



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:37 PM UTC

PDB ID : 6ZI9 / pdb_00006zi9
Title : Ultrafast Structural Response to Charge Redistribution Within a Photosynthetic Reaction Centre - 300 ps (b) structure
Authors : Baath, P.; Dods, R.; Braenden, G.; Neutze, R.
Deposited on : 2020-06-25
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

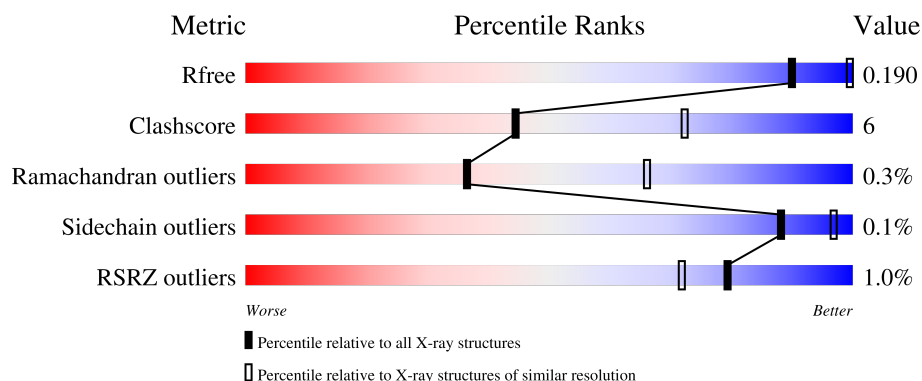
1 Overall quality at a glance ⓘ

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	% 90% 8% .
2	H	258	3% 86% 13% .
3	L	273	86% 14%
4	M	323	90% 10%

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	L	304	X	-	-	-
10	BCB	M	403[A]	X	-	-	-
10	BCB	M	403[B]	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 11472 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			

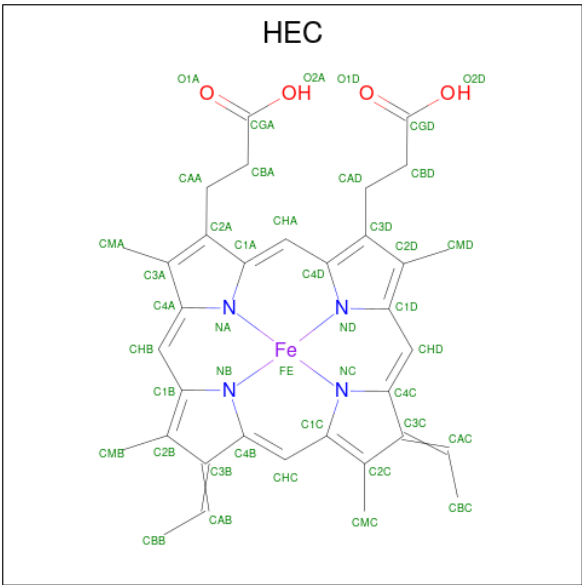
- Molecule 3 is a protein called Reaction center protein L chain.

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.

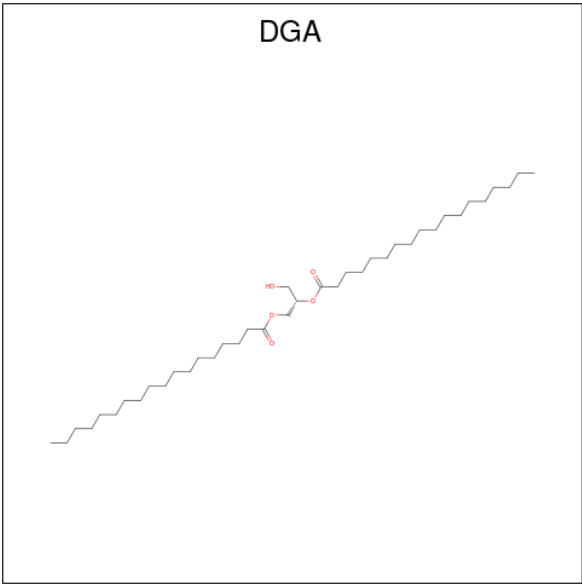
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	51	0
			2977	1983	491	490	13			

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



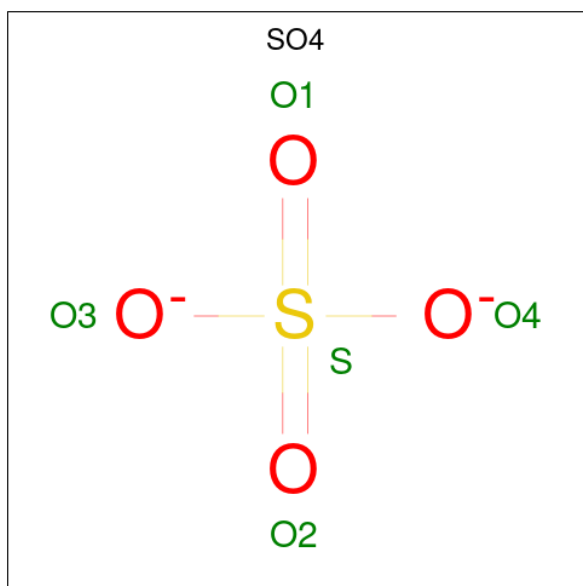
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



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).



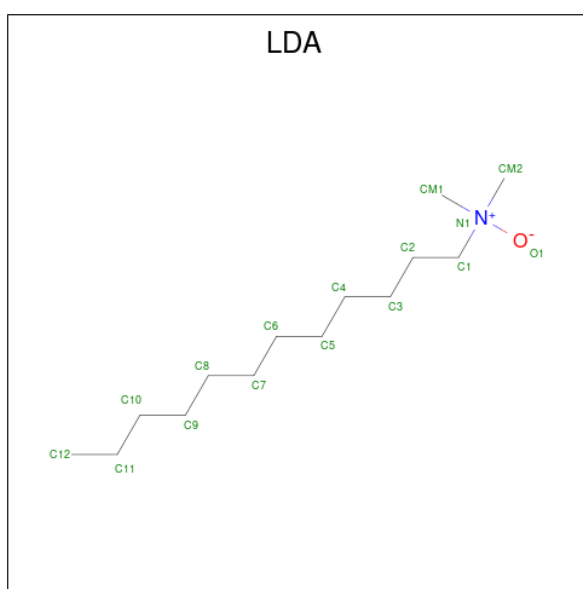
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total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

Continued on next page...

Continued from previous page...

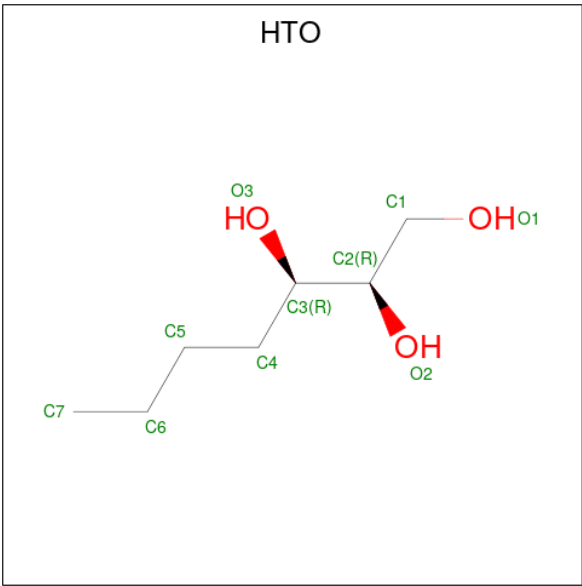
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		
7	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



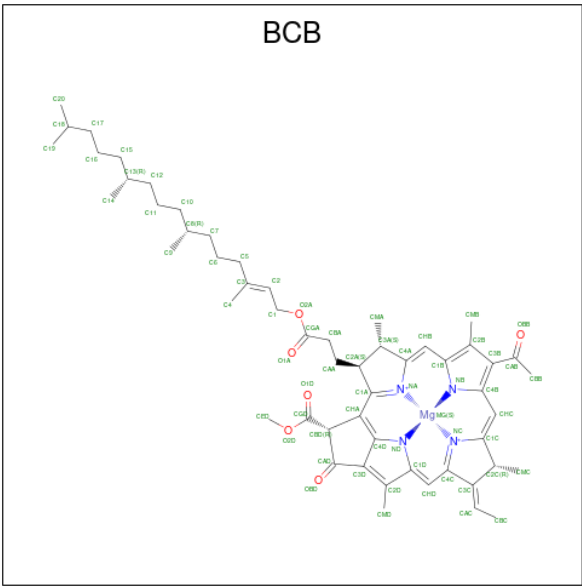
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: C₇H₁₆O₃).



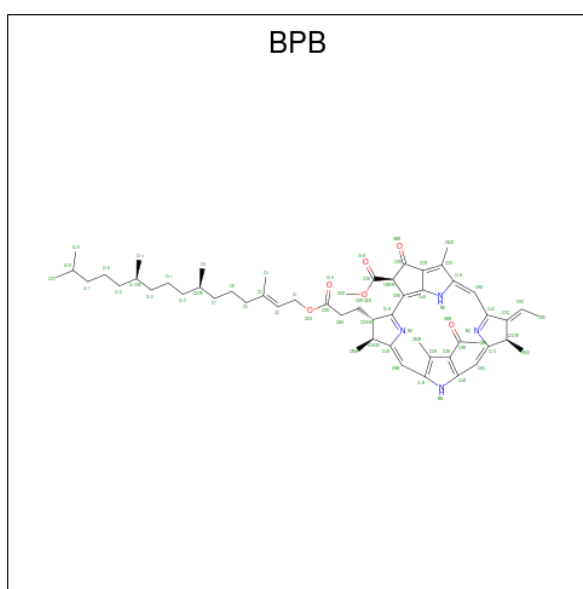
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆) (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		
10	L	1	Total	C	Mg	N	O	0	1
			132	110	2	8	12		
10	L	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).

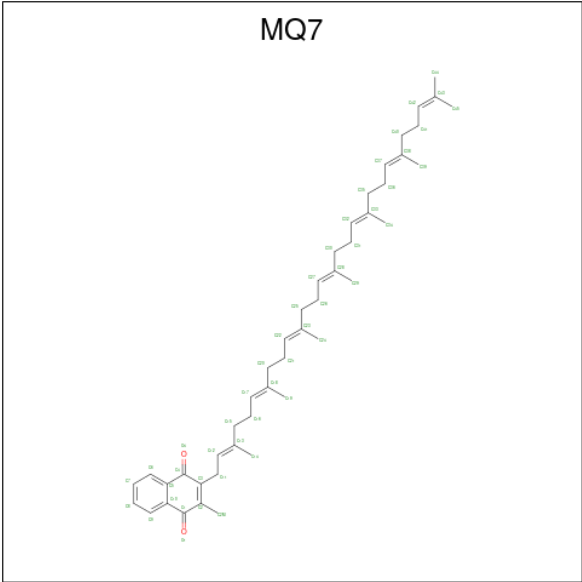


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	1
			130	110	8	12		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

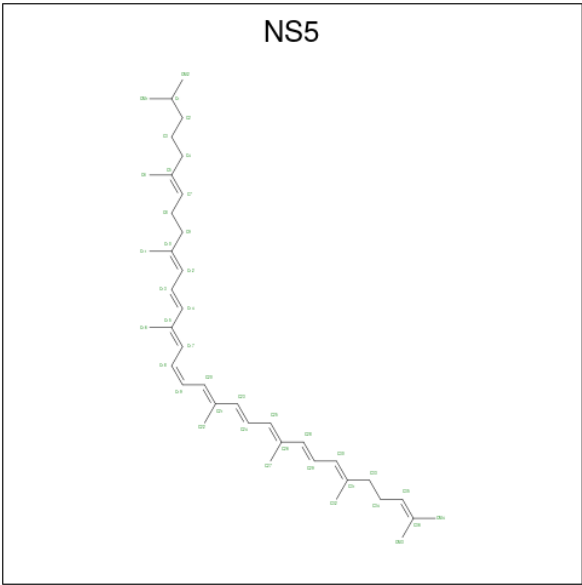
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	1
			2	2		

- 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		

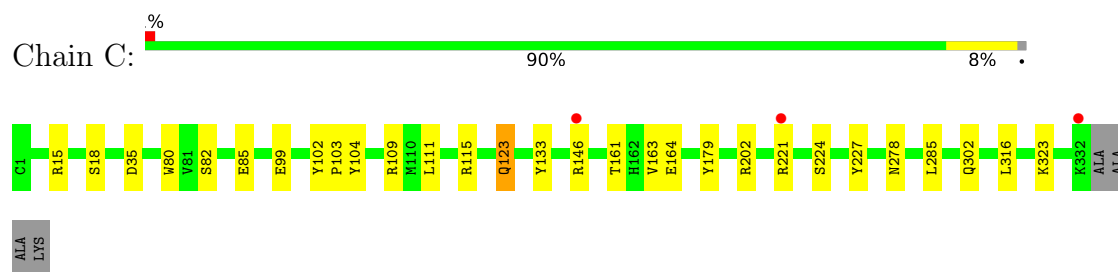
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	56	Total 56	O 56	0	0
15	H	27	Total 27	O 27	0	0
15	L	25	Total 25	O 25	0	0
15	M	38	Total 38	O 38	0	0

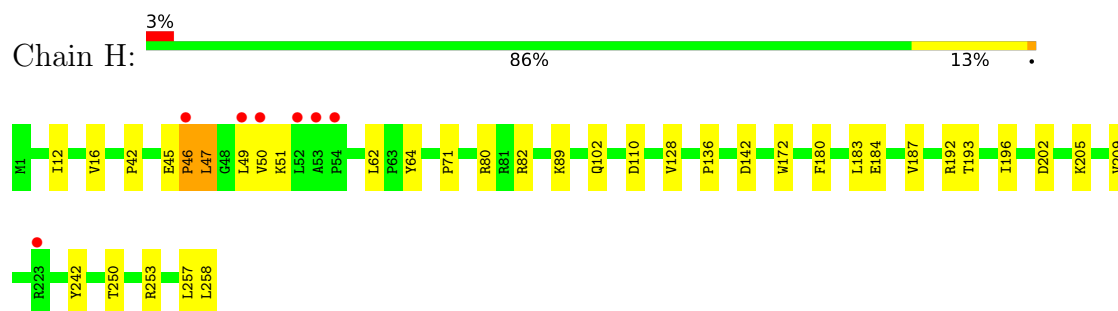
3 Residue-property plots

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.

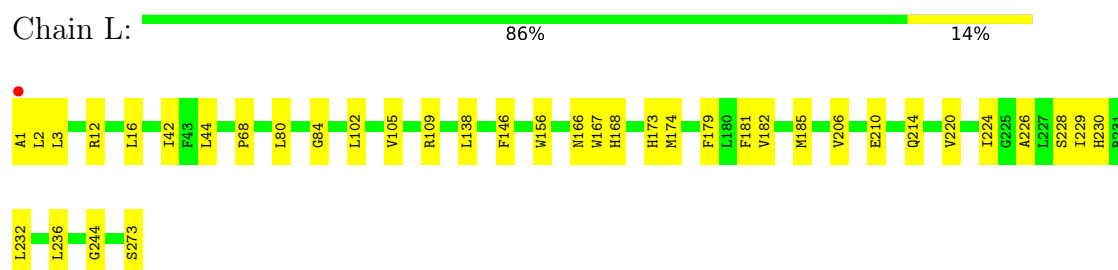
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



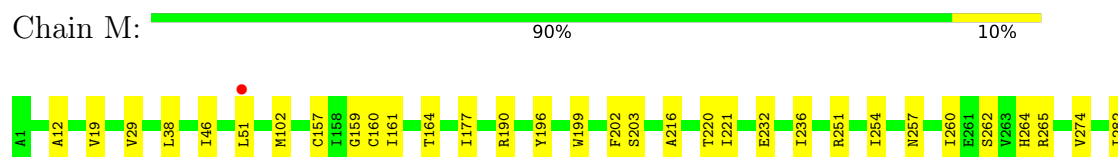
- Molecule 2: Reaction center protein H chain



- 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	226.50Å 226.50Å 113.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.31 – 2.80 34.31 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.31-2.80) 99.9 (34.31-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0158, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.166 , 0.190 0.169 , 0.190	Depositor DCC
R_{free} test set	3919 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	74.8	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11472	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: MQ7, BCB, FE, SO4, FME, HTO, HEC, LDA, BPB, NS5, DGA

