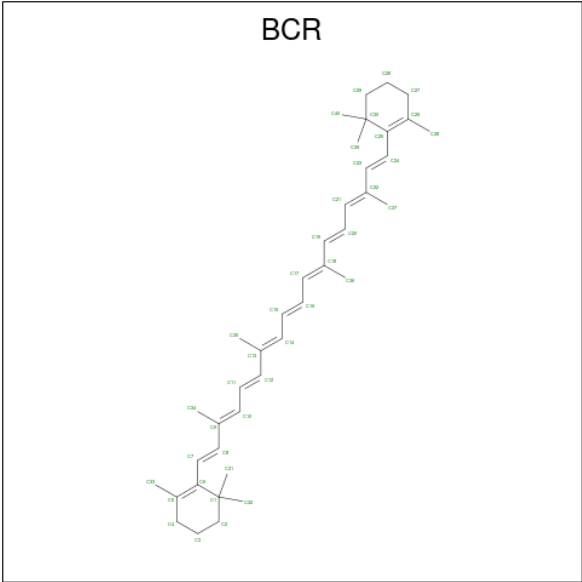
Mol	Chain	Residues	Atoms				AltConf
15	D	1	Total	C	O	S	0
			54	41	12	1	
15	K	1	Total	C	O	S	0
			54	41	12	1	

- 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	
16	L	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$) (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

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.

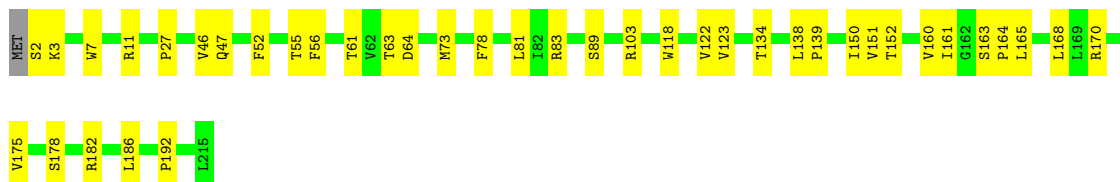
• Molecule 1: Cytochrome b6

Chain A:  80% 20%



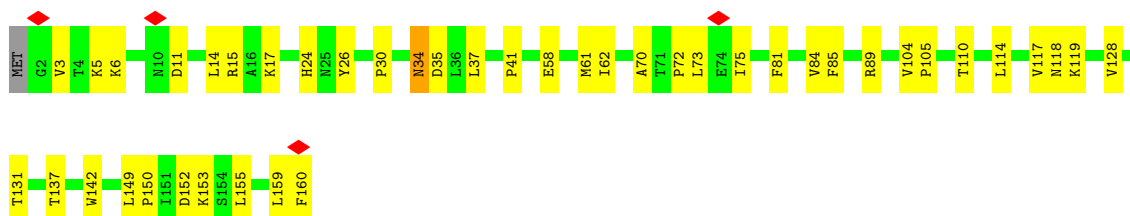
• Molecule 1: Cytochrome b6

Chain I:  81% 19%



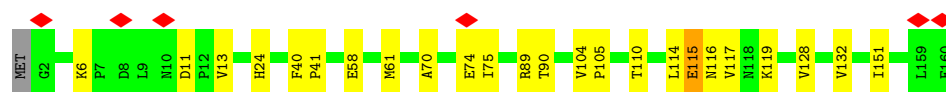
• Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:  72% 26% ..

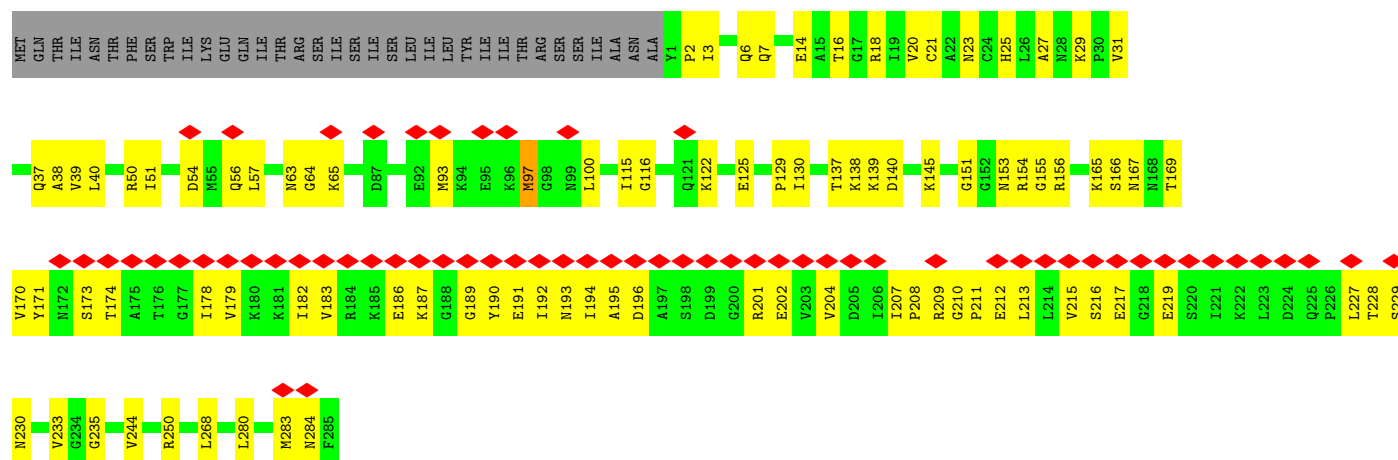


• Molecule 2: Cytochrome b6-f complex subunit 4

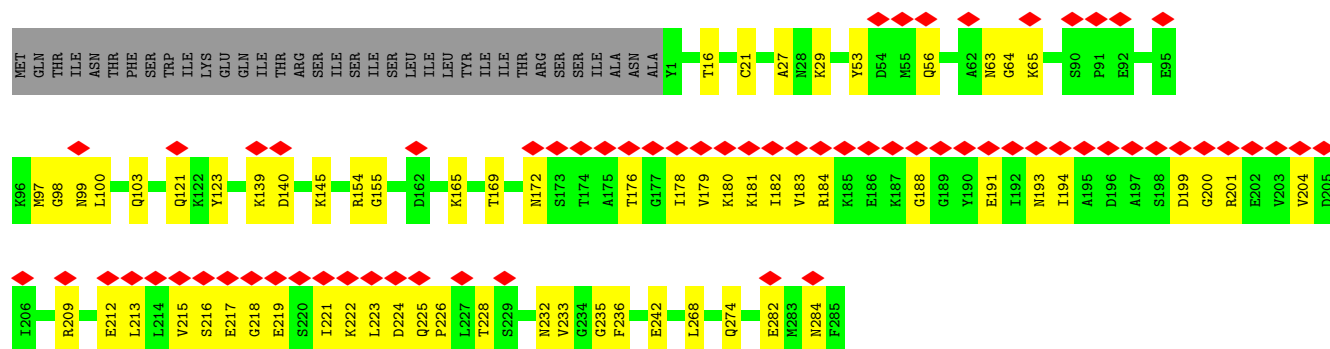
Chain J:  84% 14% ..



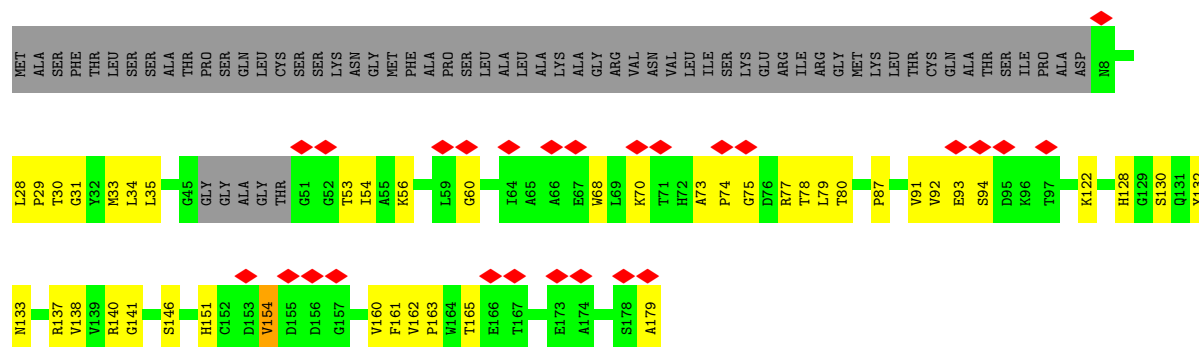
• Molecule 3: Cytochrome f



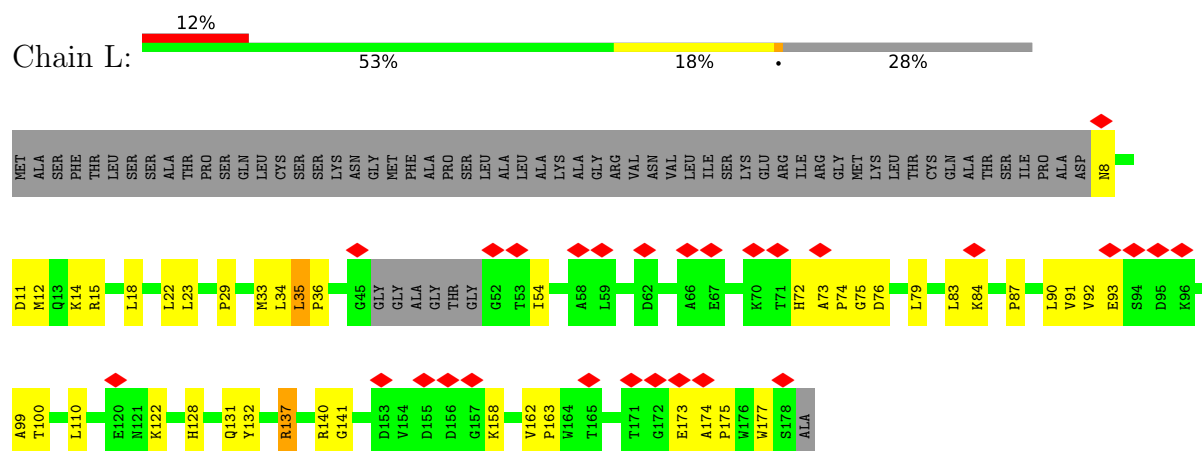
• Molecule 3: Cytochrome f



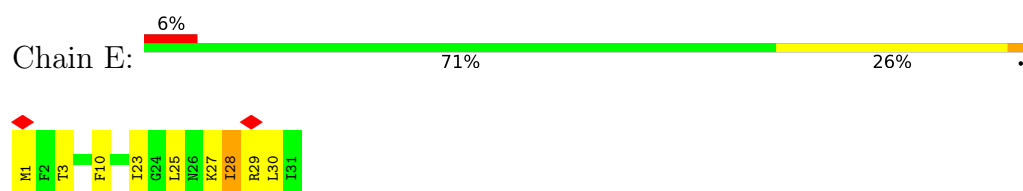
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic



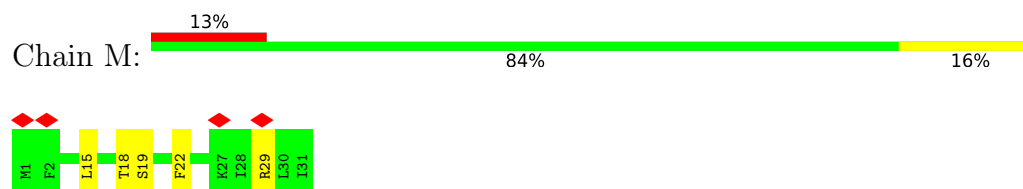
- Molecule 4: Cytochrome b6-f complex iron-sulfur subunit, chloroplastic



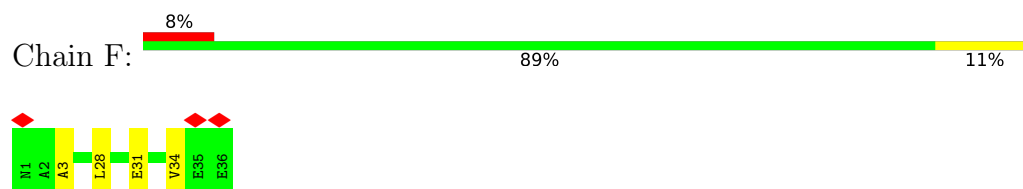
- Molecule 5: Cytochrome b6-f complex subunit 6



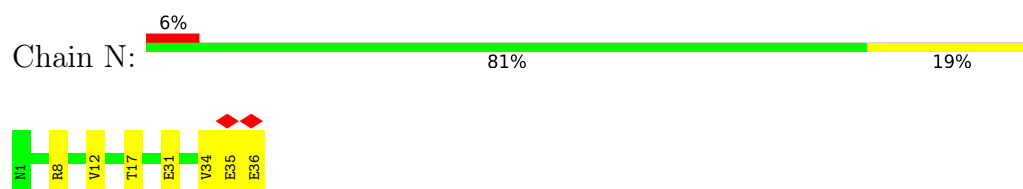
- Molecule 5: Cytochrome b6-f complex subunit 6



- Molecule 6: Cytochrome b6-f complex subunit 7

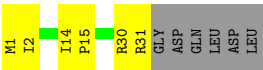


- Molecule 6: Cytochrome b6-f complex subunit 7



- Molecule 7: Cytochrome b6-f complex subunit 5

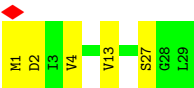
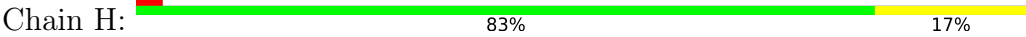




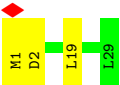
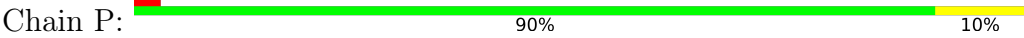
● Molecule 7: Cytochrome b6-f complex subunit 5



● Molecule 8: Cytochrome b6-f complex subunit 8



● Molecule 8: Cytochrome b6-f complex subunit 8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	97597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; 2 iteration in global CTF refinement, with an anisotropic mag. 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	2.202	Depositor
Minimum map value	-0.958	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.29	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: UMQ, SQD, BCR, PGT, CLA, HEM, FES, HEC, PL9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/1747	0.47	1/2382 (0.0%)
1	I	0.21	0/1747	0.44	0/2382
2	B	0.23	0/1262	0.53	3/1733 (0.2%)
2	J	0.18	0/1263	0.35	0/1733
3	C	0.18	0/2256	0.37	0/3058
3	K	0.16	0/2256	0.36	0/3058
4	D	0.16	0/1297	0.43	0/1774
4	L	0.15	0/1288	0.38	0/1762
5	E	0.21	0/247	0.49	0/333
5	M	0.14	0/247	0.30	0/333
6	F	0.23	0/265	0.41	0/359
6	N	0.19	0/265	0.35	0/359
7	G	0.16	0/254	0.35	0/344
7	O	0.17	0/254	0.38	0/344
8	H	0.15	0/227	0.36	0/309
8	P	0.16	0/228	0.30	0/309
All	All	0.19	0/15103	0.41	4/20572 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LEU	N-CA-C	6.64	121.45	112.88
2	B	34	ASN	N-CA-C	5.84	118.15	111.02
2	B	11	ASP	CA-C-N	5.38	125.20	119.28
2	B	11	ASP	C-N-CA	5.38	125.20	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1725	35	0
1	I	1697	0	1724	43	0
2	B	1225	0	1276	38	0
2	J	1226	0	1276	27	0
3	C	2209	0	2253	92	0
3	K	2209	0	2253	66	0
4	D	1263	0	1235	39	0
4	L	1254	0	1227	38	0
5	E	243	0	268	5	0
5	M	243	0	268	6	0
6	F	264	0	282	6	0
6	N	264	0	282	6	0
7	G	249	0	273	7	0
7	O	249	0	273	7	0
8	H	222	0	234	8	0
8	P	223	0	234	2	0
9	A	86	0	60	10	0
9	I	86	0	60	9	0
10	A	43	0	32	5	0
10	C	43	0	29	4	0
10	I	43	0	31	3	0
10	K	43	0	31	4	0
11	A	65	0	72	6	0
11	J	65	0	72	12	0
12	A	55	0	80	6	0
12	B	55	0	80	13	0
12	D	55	0	80	4	0
12	I	110	80	160	16	0
12	J	110	0	160	37	0
13	A	68	88	88	1	0
13	B	68	88	88	1	0
13	H	34	44	44	1	0
13	I	68	88	88	0	0
13	J	68	88	88	3	0
13	P	34	44	44	0	0
14	A	51	78	78	1	0
14	D	51	0	78	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	51	78	78	2	0
14	L	51	0	78	3	0
15	D	54	0	77	3	0
15	K	54	0	77	1	0
16	D	4	0	0	1	0
16	L	4	0	0	0	0
17	F	40	0	56	3	0
17	P	40	0	56	2	0
All	All	16336	676	17048	470	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 14.

