Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 07:51 am GMT

PDB ID	:	6ZIA
Title	:	Ultrafast Structural Response to Charge Redistribution Within a Photosynthetic Reaction Centre - 8 us 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 (i) 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 (i)) were used in the production of this report:

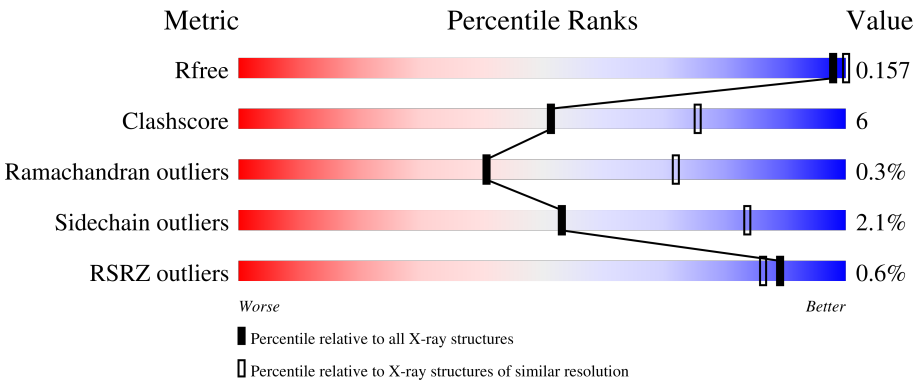
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	89% 9% ••
2	H	258	2% 84% 14% •
3	L	273	88% 12%
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	-	-	-
6	DGA	C	405	-	-	-	X
7	SO4	M	407	-	-	X	-
8	LDA	M	413	-	-	-	X

2 Entry composition (i)

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
			Total	C	N	O	S			
1	C	332	2602	1640	466	478	18	0	0	0

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

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

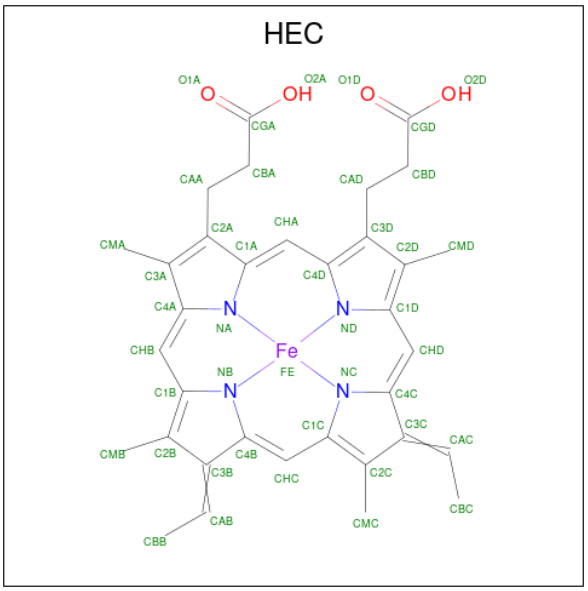
- Molecule 3 is a protein called Reaction center protein L chain.

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

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

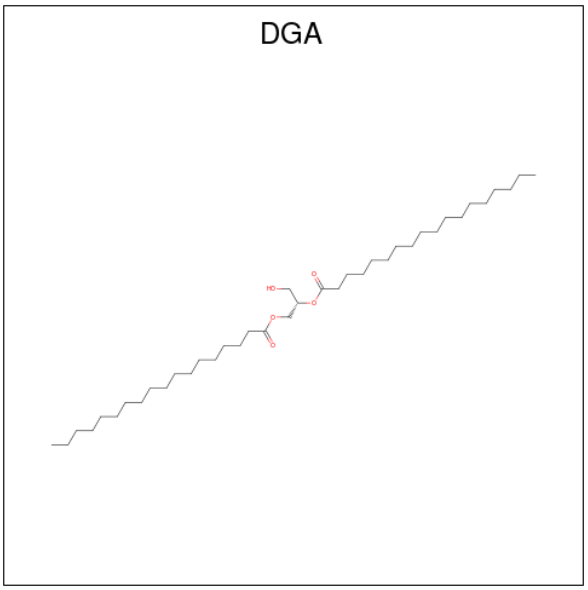
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2977	1983	491	490	13	0	51	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



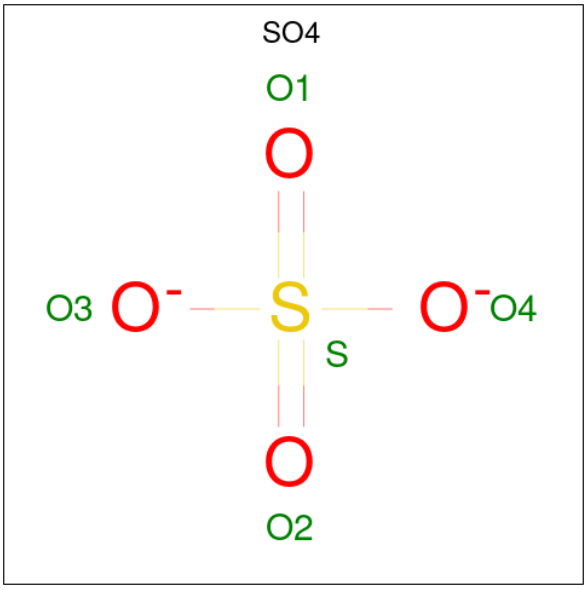
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0

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



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



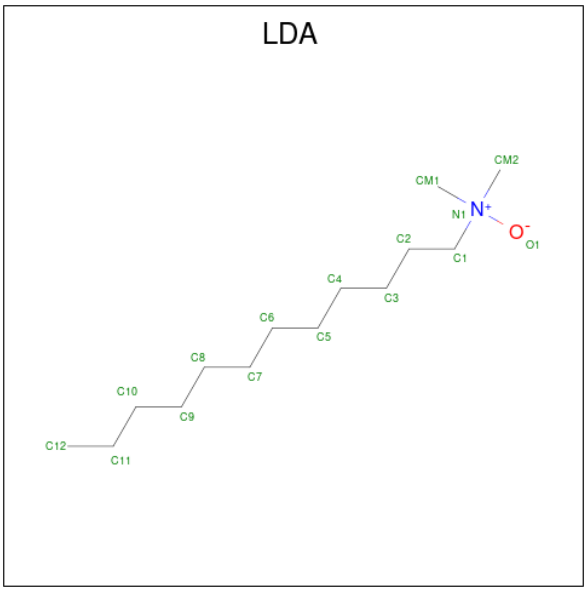
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	C	1	5	4	1	0	0
			Total	O	S		
7	C	1	5	4	1	0	0
			Total	O	S		
7	C	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O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

Continued on next page...

Continued from previous page...

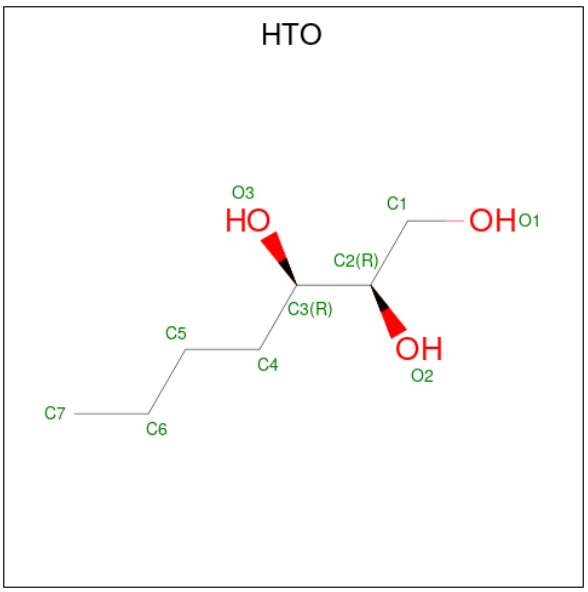
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
7	M	1	5	4	1		0	0
			Total	O	S			
7	M	1	5	4	1		0	0
			Total	O	S			
7	M	1	5	4	1		0	0
			Total	O	S			
7	M	1	5	4	1		0	0

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



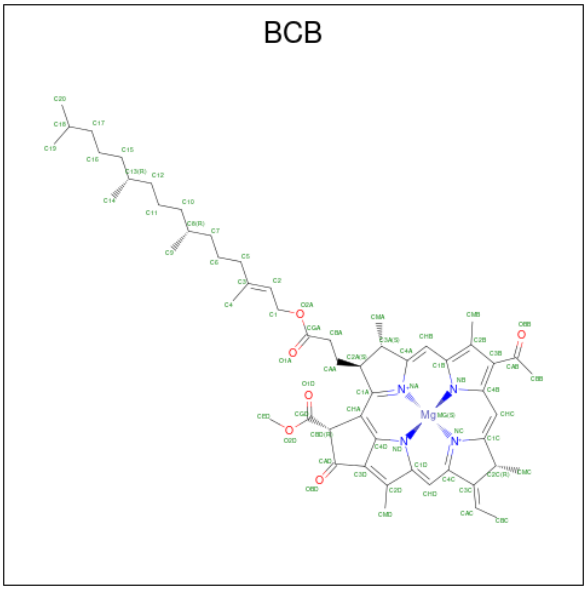
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	H	1	16	14	1	1	0	0
			Total	C	N	O		
8	H	1	16	14	1	1	0	0
			Total	C	N	O		
8	H	1	16	14	1	1	0	0
			Total	C	N	O		
8	L	1	16	14	1	1	0	0
			Total	C	N	O		
8	L	1	16	14	1	1	0	0
			Total	C	N	O		
8	M	1	16	14	1	1	0	0
			Total	C	N	O		
8	M	1	16	14	1	1	0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

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



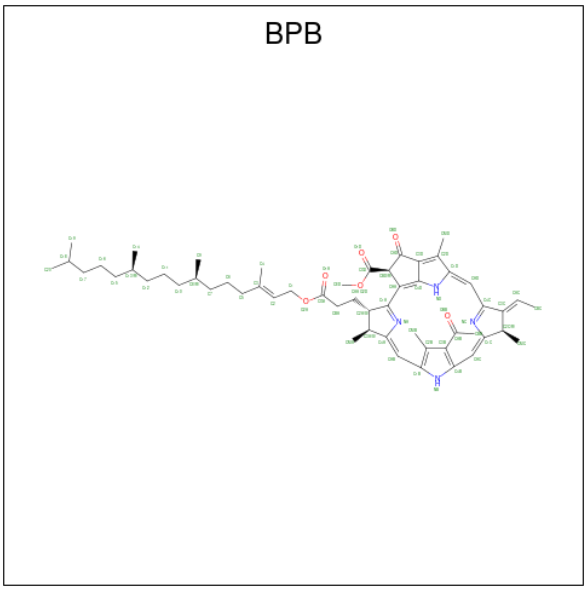
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	O		0	0
			10	7	3			
9	H	1	Total	C	O		0	0
			10	7	3			
9	L	1	Total	C	O		0	0
			10	7	3			

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



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

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

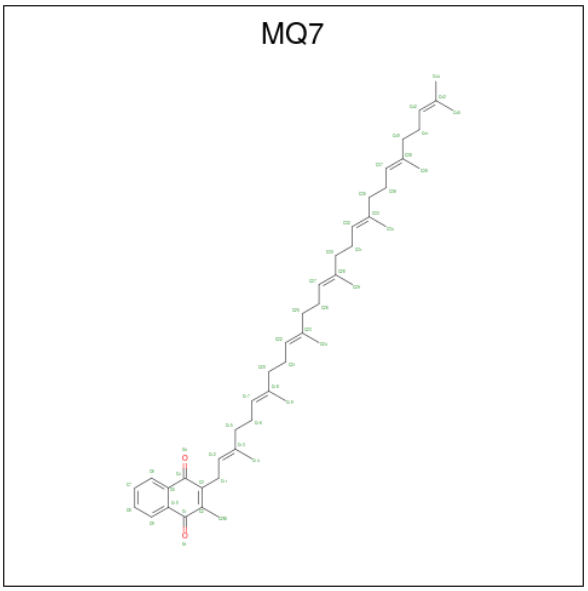


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	L	1	130	110	8	12	0	1
			Total	C	N	O		
11	L	1	65	55	4	6	0	0

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

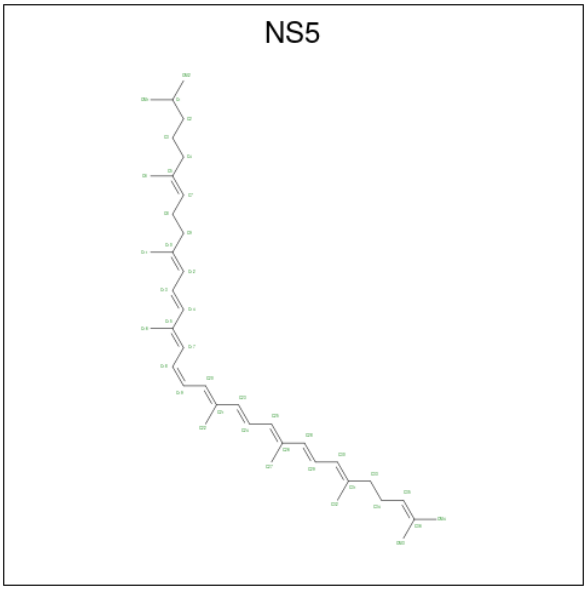
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
12	M	1	2	2	0	1

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



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

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 15 is water.

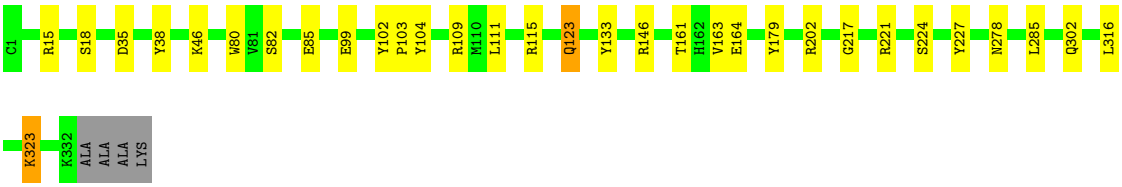
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	C	56	56	56	0	0
			Total	O		
15	H	27	27	27	0	0
			Total	O		
15	L	24	24	24	0	0
			Total	O		
15	M	39	39	39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

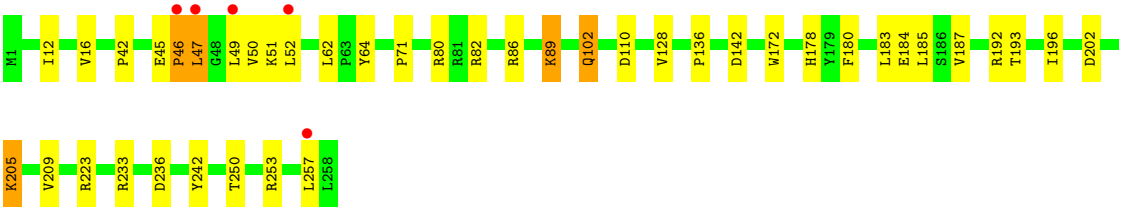
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



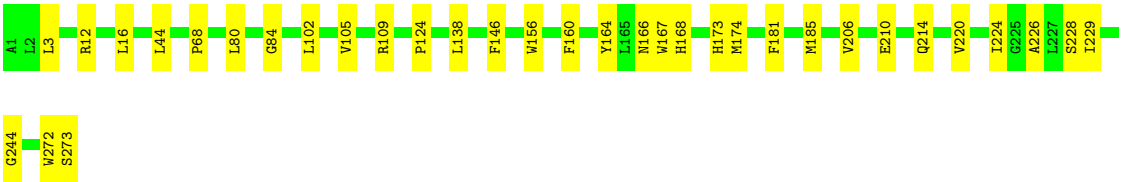
• Molecule 2: Reaction center protein H chain

Chain H:



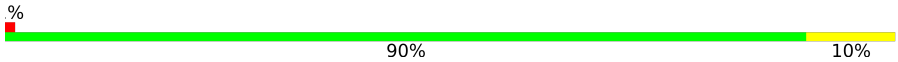
• Molecule 3: Reaction center protein L chain

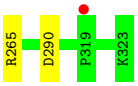
Chain L:



• Molecule 4: Reaction center protein M chain

Chain M:




