



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 PM UTC

PDB ID : 6ZI5 / pdb_00006zi5
Title : Ultrafast Structural Response to Charge Redistribution Within a Photosynthetic Reaction Centre - 300 ps (a) structure
Authors : Baath, P.; Dods, R.; Braenden, G.; Neutze, R.
Deposited on : 2020-06-24
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

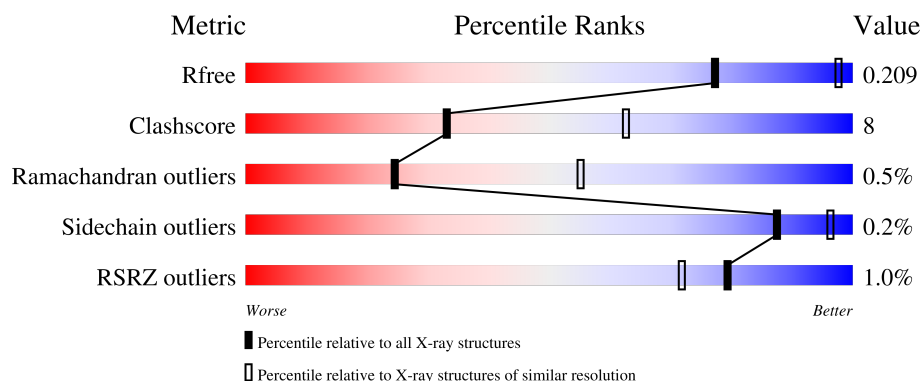
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	336	% 84% 15%
2	H	258	2% 85% 14%
3	L	273	% 78% 22%
4	M	323	% 88% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BCB	L	301[A]	X	-	-	-
10	BCB	L	301[B]	X	-	-	-
10	BCB	L	302[A]	X	-	-	-
10	BCB	L	302[B]	X	-	-	-
10	BCB	M	403	X	-	-	-
10	BCB	M	404[A]	X	-	-	-
10	BCB	M	404[B]	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 11266 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	332	Total	C	N	O	S	0	0	0
			2602	1640	466	478	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	0	0	0
			2018	1292	344	380	2			

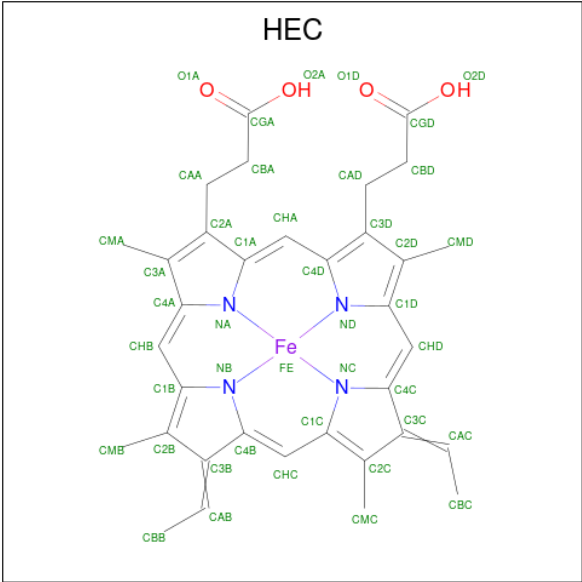
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	41	0
			2508	1678	409	413	8			

- Molecule 4 is a protein called Reaction center protein M chain.

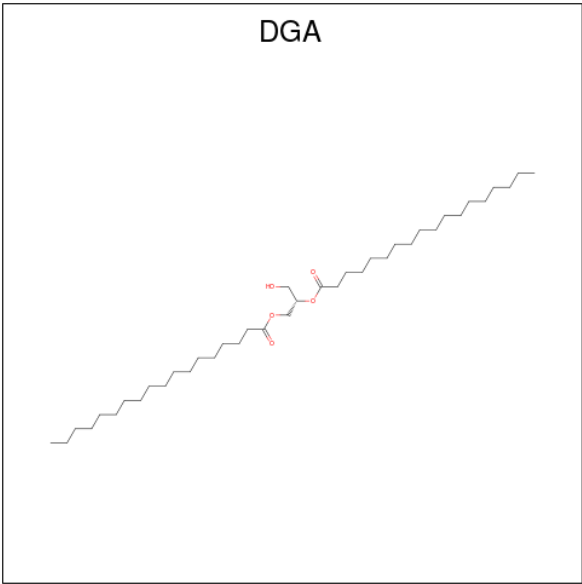
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	51	0
			2977	1983	491	490	13			

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



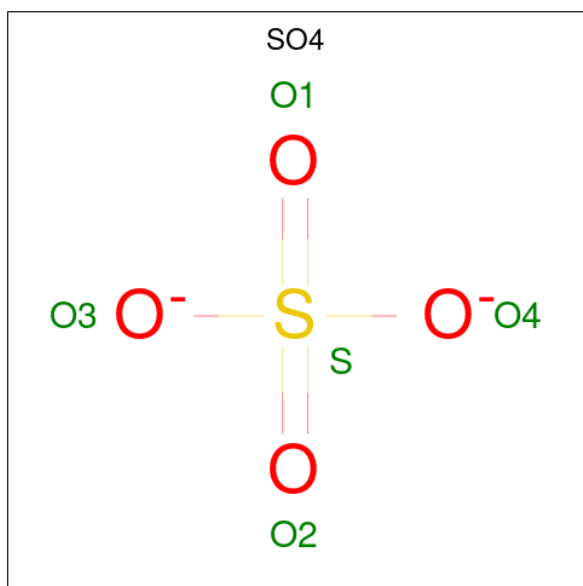
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



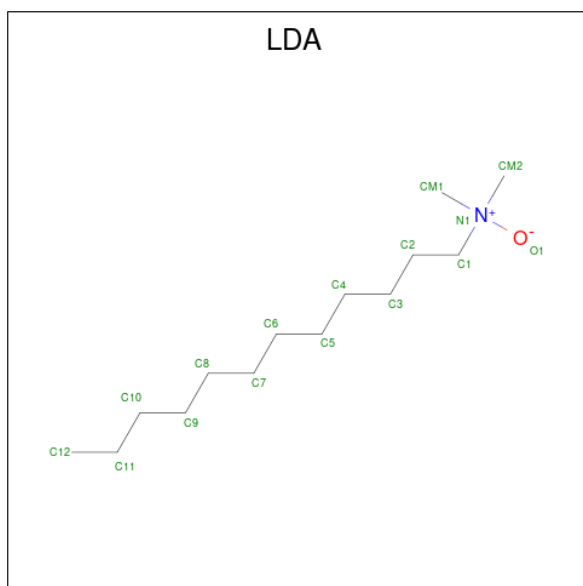
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

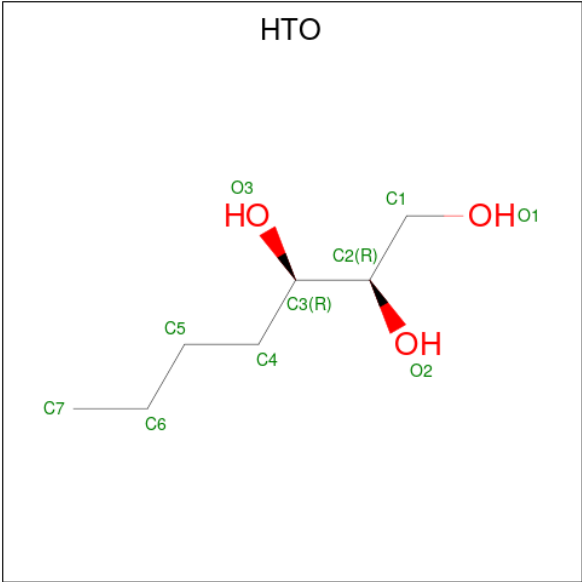
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



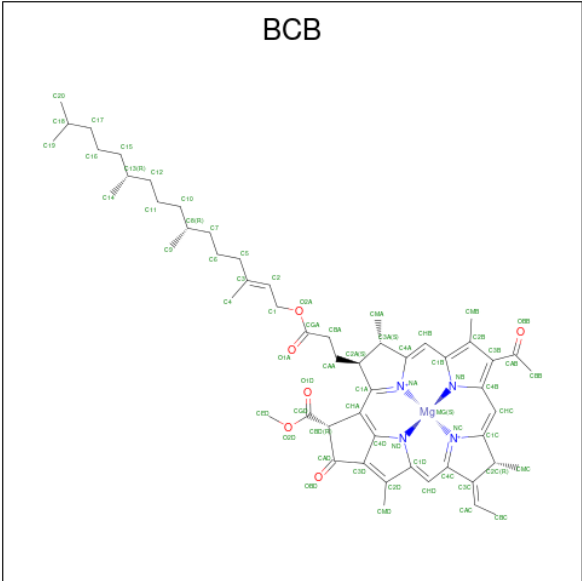
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	O		0	0
			10	7	3			
9	L	1	Total	C	O		0	0
			10	7	3			

- Molecule 10 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: $C_{55}H_{72}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



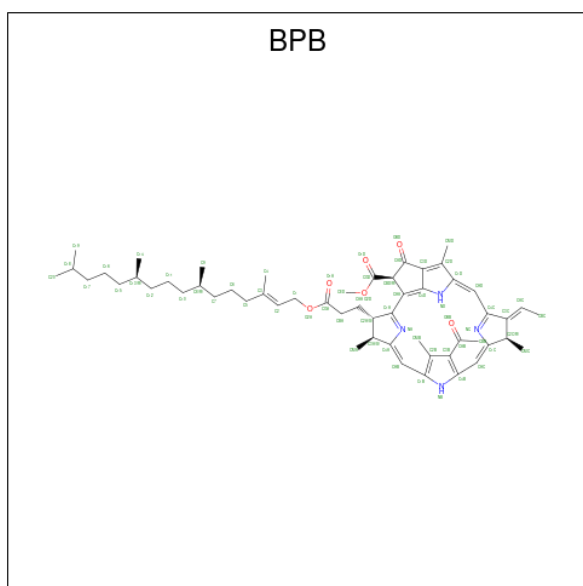
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	L	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		
10	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
10	M	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		

- Molecule 11 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

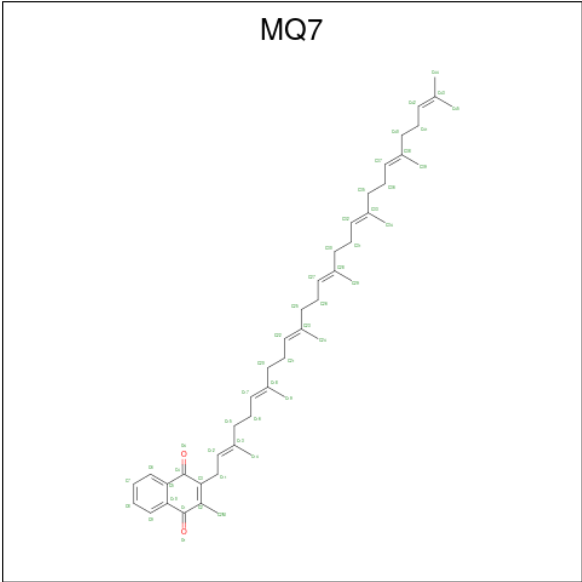


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	1
			130	110	8	12		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is FE (III) ION (CCD ID: FE) (formula: Fe).

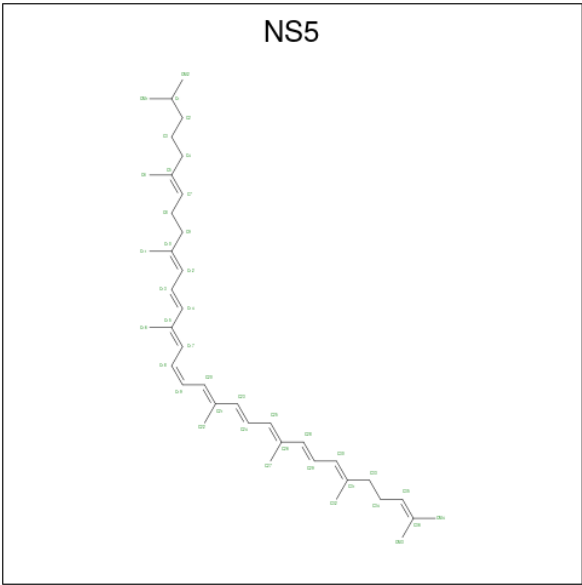
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	1
			2	2		

- Molecule 13 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C	O	0
			96	92	4	

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total	C		0
			40	40		

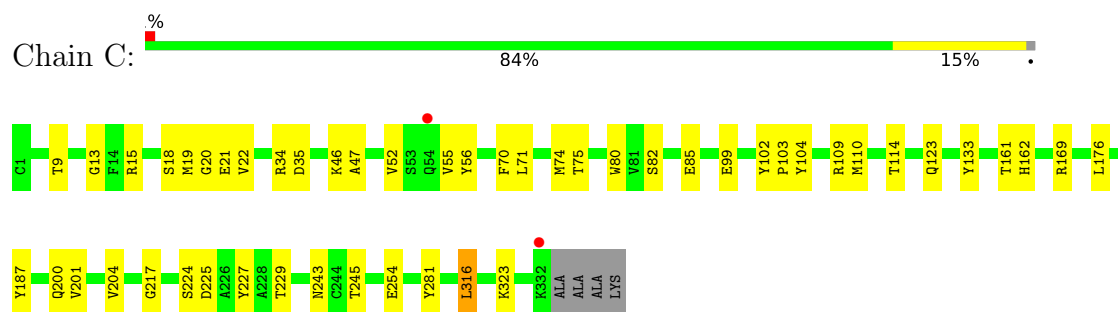
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	3	Total 3	O 3	0	0
15	H	2	Total 2	O 2	0	0
15	L	4	Total 4	O 4	0	0
15	M	4	Total 4	O 4	0	0

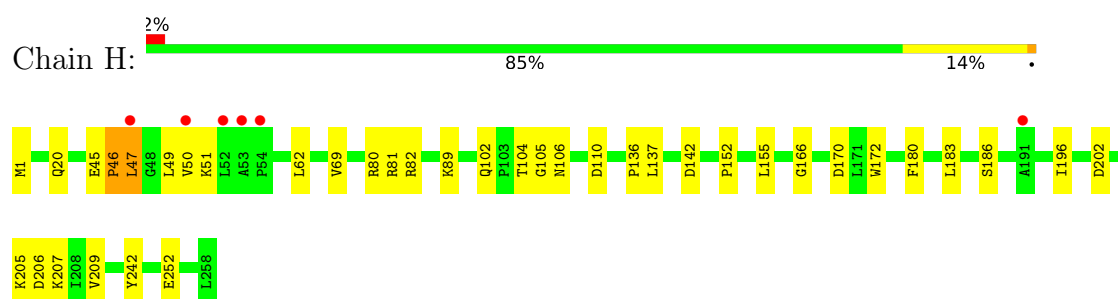
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

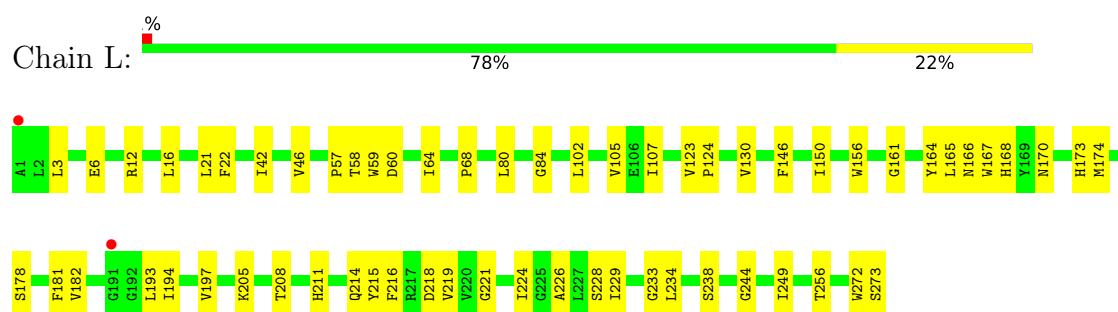
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



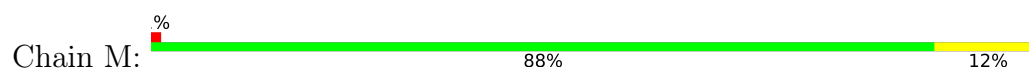
- Molecule 2: Reaction center protein H chain

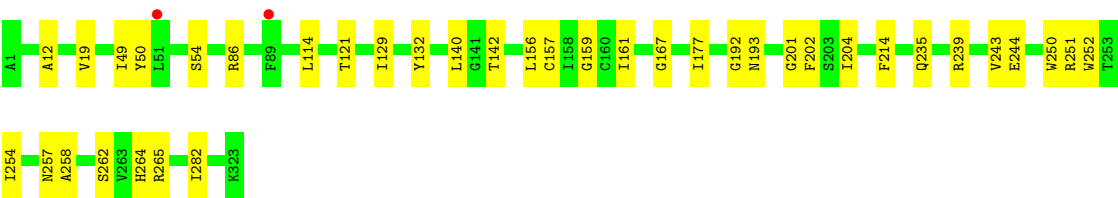


- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	226.40Å 226.40Å 113.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.75 – 2.80 37.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.75-2.80) 99.9 (37.75-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.8.01158, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.176 , 0.202 0.184 , 0.209	Depositor DCC
R_{free} test set	5696 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: HTO, DGA, LDA, BCB, NS5, BPB, FE, FME, HEC, MQ7, SO4

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	C	0.38	0/2669	0.60	0/3637
2	H	0.37	0/2055	0.58	0/2807
3	L	0.34	0/2612	0.54	0/3568
4	M	0.35	0/3101	0.52	0/4242
All	All	0.36	0/10437	0.56	0/14254

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2602	0	2578	51	0
2	H	2018	0	2020	39	0
3	L	2508	0	2390	51	0
4	M	2977	0	2832	35	0
5	C	172	0	120	3	0
6	C	37	0	58	0	0
7	C	5	0	0	0	0
7	H	20	0	0	1	0
7	M	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	48	0	93	2	0
8	L	16	0	31	1	0
9	H	10	0	16	0	0
9	L	10	0	16	0	0
10	L	264	0	288	14	0
10	M	198	0	216	7	0
11	L	130	0	148	8	0
11	M	65	0	74	5	0
12	M	2	0	0	0	0
13	M	96	0	128	3	0
14	M	40	0	60	4	0
15	C	3	0	0	0	0
15	H	2	0	0	0	0
15	L	4	0	0	0	0
15	M	4	0	0	0	0
All	All	11266	0	11068	175	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 8.