All (470) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:CYS:SG	10:A:303:HEC:HBB2	1.77	1.23
3:C:211:PRO:HB2	3:C:228:THR:HG21	1.30	1.13
3:K:182:ILE:HG23	3:K:184:ARG:HH12	1.18	1.03
3:C:173:SER:HB3	3:C:227:LEU:HD11	1.39	1.03
10:I:2004:HEC:HBD1	10:I:2004:HEC:HHA	1.38	1.01
1:A:35:CYS:SG	10:A:303:HEC:CBB	2.51	0.98
1:I:170:ARG:HG2	1:I:175:VAL:HG12	1.47	0.96
1:I:150:ILE:HG13	12:J:202:PL9:H502	1.44	0.96
13:J:205:UMQ:HO21	13:J:205:UMQ:HO3'	1.13	0.95
3:C:100:LEU:HD22	3:C:115:ILE:HD11	1.47	0.92
1:I:152:THR:HG21	1:I:170:ARG:HG3	1.49	0.92
3:C:195:ALA:HA	3:C:202:GLU:HG3	1.52	0.90
4:D:54:ILE:HD13	4:D:160:VAL:HG12	1.54	0.90
3:K:176:THR:HB	3:K:223:LEU:HB2	1.55	0.88
3:C:21:CYS:HB2	10:C:301:HEC:HAB	1.55	0.87
3:K:194:ILE:HG21	3:K:221:ILE:HD11	1.58	0.86
9:I:2003:HEM:HBC2	9:I:2003:HEM:HMC2	1.58	0.85
7:O:30:ARG:HG2	7:O:30:ARG:HH11	1.41	0.85
7:G:30:ARG:O	7:G:31:ARG:HG2	1.78	0.84
9:A:301:HEM:HMB1	9:A:301:HEM:HBB2	1.63	0.81
3:K:182:ILE:HG23	3:K:184:ARG:NH1	1.95	0.81
10:K:301:HEC:HBC3	10:K:301:HEC:HHD	1.63	0.80
9:A:302:HEM:HBC2	9:A:302:HEM:HMC2	1.62	0.80
2:B:61:MET:CE	7:G:1:MET:HE1	2.13	0.79
2:B:3:VAL:HG12	3:C:280:LEU:HD13	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:LYS:HB2	3:C:154:ARG:NH2	1.98	0.78
9:I:2002:HEM:HMC1	9:I:2002:HEM:HBC2	1.65	0.78
2:B:152:ASP:OD1	2:B:153:LYS:HG3	1.84	0.78
3:C:179:VAL:CG1	3:C:217:GLU:HA	2.14	0.77
3:K:213:LEU:HA	3:K:228:THR:HG22	1.65	0.76
7:O:30:ARG:HG2	7:O:30:ARG:NH1	1.98	0.76
3:K:21:CYS:HB3	10:K:301:HEC:HAB	1.66	0.76
11:J:201:CLA:HHC	11:J:201:CLA:HBB1	1.67	0.75
11:J:201:CLA:H143	12:J:202:PL9:H272	1.67	0.75
9:I:2002:HEM:HMB1	9:I:2002:HEM:HBB2	1.66	0.74
2:B:152:ASP:OD1	2:B:153:LYS:N	2.21	0.74
3:K:213:LEU:HD21	3:K:215:VAL:O	1.88	0.73
4:L:91:VAL:HG13	4:L:99:ALA:CB	2.19	0.73
12:B:301:PL9:H28	6:F:3:ALA:CB	2.18	0.73
9:I:2003:HEM:HMB1	9:I:2003:HEM:HBB2	1.71	0.73
4:D:132:TYR:CE2	4:D:138:VAL:HG22	2.24	0.72
4:L:91:VAL:HG13	4:L:99:ALA:HB3	1.71	0.72
1:I:27:PRO:HG3	2:J:24:HIS:O	1.90	0.72
2:J:75:ILE:HD12	12:J:202:PL9:H511	1.70	0.72
11:J:201:CLA:H18	12:J:202:PL9:H353	1.72	0.72
3:C:29:LYS:HG2	3:C:235:GLY:HA3	1.73	0.71
3:K:194:ILE:HD13	3:K:221:ILE:CD1	2.21	0.71
5:E:1:MET:HE3	5:E:3:THR:HB	1.70	0.71
3:C:186:GLU:OE1	3:C:186:GLU:N	2.21	0.71
3:C:183:VAL:HG13	3:C:191:GLU:HB2	1.72	0.70
3:K:63:ASN:OD1	3:K:64:GLY:N	2.24	0.70
10:I:2004:HEC:HBD1	10:I:2004:HEC:CHA	2.16	0.70
1:A:27:PRO:HG3	2:B:24:HIS:O	1.91	0.70
4:L:173:GLU:OE2	4:L:174:ALA:N	2.19	0.70
1:I:78:PHE:H	12:I:2008:PL9:H522	1.55	0.70
4:L:8:ASN:HB3	5:M:29:ARG:HH22	1.56	0.70
14:L:801:PGT:H331	14:L:801:PGT:H402	1.71	0.70
2:B:14:LEU:HD13	2:B:26:TYR:HD2	1.57	0.69
3:C:3:ILE:O	3:C:7:GLN:HG2	1.92	0.69
3:C:182:ILE:HD11	3:C:213:LEU:HD11	1.75	0.69
3:K:183:VAL:CG1	3:K:191:GLU:HB3	2.22	0.69
9:A:302:HEM:HBB2	9:A:302:HEM:HMB1	1.75	0.69
3:C:18:ARG:NH2	3:C:23:ASN:OD1	2.25	0.69
4:L:8:ASN:HB3	5:M:29:ARG:NH2	2.07	0.69
3:C:2:PRO:O	3:C:6:GLN:HG3	1.93	0.69
1:I:160:VAL:HG13	1:I:161:ILE:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2003:HEM:HBA1	9:I:2003:HEM:HHA	1.75	0.69
3:K:27:ALA:HB3	3:K:235:GLY:HA2	1.74	0.69
3:K:194:ILE:HD13	3:K:221:ILE:HD13	1.76	0.69
3:K:182:ILE:HD11	3:K:213:LEU:HD11	1.75	0.68
2:J:75:ILE:HD12	12:J:202:PL9:H501	1.74	0.68
4:L:140:ARG:HG2	4:L:141:GLY:N	2.07	0.68
9:A:301:HEM:HMC1	9:A:301:HEM:HBC2	1.75	0.68
1:I:73:MET:SD	1:I:83:ARG:HD3	2.34	0.68
3:K:188:GLY:O	3:K:209:ARG:HG3	1.94	0.68
3:C:155:GLY:O	10:C:301:HEC:HBA1	1.94	0.68
3:C:179:VAL:HG11	3:C:217:GLU:HA	1.75	0.67
3:C:54:ASP:HB3	3:C:57:LEU:HD22	1.75	0.67
12:I:2008:PL9:H151	12:I:2008:PL9:H202	1.76	0.67
2:J:89:ARG:HH12	12:J:203:PL9:H522	1.58	0.67
3:K:179:VAL:HG11	3:K:218:GLY:H	1.59	0.67
12:I:2008:PL9:H38	12:I:2008:PL9:H43	1.76	0.67
4:L:11:ASP:OD1	4:L:14:LYS:HG3	1.95	0.67
6:N:31:GLU:O	6:N:34:VAL:HG12	1.94	0.66
2:B:128:VAL:O	2:B:131:THR:HG22	1.95	0.66
2:B:61:MET:HE3	7:G:1:MET:HE1	1.77	0.66
3:K:181:LYS:HB3	3:K:193:ASN:HD22	1.61	0.66
1:A:22:THR:HG22	1:A:22:THR:O	1.95	0.66
3:C:29:LYS:HB2	3:C:154:ARG:HH21	1.59	0.66
3:C:201:ARG:HE	3:C:202:GLU:N	1.93	0.66
1:I:192:PRO:HB2	12:I:2001:PL9:H252	1.79	0.65
1:I:163:SER:N	1:I:164:PRO:HD2	2.12	0.65
3:K:97:MET:O	3:K:100:LEU:HD13	1.96	0.65
3:C:93:MET:O	3:C:97:MET:HG3	1.96	0.65
1:I:61:THR:HB	1:I:64:ASP:OD1	1.97	0.65
3:K:145:LYS:CE	3:K:242:GLU:HG3	2.26	0.65
4:L:54:ILE:HD11	4:L:158:LYS:HD3	1.80	0.64
3:C:193:ASN:OD1	3:C:204:VAL:HG22	1.98	0.64
2:B:14:LEU:HD13	2:B:26:TYR:CD2	2.32	0.64
2:J:41:PRO:HB2	3:K:268:LEU:HD21	1.79	0.64
3:K:29:LYS:HB2	3:K:154:ARG:NH1	2.12	0.64
6:N:35:GLU:O	6:N:36:GLU:HG3	1.97	0.64
3:C:211:PRO:HB2	3:C:228:THR:CG2	2.18	0.63
2:J:75:ILE:HB	12:J:202:PL9:H512	1.80	0.63
3:K:145:LYS:HE3	3:K:242:GLU:HG3	1.80	0.63
2:B:41:PRO:HB2	3:C:268:LEU:HD21	1.81	0.63
3:C:25:HIS:CE1	3:C:153:ASN:HD21	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:ASN:OD1	3:C:64:GLY:N	2.32	0.63
2:J:128:VAL:O	2:J:132:VAL:HG23	1.98	0.63
2:B:70:ALA:HB1	3:C:16:THR:HG22	1.81	0.62
3:C:156:ARG:NH1	3:C:167:ASN:OD1	2.32	0.62
12:A:305:PL9:H48	2:B:85:PHE:CD1	2.34	0.62
3:K:182:ILE:HD11	3:K:213:LEU:CD1	2.29	0.62
2:J:58:GLU:OE2	3:K:145:LYS:NZ	2.29	0.62
12:B:301:PL9:H28	6:F:3:ALA:HB1	1.79	0.62
3:C:37:GLN:O	13:H:201:UMQ:O6	2.14	0.62
3:K:21:CYS:CB	10:K:301:HEC:HAB	2.30	0.62
1:I:161:ILE:HG13	1:I:161:ILE:O	2.00	0.62
3:C:170:VAL:HG12	3:C:230:ASN:HA	1.80	0.62
3:C:173:SER:HB3	3:C:227:LEU:CD1	2.24	0.62
4:L:72:HIS:HB3	4:L:76:ASP:OD2	2.00	0.61
3:K:100:LEU:HD11	3:K:123:TYR:CZ	2.35	0.61
5:M:22:PHE:HE2	6:N:34:VAL:HG11	1.64	0.61
1:A:52:PHE:O	1:A:55:THR:OG1	2.13	0.61
4:D:128:HIS:HB2	16:D:203:FES:S1	2.41	0.61
3:K:100:LEU:HD11	3:K:123:TYR:CE1	2.35	0.61
4:L:54:ILE:CD1	4:L:158:LYS:HD3	2.30	0.61
4:L:99:ALA:O	4:L:100:THR:OG1	2.14	0.61
3:C:20:VAL:HG23	3:C:20:VAL:O	2.01	0.60
4:D:154:VAL:O	4:D:154:VAL:HG22	2.00	0.60
3:K:223:LEU:O	3:K:224:ASP:HB2	2.00	0.60
1:A:81:LEU:HD21	12:D:202:PL9:H221	1.83	0.60
1:A:176:GLY:O	1:A:179:THR:HG22	2.00	0.60
9:A:302:HEM:HHA	9:A:302:HEM:HBA1	1.82	0.60
3:C:182:ILE:HG23	3:C:182:ILE:O	2.01	0.60
3:C:212:GLU:O	3:C:228:THR:HG23	2.02	0.60
8:H:1:MET:HG2	8:H:2:ASP:N	2.17	0.60
11:J:201:CLA:O1D	12:J:203:PL9:H48	2.02	0.60
2:B:73:LEU:O	12:B:301:PL9:HC2	2.01	0.60
3:C:57:LEU:HD12	3:C:233:VAL:HB	1.84	0.60
4:D:79:LEU:HD11	4:D:87:PRO:HB2	1.83	0.60
1:I:170:ARG:CG	1:I:175:VAL:HG12	2.28	0.60
4:L:175:PRO:HB3	4:L:177:TRP:CH2	2.37	0.59
3:K:176:THR:HB	3:K:223:LEU:CB	2.31	0.59
14:D:204:PGT:H462	1:I:186:LEU:HD21	1.82	0.59
1:I:61:THR:HG22	1:I:63:THR:H	1.66	0.59
9:I:2002:HEM:HBC2	9:I:2002:HEM:CMC	2.33	0.59
9:I:2002:HEM:HBB2	9:I:2002:HEM:CMB	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:PRO:HG2	2:B:75:ILE:HD11	1.84	0.59
4:D:165:THR:HG22	4:D:165:THR:O	2.02	0.59
3:K:225:GLN:HG3	3:K:226:PRO:HD2	1.84	0.59
4:D:74:PRO:HA	4:D:92:VAL:CG2	2.32	0.59
4:L:131:GLN:HG3	4:L:140:ARG:HD3	1.85	0.59
1:I:134:THR:HG23	12:J:202:PL9:H253	1.84	0.59
3:K:155:GLY:O	10:K:301:HEC:HBA1	2.03	0.58
3:C:153:ASN:HD22	10:C:301:HEC:CHB	2.17	0.58
3:C:178:ILE:HD12	3:C:219:GLU:O	2.04	0.58
4:D:29:PRO:O	4:D:33:MET:HG2	2.04	0.58
14:D:204:PGT:H351	1:I:168:LEU:HD21	1.84	0.58
3:C:194:ILE:O	3:C:202:GLU:HA	2.03	0.58
3:C:153:ASN:OD1	3:C:154:ARG:N	2.37	0.58
4:L:35:LEU:HB2	4:L:36:PRO:HD3	1.86	0.58
9:A:302:HEM:HBB2	9:A:302:HEM:CMB	2.34	0.57
3:C:213:LEU:HD21	3:C:215:VAL:O	2.04	0.57
2:J:11:ASP:OD1	2:J:13:VAL:HG12	2.05	0.57
2:B:61:MET:HB3	3:C:145:LYS:HB3	1.86	0.57
3:K:193:ASN:OD1	3:K:204:VAL:HG22	2.05	0.57
4:D:74:PRO:HA	4:D:92:VAL:HG23	1.86	0.57
14:D:204:PGT:H421	14:D:204:PGT:H372	1.87	0.57
3:K:179:VAL:CG1	3:K:218:GLY:H	2.16	0.57
9:I:2003:HEM:HBC2	9:I:2003:HEM:CMC	2.33	0.57
9:A:302:HEM:HBC2	9:A:302:HEM:CMC	2.34	0.57
9:I:2003:HEM:HBB2	9:I:2003:HEM:CMB	2.34	0.56
5:M:15:LEU:O	5:M:18:THR:HG22	2.05	0.56
1:A:35:CYS:SG	10:A:303:HEC:CAB	2.93	0.56
10:I:2004:HEC:HBC3	10:I:2004:HEC:HHD	1.86	0.56
4:L:162:VAL:HG13	4:L:163:PRO:HD2	1.86	0.56
4:D:130:SER:HB3	4:D:141:GLY:HA3	1.87	0.56
3:K:233:VAL:HG22	3:K:233:VAL:O	2.04	0.56
9:A:301:HEM:HBB2	9:A:301:HEM:CMB	2.34	0.56
13:J:205:UMQ:O3'	13:J:205:UMQ:O2	2.03	0.56
3:C:57:LEU:HD23	3:C:57:LEU:H	1.71	0.55
5:E:28:ILE:O	5:E:28:ILE:HG13	2.06	0.55
4:L:75:GLY:H	4:L:92:VAL:HG23	1.72	0.55
4:D:162:VAL:HG13	4:D:163:PRO:HD2	1.88	0.55
6:F:31:GLU:O	6:F:34:VAL:HG12	2.07	0.55
3:K:139:LYS:O	3:K:140:ASP:HB2	2.05	0.55
9:A:301:HEM:HBC2	9:A:301:HEM:CMC	2.35	0.55
3:C:183:VAL:CG1	3:C:191:GLU:HB2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:ILE:HD11	3:C:213:LEU:CD1	2.37	0.55
3:K:199:ASP:HB2	3:K:201:ARG:CD	2.37	0.54
12:B:301:PL9:HC72	12:B:301:PL9:H122	1.88	0.54
4:D:30:THR:O	4:D:34:LEU:HG	2.07	0.54
7:O:26:TYR:CZ	7:O:30:ARG:HD2	2.43	0.54
1:A:22:THR:O	1:A:22:THR:CG2	2.56	0.54
1:A:103:ARG:HD2	1:A:103:ARG:C	2.33	0.54
1:A:190:VAL:HG22	12:I:2008:PL9:H501	1.90	0.54
4:D:138:VAL:HG23	4:D:146:SER:HA	1.89	0.54
1:I:81:LEU:HG	12:I:2008:PL9:H252	1.90	0.54
3:K:165:LYS:HE3	3:K:169:THR:HG21	1.90	0.54
4:D:93:GLU:HG3	4:D:94:SER:H	1.72	0.54
2:J:75:ILE:HD12	12:J:202:PL9:C51	2.36	0.54
1:I:151:VAL:HG13	12:J:202:PL9:C45	2.38	0.53
2:J:75:ILE:HB	12:J:202:PL9:C51	2.38	0.53
2:J:75:ILE:HD12	12:J:202:PL9:C50	2.39	0.53
3:K:212:GLU:O	3:K:228:THR:HB	2.08	0.53
3:C:201:ARG:HE	3:C:202:GLU:H	1.55	0.53
11:J:201:CLA:C18	12:J:202:PL9:H353	2.37	0.53
12:J:203:PL9:H351	12:J:203:PL9:C38	2.39	0.53
11:A:304:CLA:O2D	11:A:304:CLA:HBA2	2.09	0.53
4:D:163:PRO:HB3	4:D:179:ALA:O	2.09	0.53
4:L:162:VAL:CG1	4:L:163:PRO:HD2	2.39	0.53
3:C:170:VAL:HG12	3:C:229:SER:O	2.09	0.53
1:A:70:GLN:HG3	2:B:62:ILE:HD13	1.91	0.52
3:C:137:THR:HG22	3:C:137:THR:O	2.09	0.52
3:K:145:LYS:HE2	3:K:242:GLU:HG3	1.91	0.52
3:K:184:ARG:HD2	3:K:184:ARG:N	2.23	0.52
4:D:54:ILE:HD13	4:D:160:VAL:CG1	2.35	0.52
4:D:68:TRP:HZ2	4:D:78:THR:HB	1.73	0.52
2:J:41:PRO:HB2	3:K:268:LEU:CD2	2.39	0.52
2:B:89:ARG:HH11	12:B:301:PL9:H523	1.75	0.52
3:C:189:GLY:HA3	3:C:207:ILE:O	2.09	0.52
15:D:201:SQD:H262	15:D:201:SQD:O10	2.09	0.52
12:A:305:PL9:H453	2:B:84:VAL:HG23	1.92	0.52
1:I:134:THR:CG2	12:J:202:PL9:H253	2.40	0.52
2:J:74:GLU:OE2	12:J:203:PL9:H171	2.10	0.51
12:J:202:PL9:H251	12:J:202:PL9:C28	2.40	0.51
3:K:27:ALA:HB2	3:K:232:ASN:HD21	1.75	0.51
14:D:204:PGT:C47	14:D:204:PGT:H431	2.37	0.51
2:J:114:LEU:C	2:J:114:LEU:HD12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:MET:HE1	7:G:1:MET:HE1	1.92	0.51
12:B:301:PL9:C38	12:B:301:PL9:H351	2.41	0.51
3:C:179:VAL:HG13	3:C:217:GLU:HA	1.93	0.51
4:D:132:TYR:CD2	4:D:138:VAL:HG22	2.45	0.51
1:I:152:THR:CG2	1:I:170:ARG:HG3	2.30	0.51
2:J:74:GLU:HG3	12:J:203:PL9:H121	1.93	0.51
2:J:104:VAL:HB	2:J:105:PRO:CD	2.40	0.51
4:L:73:ALA:HB1	4:L:74:PRO:HD2	1.93	0.51
1:A:3:LYS:HD3	14:A:308:PGT:H31	1.91	0.51
3:C:165:LYS:CG	3:C:169:THR:HG21	2.41	0.51
1:I:3:LYS:NZ	14:I:2007:PGT:O5	2.41	0.51
3:C:2:PRO:HG2	3:C:116:GLY:HA2	1.93	0.51
1:A:195:THR:O	1:A:199:MET:HB2	2.11	0.50
4:D:28:LEU:HB2	4:D:29:PRO:HD3	1.94	0.50
1:I:78:PHE:N	12:I:2008:PL9:H522	2.23	0.50
6:N:17:THR:HG23	8:P:19:LEU:HD21	1.94	0.50
1:A:185:SER:HG	1:I:56:PHE:HE1	1.58	0.50
3:C:228:THR:HG22	3:C:229:SER:N	2.27	0.50
1:A:158:ILE:HG23	1:A:159:PRO:HD2	1.94	0.50
4:D:130:SER:HA	4:D:141:GLY:HA3	1.94	0.50
3:K:282:GLU:HB3	3:K:284:ASN:OD1	2.11	0.50
3:C:192:ILE:O	3:C:204:VAL:HA	2.11	0.50
2:J:115:GLU:HG3	13:J:205:UMQ:HA1	1.93	0.50
3:K:172:ASN:OD1	3:K:226:PRO:HA	2.12	0.49
4:L:175:PRO:HB3	4:L:177:TRP:CZ2	2.47	0.49
2:B:159:LEU:O	2:B:160:PHE:C	2.54	0.49
8:H:1:MET:HG2	8:H:2:ASP:H	1.77	0.49
4:L:131:GLN:HB2	4:L:140:ARG:HB3	1.94	0.49
5:E:10:PHE:HB2	8:H:13:VAL:HG21	1.95	0.49
1:I:78:PHE:H	12:I:2008:PL9:C52	2.21	0.49
1:I:81:LEU:HG	12:I:2008:PL9:C25	2.43	0.49
12:J:202:PL9:H251	12:J:202:PL9:H28	1.94	0.49
3:K:181:LYS:HA	3:K:217:GLU:OE2	2.12	0.49
3:K:274:GLN:OE1	4:L:18:LEU:HD23	2.13	0.49
1:A:137:SER:CB	1:A:148:VAL:HG21	2.43	0.49
11:A:304:CLA:H91	12:A:305:PL9:HC2	1.93	0.49
2:B:142:TRP:HZ2	2:B:155:LEU:O	1.95	0.49
1:I:46:VAL:HG22	12:I:2008:PL9:H303	1.95	0.49
3:K:199:ASP:OD2	3:K:201:ARG:HD3	2.13	0.49
15:D:201:SQD:H171	15:D:201:SQD:H141	1.61	0.48
1:A:175:VAL:HG13	1:A:179:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:MET:SD	1:A:83:ARG:HD3	2.53	0.48
3:C:284:ASN:OD1	3:C:284:ASN:O	2.32	0.48
11:A:304:CLA:H18	12:A:305:PL9:H252	1.95	0.48
11:J:201:CLA:H18	12:J:202:PL9:C35	2.42	0.48
12:J:202:PL9:H401	12:J:202:PL9:H421	1.60	0.48
1:A:159:PRO:O	1:A:162:GLY:N	2.44	0.48
1:I:118:TRP:O	1:I:122:VAL:HG23	2.13	0.48
11:J:201:CLA:C19	12:J:202:PL9:H353	2.43	0.48
4:D:130:SER:CB	4:D:141:GLY:HA3	2.43	0.48
4:D:56:LYS:HD3	4:D:60:GLY:O	2.14	0.48
6:F:28:LEU:HD21	8:H:27:SER:HA	1.96	0.48
11:J:201:CLA:HHC	11:J:201:CLA:CBB	2.42	0.48
3:K:139:LYS:HA	3:K:139:LYS:HE2	1.96	0.47
3:K:178:ILE:HG23	3:K:219:GLU:O	2.13	0.47
3:K:180:LYS:HB3	3:K:193:ASN:O	2.14	0.47
4:L:35:LEU:CB	4:L:36:PRO:HD3	2.44	0.47
4:L:83:LEU:O	4:L:84:LYS:HB2	2.14	0.47
1:A:14:ILE:HB	13:A:306:UMQ:HF2	1.95	0.47
3:C:63:ASN:OD1	3:C:65:LYS:N	2.44	0.47
3:C:27:ALA:HB3	3:C:235:GLY:HA2	1.96	0.47
3:C:196:ASP:HB2	3:C:201:ARG:O	2.15	0.47
1:I:52:PHE:O	1:I:55:THR:OG1	2.32	0.47
11:J:201:CLA:H141	12:J:202:PL9:H312	1.97	0.47
3:K:29:LYS:HB2	3:K:154:ARG:HH12	1.76	0.47
3:C:209:ARG:C	3:C:211:PRO:HD2	2.39	0.47
3:C:178:ILE:HG13	3:C:179:VAL:N	2.30	0.47
3:C:196:ASP:CB	3:C:201:ARG:H	2.28	0.47
4:L:93:GLU:HG2	4:L:99:ALA:HA	1.96	0.47
4:D:80:THR:O	4:D:87:PRO:HA	2.15	0.47
8:H:4:VAL:HG12	8:H:4:VAL:O	2.14	0.47
6:N:8:ARG:O	6:N:12:VAL:HG23	2.14	0.47
1:A:138:LEU:N	1:A:139:PRO:CD	2.78	0.47
2:B:89:ARG:NH1	12:B:301:PL9:H523	2.29	0.47
4:D:31:GLY:O	4:D:35:LEU:HD13	2.14	0.47
1:I:138:LEU:N	1:I:139:PRO:CD	2.78	0.47
2:B:110:THR:HG22	14:I:2007:PGT:H432	1.96	0.46
3:K:176:THR:OG1	3:K:221:ILE:O	2.30	0.46
3:C:211:PRO:CB	3:C:228:THR:HG21	2.22	0.46
4:D:122:LYS:HG2	4:D:133:ASN:HA	1.96	0.46
11:J:201:CLA:H101	11:J:201:CLA:H13	1.49	0.46
1:A:103:ARG:HD2	1:A:103:ARG:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:PRO:O	2:B:34:ASN:HB2	2.15	0.46
3:C:31:VAL:HG11	3:C:151:GLY:O	2.15	0.46
12:A:305:PL9:C28	12:A:305:PL9:H251	2.45	0.46
4:D:93:GLU:CG	4:D:94:SER:H	2.29	0.46
3:C:139:LYS:HE3	3:C:140:ASP:OD1	2.15	0.46
2:J:74:GLU:HG2	12:J:203:PL9:H112	1.97	0.46
4:D:68:TRP:CZ2	4:D:78:THR:HB	2.50	0.46
17:F:101:BCR:H331	17:F:101:BCR:C8	2.46	0.46
1:I:151:VAL:HG12	12:J:202:PL9:H43	1.98	0.46
2:J:89:ARG:HH12	12:J:203:PL9:C52	2.25	0.46
2:B:37:LEU:O	2:B:37:LEU:HG	2.16	0.46
3:C:250:ARG:HA	12:D:202:PL9:H112	1.98	0.46
4:D:75:GLY:H	4:D:92:VAL:HG23	1.81	0.46
4:D:151:HIS:HB2	4:D:162:VAL:HB	1.98	0.46
3:C:202:GLU:N	3:C:202:GLU:OE1	2.49	0.46
1:I:123:VAL:HG22	12:J:202:PL9:HC8	1.97	0.46
3:K:182:ILE:CD1	3:K:213:LEU:HD11	2.44	0.46
1:I:151:VAL:HG13	12:J:202:PL9:H452	1.98	0.46
1:A:92:MET:O	1:A:96:MET:HG2	2.16	0.45
1:I:103:ARG:C	1:I:103:ARG:HD2	2.41	0.45
1:A:11:ARG:HG3	1:A:11:ARG:HH11	1.80	0.45
3:C:171:TYR:CE2	3:C:208:PRO:HD3	2.51	0.45
3:C:173:SER:N	3:C:227:LEU:HD13	2.32	0.45
3:C:210:GLY:N	3:C:211:PRO:HD2	2.31	0.45
11:A:304:CLA:HMB1	11:A:304:CLA:HBB1	1.99	0.45
2:B:152:ASP:OD1	2:B:152:ASP:C	2.58	0.45
4:D:34:LEU:HD23	12:D:202:PL9:H352	1.98	0.45
8:P:1:MET:HG2	8:P:2:ASP:N	2.30	0.45
1:I:163:SER:N	1:I:164:PRO:CD	2.80	0.45
1:I:64:ASP:OD1	1:I:64:ASP:N	2.48	0.45
11:J:201:CLA:H162	12:J:202:PL9:C33	2.46	0.45
3:K:199:ASP:OD1	3:K:200:GLY:N	2.49	0.45
3:C:174:THR:HG22	3:C:174:THR:O	2.16	0.45
6:F:34:VAL:HG22	6:F:34:VAL:O	2.16	0.45
1:A:115:GLU:OE1	1:I:11:ARG:NH1	2.50	0.45
2:B:114:LEU:HD12	2:B:114:LEU:O	2.17	0.45
4:D:73:ALA:O	4:D:92:VAL:HG21	2.16	0.45
17:P:101:BCR:H20C	17:P:101:BCR:H361	1.82	0.45
3:C:38:ALA:HA	3:C:244:VAL:O	2.17	0.44
5:E:30:LEU:HD23	5:E:30:LEU:O	2.16	0.44
12:I:2008:PL9:H121	12:I:2008:PL9:H101	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:304:CLA:O1D	12:B:301:PL9:H502	2.17	0.44
3:C:195:ALA:CA	3:C:202:GLU:HG3	2.37	0.44
1:A:178:SER:O	1:A:182:ARG:HG3	2.18	0.44
4:L:12:MET:HE2	4:L:12:MET:HB2	1.85	0.44
3:C:166:SER:O	3:C:169:THR:HG22	2.17	0.44
1:I:2:SER:O	1:I:3:LYS:HB2	2.17	0.44
1:A:172:SER:OG	1:A:173:ALA:N	2.50	0.44
4:D:77:ARG:CZ	4:D:91:VAL:HG21	2.48	0.44
12:I:2008:PL9:H321	12:I:2008:PL9:H301	1.64	0.44
3:K:21:CYS:SG	3:K:236:PHE:CE1	3.11	0.44
3:K:53:TYR:HB3	3:K:154:ARG:HD3	1.99	0.44
3:C:156:ARG:HG2	10:C:301:HEC:HAD1	2.00	0.44
3:C:186:GLU:HG2	3:C:187:LYS:N	2.32	0.44
12:J:203:PL9:H351	12:J:203:PL9:H38	1.98	0.44
12:J:203:PL9:H122	12:J:203:PL9:H101	1.54	0.44
4:L:110:LEU:HD12	4:L:128:HIS:HE1	1.82	0.44
3:K:154:ARG:HG2	3:K:154:ARG:HH11	1.83	0.44
4:D:93:GLU:OE1	4:D:93:GLU:HA	2.16	0.43
8:H:1:MET:CG	8:H:2:ASP:N	2.80	0.43
3:C:207:ILE:HG22	3:C:208:PRO:O	2.17	0.43
5:E:10:PHE:CB	8:H:13:VAL:HG21	2.47	0.43
12:J:202:PL9:C48	12:J:202:PL9:H451	2.48	0.43
4:L:35:LEU:HD22	4:L:35:LEU:HA	1.85	0.43
1:A:133:VAL:HG23	2:B:81:PHE:CZ	2.53	0.43
3:K:222:LYS:O	3:K:222:LYS:HG3	2.18	0.43
11:A:304:CLA:H203	12:A:305:PL9:HC71	2.00	0.43
12:B:301:PL9:H28	6:F:3:ALA:HB2	1.96	0.43
1:I:3:LYS:HA	1:I:3:LYS:HE2	2.01	0.43
1:I:134:THR:HG23	12:J:202:PL9:C25	2.49	0.43
1:A:25:TYR:CZ	2:B:5:LYS:HE2	2.53	0.43
1:A:137:SER:HB3	1:A:148:VAL:CG2	2.49	0.43
3:C:50:ARG:HD3	3:C:125:GLU:OE1	2.19	0.43
3:C:51:ILE:HG23	3:C:154:ARG:NH1	2.33	0.43
2:J:40:PHE:HB2	2:J:41:PRO:HD3	2.01	0.43
12:I:2008:PL9:H351	12:I:2008:PL9:H371	1.57	0.43
4:D:53:THR:O	4:D:160:VAL:HA	2.19	0.43
11:J:201:CLA:H162	12:J:202:PL9:H33	2.01	0.43
3:K:63:ASN:CG	3:K:65:LYS:HE2	2.44	0.43
3:K:121:GLN:HA	3:K:121:GLN:OE1	2.18	0.43
4:L:12:MET:O	4:L:12:MET:HG3	2.19	0.43
12:B:301:PL9:H351	12:B:301:PL9:H38	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:VAL:HG13	3:C:179:VAL:O	2.19	0.43
4:L:79:LEU:HD22	4:L:87:PRO:HB2	2.00	0.43
4:L:90:LEU:HD23	4:L:90:LEU:HA	1.88	0.43
14:L:801:PGT:H461	14:L:801:PGT:H432	1.26	0.43
1:A:32:ILE:O	1:A:35:CYS:SG	2.76	0.42
3:C:182:ILE:CD1	3:C:213:LEU:HD11	2.47	0.42
4:D:73:ALA:HB1	4:D:74:PRO:HD2	2.00	0.42
3:K:268:LEU:HD13	4:L:22:LEU:HD11	2.00	0.42
7:O:30:ARG:HH11	7:O:30:ARG:CG	2.15	0.42
4:D:137:ARG:HE	4:D:137:ARG:HB3	1.74	0.42
5:M:18:THR:HG23	5:M:19:SER:N	2.34	0.42
8:H:1:MET:CG	8:H:2:ASP:H	2.32	0.42
1:I:7:TRP:O	1:I:11:ARG:HG2	2.19	0.42
12:I:2008:PL9:H361	12:I:2008:PL9:H322	1.77	0.42
4:L:132:TYR:HA	4:L:137:ARG:O	2.19	0.42
12:B:301:PL9:C25	7:G:2:ILE:HD13	2.49	0.42
10:A:303:HEC:HBB3	10:A:303:HEC:HMB1	2.02	0.42
12:B:301:PL9:H251	12:B:301:PL9:H271	1.57	0.42
3:C:283:MET:O	3:C:283:MET:HG3	2.20	0.42
1:A:5:TYR:CD1	1:A:14:ILE:HD11	2.54	0.42
2:B:137:THR:HA	12:B:301:PL9:H513	2.02	0.42
3:C:190:TYR:CD2	3:C:213:LEU:HD13	2.55	0.42
3:C:215:VAL:HG12	3:C:216:SER:N	2.34	0.42
1:I:47:GLN:OE1	1:I:89:SER:HB2	2.20	0.42
12:I:2008:PL9:H38	12:I:2008:PL9:C43	2.48	0.42
7:O:5:PHE:O	7:O:9:ILE:HG13	2.20	0.42
2:B:61:MET:CE	7:G:1:MET:CE	2.92	0.41
2:B:70:ALA:HB1	3:C:16:THR:CG2	2.48	0.41
1:I:178:SER:O	1:I:182:ARG:HG3	2.20	0.41
2:J:90:THR:CG2	2:J:151:ILE:HD11	2.50	0.41
12:J:203:PL9:H322	12:J:203:PL9:H301	1.68	0.41
2:B:114:LEU:HD11	13:B:302:UMQ:HF2	2.01	0.41
3:C:215:VAL:CG1	3:C:216:SER:N	2.83	0.41
3:C:250:ARG:HA	12:D:202:PL9:H13	2.01	0.41
4:L:140:ARG:CG	4:L:141:GLY:N	2.79	0.41
4:D:151:HIS:O	4:D:161:PHE:HA	2.20	0.41
10:A:303:HEC:CBB	10:A:303:HEC:HMB1	2.51	0.41
1:A:47:GLN:OE1	1:A:89:SER:HB2	2.20	0.41
3:C:129:PRO:C	3:C:130:ILE:HG13	2.45	0.41
12:I:2008:PL9:C35	4:L:34:LEU:HD12	2.50	0.41
3:K:56:GLN:HG2	3:K:56:GLN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:75:GLY:H	4:L:92:VAL:CG2	2.33	0.41
1:A:3:LYS:HE3	1:A:3:LYS:HB3	1.91	0.41
3:C:212:GLU:C	3:C:228:THR:HG23	2.45	0.41
17:F:101:BCR:H15C	17:F:101:BCR:H351	1.85	0.41
7:G:14:ILE:N	7:G:15:PRO:HD2	2.36	0.41
2:J:61:MET:SD	7:O:1:MET:HE1	2.61	0.41
2:J:70:ALA:HB1	3:K:16:THR:HG22	2.02	0.41
7:O:13:LEU:HD23	7:O:13:LEU:HA	1.89	0.41
1:I:151:VAL:CG1	12:J:202:PL9:H43	2.51	0.41
2:J:70:ALA:HB1	3:K:16:THR:CG2	2.51	0.41
4:L:29:PRO:O	4:L:33:MET:HG2	2.20	0.41
2:B:72:PRO:HG2	2:B:75:ILE:CD1	2.50	0.41
3:C:201:ARG:NE	3:C:202:GLU:H	2.17	0.41
14:L:801:PGT:H351	14:L:801:PGT:H381	1.83	0.41
5:M:22:PHE:CE2	6:N:34:VAL:HG11	2.50	0.41
17:P:101:BCR:C8	17:P:101:BCR:H331	2.51	0.41
2:B:104:VAL:HB	2:B:105:PRO:CD	2.50	0.41
3:C:39:VAL:HG22	3:C:40:LEU:N	2.36	0.41
2:J:110:THR:O	2:J:114:LEU:HG	2.21	0.41
3:C:97:MET:HE2	3:C:97:MET:HB2	1.74	0.40
2:B:149:LEU:HB3	2:B:150:PRO:HD2	2.03	0.40
15:D:201:SQD:H342	15:D:201:SQD:H372	1.90	0.40
3:K:216:SER:OG	3:K:219:GLU:OE2	2.38	0.40
3:C:14:GLU:HG3	3:C:18:ARG:O	2.21	0.40
4:D:74:PRO:HA	4:D:92:VAL:HG21	2.01	0.40
9:A:302:HEM:HMB1	9:A:302:HEM:CBB	2.49	0.40
2:B:58:GLU:OE2	3:C:37:GLN:NE2	2.54	0.40
2:B:117:VAL:HG13	2:B:118:ASN:N	2.36	0.40
17:F:101:BCR:H24C	17:F:101:BCR:H371	1.84	0.40
3:K:98:GLY:O	3:K:99:ASN:OD1	2.39	0.40
15:K:302:SQD:O8	4:L:15:ARG:NH2	2.41	0.40
4:D:77:ARG:HD2	4:D:91:VAL:HG23	2.04	0.40
2:J:104:VAL:HB	2:J:105:PRO:HD3	2.03	0.40
3:K:213:LEU:C	3:K:213:LEU:HD23	2.46	0.40
4:L:23:LEU:HD23	4:L:23:LEU:HA	1.97	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%)	203 (96%)	9 (4%)	0	100	100
1	I	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
2	B	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
2	J	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
3	C	283/320 (88%)	265 (94%)	18 (6%)	0	100	100
3	K	283/320 (88%)	274 (97%)	9 (3%)	0	100	100
4	D	163/230 (71%)	153 (94%)	10 (6%)	0	100	100
4	L	161/230 (70%)	149 (92%)	12 (8%)	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	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%)	28 (97%)	1 (3%)	0	100	100
7	O	29/37 (78%)	27 (93%)	2 (7%)	0	100	100
8	H	27/29 (93%)	27 (100%)	0	0	100	100
8	P	27/29 (93%)	27 (100%)	0	0	100	100
All	All	1866/2116 (88%)	1780 (95%)	86 (5%)	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%)	183 (99%)	2 (1%)	65	85
1	I	185/186 (100%)	184 (100%)	1 (0%)	81	92
2	B	134/135 (99%)	129 (96%)	5 (4%)	30	59
2	J	134/135 (99%)	129 (96%)	5 (4%)	30	59
3	C	242/275 (88%)	238 (98%)	4 (2%)	53	79
3	K	242/275 (88%)	241 (100%)	1 (0%)	84	93
4	D	135/183 (74%)	132 (98%)	3 (2%)	45	74
4	L	135/183 (74%)	132 (98%)	3 (2%)	45	74
5	E	26/26 (100%)	21 (81%)	5 (19%)	1	4
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%)	25 (96%)	1 (4%)	29	58
8	H	24/24 (100%)	24 (100%)	0	100	100
8	P	24/24 (100%)	24 (100%)	0	100	100
All	All	1596/1772 (90%)	1566 (98%)	30 (2%)	49	77