R265
D290
P319
K323

4 Data and refinement statistics (i)

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 – 2.38	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.31-2.80) 98.5 (34.31-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5.8.0158, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.160 , 0.154 0.162 , 0.157	Depositor DCC
R_{free} test set	5919 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	77.4	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 71.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11472	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: LDA, HTO, HEC, FE, MQ7, SO4, NS5, BPB, FME, BCB, 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	0.42	0/2669	0.57	0/3637
2	H	0.43	0/2055	0.60	0/2807
3	L	0.43	0/2612	0.56	0/3568
4	M	0.45	0/3101	0.55	0/4242
All	All	0.43	0/10437	0.57	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	25	0
2	H	2018	0	2020	34	0
3	L	2508	0	2390	35	0
4	M	2977	0	2832	25	0
5	C	172	0	120	4	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	2	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	4	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	15	0
10	M	132	0	144	6	0
11	L	195	0	222	14	0
12	M	2	0	0	0	0
13	M	96	0	128	1	0
14	M	40	0	60	2	0
15	C	56	0	0	0	0
15	H	27	0	0	0	0
15	L	24	0	0	0	0
15	M	39	0	0	0	0
All	All	11472	0	11177	126	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 (126) 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
1:C:161:THR:HG21	3:L:273:SER:O	1.83	0.78
2:H:184:GLU:OE2	2:H:193:THR:HG21	1.83	0.77
11:L:305:BPB:HHC	11:L:305:BPB:HBBB	1.67	0.77
1:C:161:THR:HB	1:C:164:GLU:HG3	1.68	0.75
2:H:42:PRO:HD3	8:H:708:LDA:H121	1.70	0.72
4:M:239:ARG:HD3	4:M:244[B]:GLU:HG2	1.71	0.72
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
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
2:H:45:GLU:HG3	2:H:46:PRO:HD2	1.81	0.61
2:H:80:ARG:CZ	2:H:82:ARG:HD2	2.31	0.60
2:H:196:ILE:HD12	2:H:242:TYR:CZ	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:265[B]:ARG:NH1	7:M:407:SO4:O1	2.32	0.58
2:H:205:LYS:H	2:H:205:LYS:CD	2.14	0.58
5:C:403:HEC:HBC1	5:C:404:HEC:HMA1	1.86	0.57
2:H:128:VAL:HG22	3:L:210:GLU:CD	2.25	0.56
4:M:190:ARG:O	4:M:190:ARG:HD2	2.05	0.56
10:M:403[B]:BCB:HBD	10:M:403[B]:BCB:HAA1	1.87	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	2.05	0.54
3:L:181:PHE:HB3	11:L:305:BPB:HBBA	1.87	0.54
3:L:224:ILE:HG12	3:L:228:SER:HB2	1.90	0.54
3:L:185:MET:CE	10:L:304:BCB:H41	2.37	0.54
2:H:89:LYS:HE3	2:H:110:ASP:HB3	1.90	0.54
3:L:244[A]:GLY:O	10:L:301[A]:BCB:HED3	2.09	0.53
3:L:181:PHE:CD2	11:L:305:BPB:HBB	2.43	0.53
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.44	0.53
2:H:142:ASP:OD1	2:H:142:ASP:N	2.35	0.53
2:H:183:LEU:HB2	2:H:196:ILE:CG2	2.39	0.53
4:M:239:ARG:HD2	4:M:244[B]:GLU:OE2	2.09	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
11:L:303[B]:BPB:HBBB	11:L:303[B]:BPB:HMB	1.92	0.52
1:C:323:LYS:H	1:C:323:LYS:CD	2.22	0.52
4:M:204[B]:ILE:HG12	10:M:403[B]:BCB:HMB3	1.92	0.52
10:L:302[B]:BCB:HMD2	10:M:403[B]:BCB:HBB3	1.91	0.52
11:L:303[B]:BPB:HEDA	4:M:254:ILE:HG21	1.92	0.52
2:H:180:PHE:CE2	4:M:12:ALA:HB2	2.45	0.52
4:M:102:MET:HE1	4:M:164:THR:HG22	1.91	0.51
5:C:401:HEC:HMB1	5:C:401:HEC:HBB3	1.93	0.51
2:H:12:ILE:O	2:H:16:VAL:HG23	2.11	0.51
10:L:302[B]:BCB:HMD1	4:M:204[B]:ILE:HD13	1.92	0.50
1:C:227:TYR:HH	4:M:183:TRP:HD1	1.60	0.50
2:H:64:TYR:CE1	8:H:708:LDA:H11	2.47	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
1:C:123:GLN:H	1:C:123:GLN:HE21	1.60	0.50
3:L:166[B]:ASN:OD1	3:L:168[B]:HIS:HB2	2.12	0.49
3:L:3:LEU:HD11	4:M:251[A]:ARG:HD2	1.94	0.49
5:C:403:HEC:HMB1	5:C:403:HEC:HBB3	1.95	0.49
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:GLU:O	2:H:47:LEU:N	2.47	0.48
10:L:301[B]:BCB:H52	11:L:303[B]:BPB:HBBA	1.95	0.48
5:C:402:HEC:HHA	5:C:402:HEC:O1D	2.14	0.47
2:H:187:VAL:CG2	2:H:192:ARG:HG3	2.44	0.47
4:M:239:ARG:HD3	4:M:244[B]:GLU:CG	2.43	0.47
4:M:29:VAL:HG21	4:M:51:LEU:HD12	1.96	0.47
2:H:62:LEU:O	8:H:708:LDA:HM21	2.14	0.47
2:H:49:LEU:O	2:H:51:LYS:N	2.48	0.47
2:H:128:VAL:CG2	3:L:210:GLU:CD	2.83	0.47
11:L:303[A]:BPB:HMB	11:L:303[A]:BPB:HBBB	1.96	0.47
3:L:168[A]:HIS:CE1	10:L:301[A]:BCB:HMC2	2.50	0.47
8:H:701:LDA:HM21	8:L:306:LDA:HM22	1.97	0.47
1:C:224:SER:HA	1:C:227:TYR:HD1	1.81	0.45
3:L:167[A]:TRP:HE1	3:L:173[A]:HIS:CD2	2.34	0.45
2:H:45:GLU:HG3	2:H:46:PRO:CD	2.45	0.45
3:L:181:PHE:HB3	11:L:305:BPB:CBB	2.46	0.45
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.17	0.45
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.98	0.45
1:C:161:THR:HG21	3:L:273:SER:C	2.36	0.45
3:L:185:MET:HE2	10:L:304:BCB:H41	1.98	0.45
3:L:124:PRO:HD3	11:L:303[B]:BPB:HAC	1.98	0.45
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:306:LDA:HM21	8:L:306:LDA:H22	1.60	0.44
4:M:159:GLY:HA3	14:M:404:NS5:H272	1.98	0.44
3:L:174[B]:MET:HA	10:L:304:BCB:OBD	2.18	0.44
11:L:305:BPB:H14	11:L:305:BPB:H16A	1.61	0.44
3:L:44:LEU:HD12	3:L:44:LEU:HA	1.70	0.44
1:C:146:ARG:HD3	1:C:179:TYR:CE1	2.53	0.44
10:L:302[B]:BCB:HMB1	10:L:302[B]:BCB:HBB2	2.00	0.43
2:H:89:LYS:HE3	2:H:110:ASP:CB	2.48	0.43
10:L:301[B]:BCB:H2C	10:M:403[B]:BCB:H2C	1.99	0.43
1:C:82:SER:HB2	1:C:85:GLU:HB2	2.00	0.43
1:C:323:LYS:H	1:C:323:LYS:HD3	1.84	0.43
3:L:214:GLN:HG2	4:M:19:VAL:HB	2.01	0.43
3:L:226:ALA:O	3:L:229:ILE:HG22	2.18	0.43
10:L:304:BCB:H43	10:L:304:BCB:H11	1.85	0.43
4:M:157:CYS:HA	4:M:161:ILE:HB	1.99	0.43
2:H:102:GLN:NE2	3:L:12:ARG:HD3	2.33	0.43
3:L:220:VAL:HG11	11:L:305:BPB:HEDA	2.00	0.43
4:M:236:ILE:HG12	4:M:260[A]:ILE:HG23	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:HD2	3:L:68:PRO:O	2.17	0.43
4:M:261[B]:GLU:OE2	4:M:265[B]:ARG:NH2	2.46	0.43
4:M:260[B]:ILE:O	4:M:264[B]:HIS:ND1	2.51	0.42
14:M:404:NS5:H18	14:M:404:NS5:H161	1.86	0.42
10:L:301[A]:BCB:H62	10:L:301[A]:BCB:H41	1.93	0.42
11:L:303[B]:BPB:HED	13:M:402[B]:MQ7:H22	2.01	0.42
1:C:202:ARG:O	1:C:221:ARG:NH2	2.47	0.42
3:L:102:LEU:O	3:L:105:VAL:HG22	2.19	0.42
10:L:301[A]:BCB:H151	11:L:303[A]:BPB:H5A	2.00	0.42
1:C:109:ARG:HG2	1:C:285:LEU:HD21	2.02	0.42
2:H:71:PRO:HD3	3:L:206:VAL:HG22	2.01	0.42
2:H:136:PRO:HA	2:H:172:TRP:HA	2.01	0.42
2:H:257:LEU:HD13	3:L:16:LEU:HD23	2.02	0.41
3:L:146:PHE:HB3	3:L:156[B]:TRP:CD2	2.55	0.41
11:L:303[A]:BPB:OBB	11:L:303[A]:BPB:HHC	2.20	0.41
1:C:18:SER:HB2	3:L:156[A]:TRP:CD1	2.55	0.41
4:M:265[A]:ARG:NH2	7:M:407:SO4:O1	2.46	0.41
2:H:128:VAL:HG22	3:L:210:GLU:HB2	2.03	0.41
1:C:217:GLY:HA2	4:M:167:GLY:O	2.20	0.41
2:H:47:LEU:CD1	2:H:49:LEU:HB3	2.51	0.41
2:H:257:LEU:HD12	2:H:257:LEU:H	1.86	0.41
4:M:120:MET:HG3	10:M:403[B]:BCB:H202	2.03	0.41
1:C:99:GLU:HG2	1:C:104:TYR:CE1	2.56	0.40
3:L:80:LEU:HA	3:L:84:GLY:HA3	2.02	0.40
4:M:248[B]:LEU:HD23	4:M:248[B]:LEU:HA	1.86	0.40
3:L:164[B]:TYR:CD1	3:L:164[B]:TYR:N	2.89	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%)	320 (97%)	10 (3%)	0	100	100
2	H	256/258 (99%)	248 (97%)	5 (2%)	3 (1%)	13	39
3	L	312/273 (114%)	300 (96%)	12 (4%)	0	100	100
4	M	372/323 (115%)	358 (96%)	13 (4%)	1 (0%)	41	72
All	All	1270/1190 (107%)	1226 (96%)	40 (3%)	4 (0%)	41	72

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 (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%)	277 (99%)	4 (1%)	67	90
2	H	212/212 (100%)	202 (95%)	10 (5%)	26	59
3	L	253/218 (116%)	250 (99%)	3 (1%)	71	92
4	M	288/249 (116%)	282 (98%)	6 (2%)	53	84
All	All	1034/961 (108%)	1011 (98%)	23 (2%)	53	83

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	46	LYS
1	C	123	GLN
1	C	323	LYS
2	H	52	LEU
2	H	86	ARG
2	H	89	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	102	GLN
2	H	178	HIS
2	H	185	LEU
2	H	205	LYS
2	H	223	ARG
2	H	233	ARG
2	H	236	ASP
3	L	160[A]	PHE
3	L	160[B]	PHE
3	L	272	TRP
4	M	27	ASP
4	M	194[A]	PHE
4	M	194[B]	PHE
4	M	214[A]	PHE
4	M	214[B]	PHE
4	M	290	ASP

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
1	C	310	GLN
2	H	102	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.98	0	7,9,11	1.08	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 monosaccharides 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	$\#\|Z\| > 2$
11	BPB	L	305	-	49,70,70	2.11	9 (18%)	47,101,101	2.09	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SO4	C	408	-	4,4,4	0.16	0	6,6,6	0.11	0
8	LDA	M	413	-	12,15,15	0.48	0	14,17,17	0.52	0
7	SO4	H	704	-	4,4,4	0.12	0	6,6,6	0.16	0
5	HEC	C	402	1	32,50,50	1.50	4 (12%)	24,82,82	2.01	8 (33%)
6	DGA	C	405	1	36,36,43	1.18	3 (8%)	38,38,45	1.17	3 (7%)
10	BCB	M	403[B]	-	63,74,74	1.89	13 (20%)	74,115,115	3.09	23 (31%)
5	HEC	C	401	1	32,50,50	1.63	6 (18%)	24,82,82	2.52	5 (20%)
7	SO4	C	407	-	4,4,4	0.16	0	6,6,6	0.14	0
7	SO4	H	702	-	4,4,4	0.23	0	6,6,6	0.33	0
10	BCB	L	302[A]	-	63,74,74	1.88	15 (23%)	74,115,115	3.14	24 (32%)
10	BCB	L	304	-	63,74,74	1.83	14 (22%)	74,115,115	3.25	25 (33%)
7	SO4	M	408	-	4,4,4	0.30	0	6,6,6	0.27	0
8	LDA	L	307	-	12,15,15	0.39	0	14,17,17	0.64	0
11	BPB	L	303[B]	-	49,70,70	2.05	9 (18%)	47,101,101	2.27	14 (29%)
7	SO4	M	410	-	4,4,4	0.28	0	6,6,6	0.33	0
7	SO4	H	703	-	4,4,4	0.22	0	6,6,6	0.12	0
8	LDA	H	707	-	12,15,15	0.36	0	14,17,17	0.82	0
9	HTO	L	308	-	9,9,9	0.72	0	10,10,10	1.20	1 (10%)
7	SO4	M	407	-	4,4,4	0.14	0	6,6,6	0.25	0
7	SO4	C	406	-	4,4,4	0.25	0	6,6,6	0.39	0
5	HEC	C	403	1	32,50,50	1.55	5 (15%)	24,82,82	1.85	8 (33%)
9	HTO	H	710	-	9,9,9	0.85	0	10,10,10	1.04	1 (10%)
8	LDA	M	412	-	12,15,15	0.42	0	14,17,17	0.55	0
7	SO4	M	406	-	4,4,4	0.16	0	6,6,6	0.17	0
8	LDA	L	306	-	12,15,15	0.39	0	14,17,17	0.70	0
10	BCB	L	301[B]	-	63,74,74	1.93	13 (20%)	74,115,115	2.92	21 (28%)
10	BCB	M	403[A]	-	63,74,74	1.87	13 (20%)	74,115,115	3.10	25 (33%)
7	SO4	M	409	-	4,4,4	0.15	0	6,6,6	0.18	0
7	SO4	M	411	-	4,4,4	0.25	0	6,6,6	0.21	0
8	LDA	H	701	-	12,15,15	0.36	0	14,17,17	0.76	0
8	LDA	H	708	-	12,15,15	0.27	0	14,17,17	0.84	0
11	BPB	L	303[A]	-	49,70,70	2.05	9 (18%)	47,101,101	2.22	13 (27%)
5	HEC	C	404	1	32,50,50	1.56	3 (9%)	24,82,82	1.67	7 (29%)
13	MQ7	M	402[B]	-	49,49,49	1.50	2 (4%)	60,63,63	1.48	11 (18%)
7	SO4	H	705	-	4,4,4	0.27	0	6,6,6	0.36	0
14	NS5	M	404	-	39,39,39	1.39	2 (5%)	44,46,46	2.04	14 (31%)
7	SO4	M	405	-	4,4,4	0.11	0	6,6,6	0.26	0
10	BCB	L	302[B]	-	63,74,74	1.87	15 (23%)	74,115,115	3.03	25 (33%)
10	BCB	L	301[A]	-	63,74,74	1.88	13 (20%)	74,115,115	3.07	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	HTO	H	709	-	9,9,9	0.85	0	10,10,10	0.59	0
7	SO4	H	706	-	4,4,4	0.18	0	6,6,6	0.09	0
13	MQ7	M	402[A]	-	49,49,49	1.53	2 (4%)	60,63,63	1.56	14 (23%)

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	305	-	-	7/37/105/105	0/5/6/6
8	LDA	M	413	-	-	4/13/13/13	-
5	HEC	C	402	1	-	3/10/54/54	-
6	DGA	C	405	1	-	15/37/37/45	-
10	BCB	M	403[B]	-	3/3/21/26	19/37/137/137	-
5	HEC	C	401	1	-	3/10/54/54	-
10	BCB	L	302[A]	-	2/2/21/26	6/37/137/137	-
10	BCB	L	304	-	3/3/21/26	14/37/137/137	-
8	LDA	L	307	-	-	10/13/13/13	-
11	BPB	L	303[B]	-	-	10/37/105/105	0/5/6/6
8	LDA	H	707	-	-	6/13/13/13	-
9	HTO	L	308	-	-	4/10/10/10	-
5	HEC	C	403	1	-	2/10/54/54	-
9	HTO	H	710	-	-	0/10/10/10	-
8	LDA	M	412	-	-	4/13/13/13	-
8	LDA	L	306	-	-	5/13/13/13	-
10	BCB	L	301[B]	-	3/3/21/26	8/37/137/137	-
10	BCB	M	403[A]	-	2/2/21/26	13/37/137/137	-
8	LDA	H	701	-	-	3/13/13/13	-
8	LDA	H	708	-	-	7/13/13/13	-
11	BPB	L	303[A]	-	-	7/37/105/105	0/5/6/6
5	HEC	C	404	1	-	0/10/54/54	-
13	MQ7	M	402[B]	-	-	1/41/61/61	0/2/2/2
14	NS5	M	404	-	-	10/43/43/43	-
10	BCB	L	302[B]	-	2/2/21/26	9/37/137/137	-
10	BCB	L	301[A]	-	3/3/21/26	8/37/137/137	-
9	HTO	H	709	-	-	4/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	MQ7	M	402[A]	-	-	0/41/61/61	0/2/2/2

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	402[A]	MQ7	C3-C2	8.56	1.50	1.35
13	M	402[B]	MQ7	C3-C2	8.09	1.50	1.35
11	L	305	BPB	CAC-C3C	7.51	1.52	1.33
14	M	404	NS5	C35-C36	7.35	1.53	1.32
11	L	303[B]	BPB	CAC-C3C	7.16	1.51	1.33
11	L	303[A]	BPB	CAC-C3C	7.12	1.51	1.33
10	L	302[A]	BCB	CAC-C3C	6.13	1.50	1.33
10	M	403[B]	BCB	CAC-C3C	6.03	1.50	1.33
10	L	302[B]	BCB	CAC-C3C	5.90	1.49	1.33
10	L	301[A]	BCB	CAC-C3C	5.89	1.49	1.33
10	M	403[A]	BCB	CAC-C3C	5.88	1.49	1.33
10	L	301[B]	BCB	CAC-C3C	5.79	1.49	1.33
10	M	403[A]	BCB	O2D-CGD	5.44	1.46	1.33
5	C	401	HEC	C2B-C3B	-5.42	1.35	1.40
10	L	304	BCB	CAC-C3C	5.38	1.48	1.33
11	L	303[B]	BPB	C3B-C2B	5.32	1.49	1.39
11	L	303[B]	BPB	O2D-CGD	5.23	1.46	1.33
11	L	303[A]	BPB	O2D-CGD	5.20	1.45	1.33
13	M	402[B]	MQ7	C10-C5	5.18	1.49	1.40
11	L	303[A]	BPB	C3B-C2B	5.15	1.48	1.39
10	M	403[B]	BCB	C3B-C2B	5.15	1.48	1.39
10	L	301[A]	BCB	C3B-C2B	5.13	1.48	1.39
11	L	305	BPB	O2A-CGA	5.10	1.48	1.33
11	L	303[B]	BPB	C3D-C2D	5.08	1.48	1.39
5	C	404	HEC	C2B-C3B	-5.07	1.35	1.40
10	L	301[B]	BCB	O2D-CGD	5.06	1.45	1.33
10	L	302[B]	BCB	O2D-CGD	5.04	1.45	1.33
10	M	403[A]	BCB	C3B-C2B	5.03	1.48	1.39
10	M	403[B]	BCB	O2D-CGD	5.02	1.45	1.33
10	L	304	BCB	O2D-CGD	5.00	1.45	1.33
10	L	302[A]	BCB	C3B-C2B	4.98	1.48	1.39
10	L	302[B]	BCB	C3B-C2B	4.97	1.48	1.39
10	L	301[B]	BCB	C3B-C2B	4.97	1.48	1.39
11	L	305	BPB	O2D-CGD	4.90	1.45	1.33
10	L	301[A]	BCB	O2D-CGD	4.90	1.45	1.33
10	L	302[A]	BCB	O2D-CGD	4.87	1.45	1.33
11	L	303[A]	BPB	C3D-C2D	4.86	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	301[B]	BCB	CHD-C1D	4.75	1.47	1.38
10	L	304	BCB	C3B-C2B	4.69	1.47	1.39
11	L	305	BPB	C3B-C2B	4.64	1.47	1.39
11	L	303[B]	BPB	OBD-CAD	4.56	1.28	1.22
11	L	305	BPB	OBD-CAD	4.55	1.28	1.22
10	L	301[B]	BCB	C2C-C3C	-4.50	1.45	1.51
13	M	402[A]	MQ7	C10-C5	4.48	1.48	1.40
5	C	402	HEC	C2B-C3B	-4.45	1.36	1.40
11	L	305	BPB	C3D-C2D	4.45	1.47	1.39
5	C	403	HEC	C2B-C3B	-4.43	1.36	1.40
10	M	403[B]	BCB	O2A-CGA	4.28	1.45	1.33
11	L	303[A]	BPB	OBD-CAD	4.25	1.28	1.22
10	L	302[A]	BCB	C2C-C3C	-4.17	1.46	1.51
10	L	301[A]	BCB	O2A-CGA	4.17	1.45	1.33
10	L	302[A]	BCB	O2A-CGA	4.14	1.45	1.33
10	L	302[B]	BCB	O2A-CGA	4.12	1.45	1.33
10	L	301[A]	BCB	C2C-C3C	-4.11	1.46	1.51
10	L	304	BCB	C2C-C3C	-4.07	1.46	1.51
10	M	403[A]	BCB	O2A-CGA	4.07	1.45	1.33
10	L	301[B]	BCB	O2A-CGA	4.05	1.45	1.33
10	L	304	BCB	O2A-CGA	3.98	1.45	1.33
10	L	302[B]	BCB	C2C-C3C	-3.97	1.46	1.51
10	L	302[A]	BCB	CHD-C1D	3.97	1.46	1.38
11	L	303[A]	BPB	O2A-CGA	3.95	1.44	1.33
10	L	301[B]	BCB	OBD-CAD	3.95	1.29	1.22
10	L	301[A]	BCB	CHD-C1D	3.93	1.46	1.38
10	M	403[B]	BCB	CHD-C1D	3.89	1.45	1.38
10	L	302[B]	BCB	CHD-C1D	3.85	1.45	1.38
10	M	403[A]	BCB	CHD-C1D	3.83	1.45	1.38
10	L	304	BCB	CHD-C1D	3.83	1.45	1.38
11	L	305	BPB	C4C-NC	-3.76	1.26	1.37
10	M	403[B]	BCB	OBD-CAD	3.75	1.28	1.22
10	L	302[B]	BCB	OBD-CAD	3.75	1.28	1.22
10	L	301[A]	BCB	OBD-CAD	3.74	1.28	1.22
11	L	303[B]	BPB	O2A-CGA	3.73	1.44	1.33
11	L	303[A]	BPB	CHA-CBD	-3.71	1.48	1.52
10	L	304	BCB	C3D-C2D	3.70	1.49	1.39
10	L	301[A]	BCB	C3D-C2D	3.68	1.49	1.39
10	M	403[B]	BCB	C2C-C3C	-3.66	1.47	1.51
10	M	403[A]	BCB	C3D-C2D	3.61	1.49	1.39
5	C	401	HEC	C3C-C2C	-3.59	1.37	1.40
11	L	305	BPB	CHA-CBD	-3.53	1.48	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	302[A]	BCB	OBD-CAD	3.52	1.28	1.22
5	C	404	HEC	C3C-C2C	-3.51	1.37	1.40
10	M	403[B]	BCB	C1D-ND	-3.48	1.33	1.37
10	L	301[B]	BCB	C3D-C2D	3.47	1.48	1.39
10	M	403[A]	BCB	OBD-CAD	3.43	1.28	1.22
10	L	302[A]	BCB	C3D-C2D	3.41	1.48	1.39
6	C	405	DGA	OG2-CB1	3.35	1.43	1.34
10	M	403[A]	BCB	C1D-ND	-3.34	1.33	1.37
11	L	303[B]	BPB	CHA-CBD	-3.34	1.48	1.52
5	C	402	HEC	C3C-C2C	-3.31	1.37	1.40
11	L	303[A]	BPB	C4C-NC	-3.28	1.27	1.37
10	M	403[B]	BCB	C3D-C2D	3.25	1.48	1.39
10	L	302[B]	BCB	C1D-ND	-3.24	1.33	1.37
10	L	301[A]	BCB	C1D-ND	-3.21	1.33	1.37
10	L	301[B]	BCB	C1D-ND	-3.20	1.33	1.37
10	L	304	BCB	OBD-CAD	3.19	1.28	1.22
10	M	403[B]	BCB	CHD-C4C	3.16	1.46	1.39
10	L	301[B]	BCB	CHD-C4C	3.15	1.46	1.39
10	L	302[B]	BCB	C3D-C2D	3.13	1.47	1.39
10	L	304	BCB	CHD-C4C	3.13	1.46	1.39
10	L	302[A]	BCB	C1D-ND	-3.02	1.34	1.37
10	M	403[A]	BCB	C2C-C3C	-3.02	1.47	1.51
10	L	304	BCB	C4B-CHC	3.02	1.49	1.41
6	C	405	DGA	OG1-CA1	3.00	1.42	1.33
11	L	305	BPB	C3A-C2A	-2.99	1.52	1.54
10	L	302[B]	BCB	CHD-C4C	2.88	1.45	1.39
5	C	403	HEC	C3C-C2C	-2.87	1.37	1.40
10	L	301[A]	BCB	CHD-C4C	2.86	1.45	1.39
11	L	303[B]	BPB	C4C-NC	-2.82	1.28	1.37
6	C	405	DGA	OG2-CG2	-2.77	1.42	1.47
10	M	403[B]	BCB	C4B-CHC	2.73	1.48	1.41
10	L	302[A]	BCB	CHD-C4C	2.73	1.45	1.39
10	L	302[A]	BCB	C1B-CHB	2.72	1.48	1.41
10	M	403[A]	BCB	CHD-C4C	2.69	1.45	1.39
10	L	301[A]	BCB	C4B-CHC	2.68	1.48	1.41
10	L	304	BCB	C1D-ND	-2.68	1.34	1.37
10	M	403[A]	BCB	C4B-CHC	2.66	1.48	1.41
11	L	303[A]	BPB	C3A-C2A	-2.66	1.52	1.54
10	L	302[B]	BCB	C4B-CHC	2.61	1.48	1.41
5	C	403	HEC	C3C-C4C	2.55	1.47	1.43
10	M	403[A]	BCB	C4D-CHA	2.54	1.47	1.38
10	L	304	BCB	C1B-CHB	2.53	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[A]	BCB	C4B-CHC	2.51	1.48	1.41
10	L	301[B]	BCB	C4D-CHA	2.50	1.47	1.38
5	C	403	HEC	CBA-CGA	2.48	1.56	1.50
10	M	403[B]	BCB	C4D-CHA	2.38	1.46	1.38
10	M	403[A]	BCB	C1B-CHB	2.37	1.47	1.41
10	L	301[B]	BCB	C4B-CHC	2.35	1.47	1.41
5	C	403	HEC	C2A-C1A	2.31	1.47	1.42
10	M	403[B]	BCB	C1B-CHB	2.31	1.47	1.41
10	L	302[B]	BCB	C4B-NB	2.30	1.37	1.35
10	L	301[A]	BCB	C4D-CHA	2.26	1.46	1.38
10	L	301[A]	BCB	C1B-CHB	2.24	1.47	1.41
10	L	302[B]	BCB	C1B-CHB	2.23	1.47	1.41
10	L	301[B]	BCB	C1B-CHB	2.20	1.47	1.41
5	C	401	HEC	CBD-CGD	2.17	1.55	1.50
11	L	303[B]	BPB	C3A-C2A	-2.17	1.52	1.54
10	L	304	BCB	C4D-CHA	2.15	1.46	1.38
10	L	302[B]	BCB	MG-NA	-2.14	2.01	2.06
5	C	401	HEC	C3C-C4C	2.13	1.46	1.43
5	C	402	HEC	C4D-ND	2.11	1.40	1.36
5	C	404	HEC	C3C-C4C	2.10	1.46	1.43
10	L	302[B]	BCB	C3D-C4D	-2.09	1.39	1.44
10	L	302[A]	BCB	C4D-CHA	2.09	1.45	1.38
10	L	302[A]	BCB	C3D-C4D	-2.07	1.39	1.44
10	L	304	BCB	C3D-C4D	-2.07	1.39	1.44
10	L	302[A]	BCB	MG-NA	-2.05	2.01	2.06
5	C	401	HEC	CBA-CGA	2.03	1.55	1.50
14	M	404	NS5	C23-C21	2.02	1.50	1.45
5	C	402	HEC	CBA-CGA	2.01	1.55	1.50
5	C	401	HEC	C2A-C1A	2.01	1.47	1.42