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	0.37	0/2669	0.55	0/3637
2	H	0.38	0/2055	0.56	0/2807
3	L	0.34	0/2612	0.52	0/3568
4	M	0.35	0/3101	0.49	0/4242
All	All	0.36	0/10437	0.53	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	23	0
2	H	2018	0	2020	36	0
3	L	2508	0	2390	46	0
4	M	2977	0	2832	24	0
5	C	172	0	120	2	0
6	C	37	0	58	0	0
7	C	15	0	0	0	0
7	H	25	0	0	0	0
7	M	35	0	0	1	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	5	0
8	L	32	0	62	2	0
8	M	32	0	62	0	0
9	H	20	0	32	0	0
9	L	10	0	16	0	0
10	L	330	0	360	17	0
10	M	132	0	144	7	0
11	L	130	0	148	6	0
11	M	65	0	74	7	0
12	M	2	0	0	0	0
13	M	96	0	128	0	0
14	M	40	0	60	2	0
15	C	56	0	0	0	0
15	H	27	0	0	0	0
15	L	25	0	0	0	0
15	M	38	0	0	0	0
All	All	11472	0	11177	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (134) 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)
2:H:205:LYS:HD3	2:H:205:LYS:H	1.46	0.80
4:M:160:CYS:O	4:M:164:THR:HG23	1.82	0.78
2:H:184:GLU:OE2	2:H:193:THR:HG21	1.82	0.77
1:C:161:THR:HG21	3:L:273:SER:O	1.85	0.77
11:M:404:BPB:HHC	11:M:404:BPB:HBBB	1.67	0.77
1:C:161:THR:HB	1:C:164:GLU:HG3	1.68	0.75
4:M:38:LEU:HD23	4:M:46:ILE:HD11	1.73	0.71
1:C:161:THR:HG22	1:C:163:VAL:H	1.56	0.69
2:H:42:PRO:HD3	8:H:708:LDA:H121	1.74	0.69
1:C:161:THR:HG22	1:C:163:VAL:N	2.12	0.65
2:H:89:LYS:H	2:H:89:LYS:HE2	1.61	0.64
2:H:250:THR:OG1	2:H:253:ARG:HG3	1.97	0.64
1:C:278:ASN:HB3	1:C:302:GLN:HE21	1.63	0.63
1:C:111:LEU:O	1:C:115:ARG:HG3	1.99	0.62
3:L:42:ILE:HG12	11:L:303[B]:BPB:H6A	1.82	0.62
4:M:216[B]:ALA:O	4:M:220[B]:THR:OG1	2.15	0.61
2:H:128:VAL:HG22	3:L:210:GLU:CD	2.25	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:GLU:HG3	2:H:46:PRO:HD2	1.81	0.61
3:L:185:MET:HE3	10:L:304:BCB:H41	1.83	0.61
3:L:168[B]:HIS:CE1	10:L:301[B]:BCB:HMC2	2.35	0.60
2:H:80:ARG:CZ	2:H:82:ARG:HD2	2.32	0.60
2:H:196:ILE:HD12	2:H:242:TYR:CZ	2.37	0.60
3:L:3:LEU:HD11	4:M:251[B]:ARG:HD2	1.84	0.59
2:H:205:LYS:H	2:H:205:LYS:CD	2.14	0.57
3:L:185:MET:HE3	10:L:304:BCB:C4	2.35	0.56
10:M:403[B]:BCB:HBD	10:M:403[B]:BCB:HAA1	1.87	0.56
4:M:190:ARG:O	4:M:190:ARG:HD2	2.05	0.56
10:L:304:BCB:HBB3	10:M:403[A]:BCB:H62	1.88	0.55
2:H:196:ILE:HD12	2:H:242:TYR:CE1	2.42	0.55
1:C:123:GLN:NE2	1:C:123:GLN:H	2.04	0.54
1:C:18:SER:HB2	3:L:156[B]:TRP:CD1	2.42	0.54
3:L:224:ILE:HG12	3:L:228:SER:HB2	1.90	0.54
2:H:64:TYR:CE1	8:H:708:LDA:H11	2.43	0.54
2:H:89:LYS:HE3	2:H:110:ASP:HB3	1.90	0.54
4:M:260[B]:ILE:O	4:M:264[B]:HIS:ND1	2.40	0.53
3:L:185:MET:CE	10:L:304:BCB:H41	2.38	0.53
4:M:102:MET:HE1	4:M:164:THR:HG22	1.89	0.53
3:L:182:VAL:HG13	3:L:236[B]:LEU:HD22	1.90	0.53
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.44	0.53
10:L:301[B]:BCB:H2C	10:M:403[B]:BCB:H2C	1.90	0.53
2:H:183:LEU:HB2	2:H:196:ILE:CG2	2.39	0.53
2:H:142:ASP:OD1	2:H:142:ASP:N	2.35	0.53
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.44	0.52
3:L:16:LEU:HD11	3:L:105:VAL:CG2	2.39	0.52
3:L:181:PHE:HB3	11:M:404:BPB:HBBA	1.89	0.52
1:C:323:LYS:H	1:C:323:LYS:CD	2.22	0.52
2:H:128:VAL:CG2	3:L:210:GLU:CD	2.83	0.52
3:L:181:PHE:CD2	11:M:404:BPB:HBB	2.45	0.52
2:H:180:PHE:CE2	4:M:12:ALA:HB2	2.46	0.51
3:L:166[B]:ASN:OD1	3:L:168[B]:HIS:HB2	2.10	0.51
4:M:262[B]:SER:HA	4:M:265[B]:ARG:HG3	1.91	0.51
2:H:12:ILE:O	2:H:16:VAL:HG23	2.11	0.51
3:L:168[A]:HIS:CE1	10:L:301[A]:BCB:HMC2	2.46	0.51
3:L:244[A]:GLY:O	10:L:301[A]:BCB:HED3	2.11	0.51
3:L:3:LEU:HD11	4:M:251[A]:ARG:HD2	1.93	0.51
11:L:303[B]:BPB:OBB	11:L:303[B]:BPB:HHC	2.12	0.50
2:H:257:LEU:HD11	3:L:109:ARG:CZ	2.42	0.50
10:L:304:BCB:HHC	10:L:304:BCB:HBB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLN:H	1:C:123:GLN:HE21	1.60	0.49
3:L:174[B]:MET:HE3	10:L:304:BCB:HED2	1.95	0.49
10:M:403[B]:BCB:H3A	10:M:403[B]:BCB:O1A	2.13	0.49
1:C:161:THR:HG21	3:L:273:SER:C	2.37	0.48
3:L:224:ILE:HG12	3:L:228:SER:CB	2.43	0.48
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.48	0.48
2:H:45:GLU:O	2:H:47:LEU:N	2.47	0.48
2:H:187:VAL:CG2	2:H:192:ARG:HG3	2.44	0.48
5:C:402:HEC:HHA	5:C:402:HEC:O1D	2.14	0.47
4:M:29:VAL:HG21	4:M:51:LEU:HD12	1.96	0.47
2:H:49:LEU:O	2:H:51:LYS:N	2.48	0.47
8:H:701:LDA:HM21	8:L:305:LDA:HM22	1.97	0.47
4:M:251[B]:ARG:NH1	4:M:257[B]:ASN:OD1	2.39	0.47
2:H:250:THR:HG1	2:H:253:ARG:HG3	1.80	0.46
10:L:301[B]:BCB:H41	10:L:301[B]:BCB:H62	1.65	0.46
4:M:282:ILE:HD11	10:M:403[B]:BCB:OBD	2.16	0.46
3:L:174[B]:MET:HA	10:L:304:BCB:OBD	2.16	0.46
1:C:224:SER:HA	1:C:227:TYR:HD1	1.81	0.46
10:M:403[B]:BCB:H52	11:M:404:BPB:CHC	2.46	0.46
2:H:45:GLU:HG3	2:H:46:PRO:CD	2.45	0.45
3:L:230[B]:HIS:CD2	4:M:221[B]:ILE:HG13	2.51	0.45
3:L:167[A]:TRP:HE1	3:L:173[A]:HIS:CD2	2.35	0.45
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.17	0.45
3:L:232:LEU:HG	3:L:236[B]:LEU:CD1	2.46	0.45
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.98	0.45
3:L:220:VAL:HG11	11:M:404:BPB:HEDA	1.99	0.45
11:L:303[B]:BPB:HEDB	4:M:254:ILE:HG21	1.99	0.44
2:H:80:ARG:NH2	2:H:82:ARG:HD2	2.33	0.44
3:L:138:LEU:HD23	3:L:138:LEU:HA	1.78	0.44
8:L:305:LDA:H22	8:L:305:LDA:HM21	1.60	0.44
4:M:159:GLY:HA3	14:M:405:NS5:H272	1.98	0.44
3:L:42:ILE:HA	11:L:303[B]:BPB:H9A	1.98	0.44
4:M:265[B]:ARG:NH2	7:M:408:SO4:O1	2.44	0.44
11:M:404:BPB:H14	11:M:404:BPB:H16A	1.61	0.44
1:C:146:ARG:HD3	1:C:179:TYR:CE1	2.53	0.44
3:L:44:LEU:HD12	3:L:44:LEU:HA	1.70	0.44
4:M:196[B]:TYR:O	4:M:292:TRP:HB3	2.17	0.44
2:H:62:LEU:O	8:H:708:LDA:HM21	2.18	0.43
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.00	0.43
2:H:89:LYS:HE3	2:H:110:ASP:CB	2.48	0.43
3:L:181:PHE:HB3	11:M:404:BPB:CBB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.01	0.43
2:H:102:GLN:NE2	3:L:12:ARG:HD3	2.33	0.43
10:L:304:BCB:H43	10:L:304:BCB:H11	1.85	0.43
3:L:226:ALA:O	3:L:229:ILE:HG22	2.18	0.43
4:M:157:CYS:HA	4:M:161:ILE:HB	1.99	0.43
10:M:403[B]:BCB:H91	10:M:403[B]:BCB:H111	1.80	0.43
1:C:323:LYS:H	1:C:323:LYS:HD3	1.84	0.43
3:L:1:ALA:C	3:L:2:LEU:HD23	2.44	0.43
3:L:232:LEU:HG	3:L:236[B]:LEU:HD11	2.00	0.42
4:M:199[B]:TRP:HA	4:M:202[B]:PHE:HB2	2.01	0.42
4:M:232[B]:GLU:O	4:M:236:ILE:HG13	2.18	0.42
10:L:301[A]:BCB:H62	10:L:301[A]:BCB:H41	1.93	0.42
4:M:203[B]:SER:OG	4:M:274:VAL:O	2.37	0.42
14:M:405:NS5:H18	14:M:405:NS5:H161	1.86	0.42
1:C:15:ARG:HD2	3:L:68:PRO:O	2.18	0.42
10:L:301[A]:BCB:H151	11:L:303[A]:BPB:H5A	2.00	0.42
3:L:102:LEU:O	3:L:105:VAL:HG22	2.19	0.42
1:C:202:ARG:O	1:C:221:ARG:NH2	2.47	0.42
2:H:257:LEU:HD13	3:L:16:LEU:HD23	2.02	0.42
1:C:109:ARG:HG2	1:C:285:LEU:HD21	2.02	0.42
2:H:136:PRO:HA	2:H:172:TRP:HA	2.01	0.42
2:H:71:PRO:HD3	3:L:206:VAL:HG22	2.01	0.41
11:L:303[A]:BPB:OBB	11:L:303[A]:BPB:HHC	2.20	0.41
4:M:236:ILE:HG12	4:M:260[A]:ILE:HG23	2.01	0.41
2:H:257:LEU:HD12	2:H:257:LEU:H	1.86	0.41
3:L:146:PHE:HB3	3:L:156[A]:TRP:CD2	2.56	0.41
3:L:244[B]:GLY:O	10:L:301[B]:BCB:HED3	2.21	0.41
5:C:403:HEC:HBC1	5:C:404:HEC:HMA3	2.03	0.41
2:H:47:LEU:CD1	2:H:49:LEU:HB3	2.51	0.41
2:H:128:VAL:HG22	3:L:210:GLU:HB2	2.03	0.41
2:H:257:LEU:C	2:H:258:LEU:HD12	2.46	0.41
8:H:707:LDA:H123	10:L:302[A]:BCB:HED3	2.03	0.40
3:L:80:LEU:HA	3:L:84:GLY:HA3	2.02	0.40
1:C:99:GLU:HG2	1:C:104:TYR:CE1	2.56	0.40
3:L:179:PHE:HA	3:L:182:VAL:HG12	2.04	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 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%)	320 (97%)	10 (3%)	0	100	100
2	H	256/258 (99%)	248 (97%)	5 (2%)	3 (1%)	10	34
3	L	312/273 (114%)	301 (96%)	11 (4%)	0	100	100
4	M	372/323 (115%)	355 (95%)	16 (4%)	1 (0%)	36	66
All	All	1270/1190 (107%)	1224 (96%)	42 (3%)	4 (0%)	36	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE
2	H	46	PRO
2	H	47	LEU
2	H	50	VAL

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 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%)	280 (100%)	1 (0%)	84	94
2	H	212/212 (100%)	212 (100%)	0	100	100
3	L	253/218 (116%)	253 (100%)	0	100	100
4	M	288/249 (116%)	288 (100%)	0	100	100
All	All	1034/961 (108%)	1033 (100%)	1 (0%)	88	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	123	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	120	ASN
1	C	123	GLN
1	C	302	GLN
2	H	72	HIS
2	H	102	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	1.02	0	8,9,11	1.03	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	-

There are no bond length outliers.

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	CA-CB-CG-SD

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 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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	$\# Z > 2$
8	LDA	M	414	-	13,15,15	1.27	1 (7%)	14,17,17	0.52	0
14	NS5	M	405	-	39,39,39	1.33	2 (5%)	46,46,46	2.09	15 (32%)
10	BCB	L	302[A]	-	60,74,74	2.95	18 (30%)	59,115,115	3.03	21 (35%)
9	HTO	H	709	-	9,9,9	0.88	0	10,10,10	0.60	0
7	SO4	H	705	-	4,4,4	0.38	0	6,6,6	0.31	0
13	MQ7	M	402[A]	-	49,49,49	1.56	2 (4%)	61,63,63	1.54	15 (24%)
5	HEC	C	402	1	46,50,50	1.68	3 (6%)	58,82,82	1.83	7 (12%)
7	SO4	C	407	-	4,4,4	0.27	0	6,6,6	0.16	0
7	SO4	H	702	-	4,4,4	0.35	0	6,6,6	0.28	0
10	BCB	L	302[B]	-	60,74,74	2.95	18 (30%)	59,115,115	2.95	21 (35%)
7	SO4	M	411	-	4,4,4	0.39	0	6,6,6	0.29	0
9	HTO	H	710	-	9,9,9	0.88	0	10,10,10	1.02	1 (10%)
11	BPB	M	404	-	57,70,70	2.56	13 (22%)	55,101,101	2.64	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	M	407	-	4,4,4	0.27	0	6,6,6	0.20	0
10	BCB	L	304	-	60,74,74	2.89	18 (30%)	59,115,115	2.84	20 (33%)
8	LDA	L	305	-	13,15,15	1.44	1 (7%)	14,17,17	0.69	0
13	MQ7	M	402[B]	-	49,49,49	1.49	2 (4%)	61,63,63	1.56	14 (22%)
7	SO4	M	409	-	4,4,4	0.40	0	6,6,6	0.26	0
7	SO4	H	703	-	4,4,4	0.34	0	6,6,6	0.13	0
9	HTO	L	307	-	9,9,9	0.75	0	10,10,10	1.19	1 (10%)
8	LDA	H	701	-	13,15,15	1.23	1 (7%)	14,17,17	0.76	0
7	SO4	M	406	-	4,4,4	0.22	0	6,6,6	0.25	0
10	BCB	L	301[A]	-	60,74,74	3.01	18 (30%)	59,115,115	2.70	17 (28%)
5	HEC	C	401	1	46,50,50	1.68	4 (8%)	58,82,82	2.15	10 (17%)
7	SO4	C	408	-	4,4,4	0.27	0	6,6,6	0.16	0
11	BPB	L	303[A]	-	57,70,70	2.52	12 (21%)	55,101,101	2.84	17 (30%)
6	DGA	C	405	1	36,36,43	1.20	3 (8%)	38,38,45	1.17	3 (7%)
5	HEC	C	404	1	46,50,50	1.71	2 (4%)	58,82,82	1.82	6 (10%)
8	LDA	H	707	-	13,15,15	1.32	1 (7%)	14,17,17	0.82	0
10	BCB	L	301[B]	-	60,74,74	3.00	18 (30%)	59,115,115	2.67	23 (38%)
11	BPB	L	303[B]	-	57,70,70	2.56	12 (21%)	55,101,101	2.98	19 (34%)
7	SO4	M	410	-	4,4,4	0.27	0	6,6,6	0.20	0
5	HEC	C	403	1	46,50,50	1.72	3 (6%)	58,82,82	2.10	9 (15%)
8	LDA	H	708	-	13,15,15	1.67	1 (7%)	14,17,17	0.84	0
7	SO4	H	706	-	4,4,4	0.30	0	6,6,6	0.12	0
10	BCB	M	403[A]	-	60,74,74	3.01	17 (28%)	59,115,115	2.68	19 (32%)
7	SO4	M	412	-	4,4,4	0.36	0	6,6,6	0.20	0
8	LDA	L	306	-	13,15,15	1.41	1 (7%)	14,17,17	0.64	0
7	SO4	M	408	-	4,4,4	0.25	0	6,6,6	0.28	0
10	BCB	M	403[B]	-	60,74,74	3.04	17 (28%)	59,115,115	2.97	21 (35%)
7	SO4	C	406	-	4,4,4	0.36	0	6,6,6	0.39	0
7	SO4	H	704	-	4,4,4	0.23	0	6,6,6	0.14	0
8	LDA	M	413	-	13,15,15	1.33	1 (7%)	14,17,17	0.55	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
8	LDA	M	414	-	-	4/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NS5	M	405	-	-	9/43/43/43	-
10	BCB	L	302[A]	-	2/2/21/26	4/37/137/137	-
9	HTO	H	709	-	-	4/10/10/10	-
13	MQ7	M	402[A]	-	-	0/41/61/61	0/2/2/2
5	HEC	C	402	1	-	6/14/54/54	-
10	BCB	L	302[B]	-	2/2/21/26	12/37/137/137	-
9	HTO	H	710	-	-	0/10/10/10	-
11	BPB	M	404	-	-	6/37/105/105	0/5/6/6
10	BCB	L	304	-	3/3/21/26	12/37/137/137	-
8	LDA	L	305	-	-	5/13/13/13	-
13	MQ7	M	402[B]	-	-	1/41/61/61	0/2/2/2
9	HTO	L	307	-	-	5/10/10/10	-
8	LDA	H	701	-	-	3/13/13/13	-
10	BCB	L	301[A]	-	3/3/21/26	8/37/137/137	-
5	HEC	C	401	1	-	7/14/54/54	-
11	BPB	L	303[A]	-	-	5/37/105/105	0/5/6/6
6	DGA	C	405	1	-	16/37/37/45	-
10	BCB	L	301[B]	-	3/3/21/26	10/37/137/137	-
8	LDA	H	707	-	-	6/13/13/13	-
5	HEC	C	404	1	-	4/14/54/54	-
11	BPB	L	303[B]	-	-	14/37/105/105	0/5/6/6
5	HEC	C	403	1	-	6/14/54/54	-
8	LDA	H	708	-	-	7/13/13/13	-
10	BCB	M	403[A]	-	2/2/21/26	11/37/137/137	-
8	LDA	L	306	-	-	10/13/13/13	-
10	BCB	M	403[B]	-	3/3/21/26	14/37/137/137	-
8	LDA	M	413	-	-	4/13/13/13	-