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	208	LYS
2	B	6	LYS
2	B	15	ARG
2	B	17	LYS
2	B	35	ASP
2	B	119	LYS
3	C	56	GLN
3	C	97	MET
3	C	122	LYS
3	C	138	LYS
4	D	70	LYS
4	D	140	ARG
4	D	154	VAL
5	E	23	ILE
5	E	25	LEU

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Mol	Chain	Res	Type
5	E	27	LYS
5	E	28	ILE
5	E	29	ARG
1	I	165	LEU
2	J	6	LYS
2	J	115	GLU
2	J	116	ASN
2	J	117	VAL
2	J	119	LYS
3	K	103	GLN
4	L	35	LEU
4	L	122	LYS
4	L	137	ARG
7	O	30	ARG

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	25	HIS
3	C	246	GLN
4	D	117	ASN
2	J	24	HIS
2	J	116	ASN
2	J	121	GLN
3	K	6	GLN
3	K	193	ASN
3	K	225	GLN
4	L	117	ASN
4	L	121	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

37 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$
13	UMQ	B	302	-	35,35,35	1.18	2 (5%)	46,46,46	1.07	2 (4%)
12	PL9	D	202	-	55,55,55	1.14	5 (9%)	68,69,69	1.50	14 (20%)
14	PGT	A	308	-	50,50,50	0.89	4 (8%)	53,56,56	1.04	2 (3%)
13	UMQ	I	2005	-	35,35,35	1.13	1 (2%)	46,46,46	0.84	1 (2%)
9	HEM	A	302	1	50,50,50	1.44	7 (14%)	67,82,82	1.14	6 (8%)
14	PGT	L	801	-	50,50,50	0.88	4 (8%)	53,56,56	1.09	2 (3%)
16	FES	D	203	4	0,4,4	-	-	-	-	-
9	HEM	A	301	1	50,50,50	1.45	8 (16%)	67,82,82	1.20	5 (7%)
12	PL9	I	2001	-	55,55,55	0.88	2 (3%)	68,69,69	1.65	11 (16%)
13	UMQ	J	205	-	35,35,35	1.21	4 (11%)	46,46,46	1.04	5 (10%)
12	PL9	I	2008	-	55,55,55	1.04	4 (7%)	68,69,69	1.53	12 (17%)
13	UMQ	P	102	-	35,35,35	1.14	2 (5%)	46,46,46	0.74	0
11	CLA	J	201	-	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
13	UMQ	A	306	-	35,35,35	1.14	2 (5%)	46,46,46	0.87	0
17	BCR	P	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	9 (16%)
13	UMQ	J	204	-	35,35,35	1.15	3 (8%)	46,46,46	0.75	1 (2%)
10	HEC	K	301	3	46,50,50	1.82	5 (10%)	58,82,82	1.98	4 (6%)
13	UMQ	A	307	-	35,35,35	1.15	3 (8%)	46,46,46	0.85	1 (2%)
15	SQD	K	302	-	52,54,54	0.99	5 (9%)	62,65,65	1.40	9 (14%)
12	PL9	A	305	-	55,55,55	0.98	4 (7%)	68,69,69	1.54	12 (17%)
10	HEC	A	303	-	46,50,50	2.51	24 (52%)	58,82,82	2.07	20 (34%)
12	PL9	J	203	-	55,55,55	1.08	4 (7%)	68,69,69	1.54	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HEC	I	2004	1	46,50,50	1.83	6 (13%)	58,82,82	2.03	6 (10%)
9	HEM	I	2002	1	50,50,50	1.44	7 (14%)	67,82,82	1.16	5 (7%)
13	UMQ	H	201	-	35,35,35	1.13	0	46,46,46	0.74	0
12	PL9	J	202	-	55,55,55	1.11	4 (7%)	68,69,69	1.50	13 (19%)
14	PGT	I	2007	-	50,50,50	0.90	4 (8%)	53,56,56	1.07	2 (3%)
13	UMQ	I	2006	-	35,35,35	1.13	2 (5%)	46,46,46	1.01	2 (4%)
16	FES	L	802	4	0,4,4	-	-	-	-	-
14	PGT	D	204	-	50,50,50	0.88	4 (8%)	53,56,56	1.09	2 (3%)
13	UMQ	B	303	-	35,35,35	1.19	3 (8%)	46,46,46	0.86	1 (2%)
17	BCR	F	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	7 (12%)
10	HEC	C	301	3	46,50,50	1.82	5 (10%)	58,82,82	2.02	6 (10%)
11	CLA	A	304	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
15	SQD	D	201	-	52,54,54	0.98	5 (9%)	62,65,65	1.47	8 (12%)
12	PL9	B	301	-	55,55,55	1.08	4 (7%)	68,69,69	1.54	13 (19%)
9	HEM	I	2003	1	50,50,50	1.43	7 (14%)	67,82,82	1.15	6 (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
13	UMQ	B	302	-	-	11/20/60/60	0/2/2/2
12	PL9	D	202	-	-	21/53/73/73	0/1/1/1
14	PGT	A	308	-	-	29/55/55/55	-
13	UMQ	I	2005	-	-	8/20/60/60	0/2/2/2
9	HEM	A	302	1	-	2/14/54/54	-
14	PGT	L	801	-	-	25/55/55/55	-
16	FES	D	203	4	-	-	0/1/1/1
9	HEM	A	301	1	-	2/14/54/54	-
12	PL9	I	2001	-	-	29/53/73/73	0/1/1/1
13	UMQ	J	205	-	-	12/20/60/60	0/2/2/2
12	PL9	I	2008	-	-	22/53/73/73	0/1/1/1
13	UMQ	P	102	-	-	6/20/60/60	0/2/2/2
11	CLA	J	201	-	1/1/15/20	16/39/115/115	-
13	UMQ	A	306	-	-	7/20/60/60	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	P	101	-	-	9/29/63/63	0/2/2/2
13	UMQ	J	204	-	-	13/20/60/60	0/2/2/2
10	HEC	K	301	3	-	8/14/54/54	-
13	UMQ	A	307	-	-	14/20/60/60	0/2/2/2
15	SQD	K	302	-	-	18/49/69/69	0/1/1/1
12	PL9	A	305	-	-	23/53/73/73	0/1/1/1
10	HEC	A	303	-	-	5/14/54/54	-
12	PL9	J	203	-	-	20/53/73/73	0/1/1/1
10	HEC	I	2004	1	-	9/14/54/54	-
9	HEM	I	2002	1	-	1/14/54/54	-
13	UMQ	H	201	-	-	3/20/60/60	0/2/2/2
12	PL9	J	202	-	-	23/53/73/73	0/1/1/1
14	PGT	I	2007	-	-	23/55/55/55	-
13	UMQ	I	2006	-	-	11/20/60/60	0/2/2/2
16	FES	L	802	4	-	-	0/1/1/1
14	PGT	D	204	-	-	36/55/55/55	-
13	UMQ	B	303	-	-	6/20/60/60	0/2/2/2
17	BCR	F	101	-	-	6/29/63/63	0/2/2/2
11	CLA	A	304	-	1/1/15/20	17/39/115/115	-
10	HEC	C	301	3	-	11/14/54/54	-
15	SQD	D	201	-	-	24/49/69/69	0/1/1/1
12	PL9	B	301	-	-	23/53/73/73	0/1/1/1
9	HEM	I	2003	1	-	2/14/54/54	-

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	2004	HEC	CAB-C3B	6.19	1.55	1.35
10	I	2004	HEC	CAC-C3C	6.16	1.55	1.35
10	K	301	HEC	CAB-C3B	6.14	1.54	1.35
10	C	301	HEC	CAB-C3B	6.11	1.54	1.35
10	K	301	HEC	CAC-C3C	6.10	1.54	1.35
10	C	301	HEC	CAC-C3C	6.03	1.54	1.35
10	C	301	HEC	C3D-C2D	5.73	1.53	1.38
10	K	301	HEC	C3D-C2D	5.66	1.53	1.38
10	I	2004	HEC	C3D-C2D	5.56	1.53	1.38
10	A	303	HEC	CHA-C1A	4.96	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	303	HEC	CHB-C4A	4.78	1.47	1.38
10	A	303	HEC	C2A-C3A	4.69	1.46	1.36
10	A	303	HEC	CHC-C4B	4.56	1.47	1.38
10	A	303	HEC	CHD-C4C	4.50	1.47	1.38
10	A	303	HEC	CAC-C3C	4.21	1.48	1.35
10	A	303	HEC	CAB-C3B	4.09	1.48	1.35
17	F	101	BCR	C1-C6	-3.83	1.48	1.53
9	A	302	HEM	FE-NB	3.73	2.06	1.94
9	I	2002	HEM	FE-NA	3.70	2.07	1.95
10	A	303	HEC	CHA-C4D	3.69	1.47	1.39
10	A	303	HEC	CHC-C1C	3.66	1.47	1.39
17	P	101	BCR	C30-C25	-3.62	1.49	1.53
9	I	2003	HEM	FE-NA	3.58	2.07	1.95
10	A	303	HEC	CHB-C1B	3.57	1.47	1.39
11	J	201	CLA	C1D-ND	3.52	1.42	1.37
9	A	301	HEM	FE-NC	3.52	2.06	1.95
9	A	301	HEM	FE-ND	3.49	2.05	1.94
10	A	303	HEC	CHD-C1D	3.47	1.47	1.39
11	A	304	CLA	C1D-ND	3.45	1.42	1.37
17	F	101	BCR	C30-C25	-3.34	1.49	1.53
9	A	301	HEM	FE-NB	3.32	2.05	1.94
17	P	101	BCR	C1-C6	-3.31	1.49	1.53
9	I	2002	HEM	FE-NB	3.31	2.05	1.94
9	A	302	HEM	FE-ND	3.29	2.05	1.94
9	I	2002	HEM	FE-ND	3.28	2.05	1.94
11	J	201	CLA	C4B-NB	3.23	1.42	1.37
12	J	202	PL9	C3-C4	-3.22	1.44	1.49
9	A	302	HEM	FE-NA	3.22	2.05	1.95
10	A	303	HEC	C3D-C2D	3.20	1.47	1.38
9	I	2003	HEM	FE-ND	3.19	2.04	1.94
9	I	2003	HEM	FE-NB	3.18	2.04	1.94
15	K	302	SQD	O48-C23	3.18	1.42	1.33
9	A	301	HEM	FE-NA	3.16	2.05	1.95
9	I	2003	HEM	FE-NC	3.15	2.05	1.95
15	D	201	SQD	O48-C23	3.09	1.42	1.33
9	I	2002	HEM	FE-NC	3.08	2.05	1.95
9	A	302	HEM	FE-NC	3.07	2.05	1.95
12	D	202	PL9	C3-C4	-3.04	1.44	1.49
12	J	202	PL9	C7-C3	-2.98	1.47	1.51
9	A	302	HEM	CAC-C3C	2.95	1.55	1.47
9	I	2002	HEM	CAB-C3B	2.94	1.55	1.47
9	I	2002	HEM	CAC-C3C	2.94	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	301	HEM	CAB-C3B	2.92	1.55	1.47
9	I	2003	HEM	CAB-C3B	2.92	1.55	1.47
9	I	2003	HEM	CAC-C3C	2.91	1.55	1.47
9	A	302	HEM	CAB-C3B	2.89	1.55	1.47
9	A	301	HEM	CAC-C3C	2.89	1.55	1.47
11	A	304	CLA	C4B-NB	2.88	1.41	1.37
15	K	302	SQD	O47-C7	2.85	1.42	1.34
12	D	202	PL9	C7-C3	-2.78	1.47	1.51
12	J	203	PL9	C3-C4	-2.76	1.45	1.49
15	D	201	SQD	O47-C7	2.76	1.42	1.34
12	B	301	PL9	C3-C4	-2.74	1.45	1.49
12	J	203	PL9	C7-C3	-2.72	1.47	1.51
12	J	202	PL9	C6-C1	-2.68	1.44	1.48
14	L	801	PGT	O2-C2	-2.68	1.40	1.46
11	A	304	CLA	C1B-C2B	2.66	1.49	1.43
14	D	204	PGT	O2-C2	-2.63	1.40	1.46
11	J	201	CLA	C1B-C2B	2.59	1.49	1.43
12	B	301	PL9	C7-C3	-2.59	1.47	1.51
14	I	2007	PGT	O2-C2	-2.58	1.40	1.46
12	I	2001	PL9	C6-C1	-2.55	1.44	1.48
10	A	303	HEC	C1C-C2C	2.48	1.48	1.43
12	A	305	PL9	C7-C3	-2.45	1.48	1.51
11	J	201	CLA	C3B-C4B	2.45	1.49	1.42
12	J	203	PL9	C6-C1	-2.44	1.44	1.48
12	D	202	PL9	C6-C1	-2.44	1.44	1.48
14	D	204	PGT	O3-C11	2.44	1.40	1.33
14	I	2007	PGT	O3-C11	2.44	1.40	1.33
14	A	308	PGT	O2-C2	-2.40	1.40	1.46
12	I	2008	PL9	C3-C4	-2.40	1.45	1.49
10	A	303	HEC	C4C-NC	-2.39	1.35	1.39
14	A	308	PGT	O3-C11	2.39	1.40	1.33
10	A	303	HEC	C1A-NA	-2.39	1.35	1.39
10	A	303	HEC	C4B-NB	-2.37	1.35	1.39
13	B	302	UMQ	O5'-C5'	2.37	1.50	1.44
12	I	2008	PL9	C7-C3	-2.35	1.48	1.51
10	A	303	HEC	C4D-ND	-2.32	1.35	1.39
13	J	205	UMQ	O5'-C1'	2.31	1.47	1.41
13	J	205	UMQ	O5'-C5'	2.30	1.50	1.44
11	J	201	CLA	CHC-C1C	2.30	1.43	1.38
12	D	202	PL9	C53-C6	-2.29	1.46	1.50
10	A	303	HEC	C1D-ND	-2.27	1.35	1.39
14	L	801	PGT	O3-C3	-2.27	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	303	HEC	C4D-C3D	2.26	1.49	1.44
14	L	801	PGT	O3-C11	2.26	1.39	1.33
10	C	301	HEC	C3C-C2C	-2.25	1.33	1.41
14	A	308	PGT	O2-C31	2.24	1.40	1.34
12	J	203	PL9	C53-C6	-2.24	1.46	1.50
12	J	202	PL9	C53-C6	-2.23	1.46	1.50
14	I	2007	PGT	O2-C31	2.22	1.40	1.34
13	J	205	UMQ	C3-C4	-2.22	1.46	1.52
10	I	2004	HEC	C3B-C2B	-2.21	1.33	1.41
12	I	2008	PL9	C53-C6	-2.21	1.46	1.50
10	A	303	HEC	C1D-C2D	2.20	1.48	1.43
10	A	303	HEC	C4A-NA	-2.20	1.35	1.39
12	A	305	PL9	C53-C6	-2.20	1.46	1.50
10	K	301	HEC	C3B-C2B	-2.20	1.33	1.41
12	A	305	PL9	C6-C1	-2.20	1.44	1.48
14	I	2007	PGT	O3-C3	-2.17	1.40	1.45
12	I	2001	PL9	C53-C6	-2.17	1.46	1.50
13	B	303	UMQ	O5'-C5'	2.17	1.49	1.44
14	L	801	PGT	O2-C31	2.17	1.40	1.34
10	I	2004	HEC	C3C-C2C	-2.17	1.33	1.41
11	A	304	CLA	C3B-C4B	2.16	1.49	1.42
13	B	303	UMQ	C3-C4	-2.16	1.46	1.52
11	A	304	CLA	CHC-C1C	2.15	1.42	1.38
15	D	201	SQD	O2-C2	-2.15	1.37	1.43
12	B	301	PL9	C6-C1	-2.14	1.45	1.48
15	K	302	SQD	O4-C4	-2.14	1.37	1.43
10	K	301	HEC	C3C-C2C	-2.14	1.33	1.41
13	B	303	UMQ	O5'-C1'	2.14	1.47	1.41
13	B	302	UMQ	C3-C4	-2.13	1.46	1.52
14	D	204	PGT	O2-C31	2.12	1.40	1.34
14	A	308	PGT	O3-C3	-2.12	1.40	1.45
15	K	302	SQD	O2-C2	-2.11	1.37	1.43
12	D	202	PL9	C16-C14	-2.11	1.46	1.51
10	A	303	HEC	C1B-C2B	2.11	1.48	1.43
13	A	307	UMQ	O5'-C5'	2.11	1.49	1.44
13	I	2005	UMQ	C3-C4	-2.10	1.46	1.52
14	D	204	PGT	O3-C3	-2.10	1.40	1.45
13	P	102	UMQ	C3-C4	-2.10	1.46	1.52
11	A	304	CLA	CMD-C2D	-2.09	1.46	1.50
10	C	301	HEC	C3B-C2B	-2.09	1.34	1.41
11	A	304	CLA	MG-NB	-2.09	2.01	2.05
12	A	305	PL9	C3-C4	-2.08	1.46	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	204	UMQ	O5'-C5'	2.08	1.49	1.44
12	I	2008	PL9	C6-C1	-2.08	1.45	1.48
13	A	306	UMQ	C3-C4	-2.07	1.47	1.52
11	J	201	CLA	CMD-C2D	-2.07	1.46	1.50
17	P	101	BCR	C33-C5	-2.05	1.47	1.50
15	D	201	SQD	O3-C3	-2.05	1.37	1.43
15	D	201	SQD	O4-C4	-2.04	1.37	1.43
12	B	301	PL9	C53-C6	-2.04	1.46	1.50
13	A	307	UMQ	C3-C4	-2.04	1.47	1.52
9	A	302	HEM	CMC-C2C	2.04	1.54	1.50
10	A	303	HEC	C1A-C2A	2.04	1.48	1.45
13	J	204	UMQ	O5'-C1'	2.03	1.47	1.41
10	A	303	HEC	C1B-NB	-2.03	1.35	1.39
11	A	304	CLA	CMB-C2B	-2.03	1.46	1.50
13	A	306	UMQ	O5'-C5'	2.03	1.49	1.44
13	J	205	UMQ	C3'-C4'	-2.03	1.46	1.52
9	A	301	HEM	CMC-C2C	2.03	1.54	1.50
9	A	301	HEM	CMA-C3A	2.03	1.54	1.50
11	A	304	CLA	CMC-C2C	-2.02	1.46	1.50
11	J	201	CLA	CMB-C2B	-2.02	1.46	1.50
13	I	2006	UMQ	O5'-C5'	2.02	1.49	1.44
15	K	302	SQD	O3-C3	-2.02	1.38	1.43
13	J	204	UMQ	C3'-C4'	-2.02	1.46	1.52
13	P	102	UMQ	O5'-C5'	2.02	1.49	1.44
9	I	2002	HEM	CMC-C2C	2.02	1.54	1.50
13	I	2006	UMQ	C3-C4	-2.02	1.47	1.52
13	A	307	UMQ	O5'-C1'	2.01	1.47	1.41
9	I	2003	HEM	CMC-C2C	2.01	1.54	1.50
10	I	2004	HEC	CMA-C3A	2.00	1.54	1.50

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	301	HEC	CBC-CAC-C3C	-9.30	108.86	127.43
10	K	301	HEC	CBC-CAC-C3C	-9.19	109.06	127.43
10	C	301	HEC	CBB-CAB-C3B	-8.96	109.52	127.43
10	K	301	HEC	CBB-CAB-C3B	-8.69	110.07	127.43
10	I	2004	HEC	CBB-CAB-C3B	-8.66	110.13	127.43
10	I	2004	HEC	CBC-CAC-C3C	-8.40	110.65	127.43
12	I	2001	PL9	C7-C3-C4	7.24	122.87	116.91
11	A	304	CLA	C4A-NA-C1A	6.47	109.63	106.68
11	J	201	CLA	C4A-NA-C1A	6.05	109.44	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	305	PL9	C7-C3-C4	5.72	121.62	116.91
12	J	203	PL9	C7-C3-C4	5.44	121.39	116.91
12	I	2008	PL9	C7-C3-C4	5.42	121.38	116.91
12	B	301	PL9	C7-C3-C4	5.16	121.16	116.91
12	I	2001	PL9	C7-C3-C2	-4.96	117.55	123.39
12	J	202	PL9	C7-C3-C4	4.87	120.92	116.91
10	A	303	HEC	C3D-C4D-ND	4.76	115.44	110.15
12	D	202	PL9	C7-C3-C4	4.73	120.81	116.91
14	I	2007	PGT	O2-C31-C32	4.49	121.20	111.48
10	A	303	HEC	C2A-C1A-NA	4.45	114.62	110.32
15	D	201	SQD	O6-C1-C2	4.35	114.87	108.27
14	A	308	PGT	O2-C31-C32	4.34	120.87	111.48
12	A	305	PL9	C7-C3-C2	-4.21	118.43	123.39
12	J	203	PL9	C7-C3-C2	-4.18	118.47	123.39
12	I	2008	PL9	C7-C3-C2	-4.15	118.49	123.39
14	L	801	PGT	O2-C31-C32	4.08	120.31	111.48
15	D	201	SQD	O9-S-O7	-4.05	100.64	113.82
14	D	204	PGT	O2-C31-C32	4.00	120.14	111.48
15	K	302	SQD	O9-S-O7	-4.00	100.81	113.82
12	B	301	PL9	C7-C3-C2	-3.95	118.73	123.39
13	B	302	UMQ	O5'-C5'-C4'	3.85	117.67	109.72
10	I	2004	HEC	C4D-ND-C1D	3.84	112.08	105.82
12	J	202	PL9	C7-C3-C2	-3.81	118.90	123.39
10	A	303	HEC	CBB-CAB-C3B	-3.78	119.87	127.43
12	D	202	PL9	C7-C3-C2	-3.73	119.00	123.39
10	A	303	HEC	C1D-C2D-C3D	-3.72	102.56	106.82
10	A	303	HEC	C2C-C1C-NC	3.69	116.05	110.14
10	A	303	HEC	C2D-C1D-ND	3.61	115.94	110.14
10	K	301	HEC	C4D-ND-C1D	3.57	111.64	105.82
10	A	303	HEC	C2B-C1B-NB	3.56	115.86	110.14
10	C	301	HEC	C4D-ND-C1D	3.52	111.55	105.82
15	D	201	SQD	O7-S-C6	3.42	111.86	106.76
15	D	201	SQD	O47-C7-C8	3.40	118.83	111.48
15	K	302	SQD	O47-C7-C8	3.39	118.83	111.48
15	K	302	SQD	O7-S-C6	3.36	111.77	106.76
11	A	304	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
12	J	203	PL9	C40-C39-C41	3.17	120.74	115.23
11	J	201	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
10	A	303	HEC	C3A-C4A-NA	3.09	115.34	109.64
10	A	303	HEC	C4A-C3A-C2A	-3.05	102.45	106.97
12	B	301	PL9	C40-C39-C41	3.03	120.50	115.23
12	B	301	PL9	C27-C28-C29	-3.02	120.70	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	201	SQD	O9-S-C6	3.02	111.26	106.76
12	A	305	PL9	C40-C39-C41	2.97	120.38	115.23
11	J	201	CLA	C3B-C4B-NB	-2.97	107.88	110.53
12	D	202	PL9	C40-C39-C41	2.96	120.37	115.23
13	B	303	UMQ	C1-O1-C4'	-2.95	110.98	117.98
10	I	2004	HEC	C2A-C1A-NA	-2.94	107.49	110.32
10	A	303	HEC	CBC-CAC-C3C	-2.93	121.57	127.43
15	K	302	SQD	O9-S-C6	2.91	111.10	106.76
12	B	301	PL9	C22-C23-C24	-2.89	121.00	127.62
17	P	101	BCR	C15-C16-C17	-2.89	117.61	123.52
12	I	2008	PL9	C27-C28-C29	-2.89	121.02	127.62
15	K	302	SQD	O6-C1-C2	2.88	112.65	108.27
12	J	202	PL9	C40-C39-C41	2.87	120.22	115.23
12	J	203	PL9	C27-C28-C29	-2.85	121.10	127.62
14	D	204	PGT	O3-C11-C12	2.84	120.49	111.83
10	A	303	HEC	C1A-C2A-C3A	-2.80	103.42	107.11
10	I	2004	HEC	CAD-C3D-C4D	2.80	130.41	124.94
12	J	202	PL9	C27-C28-C29	-2.79	121.24	127.62
12	I	2001	PL9	C40-C39-C41	2.78	120.06	115.23
15	D	201	SQD	O48-C23-C24	2.78	120.32	111.83
14	A	308	PGT	O3-C11-C12	2.77	120.30	111.83
17	F	101	BCR	C24-C23-C22	-2.76	122.16	126.23
17	P	101	BCR	C2-C1-C6	2.74	114.42	110.44
17	F	101	BCR	C27-C26-C25	2.74	126.40	122.70
12	J	203	PL9	C22-C23-C24	-2.73	121.37	127.62
12	J	202	PL9	C22-C23-C24	-2.73	121.37	127.62
15	K	302	SQD	C44-O6-C1	2.72	119.62	113.80
12	D	202	PL9	C22-C23-C24	-2.72	121.41	127.62
17	P	101	BCR	C27-C26-C25	2.70	126.36	122.70
10	A	303	HEC	C4D-C3D-C2D	-2.70	102.69	106.87
17	F	101	BCR	C33-C5-C6	-2.70	121.54	124.48
12	J	202	PL9	C7-C8-C9	-2.69	122.19	126.83
12	A	305	PL9	C22-C23-C24	-2.69	121.46	127.62
11	A	304	CLA	C3B-C4B-NB	-2.68	108.14	110.53
9	A	301	HEM	C4D-ND-C1D	2.68	108.38	105.21
12	D	202	PL9	C27-C28-C29	-2.65	121.55	127.62
9	I	2002	HEM	C1B-NB-C4B	2.65	108.35	105.21
12	I	2008	PL9	C40-C39-C41	2.63	119.80	115.23
17	F	101	BCR	C15-C16-C17	-2.63	118.14	123.52
14	L	801	PGT	O3-C11-C12	2.63	119.84	111.83
12	I	2001	PL9	C22-C23-C24	-2.62	121.63	127.62
9	A	301	HEM	C3D-C4D-ND	-2.61	107.31	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	2008	PL9	C22-C23-C24	-2.61	121.65	127.62
9	I	2003	HEM	C4D-ND-C1D	2.61	108.30	105.21
12	D	202	PL9	C7-C8-C9	-2.59	122.37	126.83
10	A	303	HEC	CMA-C3A-C4A	2.57	129.25	124.73
15	K	302	SQD	O8-S-C6	2.56	110.91	105.97
9	I	2003	HEM	C1B-NB-C4B	2.55	108.23	105.21
12	A	305	PL9	C27-C28-C29	-2.55	121.80	127.62
9	A	302	HEM	C4D-ND-C1D	2.54	108.22	105.21
17	P	101	BCR	C15-C14-C13	-2.53	123.73	127.28
12	B	301	PL9	C7-C8-C9	-2.52	122.50	126.83
9	A	302	HEM	C1B-NB-C4B	2.51	108.18	105.21
11	J	201	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
12	I	2001	PL9	C7-C8-C9	-2.51	122.51	126.83
13	A	307	UMQ	C1-O1-C4'	-2.50	112.04	117.98
10	A	303	HEC	CMC-C2C-C1C	2.49	129.21	125.42
9	I	2002	HEM	C4D-ND-C1D	2.49	108.16	105.21
14	I	2007	PGT	O3-C11-C12	2.48	119.41	111.83
9	A	301	HEM	C1B-NB-C4B	2.48	108.15	105.21
12	J	203	PL9	O2-C1-C6	2.48	124.42	120.48
13	I	2005	UMQ	C1-O1-C4'	-2.48	112.11	117.98
12	B	301	PL9	O2-C1-C6	2.46	124.39	120.48
17	P	101	BCR	C24-C23-C22	-2.45	122.61	126.23
15	D	201	SQD	O8-S-C6	2.44	110.69	105.97
12	D	202	PL9	C20-C19-C21	2.44	119.47	115.23
12	I	2008	PL9	C7-C8-C9	-2.44	122.63	126.83
12	I	2001	PL9	C36-C34-C33	-2.44	115.69	121.17
9	I	2002	HEM	C3B-C2B-C1B	2.43	108.24	106.41
17	F	101	BCR	C15-C14-C13	-2.43	123.87	127.28
15	K	302	SQD	O48-C23-C24	2.42	119.23	111.83
10	A	303	HEC	CMB-C2B-C1B	2.42	129.11	125.42
10	K	301	HEC	C2A-C1A-NA	-2.41	108.00	110.32
12	I	2008	PL9	C20-C19-C21	2.40	119.40	115.23
15	K	302	SQD	O5-C5-C4	2.40	114.02	109.70
9	I	2003	HEM	C3D-C4D-ND	-2.40	107.54	110.17
15	D	201	SQD	O5-C5-C4	2.39	114.01	109.70
9	A	302	HEM	C3B-C2B-C1B	2.39	108.20	106.41
11	A	304	CLA	CHB-C4A-NA	2.38	127.84	124.40
12	B	301	PL9	C37-C38-C39	-2.38	122.19	127.62
12	I	2008	PL9	O2-C1-C6	2.37	124.26	120.48
12	J	203	PL9	C7-C8-C9	-2.37	122.75	126.83
12	J	202	PL9	O1-C4-C3	-2.36	118.24	120.73
12	I	2001	PL9	O2-C1-C6	2.36	124.24	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	305	PL9	C20-C19-C21	2.36	119.32	115.23
13	J	204	UMQ	C1-O1-C4'	-2.35	112.40	117.98
12	J	202	PL9	O2-C1-C6	2.35	124.22	120.48
13	I	2006	UMQ	C1-O1-C4'	-2.34	112.44	117.98
9	I	2003	HEM	C3B-C2B-C1B	2.33	108.16	106.41
13	B	302	UMQ	C3'-C4'-C5'	2.33	116.09	110.93
12	J	203	PL9	C37-C38-C39	-2.33	122.30	127.62
9	A	301	HEM	C3B-C2B-C1B	2.32	108.15	106.41
12	B	301	PL9	C20-C19-C21	2.32	119.25	115.23
17	P	101	BCR	C33-C5-C6	-2.31	121.96	124.48
13	J	205	UMQ	C1'-O5'-C5'	2.31	118.24	113.72
9	A	301	HEM	C2A-C1A-NA	-2.31	107.59	110.15
12	J	202	PL9	C12-C13-C14	-2.30	122.35	127.62
9	A	302	HEM	C3D-C4D-ND	-2.30	107.65	110.17
12	A	305	PL9	O2-C1-C6	2.28	124.11	120.48
12	I	2001	PL9	C37-C38-C39	-2.28	122.40	127.62
12	B	301	PL9	C32-C33-C34	-2.28	122.41	127.62
12	A	305	PL9	C37-C38-C39	-2.27	122.42	127.62
12	I	2008	PL9	C32-C33-C34	-2.26	122.45	127.62
12	D	202	PL9	O1-C4-C3	-2.26	118.35	120.73
9	I	2002	HEM	C3B-C4B-NB	-2.26	107.85	109.47
17	P	101	BCR	C38-C26-C25	-2.25	122.03	124.48
9	A	302	HEM	C2A-C1A-NA	-2.23	107.68	110.15
10	A	303	HEC	CHB-C1B-C2B	-2.22	120.97	127.43
17	F	101	BCR	C38-C26-C25	-2.22	122.06	124.48
12	D	202	PL9	O2-C1-C6	2.22	124.01	120.48
9	I	2003	HEM	C2A-C1A-NA	-2.21	107.69	110.15
12	A	305	PL9	C12-C13-C14	-2.21	122.56	127.62
13	J	205	UMQ	C1-C2-C3	2.21	114.66	110.01
12	I	2001	PL9	C27-C28-C29	-2.21	122.57	127.62
12	I	2001	PL9	O2-C1-C2	-2.19	116.84	121.83
12	A	305	PL9	C7-C8-C9	-2.18	123.07	126.83
12	J	202	PL9	C37-C38-C39	-2.18	122.63	127.62
12	J	203	PL9	O2-C1-C2	-2.18	116.88	121.83
9	I	2002	HEM	C3D-C4D-ND	-2.18	107.78	110.17
10	C	301	HEC	CAA-CBA-CGA	-2.17	107.90	113.67
12	I	2008	PL9	C12-C13-C14	-2.17	122.66	127.62
11	J	201	CLA	CHB-C4A-NA	2.17	127.53	124.40
13	J	205	UMQ	O5'-C1'-C2'	2.17	114.82	110.37
13	J	205	UMQ	O5'-C5'-C4'	2.16	114.20	109.72
12	D	202	PL9	C42-C43-C44	-2.16	122.67	127.62
12	D	202	PL9	C37-C38-C39	-2.16	122.68	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	2003	HEM	C3B-C4B-NB	-2.15	107.92	109.47
12	B	301	PL9	O2-C1-C2	-2.15	116.93	121.83
10	C	301	HEC	CHA-C1A-NA	2.15	126.79	124.45
10	A	303	HEC	CHD-C1D-C2D	-2.14	121.20	127.43
17	P	101	BCR	C3-C4-C5	-2.14	110.24	114.06
11	A	304	CLA	C1-C2-C3	-2.14	122.69	126.20
12	B	301	PL9	O1-C4-C3	-2.14	118.48	120.73
12	A	305	PL9	O2-C1-C2	-2.12	117.00	121.83
12	D	202	PL9	C32-C33-C34	-2.12	122.76	127.62
10	A	303	HEC	CAA-C2A-C1A	2.12	129.16	124.85
12	J	203	PL9	C12-C13-C14	-2.12	122.78	127.62
12	J	202	PL9	C20-C19-C21	2.11	118.90	115.23
12	J	202	PL9	C32-C33-C34	-2.11	122.79	127.62
12	I	2008	PL9	O2-C1-C2	-2.11	117.03	121.83
12	I	2001	PL9	C8-C7-C3	2.11	117.48	112.03
12	I	2008	PL9	C37-C38-C39	-2.10	122.81	127.62
12	A	305	PL9	C42-C43-C44	-2.10	122.82	127.62
12	J	203	PL9	O1-C4-C3	-2.10	118.52	120.73
12	D	202	PL9	C12-C13-C14	-2.10	122.83	127.62
12	J	203	PL9	C32-C33-C34	-2.09	122.83	127.62
10	C	301	HEC	C2A-C1A-NA	-2.09	108.30	110.32
13	J	205	UMQ	C1-O1-C4'	-2.09	113.03	117.98
17	P	101	BCR	C7-C8-C9	-2.08	123.15	126.23
9	A	302	HEM	C3B-C4B-NB	-2.08	107.97	109.47
10	A	303	HEC	CHD-C4C-C3C	-2.07	121.72	125.21
13	I	2006	UMQ	C3-C4-C5	2.06	113.97	110.23
10	I	2004	HEC	CHB-C4A-NA	2.06	126.69	124.45
12	J	202	PL9	O2-C1-C2	-2.06	117.15	121.83
12	J	203	PL9	C42-C43-C44	-2.03	122.97	127.62
12	D	202	PL9	O2-C1-C2	-2.03	117.22	121.83
10	A	303	HEC	CAD-C3D-C4D	2.02	128.89	124.94
11	A	304	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
12	B	301	PL9	C12-C13-C14	-2.02	123.01	127.62
17	F	101	BCR	C7-C8-C9	-2.01	123.26	126.23