All (277) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	304	BCB	C1C-NC-C4C	-20.04	97.70	106.71
10	L	302[A]	BCB	C1C-NC-C4C	-19.15	98.10	106.71
10	L	301[A]	BCB	C1C-NC-C4C	-18.91	98.21	106.71
10	M	403[A]	BCB	C1C-NC-C4C	-18.26	98.50	106.71
10	M	403[B]	BCB	C1C-NC-C4C	-17.89	98.66	106.71
10	L	302[B]	BCB	C1C-NC-C4C	-17.60	98.79	106.71
10	L	301[B]	BCB	C1C-NC-C4C	-16.96	99.08	106.71
11	L	303[B]	BPB	O2D-CGD-CBD	8.19	121.37	111.00
5	C	401	HEC	CBA-CAA-C2A	-8.02	99.08	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	303[A]	BPB	O2D-CGD-CBD	7.82	120.91	111.00
11	L	305	BPB	O2D-CGD-CBD	7.62	120.65	111.00
10	M	403[A]	BCB	C4D-C3D-CAD	-7.12	99.70	108.10
11	L	303[B]	BPB	CBC-CAC-C3C	-7.10	107.86	126.70
11	L	303[A]	BPB	CBC-CAC-C3C	-6.68	108.96	126.70
10	L	304	BCB	C4D-C3D-CAD	-6.59	100.33	108.10
10	L	302[B]	BCB	CMD-C2D-C1D	6.50	136.18	124.71
10	L	302[A]	BCB	C4D-C3D-CAD	-6.33	100.63	108.10
10	M	403[B]	BCB	C4D-C3D-CAD	-6.27	100.70	108.10
10	M	403[B]	BCB	O2D-CGD-CBD	6.05	122.02	111.27
10	L	301[A]	BCB	C4D-C3D-CAD	-6.04	100.97	108.10
10	L	302[A]	BCB	O2D-CGD-CBD	5.92	121.79	111.27
11	L	305	BPB	CBC-CAC-C3C	-5.79	111.32	126.70
10	L	301[B]	BCB	CMD-C2D-C1D	5.78	134.90	124.71
5	C	402	HEC	CBA-CAA-C2A	-5.60	103.16	112.60
10	M	403[B]	BCB	CMD-C2D-C1D	5.59	134.56	124.71
10	M	403[A]	BCB	O2D-CGD-CBD	5.58	121.19	111.27
10	L	304	BCB	C1-C2-C3	-5.56	116.43	126.04
10	L	301[B]	BCB	C4D-C3D-CAD	-5.49	101.62	108.10
10	L	301[B]	BCB	O2D-CGD-CBD	5.46	120.97	111.27
5	C	401	HEC	CBD-CAD-C3D	-5.45	103.31	112.62
10	L	302[B]	BCB	O2D-CGD-CBD	5.42	120.91	111.27
10	L	301[B]	BCB	C3D-C4D-ND	5.35	118.89	110.24
10	L	302[A]	BCB	CMD-C2D-C1D	5.34	134.13	124.71
10	L	302[B]	BCB	C4D-C3D-CAD	-5.24	101.92	108.10
10	L	301[A]	BCB	O2D-CGD-CBD	5.17	120.46	111.27
10	L	304	BCB	O2D-CGD-CBD	5.11	120.34	111.27
10	M	403[A]	BCB	C3D-C4D-ND	5.09	118.47	110.24
10	L	302[B]	BCB	C3D-C4D-ND	4.98	118.30	110.24
10	M	403[B]	BCB	C3D-C4D-ND	4.96	118.27	110.24
14	M	404	NS5	C19-C20-C21	-4.93	120.27	127.31
10	L	302[A]	BCB	C3D-C4D-ND	4.83	118.05	110.24
10	L	304	BCB	C3D-C4D-ND	4.82	118.04	110.24
10	M	403[A]	BCB	CMB-C2B-C3B	4.81	133.68	124.68
10	L	304	BCB	CMD-C2D-C1D	4.80	133.16	124.71
10	L	301[A]	BCB	C3D-C4D-ND	4.78	117.98	110.24
10	L	301[A]	BCB	CMD-C2D-C1D	4.76	133.09	124.71
10	L	301[A]	BCB	CMB-C2B-C3B	4.71	133.48	124.68
10	L	302[B]	BCB	C1D-ND-C4D	-4.71	102.99	106.33
10	M	403[A]	BCB	C1D-ND-C4D	-4.65	103.03	106.33
10	L	304	BCB	OBD-CAD-C3D	-4.63	117.37	128.52
10	L	304	BCB	C1D-ND-C4D	-4.56	103.10	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403[B]	BCB	CMB-C2B-C3B	4.39	132.90	124.68
10	M	403[A]	BCB	C2C-C1C-CHC	-4.38	113.34	123.64
10	M	403[B]	BCB	O2D-CGD-O1D	-4.36	115.31	123.84
14	M	404	NS5	CM4-C36-C35	-4.36	110.05	122.65
10	L	301[B]	BCB	CMB-C2B-C3B	4.36	132.83	124.68
11	L	303[A]	BPB	CMA-C3A-C4A	-4.35	104.86	114.38
10	M	403[A]	BCB	CMD-C2D-C1D	4.29	132.27	124.71
10	L	302[A]	BCB	C2C-C1C-CHC	-4.27	113.58	123.64
11	L	303[B]	BPB	CMC-C2C-C1C	-4.26	107.19	114.36
6	C	405	DGA	OG2-CB1-CB2	4.25	120.66	111.50
10	M	403[B]	BCB	C4A-NA-C1A	4.24	108.61	106.71
10	L	301[B]	BCB	C2C-C1C-CHC	-4.21	113.73	123.64
10	L	302[A]	BCB	C1D-ND-C4D	-4.16	103.38	106.33
10	M	403[A]	BCB	O2D-CGD-O1D	-4.15	115.72	123.84
10	L	301[B]	BCB	C1D-ND-C4D	-4.14	103.39	106.33
10	L	302[B]	BCB	CMB-C2B-C3B	4.13	132.40	124.68
10	L	302[B]	BCB	C2C-C1C-CHC	-4.12	113.93	123.64
10	L	302[A]	BCB	CMB-C2B-C3B	4.11	132.38	124.68
10	L	304	BCB	C2C-C1C-CHC	-4.05	114.11	123.64
10	M	403[A]	BCB	CAD-C3D-C2D	4.01	160.16	140.80
10	M	403[B]	BCB	C1D-ND-C4D	-4.01	103.49	106.33
14	M	404	NS5	C11-C10-C9	3.99	121.99	115.27
10	L	302[B]	BCB	CMD-C2D-C3D	-3.94	118.54	127.61
10	L	302[A]	BCB	OBD-CAD-C3D	-3.89	119.15	128.52
14	M	404	NS5	C34-C35-C36	-3.89	114.47	127.75
10	M	403[B]	BCB	C2C-C1C-CHC	-3.85	114.58	123.64
10	L	301[B]	BCB	CMD-C2D-C3D	-3.82	118.83	127.61
10	L	304	BCB	CHC-C1C-NC	-3.82	119.24	124.51
11	L	303[A]	BPB	CMB-C2B-C3B	3.81	131.80	124.68
5	C	401	HEC	CMC-C2C-C1C	-3.75	122.70	128.46
10	M	403[B]	BCB	CAD-C3D-C2D	3.75	158.88	140.80
10	L	301[A]	BCB	CHC-C1C-NC	-3.73	119.35	124.51
10	L	301[A]	BCB	C1D-ND-C4D	-3.71	103.70	106.33
10	L	304	BCB	C2D-C1D-ND	3.71	112.84	110.10
10	L	301[B]	BCB	C4-C3-C5	3.69	121.48	115.27
10	L	301[B]	BCB	CAD-C3D-C2D	3.68	158.58	140.80
10	L	301[A]	BCB	C2C-C1C-CHC	-3.68	114.97	123.64
10	L	302[A]	BCB	CAD-C3D-C2D	3.68	158.56	140.80
10	L	304	BCB	CAD-C3D-C2D	3.68	158.54	140.80
14	M	404	NS5	CM3-C36-C35	-3.66	112.06	122.65
14	M	404	NS5	C18-C17-C15	-3.66	122.08	127.31
10	L	301[A]	BCB	CAD-C3D-C2D	3.65	158.41	140.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	302[B]	BCB	OBD-CAD-C3D	-3.63	119.79	128.52
10	M	403[A]	BCB	C1D-CHD-C4C	-3.62	118.24	126.06
10	M	403[B]	BCB	CHC-C1C-NC	-3.62	119.50	124.51
10	L	302[B]	BCB	C1-C2-C3	-3.57	119.86	126.04
10	L	302[A]	BCB	C6-C5-C3	-3.57	104.10	113.45
11	L	305	BPB	O2A-CGA-CBA	3.52	122.94	111.91
10	M	403[A]	BCB	C2D-C1D-ND	3.47	112.66	110.10
10	M	403[B]	BCB	CMD-C2D-C3D	-3.47	119.64	127.61
5	C	403	HEC	CMC-C2C-C1C	-3.46	123.15	128.46
10	L	304	BCB	O2A-CGA-CBA	3.44	122.70	111.91
10	L	301[A]	BCB	O2D-CGD-O1D	-3.44	117.12	123.84
13	M	402[A]	MQ7	C19-C18-C20	3.42	121.02	115.27
10	L	301[B]	BCB	O2A-CGA-CBA	3.41	122.62	111.91
13	M	402[A]	MQ7	C39-C38-C40	3.41	121.01	115.27
10	L	302[B]	BCB	CAD-C3D-C2D	3.40	157.22	140.80
10	M	403[B]	BCB	OBD-CAD-C3D	-3.39	120.36	128.52
10	L	302[B]	BCB	C2D-C1D-ND	3.36	112.58	110.10
14	M	404	NS5	C32-C31-C33	3.35	120.90	115.27
5	C	401	HEC	CMC-C2C-C3C	3.33	129.74	125.82
11	L	303[A]	BPB	C3D-CAD-CBD	3.33	111.99	107.61
11	L	303[B]	BPB	CMB-C2B-C3B	3.33	130.91	124.68
10	L	302[A]	BCB	C1-C2-C3	-3.32	120.30	126.04
10	L	301[A]	BCB	OBD-CAD-C3D	-3.31	120.54	128.52
11	L	305	BPB	C3D-CAD-CBD	3.28	111.93	107.61
10	L	301[A]	BCB	O2A-CGA-CBA	3.21	122.00	111.91
10	L	302[A]	BCB	O1D-CGD-CBD	-3.20	117.93	124.48
10	L	301[A]	BCB	C4-C3-C5	3.19	120.64	115.27
10	L	302[A]	BCB	CHC-C1C-NC	-3.19	120.10	124.51
10	L	304	BCB	C4-C3-C5	3.19	120.63	115.27
10	L	302[B]	BCB	C6-C5-C3	-3.16	105.16	113.45
10	L	302[B]	BCB	O1D-CGD-CBD	-3.16	118.01	124.48
10	M	403[B]	BCB	C1D-CHD-C4C	-3.16	119.24	126.06
11	L	305	BPB	C1-O2A-CGA	3.16	124.73	116.44
10	L	301[A]	BCB	CHD-C4C-C3C	-3.15	121.94	125.89
10	L	302[A]	BCB	CMD-C2D-C3D	-3.14	120.40	127.61
11	L	305	BPB	O1D-CGD-CBD	-3.13	119.52	124.74
11	L	305	BPB	CMD-C2D-C3D	-3.11	118.86	124.68
10	L	301[B]	BCB	O2D-CGD-O1D	-3.11	117.76	123.84
11	L	305	BPB	C1A-C2A-C3A	-3.09	99.90	102.84
10	L	304	BCB	C4-C3-C2	-3.07	115.81	123.68
5	C	403	HEC	CBA-CAA-C2A	-3.05	107.47	112.60
5	C	403	HEC	CMC-C2C-C3C	3.04	129.40	125.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	308	HTO	C5-C4-C3	-3.04	109.18	114.18
10	L	301[A]	BCB	C1D-CHD-C4C	-3.03	119.52	126.06
5	C	402	HEC	CMD-C2D-C1D	-3.00	123.85	128.46
10	L	301[A]	BCB	C2D-C1D-ND	3.00	112.32	110.10
11	L	303[B]	BPB	OBD-CAD-CBD	-2.99	121.43	125.82
10	L	302[A]	BCB	C1D-CHD-C4C	-2.99	119.60	126.06
10	L	302[A]	BCB	C2D-C1D-ND	2.99	112.31	110.10
5	C	404	HEC	CBA-CAA-C2A	-2.99	107.57	112.60
10	M	403[A]	BCB	OBD-CAD-C3D	-2.99	121.33	128.52
13	M	402[A]	MQ7	C29-C28-C30	2.98	120.28	115.27
5	C	402	HEC	CMC-C2C-C1C	-2.95	123.94	128.46
13	M	402[A]	MQ7	C21-C22-C23	-2.94	120.59	127.66
13	M	402[B]	MQ7	C19-C18-C20	2.93	120.20	115.27
5	C	404	HEC	CMA-C3A-C2A	2.92	130.44	124.94
14	M	404	NS5	C18-C19-C20	2.91	129.44	123.47
10	L	304	BCB	CHD-C4C-C3C	-2.91	122.25	125.89
13	M	402[B]	MQ7	C24-C23-C25	2.89	120.14	115.27
10	L	301[A]	BCB	O2A-CGA-O1A	-2.89	116.30	123.59
11	L	303[A]	BPB	CMC-C2C-C1C	-2.89	109.51	114.36
10	L	301[B]	BCB	O2A-CGA-O1A	-2.86	116.38	123.59
5	C	404	HEC	CAD-CBD-CGD	-2.85	105.77	113.76
11	L	303[B]	BPB	O1D-CGD-CBD	-2.82	120.03	124.74
11	L	303[A]	BPB	O2A-CGA-CBA	2.82	120.77	111.91
10	L	302[B]	BCB	CHC-C1C-NC	-2.81	120.63	124.51
10	L	302[B]	BCB	O2A-CGA-CBA	2.80	120.70	111.91
6	C	405	DGA	OG1-CA1-CA2	2.79	120.65	111.91
10	L	301[B]	BCB	CHC-C1C-NC	-2.78	120.67	124.51
5	C	404	HEC	CMC-C2C-C1C	-2.78	124.20	128.46
10	M	403[A]	BCB	CHA-C4D-ND	-2.75	126.74	132.50
13	M	402[B]	MQ7	C21-C22-C23	-2.75	121.04	127.66
11	L	305	BPB	CMC-C2C-C1C	-2.74	109.76	114.36
10	M	403[B]	BCB	CHB-C4A-NA	2.73	128.29	124.51
10	M	403[A]	BCB	C4A-NA-C1A	2.72	107.93	106.71
10	M	403[A]	BCB	CHC-C1C-NC	-2.71	120.76	124.51
10	L	304	BCB	O2A-CGA-O1A	-2.71	116.75	123.59
13	M	402[B]	MQ7	O4-C4-C5	-2.71	117.18	121.56
10	L	302[A]	BCB	C4-C3-C5	2.70	119.82	115.27
10	L	304	BCB	CMB-C2B-C3B	2.70	129.72	124.68
10	L	304	BCB	C1D-CHD-C4C	-2.69	120.26	126.06
13	M	402[B]	MQ7	C29-C28-C30	2.69	119.79	115.27
11	L	303[B]	BPB	O2D-CGD-O1D	-2.68	118.59	123.84
10	L	302[B]	BCB	C1D-CHD-C4C	-2.68	120.28	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	402	HEC	CMB-C2B-C1B	-2.67	124.36	128.46
10	M	403[B]	BCB	C4D-CHA-C1A	2.67	124.49	121.25
10	L	301[A]	BCB	CMD-C2D-C3D	-2.66	121.49	127.61
11	L	303[B]	BPB	CMD-C2D-C3D	-2.66	119.70	124.68
10	L	302[A]	BCB	O2A-CGA-CBA	2.66	120.24	111.91
11	L	303[B]	BPB	C4-C3-C5	2.65	119.73	115.27
5	C	403	HEC	CMD-C2D-C1D	-2.65	124.39	128.46
11	L	303[A]	BPB	O1D-CGD-CBD	-2.65	120.33	124.74
10	M	403[B]	BCB	C2D-C1D-ND	2.63	112.04	110.10
13	M	402[A]	MQ7	C16-C17-C18	-2.62	121.35	127.66
10	L	301[B]	BCB	OBD-CAD-C3D	-2.61	122.23	128.52
5	C	402	HEC	CAD-CBD-CGD	-2.60	106.48	113.76
11	L	303[B]	BPB	C4A-C3A-C2A	-2.60	100.37	102.84
11	L	303[A]	BPB	O2D-CGD-O1D	-2.60	118.76	123.84
10	L	302[B]	BCB	CHB-C4A-NA	2.58	128.08	124.51
14	M	404	NS5	C12-C13-C14	-2.58	115.16	123.22
10	M	403[B]	BCB	CHA-C4D-ND	-2.58	127.11	132.50
5	C	403	HEC	C1D-C2D-C3D	2.58	108.79	107.00
10	M	403[A]	BCB	C4B-CHC-C1C	-2.57	125.02	130.12
11	L	305	BPB	CMA-C3A-C4A	-2.57	108.75	114.38
10	L	302[B]	BCB	O2A-CGA-O1A	-2.57	117.12	123.59
13	M	402[B]	MQ7	C39-C38-C40	2.56	119.58	115.27
13	M	402[B]	MQ7	C34-C33-C35	2.56	119.57	115.27
13	M	402[B]	MQ7	C16-C17-C18	-2.55	121.51	127.66
10	L	304	BCB	O2D-CGD-O1D	-2.55	118.85	123.84
6	C	405	DGA	OG2-CG2-CG1	2.54	112.02	106.13
11	L	303[A]	BPB	CMD-C2D-C3D	-2.53	119.94	124.68
11	L	303[B]	BPB	O2A-CGA-CBA	2.52	119.81	111.91
10	L	301[A]	BCB	CHB-C4A-NA	2.51	127.98	124.51
10	L	302[B]	BCB	CHD-C4C-C3C	-2.51	122.75	125.89
10	L	301[B]	BCB	C1D-CHD-C4C	-2.51	120.65	126.06
10	L	304	BCB	C4B-CHC-C1C	-2.50	125.17	130.12
13	M	402[A]	MQ7	C45-C43-C44	2.49	120.11	114.60
13	M	402[A]	MQ7	C26-C27-C28	-2.47	121.71	127.66
10	L	301[A]	BCB	C1-C2-C3	-2.47	121.77	126.04
10	L	304	BCB	CMD-C2D-C3D	-2.47	121.94	127.61
10	L	302[B]	BCB	C4-C3-C5	2.47	119.42	115.27
11	L	303[B]	BPB	O2A-CGA-O1A	-2.45	117.41	123.59
10	L	302[A]	BCB	CHA-C4D-ND	-2.44	127.40	132.50
10	M	403[A]	BCB	CMD-C2D-C3D	-2.43	122.03	127.61
5	C	404	HEC	CMB-C2B-C1B	-2.43	124.73	128.46
10	L	304	BCB	CHA-C4D-ND	-2.42	127.44	132.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	302[A]	BCB	CED-O2D-CGD	2.41	121.39	115.94
10	M	403[A]	BCB	CAA-C2A-C1A	2.41	119.86	111.97
10	M	403[A]	BCB	C4D-CHA-C1A	2.40	124.17	121.25
11	L	303[A]	BPB	O2A-CGA-O1A	-2.39	117.55	123.59
10	L	302[A]	BCB	O2A-CGA-O1A	-2.39	117.57	123.59
10	L	304	BCB	C2A-C1A-CHA	-2.36	119.73	123.86
10	M	403[B]	BCB	CHD-C4C-C3C	-2.33	122.98	125.89
10	L	301[B]	BCB	CHA-C4D-ND	-2.33	127.63	132.50
13	M	402[A]	MQ7	C34-C33-C35	2.32	119.18	115.27
10	L	304	BCB	CHB-C4A-NA	2.31	127.71	124.51
10	M	403[A]	BCB	C4-C3-C5	2.29	119.12	115.27
10	M	403[B]	BCB	C6-C5-C3	-2.28	107.48	113.45
5	C	402	HEC	CMB-C2B-C3B	2.28	128.50	125.82
5	C	402	HEC	CMC-C2C-C3C	2.26	128.48	125.82
10	M	403[B]	BCB	C4B-CHC-C1C	-2.24	125.68	130.12
11	L	303[B]	BPB	CBA-CAA-C2A	-2.24	107.28	113.81
11	L	305	BPB	CED-O2D-CGD	2.23	120.98	115.94
13	M	402[A]	MQ7	C14-C13-C15	2.22	119.00	115.27
13	M	402[A]	MQ7	C12-C11-C3	-2.21	106.10	112.05
10	M	403[A]	BCB	CHD-C4C-C3C	-2.20	123.13	125.89
5	C	403	HEC	CMB-C2B-C1B	-2.19	125.10	128.46
10	L	301[A]	BCB	CHA-C4D-ND	-2.19	127.92	132.50
10	M	403[A]	BCB	C7-C6-C5	-2.18	107.42	113.36
10	M	403[A]	BCB	O2A-CGA-O1A	-2.18	118.09	123.59
10	L	302[B]	BCB	CHA-C4D-ND	-2.18	127.95	132.50
11	L	303[B]	BPB	CMA-C3A-C4A	-2.17	109.62	114.38
5	C	404	HEC	CMD-C2D-C1D	-2.17	125.13	128.46
10	L	301[B]	BCB	CHB-C4A-NA	2.17	127.51	124.51
14	M	404	NS5	C8-C7-C5	-2.16	122.45	127.66
13	M	402[B]	MQ7	C45-C43-C44	2.16	119.38	114.60
13	M	402[B]	MQ7	C14-C13-C15	2.16	118.90	115.27
10	L	301[B]	BCB	CAA-C2A-C1A	2.15	119.02	111.97
13	M	402[A]	MQ7	C5-C4-C3	2.15	122.36	118.42
5	C	404	HEC	CBD-CAD-C3D	2.14	116.27	112.62
9	H	710	HTO	C5-C4-C3	-2.14	110.66	114.18
10	L	301[A]	BCB	CAA-C2A-C1A	2.14	118.98	111.97
13	M	402[A]	MQ7	O4-C4-C5	-2.14	118.10	121.56
13	M	402[B]	MQ7	C26-C27-C28	-2.13	122.52	127.66
14	M	404	NS5	C16-C15-C14	2.13	121.43	118.08
13	M	402[A]	MQ7	C24-C23-C25	2.11	118.81	115.27
10	M	403[B]	BCB	C1-O2A-CGA	2.11	121.97	116.44
10	M	403[A]	BCB	CMB-C2B-C1B	-2.09	125.25	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	401	HEC	C2B-C3B-C4B	2.09	108.61	106.35
5	C	403	HEC	CMB-C2B-C3B	2.09	128.28	125.82
10	L	301[B]	BCB	C2D-C1D-ND	2.09	111.64	110.10
13	M	402[A]	MQ7	C41-C42-C43	-2.09	120.62	127.75
10	L	302[A]	BCB	C4A-NA-C1A	2.08	107.64	106.71
5	C	402	HEC	CMA-C3A-C2A	2.08	128.86	124.94
10	L	302[A]	BCB	CHB-C4A-NA	2.06	127.37	124.51
14	M	404	NS5	C14-C15-C17	-2.05	115.79	118.94
11	L	305	BPB	O2D-CGD-O1D	-2.05	119.83	123.84
5	C	403	HEC	O2D-CGD-CBD	2.05	120.60	114.03
14	M	404	NS5	C30-C29-C28	-2.04	116.84	123.22
10	L	302[B]	BCB	C4A-NA-C1A	2.04	107.62	106.71
11	L	303[A]	BPB	C4A-C3A-C2A	-2.03	100.91	102.84
14	M	404	NS5	C22-C21-C20	-2.02	120.09	122.92
10	L	302[B]	BCB	CHD-C1D-ND	-2.01	122.61	124.45
11	L	303[A]	BPB	C16-C15-C13	-2.00	109.44	115.92