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302[A]	BCB	C1B-C2B	9.56	1.50	1.39
11	L	303[A]	BPB	C1B-C2B	9.30	1.49	1.39
11	M	404	BPB	C1B-C2B	9.19	1.49	1.39
10	L	301[A]	BCB	C1A-CHA	9.11	1.50	1.40
10	L	302[B]	BCB	C1B-C2B	9.03	1.49	1.39
11	L	303[B]	BPB	C1B-C2B	9.03	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403[A]	BCB	C1A-CHA	8.93	1.50	1.40
13	M	402[A]	MQ7	C3-C2	8.77	1.50	1.35
10	L	304	BCB	C1B-C2B	8.52	1.49	1.39
10	M	403[B]	BCB	C1A-CHA	8.35	1.49	1.40
10	L	301[B]	BCB	C1A-CHA	8.25	1.49	1.40
10	L	301[B]	BCB	C1D-C2D	8.06	1.48	1.39
10	L	301[B]	BCB	CHC-C1C	8.03	1.48	1.38
13	M	402[B]	MQ7	C3-C2	7.98	1.49	1.35
10	L	301[A]	BCB	CHC-C1C	7.88	1.48	1.38
10	L	302[B]	BCB	CHC-C1C	7.79	1.48	1.38
10	M	403[B]	BCB	CHC-C1C	7.78	1.48	1.38
10	M	403[B]	BCB	C1B-C2B	7.77	1.48	1.39
10	L	301[A]	BCB	C1B-C2B	7.76	1.48	1.39
11	L	303[B]	BPB	C1D-C2D	7.69	1.48	1.39
10	M	403[A]	BCB	C1B-C2B	7.65	1.48	1.39
10	M	403[A]	BCB	CHC-C1C	7.63	1.47	1.38
10	M	403[B]	BCB	C1D-C2D	7.58	1.48	1.39
10	L	304	BCB	C1A-CHA	7.53	1.48	1.40
10	L	302[A]	BCB	CHC-C1C	7.51	1.47	1.38
10	L	302[B]	BCB	C1A-CHA	7.50	1.48	1.40
10	L	302[A]	BCB	C1A-CHA	7.33	1.48	1.40
10	L	301[B]	BCB	C1B-C2B	7.26	1.47	1.39
11	M	404	BPB	C1D-C2D	7.22	1.47	1.39
11	L	303[A]	BPB	C1D-C2D	7.10	1.47	1.39
10	M	403[A]	BCB	C1D-C2D	7.08	1.47	1.39
14	M	405	NS5	C35-C36	7.04	1.53	1.32
10	L	304	BCB	CHC-C1C	7.04	1.47	1.38
5	C	404	HEC	CAC-C3C	6.96	1.57	1.35
10	L	301[A]	BCB	C1D-C2D	6.82	1.47	1.39
10	L	304	BCB	C1D-C2D	6.79	1.47	1.39
5	C	401	HEC	CAC-C3C	6.70	1.56	1.35
5	C	403	HEC	CAC-C3C	6.66	1.56	1.35
5	C	402	HEC	CAC-C3C	6.57	1.56	1.35
10	L	302[A]	BCB	C1D-C2D	6.55	1.47	1.39
10	L	302[B]	BCB	C1D-C2D	6.39	1.46	1.39
11	M	404	BPB	C4D-CHA	6.33	1.49	1.39
5	C	402	HEC	CAB-C3B	6.30	1.55	1.35
5	C	403	HEC	CAB-C3B	6.28	1.55	1.35
5	C	404	HEC	CAB-C3B	6.19	1.55	1.35
11	L	303[A]	BPB	C4D-CHA	6.08	1.48	1.39
10	L	304	BCB	CHC-C4B	6.03	1.49	1.39
8	H	708	LDA	C1-N1	-5.94	1.45	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	303[B]	BPB	C3B-C2B	5.71	1.49	1.39
5	C	401	HEC	CAB-C3B	5.65	1.53	1.35
10	L	304	BCB	C3D-C2D	5.62	1.49	1.39
10	L	302[B]	BCB	CHC-C4B	5.57	1.48	1.39
10	L	301[A]	BCB	C3D-C2D	5.56	1.49	1.39
11	L	303[B]	BPB	C4D-CHA	5.56	1.47	1.39
10	M	403[B]	BCB	CHC-C4B	5.53	1.48	1.39
10	M	403[A]	BCB	C3B-C4B	5.53	1.50	1.41
10	M	403[B]	BCB	C3D-C2D	5.48	1.49	1.39
10	L	302[A]	BCB	CHB-C1B	5.48	1.48	1.39
10	M	403[A]	BCB	C3D-C2D	5.47	1.49	1.39
10	M	403[A]	BCB	CHC-C4B	5.46	1.48	1.39
10	L	302[B]	BCB	OBD-CAD	5.45	1.29	1.22
10	L	301[B]	BCB	C3B-C4B	5.43	1.50	1.41
10	M	403[A]	BCB	O2D-CGD	5.40	1.46	1.33
10	M	403[B]	BCB	C3B-C4B	5.40	1.50	1.41
10	L	301[A]	BCB	CHC-C4B	5.38	1.48	1.39
10	L	301[B]	BCB	C3B-C2B	5.35	1.48	1.39
10	M	403[B]	BCB	C3B-C2B	5.35	1.48	1.39
11	L	303[A]	BPB	C3B-C2B	5.33	1.48	1.39
10	L	301[B]	BCB	C3D-C2D	5.29	1.48	1.39
10	L	301[A]	BCB	C3B-C2B	5.27	1.48	1.39
10	L	301[A]	BCB	C3B-C4B	5.26	1.49	1.41
13	M	402[B]	MQ7	C10-C5	5.24	1.49	1.40
11	L	303[B]	BPB	O2D-CGD	5.21	1.46	1.33
10	L	302[B]	BCB	C3B-C4B	5.20	1.49	1.41
10	L	304	BCB	CHB-C1B	5.20	1.48	1.39
10	L	302[A]	BCB	CHC-C4B	5.19	1.48	1.39
10	M	403[A]	BCB	C3B-C2B	5.18	1.48	1.39
11	L	303[A]	BPB	O2D-CGD	5.16	1.45	1.33
10	L	302[A]	BCB	C3D-C2D	5.13	1.48	1.39
10	L	302[A]	BCB	C3B-C2B	5.11	1.48	1.39
11	M	404	BPB	O2A-CGA	5.11	1.48	1.33
10	L	302[B]	BCB	C3B-C2B	5.11	1.48	1.39
10	L	302[B]	BCB	C3D-C2D	5.08	1.48	1.39
11	L	303[B]	BPB	C3D-C2D	5.07	1.48	1.39
10	M	403[B]	BCB	O2D-CGD	5.07	1.45	1.33
10	L	301[A]	BCB	OBD-CAD	5.04	1.28	1.22
10	L	301[B]	BCB	CHC-C4B	5.01	1.47	1.39
10	L	302[B]	BCB	CHB-C1B	5.01	1.47	1.39
8	L	305	LDA	C1-N1	-5.01	1.46	1.51
10	M	403[B]	BCB	OBD-CAD	4.97	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	304	BCB	O2D-CGD	4.95	1.45	1.33
11	L	303[B]	BPB	OBD-CAD	4.91	1.28	1.22
11	L	303[A]	BPB	C3D-C2D	4.89	1.48	1.39
8	L	306	LDA	C1-N1	-4.89	1.46	1.51
10	M	403[A]	BCB	CHB-C1B	4.87	1.47	1.39
10	M	403[B]	BCB	CHA-CBD	-4.87	1.46	1.51
11	M	404	BPB	O2D-CGD	4.85	1.45	1.33
11	M	404	BPB	OBD-CAD	4.85	1.28	1.22
10	L	301[A]	BCB	O2D-CGD	4.83	1.45	1.33
10	L	302[A]	BCB	O2D-CGD	4.82	1.45	1.33
10	L	301[B]	BCB	OBD-CAD	4.80	1.28	1.22
10	L	304	BCB	C3B-C2B	4.80	1.47	1.39
10	L	302[A]	BCB	OBD-CAD	4.78	1.28	1.22
11	M	404	BPB	C3B-C2B	4.75	1.47	1.39
10	M	403[B]	BCB	CHB-C1B	4.73	1.47	1.39
10	L	302[A]	BCB	C3B-C4B	4.72	1.49	1.41
10	L	301[B]	BCB	O2D-CGD	4.71	1.44	1.33
10	L	301[A]	BCB	CHB-C1B	4.69	1.47	1.39
10	L	302[B]	BCB	O2D-CGD	4.69	1.44	1.33
10	M	403[A]	BCB	OBD-CAD	4.67	1.28	1.22
10	L	304	BCB	C3B-C4B	4.60	1.48	1.41
8	H	707	LDA	C1-N1	-4.58	1.46	1.51
13	M	402[A]	MQ7	C10-C5	4.56	1.48	1.40
11	M	404	BPB	C3D-C2D	4.55	1.47	1.39
11	L	303[B]	BPB	C3B-C4B	4.54	1.48	1.41
8	M	413	LDA	C1-N1	-4.54	1.46	1.51
11	L	303[A]	BPB	OBD-CAD	4.52	1.28	1.22
10	L	301[B]	BCB	CHB-C1B	4.43	1.46	1.39
10	M	403[B]	BCB	O2A-CGA	4.41	1.46	1.33
10	L	301[B]	BCB	CHB-C4A	-4.41	1.33	1.38
10	L	304	BCB	OBD-CAD	4.33	1.28	1.22
10	L	302[B]	BCB	O2A-CGA	4.32	1.45	1.33
10	L	301[B]	BCB	CHD-C1D	4.31	1.46	1.39
8	H	701	LDA	C1-N1	-4.27	1.47	1.51
11	M	404	BPB	C3B-C4B	4.26	1.48	1.41
11	L	303[A]	BPB	C3B-C4B	4.25	1.48	1.41
8	M	414	LDA	C1-N1	-4.21	1.47	1.51
10	M	403[A]	BCB	CHB-C4A	-4.20	1.33	1.38
10	M	403[B]	BCB	CHB-C4A	-4.18	1.33	1.38
10	L	301[A]	BCB	O2A-CGA	4.18	1.45	1.33
10	L	302[A]	BCB	O2A-CGA	4.15	1.45	1.33
10	L	301[B]	BCB	O2A-CGA	4.11	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	301[A]	BCB	CHB-C4A	-4.10	1.33	1.38
10	M	403[A]	BCB	O2A-CGA	4.10	1.45	1.33
10	M	403[A]	BCB	CHA-CBD	-4.10	1.46	1.51
10	L	301[A]	BCB	CHD-C1D	4.00	1.46	1.39
10	L	304	BCB	O2A-CGA	3.99	1.45	1.33
11	L	303[A]	BPB	O2A-CGA	3.97	1.44	1.33
10	L	302[B]	BCB	CHD-C1D	3.97	1.46	1.39
10	L	302[A]	BCB	CHD-C1D	3.95	1.46	1.39
10	M	403[B]	BCB	CHD-C1D	3.95	1.46	1.39
10	L	302[A]	BCB	C3A-C2A	-3.92	1.51	1.54
10	L	301[B]	BCB	C3A-C2A	-3.84	1.51	1.54
10	M	403[A]	BCB	CHD-C1D	3.83	1.45	1.39
10	L	304	BCB	CHD-C1D	3.83	1.45	1.39
11	M	404	BPB	C4C-NC	-3.76	1.26	1.37
10	L	301[B]	BCB	CHD-C4C	3.76	1.46	1.39
11	L	303[B]	BPB	O2A-CGA	3.74	1.44	1.33
10	L	302[A]	BCB	CHA-CBD	-3.68	1.47	1.51
10	L	301[A]	BCB	C3A-C2A	-3.68	1.51	1.54
10	L	304	BCB	C3A-C2A	-3.66	1.51	1.54
10	L	304	BCB	CHD-C4C	3.66	1.46	1.39
10	L	304	BCB	CHB-C4A	-3.62	1.34	1.38
10	M	403[B]	BCB	CHD-C4C	3.61	1.46	1.39
10	L	302[B]	BCB	CHB-C4A	-3.56	1.34	1.38
10	L	302[B]	BCB	C3A-C2A	-3.50	1.51	1.54
10	L	301[B]	BCB	CHA-CBD	-3.50	1.47	1.51
10	M	403[A]	BCB	C3A-C2A	-3.46	1.51	1.54
6	C	405	DGA	OG2-CB1	3.35	1.43	1.34
10	L	301[A]	BCB	CHD-C4C	3.34	1.45	1.39
10	L	302[A]	BCB	CHB-C4A	-3.30	1.34	1.38
11	L	303[A]	BPB	C4C-NC	-3.29	1.27	1.37
10	M	403[B]	BCB	C3A-C2A	-3.27	1.51	1.54
11	L	303[B]	BPB	C3A-C2A	-3.24	1.51	1.54
11	L	303[A]	BPB	CHA-CBD	-3.24	1.47	1.51
10	L	302[B]	BCB	CHD-C4C	3.21	1.45	1.39
10	L	302[A]	BCB	CHD-C4C	3.17	1.45	1.39
11	M	404	BPB	C3A-C2A	-3.16	1.52	1.54
10	L	301[A]	BCB	CHA-CBD	-3.15	1.48	1.51
10	M	403[A]	BCB	CHD-C4C	3.13	1.45	1.39
11	L	303[B]	BPB	C4C-NC	-3.04	1.28	1.37
11	L	303[B]	BPB	CHA-CBD	-3.04	1.48	1.51
10	L	302[B]	BCB	CHA-CBD	-3.01	1.48	1.51
6	C	405	DGA	OG1-CA1	3.00	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	404	BPB	CHA-CBD	-2.97	1.48	1.51
10	L	304	BCB	CHA-CBD	-2.88	1.48	1.51
6	C	405	DGA	OG2-CG2	-2.78	1.42	1.47
11	L	303[A]	BPB	C3A-C2A	-2.73	1.52	1.54
10	L	302[A]	BCB	CBD-CGD	-2.61	1.49	1.52
10	L	302[B]	BCB	CBD-CGD	-2.54	1.49	1.52
5	C	403	HEC	CBA-CGA	2.50	1.56	1.50
10	L	301[A]	BCB	CBD-CGD	-2.20	1.49	1.52
5	C	401	HEC	CBD-CGD	2.18	1.55	1.50
10	L	301[B]	BCB	CBD-CGD	-2.10	1.49	1.52
10	L	304	BCB	CBD-CGD	-2.08	1.49	1.52
5	C	401	HEC	CBA-CGA	2.04	1.55	1.50
14	M	405	NS5	C23-C21	2.03	1.50	1.46
11	M	404	BPB	C1D-ND	-2.03	1.35	1.38
5	C	402	HEC	CBA-CGA	2.02	1.55	1.50