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	304	CLA	ND
11	J	201	CLA	ND

All (495) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	302	HEM	C1A-C2A-CAA-CBA
9	I	2003	HEM	C1A-C2A-CAA-CBA
10	C	301	HEC	C2B-C3B-CAB-CBB
10	C	301	HEC	C4B-C3B-CAB-CBB
10	C	301	HEC	C2C-C3C-CAC-CBC
10	C	301	HEC	C2D-C3D-CAD-CBD
10	I	2004	HEC	C2B-C3B-CAB-CBB
10	I	2004	HEC	C4B-C3B-CAB-CBB
10	I	2004	HEC	C2C-C3C-CAC-CBC
10	I	2004	HEC	C4C-C3C-CAC-CBC
10	K	301	HEC	C2B-C3B-CAB-CBB
10	K	301	HEC	C4B-C3B-CAB-CBB
10	K	301	HEC	C2C-C3C-CAC-CBC
10	K	301	HEC	C4C-C3C-CAC-CBC
11	A	304	CLA	C1A-C2A-CAA-CBA
11	A	304	CLA	C3A-C2A-CAA-CBA
11	A	304	CLA	C11-C10-C8-C9
11	J	201	CLA	C1A-C2A-CAA-CBA
11	J	201	CLA	C3A-C2A-CAA-CBA
11	J	201	CLA	CBA-CGA-O2A-C1
11	J	201	CLA	O1A-CGA-O2A-C1
12	A	305	PL9	C4-C3-C7-C8
12	A	305	PL9	C7-C8-C9-C10
12	A	305	PL9	C7-C8-C9-C11
12	A	305	PL9	C23-C24-C26-C27
12	B	301	PL9	C7-C8-C9-C11
12	B	301	PL9	C17-C18-C19-C20
12	B	301	PL9	C17-C18-C19-C21
12	B	301	PL9	C27-C28-C29-C31
12	D	202	PL9	C7-C8-C9-C11
12	D	202	PL9	C12-C13-C14-C16
12	D	202	PL9	C15-C14-C16-C17
12	D	202	PL9	C14-C16-C17-C18
12	D	202	PL9	C37-C38-C39-C40
12	I	2001	PL9	C2-C3-C7-C8
12	I	2001	PL9	C4-C3-C7-C8
12	I	2001	PL9	C7-C8-C9-C11
12	I	2001	PL9	C17-C18-C19-C20
12	I	2001	PL9	C17-C18-C19-C21
12	I	2001	PL9	C22-C23-C24-C26
12	I	2001	PL9	C27-C28-C29-C31
12	I	2001	PL9	C32-C33-C34-C35
12	I	2001	PL9	C32-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
12	I	2001	PL9	C37-C38-C39-C40
12	I	2001	PL9	C37-C38-C39-C41
12	I	2001	PL9	C42-C43-C44-C46
12	I	2008	PL9	C27-C28-C29-C30
12	I	2008	PL9	C27-C28-C29-C31
12	I	2008	PL9	C33-C34-C36-C37
12	I	2008	PL9	C42-C43-C44-C46
12	J	202	PL9	C3-C7-C8-C9
12	J	202	PL9	C7-C8-C9-C10
12	J	202	PL9	C7-C8-C9-C11
12	J	202	PL9	C40-C39-C41-C42
12	J	202	PL9	C42-C43-C44-C46
12	J	203	PL9	C7-C8-C9-C11
12	J	203	PL9	C12-C13-C14-C15
12	J	203	PL9	C22-C23-C24-C26
12	J	203	PL9	C35-C34-C36-C37
13	A	307	UMQ	C2'-C1'-O1'-CA
13	A	307	UMQ	O5'-C1'-O1'-CA
13	I	2005	UMQ	O5'-C1'-O1'-CA
13	J	205	UMQ	O5'-C1'-O1'-CA
14	A	308	PGT	C1-O3P-P-O1P
14	A	308	PGT	C1-O3P-P-O4P
14	A	308	PGT	C4-O4P-P-O3P
14	A	308	PGT	C4-O4P-P-O1P
14	D	204	PGT	C32-C31-O2-C2
14	D	204	PGT	C1-O3P-P-O1P
14	D	204	PGT	C1-O3P-P-O2P
14	D	204	PGT	C1-O3P-P-O4P
14	D	204	PGT	C4-O4P-P-O3P
14	D	204	PGT	C4-O4P-P-O1P
14	D	204	PGT	C4-O4P-P-O2P
14	D	204	PGT	C5-C4-O4P-P
14	D	204	PGT	C4-C5-C6-O6
14	I	2007	PGT	C32-C31-O2-C2
14	I	2007	PGT	C1-O3P-P-O1P
14	I	2007	PGT	C1-O3P-P-O2P
14	I	2007	PGT	C1-O3P-P-O4P
14	I	2007	PGT	C4-O4P-P-O2P
14	L	801	PGT	C32-C31-O2-C2
14	L	801	PGT	C2-C1-O3P-P
14	L	801	PGT	C1-O3P-P-O1P
14	L	801	PGT	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
14	L	801	PGT	C1-O3P-P-O4P
15	K	302	SQD	O49-C7-O47-C45
15	K	302	SQD	C8-C7-O47-C45
13	J	205	UMQ	O5-C1-O1-C4'
12	I	2001	PL9	C47-C48-C49-C50
12	I	2001	PL9	C47-C48-C49-C51
13	J	205	UMQ	C2-C1-O1-C4'
14	D	204	PGT	O11-C11-O3-C3
15	D	201	SQD	O10-C23-O48-C46
11	J	201	CLA	C10-C11-C12-C13
14	D	204	PGT	O31-C31-O2-C2
14	I	2007	PGT	O31-C31-O2-C2
14	L	801	PGT	O31-C31-O2-C2
14	D	204	PGT	C12-C11-O3-C3
15	D	201	SQD	C24-C23-O48-C46
15	K	302	SQD	O10-C23-O48-C46
13	A	307	UMQ	C4-C5-C6-O6
12	A	305	PL9	C25-C24-C26-C27
12	B	301	PL9	C25-C24-C26-C27
12	B	301	PL9	C45-C44-C46-C47
12	I	2001	PL9	C25-C24-C26-C27
12	I	2008	PL9	C15-C14-C16-C17
12	I	2008	PL9	C30-C29-C31-C32
12	I	2008	PL9	C35-C34-C36-C37
12	J	202	PL9	C30-C29-C31-C32
12	J	203	PL9	C12-C11-C9-C10
12	A	305	PL9	C13-C14-C16-C17
12	I	2008	PL9	C12-C11-C9-C8
12	J	202	PL9	C28-C29-C31-C32
12	J	202	PL9	C33-C34-C36-C37
12	J	202	PL9	C38-C39-C41-C42
12	J	203	PL9	C28-C29-C31-C32
11	A	304	CLA	O1A-CGA-O2A-C1
15	K	302	SQD	C24-C23-O48-C46
12	A	305	PL9	C12-C13-C14-C15
12	I	2001	PL9	C7-C8-C9-C10
12	I	2001	PL9	C42-C43-C44-C45
12	J	202	PL9	C42-C43-C44-C45
12	J	203	PL9	C7-C8-C9-C10
12	D	202	PL9	C37-C38-C39-C41
12	J	202	PL9	C32-C33-C34-C36
12	J	203	PL9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
12	J	203	PL9	C17-C18-C19-C21
14	A	308	PGT	O4P-C4-C5-O5
11	A	304	CLA	CBA-CGA-O2A-C1
13	I	2005	UMQ	O5'-C5'-C6'-O6'
13	I	2005	UMQ	O5-C5-C6-O6
12	A	305	PL9	C15-C14-C16-C17
12	A	305	PL9	C40-C39-C41-C42
12	B	301	PL9	C35-C34-C36-C37
12	I	2008	PL9	C12-C11-C9-C10
12	J	202	PL9	C35-C34-C36-C37
12	A	305	PL9	C38-C39-C41-C42
12	B	301	PL9	C43-C44-C46-C47
12	I	2001	PL9	C23-C24-C26-C27
12	J	203	PL9	C12-C11-C9-C8
12	A	305	PL9	C14-C16-C17-C18
12	A	305	PL9	C29-C31-C32-C33
12	B	301	PL9	C19-C21-C22-C23
12	D	202	PL9	C9-C11-C12-C13
12	D	202	PL9	C24-C26-C27-C28
12	D	202	PL9	C29-C31-C32-C33
12	I	2001	PL9	C9-C11-C12-C13
12	I	2001	PL9	C29-C31-C32-C33
12	I	2001	PL9	C39-C41-C42-C43
12	I	2001	PL9	C44-C46-C47-C48
12	I	2008	PL9	C14-C16-C17-C18
12	I	2008	PL9	C29-C31-C32-C33
12	J	202	PL9	C19-C21-C22-C23
12	J	202	PL9	C44-C46-C47-C48
12	J	203	PL9	C24-C26-C27-C28
12	J	203	PL9	C39-C41-C42-C43
10	C	301	HEC	C4D-C3D-CAD-CBD
10	I	2004	HEC	C4D-C3D-CAD-CBD
13	I	2005	UMQ	C4'-C5'-C6'-O6'
13	J	204	UMQ	O5'-C1'-O1'-CA
13	A	307	UMQ	O5-C5-C6-O6
13	B	302	UMQ	O5-C5-C6-O6
12	I	2001	PL9	C27-C28-C29-C30
12	A	305	PL9	C32-C33-C34-C36
12	B	301	PL9	C12-C13-C14-C16
12	J	202	PL9	C22-C23-C24-C26
12	A	305	PL9	C47-C48-C49-C51
14	A	308	PGT	O4P-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
14	D	204	PGT	O4P-C4-C5-C6
14	L	801	PGT	C43-C44-C45-C46
13	J	204	UMQ	C4'-C5'-C6'-O6'
12	I	2001	PL9	C33-C34-C36-C37
13	B	302	UMQ	C4-C5-C6-O6
13	J	204	UMQ	C2'-C1'-O1'-CA
13	J	205	UMQ	C2'-C1'-O1'-CA
14	D	204	PGT	O4P-C4-C5-O5
10	I	2004	HEC	C2D-C3D-CAD-CBD
13	I	2006	UMQ	O5-C5-C6-O6
12	I	2008	PL9	C42-C43-C44-C45
14	D	204	PGT	C43-C44-C45-C46
15	D	201	SQD	C14-C15-C16-C17
13	P	102	UMQ	O5-C5-C6-O6
14	D	204	PGT	O5-C5-C6-O6
12	J	203	PL9	C27-C28-C29-C31
13	A	306	UMQ	O5-C5-C6-O6
12	B	301	PL9	C14-C16-C17-C18
12	I	2001	PL9	C14-C16-C17-C18
12	J	203	PL9	C14-C16-C17-C18
12	J	203	PL9	C19-C21-C22-C23
12	J	203	PL9	C44-C46-C47-C48
13	J	205	UMQ	O1'-CA-CB-CC
13	J	205	UMQ	O5'-C5'-C6'-O6'
13	P	102	UMQ	C4-C5-C6-O6
10	C	301	HEC	C3D-CAD-CBD-CGD
15	D	201	SQD	C34-C35-C36-C37
13	I	2005	UMQ	C4-C5-C6-O6
12	B	301	PL9	C27-C28-C29-C30
13	J	204	UMQ	O5'-C5'-C6'-O6'
12	I	2008	PL9	C13-C14-C16-C17
14	D	204	PGT	C11-C12-C13-C14
15	K	302	SQD	C11-C10-C9-C8
10	C	301	HEC	C3A-C2A-CAA-CBA
14	L	801	PGT	C12-C11-O3-C3
9	I	2003	HEM	C3A-C2A-CAA-CBA
11	A	304	CLA	C13-C15-C16-C17
11	A	304	CLA	C15-C16-C17-C18
13	B	302	UMQ	C3'-C4'-O1-C1
12	A	305	PL9	C2-C3-C7-C8
12	D	202	PL9	C12-C13-C14-C15
12	I	2001	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
13	B	302	UMQ	C5'-C4'-O1-C1
12	B	301	PL9	C34-C36-C37-C38
12	J	202	PL9	C24-C26-C27-C28
12	J	203	PL9	C9-C11-C12-C13
12	J	203	PL9	C34-C36-C37-C38
17	P	101	BCR	C20-C21-C22-C37
17	P	101	BCR	C37-C22-C23-C24
14	D	204	PGT	C41-C42-C43-C44
9	A	301	HEM	C2A-CAA-CBA-CGA
9	I	2002	HEM	C2A-CAA-CBA-CGA
10	A	303	HEC	C2A-CAA-CBA-CGA
14	I	2007	PGT	C4-C5-C6-O6
10	C	301	HEC	C1A-C2A-CAA-CBA
17	P	101	BCR	C11-C10-C9-C8
17	P	101	BCR	C20-C21-C22-C23
13	H	201	UMQ	CA-CB-CC-CD
13	A	306	UMQ	CC-CD-CF-CG
13	I	2006	UMQ	CD-CF-CG-CH
14	D	204	PGT	C32-C33-C34-C35
13	J	204	UMQ	CC-CD-CF-CG
13	H	201	UMQ	CF-CG-CH-CI
13	J	204	UMQ	CD-CF-CG-CH
13	B	302	UMQ	CA-CB-CC-CD
14	D	204	PGT	C44-C45-C46-C47
14	L	801	PGT	O11-C11-O3-C3
14	A	308	PGT	C33-C34-C35-C36
13	I	2006	UMQ	CG-CH-CI-CJ
13	J	204	UMQ	C3'-C4'-O1-C1
14	L	801	PGT	C44-C45-C46-C47
15	D	201	SQD	C11-C12-C13-C14
15	D	201	SQD	C16-C17-C18-C19
13	P	102	UMQ	CC-CD-CF-CG
14	I	2007	PGT	C20-C21-C22-C23
15	K	302	SQD	C26-C27-C28-C29
14	D	204	PGT	C12-C13-C14-C15
15	K	302	SQD	C17-C18-C19-C20
14	L	801	PGT	C5-C4-O4P-P
14	L	801	PGT	C32-C33-C34-C35
13	P	102	UMQ	CB-CC-CD-CF
14	L	801	PGT	C13-C14-C15-C16
14	I	2007	PGT	C41-C42-C43-C44
14	L	801	PGT	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
13	J	204	UMQ	O1'-CA-CB-CC
13	B	302	UMQ	CB-CC-CD-CF
15	D	201	SQD	C26-C27-C28-C29
13	J	204	UMQ	CB-CC-CD-CF
15	D	201	SQD	C12-C13-C14-C15
17	F	101	BCR	C22-C23-C24-C25
13	B	302	UMQ	C2'-C1'-O1'-CA
15	D	201	SQD	C9-C10-C11-C12
13	B	302	UMQ	CC-CD-CF-CG
13	J	204	UMQ	C5'-C4'-O1-C1
14	L	801	PGT	C17-C18-C19-C20
13	B	303	UMQ	CA-CB-CC-CD
9	A	302	HEM	C3A-C2A-CAA-CBA
12	D	202	PL9	C44-C46-C47-C48
13	I	2006	UMQ	O1'-CA-CB-CC
15	D	201	SQD	O47-C45-C46-O48
14	D	204	PGT	C42-C43-C44-C45
13	B	302	UMQ	O1'-CA-CB-CC
13	B	303	UMQ	O5-C5-C6-O6
15	D	201	SQD	C32-C33-C34-C35
15	K	302	SQD	C16-C17-C18-C19
10	I	2004	HEC	C3D-CAD-CBD-CGD
13	A	307	UMQ	CC-CD-CF-CG
11	A	304	CLA	C2A-CAA-CBA-CGA
13	A	307	UMQ	CG-CH-CI-CJ
14	I	2007	PGT	C14-C15-C16-C17
13	I	2005	UMQ	CB-CC-CD-CF
14	A	308	PGT	O3P-C1-C2-C3
15	K	302	SQD	C12-C13-C14-C15
11	J	201	CLA	C11-C10-C8-C7
13	B	302	UMQ	O5'-C5'-C6'-O6'
12	J	202	PL9	C15-C14-C16-C17
12	I	2008	PL9	C23-C24-C26-C27
12	I	2008	PL9	C47-C48-C49-C51
15	K	302	SQD	C34-C35-C36-C37
13	B	303	UMQ	O5'-C5'-C6'-O6'
13	J	205	UMQ	O5-C5-C6-O6
10	A	303	HEC	C1A-C2A-CAA-CBA
12	A	305	PL9	C24-C26-C27-C28
12	D	202	PL9	C39-C41-C42-C43
14	A	308	PGT	C1-C2-C3-O3
15	D	201	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
15	K	302	SQD	C44-C45-C46-O48
14	A	308	PGT	C12-C11-O3-C3
13	I	2006	UMQ	O5'-C5'-C6'-O6'
11	J	201	CLA	C16-C17-C18-C20
12	A	305	PL9	C12-C11-C9-C10
13	B	303	UMQ	CG-CH-CI-CJ
14	I	2007	PGT	C31-C32-C33-C34
13	A	307	UMQ	O1'-CA-CB-CC
11	A	304	CLA	CBD-CGD-O2D-CED
15	D	201	SQD	C28-C29-C30-C31
13	I	2006	UMQ	C4-C5-C6-O6
12	I	2008	PL9	C25-C24-C26-C27
15	D	201	SQD	C25-C26-C27-C28
14	I	2007	PGT	C34-C35-C36-C37
14	A	308	PGT	C21-C22-C23-C24
14	I	2007	PGT	C12-C13-C14-C15
15	D	201	SQD	O6-C44-C45-O47
12	B	301	PL9	C29-C31-C32-C33
13	A	306	UMQ	CB-CC-CD-CF
14	D	204	PGT	C19-C20-C21-C22
15	K	302	SQD	C9-C10-C11-C12
14	A	308	PGT	C17-C18-C19-C20
14	D	204	PGT	C39-C40-C41-C42
13	I	2006	UMQ	CI-CJ-CK-CL
11	A	304	CLA	C2C-C3C-CAC-CBC
13	A	306	UMQ	CB-CA-O1'-C1'
13	J	205	UMQ	CB-CA-O1'-C1'
11	A	304	CLA	C11-C12-C13-C14
11	J	201	CLA	C11-C10-C8-C9
13	J	205	UMQ	CA-CB-CC-CD
13	A	306	UMQ	O1'-CA-CB-CC
13	P	102	UMQ	CD-CF-CG-CH
14	L	801	PGT	O3P-C1-C2-C3
11	A	304	CLA	C11-C12-C13-C15
11	J	201	CLA	C16-C17-C18-C19
13	A	307	UMQ	CD-CF-CG-CH
12	I	2001	PL9	C35-C34-C36-C37
12	I	2008	PL9	C40-C39-C41-C42
14	A	308	PGT	O11-C11-O3-C3
14	D	204	PGT	C21-C22-C23-C24
13	H	201	UMQ	CB-CC-CD-CF
12	D	202	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
14	D	204	PGT	C1-C2-C3-O3
17	F	101	BCR	C23-C24-C25-C30
14	L	801	PGT	C34-C35-C36-C37
14	D	204	PGT	O2-C2-C3-O3
14	L	801	PGT	O2-C2-C3-O3
12	B	301	PL9	C4-C3-C7-C8
12	D	202	PL9	C4-C3-C7-C8
12	I	2008	PL9	C4-C3-C7-C8
12	D	202	PL9	C45-C44-C46-C47
12	B	301	PL9	C23-C24-C26-C27
12	J	202	PL9	C23-C24-C26-C27
14	A	308	PGT	C36-C37-C38-C39
14	A	308	PGT	C34-C35-C36-C37
15	D	201	SQD	C29-C30-C31-C32
12	A	305	PL9	C34-C36-C37-C38
14	L	801	PGT	C19-C20-C21-C22
15	D	201	SQD	C13-C14-C15-C16
13	A	306	UMQ	CF-CG-CH-CI
13	A	307	UMQ	O5'-C5'-C6'-O6'
12	B	301	PL9	C7-C8-C9-C10
12	D	202	PL9	C27-C28-C29-C30
14	A	308	PGT	C16-C17-C18-C19
13	J	205	UMQ	CC-CD-CF-CG
15	D	201	SQD	C8-C7-O47-C45
11	J	201	CLA	C2C-C3C-CAC-CBC
12	I	2008	PL9	C24-C26-C27-C28
15	D	201	SQD	O6-C44-C45-C46
12	J	202	PL9	C32-C33-C34-C35
13	A	307	UMQ	C4'-C5'-C6'-O6'
12	J	202	PL9	C18-C19-C21-C22
14	I	2007	PGT	C36-C37-C38-C39
14	A	308	PGT	O2-C2-C3-O3
15	K	302	SQD	O6-C44-C45-O47
11	J	201	CLA	C13-C15-C16-C17
14	I	2007	PGT	C18-C19-C20-C21
14	D	204	PGT	C33-C34-C35-C36
10	A	303	HEC	C3A-C2A-CAA-CBA
12	B	301	PL9	C13-C14-C16-C17
14	D	204	PGT	C37-C38-C39-C40
13	I	2006	UMQ	CB-CA-O1'-C1'
12	A	305	PL9	C9-C11-C12-C13
11	J	201	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	P	101	BCR	C22-C23-C24-C25
12	J	203	PL9	C32-C33-C34-C36
15	D	201	SQD	C5-C6-S-O9
15	K	302	SQD	C5-C6-S-O9
14	D	204	PGT	C40-C41-C42-C43
14	A	308	PGT	C19-C20-C21-C22
10	C	301	HEC	C4C-C3C-CAC-CBC
14	A	308	PGT	O3P-C1-C2-O2
14	L	801	PGT	O3P-C1-C2-O2
14	D	204	PGT	C36-C37-C38-C39
14	D	204	PGT	C13-C14-C15-C16
15	K	302	SQD	O47-C45-C46-O48
13	I	2006	UMQ	CC-CD-CF-CG
15	K	302	SQD	C15-C16-C17-C18
15	D	201	SQD	C30-C31-C32-C33
14	L	801	PGT	C38-C39-C40-C41
14	I	2007	PGT	C4-O4P-P-O3P
14	I	2007	PGT	C4-O4P-P-O1P
14	L	801	PGT	C4-O4P-P-O3P
12	D	202	PL9	C12-C11-C9-C10
13	I	2005	UMQ	CG-CH-CI-CJ
11	A	304	CLA	C4C-C3C-CAC-CBC
12	I	2008	PL9	C28-C29-C31-C32
13	I	2005	UMQ	CF-CG-CH-CI
10	K	301	HEC	C1A-C2A-CAA-CBA
17	F	101	BCR	C11-C10-C9-C8
13	I	2006	UMQ	CB-CC-CD-CF
12	A	305	PL9	C37-C38-C39-C41
12	A	305	PL9	C42-C43-C44-C46
15	D	201	SQD	C19-C20-C21-C22
15	K	302	SQD	C7-C8-C9-C10
13	A	307	UMQ	C3'-C4'-O1-C1
17	F	101	BCR	C7-C8-C9-C34
13	A	307	UMQ	C5'-C4'-O1-C1
10	K	301	HEC	C3A-C2A-CAA-CBA
14	L	801	PGT	C42-C43-C44-C45
12	D	202	PL9	C2-C3-C7-C8
11	A	304	CLA	O1D-CGD-O2D-CED
14	A	308	PGT	C2-C1-O3P-P
13	J	204	UMQ	CG-CH-CI-CJ
12	J	202	PL9	C20-C19-C21-C22
11	A	304	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	D	204	PGT	C16-C17-C18-C19
12	I	2001	PL9	C12-C13-C14-C15
14	I	2007	PGT	C39-C40-C41-C42
12	J	202	PL9	C45-C44-C46-C47
11	J	201	CLA	C2-C3-C5-C6
11	J	201	CLA	C4C-C3C-CAC-CBC
17	F	101	BCR	C11-C10-C9-C34
17	P	101	BCR	C11-C10-C9-C34
12	B	301	PL9	C15-C14-C16-C17
10	I	2004	HEC	C2A-CAA-CBA-CGA
13	I	2006	UMQ	CH-CI-CJ-CK
14	L	801	PGT	C39-C40-C41-C42
11	J	201	CLA	C2A-CAA-CBA-CGA
13	J	205	UMQ	C4'-C5'-C6'-O6'
13	J	204	UMQ	CH-CI-CJ-CK
11	A	304	CLA	C14-C13-C15-C16
14	A	308	PGT	C41-C42-C43-C44
14	I	2007	PGT	O5-C5-C6-O6
17	F	101	BCR	C23-C24-C25-C26
17	P	101	BCR	C23-C24-C25-C30
14	A	308	PGT	C15-C16-C17-C18
12	A	305	PL9	C39-C41-C42-C43
12	I	2008	PL9	C39-C41-C42-C43
13	B	303	UMQ	CB-CC-CD-CF
10	C	301	HEC	CAD-CBD-CGD-O1D
14	D	204	PGT	C14-C15-C16-C17
12	B	301	PL9	C12-C11-C9-C10
12	I	2008	PL9	C38-C39-C41-C42
14	A	308	PGT	C42-C43-C44-C45
12	B	301	PL9	C20-C19-C21-C22
12	D	202	PL9	C25-C24-C26-C27
12	I	2001	PL9	C40-C39-C41-C42
12	J	203	PL9	C30-C29-C31-C32
10	C	301	HEC	CAD-CBD-CGD-O2D
14	A	308	PGT	O2-C31-C32-C33
10	K	301	HEC	CAA-CBA-CGA-O2A
12	B	301	PL9	C30-C29-C31-C32
14	I	2007	PGT	C17-C18-C19-C20
13	A	307	UMQ	CH-CI-CJ-CK
13	J	205	UMQ	CB-CC-CD-CF
14	A	308	PGT	C14-C15-C16-C17
10	K	301	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	D	201	SQD	C18-C19-C20-C21
13	J	204	UMQ	C4-C5-C6-O6
11	A	304	CLA	C11-C10-C8-C7
17	P	101	BCR	C23-C24-C25-C26
12	B	301	PL9	C39-C41-C42-C43
14	A	308	PGT	O3-C11-C12-C13
12	J	202	PL9	C13-C14-C16-C17
14	A	308	PGT	C38-C39-C40-C41
10	A	303	HEC	CAD-CBD-CGD-O2D
13	B	303	UMQ	CC-CD-CF-CG
14	A	308	PGT	C39-C40-C41-C42
12	D	202	PL9	C22-C23-C24-C26
13	A	307	UMQ	CB-CA-O1'-C1'
13	B	302	UMQ	CB-CA-O1'-C1'
14	D	204	PGT	O3-C11-C12-C13
14	L	801	PGT	C1-C2-C3-O3
15	K	302	SQD	O6-C44-C45-C46
17	P	101	BCR	C21-C22-C23-C24
14	I	2007	PGT	O2-C31-C32-C33
14	A	308	PGT	O11-C11-C12-C13
10	A	303	HEC	CAD-CBD-CGD-O1D
12	A	305	PL9	C17-C18-C19-C21
15	D	201	SQD	C27-C28-C29-C30
14	D	204	PGT	O11-C11-C12-C13
14	I	2007	PGT	O31-C31-C32-C33
13	A	306	UMQ	C4-C5-C6-O6
12	D	202	PL9	C11-C12-C13-C14
13	P	102	UMQ	CG-CH-CI-CJ
11	J	201	CLA	CAD-CBD-CGD-O2D
10	I	2004	HEC	CAD-CBD-CGD-O2D
9	A	301	HEM	CAD-CBD-CGD-O2D
14	I	2007	PGT	C33-C34-C35-C36