All (175) 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:C:13:GLY:CA	1:C:19:MET:HE2	1.69	1.21
1:C:13:GLY:HA3	1:C:19:MET:HE2	1.17	1.08
2:H:89:LYS:HE2	2:H:110:ASP:CB	1.96	0.95
4:M:262[B]:SER:HA	4:M:265[B]:ARG:HG3	1.49	0.92
2:H:89:LYS:HE2	2:H:110:ASP:HB2	1.55	0.86
1:C:13:GLY:HA3	1:C:19:MET:CE	2.05	0.86
2:H:152:PRO:HA	2:H:155:LEU:HD13	1.60	0.80
1:C:13:GLY:CA	1:C:19:MET:CE	2.59	0.78
11:M:405:BPB:HHC	11:M:405:BPB:HBBB	1.66	0.78
4:M:54:SER:HB3	4:M:129:ILE:HD11	1.64	0.77
1:C:20:GLY:N	1:C:245:THR:HG21	1.99	0.77
1:C:200:GLN:HE21	1:C:201:VAL:H	1.31	0.77
2:H:205:LYS:HD3	2:H:205:LYS:H	1.48	0.76
1:C:52:VAL:HA	1:C:55:VAL:HG12	1.68	0.75
3:L:233:GLY:HA3	4:M:214[A]:PHE:CZ	2.23	0.74
3:L:208:THR:HG22	3:L:211:HIS:ND1	2.04	0.72
1:C:110:MET:O	1:C:114:THR:HG23	1.88	0.72
1:C:243:ASN:OD1	1:C:245:THR:HB	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:257[B]:ASN:ND2	4:M:258[B]:ALA:O	2.25	0.70
1:C:200:GLN:HE21	1:C:201:VAL:N	1.88	0.70
3:L:233:GLY:HA3	4:M:214[A]:PHE:CE1	2.27	0.69
1:C:20:GLY:H	1:C:245:THR:HG21	1.55	0.69
1:C:204:VAL:HG11	1:C:254:GLU:HB3	1.76	0.69
1:C:204:VAL:CG1	1:C:254:GLU:HB3	2.24	0.68
1:C:169:ARG:HG3	1:C:169:ARG:HH11	1.58	0.67
1:C:13:GLY:N	1:C:19:MET:HE2	2.09	0.67
1:C:46:LYS:HD3	1:C:47:ALA:H	1.59	0.66
1:C:46:LYS:HA	1:C:46:LYS:HE2	1.77	0.65
2:H:47:LEU:C	2:H:47:LEU:HD13	2.21	0.65
2:H:89:LYS:HE2	2:H:110:ASP:HB3	1.77	0.63
3:L:42:ILE:O	3:L:46:VAL:HG12	1.98	0.63
2:H:252:GLU:OE2	2:H:252:GLU:N	2.27	0.63
8:H:701:LDA:HM11	8:L:304:LDA:HM21	1.81	0.62
7:H:702:SO4:O1	4:M:251[B]:ARG:NH2	2.26	0.61
2:H:89:LYS:HZ3	2:H:106:ASN:C	2.09	0.61
1:C:201:VAL:O	1:C:229:THR:HG21	2.01	0.60
2:H:205:LYS:H	2:H:205:LYS:CD	2.14	0.60
2:H:45:GLU:HG3	2:H:46:PRO:HD2	1.85	0.58
2:H:89:LYS:HZ2	2:H:105:GLY:C	2.10	0.58
1:C:52:VAL:HA	1:C:55:VAL:CG1	2.34	0.58
4:M:54:SER:HB3	4:M:129:ILE:CD1	2.33	0.58
1:C:19:MET:HB3	1:C:245:THR:HG23	1.86	0.57
3:L:197:VAL:HA	4:M:140:LEU:HD22	1.85	0.57
1:C:161:THR:HG21	3:L:273:SER:O	2.05	0.57
3:L:181:PHE:HB3	11:M:405:BPB:HBBA	1.86	0.57
3:L:60:ASP:O	3:L:64:ILE:HD12	2.06	0.56
3:L:224:ILE:HG12	3:L:228:SER:HB2	1.86	0.56
1:C:114:THR:HG21	5:C:402:HEC:HHC	1.87	0.56
1:C:34:ARG:HD2	1:C:35:ASP:OD1	2.06	0.54
1:C:323:LYS:HD3	1:C:323:LYS:H	1.72	0.54
3:L:168[B]:HIS:CE1	10:L:301[B]:BCB:HMC2	2.43	0.54
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.43	0.54
1:C:82:SER:HB2	1:C:85:GLU:HB2	1.89	0.54
1:C:109:ARG:HH11	1:C:281:TYR:HA	1.73	0.54
1:C:169:ARG:HG3	1:C:169:ARG:NH1	2.21	0.54
2:H:136:PRO:HA	2:H:172:TRP:HA	1.89	0.53
4:M:159:GLY:HA3	14:M:406:NS5:H272	1.89	0.53
1:C:225:ASP:O	1:C:229:THR:HG23	2.08	0.52
3:L:181:PHE:HB3	11:M:405:BPB:CBB	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:215:TYR:O	3:L:219:VAL:HG12	2.10	0.52
2:H:196:ILE:HD12	2:H:242:TYR:CZ	2.45	0.51
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.92	0.51
3:L:16:LEU:HD11	3:L:105:VAL:CG2	2.41	0.51
10:M:403:BCB:HHC	10:M:403:BCB:HBB2	1.92	0.51
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.45	0.51
2:H:155:LEU:HD23	2:H:206:ASP:C	2.35	0.51
11:L:303[B]:BPB:OBB	11:L:303[B]:BPB:HHC	2.10	0.51
2:H:142:ASP:OD1	2:H:142:ASP:N	2.36	0.51
3:L:80:LEU:HA	3:L:84:GLY:HA3	1.93	0.51
2:H:20:GLN:HG2	4:M:202[B]:PHE:CE2	2.46	0.51
3:L:226:ALA:O	3:L:229:ILE:HG22	2.11	0.51
1:C:99:GLU:HG2	1:C:104:TYR:CE1	2.45	0.50
4:M:157:CYS:HA	4:M:161:ILE:HB	1.92	0.50
10:M:403:BCB:HBB3	10:M:404[A]:BCB:H62	1.94	0.50
4:M:121:THR:HG23	4:M:156:LEU:HD21	1.94	0.50
1:C:20:GLY:N	1:C:245:THR:CG2	2.72	0.50
1:C:18:SER:HB2	3:L:156[A]:TRP:CD1	2.47	0.50
10:M:404[B]:BCB:H141	11:M:405:BPB:H1A	1.94	0.49
3:L:214:GLN:HG2	4:M:19:VAL:HB	1.94	0.49
2:H:89:LYS:HB2	2:H:104:THR:OG1	2.12	0.49
5:C:402:HEC:HHA	5:C:402:HEC:O1D	2.13	0.49
2:H:62:LEU:O	8:H:707:LDA:HM21	2.13	0.49
3:L:181:PHE:CD2	11:M:405:BPB:HBB	2.48	0.49
10:L:302[B]:BCB:OBD	4:M:201[B]:GLY:HA2	2.13	0.49
1:C:46:LYS:HD3	1:C:47:ALA:N	2.25	0.48
2:H:69:VAL:CG2	3:L:205:LYS:HA	2.43	0.48
3:L:194:ILE:HG21	4:M:264[B]:HIS:ND1	2.29	0.48
2:H:166:GLY:HA3	2:H:186:SER:O	2.14	0.48
2:H:45:GLU:HG3	2:H:46:PRO:CD	2.43	0.48
3:L:178[A]:SER:O	3:L:182:VAL:HG12	2.14	0.47
10:L:301[A]:BCB:H202	13:M:402[A]:MQ7:H261	1.96	0.47
10:L:301[B]:BCB:O1A	10:L:301[B]:BCB:HBD	2.15	0.47
3:L:233:GLY:CA	4:M:214[A]:PHE:CZ	2.96	0.47
2:H:47:LEU:C	2:H:47:LEU:CD1	2.86	0.47
3:L:174[A]:MET:HE3	10:M:403:BCB:HED2	1.96	0.47
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.50	0.47
3:L:234:LEU:O	3:L:238[B]:SER:OG	2.22	0.47
4:M:132:TYR:CE2	4:M:142:THR:HG21	2.50	0.47
3:L:174[B]:MET:HA	10:M:403:BCB:OBD	2.15	0.46
3:L:166[B]:ASN:OD1	3:L:168[B]:HIS:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:244[A]:GLY:O	10:L:301[A]:BCB:HED3	2.15	0.46
11:L:303[B]:BPB:HEDB	4:M:250[B]:TRP:CZ3	2.50	0.46
4:M:254:ILE:HD11	13:M:402[A]:MQ7:H142	1.97	0.46
10:L:301[B]:BCB:CAD	10:L:302[B]:BCB:HBC1	2.46	0.46
2:H:80:ARG:NH2	2:H:82:ARG:HD2	2.31	0.46
1:C:109:ARG:NH1	1:C:281:TYR:HA	2.31	0.45
2:H:49:LEU:O	2:H:51:LYS:N	2.50	0.45
4:M:262[B]:SER:HA	4:M:265[B]:ARG:CG	2.35	0.45
2:H:47:LEU:CD1	2:H:49:LEU:HB3	2.46	0.45
2:H:196:ILE:HD12	2:H:242:TYR:CE1	2.50	0.45
11:L:303[A]:BPB:HEDB	4:M:254:ILE:HG21	1.97	0.45
11:L:303[B]:BPB:H14	11:L:303[B]:BPB:H16A	1.77	0.45
1:C:56:TYR:HB3	5:C:401:HEC:O2A	2.16	0.45
2:H:137:LEU:HB2	2:H:170:ASP:OD1	2.16	0.45
2:H:80:ARG:CZ	2:H:82:ARG:HD2	2.47	0.44
2:H:89:LYS:CD	2:H:105:GLY:H	2.31	0.44
1:C:71:LEU:O	1:C:75:THR:HG23	2.17	0.44
3:L:3:LEU:HB2	3:L:6:GLU:HB2	1.99	0.44
1:C:22:VAL:HG22	3:L:256:THR:HG22	2.00	0.44
3:L:124:PRO:HD3	11:L:303[A]:BPB:HAC	1.99	0.44
10:L:301[B]:BCB:H61	10:L:302[B]:BCB:HBB2	2.00	0.44
2:H:81:ARG:HD2	2:H:81:ARG:H	1.83	0.44
14:M:406:NS5:H18	14:M:406:NS5:H161	1.82	0.44
2:H:20:GLN:HG2	4:M:202[A]:PHE:CE2	2.52	0.43
3:L:146:PHE:HB3	3:L:156[A]:TRP:CD2	2.54	0.43
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.19	0.43
11:L:303[A]:BPB:OBB	11:L:303[A]:BPB:HHC	2.18	0.43
1:C:176:LEU:HD11	1:C:187:TYR:O	2.19	0.43
3:L:130:VAL:HG13	3:L:249:ILE:HG12	2.01	0.43
1:C:19:MET:HA	1:C:245:THR:HG21	2.00	0.43
2:H:89:LYS:HD2	2:H:105:GLY:H	1.84	0.43
14:M:406:NS5:H29	14:M:406:NS5:H271	1.86	0.43
1:C:204:VAL:HG13	1:C:254:GLU:HB3	2.01	0.42
1:C:217:GLY:HA2	4:M:167:GLY:O	2.19	0.42
3:L:221:GLY:N	4:M:49:ILE:HD13	2.34	0.42
3:L:150:ILE:HG23	10:L:302[B]:BCB:HED1	2.01	0.42
1:C:15:ARG:HD2	3:L:68:PRO:O	2.19	0.42
1:C:161:THR:OG1	1:C:162:HIS:N	2.52	0.42
3:L:102:LEU:O	3:L:105:VAL:HG22	2.20	0.42
4:M:239:ARG:HD3	4:M:244[A]:GLU:HG2	2.00	0.42
3:L:16:LEU:HD11	3:L:105:VAL:HG23	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:302[B]:BCB:HMD2	4:M:204[B]:ILE:HD13	2.01	0.42
3:L:161[A]:GLY:HA3	10:L:301[A]:BCB:HAC1	2.01	0.42
4:M:235:GLN:OE1	4:M:243[B]:VAL:HG22	2.19	0.42
1:C:18:SER:HB2	3:L:156[B]:TRP:CD1	2.55	0.42
10:L:301[B]:BCB:H152	11:L:303[B]:BPB:H44	2.02	0.42
2:H:183:LEU:HB2	2:H:196:ILE:CG2	2.50	0.41
1:C:9:THR:HA	1:C:21:GLU:O	2.19	0.41
1:C:323:LYS:H	1:C:323:LYS:CD	2.32	0.41
3:L:21:LEU:HD12	3:L:22:PHE:CE2	2.55	0.41
4:M:282:ILE:HD11	10:M:404[B]:BCB:OBD	2.20	0.41
1:C:224:SER:HA	1:C:227:TYR:HD1	1.85	0.41
3:L:167[B]:TRP:HB3	10:L:301[B]:BCB:HMC3	2.02	0.41
2:H:102:GLN:HE21	3:L:12:ARG:HD3	1.86	0.41
3:L:58:THR:OG1	3:L:59:TRP:N	2.54	0.41
3:L:193:LEU:HD22	3:L:216:PHE:HE2	1.84	0.41
11:L:303[A]:BPB:HMBB	11:L:303[A]:BPB:HBBB	2.03	0.41
4:M:114:LEU:HD11	14:M:406:NS5:H351	2.02	0.41
2:H:45:GLU:O	2:H:47:LEU:N	2.54	0.41
2:H:155:LEU:HD23	2:H:207:LYS:N	2.36	0.41
2:H:180:PHE:CE2	4:M:12:ALA:HB2	2.56	0.41
3:L:123:VAL:HG22	3:L:124:PRO:HD3	2.02	0.41
10:L:301[B]:BCB:H192	10:L:301[B]:BCB:H162	1.67	0.41
4:M:250[A]:TRP:CD1	13:M:402[A]:MQ7:C3	3.03	0.41
2:H:47:LEU:HD12	2:H:49:LEU:HB3	2.02	0.41
10:L:302[B]:BCB:H112	10:L:302[B]:BCB:H142	1.85	0.41
3:L:170[B]:ASN:HB3	3:L:173[B]:HIS:HB2	2.03	0.40
3:L:218:ASP:O	4:M:50:TYR:HB3	2.20	0.40
10:M:404[B]:BCB:H202	10:M:404[B]:BCB:H161	1.93	0.40
3:L:107:ILE:HG23	4:M:252[B]:TRP:HE3	1.85	0.40
3:L:167[A]:TRP:HE1	3:L:173[A]:HIS:CD2	2.40	0.40
3:L:272:TRP:CE2	4:M:86:ARG:HG3	2.56	0.40
4:M:192:GLY:O	4:M:193[B]:ASN:HB3	2.21	0.40
1:C:70:PHE:CZ	1:C:74:MET:HE3	2.56	0.40
3:L:164[A]:TYR:O	3:L:166[A]:ASN:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	C	330/336 (98%)	319 (97%)	11 (3%)	0	100	100
2	H	256/258 (99%)	245 (96%)	8 (3%)	3 (1%)	10	34
3	L	312/273 (114%)	297 (95%)	12 (4%)	3 (1%)	12	38
4	M	372/323 (115%)	355 (95%)	16 (4%)	1 (0%)	36	66
All	All	1270/1190 (107%)	1216 (96%)	47 (4%)	7 (1%)	24	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	47	LEU
2	H	50	VAL
2	H	46	PRO
3	L	165[A]	LEU
3	L	165[B]	LEU
4	M	177	ILE
3	L	57	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	C	281/282 (100%)	279 (99%)	2 (1%)	76	91
2	H	212/212 (100%)	212 (100%)	0	100	100
3	L	253/218 (116%)	253 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M	288/249 (116%)	288 (100%)	0	100	100
All	All	1034/961 (108%)	1032 (100%)	2 (0%)	87	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	123	GLN
1	C	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	24	HIS
1	C	123	GLN
1	C	200	GLN
2	H	8	GLN
2	H	72	HIS
2	H	102	GLN
2	H	106	ASN
4	M	26	ASN
4	M	87	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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
2	FME	H	1	2	8,9,10	1.05	1 (12%)	8,9,11	0.94	0

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
2	FME	H	1	2	-	1/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	CA-N	-2.03	1.43	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	BPB	L	303[B]	-	57,70,70	2.63	12 (21%)	55,101,101	2.67	15 (27%)
10	BCB	L	302[A]	-	60,74,74	2.90	18 (30%)	59,115,115	2.99	23 (38%)
8	LDA	H	706	-	13,15,15	1.33	1 (7%)	14,17,17	0.80	0
9	HTO	L	305	-	9,9,9	0.78	0	10,10,10	0.89	1 (10%)
13	MQ7	M	402[A]	-	49,49,49	1.57	2 (4%)	61,63,63	1.47	10 (16%)
6	DGA	C	405	1	36,36,43	1.18	3 (8%)	38,38,45	1.23	4 (10%)
7	SO4	M	408	-	4,4,4	0.23	0	6,6,6	0.15	0
7	SO4	C	406	-	4,4,4	0.35	0	6,6,6	0.21	0
10	BCB	L	301[A]	-	60,74,74	3.04	17 (28%)	59,115,115	2.68	20 (33%)
5	HEC	C	403	1	46,50,50	1.68	3 (6%)	58,82,82	2.09	11 (18%)
9	HTO	H	708	-	9,9,9	0.81	0	10,10,10	0.80	0
8	LDA	H	701	-	13,15,15	1.25	1 (7%)	14,17,17	0.68	0
7	SO4	M	413	-	4,4,4	0.33	0	6,6,6	0.12	0
11	BPB	L	303[A]	-	57,70,70	2.56	12 (21%)	55,101,101	2.82	19 (34%)
7	SO4	M	412	-	4,4,4	0.43	0	6,6,6	0.28	0
7	SO4	H	705	-	4,4,4	0.27	0	6,6,6	0.18	0
8	LDA	H	707	-	13,15,15	1.74	1 (7%)	14,17,17	1.17	1 (7%)
10	BCB	M	404[B]	-	60,74,74	3.13	17 (28%)	59,115,115	2.98	20 (33%)
7	SO4	M	409	-	4,4,4	0.29	0	6,6,6	0.29	0
7	SO4	H	703	-	4,4,4	0.33	0	6,6,6	0.13	0
7	SO4	M	407	-	4,4,4	0.24	0	6,6,6	0.43	0
7	SO4	M	410	-	4,4,4	0.37	0	6,6,6	0.21	0
5	HEC	C	402	1	46,50,50	1.65	3 (6%)	58,82,82	1.97	7 (12%)
7	SO4	H	702	-	4,4,4	0.33	0	6,6,6	0.29	0
11	BPB	M	405	-	57,70,70	2.58	12 (21%)	55,101,101	2.79	17 (30%)
10	BCB	M	403	-	60,74,74	2.93	18 (30%)	59,115,115	2.72	18 (30%)
10	BCB	M	404[A]	-	60,74,74	3.11	17 (28%)	59,115,115	2.72	19 (32%)
13	MQ7	M	402[B]	-	49,49,49	1.46	2 (4%)	61,63,63	1.43	10 (16%)
7	SO4	H	704	-	4,4,4	0.22	0	6,6,6	0.11	0
10	BCB	L	302[B]	-	60,74,74	2.95	17 (28%)	59,115,115	2.87	20 (33%)
14	NS5	M	406	-	39,39,39	1.33	1 (2%)	46,46,46	2.17	15 (32%)
8	LDA	L	304	-	13,15,15	1.43	1 (7%)	14,17,17	0.73	0
10	BCB	L	301[B]	-	60,74,74	3.05	17 (28%)	59,115,115	2.70	18 (30%)
5	HEC	C	401	1	46,50,50	1.64	3 (6%)	58,82,82	1.95	9 (15%)
5	HEC	C	404	1	46,50,50	1.72	2 (4%)	58,82,82	2.24	10 (17%)
7	SO4	M	411	-	4,4,4	0.38	0	6,6,6	0.21	0

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
11	BPB	L	303[B]	-	-	7/37/105/105	0/5/6/6
10	BCB	L	302[A]	-	2/2/21/26	5/37/137/137	-
8	LDA	H	706	-	-	6/13/13/13	-
9	HTO	L	305	-	-	4/10/10/10	-
13	MQ7	M	402[A]	-	-	0/41/61/61	0/2/2/2
6	DGA	C	405	1	-	16/37/37/45	-
10	BCB	L	301[A]	-	3/3/21/26	8/37/137/137	-
5	HEC	C	403	1	-	4/14/54/54	-
9	HTO	H	708	-	-	1/10/10/10	-
8	LDA	H	701	-	-	4/13/13/13	-
11	BPB	L	303[A]	-	-	7/37/105/105	0/5/6/6
10	BCB	M	404[B]	-	3/3/21/26	11/37/137/137	-
8	LDA	H	707	-	-	11/13/13/13	-
5	HEC	C	402	1	-	6/14/54/54	-
11	BPB	M	405	-	-	8/37/105/105	0/5/6/6
10	BCB	M	403	-	3/3/21/26	11/37/137/137	-
10	BCB	M	404[A]	-	3/3/21/26	10/37/137/137	-
13	MQ7	M	402[B]	-	-	2/41/61/61	0/2/2/2
10	BCB	L	302[B]	-	2/2/21/26	7/37/137/137	-
14	NS5	M	406	-	-	11/43/43/43	-
10	BCB	L	301[B]	-	3/3/21/26	10/37/137/137	-
8	LDA	L	304	-	-	6/13/13/13	-
5	HEC	C	401	1	-	7/14/54/54	-
5	HEC	C	404	1	-	9/14/54/54	-