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	L	301[A]	BCB	NA
10	L	301[A]	BCB	ND
10	L	301[A]	BCB	NC
10	L	301[B]	BCB	NA
10	L	301[B]	BCB	ND
10	L	301[B]	BCB	NC
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	ND
10	L	304	BCB	NC
10	M	403[A]	BCB	NA
10	M	403[A]	BCB	NC
10	M	403[B]	BCB	NA
10	M	403[B]	BCB	ND
10	M	403[B]	BCB	NC

All (182) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3
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
8	L	307	LDA	C2-C1-N1-O1
8	L	307	LDA	C2-C1-N1-CM1
8	M	413	LDA	C2-C1-N1-CM1
8	M	413	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	308	HTO	O2-C2-C3-C4
10	L	301[A]	BCB	C2-C3-C5-C6
10	L	301[A]	BCB	C4-C3-C5-C6
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	L	304	BCB	C2C-C3C-CAC-CBC
10	M	403[A]	BCB	C2A-CAA-CBA-CGA
10	M	403[A]	BCB	C2C-C3C-CAC-CBC
10	M	403[A]	BCB	CHA-CBD-CGD-O1D
10	M	403[A]	BCB	CHA-CBD-CGD-O2D
10	M	403[A]	BCB	CAD-CBD-CGD-O1D
10	M	403[A]	BCB	CAD-CBD-CGD-O2D
10	M	403[B]	BCB	C2C-C3C-CAC-CBC
10	M	403[B]	BCB	CHA-CBD-CGD-O1D
10	M	403[B]	BCB	CHA-CBD-CGD-O2D
10	M	403[B]	BCB	CAD-CBD-CGD-O1D
10	M	403[B]	BCB	CAD-CBD-CGD-O2D
11	L	303[A]	BPB	O2A-C1-C2-C3
11	L	303[A]	BPB	C2C-C3C-CAC-CBC
11	L	303[B]	BPB	C2C-C3C-CAC-CBC
11	L	305	BPB	C2C-C3C-CAC-CBC
14	M	404	NS5	C34-C35-C36-CM3
10	L	304	BCB	CBD-CGD-O2D-CED
10	L	301[B]	BCB	C4-C3-C5-C6
10	L	301[B]	BCB	C2-C3-C5-C6
11	L	305	BPB	CBA-CGA-O2A-C1
10	M	403[B]	BCB	C11-C12-C13-C14
14	M	404	NS5	C13-C14-C15-C16
10	L	304	BCB	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
11	L	305	BPB	O1A-CGA-O2A-C1
10	L	301[A]	BCB	C13-C15-C16-C17
10	M	403[A]	BCB	C8-C10-C11-C12
10	L	304	BCB	C3-C5-C6-C7
11	L	303[B]	BPB	C8-C10-C11-C12
8	H	708	LDA	C3-C4-C5-C6
10	M	403[B]	BCB	C16-C17-C18-C19
8	L	306	LDA	C2-C3-C4-C5
8	M	412	LDA	C5-C6-C7-C8
6	C	405	DGA	CA2-CA1-OG1-CG1
10	M	403[B]	BCB	CBA-CGA-O2A-C1
6	C	405	DGA	CBB-CAB-CB9-CB8
8	H	708	LDA	C5-C6-C7-C8
10	L	302[B]	BCB	C13-C15-C16-C17
8	L	307	LDA	C7-C8-C9-C10
6	C	405	DGA	CCB-CDB-CEB-CFB
11	L	303[B]	BPB	O2A-C1-C2-C3
11	L	303[A]	BPB	C2-C3-C5-C6
11	L	303[B]	BPB	C2-C3-C5-C6
6	C	405	DGA	OA1-CA1-OG1-CG1
8	M	413	LDA	C6-C7-C8-C9
8	L	307	LDA	C3-C4-C5-C6
10	M	403[B]	BCB	O1A-CGA-O2A-C1
11	L	303[B]	BPB	C3-C5-C6-C7
8	L	306	LDA	C5-C6-C7-C8
11	L	303[B]	BPB	C4-C3-C5-C6
10	L	302[A]	BCB	C12-C13-C15-C16
10	L	302[B]	BCB	C12-C13-C15-C16
14	M	404	NS5	C34-C35-C36-CM4
10	M	403[B]	BCB	C8-C10-C11-C12
11	L	305	BPB	C13-C15-C16-C17
8	L	307	LDA	C6-C7-C8-C9
11	L	303[A]	BPB	C4-C3-C5-C6
10	L	302[B]	BCB	C14-C13-C15-C16
8	L	306	LDA	C3-C4-C5-C6
10	M	403[B]	BCB	C1A-C2A-CAA-CBA
11	L	303[A]	BPB	C8-C10-C11-C12
8	H	701	LDA	C6-C7-C8-C9
8	L	307	LDA	C4-C5-C6-C7
10	M	403[A]	BCB	C13-C15-C16-C17
8	L	306	LDA	C1-C2-C3-C4
8	H	708	LDA	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	M	404	NS5	C7-C8-C9-C10
9	H	709	HTO	C4-C5-C6-C7
8	H	701	LDA	C4-C5-C6-C7
9	L	308	HTO	O2-C2-C3-O3
10	M	403[A]	BCB	C12-C13-C15-C16
10	M	403[A]	BCB	C14-C13-C15-C16
6	C	405	DGA	CB9-CAB-CBB-CCB
8	H	708	LDA	N1-C1-C2-C3
10	L	302[A]	BCB	C13-C15-C16-C17
8	L	307	LDA	C9-C10-C11-C12
10	M	403[B]	BCB	C3A-C2A-CAA-CBA
9	L	308	HTO	C1-C2-C3-O3
8	H	707	LDA	C1-C2-C3-C4
14	M	404	NS5	C3-C4-C5-C6
8	L	307	LDA	C1-C2-C3-C4
9	L	308	HTO	C4-C5-C6-C7
8	H	707	LDA	C6-C7-C8-C9
10	L	302[A]	BCB	C14-C13-C15-C16
10	M	403[B]	BCB	C16-C17-C18-C20
10	L	301[B]	BCB	C12-C13-C15-C16
10	M	403[B]	BCB	C12-C13-C15-C16
11	L	303[B]	BPB	C6-C7-C8-C10
10	L	304	BCB	C5-C6-C7-C8
8	H	708	LDA	C6-C7-C8-C9
10	L	304	BCB	CAD-CBD-CGD-O2D
11	L	303[A]	BPB	CAD-CBD-CGD-O2D
11	L	305	BPB	CAD-CBD-CGD-O2D
6	C	405	DGA	CA3-CA4-CA5-CA6
8	L	307	LDA	C2-C1-N1-CM2
6	C	405	DGA	CA9-CAA-CBA-CCA
10	L	301[B]	BCB	C16-C17-C18-C20
8	L	306	LDA	C4-C5-C6-C7
6	C	405	DGA	CB6-CB7-CB8-CB9
8	M	413	LDA	C2-C1-N1-O1
10	L	301[A]	BCB	CAD-CBD-CGD-O1D
5	C	402	HEC	C3D-CAD-CBD-CGD
10	M	403[B]	BCB	C11-C12-C13-C15
8	H	708	LDA	C7-C8-C9-C10
8	L	307	LDA	C11-C10-C9-C8
10	L	301[B]	BCB	C14-C13-C15-C16
10	M	403[B]	BCB	C14-C13-C15-C16
11	L	303[B]	BPB	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	L	301[A]	BCB	C16-C17-C18-C20
14	M	404	NS5	C13-C14-C15-C17
6	C	405	DGA	CB2-CB3-CB4-CB5
11	L	305	BPB	C4-C3-C5-C6
10	L	302[B]	BCB	C8-C10-C11-C12
11	L	303[B]	BPB	CHA-CBD-CGD-O1D
11	L	303[B]	BPB	CHA-CBD-CGD-O2D
14	M	404	NS5	C10-C12-C13-C14
14	M	404	NS5	C23-C24-C25-C26
6	C	405	DGA	CAB-CBB-CCB-CDB
10	L	301[A]	BCB	C16-C17-C18-C19
10	L	304	BCB	C8-C10-C11-C12
10	M	403[A]	BCB	O2A-C1-C2-C3
8	H	708	LDA	C2-C3-C4-C5
8	H	701	LDA	C9-C10-C11-C12
10	L	304	BCB	C11-C10-C8-C7
5	C	401	HEC	CAA-CBA-CGA-O1A
5	C	401	HEC	CAA-CBA-CGA-O2A
10	M	403[B]	BCB	C2A-CAA-CBA-CGA
10	L	304	BCB	C10-C11-C12-C13
10	L	302[B]	BCB	C11-C10-C8-C7
10	L	304	BCB	C4-C3-C5-C6
10	L	301[B]	BCB	C11-C12-C13-C14
10	L	302[B]	BCB	C11-C10-C8-C9
10	L	304	BCB	C11-C10-C8-C9
10	L	301[B]	BCB	CAD-CBD-CGD-O2D
10	M	403[A]	BCB	C15-C16-C17-C18
8	M	412	LDA	C3-C4-C5-C6
10	L	301[A]	BCB	CHA-CBD-CGD-O1D
10	L	302[A]	BCB	CHA-CBD-CGD-O1D
10	L	302[B]	BCB	CHA-CBD-CGD-O1D
10	L	302[B]	BCB	CHA-CBD-CGD-O2D
10	L	304	BCB	CHA-CBD-CGD-O1D
10	L	304	BCB	CHA-CBD-CGD-O2D
10	M	403[B]	BCB	CAA-CBA-CGA-O2A
11	L	303[A]	BPB	CHA-CBD-CGD-O1D
8	M	412	LDA	C6-C7-C8-C9
14	M	404	NS5	C3-C4-C5-C7
10	M	403[A]	BCB	C16-C17-C18-C20
6	C	405	DGA	CBB-CCB-CDB-CEB
5	C	402	HEC	CAA-CBA-CGA-O1A
6	C	405	DGA	OB1-CB1-OG2-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	M	403[B]	BCB	CAA-CBA-CGA-O1A
10	L	304	BCB	C2-C3-C5-C6
11	L	305	BPB	C2-C3-C5-C6
10	L	301[A]	BCB	C15-C16-C17-C18
10	L	302[A]	BCB	C8-C10-C11-C12
8	M	412	LDA	C4-C5-C6-C7
13	M	402[B]	MQ7	C39-C38-C40-C41
6	C	405	DGA	CB1-CB2-CB3-CB4
5	C	403	HEC	CAD-CBD-CGD-O2D
5	C	401	HEC	CAD-CBD-CGD-O2D
5	C	403	HEC	CAA-CBA-CGA-O2A
14	M	404	NS5	C31-C33-C34-C35
5	C	402	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