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	HEC	CBB-CAB-C3B	-12.34	102.78	127.43
5	C	401	HEC	CBB-CAB-C3B	-11.28	104.88	127.43
10	L	302[A]	BCB	C4B-CHC-C1C	10.25	127.92	121.32
11	L	303[B]	BPB	O2D-CGD-CBD	10.18	122.13	110.95
10	L	302[B]	BCB	O2D-CGD-CBD	9.89	121.81	110.95
10	L	302[A]	BCB	O2D-CGD-CBD	9.83	121.75	110.95
10	L	302[B]	BCB	C4B-CHC-C1C	9.30	127.31	121.32
10	M	403[A]	BCB	O2D-CGD-CBD	9.29	121.15	110.95
11	L	303[B]	BPB	C3D-C4D-ND	9.22	119.53	107.71
10	M	403[B]	BCB	O2D-CGD-CBD	9.20	121.06	110.95
11	L	303[A]	BPB	O2D-CGD-CBD	9.01	120.84	110.95
11	L	303[A]	BPB	C3D-C4D-ND	8.96	119.20	107.71
11	M	404	BPB	O2D-CGD-CBD	8.83	120.65	110.95
10	L	302[B]	BCB	C1B-CHB-C4A	8.76	126.96	121.32
11	M	404	BPB	C3D-C4D-ND	8.70	118.87	107.71
10	L	301[A]	BCB	O2D-CGD-CBD	8.66	120.46	110.95
10	M	403[B]	BCB	C4B-CHC-C1C	8.65	126.88	121.32
10	L	301[B]	BCB	C1B-CHB-C4A	8.61	126.86	121.32
10	L	304	BCB	O2D-CGD-CBD	8.55	120.34	110.95
10	L	301[A]	BCB	C1B-CHB-C4A	8.42	126.74	121.32
11	L	303[B]	BPB	C2B-C1B-NB	8.41	115.51	109.43
10	L	302[A]	BCB	C1B-CHB-C4A	8.36	126.70	121.32
10	M	403[A]	BCB	C1B-CHB-C4A	8.28	126.65	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	303[A]	BPB	C2B-C1B-NB	8.15	115.32	109.43
5	C	404	HEC	CBB-CAB-C3B	-8.14	111.16	127.43
10	L	304	BCB	C1B-CHB-C4A	8.00	126.47	121.32
10	L	301[B]	BCB	O2D-CGD-CBD	7.95	119.69	110.95
10	M	403[B]	BCB	C1B-CHB-C4A	7.95	126.44	121.32
10	L	301[A]	BCB	C4B-CHC-C1C	7.82	126.35	121.32
10	L	301[B]	BCB	C4B-CHC-C1C	7.29	126.01	121.32
5	C	402	HEC	CBB-CAB-C3B	-7.04	113.36	127.43
5	C	402	HEC	CBC-CAC-C3C	-6.95	113.54	127.43
5	C	404	HEC	CBC-CAC-C3C	-6.95	113.55	127.43
10	L	304	BCB	C3D-CAD-CBD	6.88	116.66	107.61
10	L	304	BCB	OBD-CAD-C3D	-6.74	117.37	127.89
10	M	403[B]	BCB	C3D-CAD-CBD	6.62	116.32	107.61
10	M	403[A]	BCB	C3D-CAD-CBD	6.53	116.21	107.61
11	L	303[A]	BPB	C4D-ND-C1D	-6.38	101.22	108.87
11	M	404	BPB	C2B-C1B-NB	6.12	113.85	109.43
11	L	303[B]	BPB	C4D-ND-C1D	-6.10	101.56	108.87
10	L	302[A]	BCB	C3D-CAD-CBD	6.06	115.58	107.61
10	L	304	BCB	C4B-CHC-C1C	5.97	125.17	121.32
10	L	304	BCB	C1-C2-C3	-5.96	116.43	126.20
11	M	404	BPB	C4D-ND-C1D	-5.91	101.79	108.87
10	L	304	BCB	CHA-C1A-C2A	-5.78	119.73	133.31
10	M	403[A]	BCB	C4B-CHC-C1C	5.76	125.03	121.32
10	L	301[A]	BCB	C3D-CAD-CBD	5.72	115.13	107.61
10	L	302[A]	BCB	OBD-CAD-C3D	-5.60	119.15	127.89
10	L	302[B]	BCB	CHA-C1A-C2A	-5.43	120.56	133.31
11	L	303[B]	BPB	OBD-CAD-C3D	-5.38	119.50	127.89
10	L	301[B]	BCB	C3D-CAD-CBD	5.35	114.65	107.61
10	L	302[B]	BCB	C3D-CAD-CBD	5.27	114.54	107.61
10	L	302[A]	BCB	CHA-C1A-C2A	-5.25	120.99	133.31
10	L	302[B]	BCB	OBD-CAD-C3D	-5.10	119.94	127.89
14	M	405	NS5	C19-C20-C21	-5.00	120.27	127.28
11	L	303[A]	BPB	C2D-C1D-ND	4.93	112.99	109.43
5	C	401	HEC	CBA-CAA-C2A	-4.87	99.08	112.53
10	L	301[B]	BCB	CMB-C2B-C3B	4.83	134.34	124.68
10	M	403[B]	BCB	CHA-C1A-C2A	-4.76	122.12	133.31
10	L	301[A]	BCB	OBD-CAD-C3D	-4.73	120.52	127.89
10	M	403[B]	BCB	CMB-C2B-C3B	4.62	133.91	124.68
10	M	403[B]	BCB	O2D-CGD-O1D	-4.56	114.97	123.85
11	L	303[A]	BPB	CMA-C3A-C4A	-4.55	104.80	114.61
10	M	403[B]	BCB	C1-O2A-CGA	4.53	127.61	116.65
10	M	403[A]	BCB	CMB-C2B-C3B	4.49	133.65	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	302[A]	BCB	O1D-CGD-CBD	-4.48	117.92	124.72
10	L	301[B]	BCB	CHA-C1A-C2A	-4.46	122.83	133.31
10	M	403[B]	BCB	O2A-CGA-CBA	4.42	125.32	111.83
10	L	301[A]	BCB	CMB-C2B-C3B	4.39	133.45	124.68
10	L	301[A]	BCB	CHA-C1A-C2A	-4.38	123.03	133.31
5	C	401	HEC	C2A-C1A-NA	-4.31	106.16	110.32
10	L	302[B]	BCB	O1D-CGD-CBD	-4.31	118.19	124.72
11	M	404	BPB	C2D-C1D-ND	4.27	112.52	109.43
6	C	405	DGA	OG2-CB1-CB2	4.24	120.66	111.48
10	M	403[A]	BCB	OBD-CAD-C3D	-4.22	121.31	127.89
10	M	403[B]	BCB	OBD-CAD-C3D	-4.20	121.34	127.89
14	M	405	NS5	CM4-C36-C35	-4.20	110.05	122.66
10	M	403[A]	BCB	O2D-CGD-O1D	-4.19	115.70	123.85
10	L	302[B]	BCB	C1-C2-C3	-4.16	119.39	126.20
10	M	403[A]	BCB	C3D-C4D-CHA	4.08	114.75	108.54
14	M	405	NS5	C13-C12-C10	-4.04	122.01	127.69
10	M	403[B]	BCB	C3D-C4D-CHA	4.02	114.65	108.54
11	L	303[B]	BPB	C2D-C1D-ND	4.01	112.33	109.43
10	L	302[A]	BCB	C3D-C4D-CHA	3.99	114.61	108.54
10	M	403[A]	BCB	CHA-C1A-C2A	-3.99	123.94	133.31
5	C	401	HEC	CBC-CAC-C3C	-3.98	119.49	127.43
14	M	405	NS5	C34-C35-C36	-3.95	114.47	127.64
10	L	304	BCB	C3D-C4D-CHA	3.93	114.52	108.54
14	M	405	NS5	C11-C10-C9	3.89	121.99	115.23
11	L	303[B]	BPB	CMB-C2B-C3B	3.89	132.46	124.68
10	L	302[A]	BCB	CMB-C2B-C3B	3.85	132.38	124.68
11	M	404	BPB	OBD-CAD-C3D	-3.85	121.89	127.89
10	M	403[B]	BCB	O2A-CGA-O1A	-3.84	114.03	123.63
10	L	302[A]	BCB	C6-C5-C3	-3.83	104.14	113.47
10	L	302[B]	BCB	CMB-C2B-C3B	3.81	132.30	124.68
10	L	302[B]	BCB	C6-C5-C3	-3.81	104.18	113.47
5	C	402	HEC	C2A-C1A-NA	-3.75	106.71	110.32
14	M	405	NS5	C18-C17-C15	-3.70	122.08	127.28
10	L	301[B]	BCB	C3D-C4D-ND	3.68	118.84	112.94
10	L	301[A]	BCB	C3D-C4D-CHA	3.66	114.11	108.54
10	L	302[B]	BCB	C3D-C4D-CHA	3.66	114.10	108.54
11	M	404	BPB	O2A-CGA-CBA	3.64	122.94	111.83
10	L	301[B]	BCB	C4-C3-C5	3.62	121.51	115.23
10	M	403[B]	BCB	C3D-C4D-ND	3.61	118.72	112.94
10	L	302[A]	BCB	C1-C2-C3	-3.58	120.34	126.20
11	L	303[A]	BPB	CMB-C2B-C3B	3.58	131.83	124.68
11	L	303[A]	BPB	OBD-CAD-C3D	-3.57	122.33	127.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	304	BCB	O2A-CGA-CBA	3.56	122.70	111.83
11	L	303[B]	BPB	C3B-C4B-NB	3.56	113.22	108.05
11	L	303[B]	BPB	O1D-CGD-CBD	-3.54	119.35	124.72
14	M	405	NS5	CM3-C36-C35	-3.53	112.06	122.66
10	M	403[B]	BCB	C1A-CHA-C4D	3.52	124.86	118.98
10	M	403[A]	BCB	CHC-C1C-C2C	-3.50	113.31	122.69
10	M	403[A]	BCB	C3D-C4D-ND	3.48	118.52	112.94
10	L	301[A]	BCB	O2D-CGD-O1D	-3.45	117.14	123.85
11	M	404	BPB	O1D-CGD-CBD	-3.43	119.52	124.72
10	L	302[A]	BCB	CHC-C1C-C2C	-3.42	113.54	122.69
10	L	302[B]	BCB	C3D-C4D-ND	3.40	118.40	112.94
5	C	402	HEC	CBA-CAA-C2A	-3.39	103.16	112.53
11	L	303[A]	BPB	C3B-C4B-NB	3.39	112.98	108.05
10	L	301[B]	BCB	C3D-C4D-CHA	3.38	113.68	108.54
13	M	402[B]	MQ7	C16-C17-C18	-3.38	119.89	127.62
11	M	404	BPB	C1-O2A-CGA	3.34	124.73	116.65
13	M	402[A]	MQ7	C19-C18-C20	3.34	121.02	115.23
5	C	401	HEC	CBD-CAD-C3D	-3.33	103.31	112.53
10	L	301[B]	BCB	OBD-CAD-C3D	-3.33	122.70	127.89
10	L	301[A]	BCB	O2A-CGA-CBA	3.33	121.98	111.83
13	M	402[A]	MQ7	C39-C38-C40	3.33	121.00	115.23
11	L	303[A]	BPB	C3D-CAD-CBD	3.32	111.98	107.61
11	M	404	BPB	C3D-CAD-CBD	3.28	111.93	107.61
10	M	403[B]	BCB	C4-C3-C5	3.28	120.92	115.23
10	L	301[B]	BCB	CMD-C2D-C3D	-3.27	118.15	124.68
14	M	405	NS5	C32-C31-C33	3.27	120.90	115.23
10	L	304	BCB	CHC-C1C-C2C	-3.20	114.11	122.69
10	L	301[B]	BCB	O2A-CGA-CBA	3.19	121.57	111.83
5	C	403	HEC	CBC-CAC-C3C	3.18	133.80	127.43
10	L	304	BCB	C3D-C4D-ND	3.18	118.04	112.94
10	L	302[A]	BCB	C3D-C4D-ND	3.17	118.03	112.94
5	C	403	HEC	C2A-C1A-NA	-3.16	107.27	110.32
10	L	302[B]	BCB	CHC-C1C-C2C	-3.15	114.25	122.69
10	L	301[A]	BCB	C3D-C4D-ND	3.12	117.95	112.94
10	M	403[A]	BCB	C1A-CHA-C4D	3.11	124.17	118.98
10	L	304	BCB	C4-C3-C5	3.11	120.63	115.23
13	M	402[B]	MQ7	C34-C33-C35	3.10	120.61	115.23
11	M	404	BPB	C1A-C2A-C3A	-3.09	99.90	102.84
10	L	301[A]	BCB	C4-C3-C5	3.09	120.59	115.23
10	L	301[B]	BCB	CHC-C1C-C2C	-3.08	114.44	122.69
13	M	402[A]	MQ7	C21-C22-C23	-3.08	120.58	127.62
10	L	304	BCB	C4-C3-C2	-3.04	115.81	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	303[B]	BPB	OBD-CAD-CBD	-3.04	121.37	125.82
13	M	402[B]	MQ7	C19-C18-C20	3.01	120.45	115.23
9	L	307	HTO	C5-C4-C3	-3.01	109.18	114.11
10	M	403[B]	BCB	CHC-C1C-C2C	-3.00	114.65	122.69
5	C	404	HEC	C2A-C1A-NA	-3.00	107.43	110.32
11	L	303[B]	BPB	CMA-C3A-C4A	-2.99	108.16	114.61
13	M	402[B]	MQ7	C21-C22-C23	-2.99	120.78	127.62
5	C	404	HEC	CAD-CBD-CGD	-2.98	105.77	113.67
11	L	303[B]	BPB	CMD-C2D-C3D	-2.95	118.79	124.68
11	L	303[A]	BPB	O2A-CGA-CBA	2.93	120.78	111.83
13	M	402[B]	MQ7	C24-C23-C25	2.93	120.32	115.23
10	L	301[A]	BCB	O2A-CGA-O1A	-2.92	116.31	123.63
11	M	404	BPB	CMD-C2D-C3D	-2.91	118.86	124.68
13	M	402[A]	MQ7	C29-C28-C30	2.91	120.28	115.23
14	M	405	NS5	C18-C19-C20	2.90	129.44	123.52
6	C	405	DGA	OG1-CA1-CA2	2.89	120.65	111.83
10	M	403[A]	BCB	C4D-ND-C1D	-2.89	103.02	105.22
11	L	303[A]	BPB	O1D-CGD-CBD	-2.89	120.34	124.72
10	L	301[A]	BCB	CHC-C1C-C2C	-2.88	114.99	122.69
11	M	404	BPB	C3B-C4B-NB	2.80	112.12	108.05
10	L	304	BCB	C4D-ND-C1D	-2.80	103.10	105.22
14	M	405	NS5	C29-C30-C31	-2.79	123.76	127.69
14	M	405	NS5	C12-C13-C14	-2.77	115.16	123.20
11	L	303[B]	BPB	O2D-CGD-O1D	-2.75	118.49	123.85
10	L	304	BCB	O2A-CGA-O1A	-2.75	116.75	123.63
10	L	302[A]	BCB	O2A-CGA-CBA	2.74	120.20	111.83
13	M	402[A]	MQ7	C16-C17-C18	-2.74	121.36	127.62
11	M	404	BPB	CMA-C3A-C4A	-2.72	108.75	114.61
11	L	303[B]	BPB	C4A-C3A-C2A	-2.72	100.25	102.84
5	C	402	HEC	CAD-CBD-CGD	-2.71	106.48	113.67
10	L	301[A]	BCB	CHD-C4C-C3C	-2.71	121.95	130.04
10	L	301[A]	BCB	C1-C2-C3	-2.69	121.78	126.20
10	L	302[A]	BCB	C4-C3-C5	2.66	119.85	115.23
10	L	302[A]	BCB	C1A-CHA-C4D	2.66	123.42	118.98
10	L	302[B]	BCB	CMD-C2D-C3D	-2.66	119.38	124.68
5	C	404	HEC	C3D-C4D-ND	-2.64	107.22	110.15
13	M	402[B]	MQ7	C39-C38-C40	2.61	119.76	115.23
5	C	401	HEC	C3D-C4D-ND	-2.61	107.25	110.15
10	L	304	BCB	CHD-C4C-C3C	-2.61	122.25	130.04
5	C	403	HEC	C3D-C4D-ND	-2.61	107.26	110.15
10	L	301[B]	BCB	O2D-CGD-O1D	-2.60	118.78	123.85
10	L	302[B]	BCB	C4D-ND-C1D	-2.60	103.24	105.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	303[B]	BPB	C4-C3-C5	2.60	119.73	115.23
10	L	304	BCB	O1D-CGD-CBD	-2.59	120.79	124.72
11	L	303[A]	BPB	O2D-CGD-O1D	-2.59	118.81	123.85
13	M	402[B]	MQ7	C26-C27-C28	-2.58	121.71	127.62
10	L	301[B]	BCB	C1A-CHA-C4D	2.57	123.28	118.98
10	L	304	BCB	O2D-CGD-O1D	-2.57	118.85	123.85
13	M	402[A]	MQ7	C26-C27-C28	-2.57	121.74	127.62
6	C	405	DGA	OG2-CG2-CG1	2.52	112.02	106.21
10	L	304	BCB	CMB-C2B-C3B	2.52	129.72	124.68
10	L	302[B]	BCB	CMA-C3A-C4A	-2.50	109.21	114.61
13	M	402[B]	MQ7	C11-C3-C2	-2.47	120.65	124.89
10	M	403[B]	BCB	OBD-CAD-CBD	-2.46	122.21	125.82
10	L	302[A]	BCB	C4D-ND-C1D	-2.45	103.36	105.22
13	M	402[A]	MQ7	C12-C11-C3	-2.44	106.07	112.08
11	L	303[A]	BPB	O2A-CGA-O1A	-2.43	117.55	123.63
5	C	401	HEC	CHB-C4A-NA	2.43	127.09	124.45
10	L	301[B]	BCB	O2A-CGA-O1A	-2.42	117.57	123.63
10	L	302[A]	BCB	O2A-CGA-O1A	-2.42	117.58	123.63
13	M	402[A]	MQ7	C45-C43-C44	2.42	120.15	114.59
11	L	303[B]	BPB	CBA-CAA-C2A	-2.41	106.68	113.78
10	L	302[A]	BCB	CED-O2D-CGD	2.40	121.36	115.92
5	C	401	HEC	CHA-C1A-C2A	2.39	128.64	124.86
10	L	301[B]	BCB	CAA-C2A-C3A	-2.39	106.55	113.00
11	L	303[B]	BPB	O2A-CGA-CBA	2.38	119.10	111.83
13	M	402[B]	MQ7	C2M-C2-C3	-2.38	120.54	124.45
10	L	301[A]	BCB	C1A-CHA-C4D	2.37	122.94	118.98
5	C	403	HEC	C4D-ND-C1D	2.37	109.68	105.82
11	L	303[A]	BPB	CMD-C2D-C3D	-2.37	119.95	124.68
13	M	402[B]	MQ7	C12-C11-C3	-2.37	106.25	112.08
10	L	302[B]	BCB	CHD-C4C-C3C	-2.36	122.99	130.04
10	L	301[B]	BCB	CAA-CBA-CGA	-2.36	106.51	113.21
10	M	403[A]	BCB	OBD-CAD-CBD	-2.35	122.37	125.82
10	L	302[B]	BCB	O2A-CGA-CBA	2.34	118.97	111.83
10	L	302[B]	BCB	C1A-CHA-C4D	2.32	122.85	118.98
11	L	303[A]	BPB	C4B-NB-C1B	-2.32	105.44	108.82
10	L	302[B]	BCB	O2A-CGA-O1A	-2.31	117.84	123.63
10	M	403[A]	BCB	CHD-C4C-C3C	-2.30	123.16	130.04
5	C	404	HEC	CHA-C1A-NA	2.30	126.96	124.45
11	L	303[B]	BPB	O2A-CGA-O1A	-2.30	117.88	123.63
10	M	403[B]	BCB	C1A-CHA-CBD	-2.29	126.49	132.36
11	L	303[B]	BPB	C4B-NB-C1B	-2.29	105.48	108.82
5	C	402	HEC	C4A-NA-C1A	2.28	109.54	105.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	402[A]	MQ7	C34-C33-C35	2.26	119.16	115.23
14	M	405	NS5	C8-C7-C5	-2.26	122.45	127.62
10	M	403[A]	BCB	C4-C3-C5	2.25	119.13	115.23
5	C	403	HEC	CHB-C4A-NA	2.24	126.90	124.45
10	M	403[A]	BCB	O2A-CGA-O1A	-2.24	118.03	123.63
13	M	402[A]	MQ7	C5-C4-C3	2.23	122.36	118.27
11	M	404	BPB	CED-O2D-CGD	2.23	120.98	115.92
10	M	403[B]	BCB	CMD-C2D-C3D	-2.22	120.24	124.68
10	L	301[B]	BCB	C4D-ND-C1D	-2.22	103.53	105.22
13	M	402[B]	MQ7	C14-C13-C15	2.22	119.07	115.23
10	L	302[A]	BCB	CHD-C4C-C3C	-2.21	123.44	130.04
10	M	403[A]	BCB	C7-C6-C5	-2.20	107.39	113.26
14	M	405	NS5	C30-C29-C28	-2.19	116.84	123.20
14	M	405	NS5	C16-C15-C14	2.19	121.43	118.09
10	L	302[A]	BCB	CMD-C2D-C3D	-2.17	120.35	124.68
10	L	301[B]	BCB	OBD-CAD-CBD	-2.16	122.65	125.82
10	L	301[B]	BCB	CHD-C4C-C3C	-2.15	123.62	130.04
13	M	402[A]	MQ7	C14-C13-C15	2.15	118.96	115.23
13	M	402[A]	MQ7	O4-C4-C5	-2.13	118.16	121.57
11	L	303[A]	BPB	C4A-C3A-C2A	-2.11	100.83	102.84
9	H	710	HTO	C5-C4-C3	-2.11	110.66	114.11
10	L	301[B]	BCB	O1D-CGD-CBD	-2.10	121.53	124.72
13	M	402[A]	MQ7	C41-C42-C43	-2.10	120.62	127.64
10	M	403[B]	BCB	CHD-C4C-C3C	-2.10	123.75	130.04
5	C	403	HEC	O2D-CGD-CBD	2.09	120.60	114.00
13	M	402[A]	MQ7	C24-C23-C25	2.09	118.85	115.23
5	C	403	HEC	C2D-C1D-ND	-2.08	106.81	110.14
5	C	401	HEC	CAA-C2A-C3A	-2.07	123.98	127.87
10	L	302[B]	BCB	C4-C3-C5	2.06	118.81	115.23
11	M	404	BPB	O2D-CGD-O1D	-2.06	119.83	123.85
10	L	304	BCB	C1A-CHA-C4D	2.05	122.41	118.98
10	M	403[B]	BCB	C4D-ND-C1D	-2.05	103.66	105.22
10	L	301[B]	BCB	C6-C7-C8	-2.05	109.16	115.97
14	M	405	NS5	C14-C15-C17	-2.05	115.79	119.01
5	C	401	HEC	C4A-NA-C1A	2.04	109.15	105.82
13	M	402[A]	MQ7	C31-C32-C33	-2.04	122.96	127.62
5	C	403	HEC	O2A-CGA-CBA	2.03	120.42	114.00
13	M	402[B]	MQ7	C29-C28-C30	2.03	118.76	115.23
13	M	402[B]	MQ7	C41-C42-C43	-2.03	120.86	127.64
5	C	402	HEC	CHB-C4A-NA	2.02	126.65	124.45
13	M	402[B]	MQ7	C45-C43-C44	2.02	119.23	114.59
10	M	403[A]	BCB	O2A-CGA-CBA	2.01	117.97	111.83

All (18) 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	L	304	BCB	NA
10	L	304	BCB	NC
10	L	304	BCB	ND
10	M	403[A]	BCB	NA
10	M	403[A]	BCB	NC
10	M	403[B]	BCB	NA
10	M	403[B]	BCB	NC
10	M	403[B]	BCB	ND