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	303[B]	BPB	C1B-C2B	9.84	1.50	1.39
10	M	404[A]	BCB	C1A-CHA	9.65	1.51	1.40
11	L	303[A]	BPB	C1B-C2B	9.52	1.50	1.39
10	L	302[A]	BCB	C1B-C2B	9.20	1.50	1.39
11	M	405	BPB	C1B-C2B	9.00	1.49	1.39
10	M	404[B]	BCB	C1A-CHA	8.82	1.50	1.40
10	L	301[B]	BCB	C1A-CHA	8.78	1.50	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	301[A]	BCB	CHC-C1C	8.76	1.49	1.38
10	L	301[A]	BCB	C1A-CHA	8.67	1.49	1.40
10	L	302[B]	BCB	CHC-C1C	8.58	1.49	1.38
10	M	404[B]	BCB	C1B-C2B	8.44	1.49	1.39
10	L	301[B]	BCB	C1B-C2B	8.43	1.49	1.39
10	M	404[B]	BCB	C1D-C2D	8.36	1.49	1.39
10	M	404[A]	BCB	C1B-C2B	8.35	1.49	1.39
13	M	402[A]	MQ7	C3-C2	8.22	1.49	1.35
10	L	302[B]	BCB	C1B-C2B	8.19	1.48	1.39
10	L	301[B]	BCB	CHC-C1C	8.13	1.48	1.38
10	L	301[A]	BCB	C1B-C2B	8.09	1.48	1.39
10	M	403	BCB	C1B-C2B	8.08	1.48	1.39
13	M	402[B]	MQ7	C3-C2	8.04	1.49	1.35
11	L	303[B]	BPB	C1D-C2D	8.02	1.48	1.39
10	M	404[B]	BCB	CHC-C1C	7.94	1.48	1.38
10	M	403	BCB	C1A-CHA	7.86	1.48	1.40
10	M	404[A]	BCB	C1D-C2D	7.62	1.48	1.39
10	M	404[A]	BCB	CHC-C1C	7.60	1.47	1.38
10	M	403	BCB	C1D-C2D	7.44	1.48	1.39
11	L	303[A]	BPB	C1D-C2D	7.32	1.47	1.39
10	L	302[A]	BCB	CHC-C1C	7.24	1.47	1.38
11	M	405	BPB	C1D-C2D	7.24	1.47	1.39
10	L	302[B]	BCB	C1A-CHA	7.19	1.48	1.40
10	L	301[B]	BCB	C1D-C2D	7.16	1.47	1.39
14	M	406	NS5	C35-C36	7.03	1.53	1.32
10	L	302[A]	BCB	C1D-C2D	7.00	1.47	1.39
10	M	403	BCB	CHC-C1C	6.94	1.47	1.38
5	C	404	HEC	CAC-C3C	6.89	1.57	1.35
5	C	403	HEC	CAC-C3C	6.81	1.57	1.35
10	L	302[A]	BCB	C1A-CHA	6.69	1.47	1.40
10	L	302[B]	BCB	C1D-C2D	6.68	1.47	1.39
5	C	402	HEC	CAC-C3C	6.65	1.56	1.35
10	L	301[A]	BCB	C1D-C2D	6.62	1.47	1.39
5	C	401	HEC	CAC-C3C	6.56	1.56	1.35
5	C	402	HEC	CAB-C3B	6.38	1.55	1.35
11	L	303[A]	BPB	C4D-CHA	6.24	1.48	1.39
5	C	404	HEC	CAB-C3B	6.22	1.55	1.35
8	H	707	LDA	C1-N1	-6.17	1.45	1.51
11	M	405	BPB	C4D-CHA	6.14	1.48	1.39
5	C	403	HEC	CAB-C3B	5.98	1.54	1.35
10	M	404[A]	BCB	C3D-C2D	5.97	1.49	1.39
10	M	404[B]	BCB	C3B-C4B	5.95	1.51	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403	BCB	CHC-C4B	5.95	1.49	1.39
5	C	401	HEC	CAB-C3B	5.88	1.54	1.35
11	L	303[B]	BPB	C3B-C2B	5.82	1.49	1.39
10	M	403	BCB	C3D-C2D	5.81	1.49	1.39
10	L	301[A]	BCB	CHC-C4B	5.79	1.49	1.39
11	L	303[B]	BPB	C4D-CHA	5.76	1.48	1.39
10	L	301[A]	BCB	C3D-C2D	5.75	1.49	1.39
10	M	404[B]	BCB	CHC-C4B	5.71	1.48	1.39
10	L	301[B]	BCB	OBD-CAD	5.67	1.29	1.22
10	M	404[A]	BCB	C3B-C2B	5.56	1.49	1.39
10	L	301[B]	BCB	CHC-C4B	5.51	1.48	1.39
10	L	301[B]	BCB	C3B-C2B	5.46	1.49	1.39
13	M	402[A]	MQ7	C10-C5	5.46	1.49	1.40
10	M	404[A]	BCB	CHC-C4B	5.43	1.48	1.39
10	L	302[B]	BCB	C3B-C4B	5.42	1.50	1.41
10	M	404[A]	BCB	C3B-C4B	5.40	1.50	1.41
10	M	404[A]	BCB	O2D-CGD	5.39	1.46	1.33
10	L	301[A]	BCB	O2D-CGD	5.37	1.46	1.33
11	M	405	BPB	O2A-CGA	5.37	1.49	1.33
10	L	302[B]	BCB	CHC-C4B	5.36	1.48	1.39
10	L	302[B]	BCB	C3D-C2D	5.35	1.48	1.39
10	M	403	BCB	CHB-C1B	5.34	1.48	1.39
10	L	301[A]	BCB	C3B-C4B	5.30	1.50	1.41
10	L	301[A]	BCB	OBD-CAD	5.28	1.29	1.22
10	L	301[B]	BCB	C3D-C2D	5.28	1.48	1.39
10	L	302[A]	BCB	CHC-C4B	5.28	1.48	1.39
10	M	404[B]	BCB	O2D-CGD	5.27	1.46	1.33
10	L	301[B]	BCB	O2D-CGD	5.26	1.46	1.33
10	L	301[A]	BCB	C3B-C2B	5.26	1.48	1.39
10	L	302[A]	BCB	C3B-C2B	5.24	1.48	1.39
11	L	303[B]	BPB	OBD-CAD	5.23	1.29	1.22
11	L	303[A]	BPB	C3B-C2B	5.21	1.48	1.39
10	L	302[A]	BCB	C3D-C2D	5.19	1.48	1.39
10	M	404[B]	BCB	C3B-C2B	5.19	1.48	1.39
11	M	405	BPB	C3D-C2D	5.17	1.48	1.39
10	L	302[B]	BCB	OBD-CAD	5.15	1.29	1.22
10	L	302[A]	BCB	C3B-C4B	5.10	1.49	1.41
11	M	405	BPB	OBD-CAD	5.05	1.28	1.22
11	L	303[A]	BPB	O2D-CGD	5.04	1.45	1.33
10	M	404[A]	BCB	OBD-CAD	5.04	1.28	1.22
11	L	303[A]	BPB	C3D-C2D	5.03	1.48	1.39
11	L	303[B]	BPB	O2D-CGD	5.02	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	303[B]	BPB	C3D-C2D	5.00	1.48	1.39
8	L	304	LDA	C1-N1	-4.99	1.46	1.51
10	M	404[B]	BCB	C3D-C2D	4.96	1.48	1.39
10	L	302[A]	BCB	OBD-CAD	4.93	1.28	1.22
13	M	402[B]	MQ7	C10-C5	4.93	1.48	1.40
11	M	405	BPB	O2D-CGD	4.91	1.45	1.33
10	M	403	BCB	C3B-C2B	4.89	1.48	1.39
11	M	405	BPB	C3B-C2B	4.87	1.47	1.39
10	L	301[B]	BCB	C3B-C4B	4.85	1.49	1.41
10	M	404[B]	BCB	OBD-CAD	4.82	1.28	1.22
10	M	403	BCB	O2D-CGD	4.78	1.45	1.33
10	M	404[A]	BCB	CHB-C1B	4.77	1.47	1.39
10	L	302[A]	BCB	CHB-C1B	4.76	1.47	1.39
10	L	302[A]	BCB	O2D-CGD	4.71	1.44	1.33
10	L	301[A]	BCB	CHB-C1B	4.63	1.47	1.39
10	L	302[B]	BCB	C3B-C2B	4.62	1.47	1.39
10	L	302[B]	BCB	CHB-C1B	4.61	1.47	1.39
10	L	302[B]	BCB	O2D-CGD	4.59	1.44	1.33
8	H	706	LDA	C1-N1	-4.59	1.46	1.51
11	L	303[A]	BPB	OBD-CAD	4.57	1.28	1.22
10	M	403	BCB	C3B-C4B	4.54	1.48	1.41
10	M	403	BCB	OBD-CAD	4.53	1.28	1.22
10	M	404[B]	BCB	O2A-CGA	4.51	1.46	1.33
10	M	404[B]	BCB	CHA-CBD	-4.41	1.46	1.51
10	M	404[A]	BCB	O2A-CGA	4.36	1.46	1.33
10	L	301[A]	BCB	O2A-CGA	4.35	1.46	1.33
10	L	302[B]	BCB	CHB-C4A	-4.34	1.33	1.38
11	L	303[B]	BPB	C3B-C4B	4.33	1.48	1.41
10	L	301[B]	BCB	O2A-CGA	4.33	1.46	1.33
8	H	701	LDA	C1-N1	-4.32	1.47	1.51
10	L	302[B]	BCB	O2A-CGA	4.31	1.45	1.33
11	L	303[B]	BPB	O2A-CGA	4.28	1.45	1.33
10	M	403	BCB	O2A-CGA	4.27	1.45	1.33
10	M	404[B]	BCB	CHB-C1B	4.26	1.46	1.39
11	L	303[A]	BPB	C3B-C4B	4.22	1.48	1.41
10	L	301[B]	BCB	CHB-C4A	-4.20	1.33	1.38
11	L	303[A]	BPB	O2A-CGA	4.19	1.45	1.33
10	M	404[B]	BCB	CHD-C1D	4.18	1.46	1.39
10	L	301[B]	BCB	CHB-C1B	4.17	1.46	1.39
10	M	404[B]	BCB	C3A-C2A	-4.12	1.51	1.54
10	L	301[B]	BCB	C3A-C2A	-4.08	1.51	1.54
11	M	405	BPB	C3B-C4B	4.05	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302[B]	BCB	C3A-C2A	-4.02	1.51	1.54
10	L	301[A]	BCB	CHB-C4A	-3.97	1.33	1.38
10	L	302[B]	BCB	CHD-C1D	3.97	1.46	1.39
10	L	302[B]	BCB	CHD-C4C	3.92	1.46	1.39
10	M	403	BCB	CHB-C4A	-3.91	1.33	1.38
10	L	302[A]	BCB	CHD-C1D	3.91	1.46	1.39
10	M	403	BCB	C3A-C2A	-3.91	1.51	1.54
10	L	302[A]	BCB	O2A-CGA	3.90	1.44	1.33
10	M	404[B]	BCB	CHD-C4C	3.89	1.46	1.39
10	M	404[A]	BCB	CHD-C1D	3.82	1.45	1.39
10	M	404[A]	BCB	CHB-C4A	-3.79	1.34	1.38
11	M	405	BPB	CHA-CBD	-3.74	1.47	1.51
10	L	301[B]	BCB	CHD-C1D	3.68	1.45	1.39
10	M	403	BCB	CHD-C1D	3.65	1.45	1.39
10	L	301[A]	BCB	CHD-C1D	3.65	1.45	1.39
10	M	404[A]	BCB	CHA-CBD	-3.62	1.47	1.51
10	L	302[A]	BCB	CHA-CBD	-3.59	1.47	1.51
10	M	404[B]	BCB	CHB-C4A	-3.56	1.34	1.38
10	L	301[B]	BCB	CHA-CBD	-3.54	1.47	1.51
10	L	302[A]	BCB	CHB-C4A	-3.54	1.34	1.38
10	M	403	BCB	CHD-C4C	3.53	1.46	1.39
10	L	302[A]	BCB	CHD-C4C	3.51	1.46	1.39
10	L	301[A]	BCB	C3A-C2A	-3.48	1.51	1.54
10	L	301[B]	BCB	CHD-C4C	3.45	1.46	1.39
11	M	405	BPB	C4C-NC	-3.41	1.27	1.37
11	L	303[A]	BPB	C3A-C2A	-3.38	1.51	1.54
10	M	404[A]	BCB	CHD-C4C	3.36	1.45	1.39
10	L	301[A]	BCB	CHA-CBD	-3.30	1.47	1.51
10	M	404[A]	BCB	C3A-C2A	-3.27	1.51	1.54
11	L	303[B]	BPB	C4C-NC	-3.20	1.27	1.37
6	C	405	DGA	OG1-CA1	3.12	1.42	1.33
6	C	405	DGA	OG2-CB1	3.09	1.43	1.34
11	L	303[A]	BPB	C4C-NC	-3.07	1.28	1.37
10	L	302[A]	BCB	C3A-C2A	-3.06	1.52	1.54
10	L	302[B]	BCB	CHA-CBD	-3.04	1.48	1.51
11	L	303[A]	BPB	CHA-CBD	-3.03	1.48	1.51
10	M	403	BCB	CHA-CBD	-3.03	1.48	1.51
11	L	303[B]	BPB	CHA-CBD	-3.02	1.48	1.51
10	L	302[A]	BCB	CBD-CGD	-2.84	1.48	1.52
10	L	301[A]	BCB	CHD-C4C	2.81	1.44	1.39
6	C	405	DGA	OG2-CG2	-2.77	1.42	1.47
11	L	303[B]	BPB	C3A-C2A	-2.42	1.52	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	403	HEC	CBA-CGA	2.36	1.56	1.50
11	M	405	BPB	C3A-C2A	-2.14	1.52	1.54
10	M	403	BCB	CBD-CGD	-2.12	1.49	1.52
5	C	401	HEC	CBD-CGD	2.11	1.55	1.50
5	C	402	HEC	CBA-CGA	2.02	1.55	1.50