19 monomers are involved in 43 short contacts:

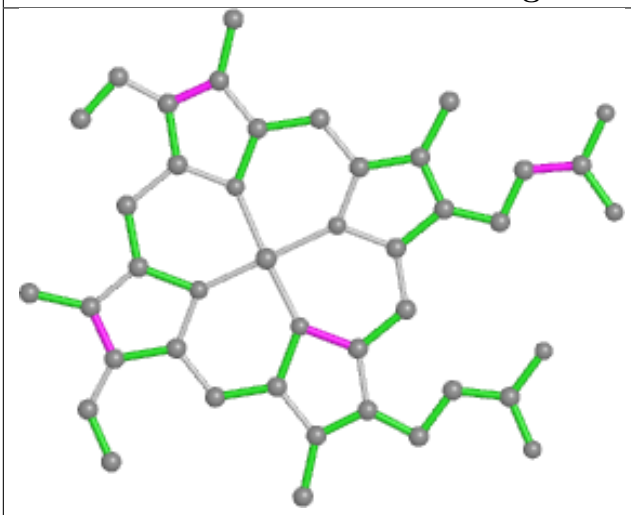
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	305	BPB	6	0
5	C	402	HEC	1	0
10	M	403[B]	BCB	5	0
5	C	401	HEC	1	0
10	L	304	BCB	6	0
11	L	303[B]	BPB	5	0
7	M	407	SO4	2	0
5	C	403	HEC	2	0
8	L	306	LDA	2	0
10	L	301[B]	BCB	2	0
10	M	403[A]	BCB	1	0
8	H	701	LDA	1	0
8	H	708	LDA	3	0
11	L	303[A]	BPB	3	0
5	C	404	HEC	1	0
13	M	402[B]	MQ7	1	0
14	M	404	NS5	2	0
10	L	302[B]	BCB	3	0
10	L	301[A]	BCB	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

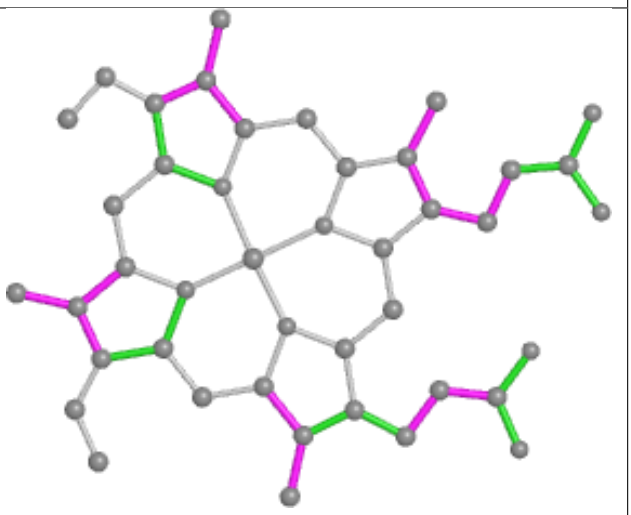
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 BPB L 305

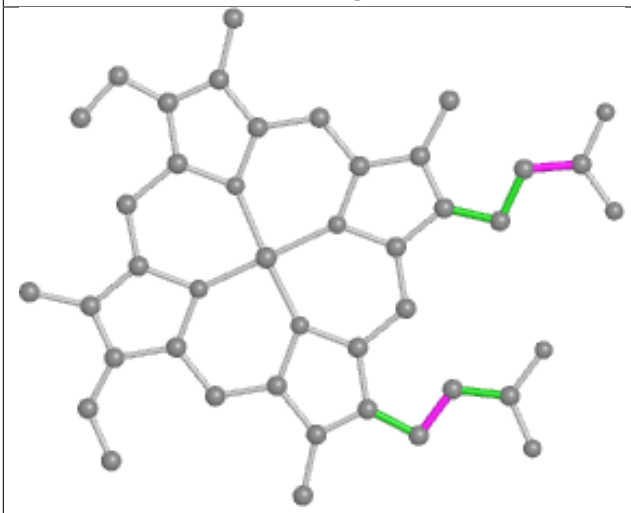
Ligand HEC C 402



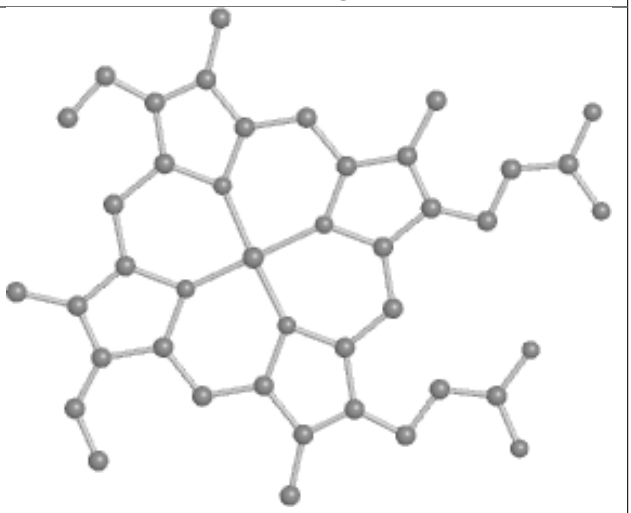
Bond lengths



Bond angles

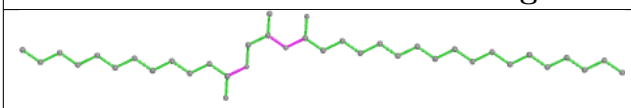


Torsions

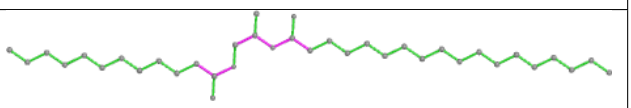


Rings

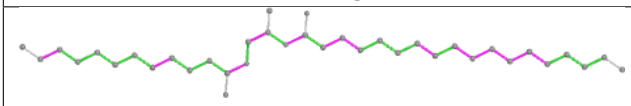
Ligand DGA C 405



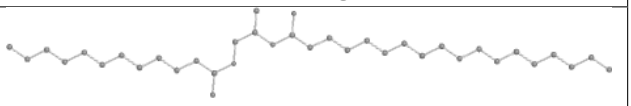
Bond lengths



Bond angles

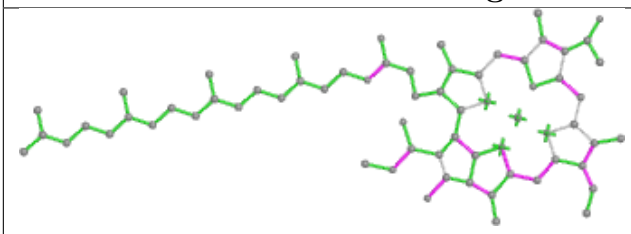


Torsions

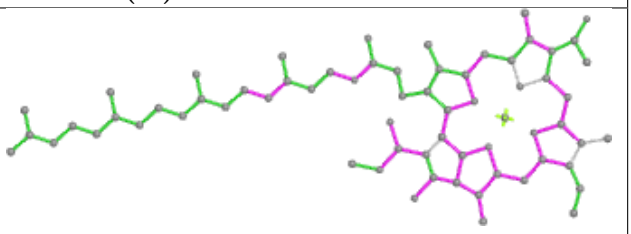


Rings

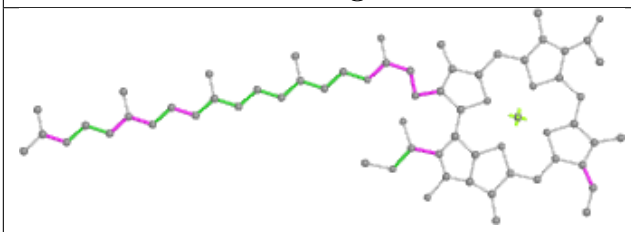
Ligand BCB M 403 (B)



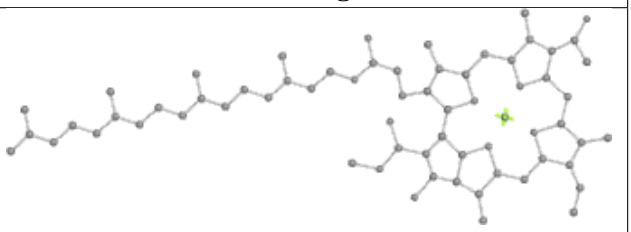
Bond lengths



Bond angles

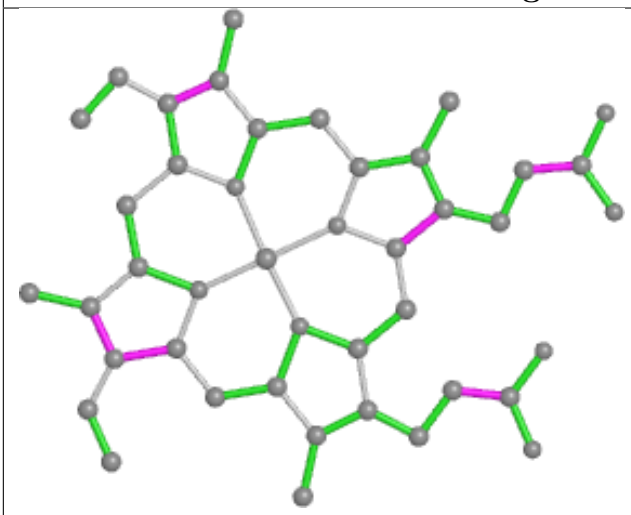


Torsions

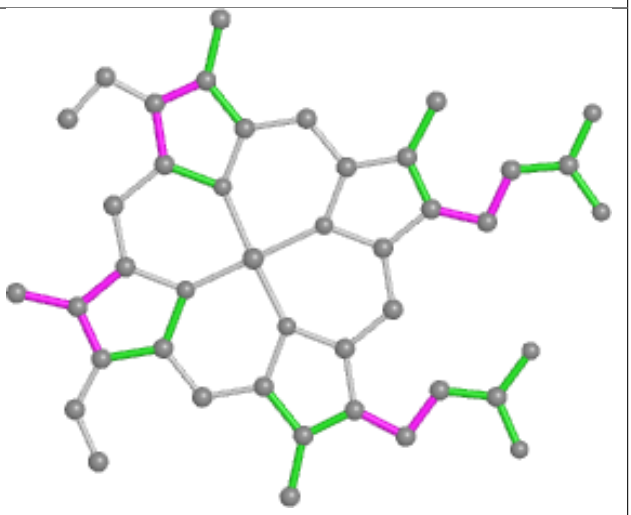


Rings

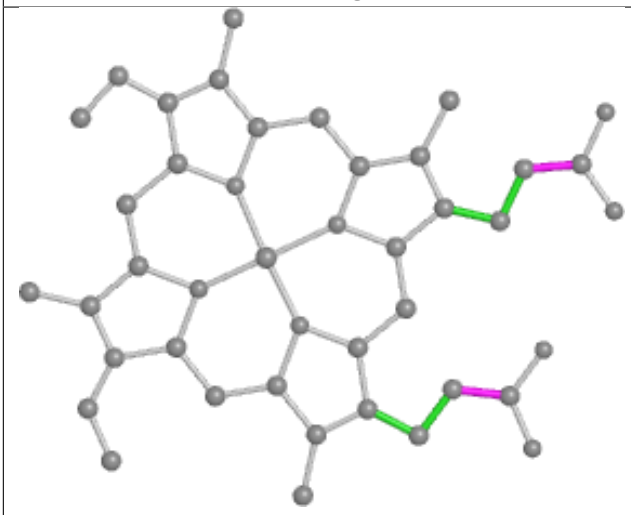
Ligand HEC C 401



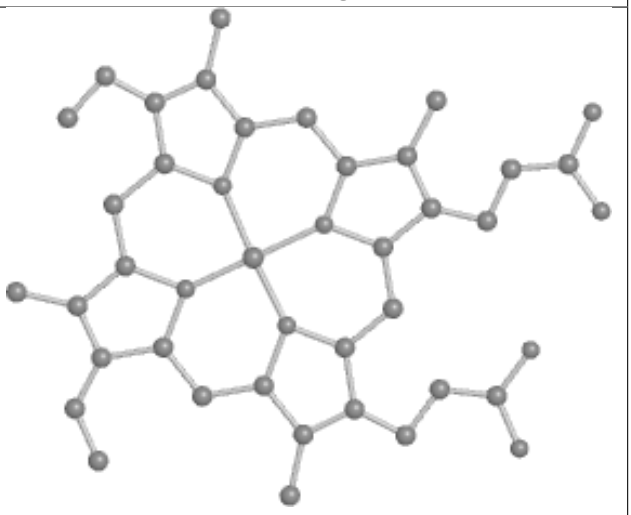
Bond lengths



Bond angles

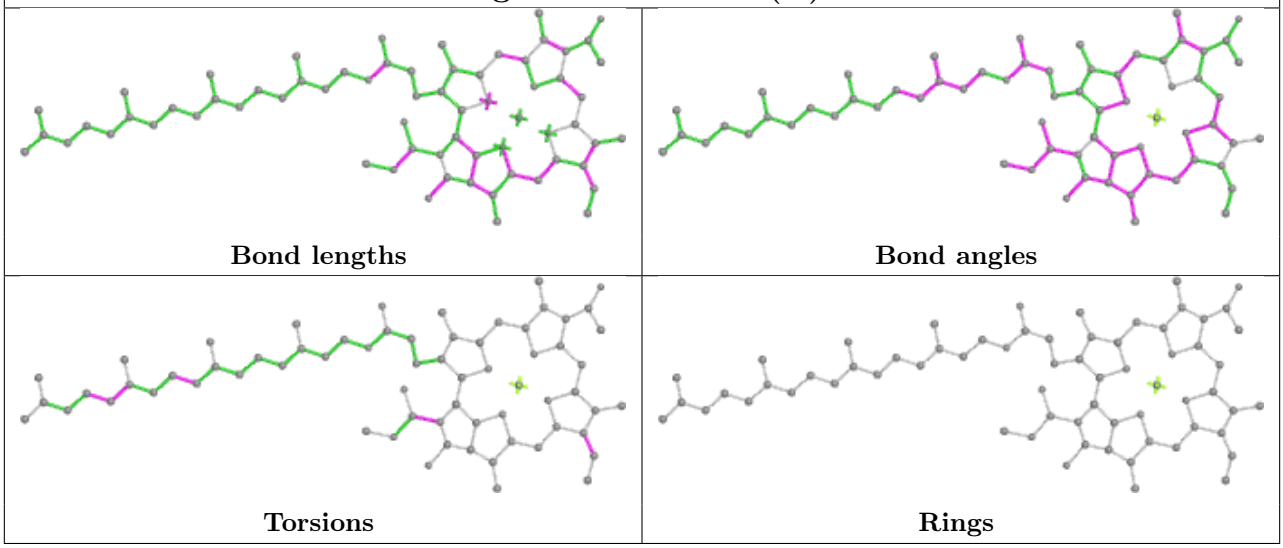


Torsions

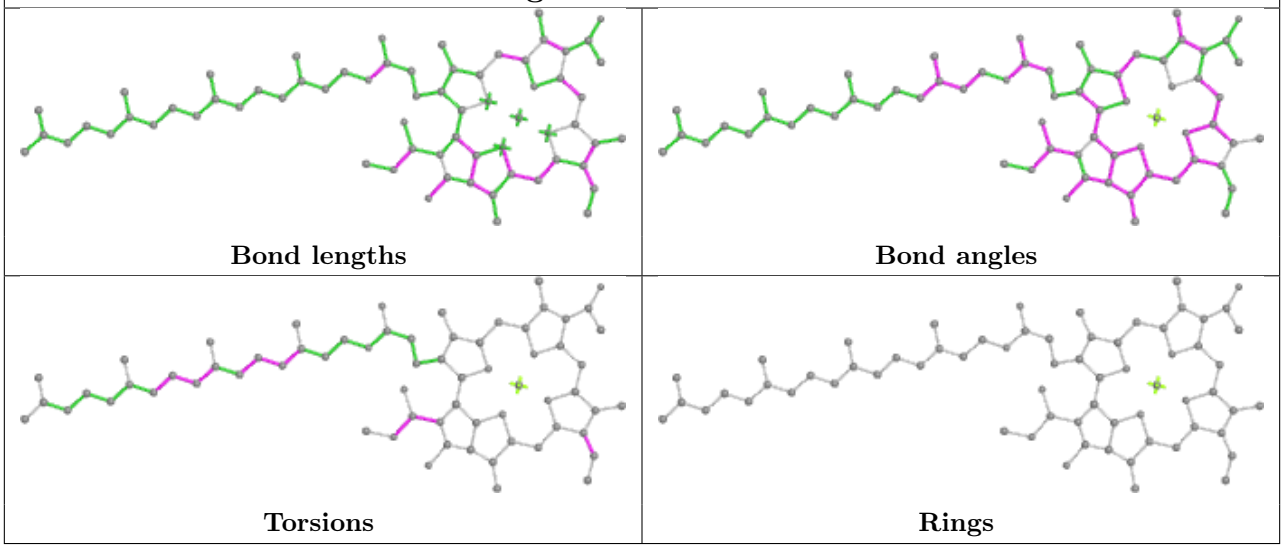


Rings

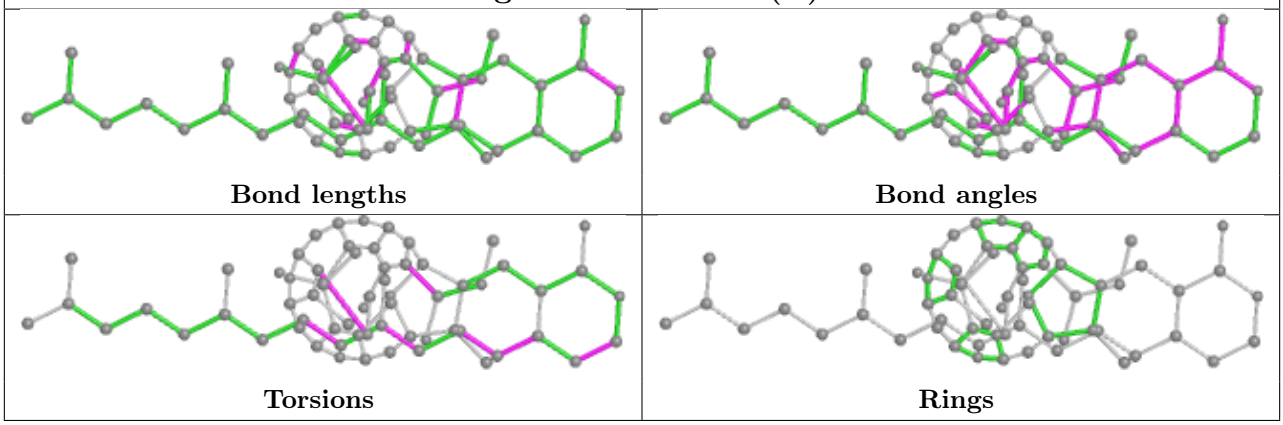
Ligand BCB L 302 (A)