All (193) 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
8	H	707	LDA	C2-C1-N1-O1
8	H	707	LDA	C2-C1-N1-CM1
8	H	707	LDA	C2-C1-N1-CM2
8	H	707	LDA	N1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	L	306	LDA	C2-C1-N1-O1
8	L	306	LDA	C2-C1-N1-CM1
8	M	414	LDA	C2-C1-N1-CM1
8	M	414	LDA	C2-C1-N1-CM2
9	H	709	HTO	C1-C2-C3-O3
9	H	709	HTO	O2-C2-C3-O3
9	H	709	HTO	O2-C2-C3-C4
9	L	307	HTO	O2-C2-C3-C4
10	L	302[A]	BCB	C2C-C3C-CAC-CBC
10	L	302[B]	BCB	C2C-C3C-CAC-CBC
10	L	304	BCB	C2C-C3C-CAC-CBC
10	M	403[A]	BCB	C2C-C3C-CAC-CBC
10	M	403[A]	BCB	CAD-CBD-CGD-O1D
10	M	403[A]	BCB	CAD-CBD-CGD-O2D
10	M	403[B]	BCB	CBA-CGA-O2A-C1
10	M	403[B]	BCB	C2C-C3C-CAC-CBC
10	M	403[B]	BCB	CAD-CBD-CGD-O1D
10	M	403[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	404	BPB	C2C-C3C-CAC-CBC
11	L	303[B]	BPB	CBD-CGD-O2D-CED
10	M	403[B]	BCB	O1A-CGA-O2A-C1
14	M	405	NS5	C34-C35-C36-CM3
10	L	302[B]	BCB	CBD-CGD-O2D-CED
10	L	304	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
10	L	301[B]	BCB	C2-C3-C5-C6
10	M	403[A]	BCB	C2A-CAA-CBA-CGA
11	M	404	BPB	CBA-CGA-O2A-C1
11	L	303[B]	BPB	O1D-CGD-O2D-CED
11	M	404	BPB	O1A-CGA-O2A-C1
10	L	304	BCB	O1D-CGD-O2D-CED
10	L	302[B]	BCB	O1D-CGD-O2D-CED
10	L	302[B]	BCB	C8-C10-C11-C12
10	M	403[A]	BCB	C8-C10-C11-C12
10	L	301[A]	BCB	C13-C15-C16-C17
10	L	301[B]	BCB	C13-C15-C16-C17
10	L	304	BCB	C3-C5-C6-C7
10	L	302[B]	BCB	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	CA2-CA1-OG1-CG1
14	M	405	NS5	C13-C14-C15-C16
8	H	708	LDA	C3-C4-C5-C6
8	M	413	LDA	C5-C6-C7-C8
8	L	305	LDA	C2-C3-C4-C5
10	M	403[B]	BCB	C12-C13-C15-C16
6	C	405	DGA	CBB-CAB-CB9-CB8
6	C	405	DGA	OA1-CA1-OG1-CG1
8	H	708	LDA	C5-C6-C7-C8
8	L	306	LDA	C7-C8-C9-C10
6	C	405	DGA	CCB-CDB-CEB-CFB
10	M	403[B]	BCB	C2A-CAA-CBA-CGA
10	L	301[B]	BCB	C15-C16-C17-C18
10	M	403[B]	BCB	C8-C10-C11-C12
11	M	404	BPB	C13-C15-C16-C17
11	L	303[B]	BPB	C4-C3-C5-C6
8	L	306	LDA	C6-C7-C8-C9
8	M	414	LDA	C6-C7-C8-C9
8	L	306	LDA	C3-C4-C5-C6
14	M	405	NS5	C34-C35-C36-CM4
8	L	305	LDA	C5-C6-C7-C8
11	L	303[A]	BPB	C8-C10-C11-C12
10	M	403[A]	BCB	C12-C13-C15-C16
11	L	303[B]	BPB	C11-C12-C13-C15
11	L	303[B]	BPB	C2-C3-C5-C6
10	M	403[A]	BCB	C14-C13-C15-C16
10	M	403[B]	BCB	C14-C13-C15-C16
11	L	303[B]	BPB	C11-C12-C13-C14
10	M	403[A]	BCB	C13-C15-C16-C17
8	L	306	LDA	C4-C5-C6-C7
8	L	305	LDA	C1-C2-C3-C4
9	L	307	HTO	O2-C2-C3-O3
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	L	305	LDA	C3-C4-C5-C6
8	H	701	LDA	C6-C7-C8-C9
10	L	302[A]	BCB	C13-C15-C16-C17
9	H	709	HTO	C4-C5-C6-C7
8	H	708	LDA	C9-C10-C11-C12
8	H	701	LDA	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	L	303[B]	BPB	C15-C16-C17-C18
10	L	301[B]	BCB	C6-C7-C8-C10
11	L	303[A]	BPB	C2-C3-C5-C6
6	C	405	DGA	OG1-CG1-CG2-CG3
8	L	306	LDA	C9-C10-C11-C12
6	C	405	DGA	CB9-CAB-CBB-CCB
14	M	405	NS5	C7-C8-C9-C10
11	L	303[A]	BPB	C4-C3-C5-C6
14	M	405	NS5	C3-C4-C5-C6
6	C	405	DGA	OG1-CG1-CG2-OG2
10	L	301[B]	BCB	C16-C17-C18-C19
11	L	303[B]	BPB	C16-C17-C18-C19
8	L	306	LDA	C1-C2-C3-C4
9	L	307	HTO	C4-C5-C6-C7
8	H	707	LDA	C6-C7-C8-C9
8	H	707	LDA	C1-C2-C3-C4
5	C	402	HEC	C3D-CAD-CBD-CGD
10	L	304	BCB	C5-C6-C7-C8
10	L	302[B]	BCB	C16-C17-C18-C19
8	H	708	LDA	C6-C7-C8-C9
10	L	301[B]	BCB	C16-C17-C18-C20
10	M	403[B]	BCB	C16-C17-C18-C20
6	C	405	DGA	CA3-CA4-CA5-CA6
8	L	306	LDA	C2-C1-N1-CM2
9	L	307	HTO	C1-C2-C3-O3
11	L	303[B]	BPB	C12-C13-C15-C16
8	L	305	LDA	C4-C5-C6-C7
6	C	405	DGA	CA9-CAA-CBA-CCA
14	M	405	NS5	C10-C12-C13-C14
14	M	405	NS5	C23-C24-C25-C26
8	M	414	LDA	C2-C1-N1-O1
6	C	405	DGA	CB6-CB7-CB8-CB9
10	L	301[A]	BCB	CAD-CBD-CGD-O2D
10	L	301[A]	BCB	C16-C17-C18-C20
6	C	405	DGA	CG1-CG2-OG2-CB1
10	L	301[A]	BCB	CAD-CBD-CGD-O1D
8	H	708	LDA	C7-C8-C9-C10
11	M	404	BPB	C4-C3-C5-C6
8	L	306	LDA	C11-C10-C9-C8
11	L	303[B]	BPB	C16-C17-C18-C20
6	C	405	DGA	CB2-CB3-CB4-CB5
10	L	301[A]	BCB	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	H	708	LDA	N1-C1-C2-C3
14	M	405	NS5	C13-C14-C15-C17
6	C	405	DGA	CAB-CBB-CCB-CDB
10	L	301[B]	BCB	C3-C5-C6-C7
10	L	302[B]	BCB	C11-C12-C13-C14
10	L	304	BCB	C8-C10-C11-C12
10	L	302[B]	BCB	C11-C10-C8-C7
10	L	304	BCB	C11-C10-C8-C7
11	L	303[B]	BPB	C11-C10-C8-C7
5	C	401	HEC	CAA-CBA-CGA-O1A
8	H	708	LDA	C2-C3-C4-C5
8	H	701	LDA	C9-C10-C11-C12
5	C	401	HEC	CAA-CBA-CGA-O2A
10	L	304	BCB	C4-C3-C5-C6
10	L	304	BCB	C10-C11-C12-C13
10	M	403[B]	BCB	C4-C3-C5-C6
10	L	302[B]	BCB	C16-C17-C18-C20
10	M	403[B]	BCB	CHA-CBD-CGD-O1D
10	M	403[B]	BCB	CHA-CBD-CGD-O2D
10	L	301[B]	BCB	C11-C10-C8-C9
13	M	402[B]	MQ7	C39-C38-C40-C41
14	M	405	NS5	C3-C4-C5-C7
10	M	403[A]	BCB	O2A-C1-C2-C3
10	L	304	BCB	C2-C3-C5-C6
11	M	404	BPB	C2-C3-C5-C6
10	L	301[B]	BCB	C6-C7-C8-C9
8	M	413	LDA	C3-C4-C5-C6
10	M	403[A]	BCB	C15-C16-C17-C18
10	L	302[A]	BCB	C12-C13-C15-C16
8	M	413	LDA	C6-C7-C8-C9
10	M	403[B]	BCB	C2-C3-C5-C6
10	L	302[B]	BCB	C11-C10-C8-C9
10	L	304	BCB	C11-C10-C8-C9
10	M	403[A]	BCB	C16-C17-C18-C20
10	L	301[A]	BCB	C15-C16-C17-C18
6	C	405	DGA	CBB-CCB-CDB-CEB
10	L	302[A]	BCB	C8-C10-C11-C12
9	L	307	HTO	C1-C2-C3-C4
11	L	303[B]	BPB	C14-C13-C15-C16
8	M	413	LDA	C4-C5-C6-C7
5	C	403	HEC	CAA-CBA-CGA-O2A
5	C	402	HEC	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

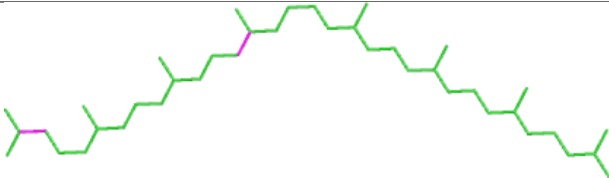
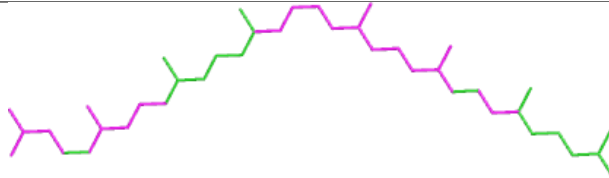
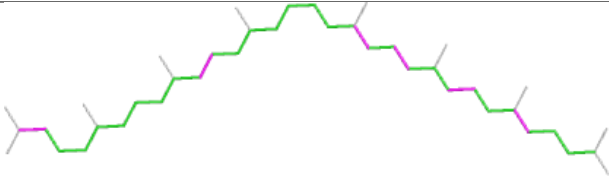
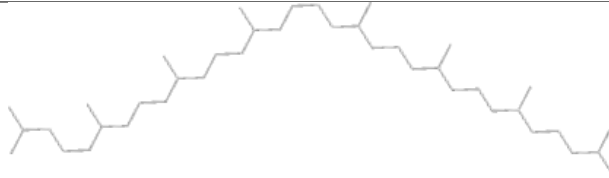
Mol	Chain	Res	Type	Atoms
6	C	405	DGA	OB1-CB1-OG2-CG2
10	L	304	BCB	CAD-CBD-CGD-O2D
5	C	401	HEC	CAD-CBD-CGD-O2D
5	C	403	HEC	CAD-CBD-CGD-O2D
6	C	405	DGA	CB1-CB2-CB3-CB4

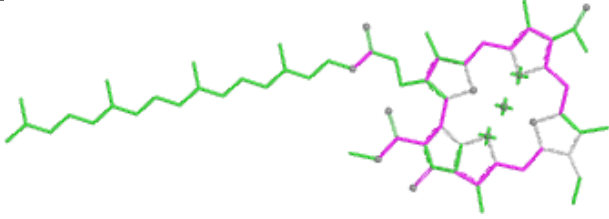
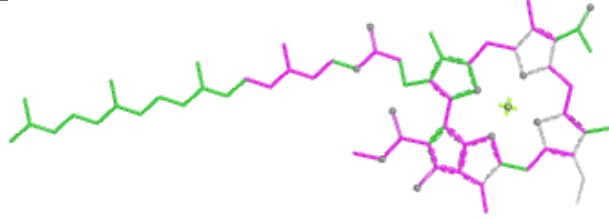
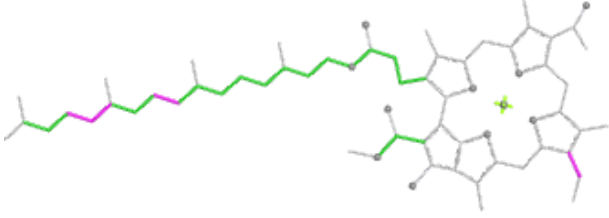
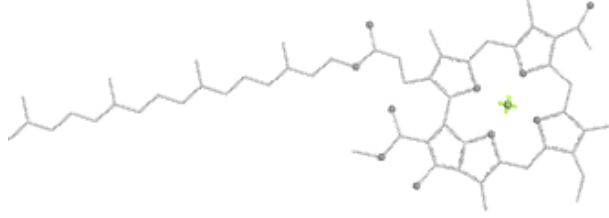
There are no ring outliers.

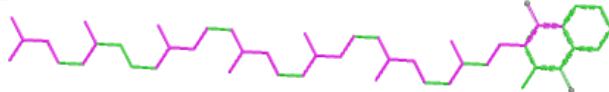
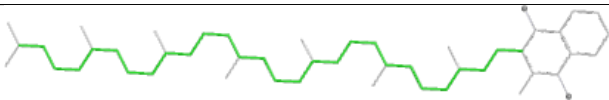
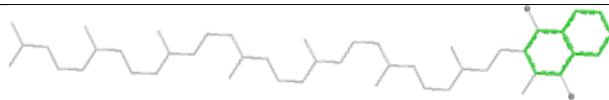
18 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	405	NS5	2	0
10	L	302[A]	BCB	1	0
5	C	402	HEC	1	0
11	M	404	BPB	7	0
10	L	304	BCB	8	0
8	L	305	LDA	2	0
8	H	701	LDA	1	0
10	L	301[A]	BCB	4	0
11	L	303[A]	BPB	2	0
5	C	404	HEC	1	0
8	H	707	LDA	1	0
10	L	301[B]	BCB	4	0
11	L	303[B]	BPB	4	0
5	C	403	HEC	1	0
8	H	708	LDA	3	0
10	M	403[A]	BCB	1	0
7	M	408	SO4	1	0
10	M	403[B]	BCB	6	0

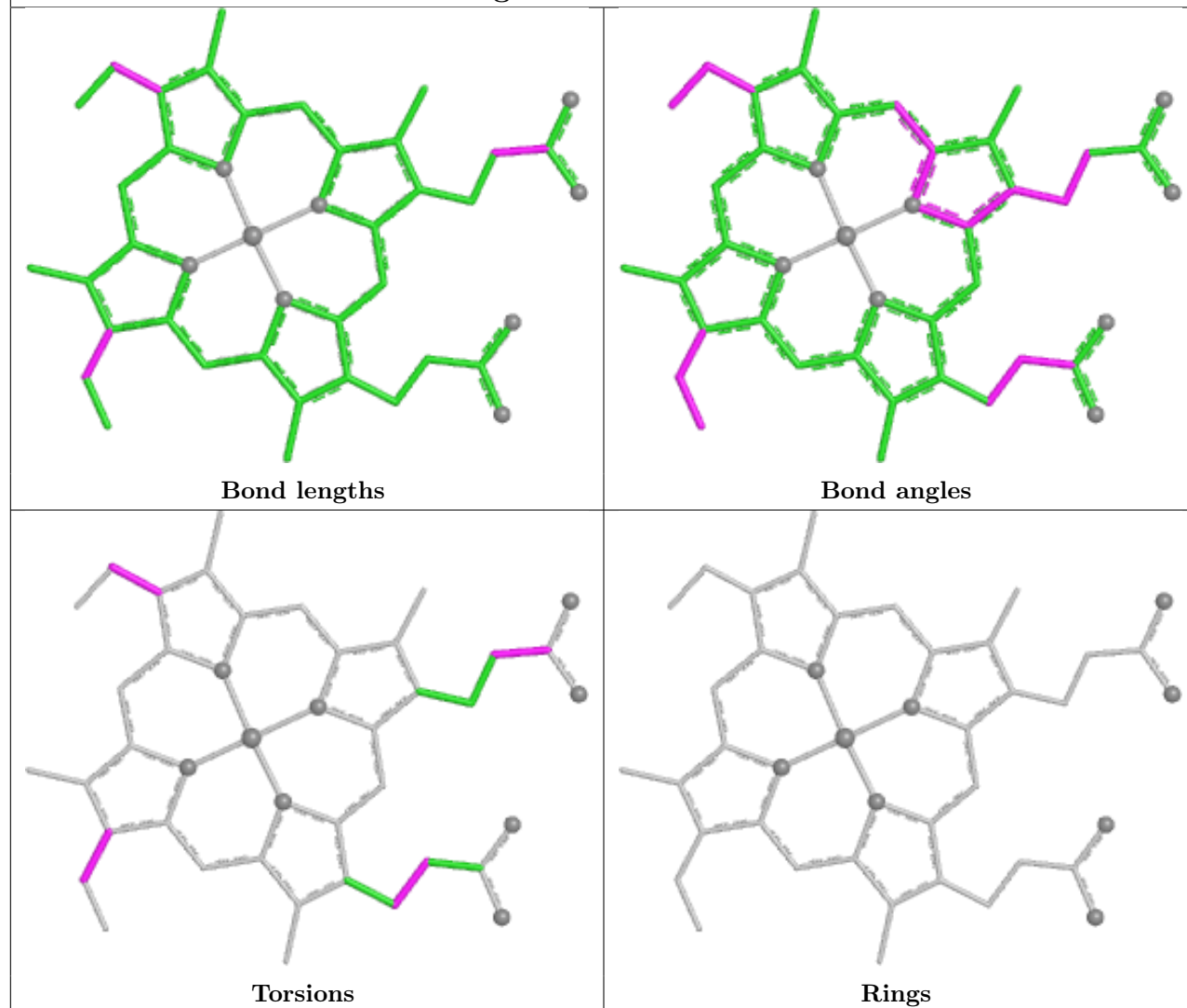
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 NS5 M 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

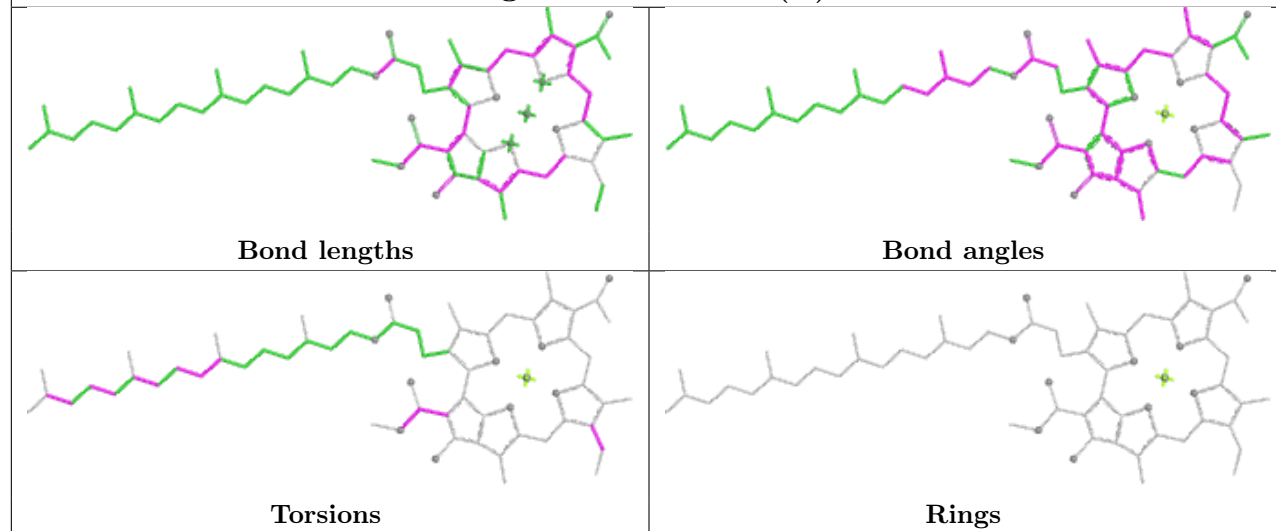
Ligand BCB L 302 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

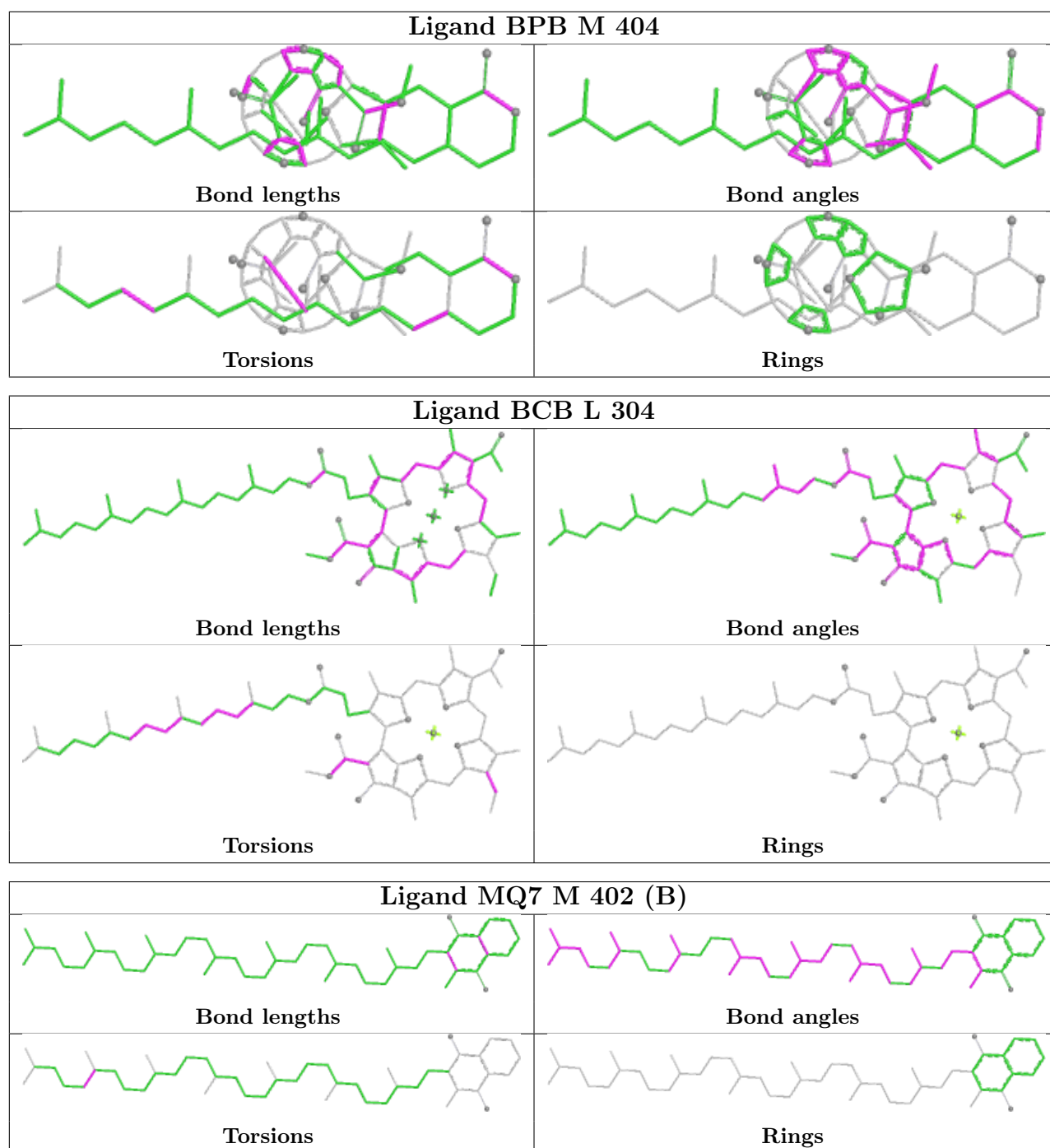
Ligand MQ7 M 402 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