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	HEC	CBB-CAB-C3B	-12.68	102.09	127.43
10	M	404[B]	BCB	O2D-CGD-CBD	11.61	123.70	110.95
5	C	404	HEC	CBB-CAB-C3B	-11.51	104.42	127.43
10	M	404[A]	BCB	O2D-CGD-CBD	10.73	122.73	110.95
5	C	401	HEC	CBB-CAB-C3B	-10.65	106.15	127.43
11	M	405	BPB	O2D-CGD-CBD	10.48	122.46	110.95
10	L	302[A]	BCB	O2D-CGD-CBD	10.08	122.02	110.95
10	L	302[B]	BCB	O2D-CGD-CBD	10.03	121.97	110.95
11	L	303[A]	BPB	O2D-CGD-CBD	9.44	121.32	110.95
5	C	402	HEC	CBB-CAB-C3B	-9.11	109.22	127.43
10	M	404[B]	BCB	C1B-CHB-C4A	8.90	127.05	121.32
10	L	302[A]	BCB	C4B-CHC-C1C	8.76	126.96	121.32
11	M	405	BPB	C3D-C4D-ND	8.75	118.92	107.71
11	L	303[B]	BPB	C3D-C4D-ND	8.73	118.90	107.71
10	M	404[B]	BCB	C4B-CHC-C1C	8.69	126.91	121.32
11	L	303[A]	BPB	C2B-C1B-NB	8.55	115.61	109.43
10	L	302[B]	BCB	C1B-CHB-C4A	8.35	126.69	121.32
10	L	301[B]	BCB	C4B-CHC-C1C	8.32	126.67	121.32
10	M	403	BCB	O2D-CGD-CBD	8.32	120.08	110.95
11	L	303[A]	BPB	C3D-C4D-ND	8.26	118.29	107.71
11	L	303[B]	BPB	O2D-CGD-CBD	8.16	119.91	110.95
10	L	301[B]	BCB	O2D-CGD-CBD	8.11	119.86	110.95
10	L	302[A]	BCB	C1B-CHB-C4A	8.00	126.47	121.32
10	L	301[A]	BCB	O2D-CGD-CBD	7.98	119.72	110.95
10	L	301[A]	BCB	C1B-CHB-C4A	7.93	126.42	121.32
5	C	404	HEC	CBC-CAC-C3C	-7.87	111.70	127.43
10	L	301[B]	BCB	C1B-CHB-C4A	7.85	126.37	121.32
10	L	302[B]	BCB	C4B-CHC-C1C	7.67	126.26	121.32
10	M	403	BCB	C4B-CHC-C1C	7.53	126.17	121.32
10	M	403	BCB	C1B-CHB-C4A	7.52	126.16	121.32
11	L	303[B]	BPB	C2B-C1B-NB	7.49	114.84	109.43
10	L	301[A]	BCB	C4B-CHC-C1C	7.38	126.07	121.32
10	M	404[A]	BCB	C4B-CHC-C1C	7.09	125.89	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	404[A]	BCB	C1B-CHB-C4A	6.78	125.68	121.32
11	M	405	BPB	C2B-C1B-NB	6.72	114.29	109.43
10	M	403	BCB	C3D-CAD-CBD	6.52	116.19	107.61
5	C	402	HEC	CBC-CAC-C3C	-6.40	114.65	127.43
10	L	302[B]	BCB	C3D-CAD-CBD	6.16	115.72	107.61
10	M	404[A]	BCB	C3D-CAD-CBD	6.05	115.57	107.61
10	M	403	BCB	CHA-C1A-C2A	-5.95	119.33	133.31
10	M	404[B]	BCB	C3D-CAD-CBD	5.95	115.44	107.61
10	L	302[A]	BCB	C3D-CAD-CBD	5.86	115.32	107.61
11	L	303[A]	BPB	C4D-ND-C1D	-5.68	102.07	108.87
10	L	301[A]	BCB	C3D-CAD-CBD	5.65	115.04	107.61
11	M	405	BPB	C4D-ND-C1D	-5.64	102.12	108.87
10	M	403	BCB	OBD-CAD-C3D	-5.62	119.13	127.89
14	M	406	NS5	C19-C20-C21	-5.59	119.44	127.28
10	L	302[B]	BCB	CHA-C1A-C2A	-5.57	120.23	133.31
11	L	303[B]	BPB	C4D-ND-C1D	-5.52	102.25	108.87
14	M	406	NS5	C13-C12-C10	-5.45	120.03	127.69
10	L	301[B]	BCB	C3D-CAD-CBD	5.43	114.75	107.61
10	L	302[A]	BCB	CHA-C1A-C2A	-5.35	120.74	133.31
11	L	303[B]	BPB	OBD-CAD-C3D	-5.26	119.69	127.89
10	L	302[A]	BCB	OBD-CAD-C3D	-4.99	120.10	127.89
10	L	302[A]	BCB	C1-C2-C3	-4.99	118.03	126.20
10	L	302[B]	BCB	OBD-CAD-C3D	-4.96	120.16	127.89
10	L	302[A]	BCB	O1D-CGD-CBD	-4.92	117.26	124.72
10	L	301[A]	BCB	CMB-C2B-C3B	4.69	134.05	124.68
10	L	301[B]	BCB	CMB-C2B-C3B	4.65	133.97	124.68
10	L	301[A]	BCB	CHA-C1A-C2A	-4.56	122.59	133.31
10	L	301[A]	BCB	OBD-CAD-C3D	-4.47	120.92	127.89
10	M	404[B]	BCB	O2D-CGD-O1D	-4.38	115.31	123.85
10	M	404[B]	BCB	OBD-CAD-C3D	-4.36	121.09	127.89
6	C	405	DGA	OG2-CB1-CB2	4.33	120.84	111.48
10	L	301[B]	BCB	CHA-C1A-C2A	-4.31	123.19	133.31
10	L	301[B]	BCB	OBD-CAD-C3D	-4.29	121.19	127.89
10	M	404[A]	BCB	O2D-CGD-O1D	-4.29	115.51	123.85
10	M	404[A]	BCB	OBD-CAD-C3D	-4.13	121.45	127.89
14	M	406	NS5	CM4-C36-C35	-4.11	110.32	122.66
14	M	406	NS5	C18-C17-C15	-4.11	121.52	127.28
11	L	303[A]	BPB	OBD-CAD-C3D	-4.09	121.51	127.89
11	M	405	BPB	C2D-C1D-ND	4.07	112.38	109.43
5	C	402	HEC	C2A-C1A-NA	-4.06	106.40	110.32
11	M	405	BPB	OBD-CAD-C3D	-4.06	121.57	127.89
11	L	303[A]	BPB	C2D-C1D-ND	4.04	112.35	109.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	404[A]	BCB	CHA-C1A-C2A	-4.00	123.92	133.31
10	M	404[B]	BCB	CHA-C1A-C2A	-3.99	123.94	133.31
14	M	406	NS5	C34-C35-C36	-3.99	114.34	127.64
11	M	405	BPB	C1A-C2A-C3A	-3.93	99.10	102.84
10	M	404[A]	BCB	C3D-C4D-CHA	3.92	114.50	108.54
10	L	301[A]	BCB	C4-C3-C5	3.92	122.03	115.23
10	M	404[B]	BCB	CMB-C2B-C3B	3.88	132.43	124.68
10	M	404[B]	BCB	C3D-C4D-CHA	3.86	114.41	108.54
10	L	301[B]	BCB	C3D-C4D-CHA	3.81	114.33	108.54
11	M	405	BPB	O2A-CGA-CBA	3.81	123.45	111.83
11	M	405	BPB	O1D-CGD-CBD	-3.77	119.00	124.72
5	C	401	HEC	C2A-C1A-NA	-3.75	106.70	110.32
10	L	301[A]	BCB	C3D-C4D-CHA	3.74	114.22	108.54
14	M	406	NS5	CM3-C36-C35	-3.72	111.49	122.66
10	M	403	BCB	C3D-C4D-ND	3.70	118.87	112.94
10	L	302[B]	BCB	C3D-C4D-ND	3.69	118.86	112.94
10	M	403	BCB	C3D-C4D-CHA	3.69	114.15	108.54
10	L	302[A]	BCB	C3D-C4D-ND	3.69	118.86	112.94
10	L	302[B]	BCB	C1-C2-C3	-3.66	120.19	126.20
11	L	303[B]	BPB	CMD-C2D-C3D	-3.65	117.39	124.68
10	L	301[A]	BCB	O2A-CGA-CBA	3.63	122.89	111.83
10	L	302[B]	BCB	O2D-CGD-O1D	-3.56	116.92	123.85
11	L	303[A]	BPB	CMB-C2B-C3B	3.55	131.78	124.68
10	M	404[A]	BCB	CMB-C2B-C3B	3.55	131.78	124.68
11	L	303[B]	BPB	CMB-C2B-C3B	3.55	131.77	124.68
10	L	302[A]	BCB	C3D-C4D-CHA	3.54	113.93	108.54
10	M	404[B]	BCB	CMD-C2D-C3D	-3.53	117.63	124.68
14	M	406	NS5	C11-C10-C9	3.53	121.35	115.23
10	L	301[A]	BCB	C3D-C4D-ND	3.47	118.51	112.94
10	L	302[B]	BCB	C3D-C4D-CHA	3.46	113.80	108.54
10	L	301[B]	BCB	C4-C3-C5	3.46	121.23	115.23
10	L	301[B]	BCB	O2D-CGD-O1D	-3.45	117.13	123.85
11	L	303[A]	BPB	C3B-C4B-NB	3.45	113.06	108.05
10	L	301[B]	BCB	O2A-CGA-CBA	3.43	122.31	111.83
10	L	302[B]	BCB	CHC-C1C-C2C	-3.41	113.56	122.69
10	L	302[A]	BCB	CMB-C2B-C3B	3.41	131.49	124.68
5	C	404	HEC	CAD-CBD-CGD	-3.40	104.65	113.67
10	L	301[B]	BCB	C3D-C4D-ND	3.37	118.35	112.94
13	M	402[B]	MQ7	C21-C22-C23	-3.37	119.91	127.62
11	L	303[A]	BPB	C3D-CAD-CBD	3.37	112.04	107.61
10	L	302[A]	BCB	CHC-C1C-C2C	-3.36	113.69	122.69
10	M	404[B]	BCB	C3D-C4D-ND	3.34	118.30	112.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	404[A]	BCB	C3D-C4D-ND	3.32	118.26	112.94
11	M	405	BPB	C1-O2A-CGA	3.31	124.67	116.65
10	M	404[B]	BCB	C1A-CHA-C4D	3.31	124.50	118.98
11	L	303[A]	BPB	C4A-C3A-C2A	-3.30	99.70	102.84
10	M	403	BCB	C1-C2-C3	-3.29	120.80	126.20
10	M	403	BCB	CHC-C1C-C2C	-3.28	113.89	122.69
13	M	402[B]	MQ7	C29-C28-C30	3.28	120.92	115.23
10	M	403	BCB	C4D-ND-C1D	-3.23	102.77	105.22
10	M	404[A]	BCB	CHC-C1C-C2C	-3.23	114.05	122.69
10	L	302[A]	BCB	C6-C5-C3	-3.22	105.63	113.47
10	L	301[B]	BCB	CHC-C1C-C2C	-3.21	114.09	122.69
5	C	401	HEC	CBA-CAA-C2A	-3.21	103.66	112.53
10	L	302[B]	BCB	CMB-C2B-C3B	3.20	131.08	124.68
10	M	404[B]	BCB	CHC-C1C-C2C	-3.20	114.13	122.69
11	L	303[B]	BPB	C3B-C4B-NB	3.19	112.69	108.05
11	L	303[B]	BPB	C2D-C1D-ND	3.17	111.72	109.43
13	M	402[A]	MQ7	C39-C38-C40	3.15	120.70	115.23
11	M	405	BPB	C3B-C4B-NB	3.13	112.61	108.05
10	L	302[A]	BCB	C4D-ND-C1D	-3.13	102.85	105.22
13	M	402[A]	MQ7	C29-C28-C30	3.11	120.63	115.23
6	C	405	DGA	OG1-CA1-CA2	3.09	121.24	111.83
11	L	303[A]	BPB	O1D-CGD-CBD	-3.07	120.06	124.72
13	M	402[B]	MQ7	C14-C13-C15	3.07	120.56	115.23
10	L	302[B]	BCB	O2A-CGA-CBA	3.06	121.16	111.83
11	L	303[B]	BPB	O1D-CGD-CBD	-3.05	120.10	124.72
11	L	303[B]	BPB	O2A-CGA-CBA	3.04	121.11	111.83
10	M	403	BCB	O2A-CGA-CBA	3.00	120.99	111.83
10	L	301[A]	BCB	O2D-CGD-O1D	-2.98	118.04	123.85
5	C	401	HEC	CBD-CAD-C3D	-2.98	104.29	112.53
10	L	302[B]	BCB	C6-C5-C3	-2.89	106.43	113.47
10	M	403	BCB	CMB-C2B-C3B	2.89	130.45	124.68
13	M	402[B]	MQ7	C39-C38-C40	2.88	120.23	115.23
10	L	302[B]	BCB	C4D-ND-C1D	-2.87	103.04	105.22
10	L	302[A]	BCB	CMD-C2D-C3D	-2.86	118.96	124.68
13	M	402[A]	MQ7	C12-C11-C3	-2.85	105.06	112.08
14	M	406	NS5	C32-C31-C33	2.85	120.18	115.23
13	M	402[A]	MQ7	C16-C17-C18	-2.85	121.10	127.62
11	L	303[A]	BPB	CMA-C3A-C4A	-2.85	108.48	114.61
11	L	303[A]	BPB	O2A-CGA-CBA	2.84	120.50	111.83
13	M	402[A]	MQ7	C34-C33-C35	2.84	120.16	115.23
10	L	302[B]	BCB	CMD-C2D-C3D	-2.83	119.02	124.68
13	M	402[B]	MQ7	C16-C17-C18	-2.83	121.16	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	405	BPB	CMD-C2D-C3D	-2.82	119.05	124.68
10	M	403	BCB	C4-C3-C5	2.82	120.12	115.23
11	L	303[A]	BPB	CMD-C2D-C3D	-2.79	119.10	124.68
10	M	404[A]	BCB	O2A-CGA-O1A	-2.79	116.64	123.63
10	L	301[B]	BCB	CAA-CBA-CGA	-2.78	105.31	113.21
5	C	402	HEC	CBA-CAA-C2A	-2.78	104.84	112.53
10	L	301[A]	BCB	C4D-ND-C1D	-2.77	103.12	105.22
10	M	404[A]	BCB	O2A-CGA-CBA	2.75	120.22	111.83
6	C	405	DGA	OG2-CG2-CG1	2.74	112.52	106.21
14	M	406	NS5	C29-C30-C31	-2.74	123.83	127.69
10	L	302[A]	BCB	C1A-CHA-C4D	2.73	123.55	118.98
11	M	405	BPB	O2D-CGD-O1D	-2.73	118.54	123.85
10	L	301[B]	BCB	C4D-ND-C1D	-2.72	103.16	105.22
10	M	404[A]	BCB	C1A-CHA-C4D	2.69	123.47	118.98
10	L	301[A]	BCB	CHD-C4C-C3C	-2.69	122.00	130.04
11	L	303[A]	BPB	O2D-CGD-O1D	-2.69	118.62	123.85
11	M	405	BPB	CMA-C3A-C4A	-2.69	108.82	114.61
13	M	402[B]	MQ7	C26-C27-C28	-2.69	121.48	127.62
5	C	403	HEC	C2A-C1A-NA	-2.67	107.74	110.32
10	L	301[A]	BCB	CHC-C1C-C2C	-2.66	115.56	122.69
10	L	302[A]	BCB	CMA-C3A-C4A	-2.66	108.89	114.61
11	L	303[A]	BPB	C4B-NB-C1B	-2.64	104.97	108.82
11	M	405	BPB	C3D-CAD-CBD	2.64	111.08	107.61
10	L	302[A]	BCB	O2A-CGA-CBA	2.63	119.84	111.83
10	L	302[A]	BCB	O2A-CGA-O1A	-2.62	117.06	123.63
13	M	402[A]	MQ7	C19-C18-C20	2.62	119.78	115.23
5	C	404	HEC	C2A-C1A-NA	-2.60	107.81	110.32
10	M	404[A]	BCB	C4D-ND-C1D	-2.56	103.28	105.22
5	C	402	HEC	C3D-C4D-ND	-2.56	107.31	110.15
10	M	403	BCB	O1D-CGD-CBD	-2.56	120.84	124.72
11	L	303[B]	BPB	C4A-C3A-C2A	-2.55	100.41	102.84
10	L	301[A]	BCB	O2A-CGA-O1A	-2.55	117.25	123.63
13	M	402[B]	MQ7	C34-C33-C35	2.55	119.65	115.23
5	C	402	HEC	CAD-CBD-CGD	-2.55	106.91	113.67
10	L	302[B]	BCB	CMA-C3A-C4A	-2.54	109.14	114.61
10	M	404[B]	BCB	O2A-CGA-CBA	2.51	119.50	111.83
14	M	406	NS5	C12-C13-C14	-2.49	115.98	123.20
10	M	404[B]	BCB	O1D-CGD-CBD	-2.49	120.95	124.72
10	L	302[A]	BCB	C4-C3-C5	2.49	119.54	115.23
10	M	403	BCB	O2D-CGD-O1D	-2.46	119.05	123.85
10	M	404[B]	BCB	O2A-CGA-O1A	-2.46	117.47	123.63
10	L	301[B]	BCB	CMD-C2D-C3D	-2.46	119.76	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	301[A]	BCB	CED-O2D-CGD	2.46	121.50	115.92
11	L	303[B]	BPB	C16-C15-C13	-2.43	107.88	115.97
10	M	404[B]	BCB	C1-C2-C3	-2.43	122.22	126.20
13	M	402[B]	MQ7	C24-C23-C25	2.42	119.44	115.23
14	M	406	NS5	C18-C19-C20	2.41	128.46	123.52
10	M	404[B]	BCB	C4D-ND-C1D	-2.41	103.39	105.22
14	M	406	NS5	C6-C5-C4	2.40	119.39	115.23
10	L	301[A]	BCB	CAA-CBA-CGA	-2.40	106.40	113.21
10	L	301[B]	BCB	C1A-CHA-C4D	2.40	122.98	118.98
13	M	402[A]	MQ7	C45-C43-C44	2.39	120.08	114.59
5	C	403	HEC	CHB-C4A-NA	2.38	127.05	124.45
10	L	302[B]	BCB	O1D-CGD-CBD	-2.38	121.11	124.72
13	M	402[B]	MQ7	C19-C18-C20	2.38	119.36	115.23
10	L	302[B]	BCB	O2A-CGA-O1A	-2.36	117.74	123.63
5	C	403	HEC	CBD-CAD-C3D	-2.34	106.06	112.53
5	C	401	HEC	C3D-C4D-ND	-2.34	107.56	110.15
10	M	404[A]	BCB	CHD-C4C-C3C	-2.33	123.09	130.04
13	M	402[A]	MQ7	C26-C27-C28	-2.33	122.30	127.62
13	M	402[A]	MQ7	C24-C23-C25	2.31	119.24	115.23
5	C	402	HEC	C4A-NA-C1A	2.31	109.59	105.82
10	L	301[B]	BCB	CHD-C4C-C3C	-2.30	123.16	130.04
11	L	303[A]	BPB	C4-C3-C5	2.28	119.19	115.23
9	L	305	HTO	C5-C4-C3	-2.28	110.37	114.11
10	M	403	BCB	CHD-C4C-C3C	-2.27	123.25	130.04
14	M	406	NS5	C8-C9-C10	-2.27	105.66	113.19
10	L	301[A]	BCB	C1-C2-C3	-2.27	122.48	126.20
8	H	707	LDA	CM2-N1-C1	-2.26	105.49	110.23
10	M	404[B]	BCB	C4-C3-C5	2.26	119.15	115.23
5	C	403	HEC	CAA-CBA-CGA	-2.24	107.71	113.67
10	L	302[A]	BCB	CHD-C4C-C3C	-2.23	123.36	130.04
5	C	403	HEC	C3D-C4D-ND	-2.21	107.69	110.15
5	C	403	HEC	O2D-CGD-CBD	2.18	120.88	114.00
5	C	404	HEC	CBD-CAD-C3D	2.17	118.54	112.53
13	M	402[A]	MQ7	C14-C13-C15	2.17	119.00	115.23
11	L	303[A]	BPB	CBA-CAA-C2A	-2.17	107.39	113.78
10	L	302[A]	BCB	CED-O2D-CGD	2.16	120.81	115.92
5	C	404	HEC	CHC-C4B-NB	2.15	126.80	124.45
10	L	302[B]	BCB	C4-C3-C5	2.15	118.95	115.23
5	C	404	HEC	CHB-C4A-NA	2.14	126.78	124.45
10	L	302[A]	BCB	C1A-CHA-CBD	-2.14	126.88	132.36
13	M	402[B]	MQ7	C45-C43-C44	2.13	119.50	114.59
5	C	401	HEC	CMC-C2C-C1C	-2.12	122.19	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	401	HEC	O2D-CGD-CBD	2.11	120.68	114.00
10	M	404[B]	BCB	CHD-C4C-C3C	-2.11	123.74	130.04
11	L	303[A]	BPB	CAA-C2A-C3A	-2.11	107.31	113.00
5	C	404	HEC	C3D-C4D-ND	-2.10	107.82	110.15
11	M	405	BPB	C4A-C3A-C2A	-2.09	100.85	102.84
14	M	406	NS5	C8-C7-C5	-2.08	122.86	127.62
5	C	403	HEC	CBC-CAC-C3C	2.08	131.59	127.43
5	C	403	HEC	O2A-CGA-CBA	2.07	120.53	114.00
11	M	405	BPB	C4B-NB-C1B	-2.06	105.81	108.82
6	C	405	DGA	OG1-CA1-OA1	-2.06	118.48	123.63
10	L	301[A]	BCB	C1A-CHA-C4D	2.05	122.40	118.98
5	C	401	HEC	CBC-CAC-C3C	-2.05	123.34	127.43
10	M	403	BCB	C1A-CHA-C4D	2.05	122.40	118.98
11	L	303[B]	BPB	CED-O2D-CGD	2.05	120.56	115.92
10	M	404[A]	BCB	OB D-CAD-CBD	-2.04	122.83	125.82
5	C	404	HEC	CBA-CAA-C2A	-2.04	106.89	112.53
5	C	401	HEC	CHB-C4A-NA	2.02	126.66	124.45
5	C	404	HEC	C4B-NB-C1B	2.02	109.12	105.82
10	M	404[A]	BCB	C1-O2A-CGA	2.02	121.54	116.65
10	M	404[A]	BCB	O1D-CGD-CBD	-2.01	121.68	124.72
5	C	403	HEC	O1D-CGD-CBD	-2.01	116.72	123.09
14	M	406	NS5	C16-C15-C14	2.00	121.15	118.09
5	C	403	HEC	O1A-CGA-CBA	-2.00	116.74	123.09
11	L	303[B]	BPB	O2A-CGA-O1A	-2.00	118.62	123.63

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	L	301[A]	BCB	NA
10	L	301[A]	BCB	NC
10	L	301[A]	BCB	ND
10	L	301[B]	BCB	NA
10	L	301[B]	BCB	NC
10	L	301[B]	BCB	ND
10	L	302[A]	BCB	NA
10	L	302[A]	BCB	NC
10	L	302[B]	BCB	NA
10	L	302[B]	BCB	NC
10	M	403	BCB	NA
10	M	403	BCB	NC
10	M	403	BCB	ND
10	M	404[A]	BCB	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	M	404[A]	BCB	NC
10	M	404[A]	BCB	ND
10	M	404[B]	BCB	NA
10	M	404[B]	BCB	NC
10	M	404[B]	BCB	ND