There are no ring outliers.

30 monomers are involved in 142 short contacts:

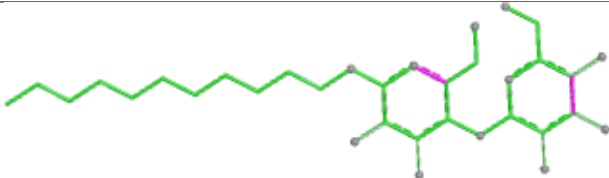
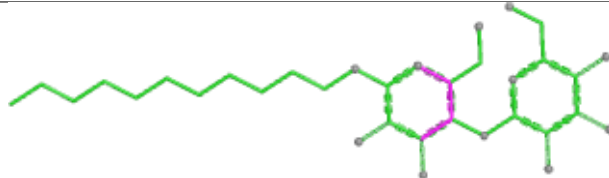
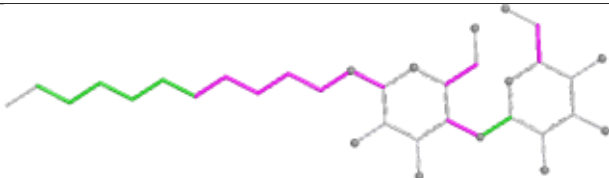
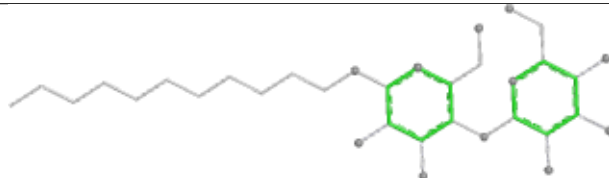
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	302	UMQ	1	0
12	D	202	PL9	4	0
14	A	308	PGT	1	0
9	A	302	HEM	6	0
14	L	801	PGT	3	0

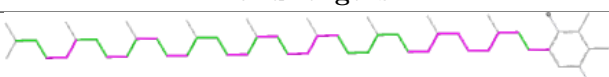
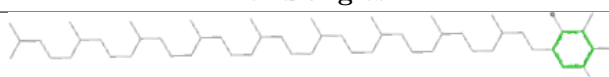
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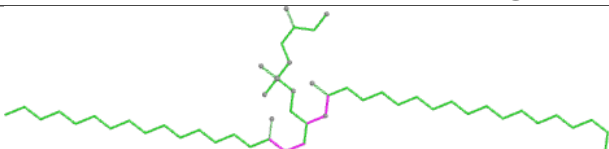
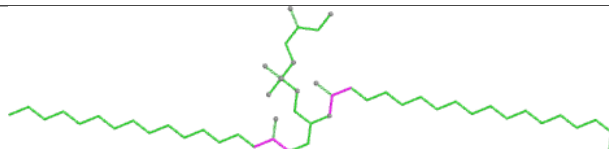
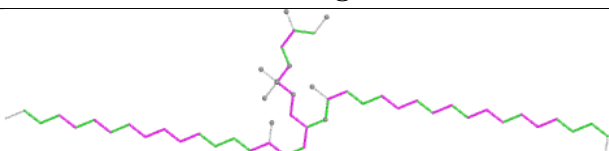
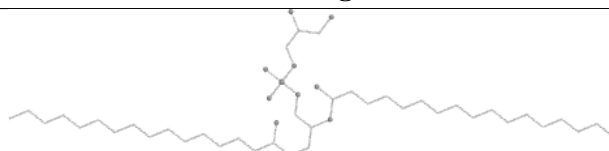
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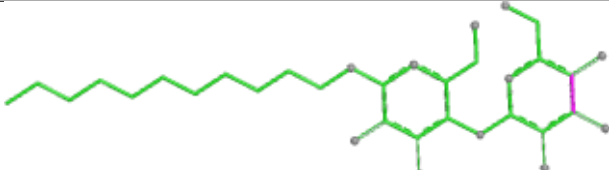
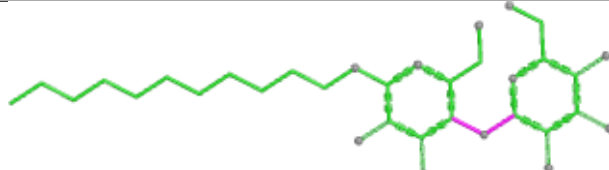
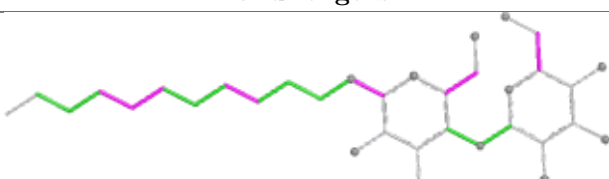
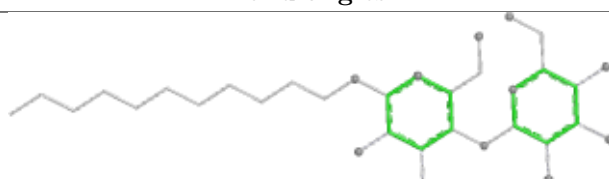
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	203	FES	1	0
9	A	301	HEM	4	0
12	I	2001	PL9	1	0
13	J	205	UMQ	3	0
12	I	2008	PL9	15	0
11	J	201	CLA	12	0
13	A	306	UMQ	1	0
17	P	101	BCR	2	0
10	K	301	HEC	4	0
15	K	302	SQD	1	0
12	A	305	PL9	6	0
10	A	303	HEC	5	0
12	J	203	PL9	10	0
10	I	2004	HEC	3	0
9	I	2002	HEM	4	0
13	H	201	UMQ	1	0
12	J	202	PL9	27	0
14	I	2007	PGT	2	0
14	D	204	PGT	4	0
17	F	101	BCR	3	0
10	C	301	HEC	4	0
11	A	304	CLA	6	0
15	D	201	SQD	3	0
12	B	301	PL9	13	0
9	I	2003	HEM	5	0

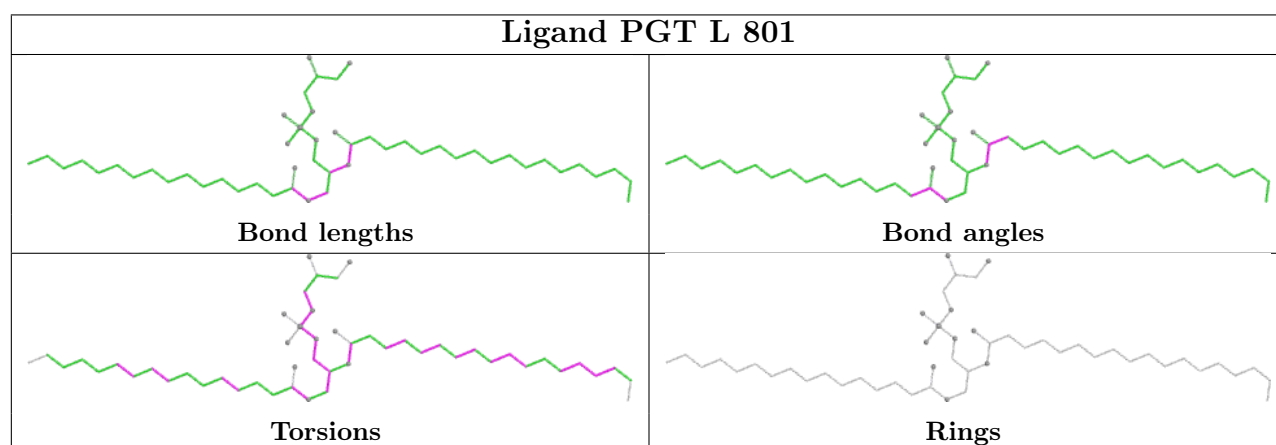
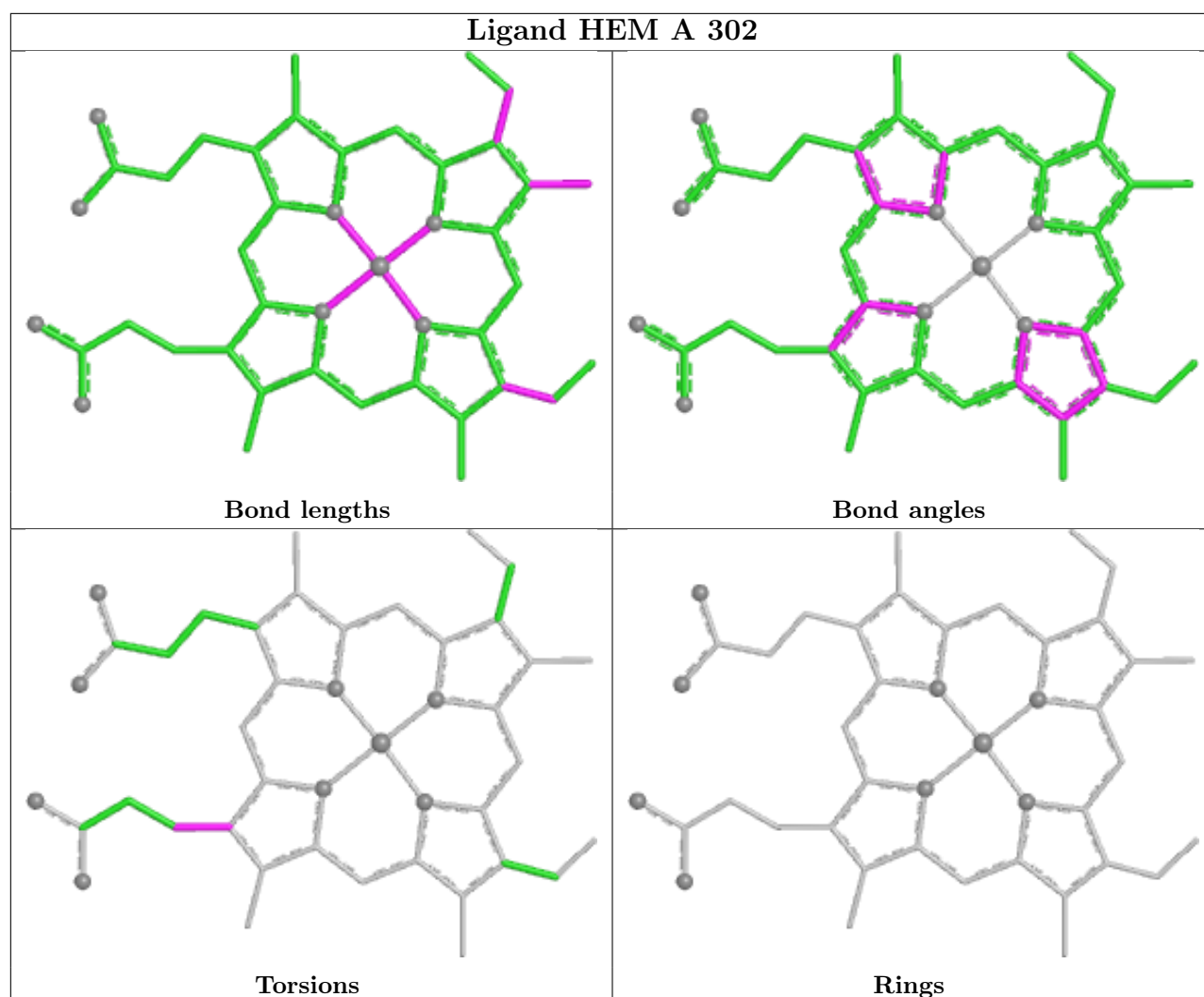
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

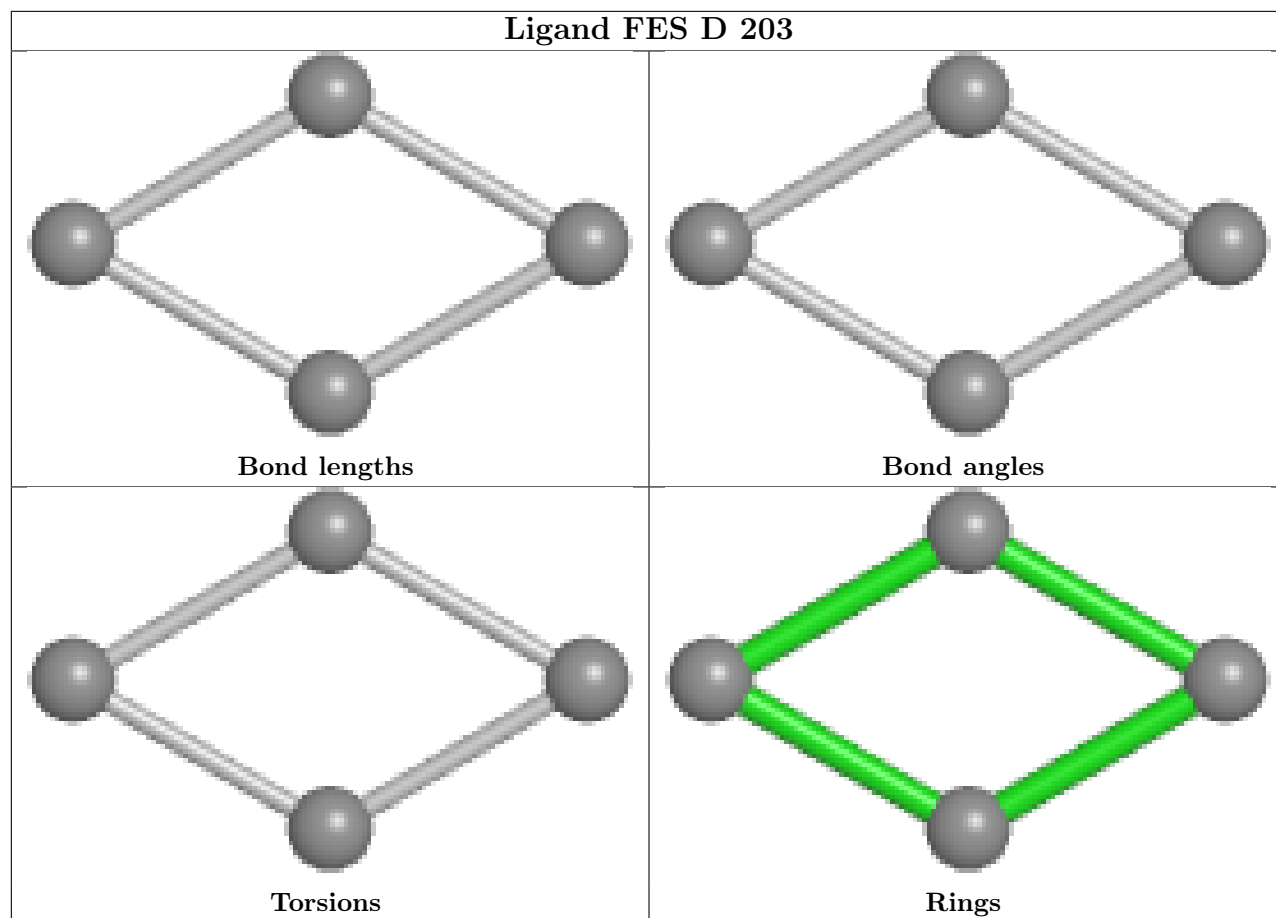
Ligand UMQ B 302	
	
Bond lengths	Bond angles
	
Torsions	Rings

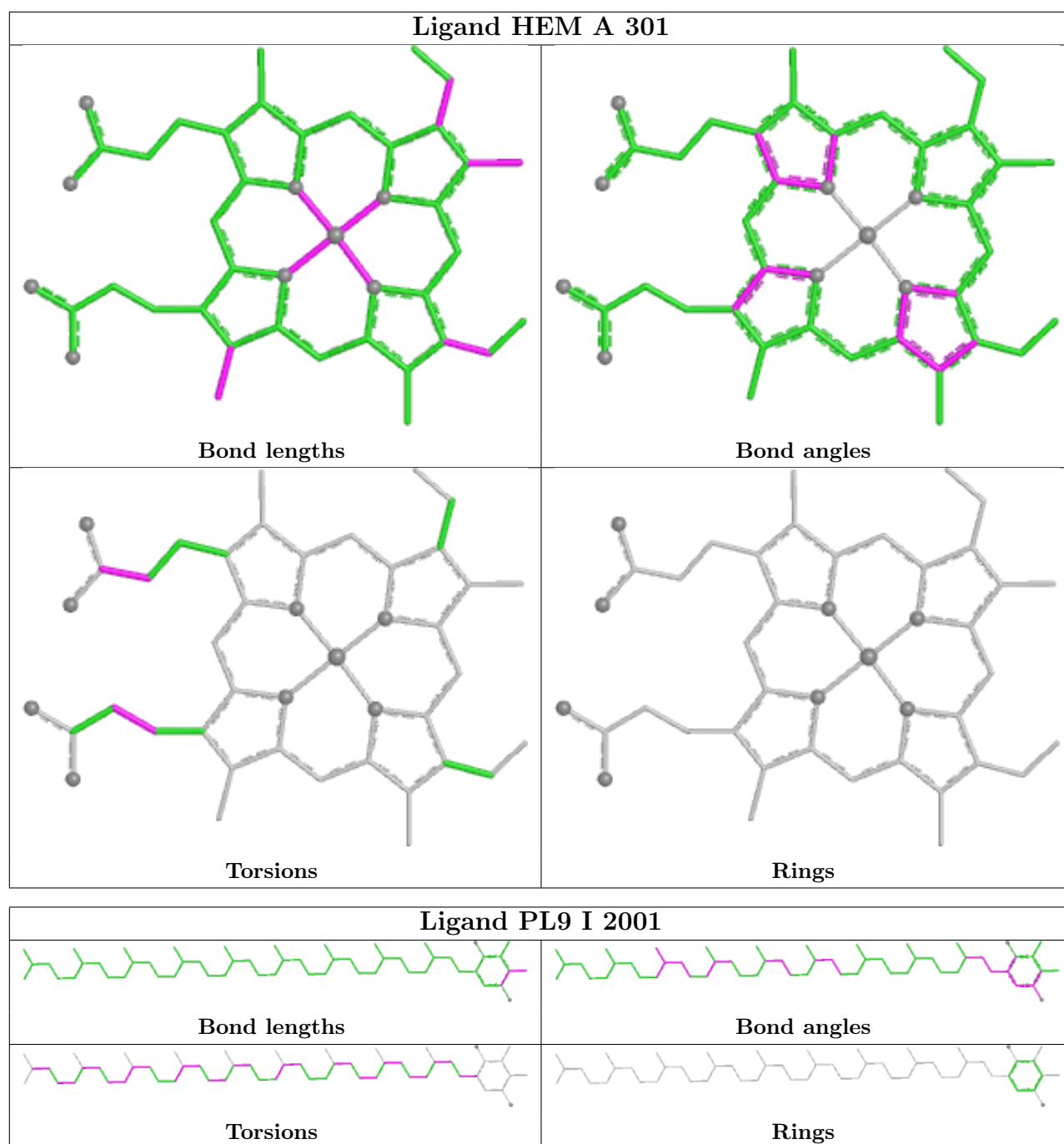
Ligand PL9 D 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

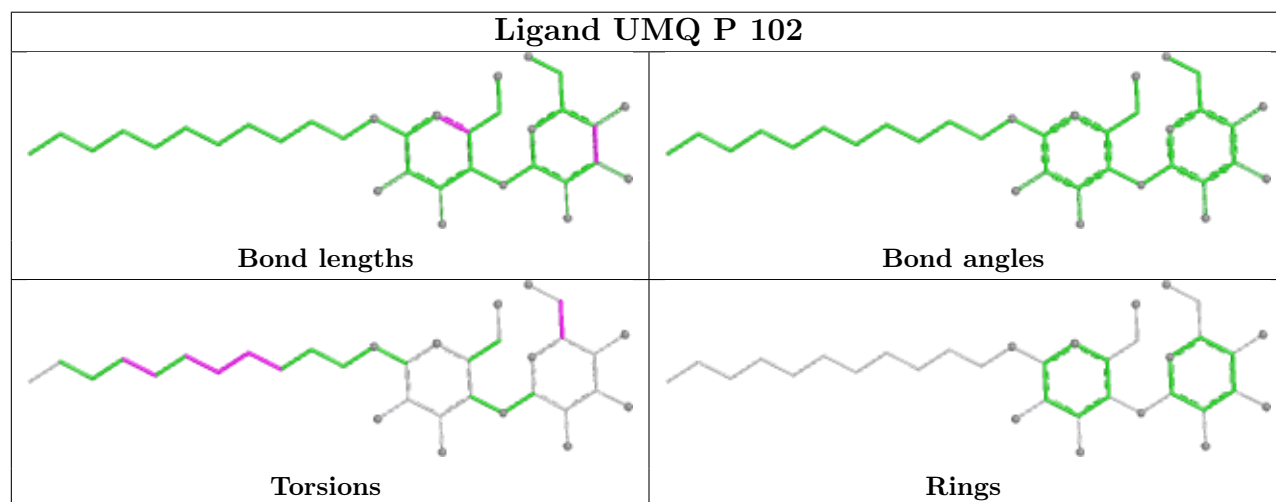
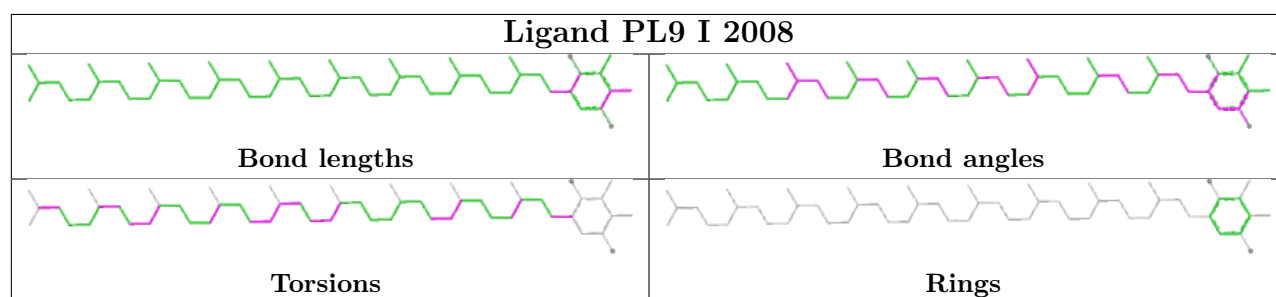
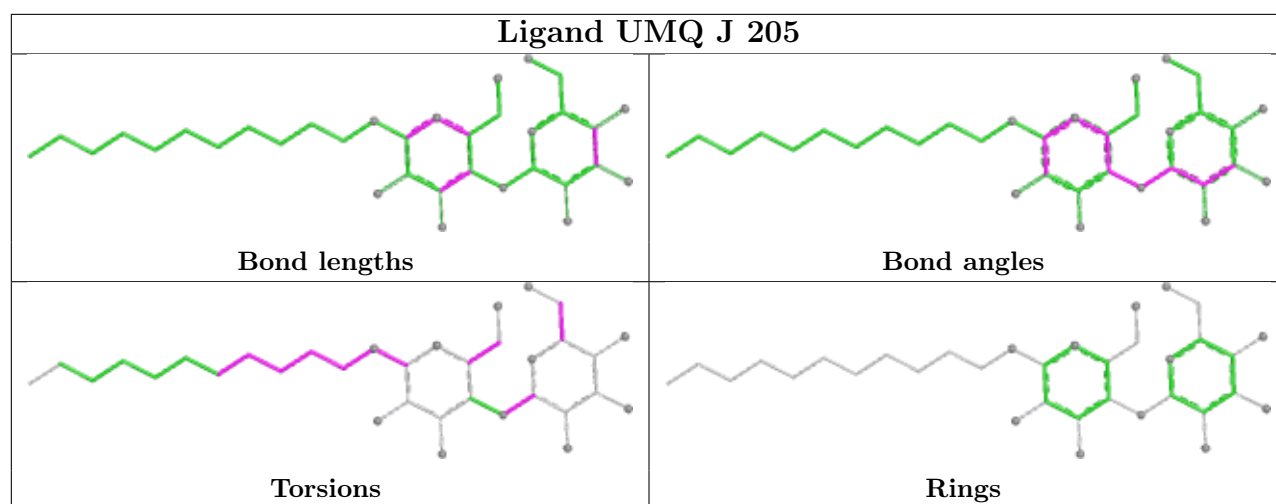
Ligand PGT A 308	
	