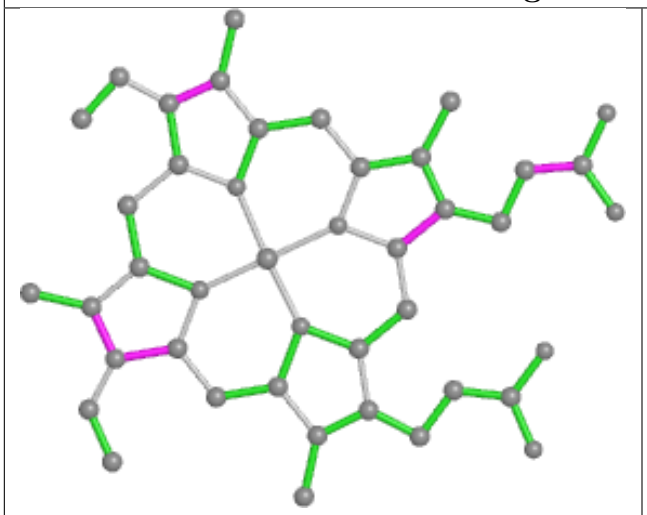
Ligand BCB L 304



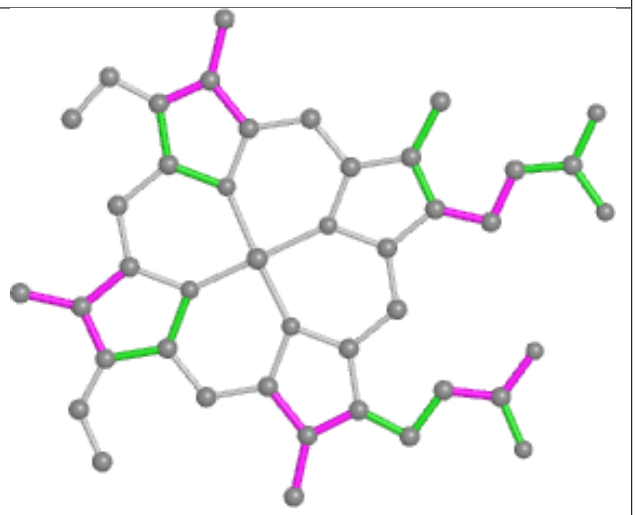
Ligand BPB L 303 (B)



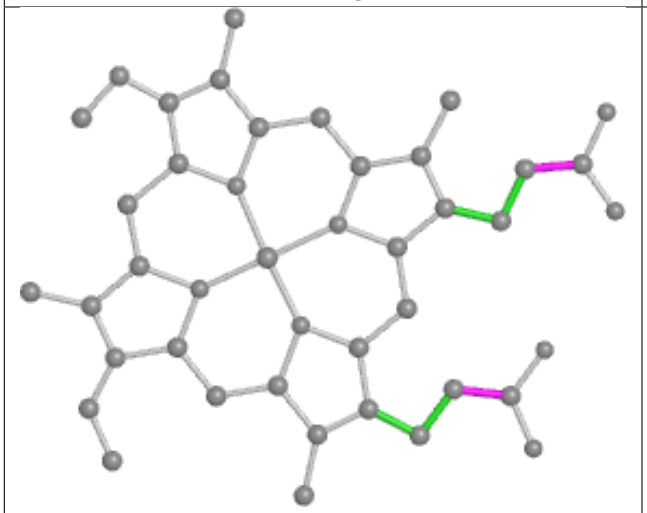
Ligand HEC C 403



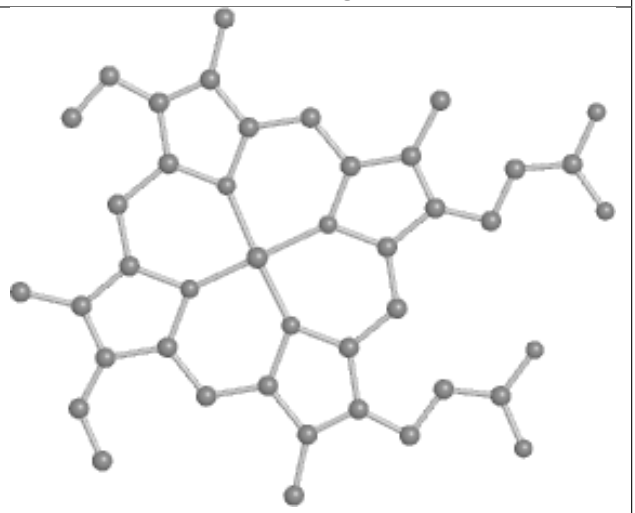
Bond lengths



Bond angles

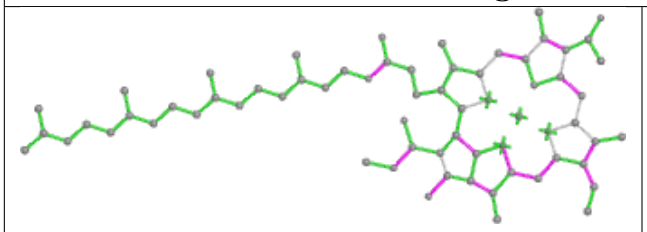


Torsions

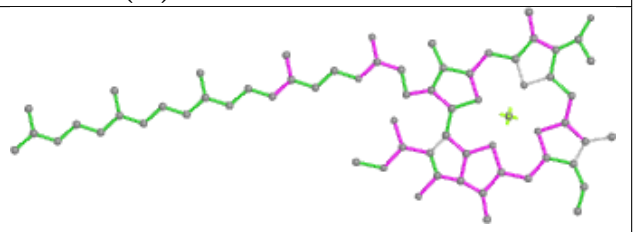


Rings

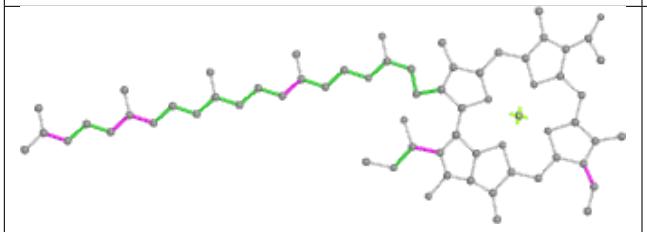
Ligand BCB L 301 (B)



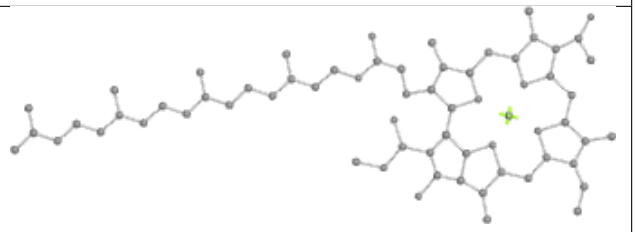
Bond lengths



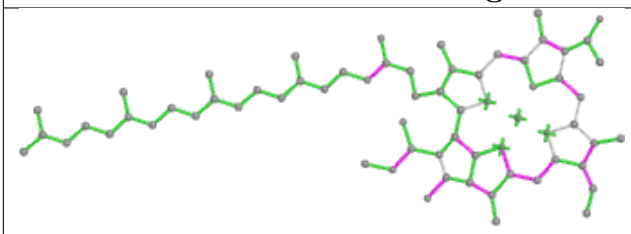
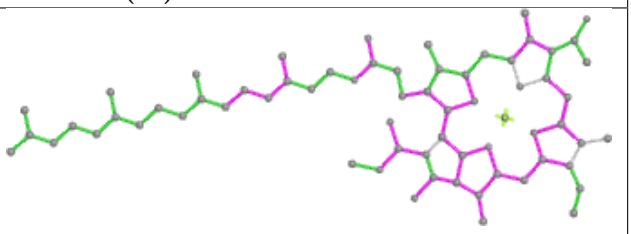
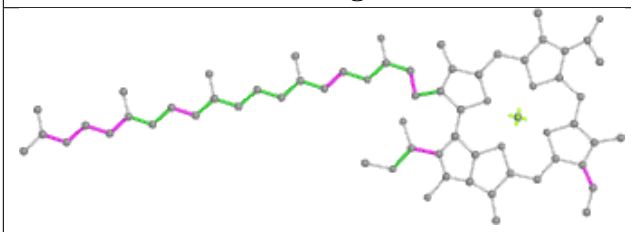
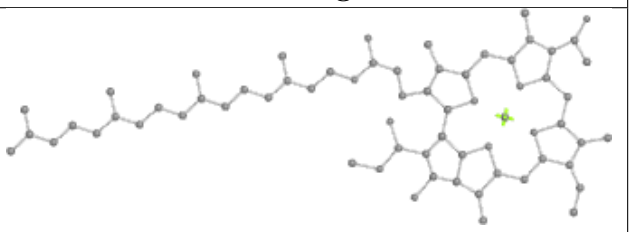
Bond angles

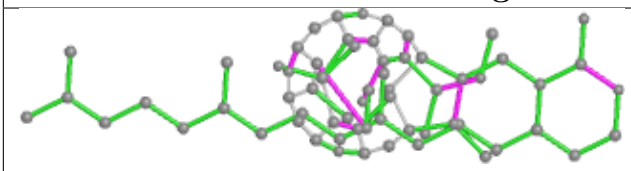
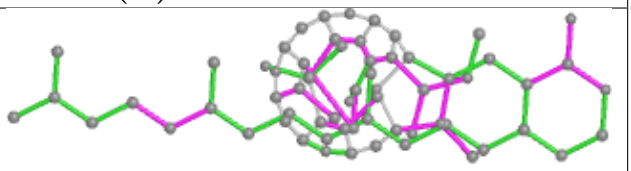
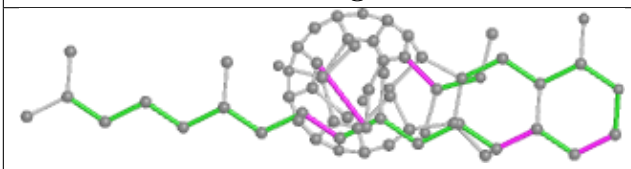
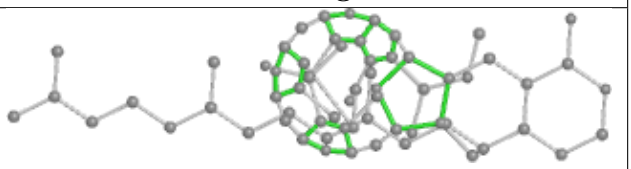


Torsions

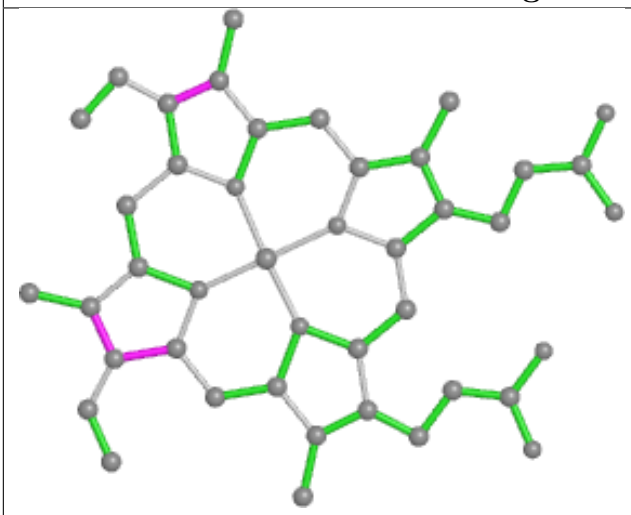


Rings

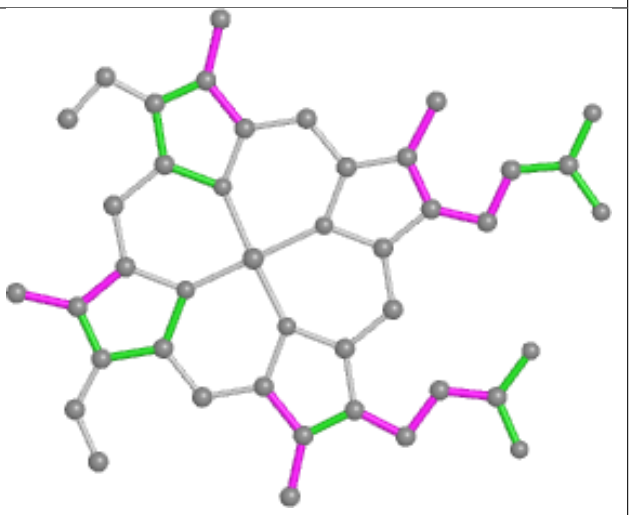
Ligand BCB M 403 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

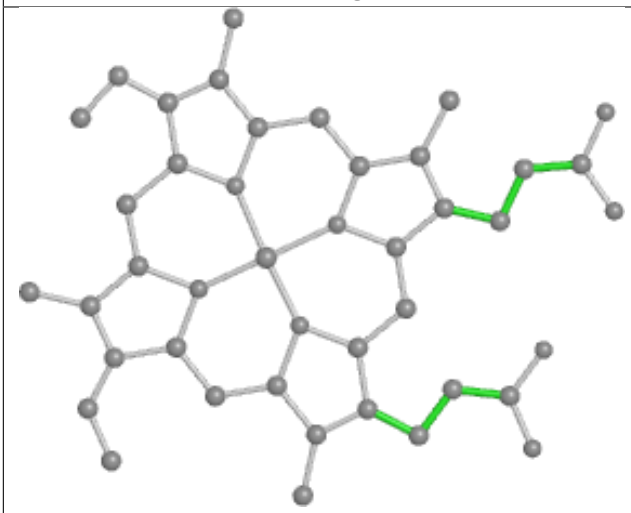
Ligand HEC C 404



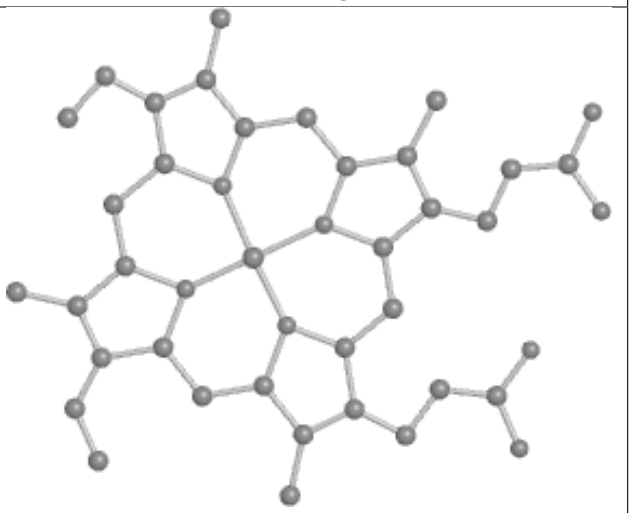
Bond lengths



Bond angles

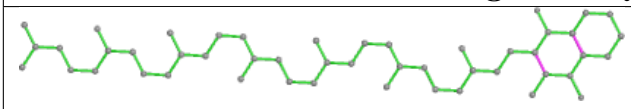


Torsions

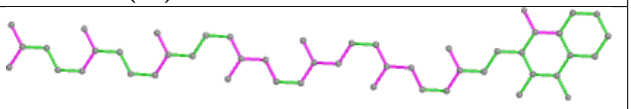


Rings

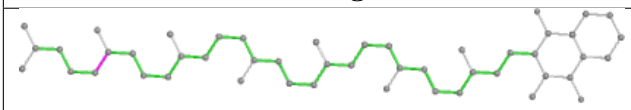
Ligand MQ7 M 402 (B)



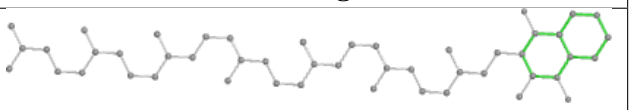
Bond lengths



Bond angles

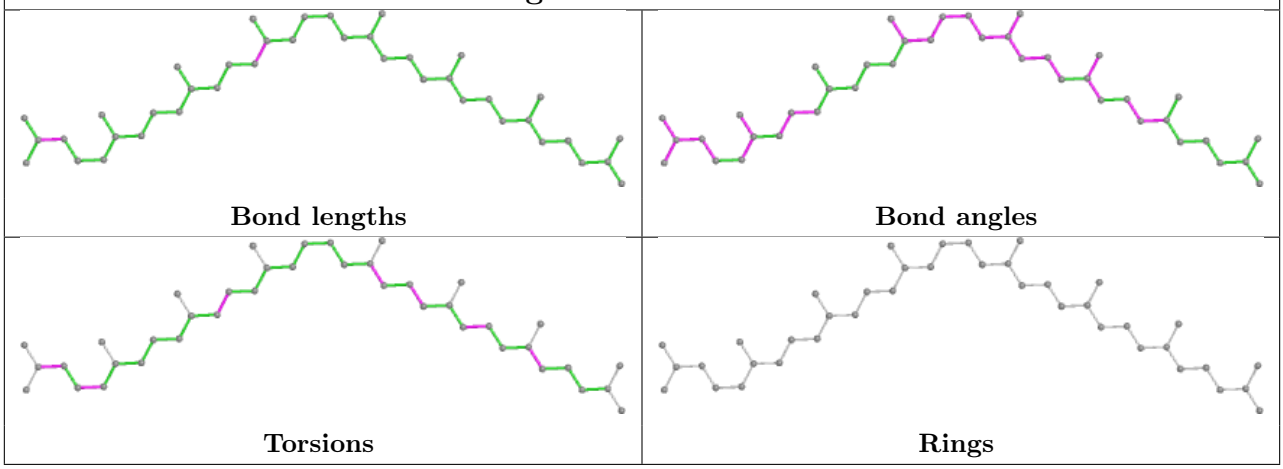


Torsions

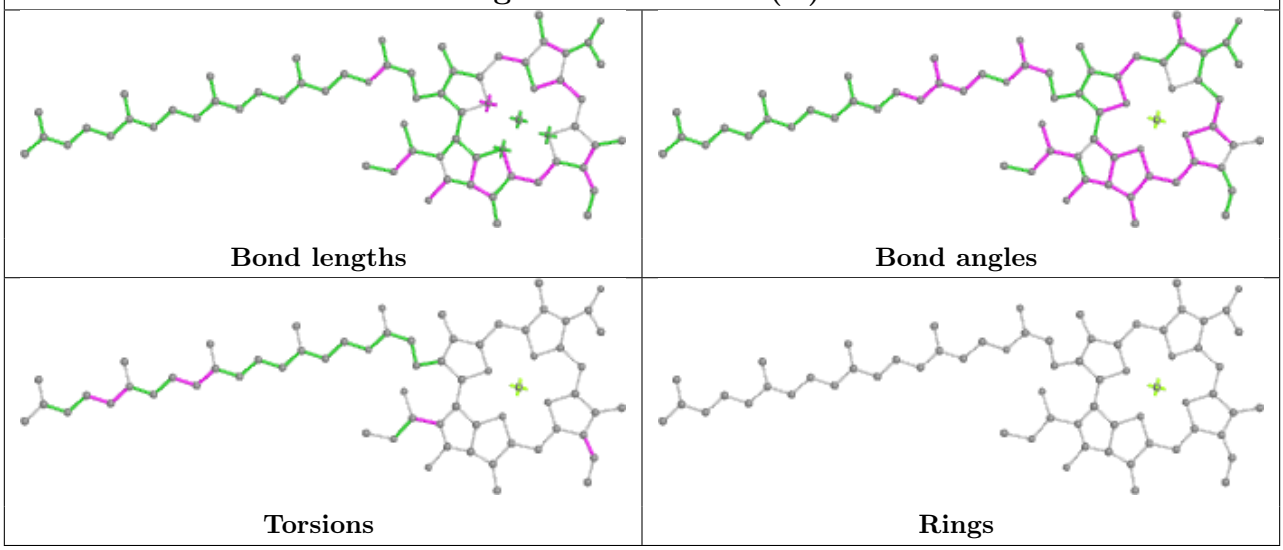


Rings

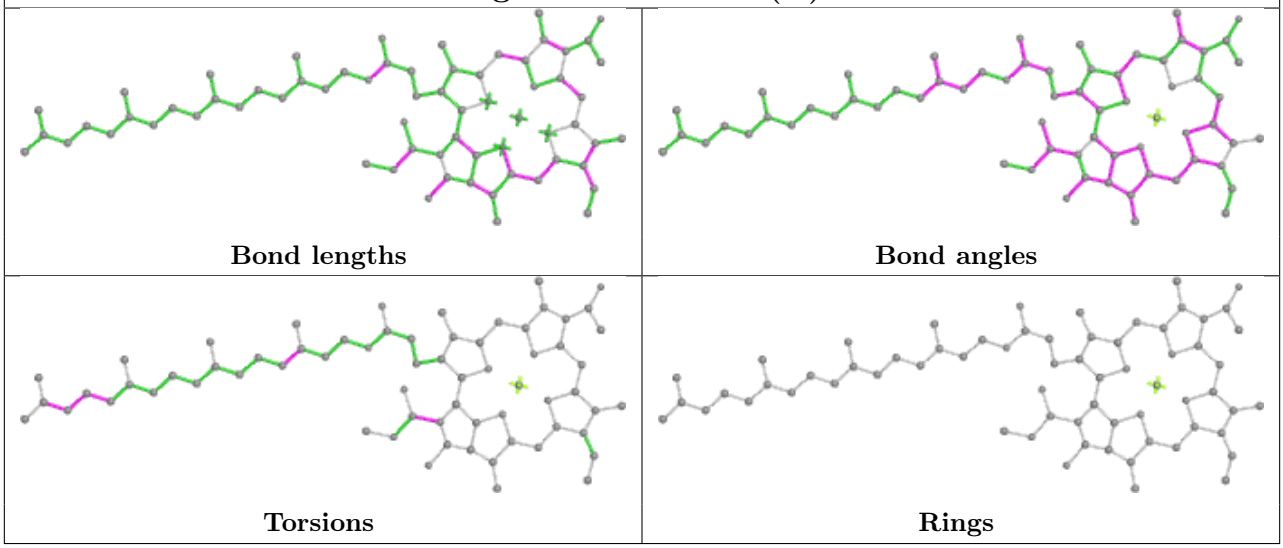
Ligand NS5 M 404

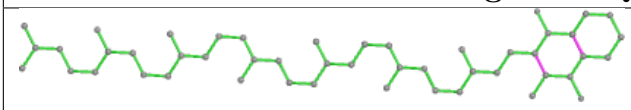
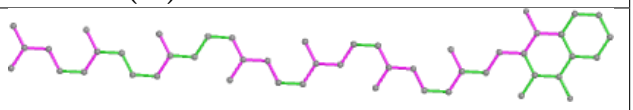
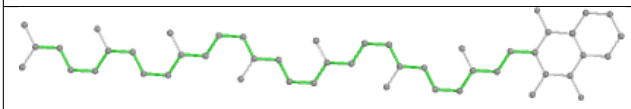
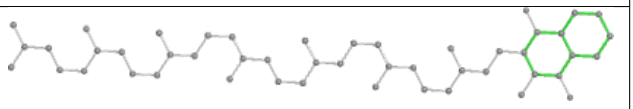