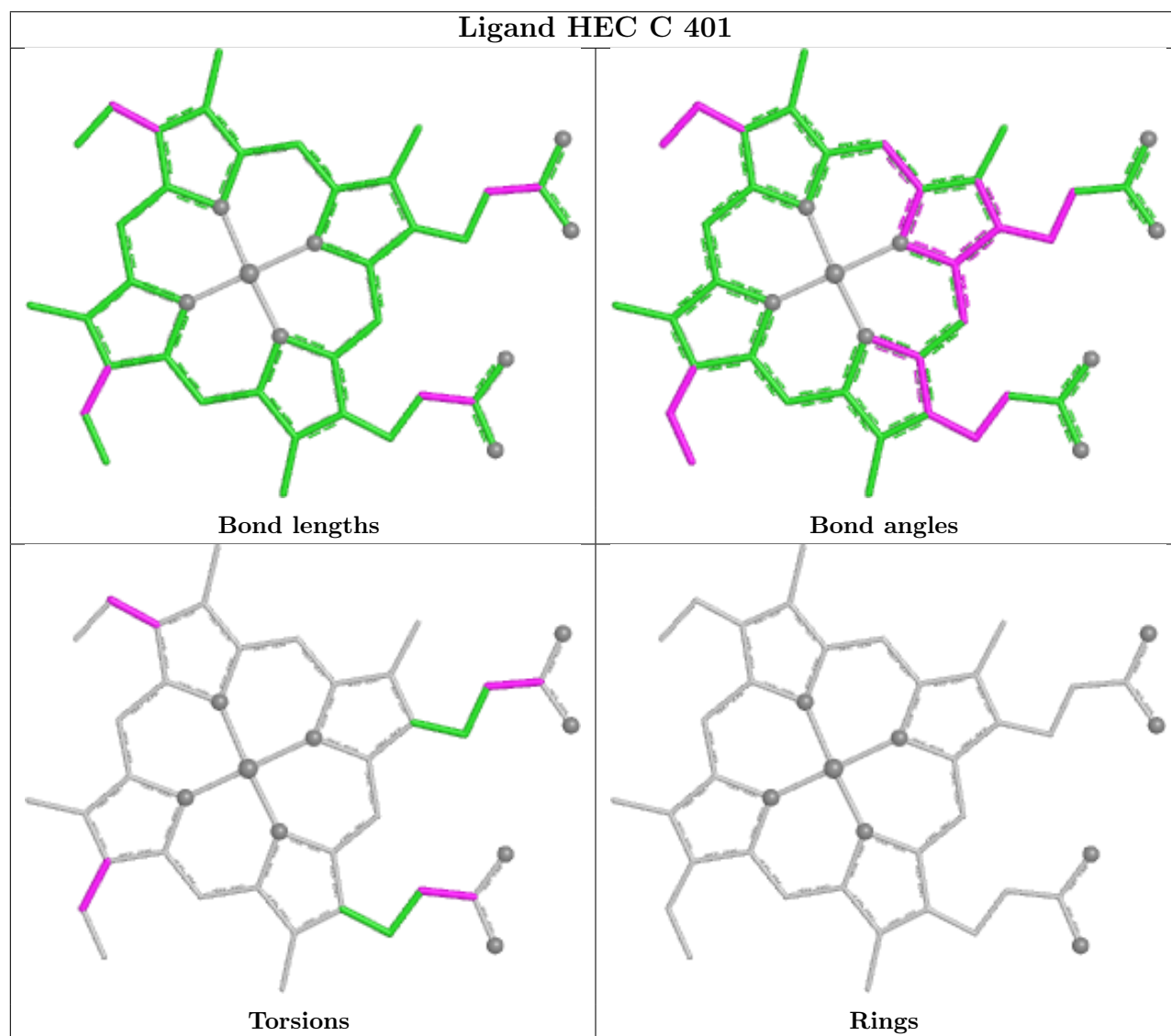
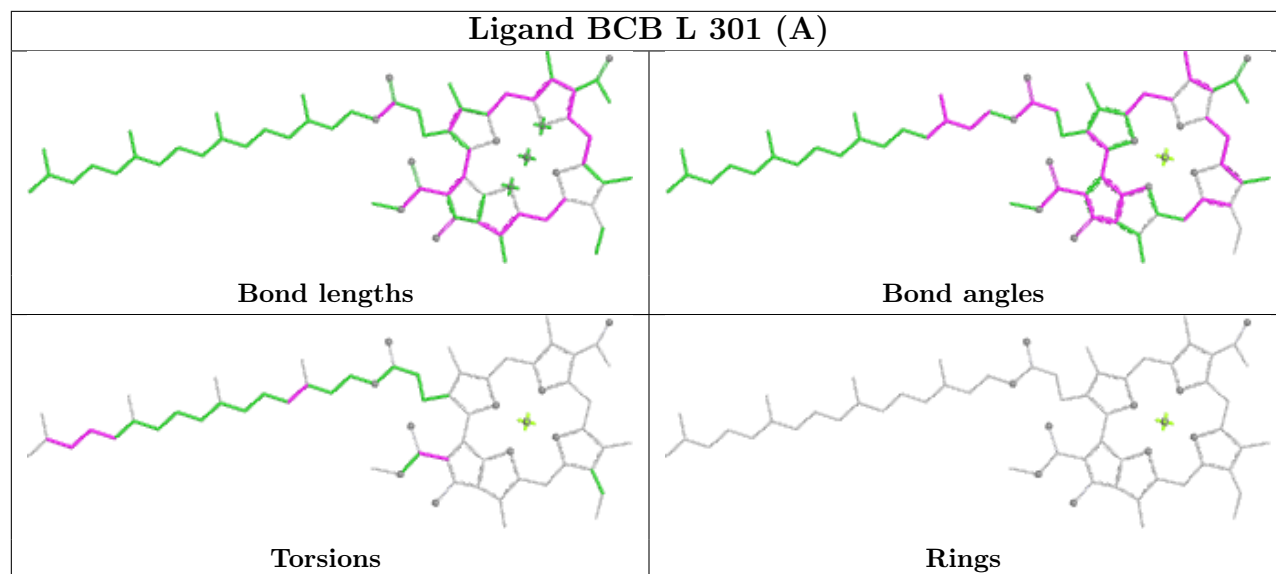
Ligand HEC C 402

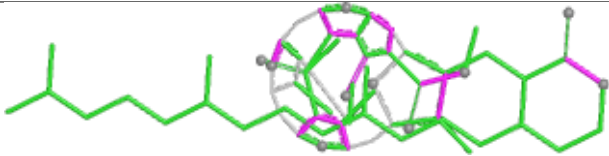
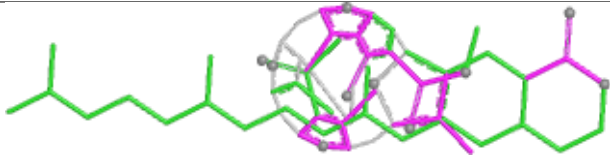
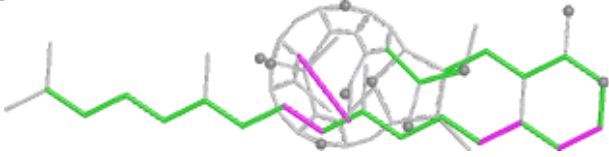
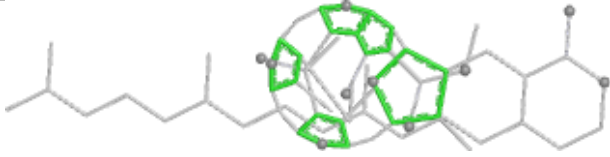
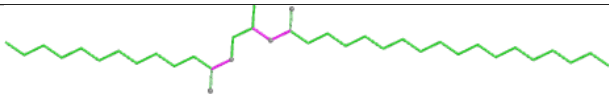
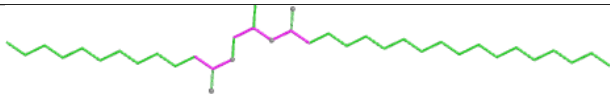
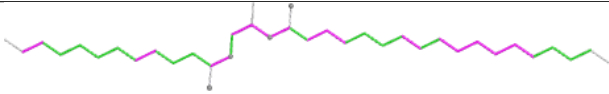
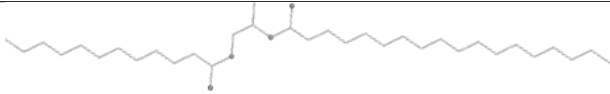


Ligand BCB L 302 (B)

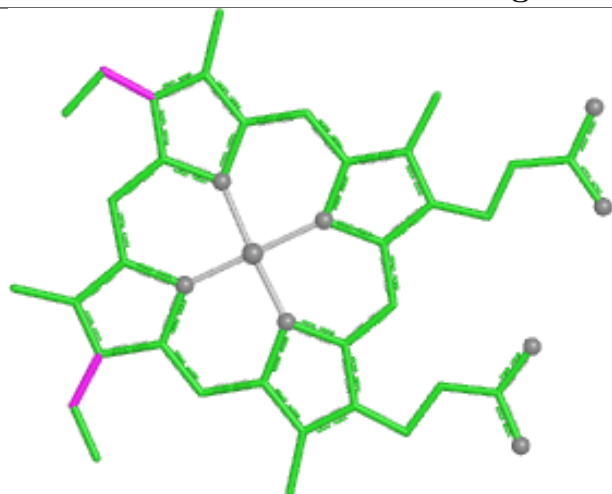




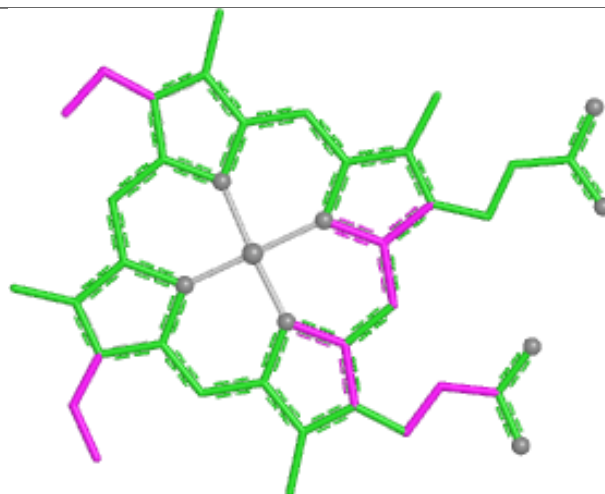


Ligand BPB L 303 (A)			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand DGA C 405			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

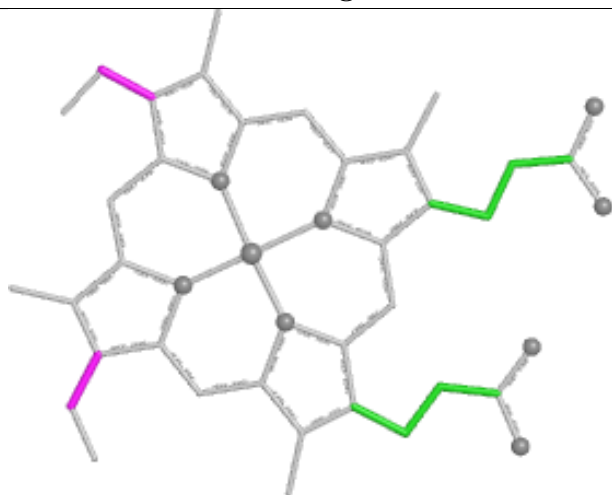
Ligand HEC C 404



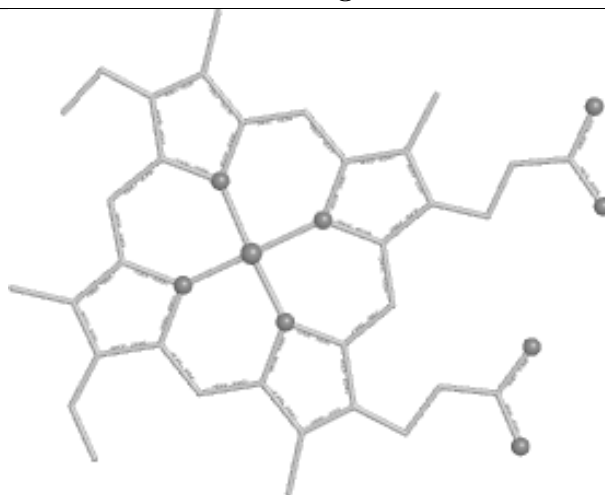
Bond lengths



Bond angles

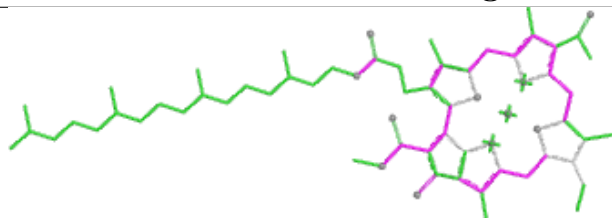


Torsions

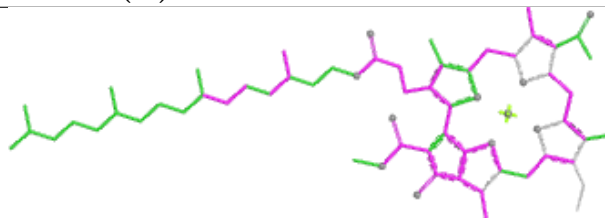


Rings

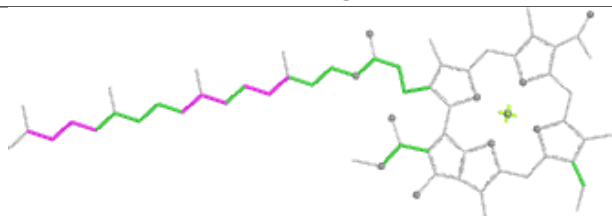
Ligand BCB L 301 (B)