Bond lengths	Bond angles
	
Torsions	Rings

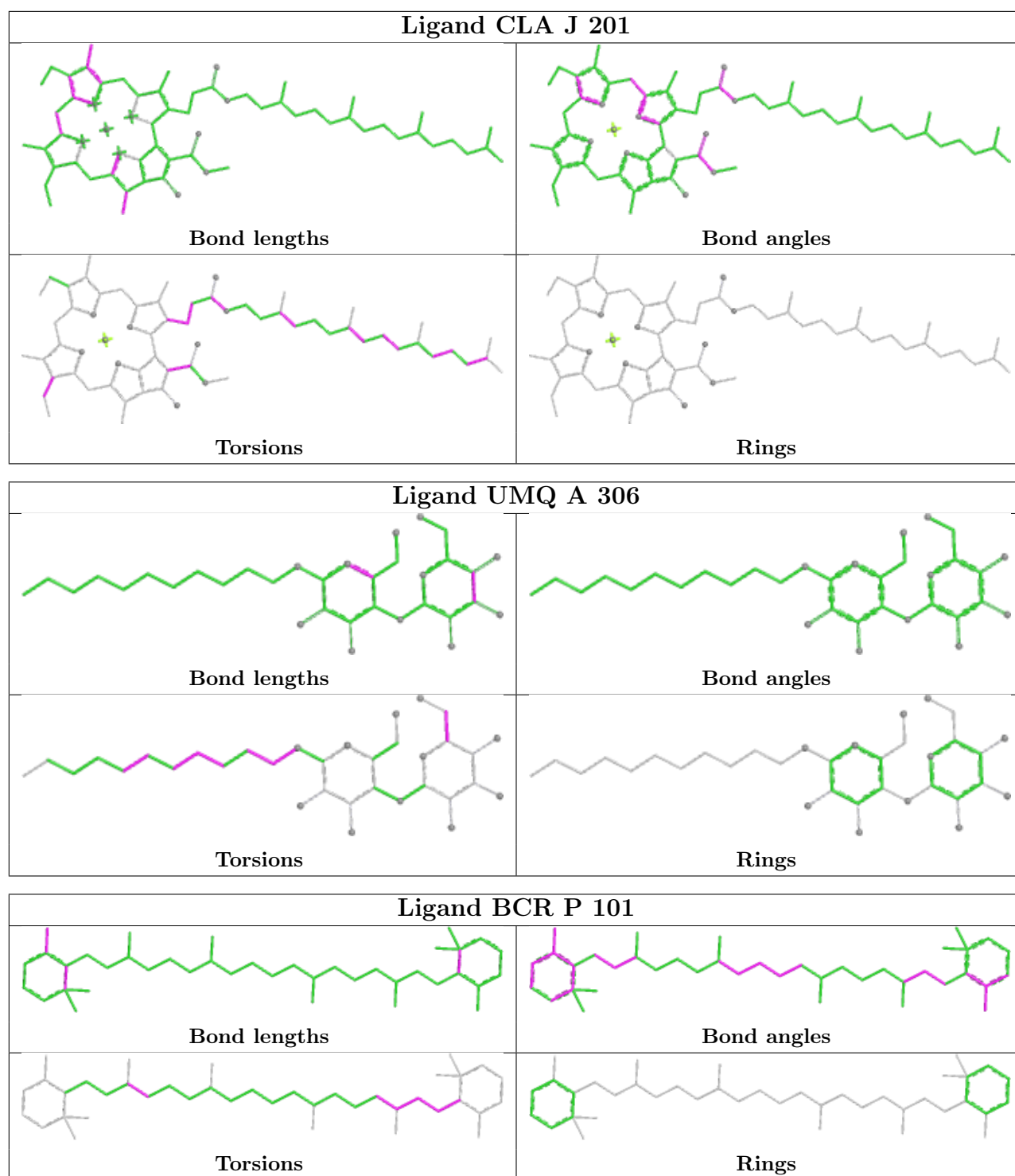
Ligand UMQ I 2005	
	
Bond lengths	Bond angles
	
Torsions	Rings

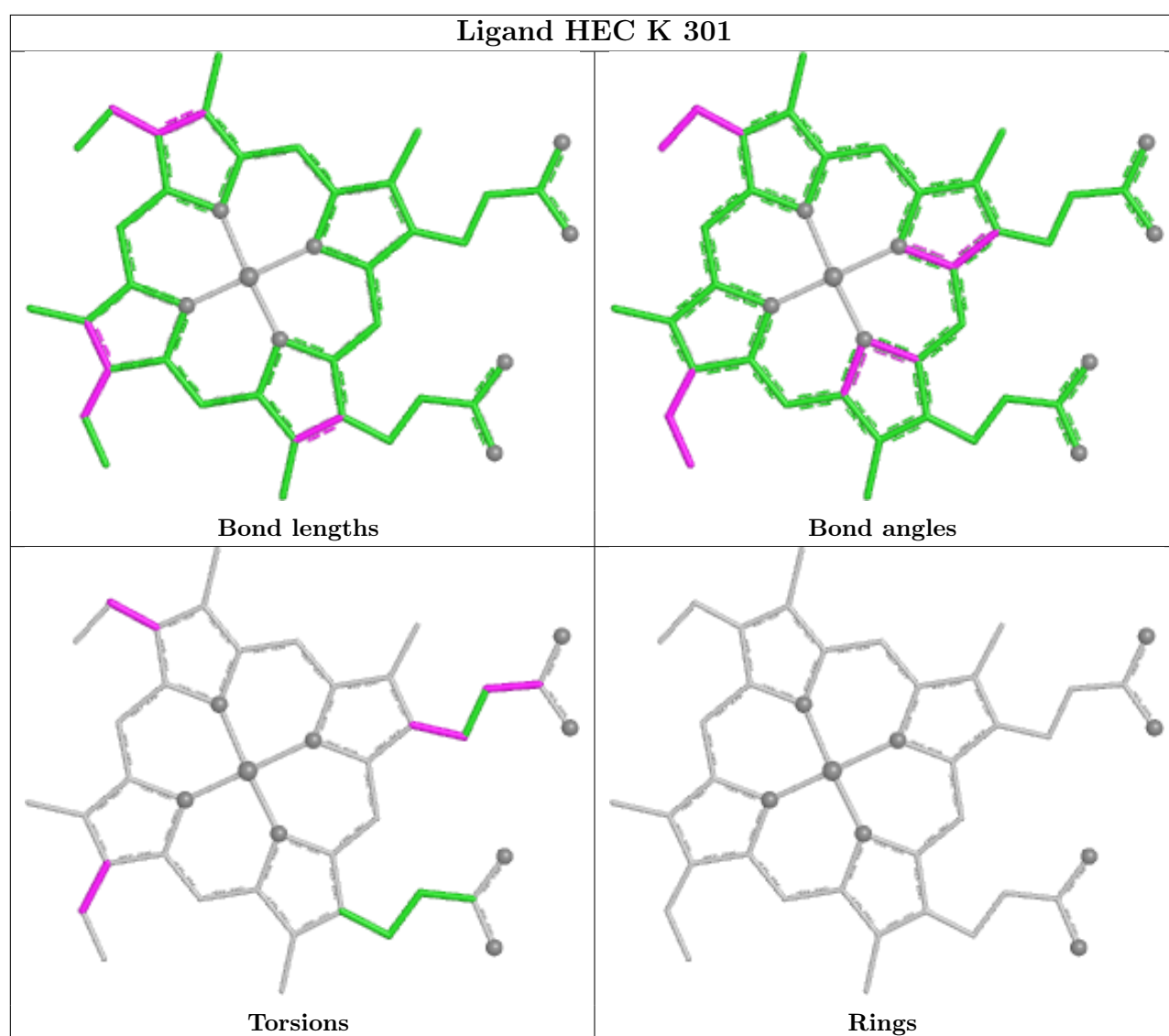
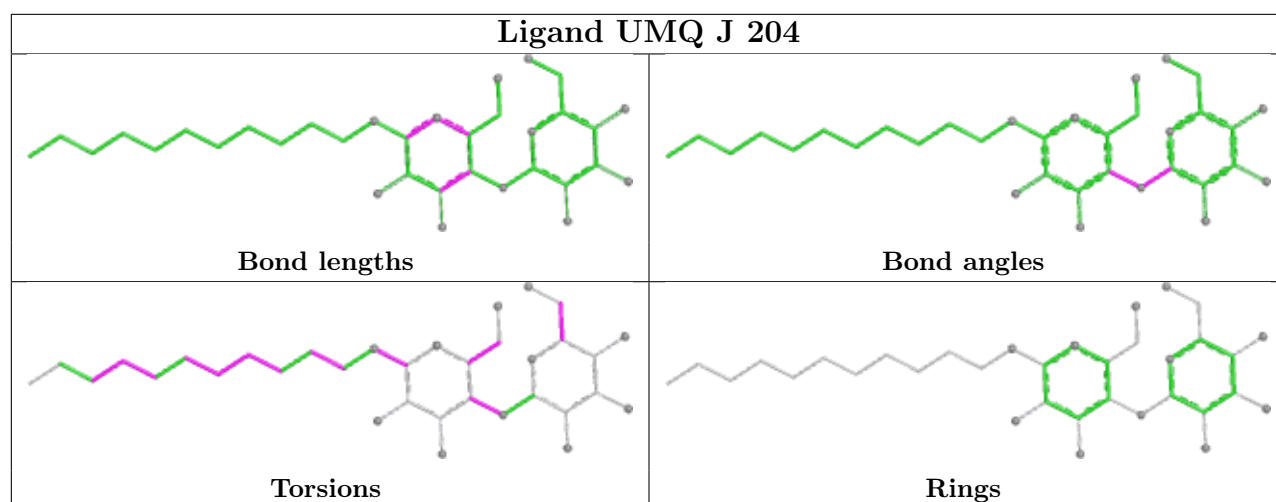


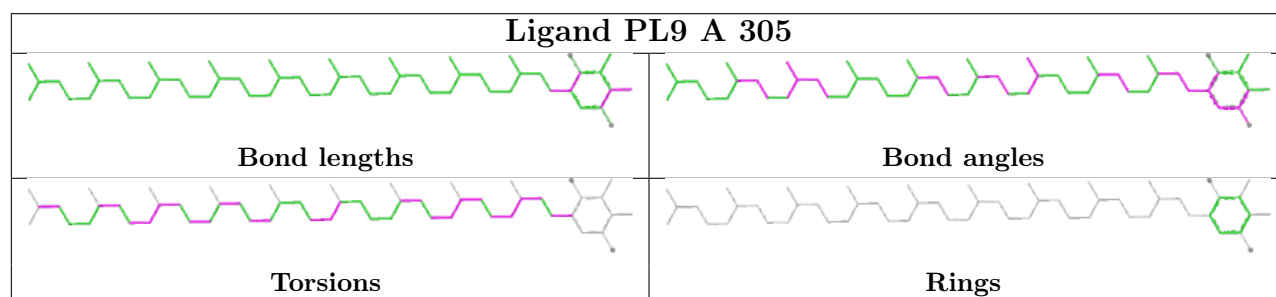
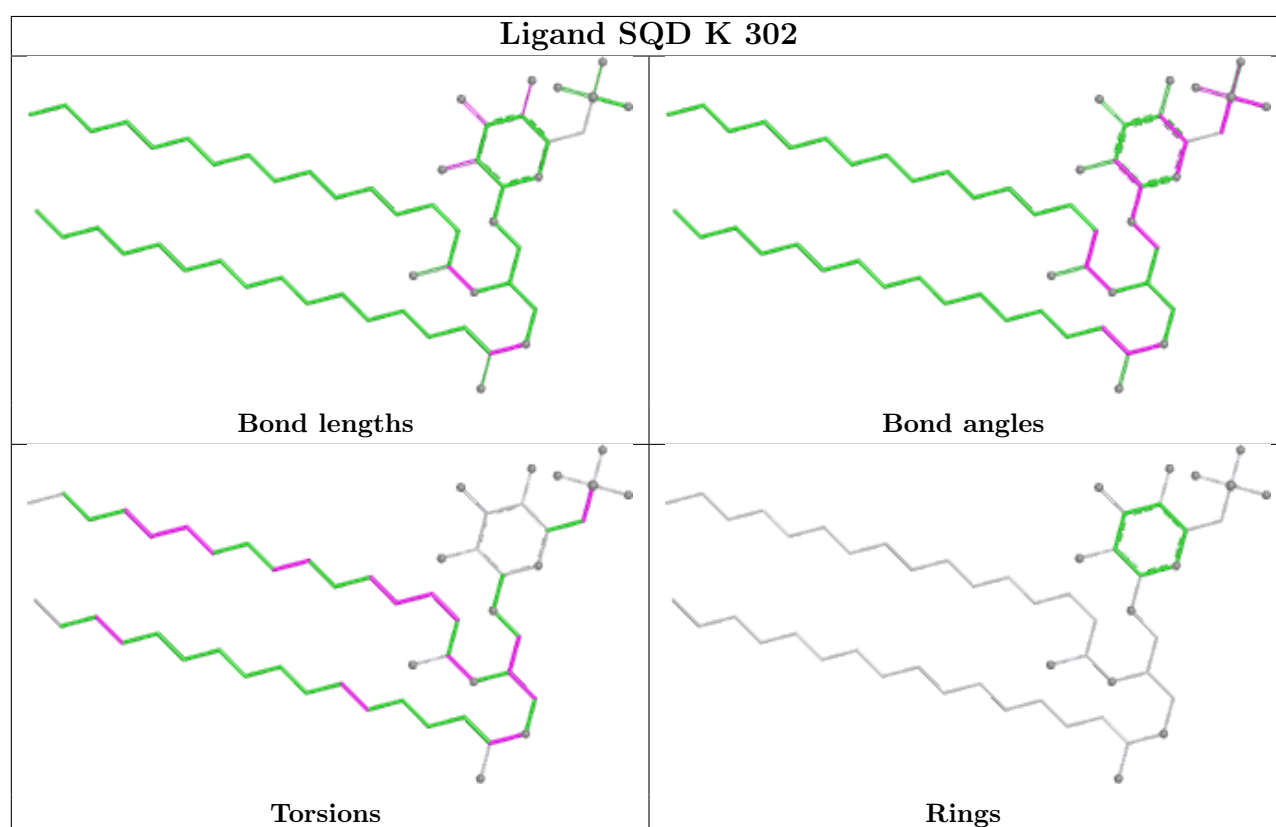
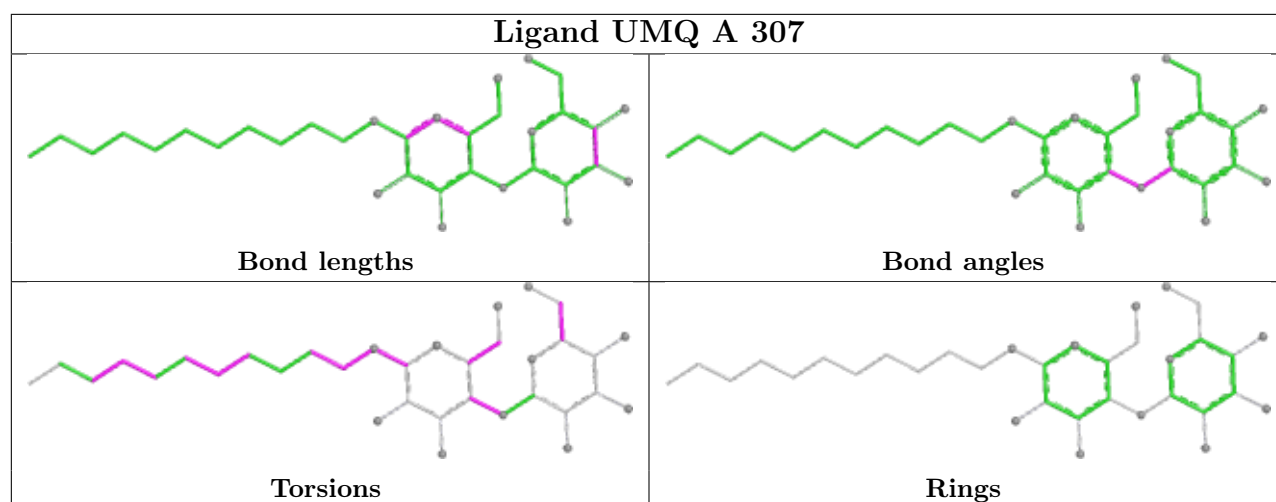


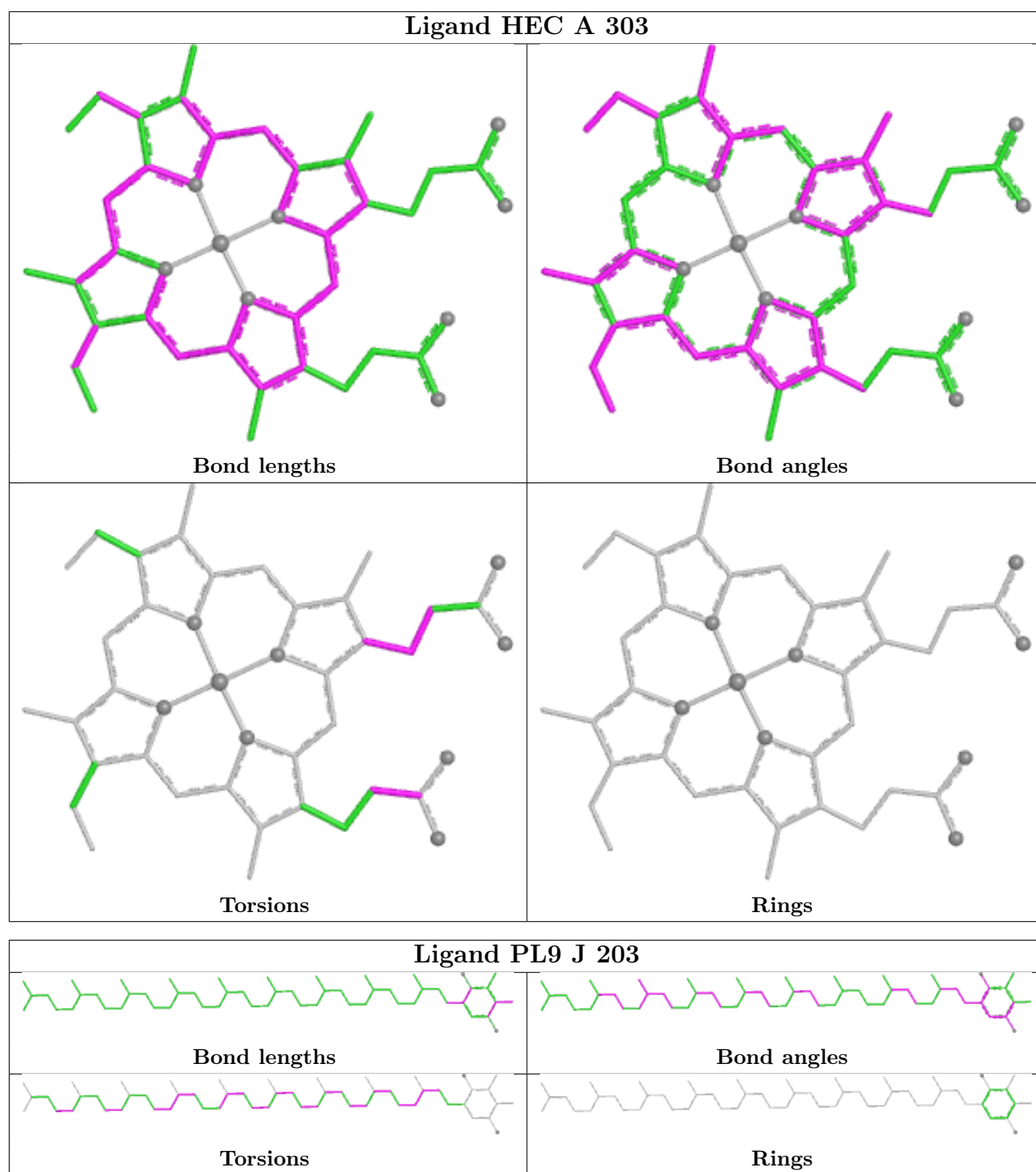


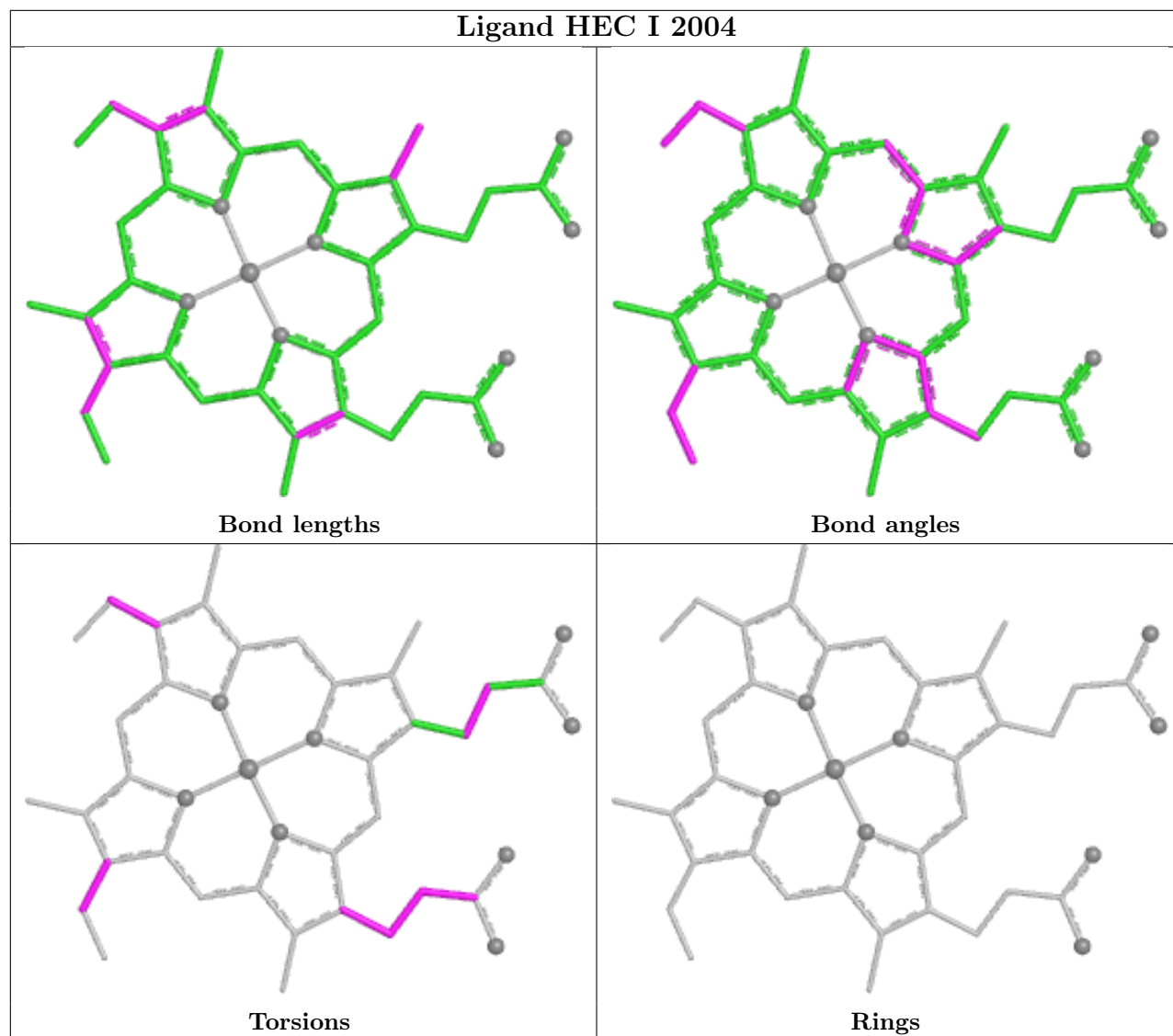




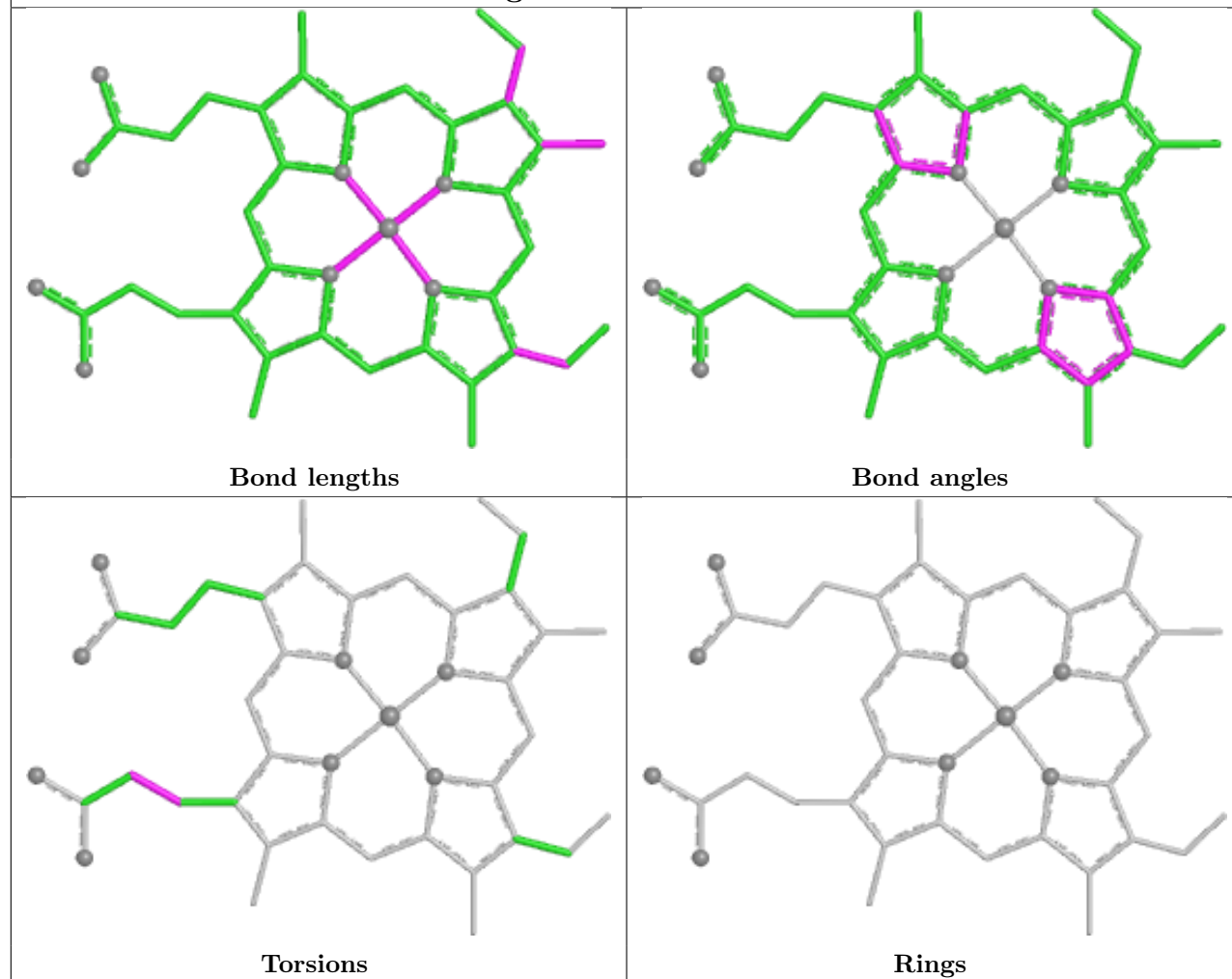




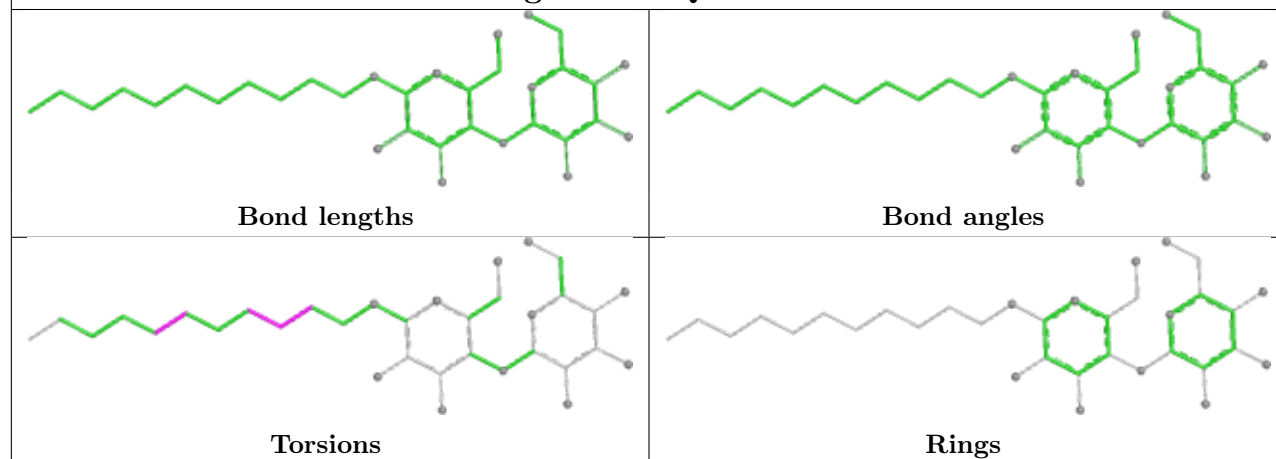


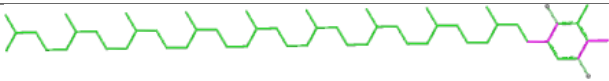
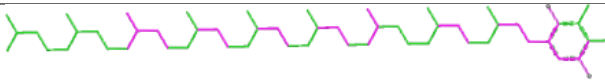
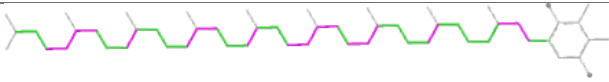
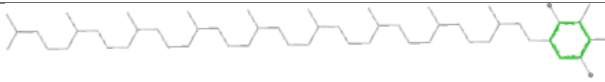