All (171) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	401	HEC	C4B-C3B-CAB-CBB
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	401	HEC	C4C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB
5	C	402	HEC	C4B-C3B-CAB-CBB
5	C	402	HEC	C2C-C3C-CAC-CBC
5	C	402	HEC	C4C-C3C-CAC-CBC
5	C	403	HEC	C2B-C3B-CAB-CBB
5	C	403	HEC	C4B-C3B-CAB-CBB
5	C	403	HEC	C2C-C3C-CAC-CBC
5	C	403	HEC	C4C-C3C-CAC-CBC
5	C	404	HEC	C2B-C3B-CAB-CBB
5	C	404	HEC	C4B-C3B-CAB-CBB
5	C	404	HEC	C2C-C3C-CAC-CBC
5	C	404	HEC	C4C-C3C-CAC-CBC
6	C	405	DGA	OG1-CG1-CG2-CG3
6	C	405	DGA	CG1-CG2-OG2-CB1
8	H	706	LDA	C2-C1-N1-O1
8	H	706	LDA	C2-C1-N1-CM1
8	H	706	LDA	C2-C1-N1-CM2
8	H	706	LDA	N1-C1-C2-C3
8	H	707	LDA	C2-C1-N1-O1
8	H	707	LDA	C2-C1-N1-CM1
8	H	707	LDA	N1-C1-C2-C3
9	L	305	HTO	O2-C2-C3-C4
10	L	301[B]	BCB	C2C-C3C-CAC-CBC
10	L	302[A]	BCB	C2C-C3C-CAC-CBC
10	L	302[B]	BCB	C2C-C3C-CAC-CBC
10	M	404[A]	BCB	C2C-C3C-CAC-CBC
10	M	404[A]	BCB	CAD-CBD-CGD-O1D
10	M	404[A]	BCB	CAD-CBD-CGD-O2D
10	M	404[B]	BCB	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	M	404[B]	BCB	CAD-CBD-CGD-O1D
10	M	404[B]	BCB	CAD-CBD-CGD-O2D
11	L	303[A]	BPB	C2C-C3C-CAC-CBC
11	L	303[B]	BPB	C2C-C3C-CAC-CBC
11	M	405	BPB	C2C-C3C-CAC-CBC
14	M	406	NS5	C13-C14-C15-C17
14	M	406	NS5	C34-C35-C36-CM3
10	M	403	BCB	CBD-CGD-O2D-CED
10	L	301[A]	BCB	C4-C3-C5-C6
10	L	301[B]	BCB	C4-C3-C5-C6
10	L	301[A]	BCB	C2-C3-C5-C6
11	M	405	BPB	CBA-CGA-O2A-C1
14	M	406	NS5	C34-C35-C36-CM4
11	M	405	BPB	O1A-CGA-O2A-C1
10	M	403	BCB	O1D-CGD-O2D-CED
6	C	405	DGA	CA2-CA1-OG1-CG1
10	L	301[B]	BCB	C2-C3-C5-C6
6	C	405	DGA	OA1-CA1-OG1-CG1
14	M	406	NS5	C13-C14-C15-C16
10	M	404[B]	BCB	C2A-CAA-CBA-CGA
10	M	404[A]	BCB	C2A-CAA-CBA-CGA
10	M	403	BCB	C5-C6-C7-C8
10	M	404[B]	BCB	C8-C10-C11-C12
10	L	302[B]	BCB	CBD-CGD-O2D-CED
10	M	404[A]	BCB	C15-C16-C17-C18
10	M	403	BCB	C3-C5-C6-C7
10	L	301[B]	BCB	C15-C16-C17-C18
10	L	301[A]	BCB	C13-C15-C16-C17
14	M	406	NS5	C7-C8-C9-C10
10	M	404[B]	BCB	C16-C17-C18-C19
8	L	304	LDA	C2-C3-C4-C5
8	H	707	LDA	C2-C3-C4-C5
8	H	707	LDA	C4-C5-C6-C7
6	C	405	DGA	CCB-CDB-CEB-CFB
6	C	405	DGA	CBB-CAB-CB9-CB8
11	L	303[A]	BPB	C8-C10-C11-C12
8	H	707	LDA	C6-C7-C8-C9
10	M	404[B]	BCB	C16-C17-C18-C20
10	M	404[A]	BCB	C8-C10-C11-C12
8	L	304	LDA	C1-C2-C3-C4
11	L	303[A]	BPB	CBD-CGD-O2D-CED
11	L	303[A]	BPB	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	M	406	NS5	C3-C4-C5-C6
10	L	302[B]	BCB	C13-C15-C16-C17
10	M	404[A]	BCB	C13-C15-C16-C17
6	C	405	DGA	CAB-CBB-CCB-CDB
14	M	406	NS5	C31-C33-C34-C35
8	H	706	LDA	C3-C4-C5-C6
5	C	401	HEC	C2A-CAA-CBA-CGA
11	L	303[A]	BPB	C2-C3-C5-C6
10	M	404[A]	BCB	C12-C13-C15-C16
9	H	708	HTO	O1-C1-C2-O2
10	L	302[B]	BCB	CHA-CBD-CGD-O1D
10	L	302[B]	BCB	CHA-CBD-CGD-O2D
11	L	303[A]	BPB	O2A-C1-C2-C3
11	L	303[B]	BPB	O2A-C1-C2-C3
8	H	701	LDA	C6-C7-C8-C9
8	L	304	LDA	C5-C6-C7-C8
14	M	406	NS5	C10-C12-C13-C14
10	L	302[B]	BCB	O1D-CGD-O2D-CED
10	M	404[A]	BCB	C14-C13-C15-C16
10	L	301[A]	BCB	C15-C16-C17-C18
10	L	301[B]	BCB	C11-C12-C13-C15
9	L	305	HTO	C4-C5-C6-C7
8	H	706	LDA	C6-C7-C8-C9
6	C	405	DGA	OG1-CG1-CG2-OG2
9	L	305	HTO	O1-C1-C2-O2
8	H	707	LDA	C11-C10-C9-C8
11	L	303[B]	BPB	C4-C3-C5-C6
10	L	302[A]	BCB	C13-C15-C16-C17
11	L	303[B]	BPB	C2-C3-C5-C6
8	L	304	LDA	C4-C5-C6-C7
10	L	301[B]	BCB	C11-C12-C13-C14
11	M	405	BPB	C16-C17-C18-C20
11	M	405	BPB	C10-C11-C12-C13
5	C	404	HEC	C4D-C3D-CAD-CBD
10	M	403	BCB	C11-C10-C8-C7
5	C	402	HEC	C3D-CAD-CBD-CGD
11	L	303[A]	BPB	O1D-CGD-O2D-CED
11	M	405	BPB	C15-C16-C17-C18
10	L	301[B]	BCB	C8-C10-C11-C12
6	C	405	DGA	CBB-CCB-CDB-CEB
8	H	707	LDA	C2-C1-N1-CM2
10	L	301[A]	BCB	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	CB9-CAB-CBB-CCB
10	M	404[B]	BCB	C12-C13-C15-C16
10	M	403	BCB	C8-C10-C11-C12
8	H	707	LDA	C5-C6-C7-C8
10	M	403	BCB	C4-C3-C5-C6
11	L	303[B]	BPB	C8-C10-C11-C12
10	L	301[A]	BCB	CAD-CBD-CGD-O2D
10	L	301[B]	BCB	CAD-CBD-CGD-O2D
10	L	301[B]	BCB	C16-C17-C18-C19
9	L	305	HTO	O2-C2-C3-O3
10	L	301[A]	BCB	CAD-CBD-CGD-O1D
10	L	301[B]	BCB	CAD-CBD-CGD-O1D
14	M	406	NS5	C23-C24-C25-C26
14	M	406	NS5	C3-C4-C5-C7
11	L	303[B]	BPB	C16-C17-C18-C19
10	M	403	BCB	C11-C10-C8-C9
11	M	405	BPB	C16-C17-C18-C19
8	H	701	LDA	C2-C3-C4-C5
10	L	302[B]	BCB	C16-C17-C18-C19
5	C	404	HEC	C3D-CAD-CBD-CGD
5	C	404	HEC	C2D-C3D-CAD-CBD
6	C	405	DGA	CA6-CA7-CA8-CA9
8	H	701	LDA	C9-C10-C11-C12
6	C	405	DGA	CA7-CA8-CA9-CAA
10	M	403	BCB	C2-C3-C5-C6
6	C	405	DGA	CB2-CB3-CB4-CB5
8	L	304	LDA	C3-C4-C5-C6
10	M	404[B]	BCB	C14-C13-C15-C16
10	M	404[B]	BCB	C1A-C2A-CAA-CBA
11	M	405	BPB	C14-C13-C15-C16
11	L	303[B]	BPB	C16-C17-C18-C20
5	C	401	HEC	CAA-CBA-CGA-O2A
6	C	405	DGA	CB6-CB7-CB8-CB9
13	M	402[B]	MQ7	C39-C38-C40-C41
10	M	404[B]	BCB	O2A-C1-C2-C3
8	H	707	LDA	C3-C4-C5-C6
10	M	404[A]	BCB	C5-C6-C7-C8
5	C	401	HEC	CAA-CBA-CGA-O1A
8	H	701	LDA	C5-C6-C7-C8
10	L	302[A]	BCB	CBD-CGD-O2D-CED
10	L	302[A]	BCB	C14-C13-C15-C16
6	C	405	DGA	CB4-CB5-CB6-CB7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	L	302[A]	BCB	C12-C13-C15-C16
10	M	403	BCB	C2C-C3C-CAC-CBC
5	C	404	HEC	CAD-CBD-CGD-O2D
10	L	301[A]	BCB	C6-C7-C8-C10
14	M	406	NS5	C11-C10-C9-C8
8	L	304	LDA	C2-C1-N1-O1
6	C	405	DGA	CA3-CA4-CA5-CA6
13	M	402[B]	MQ7	C18-C20-C21-C22
5	C	402	HEC	CAA-CBA-CGA-O1A
5	C	404	HEC	CAD-CBD-CGD-O1D
10	M	403	BCB	CAD-CBD-CGD-O2D
8	H	707	LDA	C9-C10-C11-C12

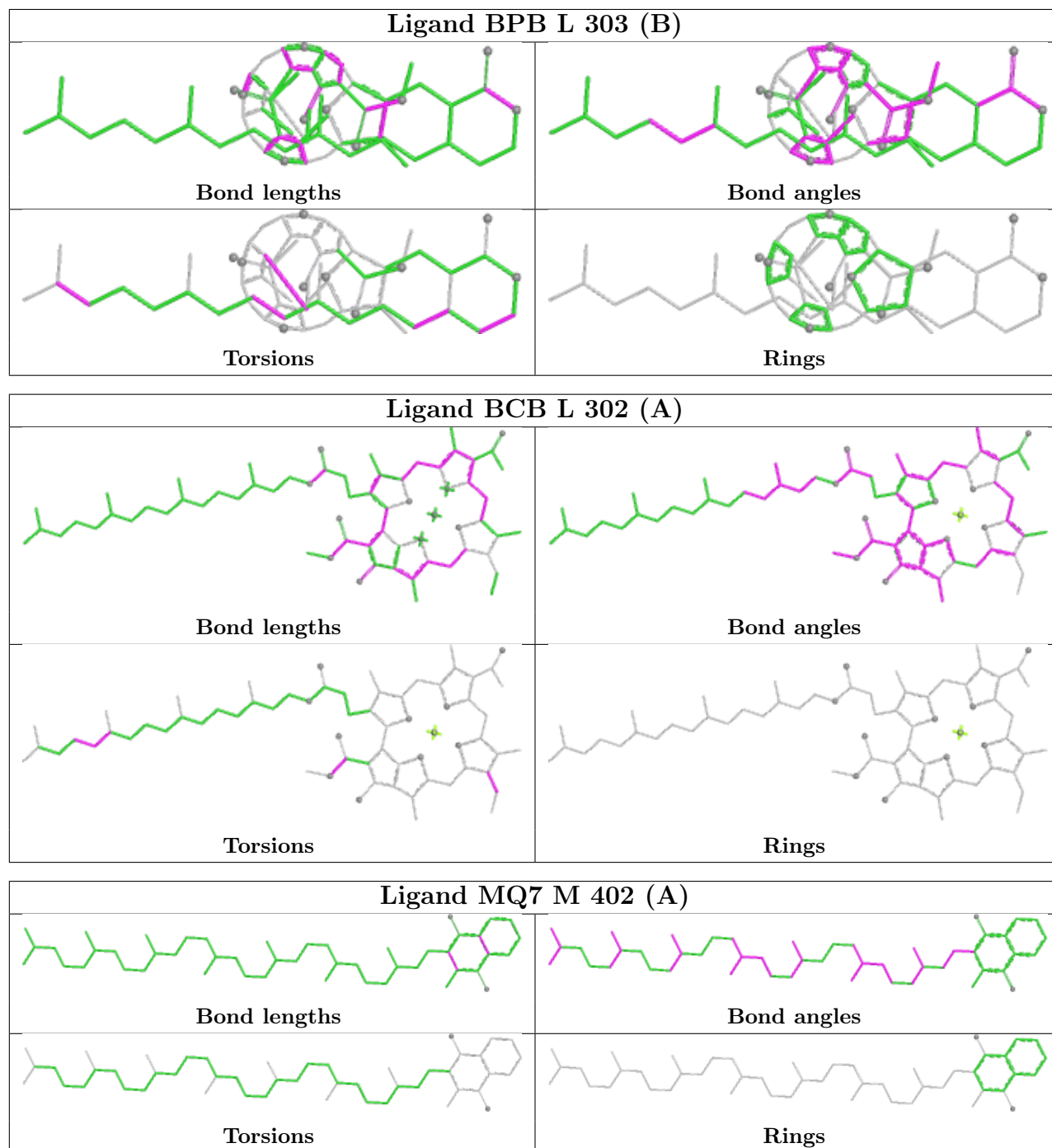
There are no ring outliers.

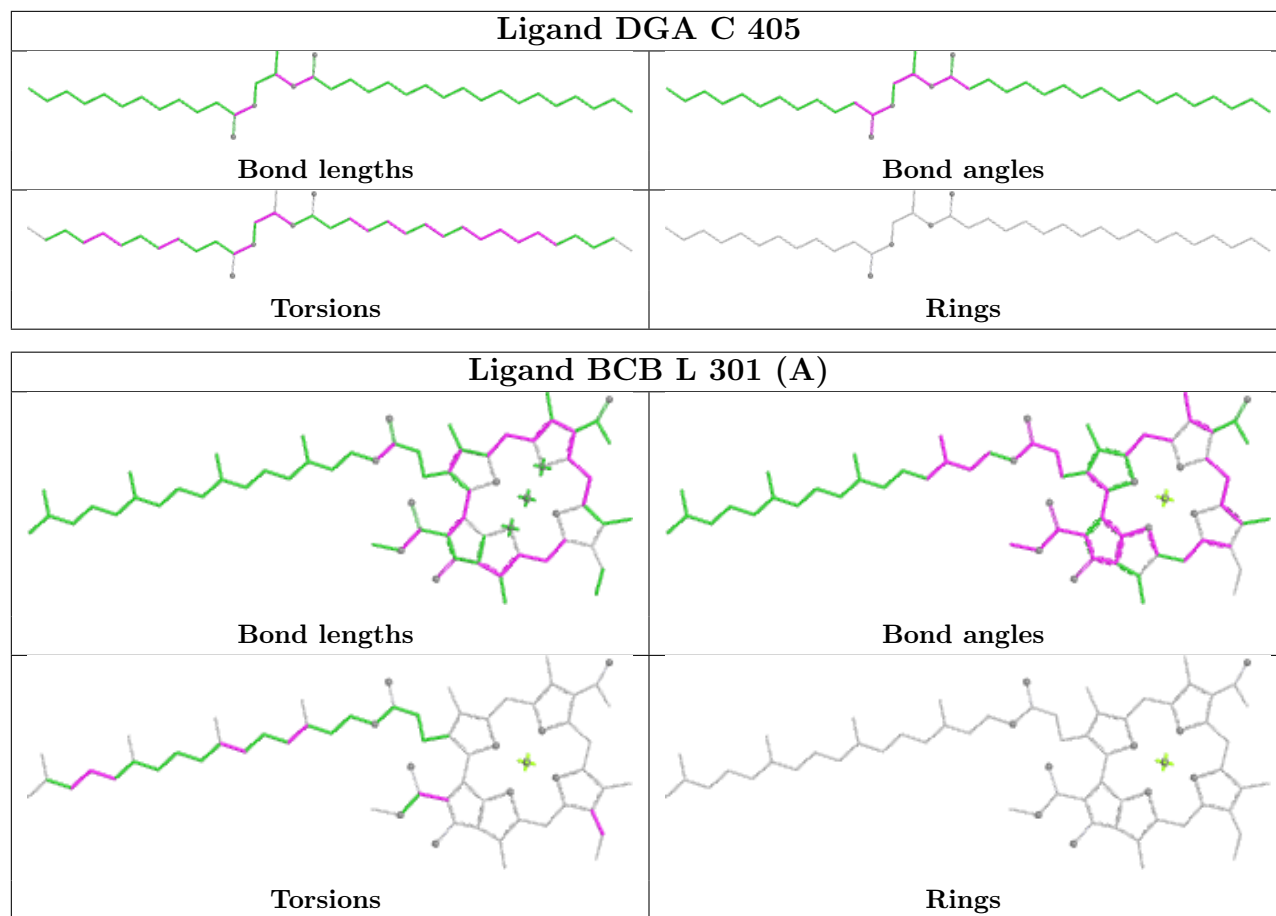
17 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	303[B]	BPB	4	0
13	M	402[A]	MQ7	3	0
10	L	301[A]	BCB	3	0
8	H	701	LDA	1	0
11	L	303[A]	BPB	4	0
8	H	707	LDA	1	0
10	M	404[B]	BCB	3	0
5	C	402	HEC	2	0
7	H	702	SO4	1	0
11	M	405	BPB	5	0
10	M	403	BCB	4	0
10	M	404[A]	BCB	1	0
10	L	302[B]	BCB	6	0
14	M	406	NS5	4	0
8	L	304	LDA	1	0
10	L	301[B]	BCB	7	0
5	C	401	HEC	1	0

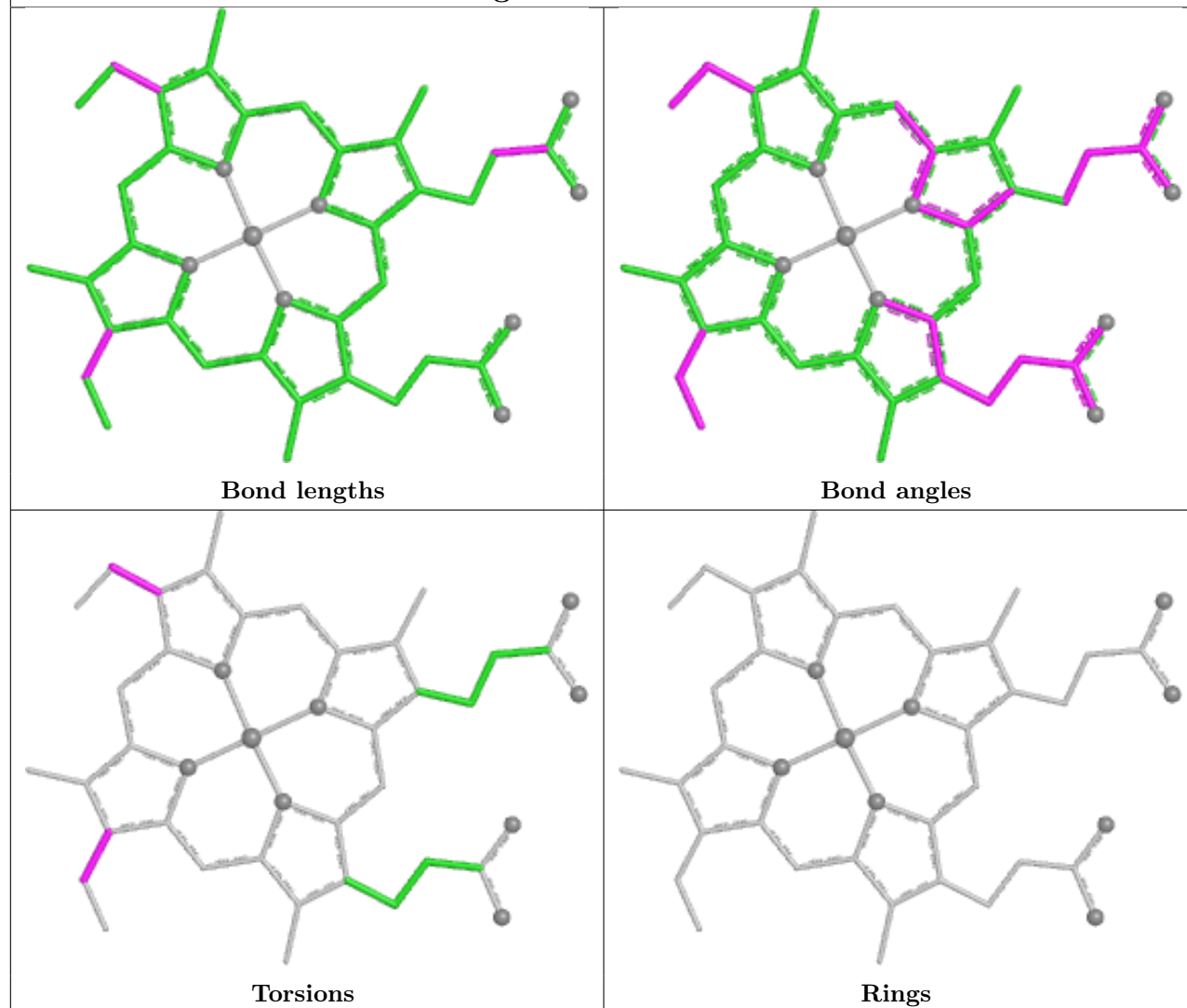
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