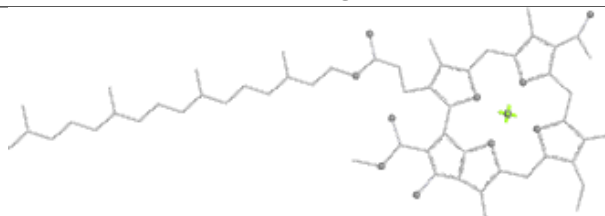
Bond lengths



Bond angles

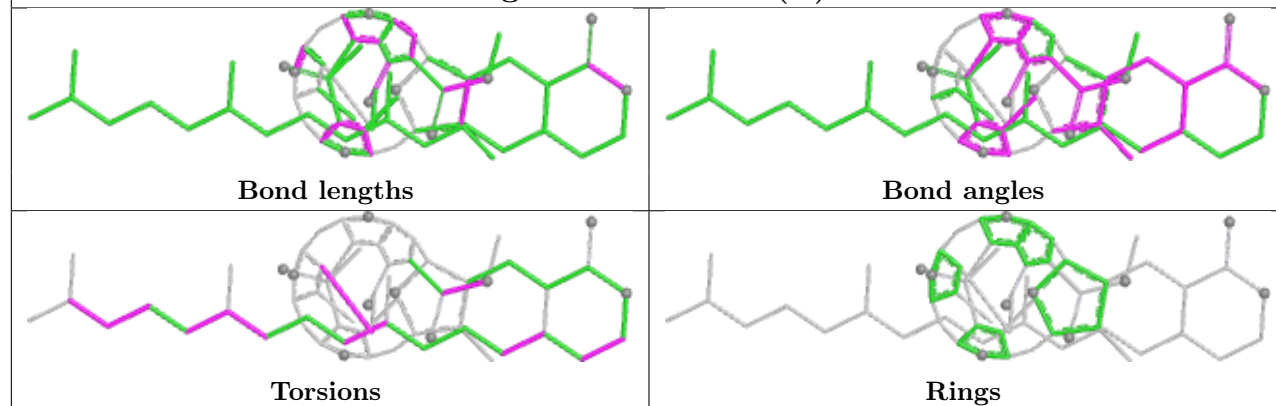


Torsions

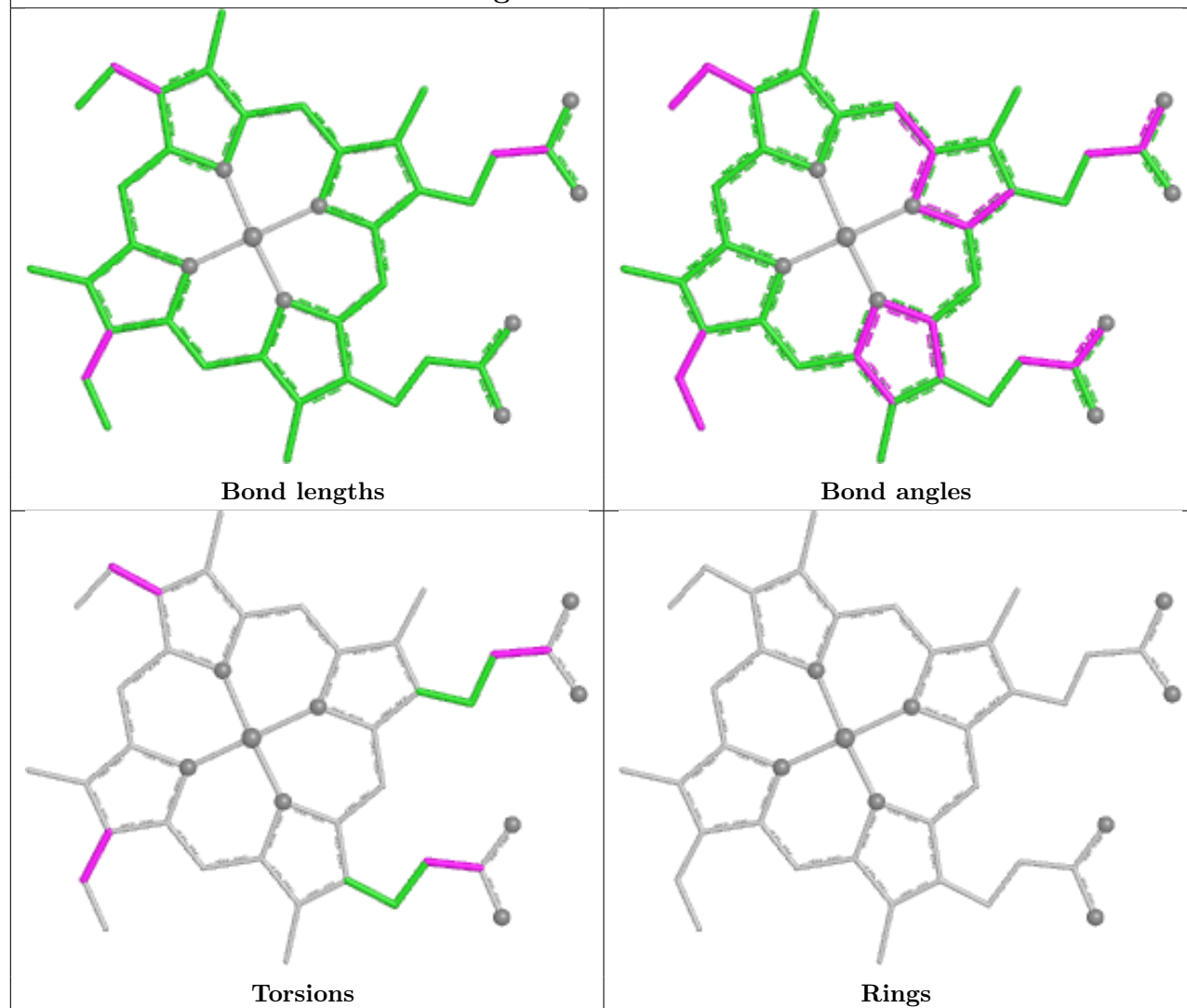


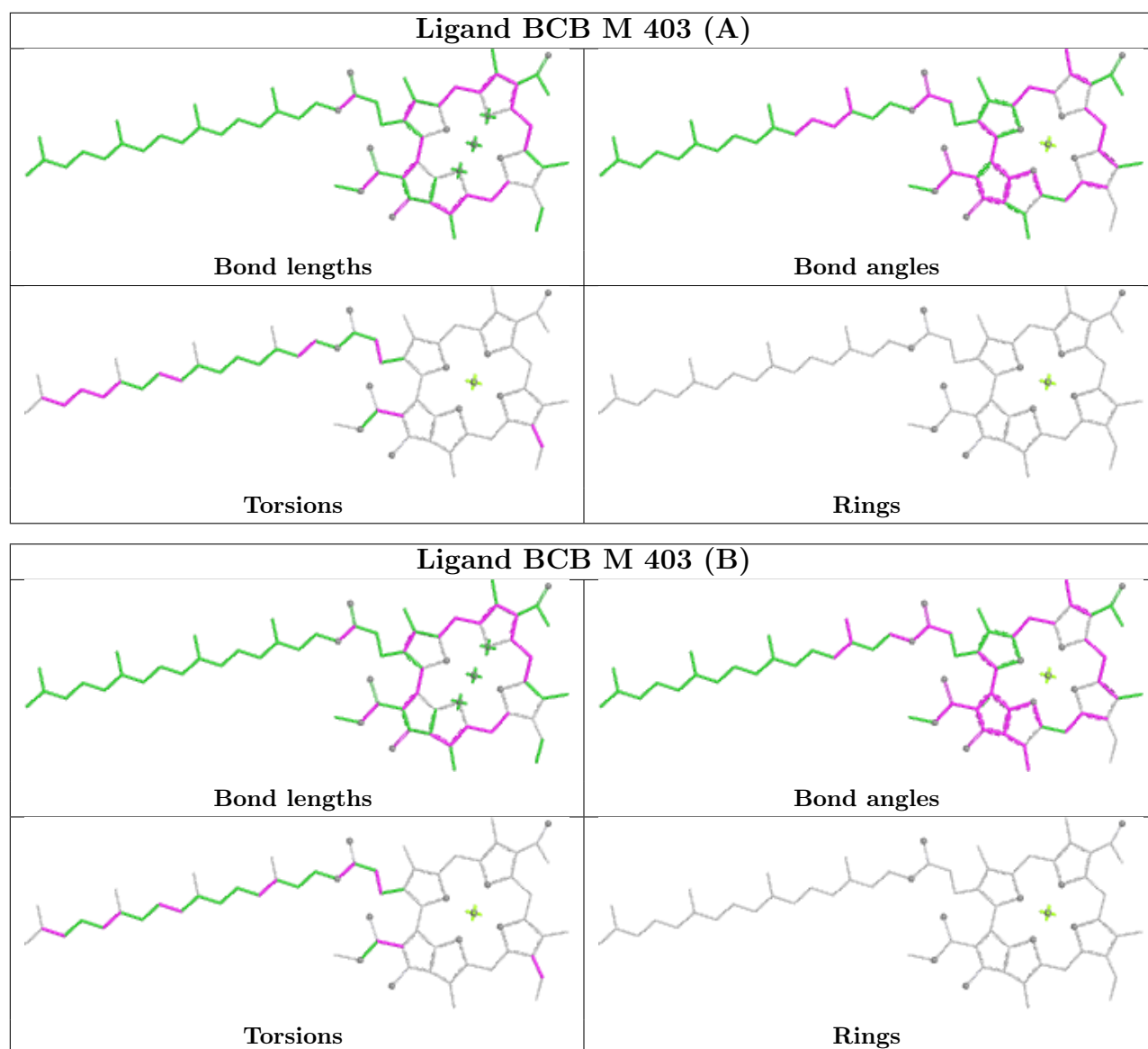
Rings

Ligand BPB L 303 (B)



Ligand HEC C 403





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.64	3 (0%) 81 74	62, 78, 103, 128	0
2	H	257/258 (99%)	-0.26	7 (2%) 56 46	68, 89, 129, 177	0
3	L	273/273 (100%)	-0.60	1 (0%) 88 84	31, 75, 99, 112	41 (15%)
4	M	323/323 (100%)	-0.52	1 (0%) 90 86	31, 75, 99, 123	51 (15%)
All	All	1185/1190 (99%)	-0.52	12 (1%) 79 72	31, 78, 108, 177	92 (7%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	52	LEU	5.1
2	H	50	VAL	3.9
2	H	54	PRO	3.0
2	H	53	ALA	2.9
2	H	46	PRO	2.8
3	L	1	ALA	2.5
1	C	332	LYS	2.3
4	M	51	LEU	2.3
2	H	49	LEU	2.3
1	C	221	ARG	2.2
1	C	146	ARG	2.1
2	H	223	ARG	2.0

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

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	0.11	73,89,102,109	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	412	5/5	0.50	0.14	137,140,144,158	0
7	SO4	M	411	5/5	0.53	0.12	128,135,147,150	0
7	SO4	M	409	5/5	0.58	0.12	117,117,131,137	0
7	SO4	C	408	5/5	0.61	0.15	98,101,106,106	5
7	SO4	H	703	5/5	0.65	0.12	147,147,156,157	0
9	HTO	L	307	10/10	0.72	0.30	87,99,108,114	0
7	SO4	H	705	5/5	0.73	0.12	119,126,134,140	0
9	HTO	H	709	10/10	0.74	0.27	89,105,115,115	0
7	SO4	C	406	5/5	0.75	0.11	119,133,138,142	0
9	HTO	H	710	10/10	0.80	0.24	89,97,109,110	0
6	DGA	C	405	37/44	0.82	0.21	87,114,152,154	0
7	SO4	C	407	5/5	0.84	0.20	106,111,116,117	5
8	LDA	M	414	16/16	0.85	0.24	75,104,135,137	0
8	LDA	L	305	16/16	0.87	0.27	93,105,128,129	0
8	LDA	L	306	16/16	0.89	0.23	104,110,139,140	0
7	SO4	M	407	5/5	0.90	0.11	98,101,114,118	0
8	LDA	M	413	16/16	0.91	0.21	92,97,134,135	0
8	LDA	H	707	16/16	0.94	0.16	68,82,141,145	0
7	SO4	M	410	5/5	0.94	0.14	89,96,100,104	5
11	BPB	M	404	65/65	0.94	0.15	66,77,159,165	0
13	MQ7	M	402[A]	48/48	0.95	0.12	64,71,114,126	48
13	MQ7	M	402[B]	48/48	0.95	0.12	64,71,114,126	48
14	NS5	M	405	40/40	0.95	0.16	65,83,123,123	0
8	LDA	H	708	16/16	0.96	0.14	82,98,122,123	0
7	SO4	H	706	5/5	0.96	0.06	86,88,103,105	5
7	SO4	M	406	5/5	0.96	0.06	88,95,107,108	0
7	SO4	H	704	5/5	0.97	0.14	86,89,93,94	5
7	SO4	H	702	5/5	0.97	0.10	90,95,102,107	0

Continued on next page...

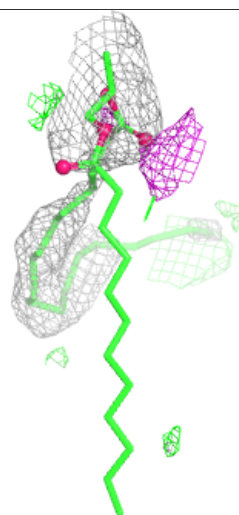
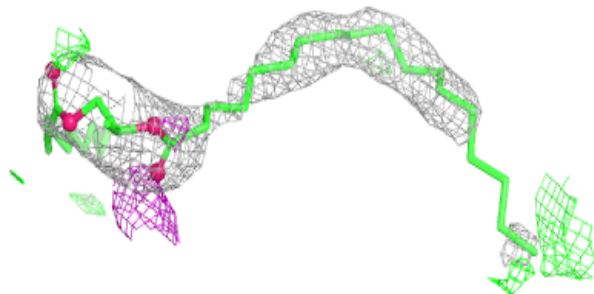
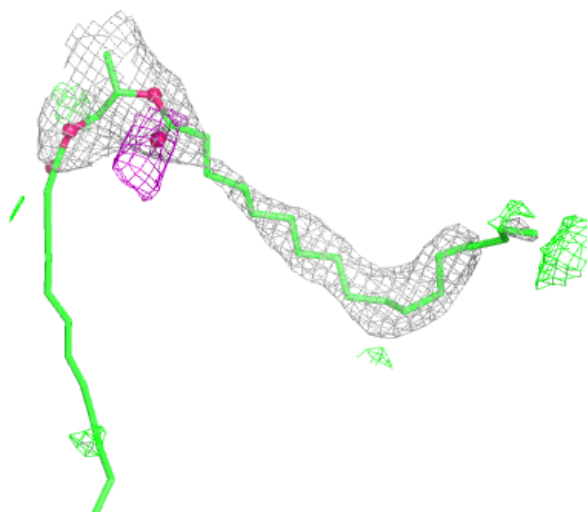
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	BCB	L	302[A]	66/66	0.98	0.09	60,65,106,109	66
10	BCB	L	302[B]	66/66	0.98	0.09	60,65,106,109	66
10	BCB	L	304	66/66	0.98	0.10	60,70,151,157	0
10	BCB	M	403[A]	66/66	0.98	0.10	54,63,96,99	66
10	BCB	M	403[B]	66/66	0.98	0.10	54,63,96,99	66
11	BPB	L	303[A]	65/65	0.98	0.08	61,67,78,81	65
11	BPB	L	303[B]	65/65	0.98	0.08	61,67,78,81	65
8	LDA	H	701	16/16	0.98	0.10	70,85,97,98	0
7	SO4	M	408	5/5	0.98	0.05	81,87,90,93	0
10	BCB	L	301[A]	66/66	0.98	0.08	55,61,78,92	66
10	BCB	L	301[B]	66/66	0.98	0.08	55,61,78,92	66
5	HEC	C	404	43/43	0.99	0.05	61,69,88,106	0
5	HEC	C	401	43/43	0.99	0.07	72,85,93,101	0
5	HEC	C	402	43/43	0.99	0.07	71,78,89,97	0
5	HEC	C	403	43/43	0.99	0.05	53,65,72,80	0
12	FE	M	401[B]	1/1	1.00	0.02	69,69,69,69	1
12	FE	M	401[A]	1/1	1.00	0.02	69,69,69,69	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.

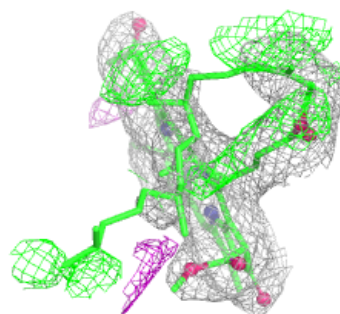
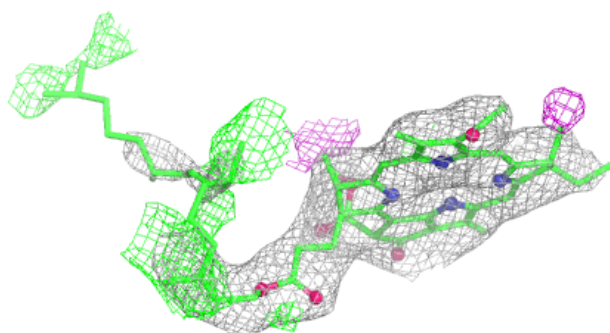
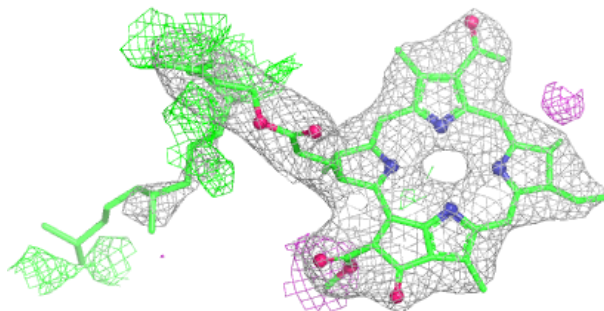
Electron density around DGA C 405:

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

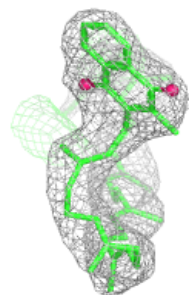
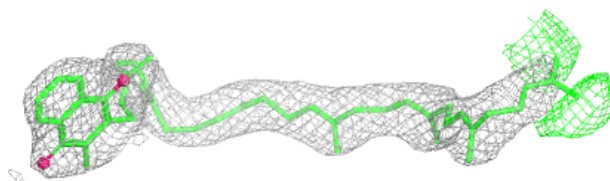
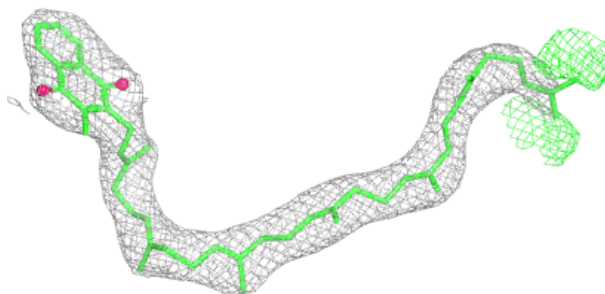


Electron density around BPB M 404:

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

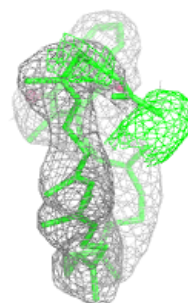
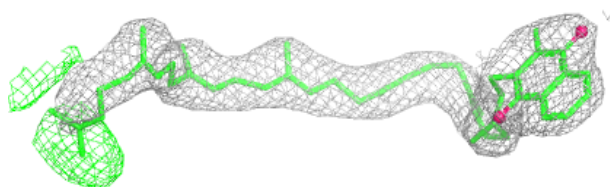
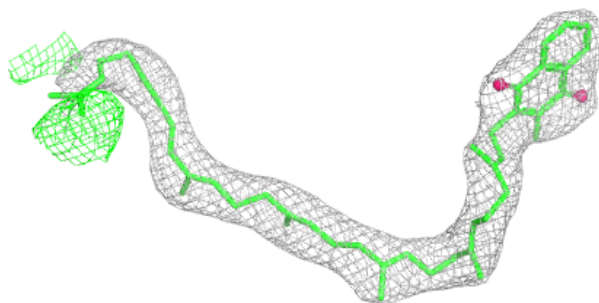
**Electron density around MQ7 M 402 (A):**

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

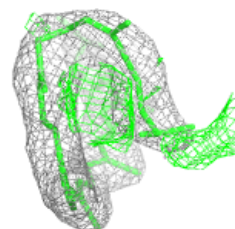
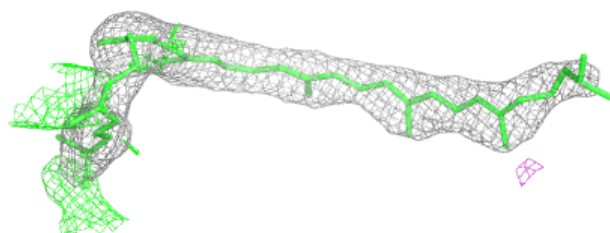
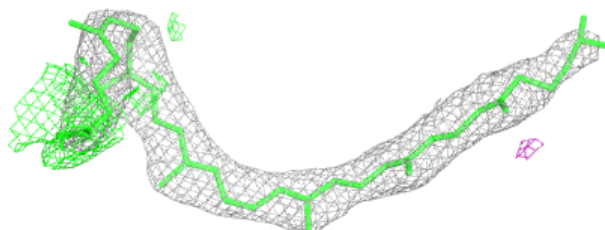


Electron density around MQ7 M 402 (B):

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

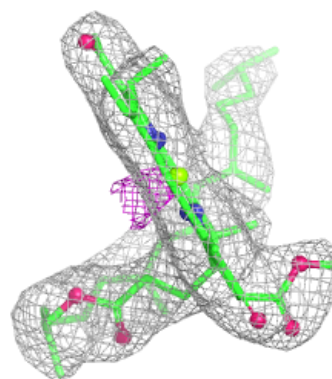
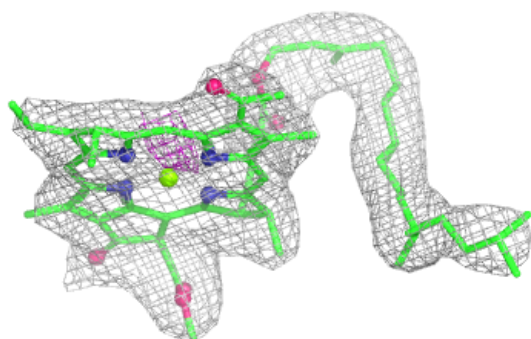
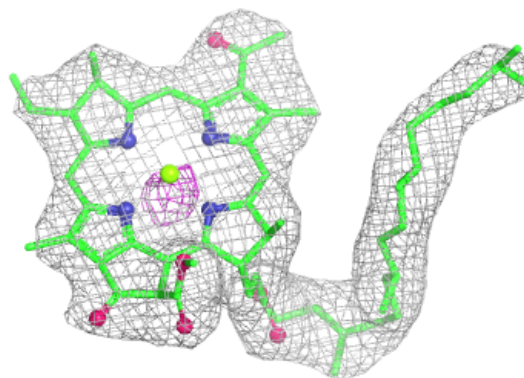
**Electron density around NS5 M 405:**