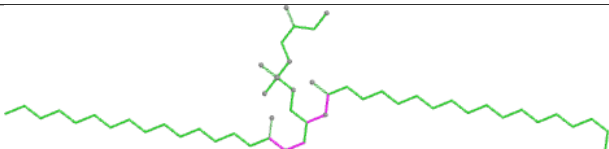
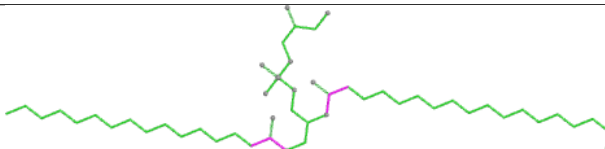
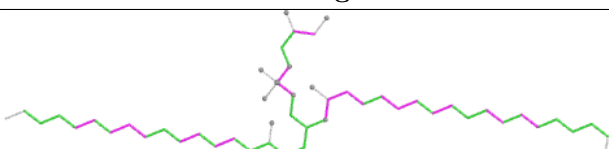
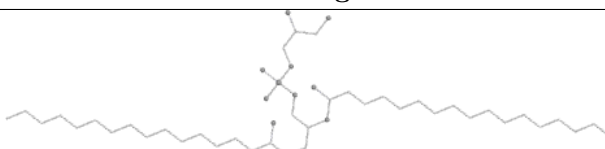
Ligand HEM I 2002

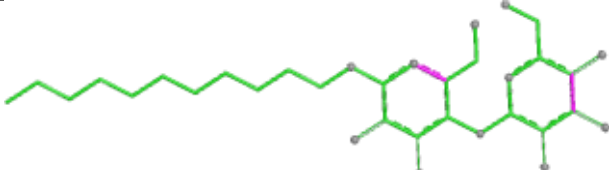
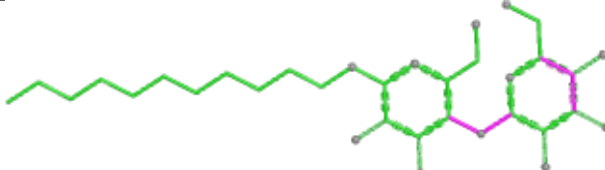
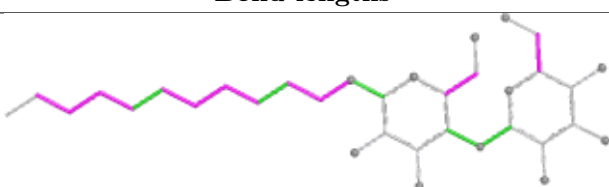
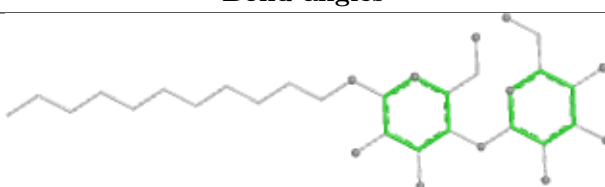


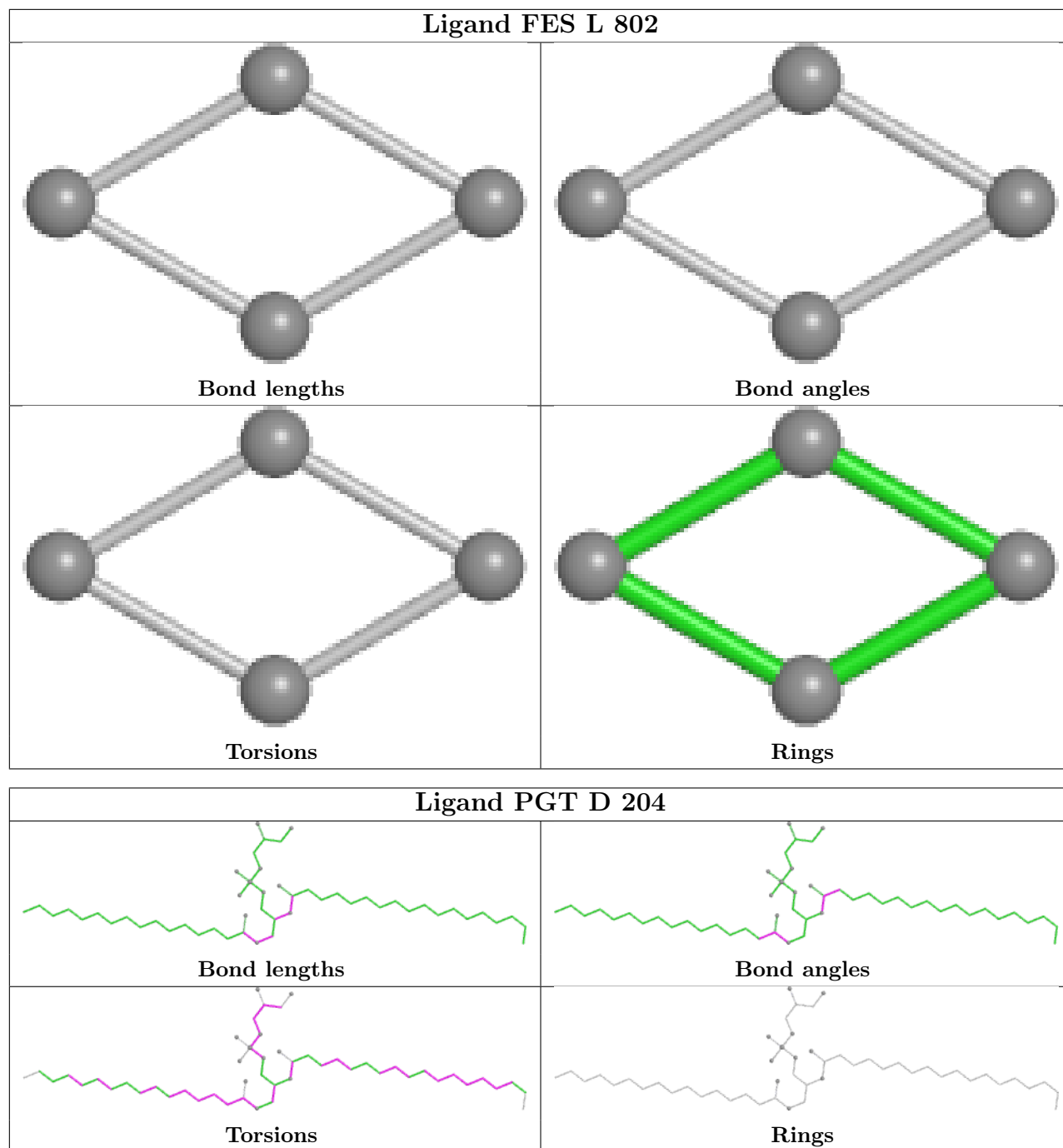
Ligand UMQ H 201

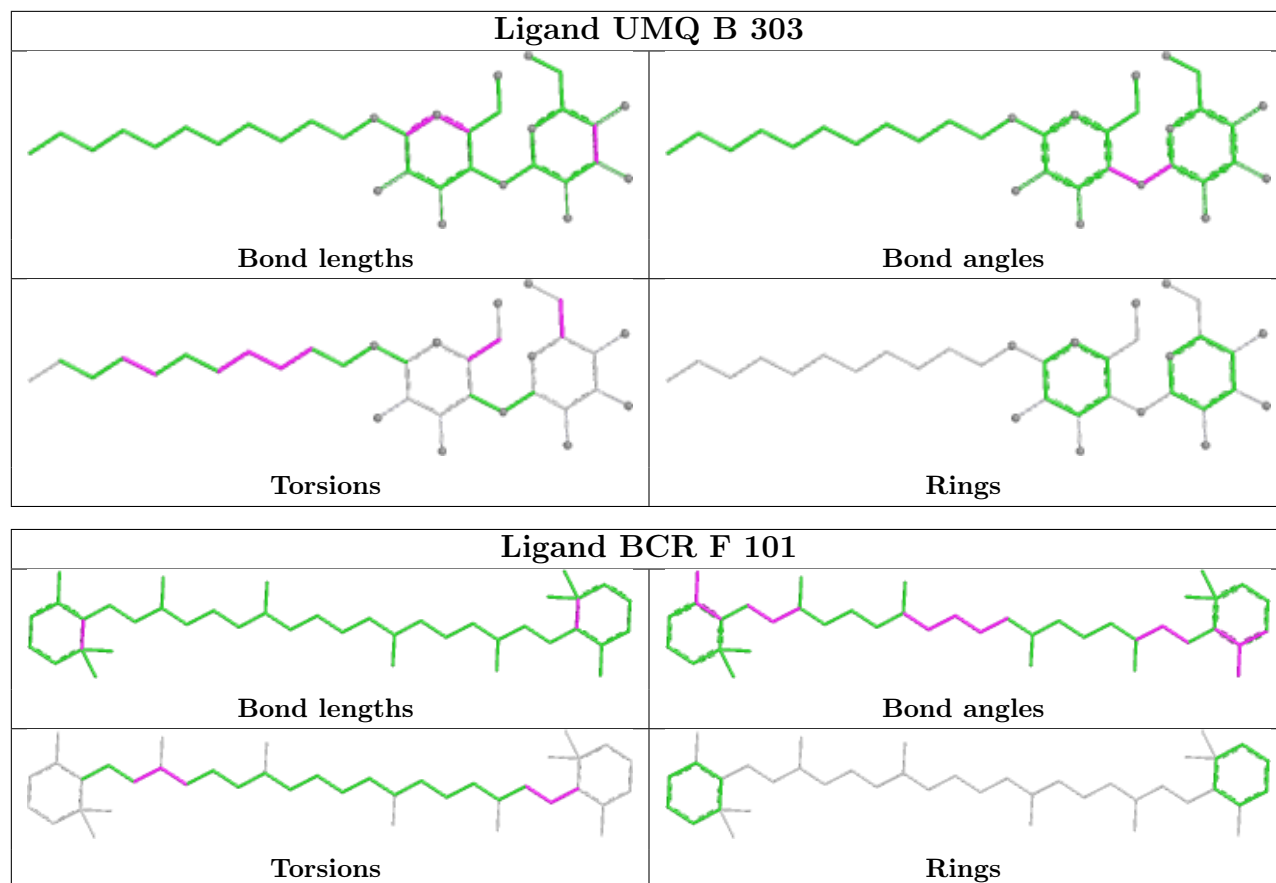


Ligand PL9 J 202	
 Bond lengths	 Bond angles
 Torsions	 Rings

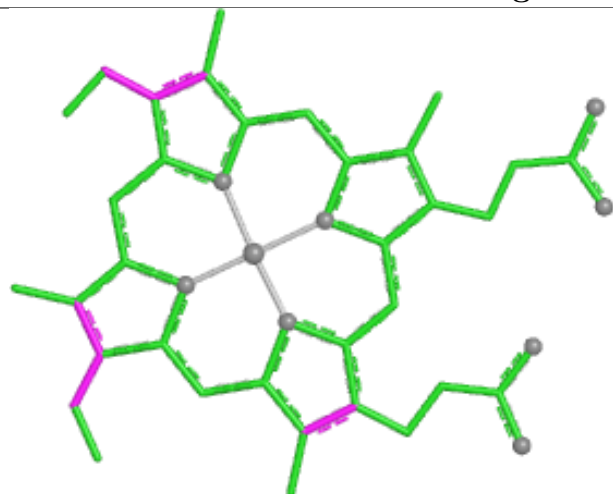
Ligand PGT I 2007	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand UMQ I 2006	
 Bond lengths	 Bond angles
 Torsions	 Rings

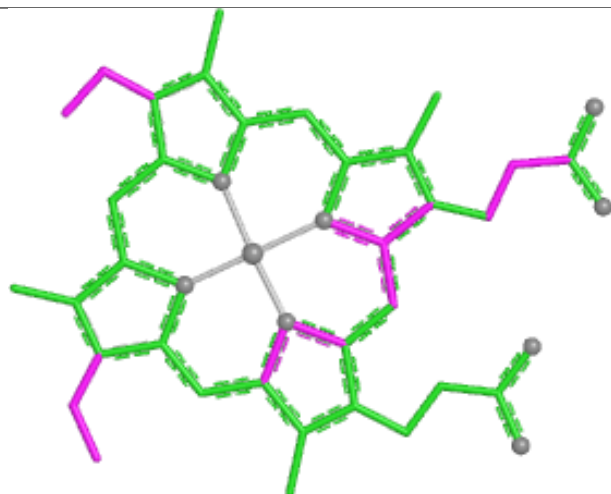




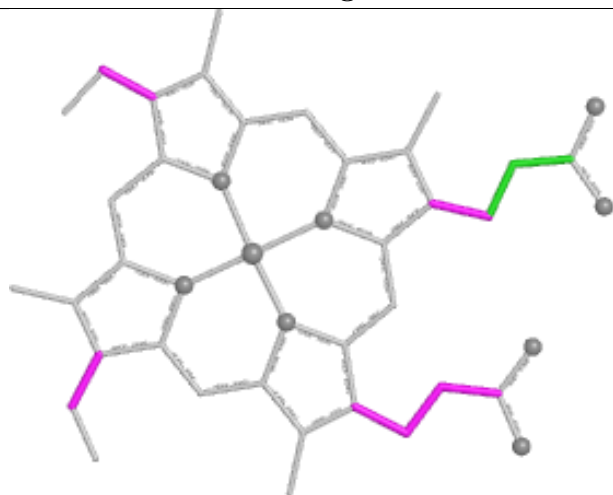
Ligand HEC C 301



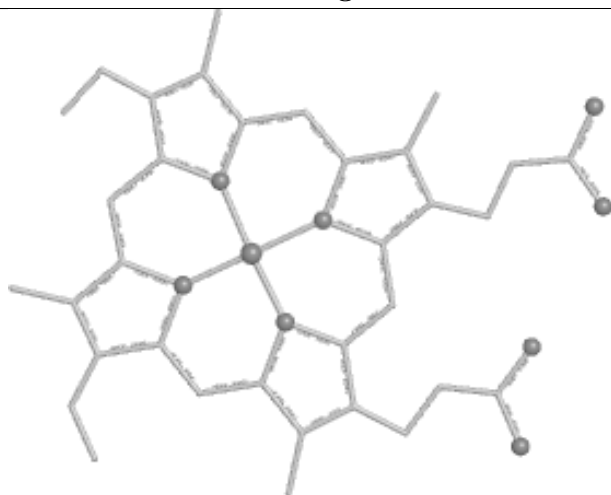
Bond lengths



Bond angles

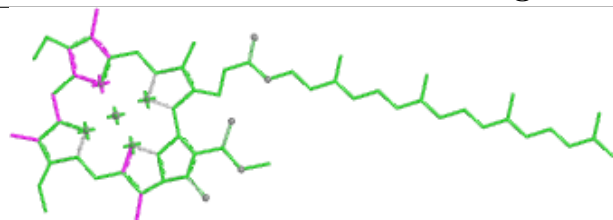


Torsions

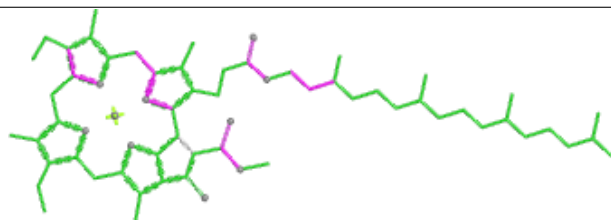


Rings

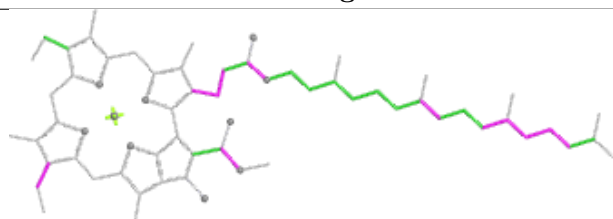
Ligand CLA A 304



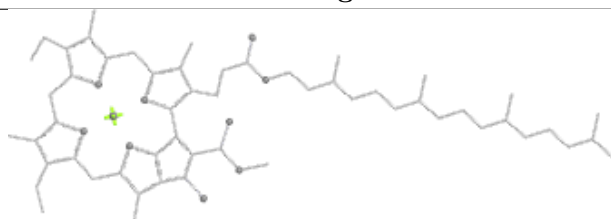
Bond lengths



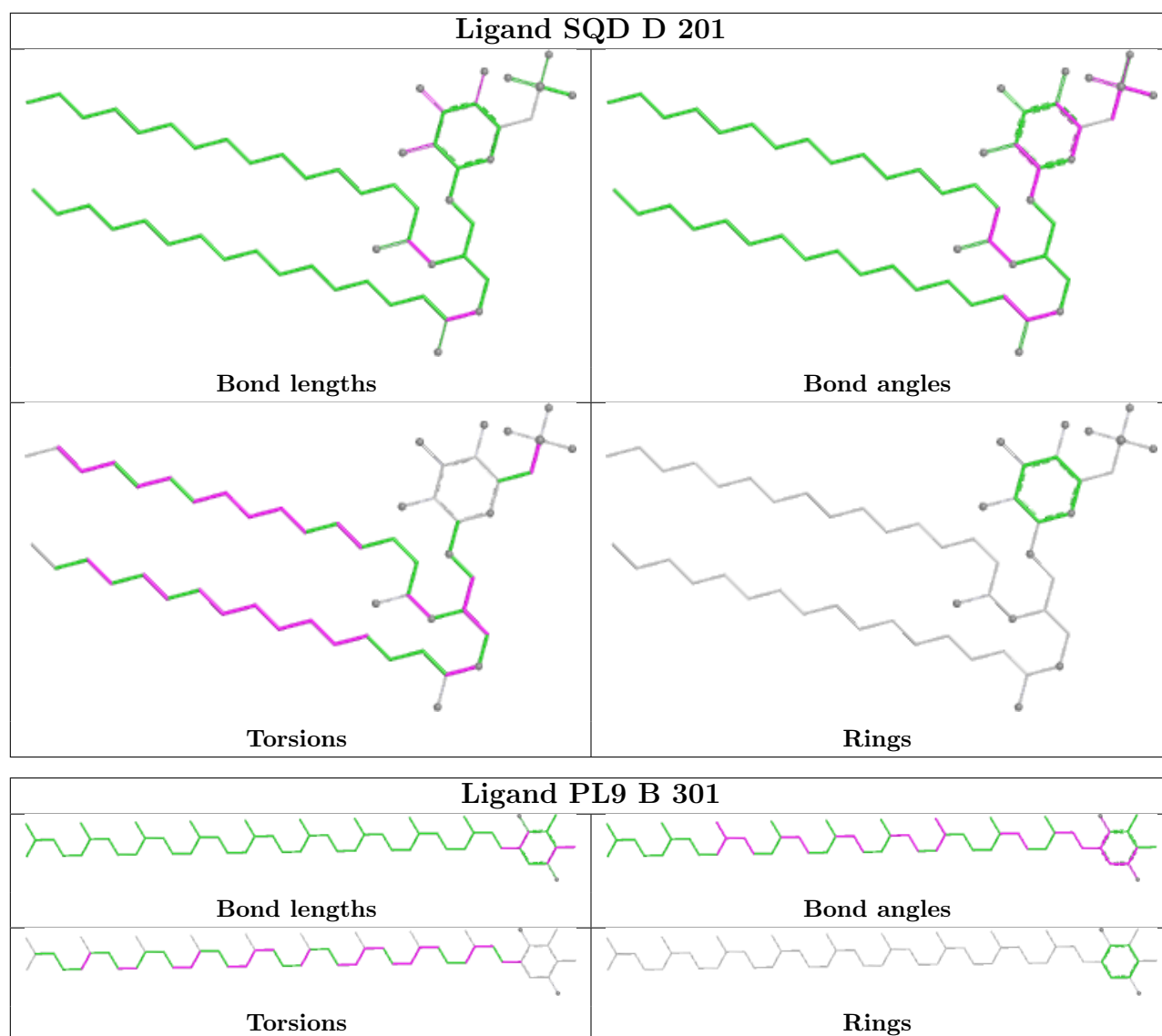
Bond angles

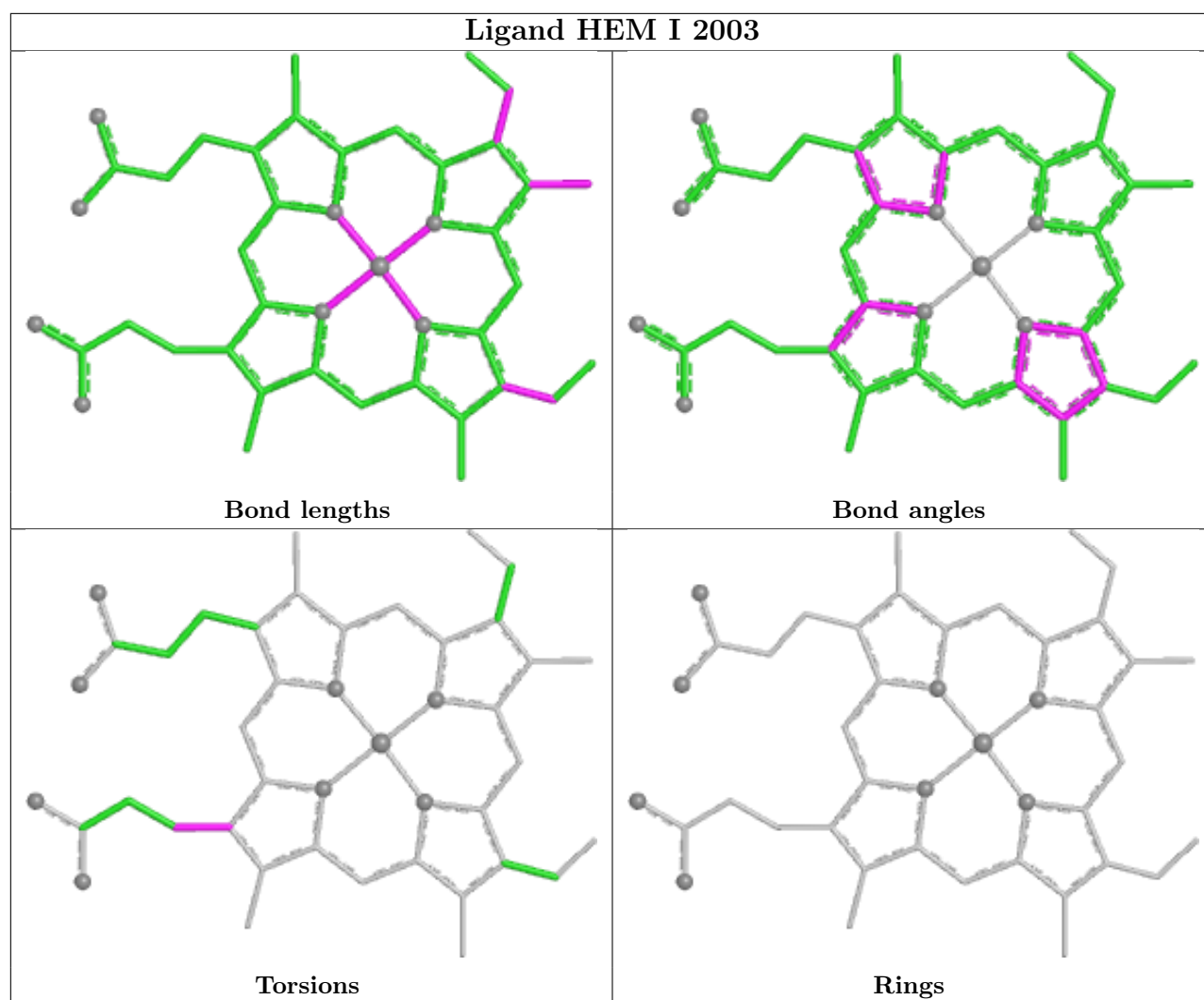


Torsions



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.

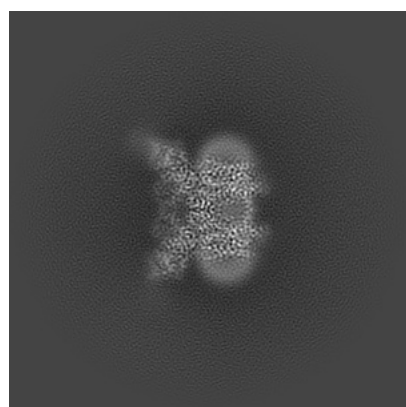
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14123. These allow visual inspection of the internal detail of the map and identification of artifacts.

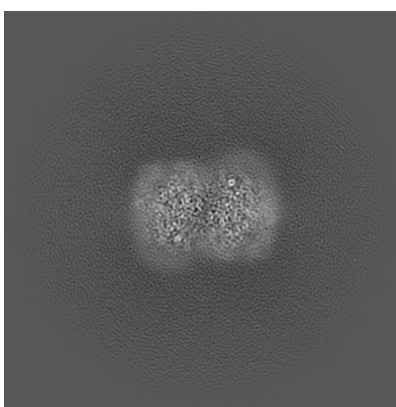
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

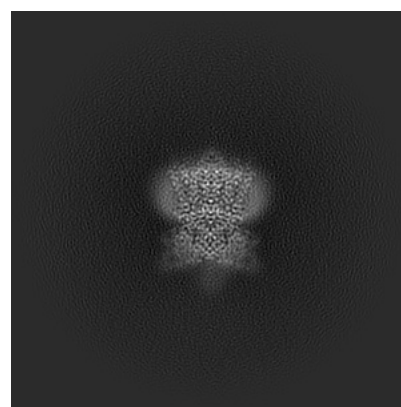
6.1.1 Primary map



X



Y

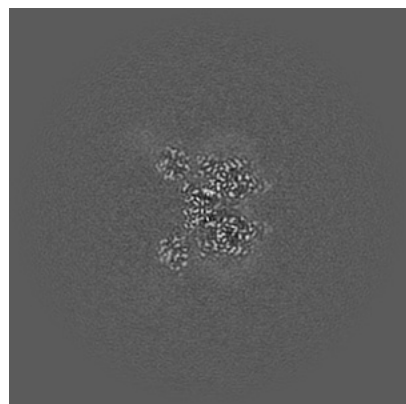


Z

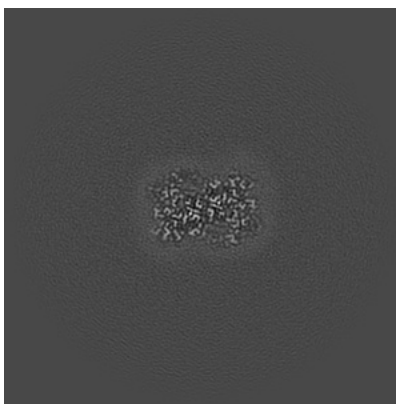
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

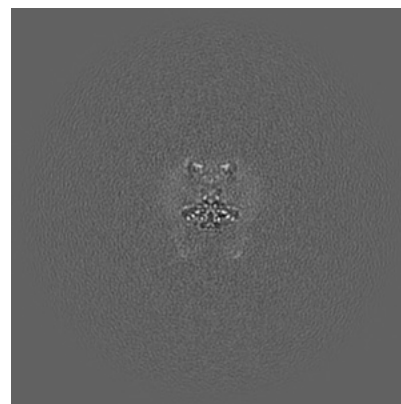
6.2.1 Primary map



X Index: 200



Y Index: 200

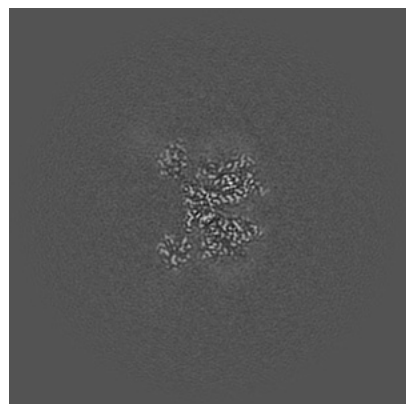


Z Index: 200

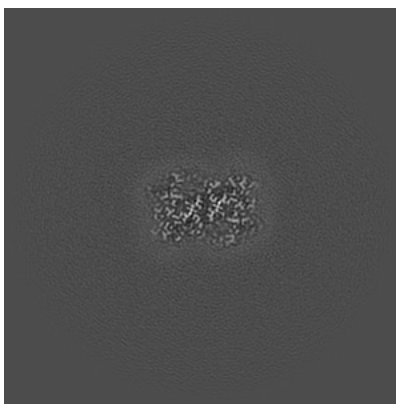
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

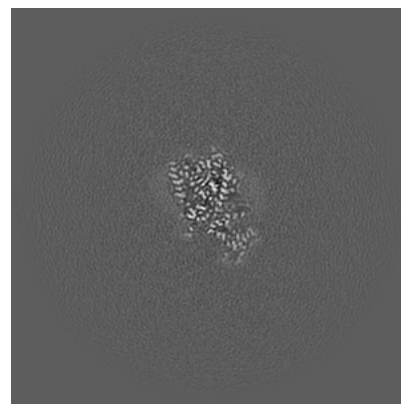
6.3.1 Primary map



X Index: 196



Y Index: 199

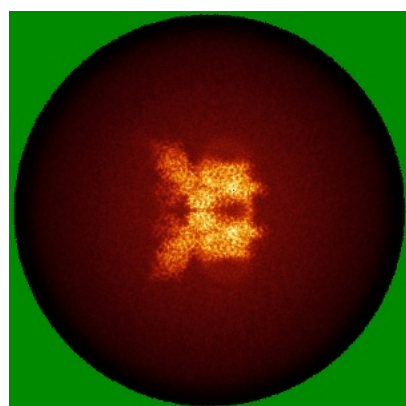


Z Index: 181

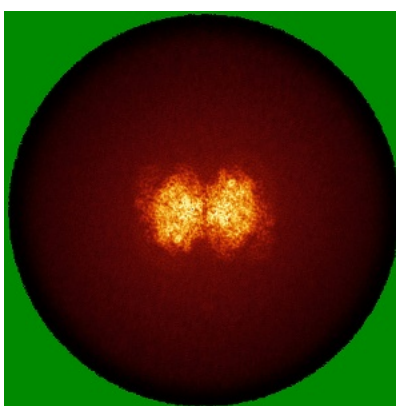
The images above show the largest variance slices of the map in three orthogonal directions.