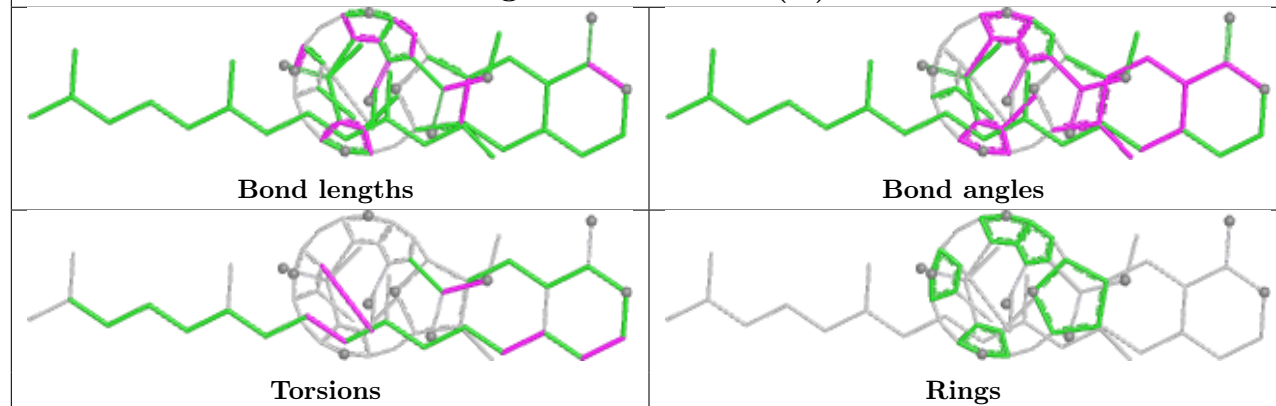


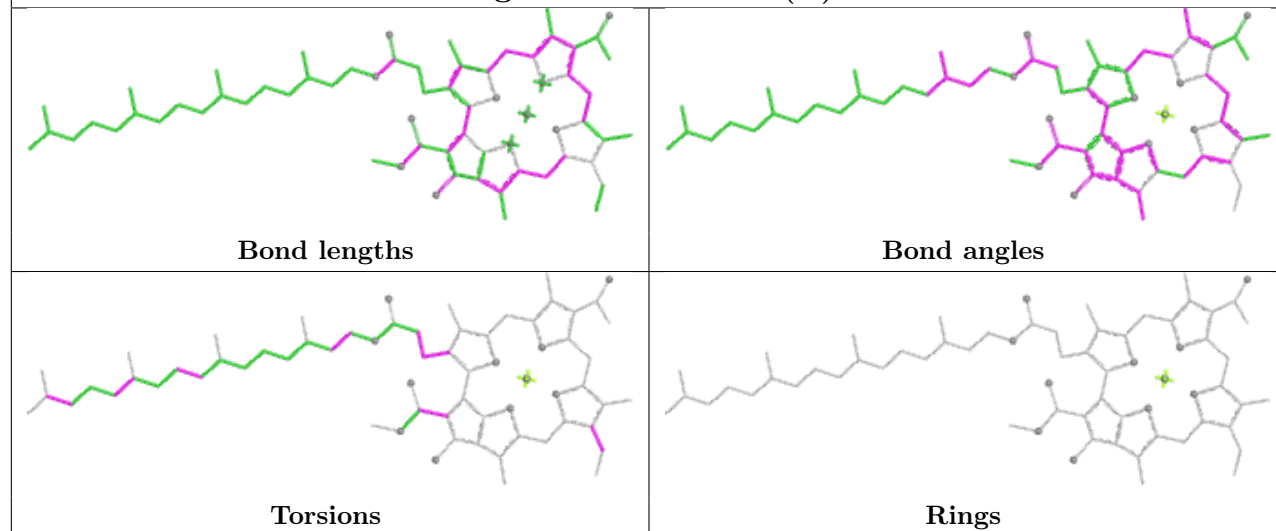
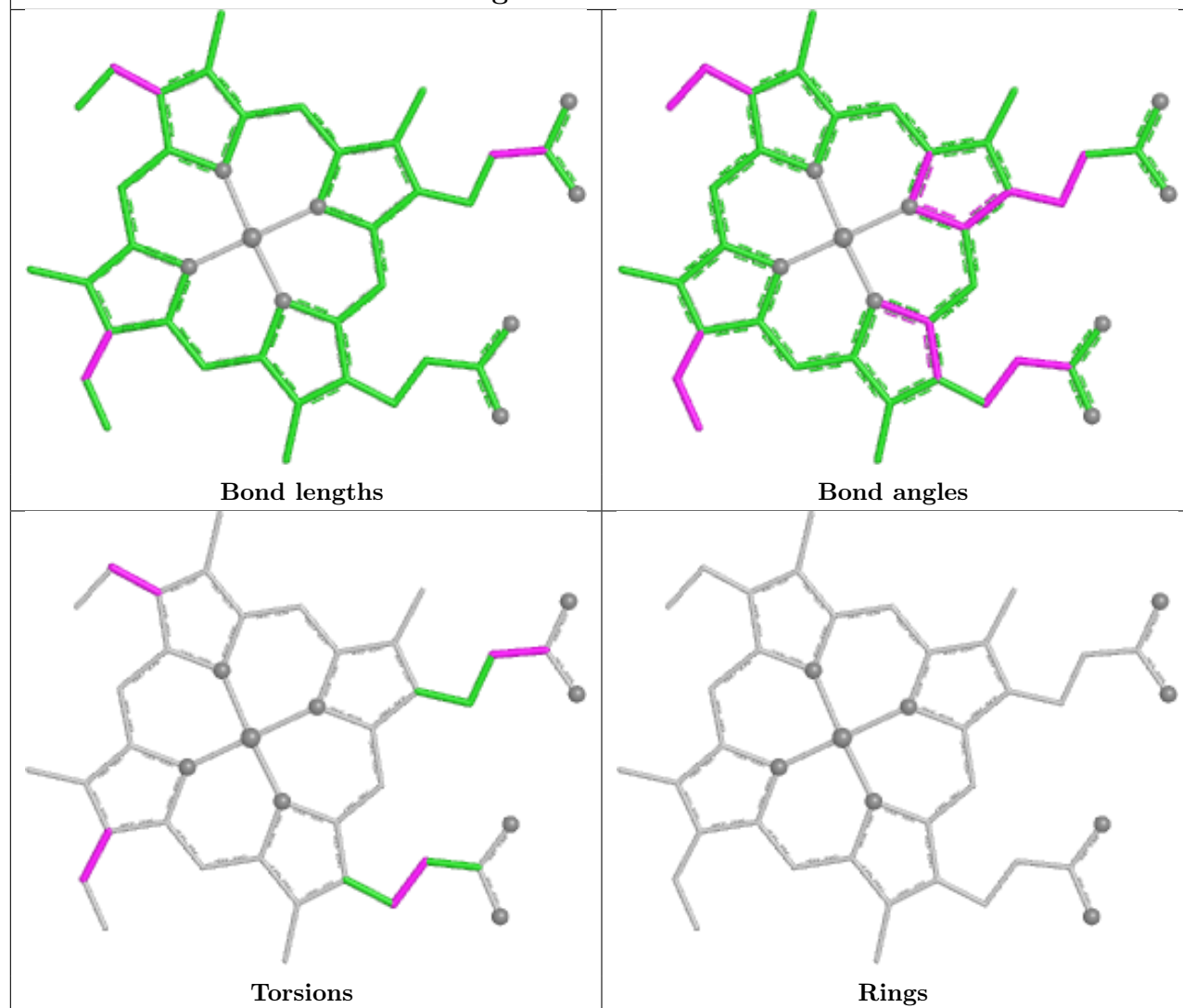


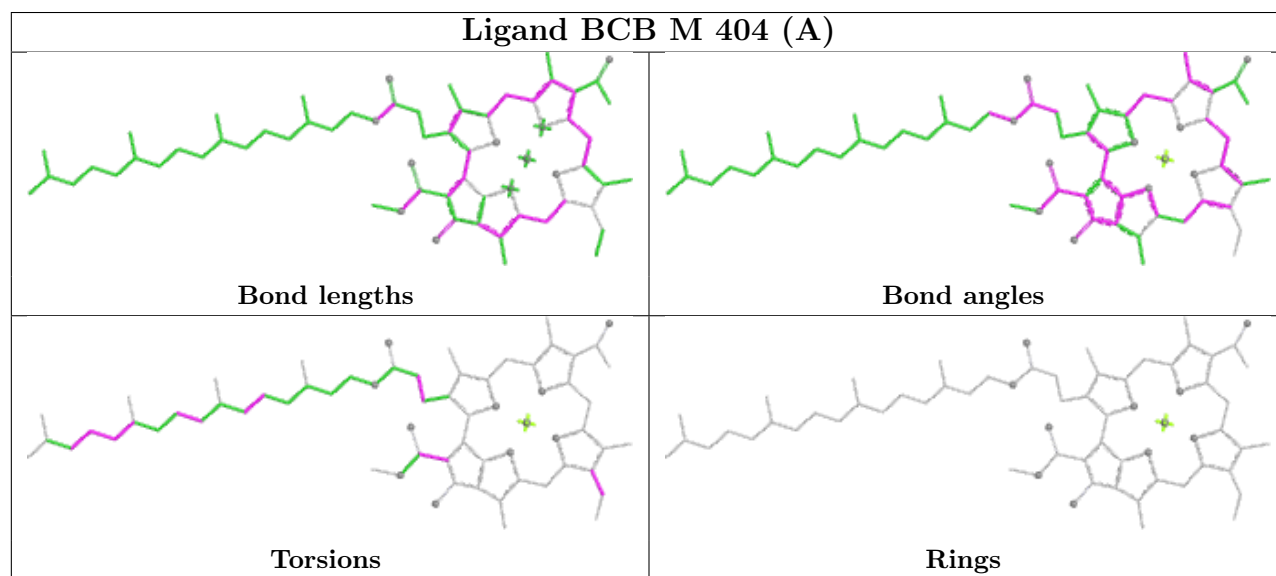
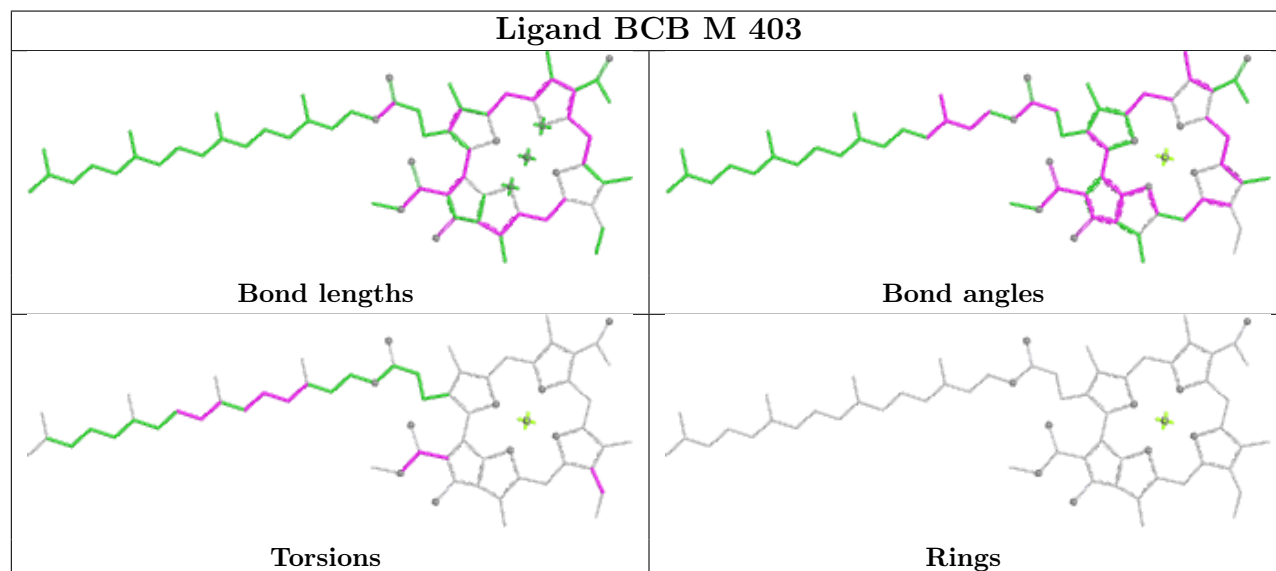
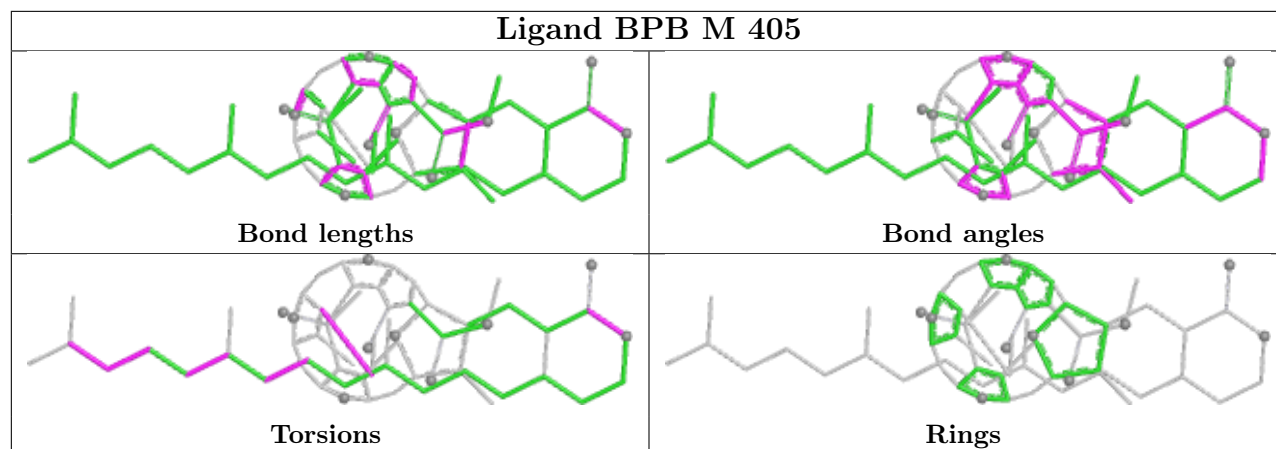
Ligand HEC C 403



Ligand BPB L 303 (A)