Ligand BCB L 302 (B)



Ligand BCB L 301 (A)



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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 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%)	-0.73	0	100	100	66, 81, 106, 131	0
2	H	257/258 (99%)	-0.65	5 (1%)	66	59	72, 92, 135, 172	0
3	L	273/273 (100%)	-0.83	0	100	100	66, 79, 104, 114	0
4	M	323/323 (100%)	-0.56	2 (0%)	89	86	65, 79, 105, 128	0
All	All	1185/1190 (99%)	-0.69	7 (0%)	89	86	65, 82, 113, 172	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	46	PRO	3.0
4	M	185	THR	2.7
2	H	49	LEU	2.5
2	H	52	LEU	2.4
2	H	257	LEU	2.3
2	H	47	LEU	2.3
4	M	319	PRO	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(Å^2)	Q<0.9
2	FME	H	1	10/11	0.97	0.11	76,92,104,112	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
6	DGA	C	405	37/44	0.65	0.46	91,118,156,158	0
8	LDA	L	306	16/16	0.73	0.27	97,108,131,133	0
8	LDA	H	707	16/16	0.76	0.34	72,87,146,150	0
8	LDA	M	413	16/16	0.77	0.54	81,109,141,142	0
9	HTO	L	308	10/10	0.80	0.39	92,104,112,119	0
7	SO4	C	408	5/5	0.83	0.41	102,105,111,111	5
8	LDA	L	307	16/16	0.84	0.45	109,115,145,146	0
7	SO4	C	407	5/5	0.87	0.68	109,113,118,120	5
14	NS5	M	404	40/40	0.87	0.23	69,88,127,127	0
7	SO4	H	705	5/5	0.89	0.52	121,129,137,143	0
7	SO4	M	410	5/5	0.89	0.40	125,132,144,146	0
9	HTO	H	709	10/10	0.90	0.47	92,108,118,119	0
9	HTO	H	710	10/10	0.90	0.14	93,101,114,114	0
8	LDA	M	412	16/16	0.90	0.46	96,101,138,140	0
7	SO4	H	704	5/5	0.90	0.37	88,91,95,96	5
7	SO4	M	408	5/5	0.91	0.36	118,118,132,138	0
7	SO4	M	409	5/5	0.91	0.20	91,99,102,106	5
7	SO4	C	406	5/5	0.91	0.22	121,136,141,144	0
7	SO4	M	411	5/5	0.93	0.46	134,137,142,156	0
13	MQ7	M	402[A]	48/48	0.95	0.20	67,74,117,130	48
13	MQ7	M	402[B]	48/48	0.95	0.20	67,74,117,130	48
10	BCB	L	304	66/66	0.95	0.20	63,73,154,160	0
7	SO4	H	703	5/5	0.96	0.45	141,141,150,151	0
11	BPB	L	305	65/65	0.97	0.18	70,81,163,168	0
8	LDA	H	708	16/16	0.97	0.27	88,103,127,128	0
8	LDA	H	701	16/16	0.97	0.16	74,88,101,102	0
7	SO4	M	406	5/5	0.97	0.07	102,105,118,122	0
10	BCB	L	301[A]	66/66	0.98	0.19	59,65,82,95	66
10	BCB	L	301[B]	66/66	0.98	0.19	59,65,82,95	66
10	BCB	L	302[A]	66/66	0.98	0.17	63,68,109,112	66
10	BCB	L	302[B]	66/66	0.98	0.17	63,68,109,112	66
7	SO4	H	702	5/5	0.98	0.07	94,99,106,111	0

Continued on next page...

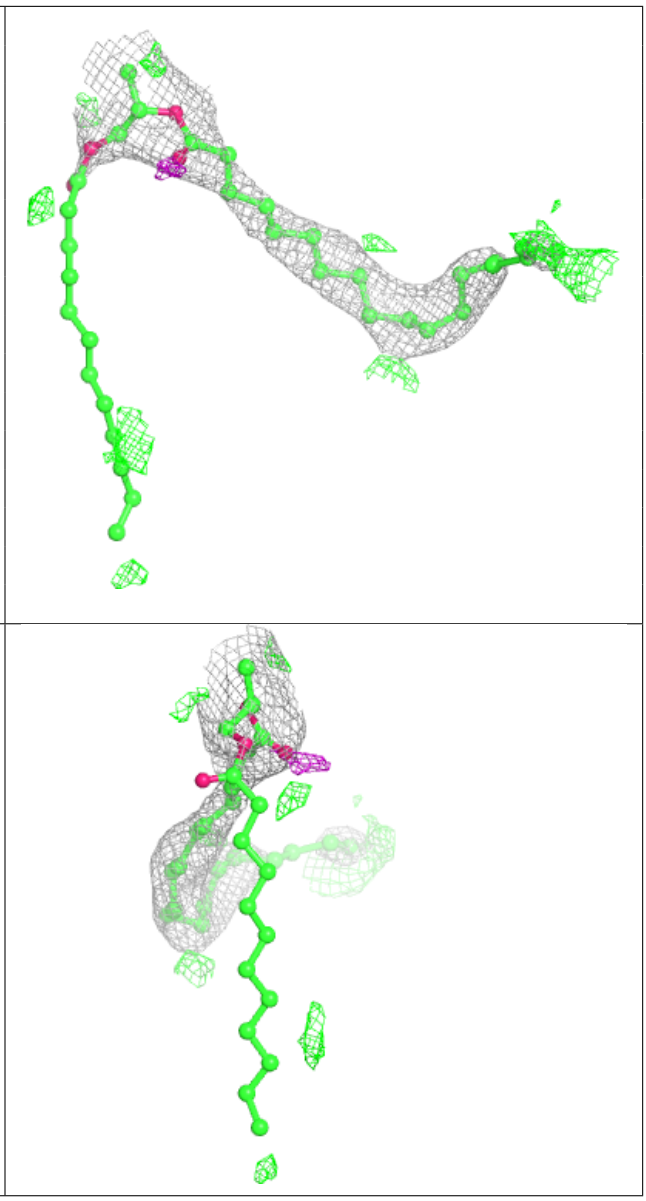
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	BCB	M	403[A]	66/66	0.98	0.24	59,68,100,104	66
10	BCB	M	403[B]	66/66	0.98	0.24	59,68,100,104	66
11	BPB	L	303[A]	65/65	0.98	0.18	65,71,81,84	65
11	BPB	L	303[B]	65/65	0.98	0.18	65,71,81,84	65
5	HEC	C	403	43/43	0.98	0.17	57,68,75,83	0
5	HEC	C	404	43/43	0.98	0.12	65,73,91,110	0
5	HEC	C	401	43/43	0.98	0.12	76,88,97,105	0
7	SO4	H	706	5/5	0.98	0.06	89,90,105,107	5
7	SO4	M	405	5/5	0.99	0.08	92,99,111,112	0
5	HEC	C	402	43/43	0.99	0.14	75,82,92,100	0
7	SO4	M	407	5/5	0.99	0.08	82,88,91,95	0
12	FE	M	401[B]	1/1	1.00	0.12	72,72,72,72	1
12	FE	M	401[A]	1/1	1.00	0.12	72,72,72,72	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.

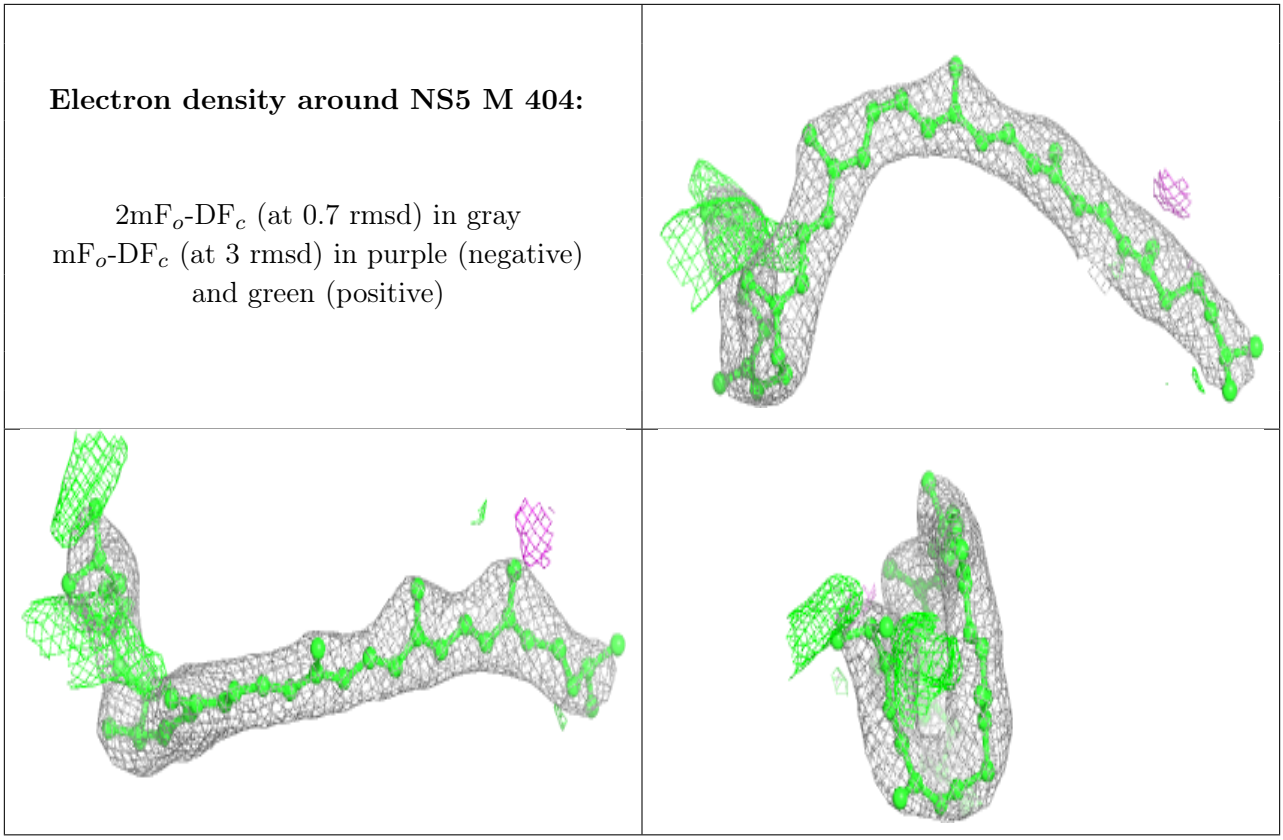
Electron density around DGA C 405:

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



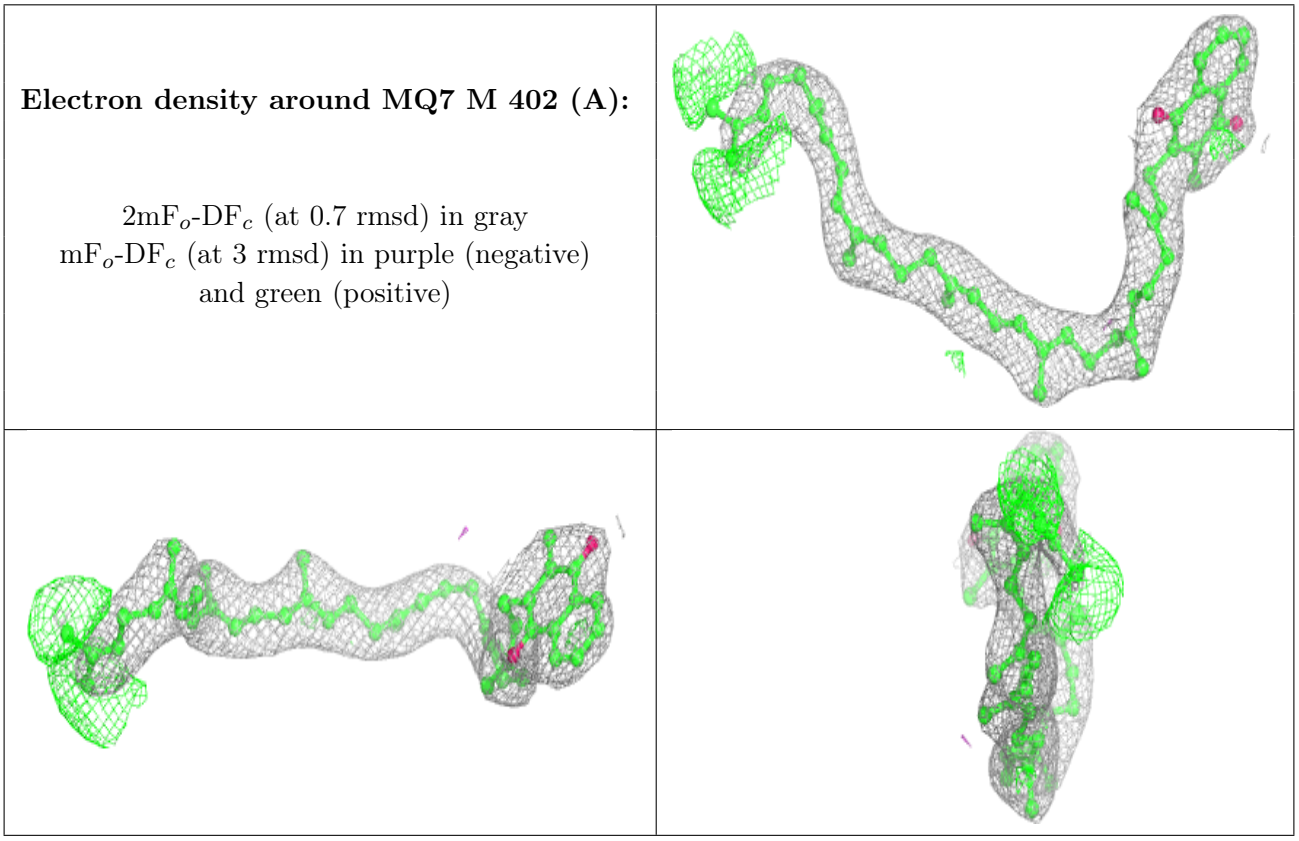
Electron density around NS5 M 404:

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



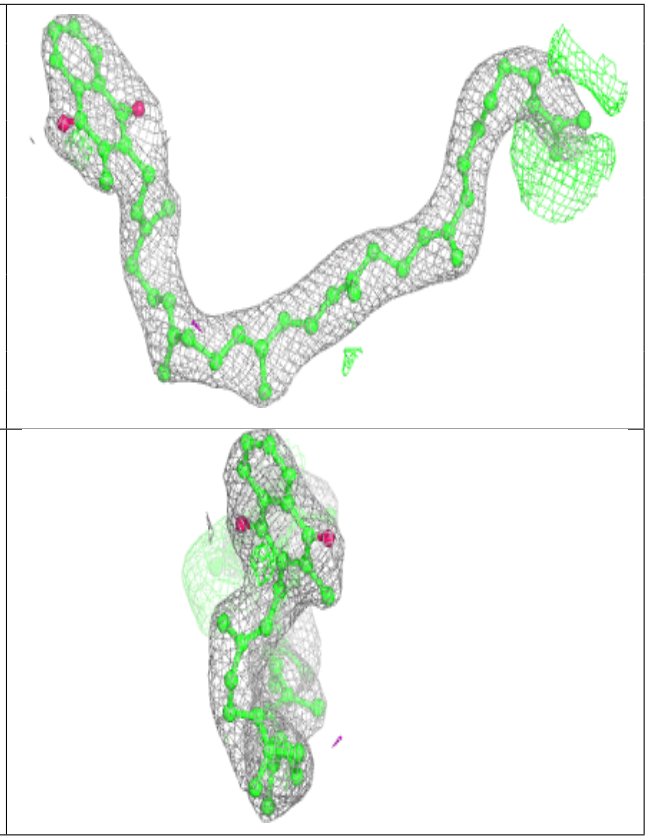
Electron density around MQ7 M 402 (A):

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



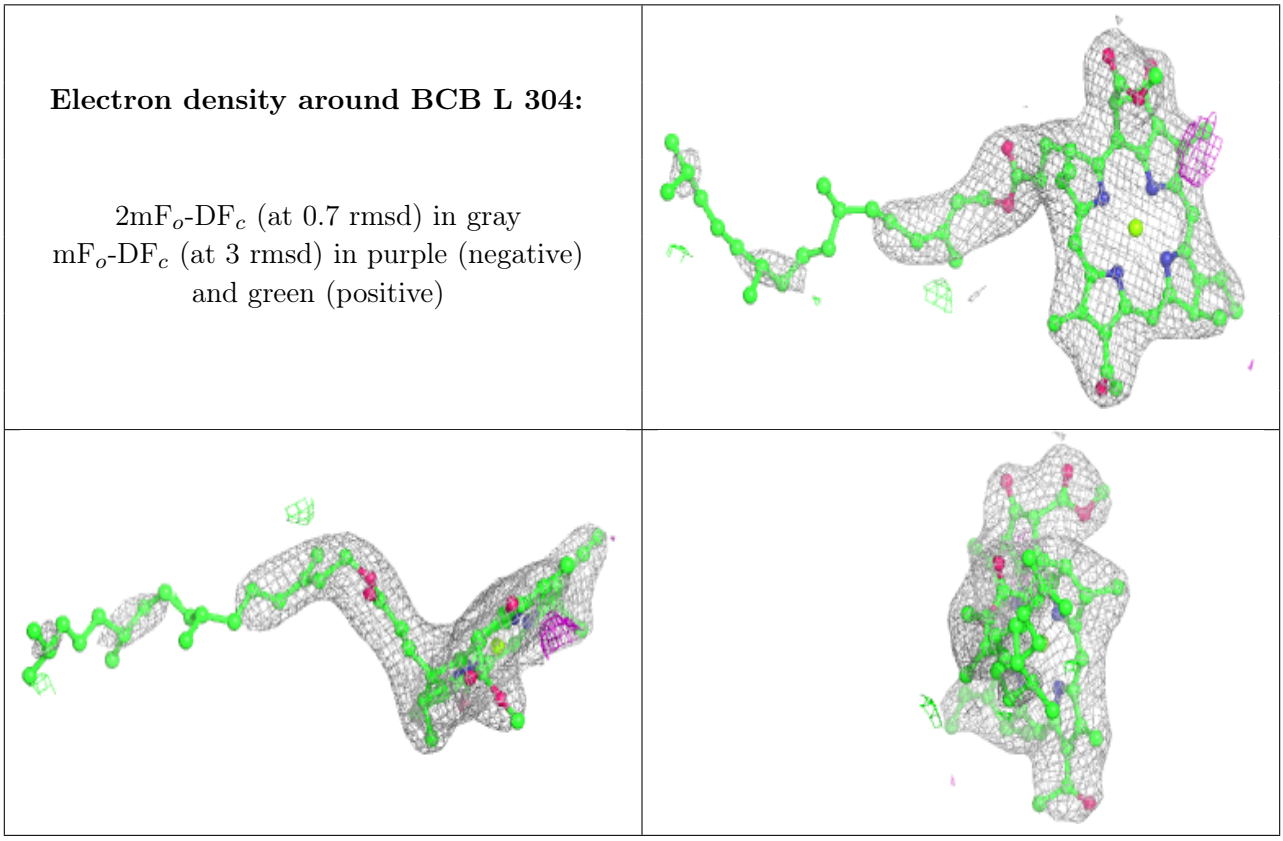
Electron density around MQ7 M 402 (B):