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

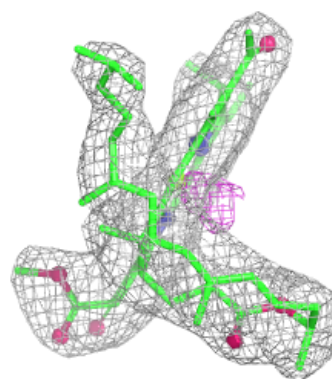
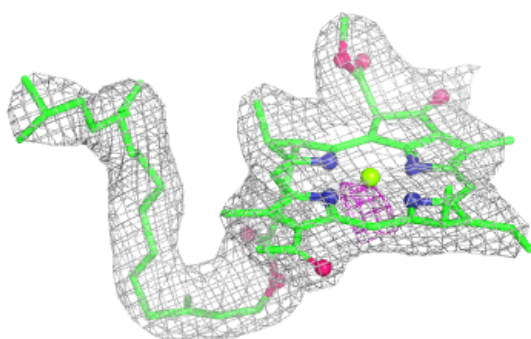
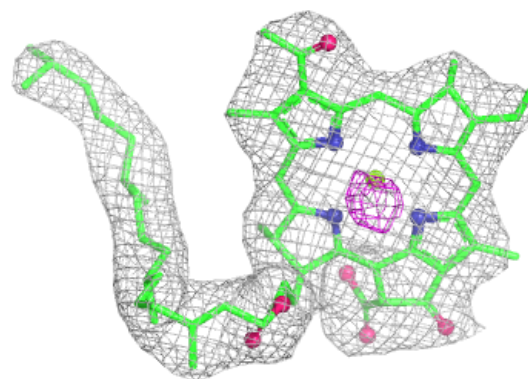


Electron density around BCB L 302 (A):

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

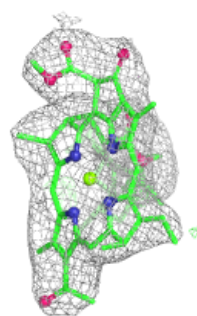
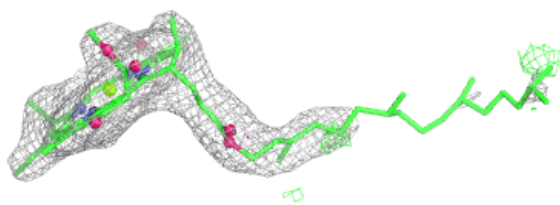
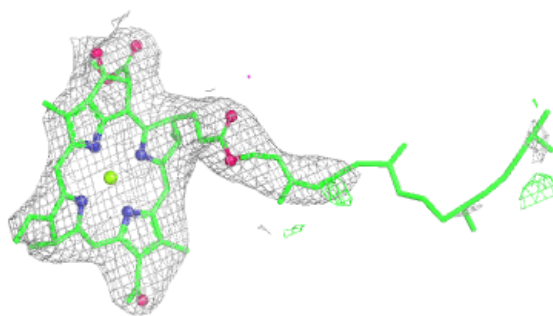
**Electron density around BCB L 302 (B):**

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

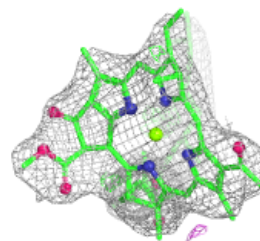
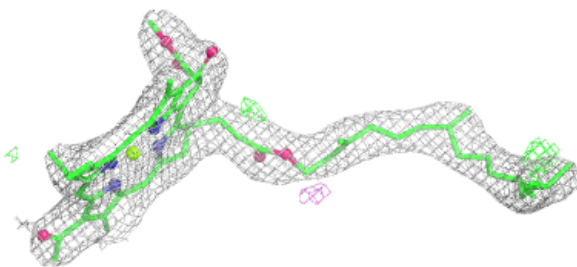
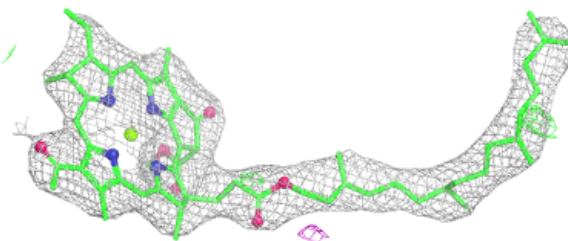


Electron density around BCB L 304:

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

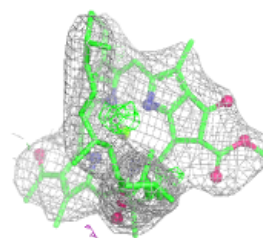
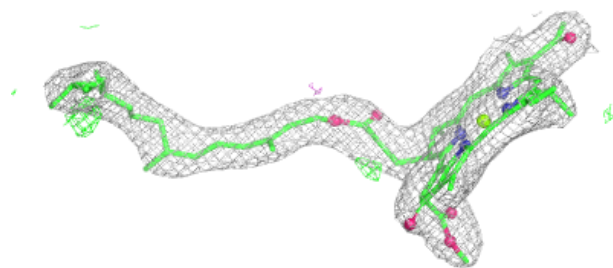
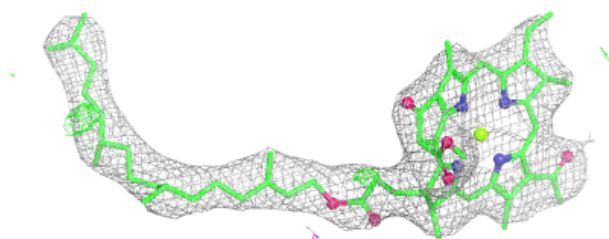
**Electron density around BCB M 403 (A):**

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



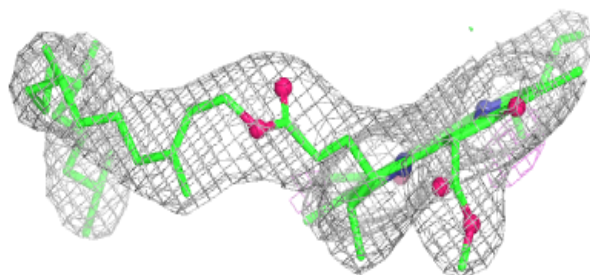
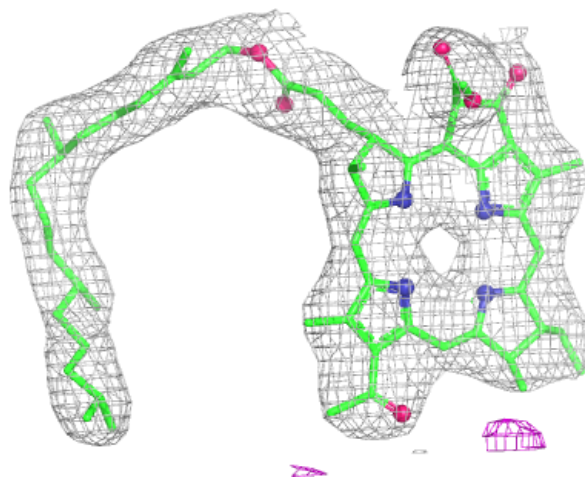
Electron density around BCB M 403 (B):

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



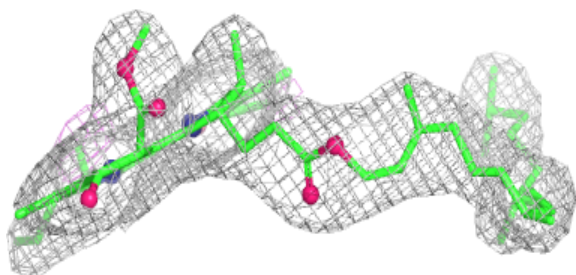
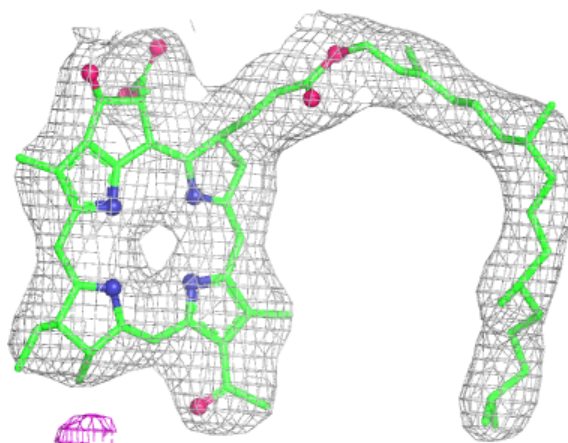
Electron density around BPB L 303 (A):

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



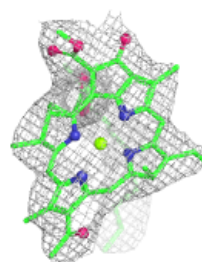
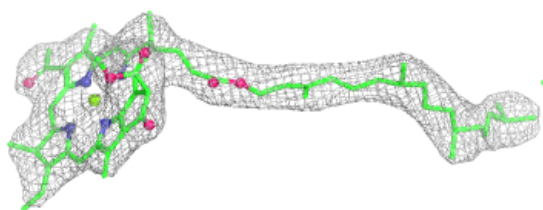
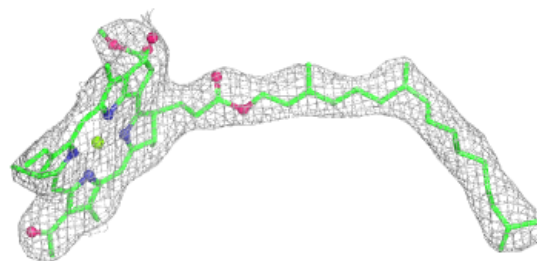
Electron density around BPB L 303 (B):

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

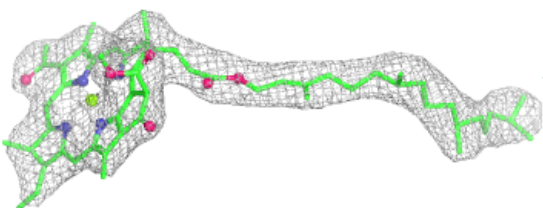
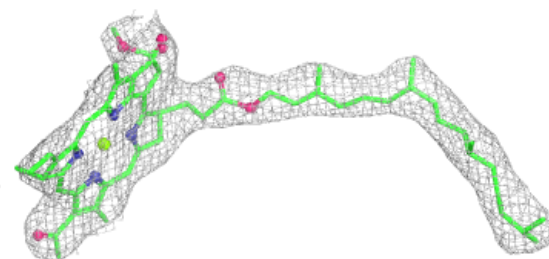


Electron density around BCB L 301 (A):

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

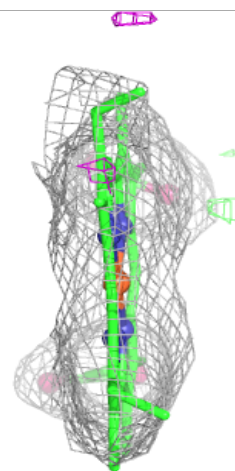
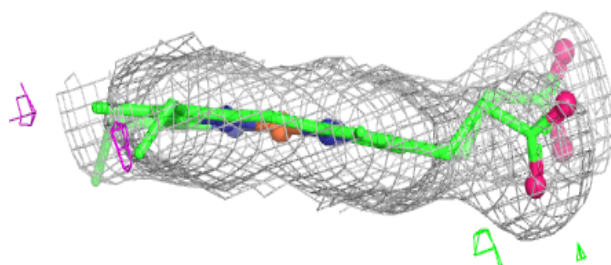
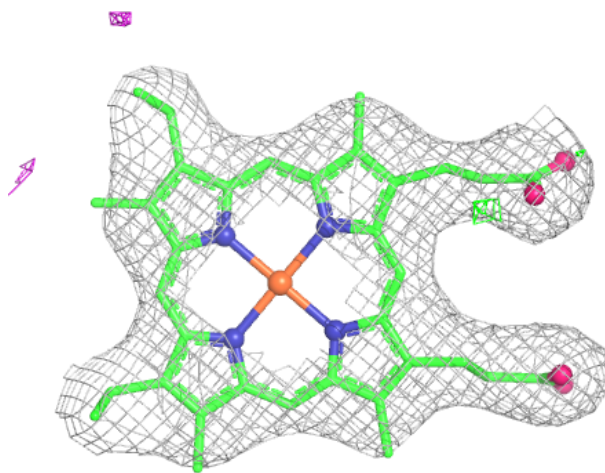
**Electron density around BCB L 301 (B):**

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



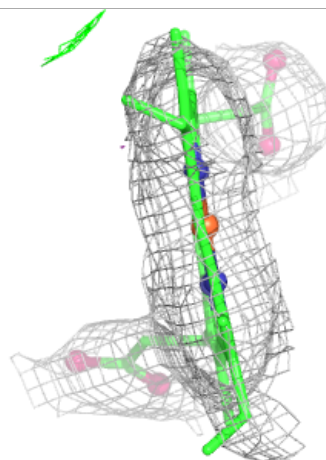
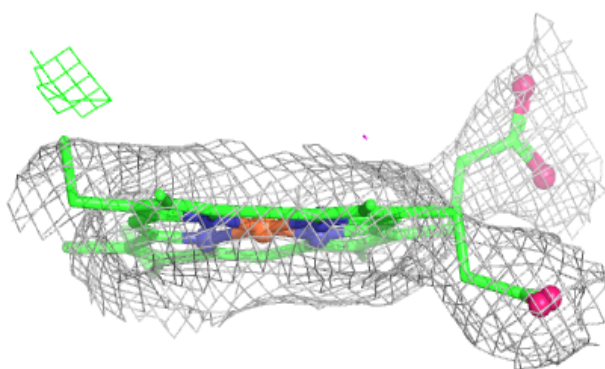
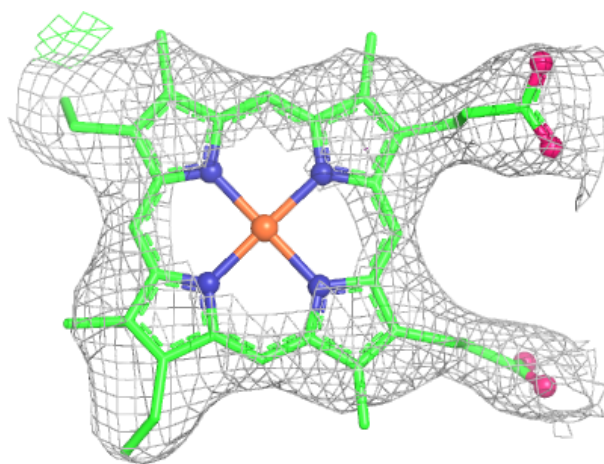
Electron density around HEC C 404:

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



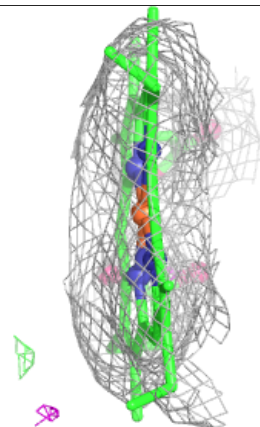
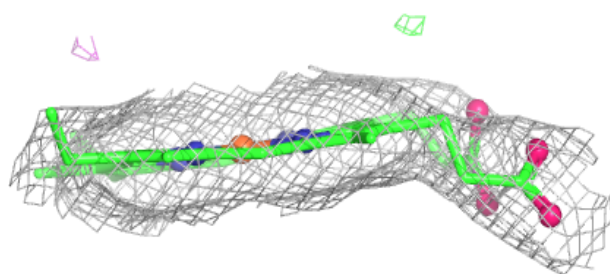
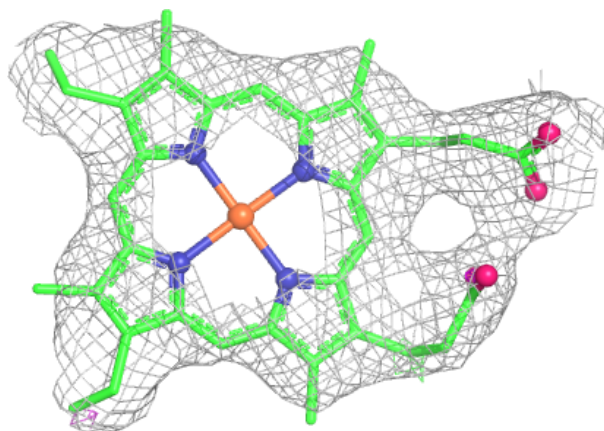
Electron density around HEC C 401:

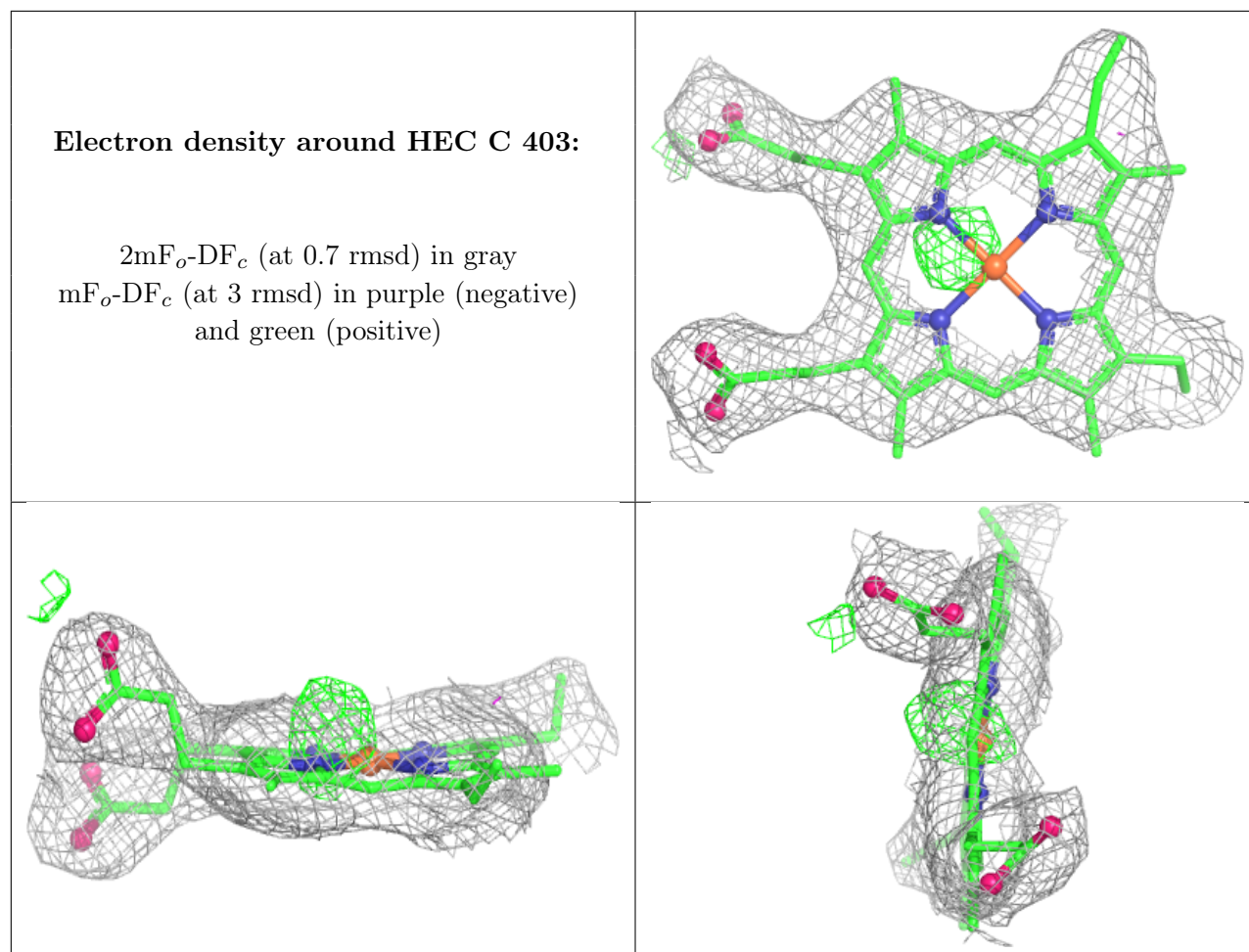
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.