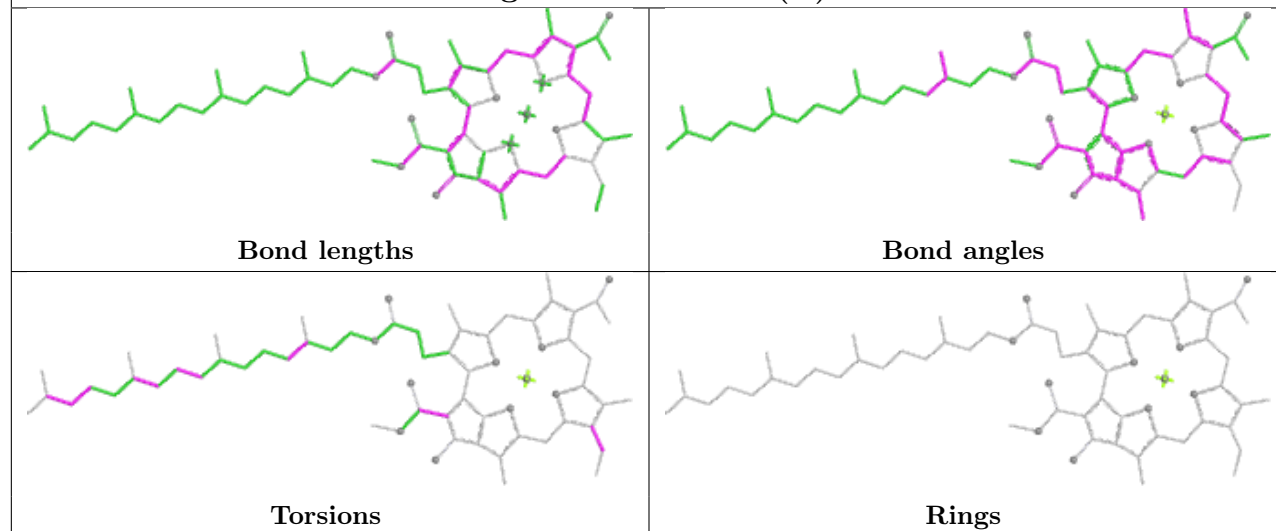


Ligand BCB M 404 (B)**Ligand HEC C 402**

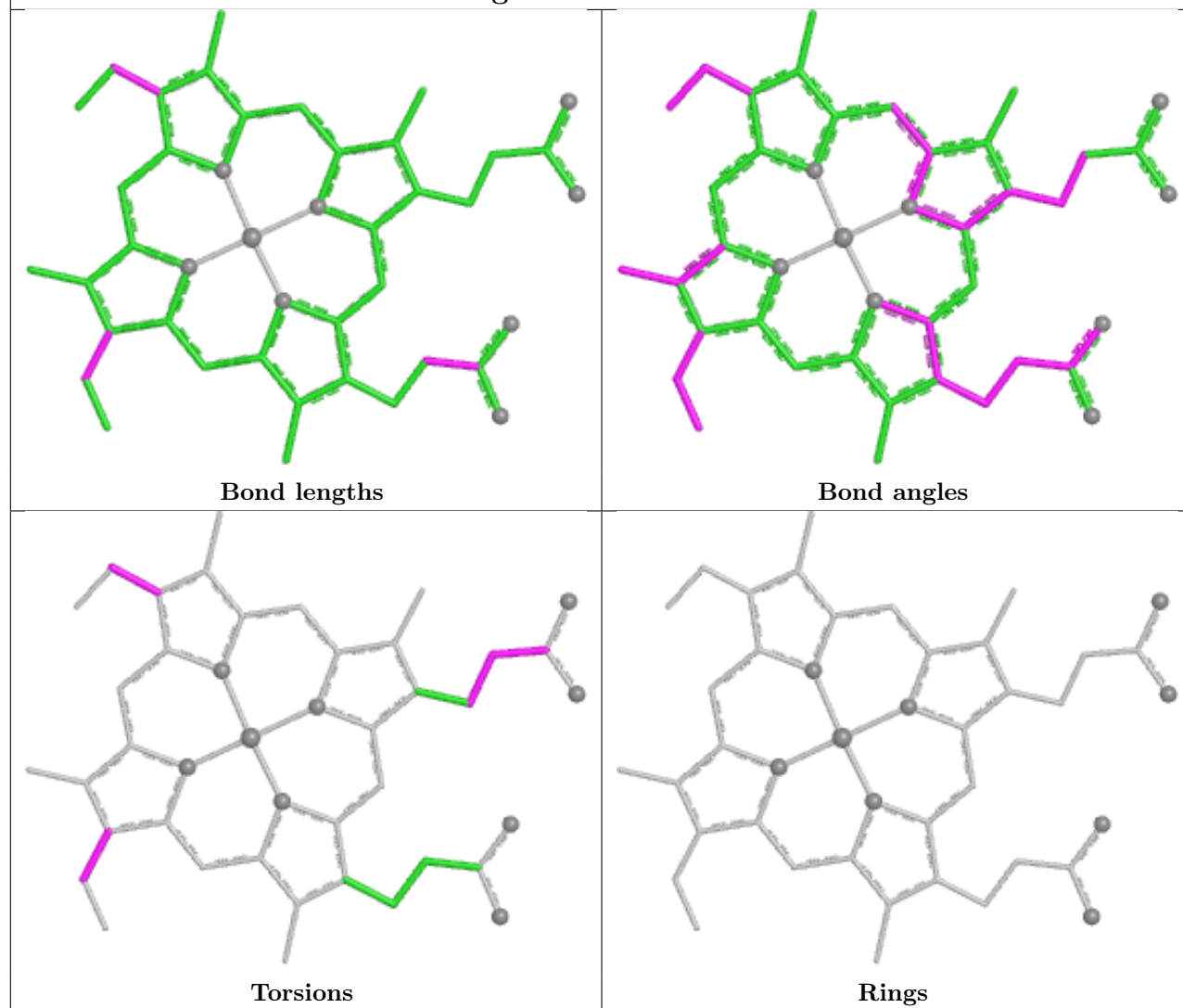


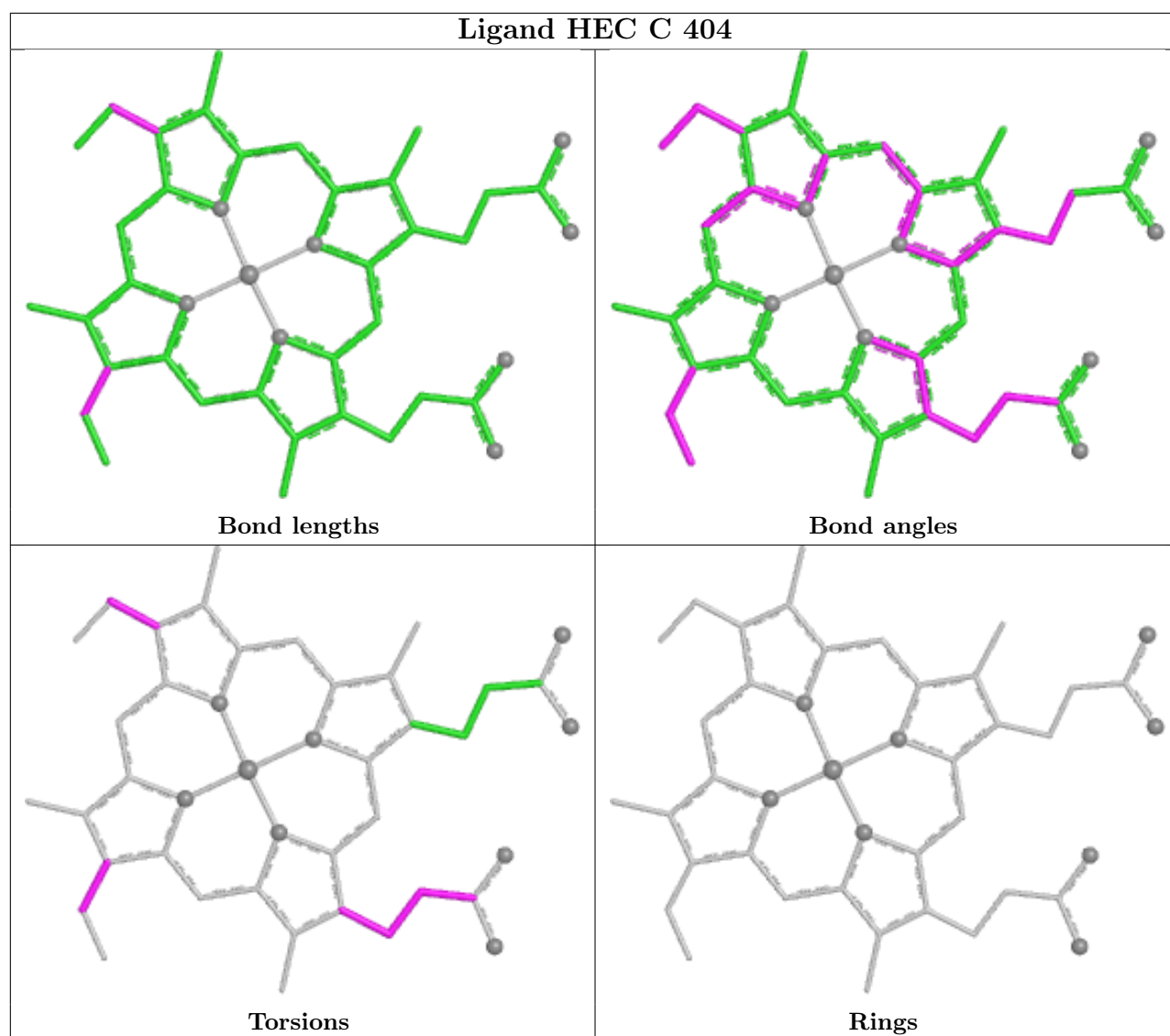
Ligand MQ7 M 402 (B)	
Bond lengths	Bond angles
Torsions	Rings
Ligand BCB L 302 (B)	
Bond lengths	Bond angles
Torsions	Rings
Ligand NS5 M 406	
Bond lengths	Bond angles
Torsions	Rings

Ligand BCB L 301 (B)



Ligand HEC C 401





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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	332/336 (98%)	-0.40	2 (0%) 85 80	74, 93, 120, 146	0
2	H	257/258 (99%)	-0.07	6 (2%) 61 51	78, 103, 147, 193	0
3	L	273/273 (100%)	-0.39	2 (0%) 84 77	38, 90, 115, 134	41 (15%)
4	M	323/323 (100%)	-0.34	2 (0%) 85 80	38, 90, 115, 139	51 (15%)
All	All	1185/1190 (99%)	-0.31	12 (1%) 79 72	38, 94, 125, 193	92 (7%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	50	VAL	4.0
2	H	52	LEU	4.0
2	H	53	ALA	3.9
3	L	1	ALA	3.5
4	M	89	PHE	3.3
2	H	54	PRO	2.8
1	C	332	LYS	2.7
1	C	54	GLN	2.4
4	M	51	LEU	2.3
2	H	191	ALA	2.2
2	H	47	LEU	2.1
3	L	191	GLY	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FME	H	1	10/11	0.95	0.12	90,102,112,127	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

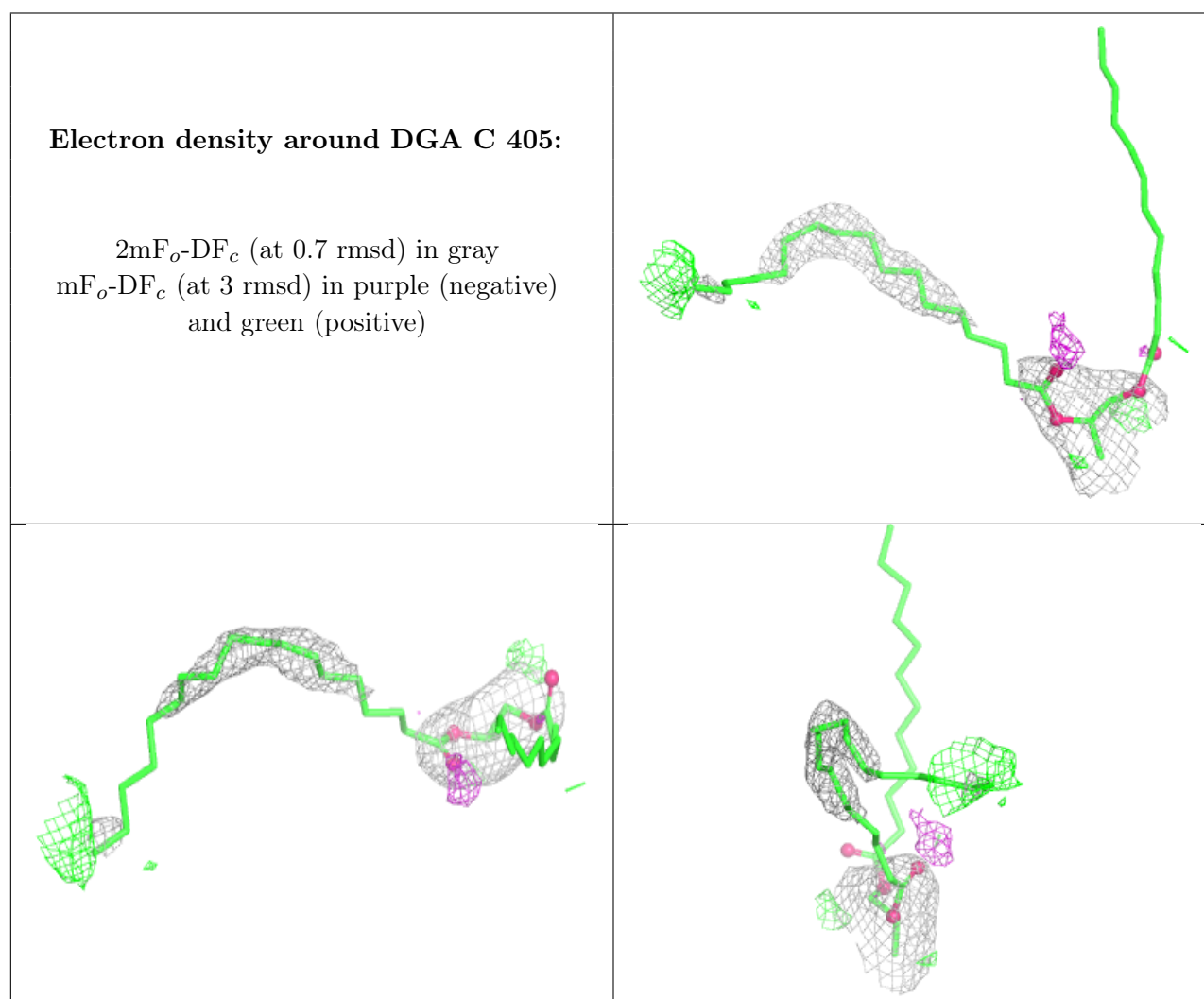
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	M	413	5/5	0.51	0.14	145,160,166,179	0
7	SO4	M	411	5/5	0.61	0.11	130,156,170,175	0
7	SO4	M	410	5/5	0.63	0.11	127,133,147,161	0
9	HTO	L	305	10/10	0.63	0.31	96,120,130,131	0
7	SO4	H	703	5/5	0.68	0.11	149,152,158,170	0
7	SO4	M	412	5/5	0.69	0.13	125,128,152,179	0
7	SO4	C	406	5/5	0.75	0.10	129,143,150,163	0
7	SO4	M	408	5/5	0.79	0.11	114,115,124,146	0
9	HTO	H	708	10/10	0.85	0.23	102,115,129,131	0
6	DGA	C	405	37/44	0.85	0.22	97,131,165,170	0
8	LDA	L	304	16/16	0.89	0.27	102,125,150,154	0
8	LDA	H	706	16/16	0.94	0.18	83,99,167,169	0
11	BPB	M	405	65/65	0.94	0.15	78,91,172,180	0
7	SO4	H	702	5/5	0.96	0.09	104,114,121,125	0
7	SO4	H	705	5/5	0.96	0.06	107,107,119,119	5
7	SO4	M	407	5/5	0.96	0.06	99,112,123,124	0
8	LDA	H	707	16/16	0.96	0.13	97,115,132,136	0
14	NS5	M	406	40/40	0.96	0.16	80,96,136,138	0
7	SO4	H	704	5/5	0.97	0.17	97,101,115,115	5
13	MQ7	M	402[A]	48/48	0.97	0.13	78,86,123,146	48
13	MQ7	M	402[B]	48/48	0.97	0.13	78,86,123,146	48
10	BCB	M	403	66/66	0.97	0.11	75,84,166,177	0
10	BCB	L	302[B]	66/66	0.98	0.10	72,80,112,115	66
8	LDA	H	701	16/16	0.98	0.11	81,96,111,111	0
10	BCB	M	404[A]	66/66	0.98	0.10	60,75,106,112	66
10	BCB	M	404[B]	66/66	0.98	0.10	60,75,106,112	66
11	BPB	L	303[A]	65/65	0.98	0.09	77,83,92,97	65
11	BPB	L	303[B]	65/65	0.98	0.09	77,83,92,97	65

Continued on next page...

Continued from previous page...

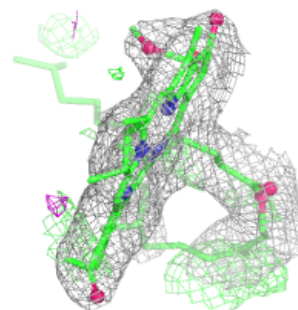
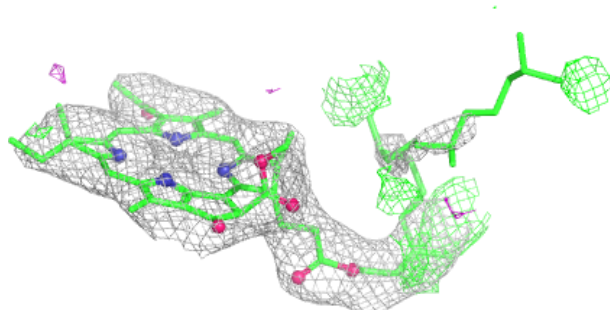
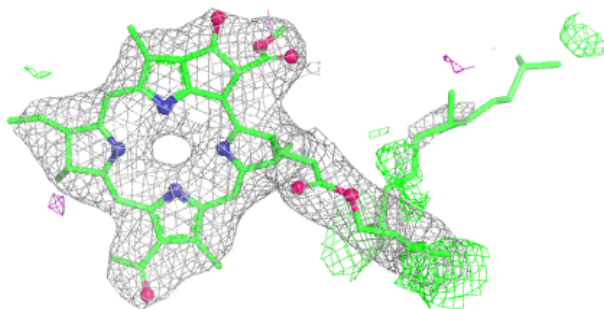
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	M	409	5/5	0.98	0.05	89,97,103,104	0
10	BCB	L	301[A]	66/66	0.98	0.10	65,75,91,109	66
10	BCB	L	301[B]	66/66	0.98	0.10	65,75,91,109	66
10	BCB	L	302[A]	66/66	0.98	0.10	72,80,112,115	66
5	HEC	C	401	43/43	0.99	0.08	90,98,112,127	0
5	HEC	C	402	43/43	0.99	0.07	82,94,105,131	0
5	HEC	C	403	43/43	0.99	0.07	73,82,93,96	0
5	HEC	C	404	43/43	0.99	0.06	75,84,101,123	0
12	FE	M	401[B]	1/1	1.00	0.02	88,88,88,88	1
12	FE	M	401[A]	1/1	1.00	0.02	88,88,88,88	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

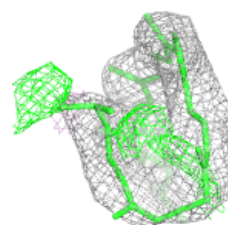
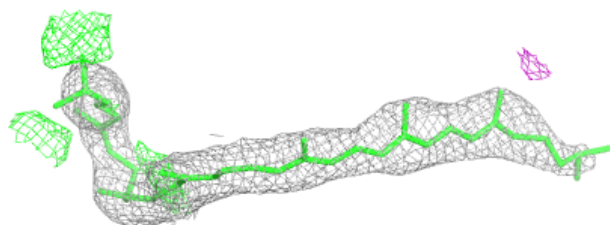
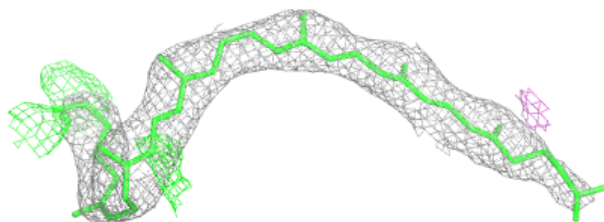


Electron density around BPB M 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

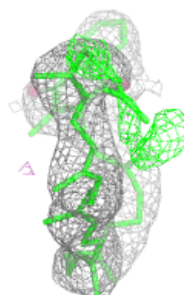
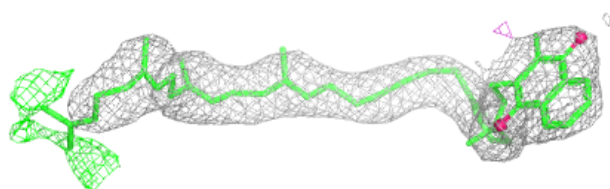
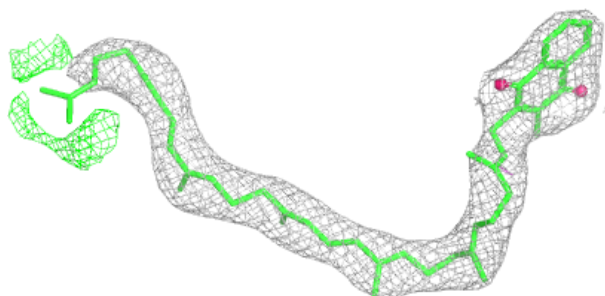
**Electron density around NS5 M 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

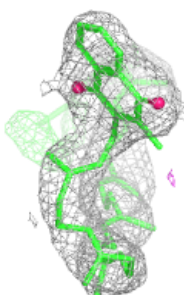
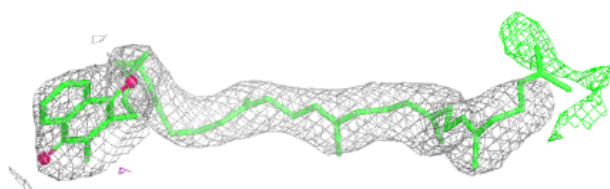
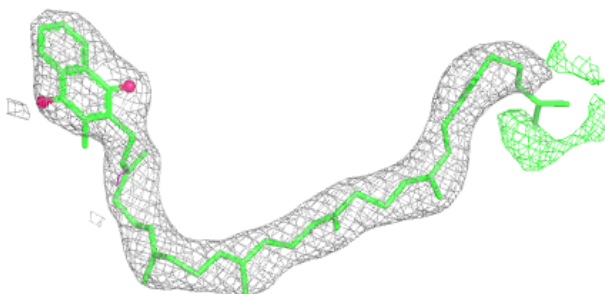


Electron density around MQ7 M 402 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

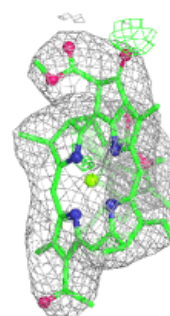
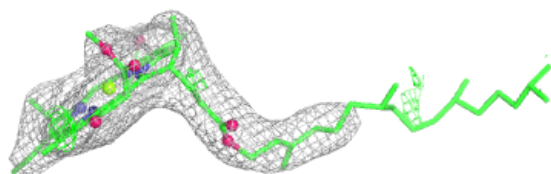
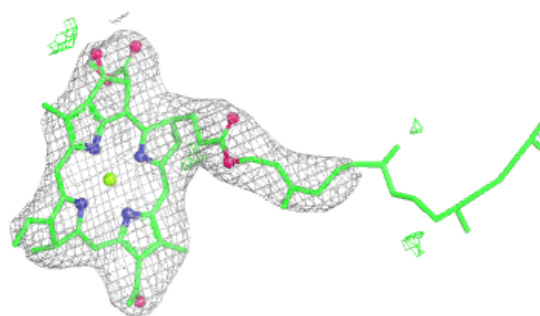
**Electron density around MQ7 M 402 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