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

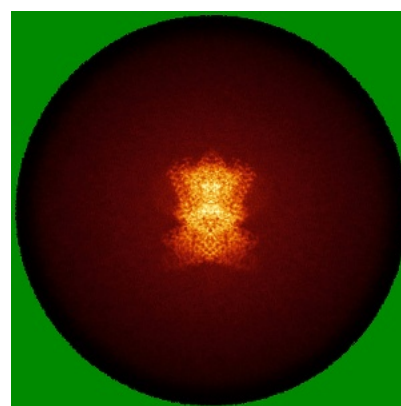
6.4.1 Primary map



X



Y

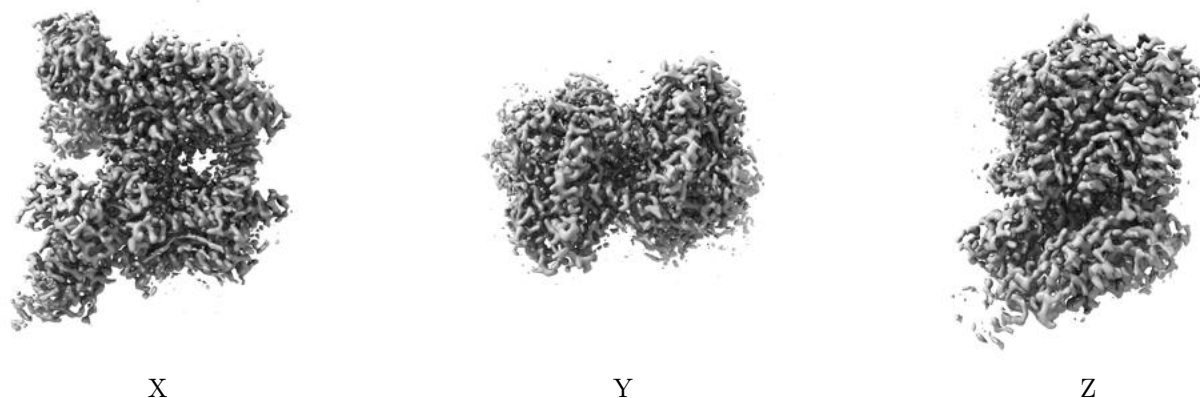


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

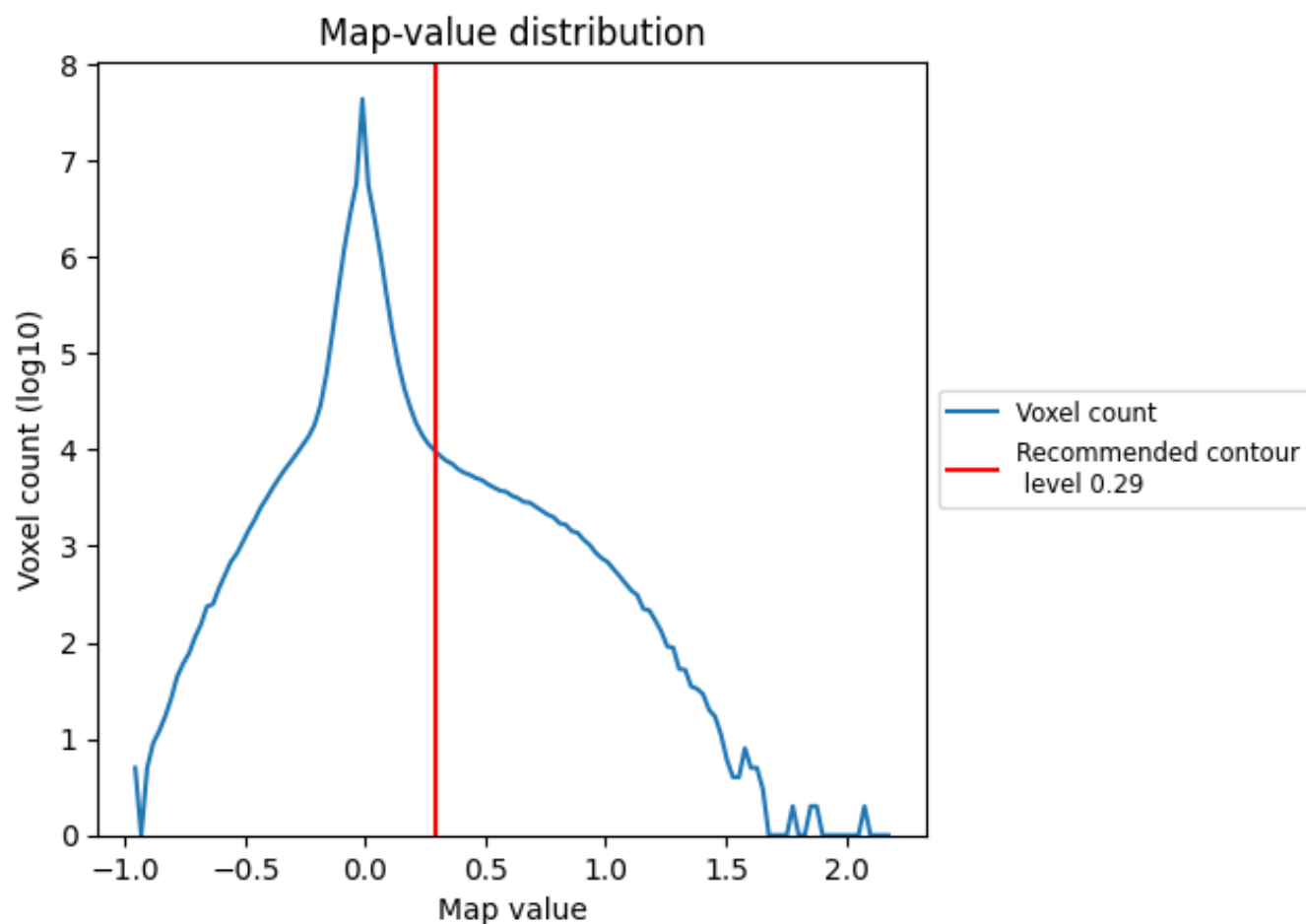
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

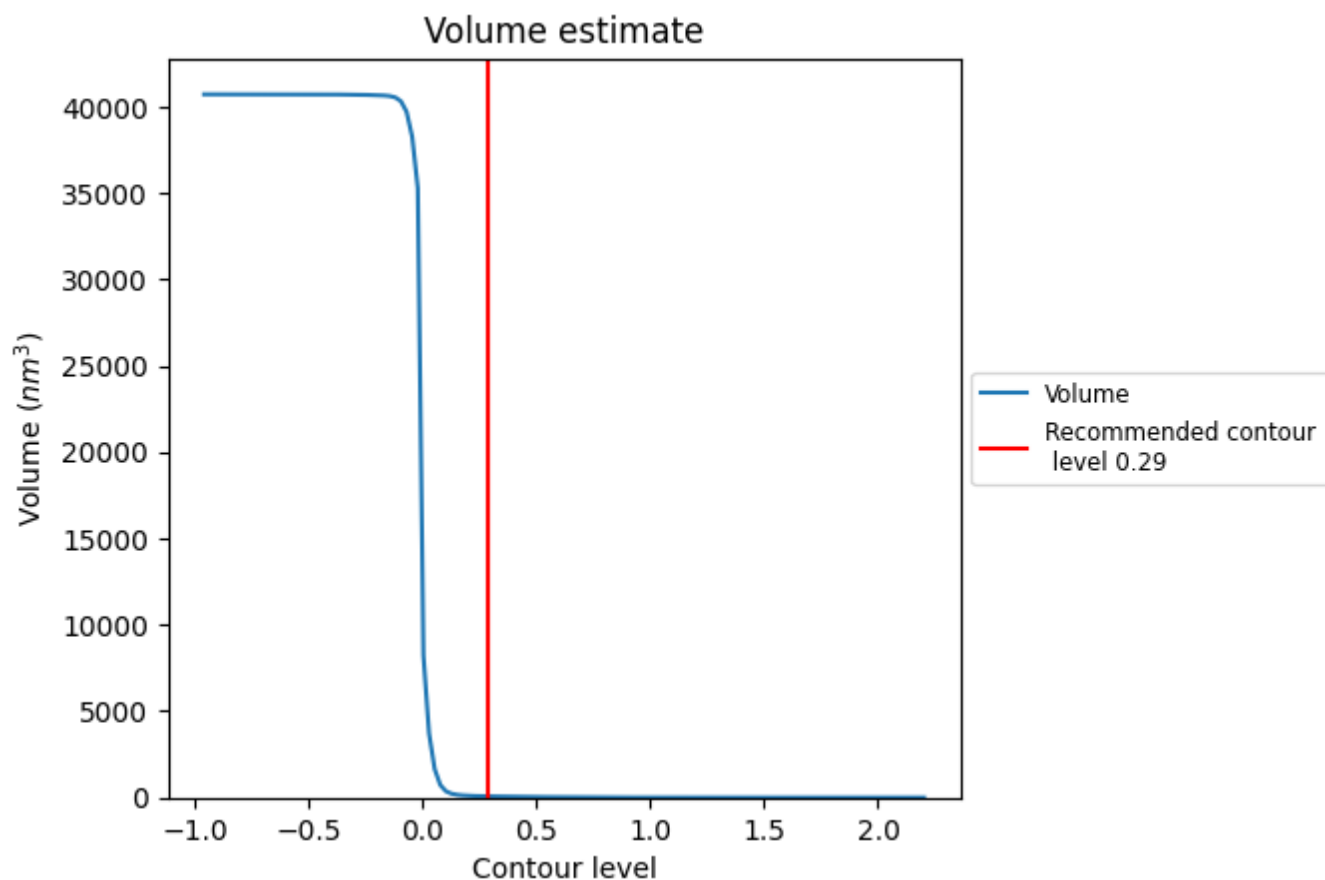
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

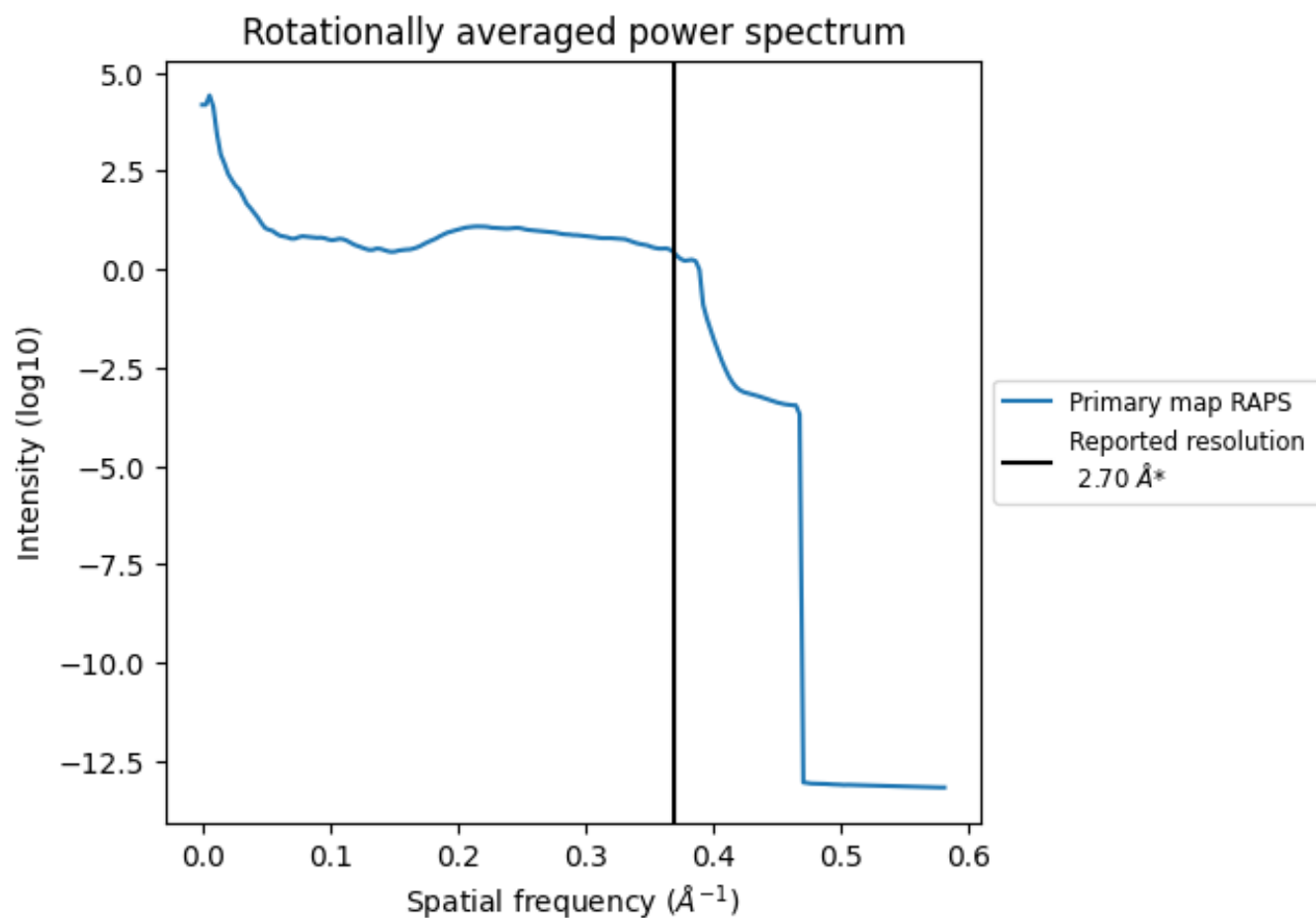
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 70 nm^3 ; this corresponds to an approximate mass of 63 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 ⓘ

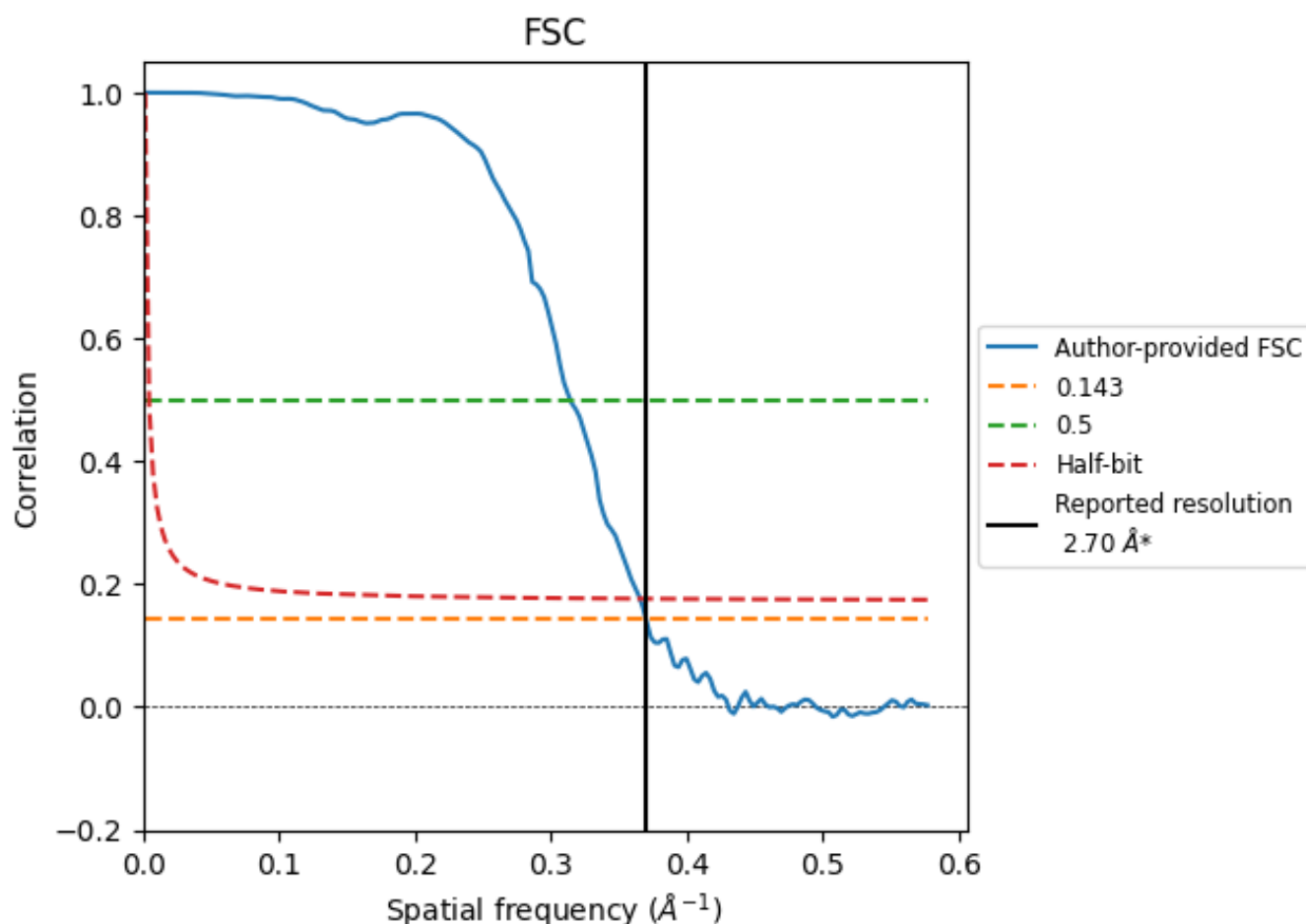


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

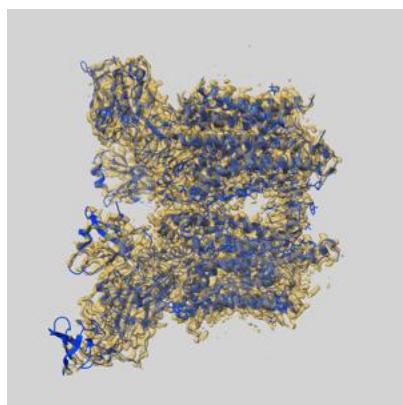
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	3.18	2.74
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

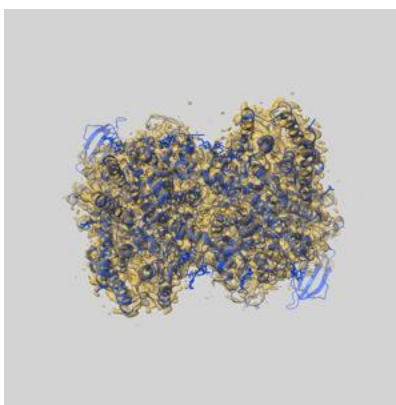
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14123 and PDB model 7QRM. Per-residue inclusion information can be found in section [3](#) on page [13](#).

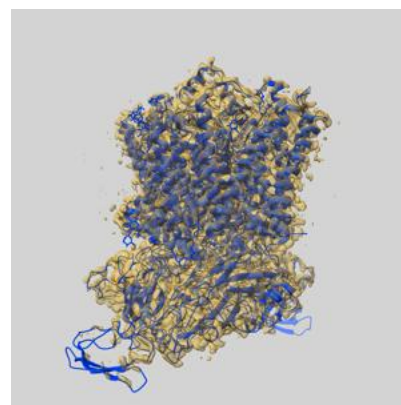
9.1 Map-model overlay [i](#)



X



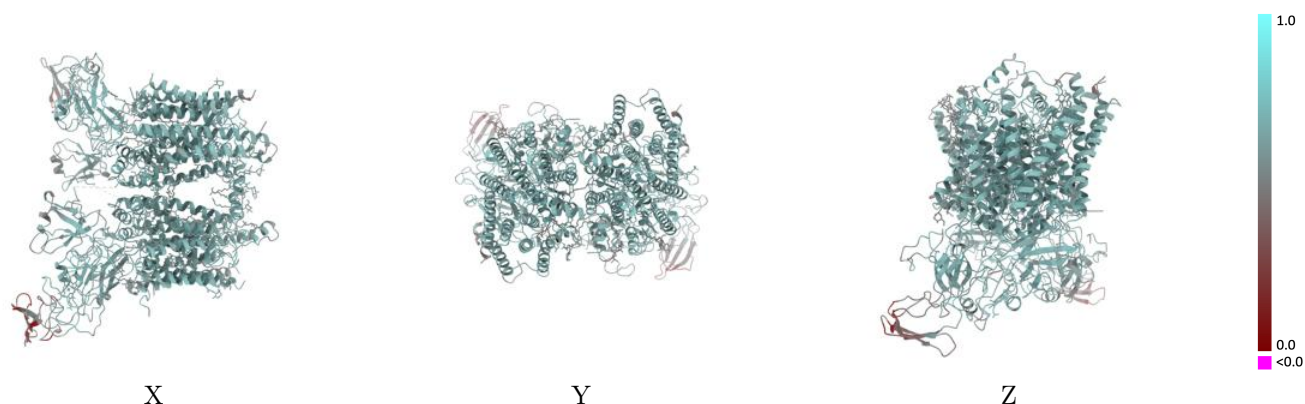
Y



Z

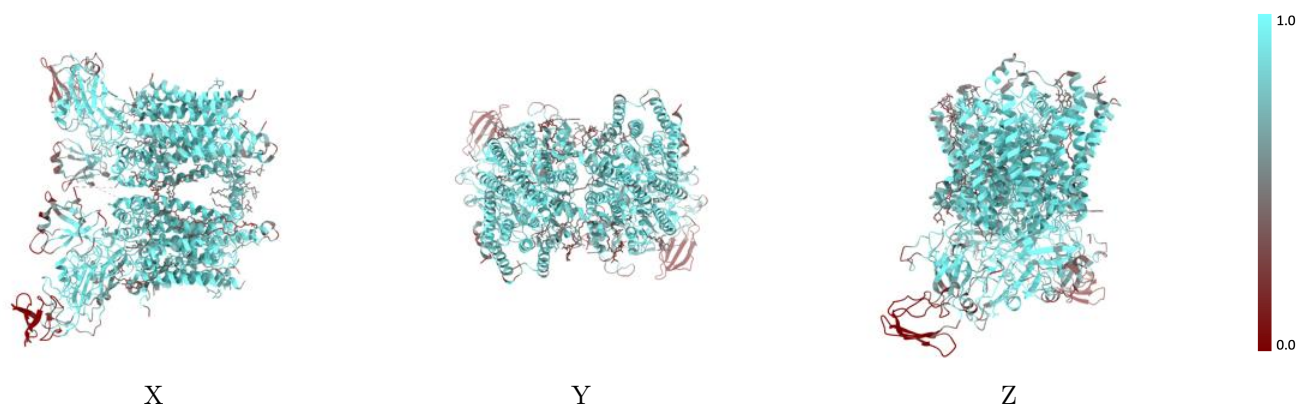
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



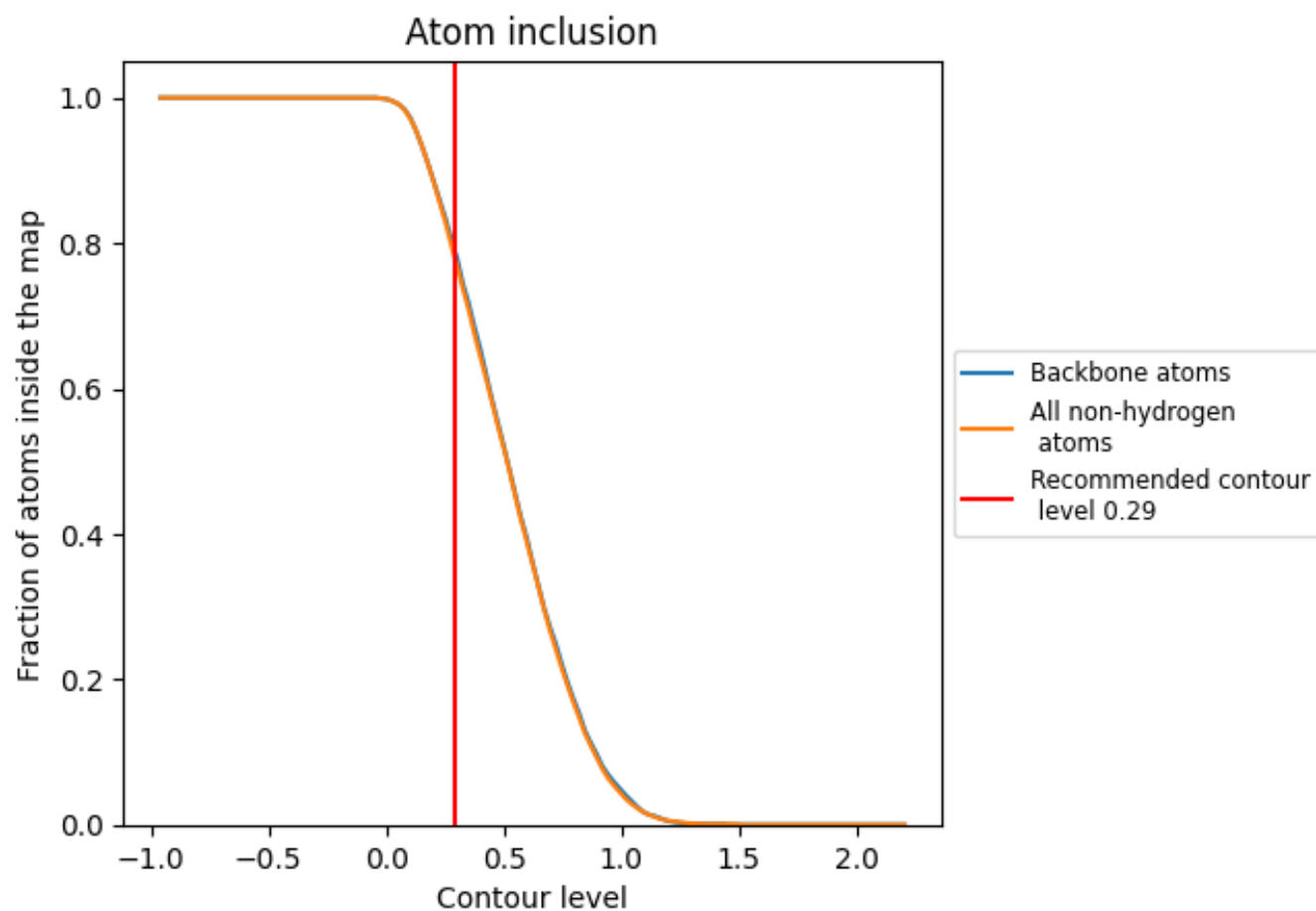
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.29).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.6170
A	0.8970	0.6530
B	0.8330	0.6280
C	0.6780	0.5800
D	0.6930	0.6040
E	0.7750	0.6100
F	0.8000	0.6200
G	0.9090	0.6330
H	0.9040	0.6470
I	0.8850	0.6500
J	0.8140	0.6260
K	0.6940	0.5840
L	0.6980	0.6020
M	0.7380	0.6110
N	0.8040	0.6090
O	0.9340	0.6500
P	0.8730	0.6400

1.0

0.0

<0.0