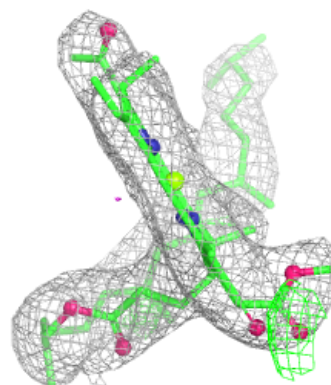
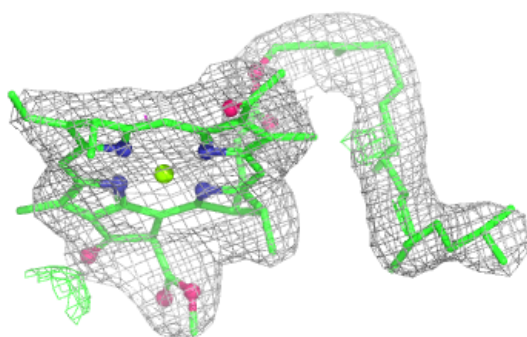
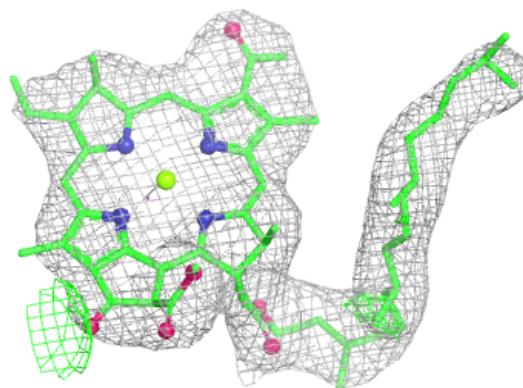


Electron density around BCB M 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

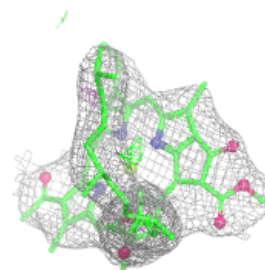
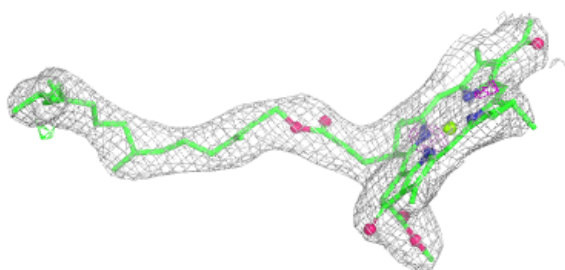
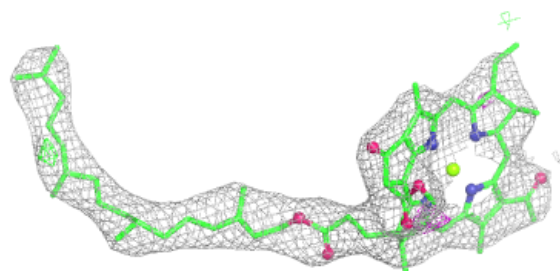
**Electron density around BCB L 302 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

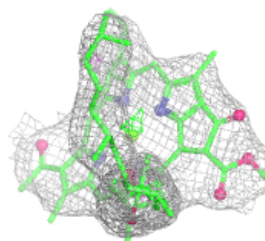
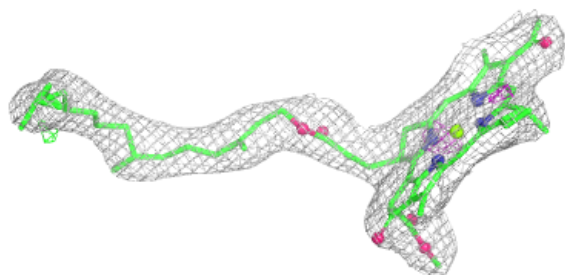
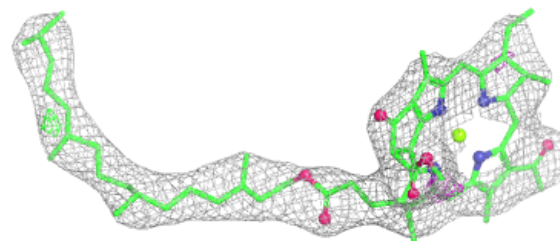


Electron density around BCB M 404 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

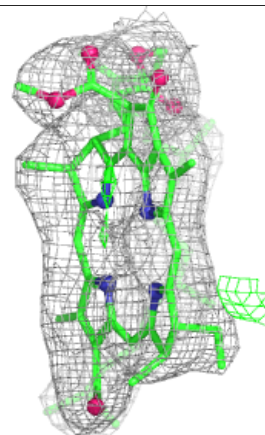
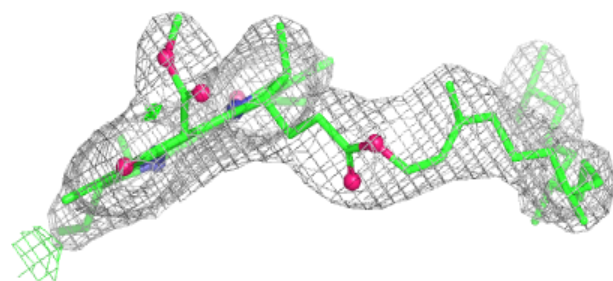
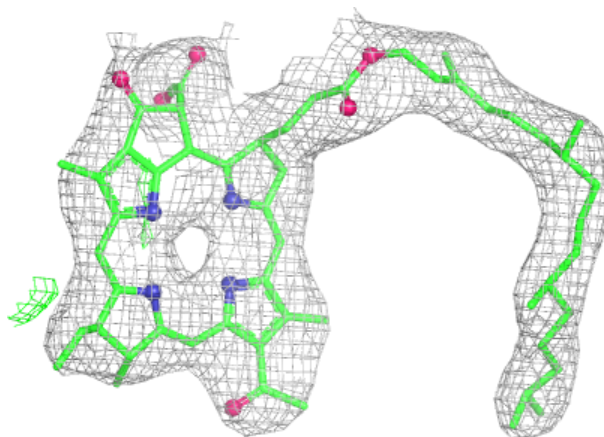
**Electron density around BCB M 404 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



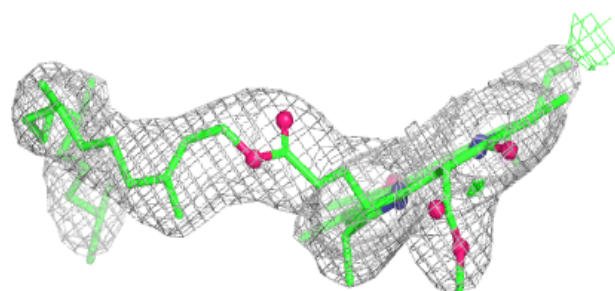
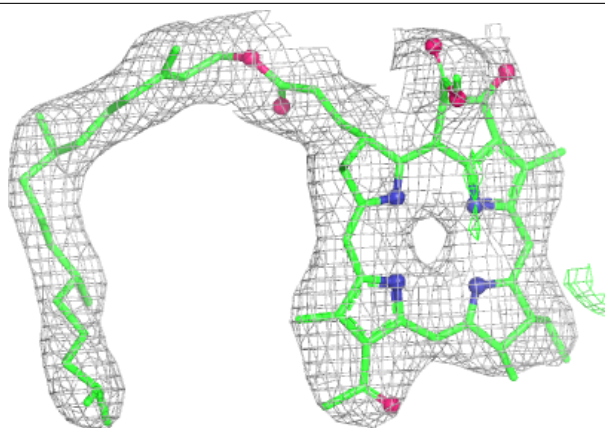
Electron density around BPB L 303 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



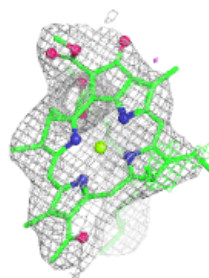
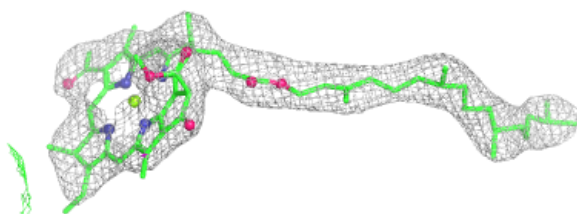
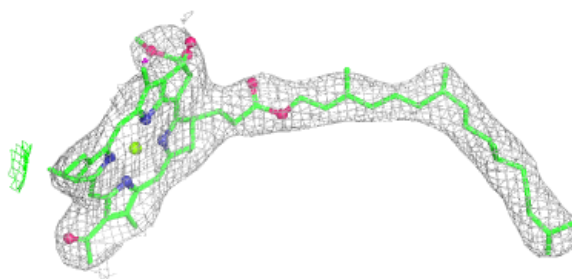
Electron density around BPB L 303 (B):

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

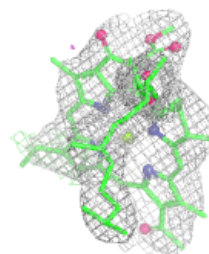
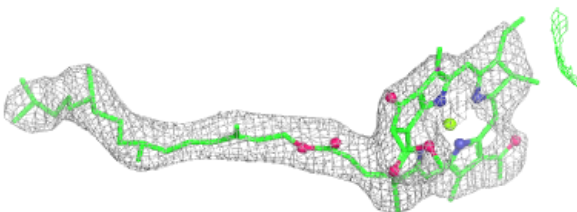
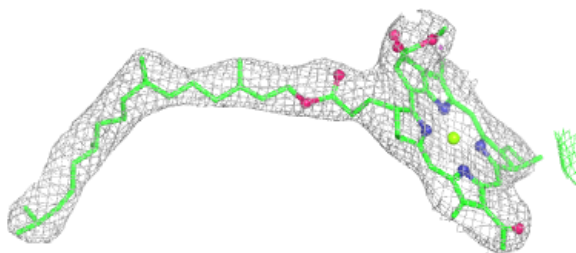


Electron density around BCB L 301 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

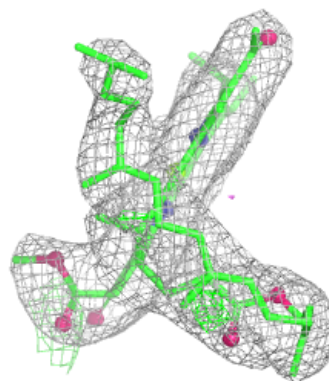
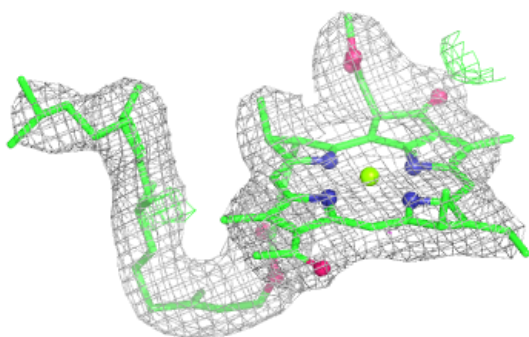
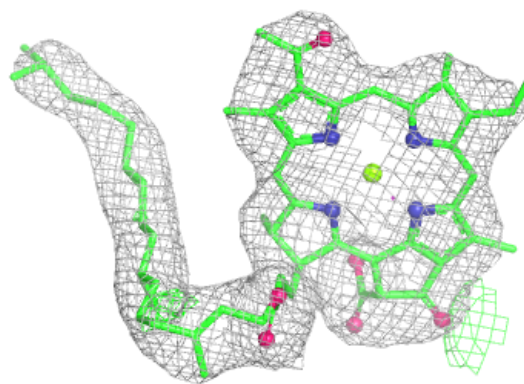
**Electron density around BCB L 301 (B):**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



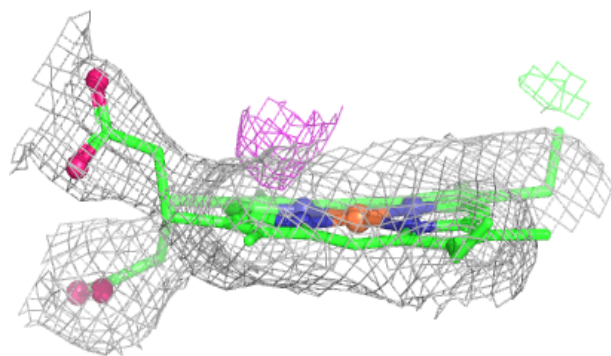
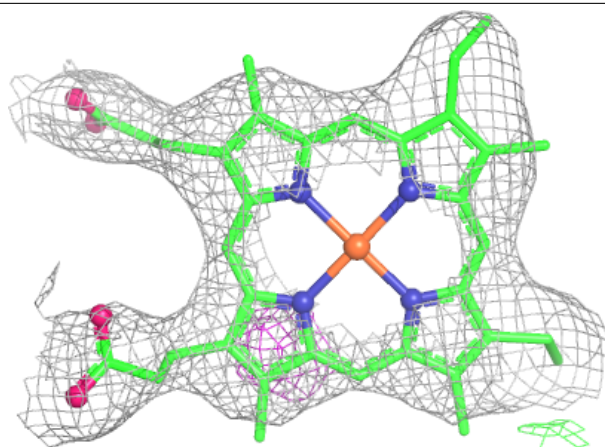
Electron density around BCB L 302 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



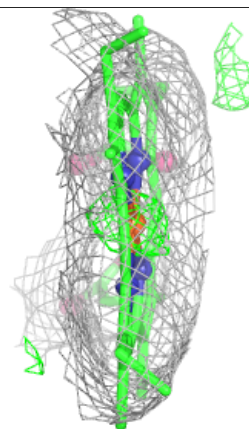
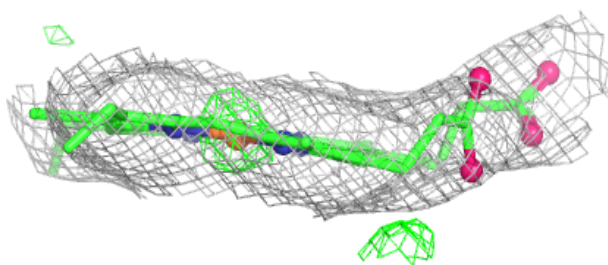
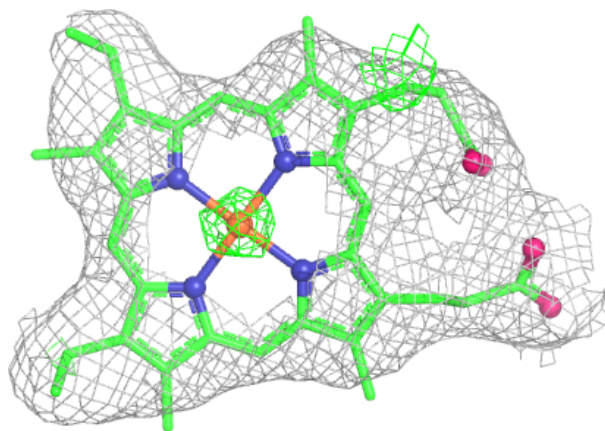
Electron density around HEC C 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



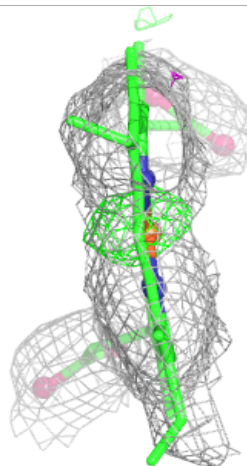
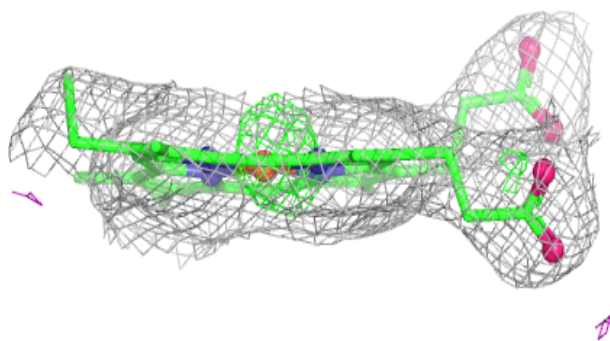
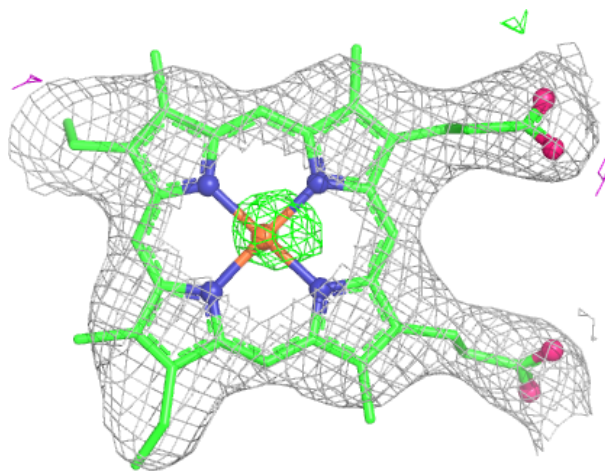
Electron density around HEC C 402:

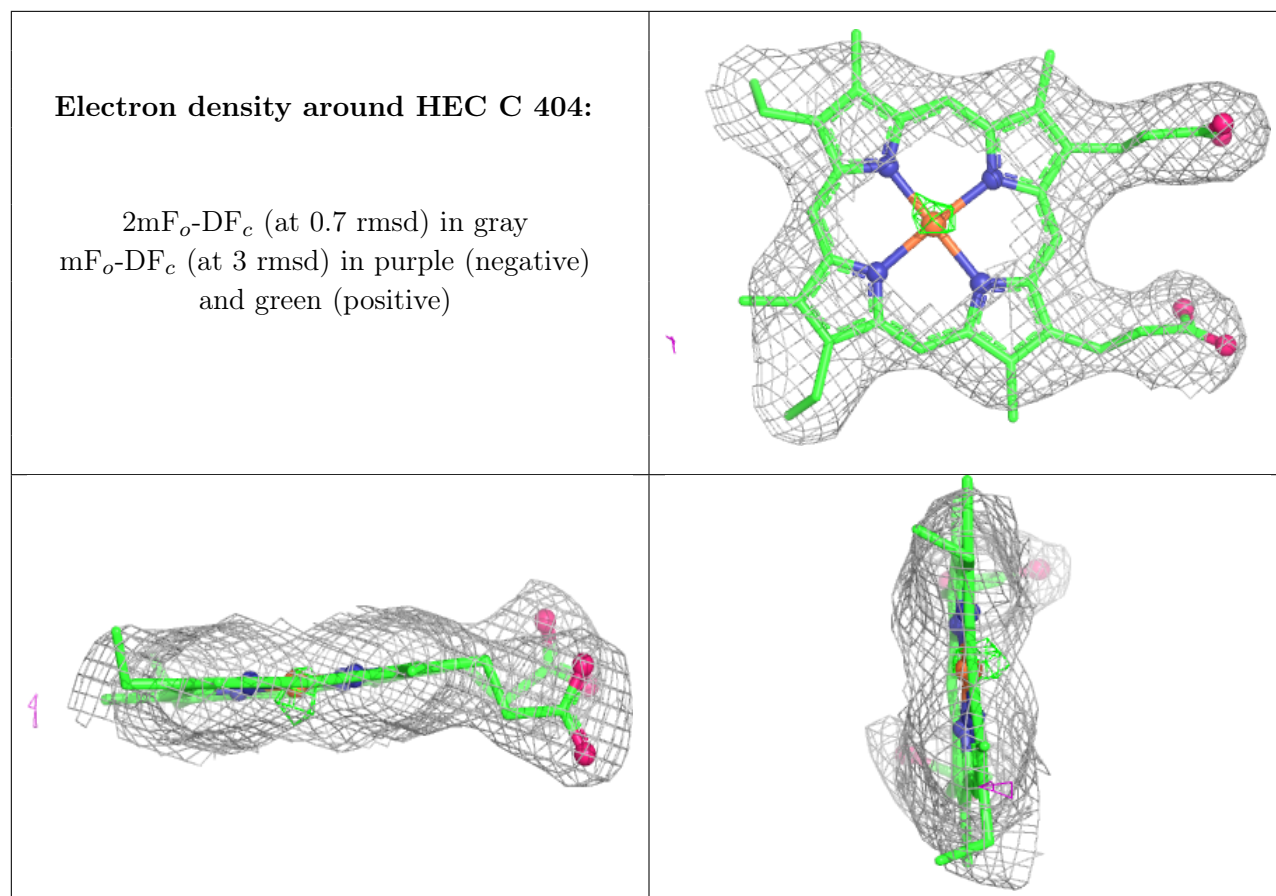
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.