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



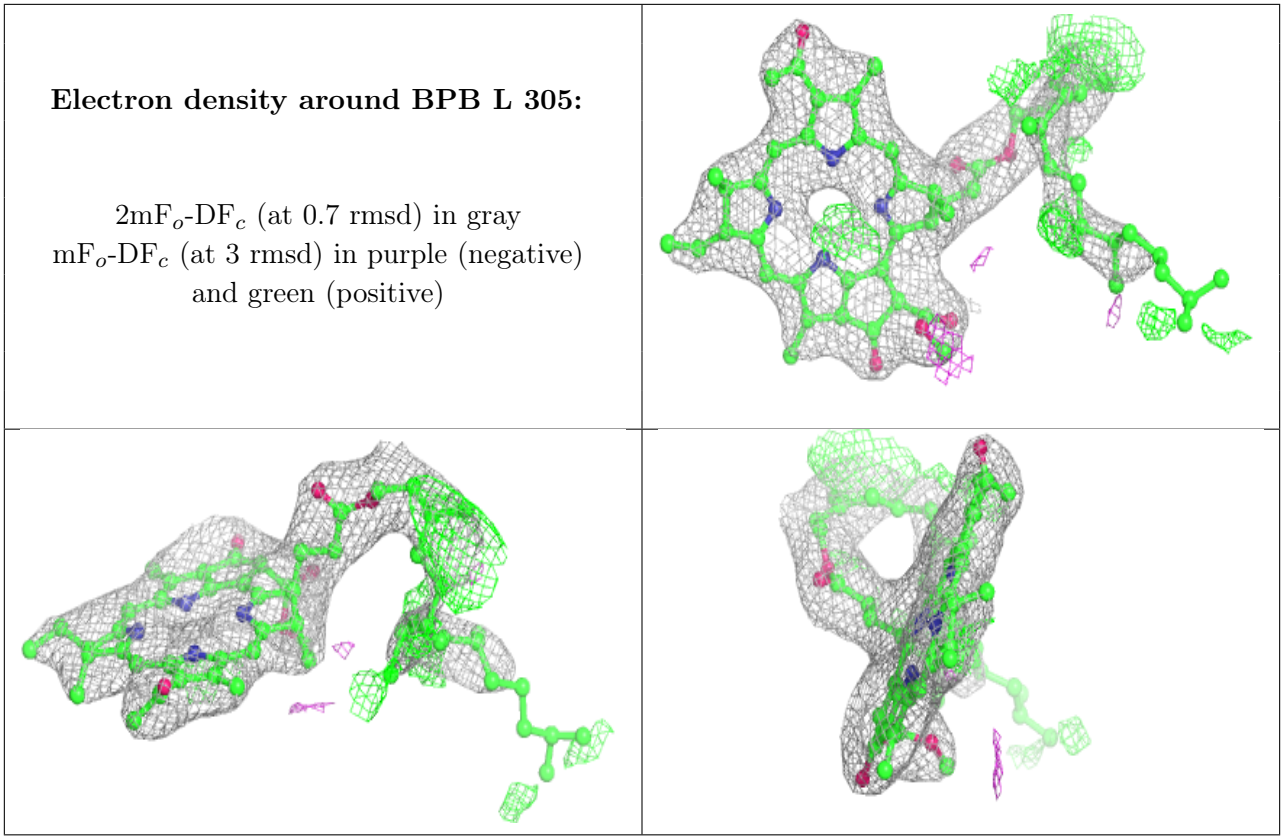
Electron density around BCB L 304:

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



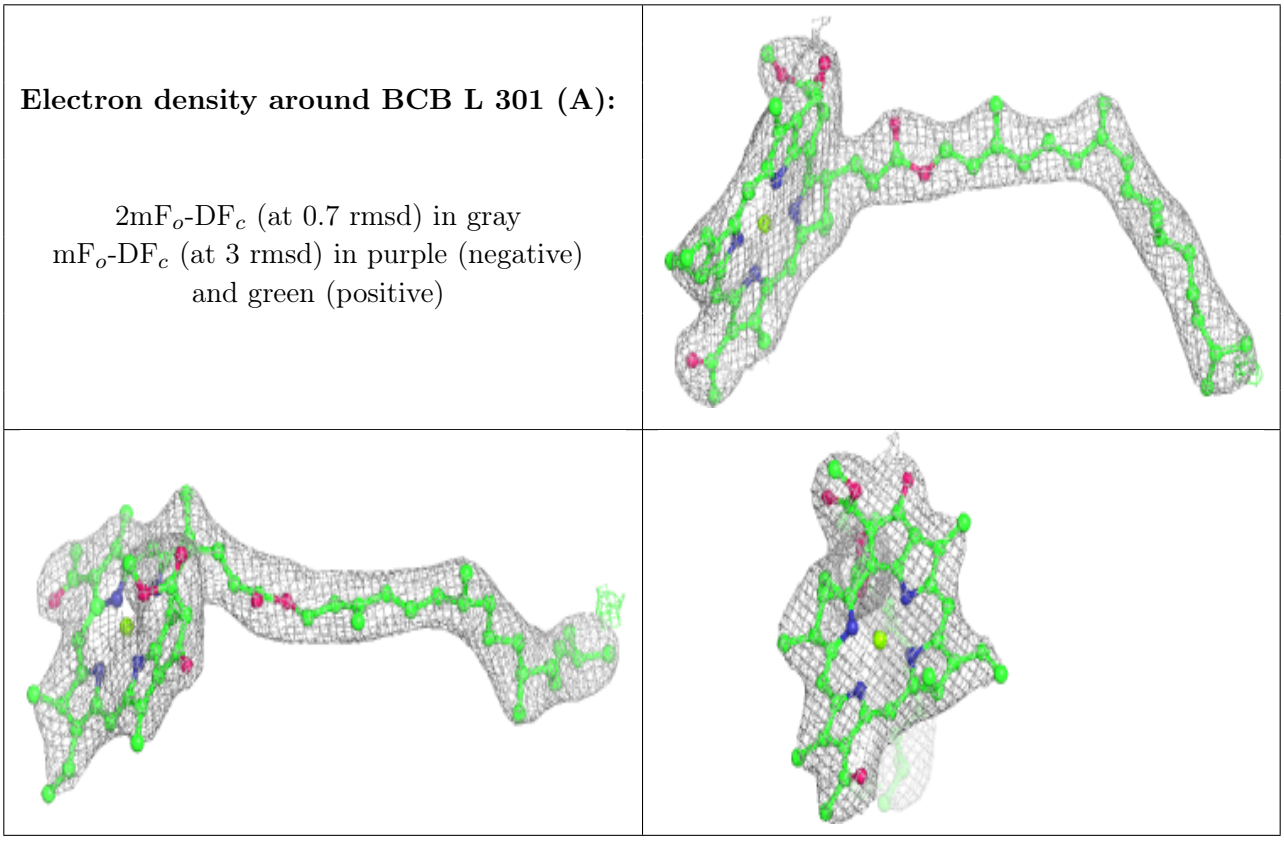
Electron density around BPB L 305:

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



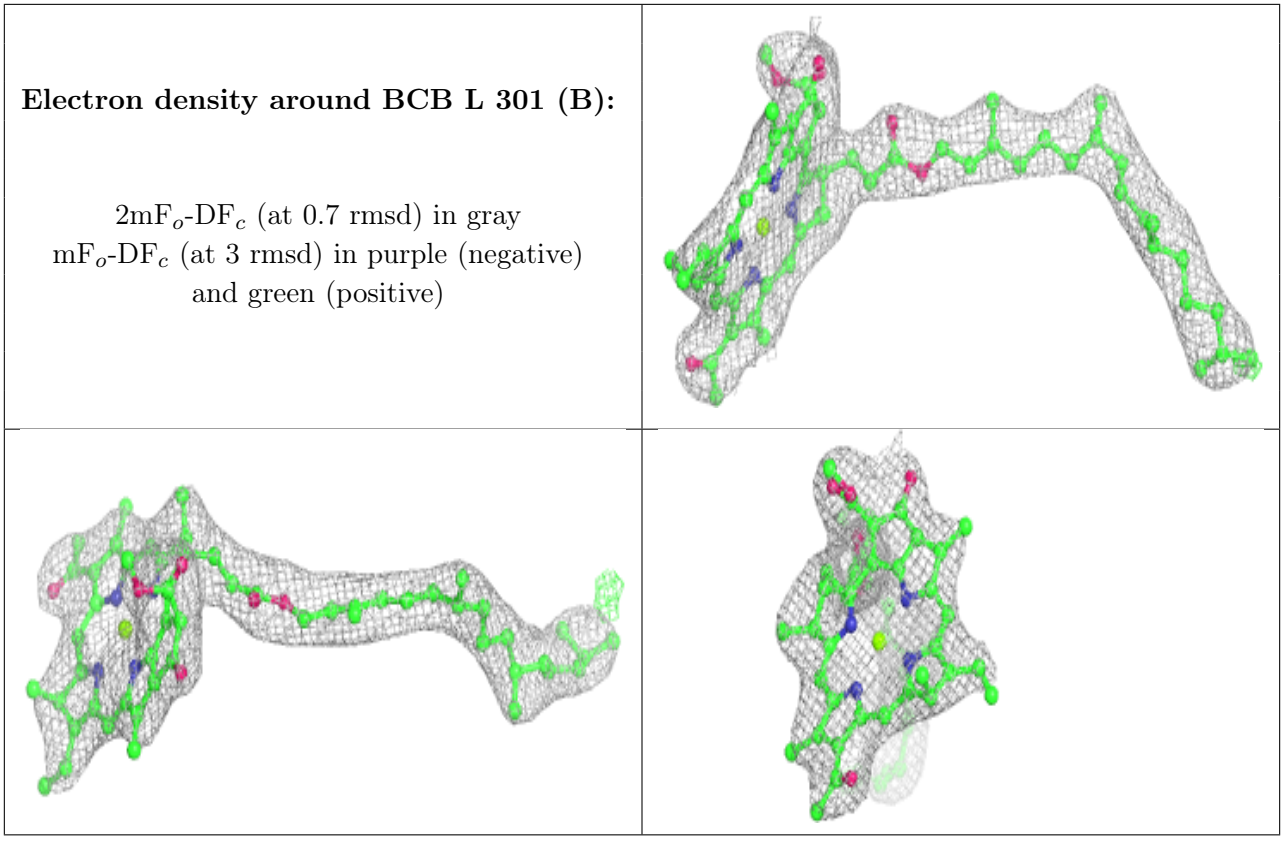
Electron density around BCB L 301 (A):

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



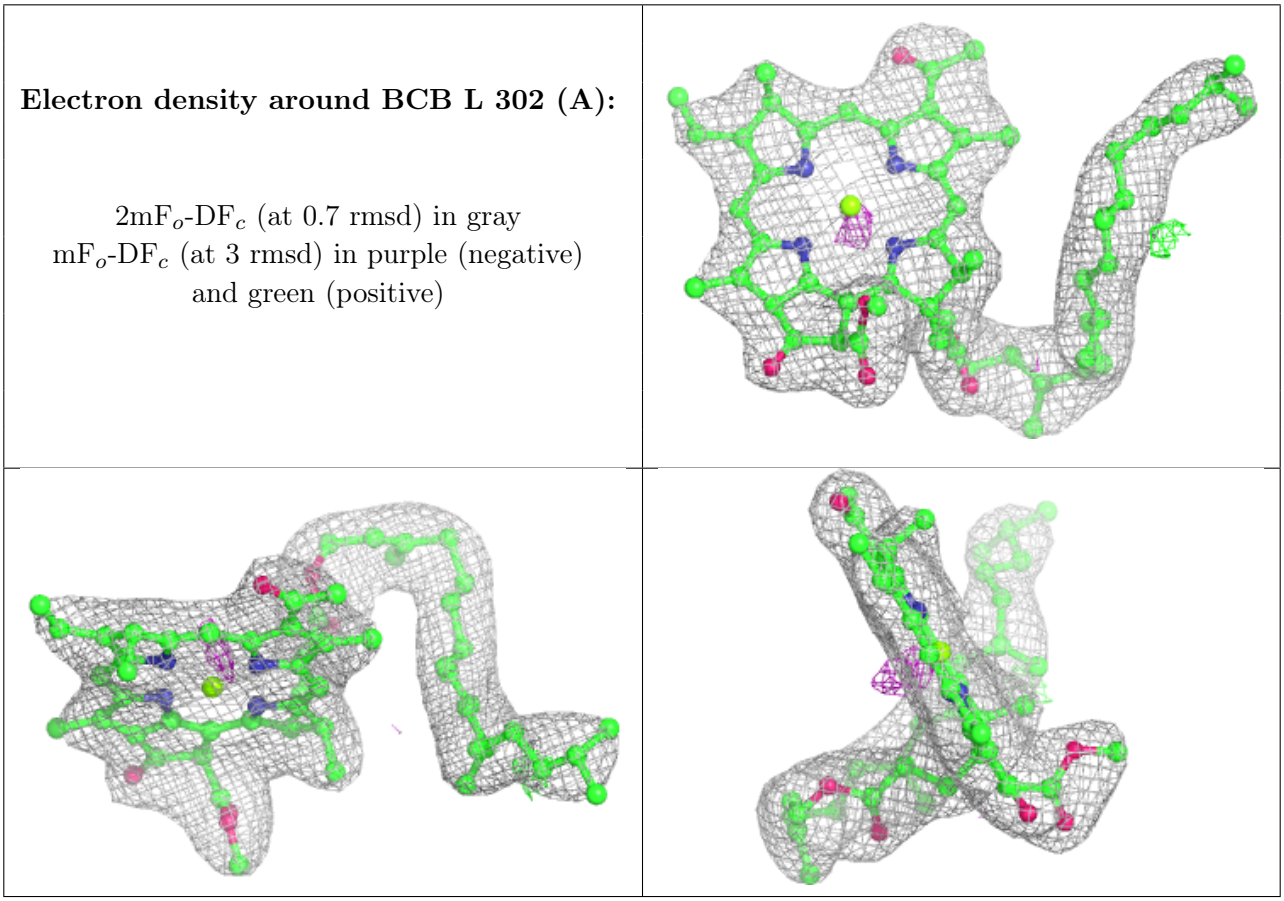
Electron density around BCB L 301 (B):

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



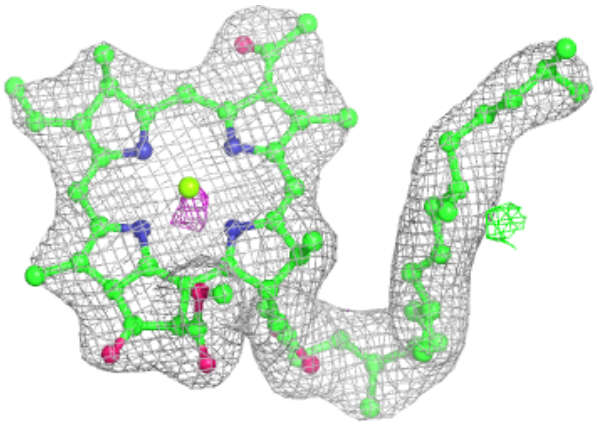
Electron density around BCB L 302 (A):

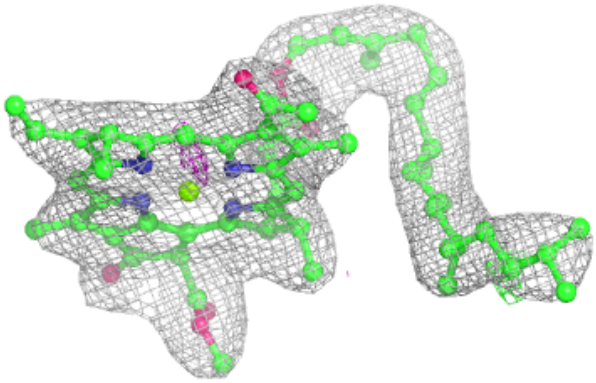
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

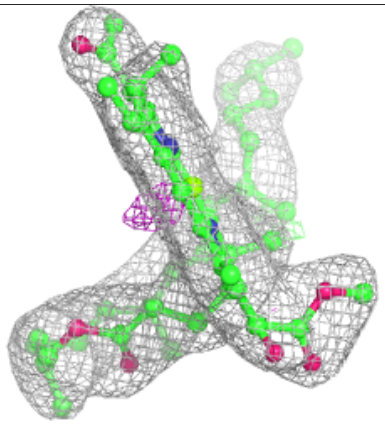


Electron density around BCB L 302 (B):

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

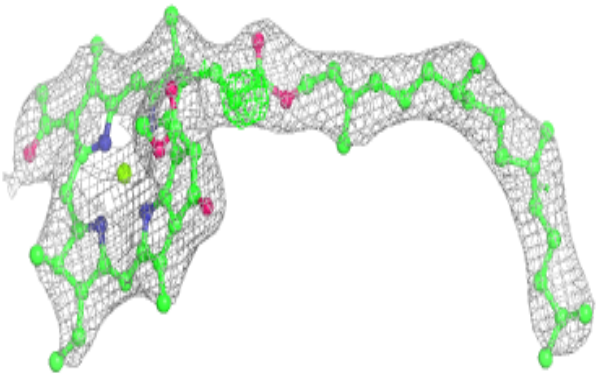


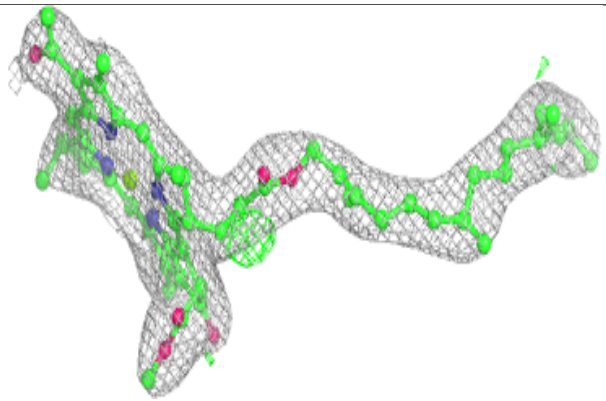


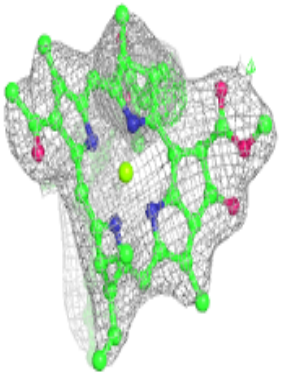


Electron density around BCB M 403 (A):

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

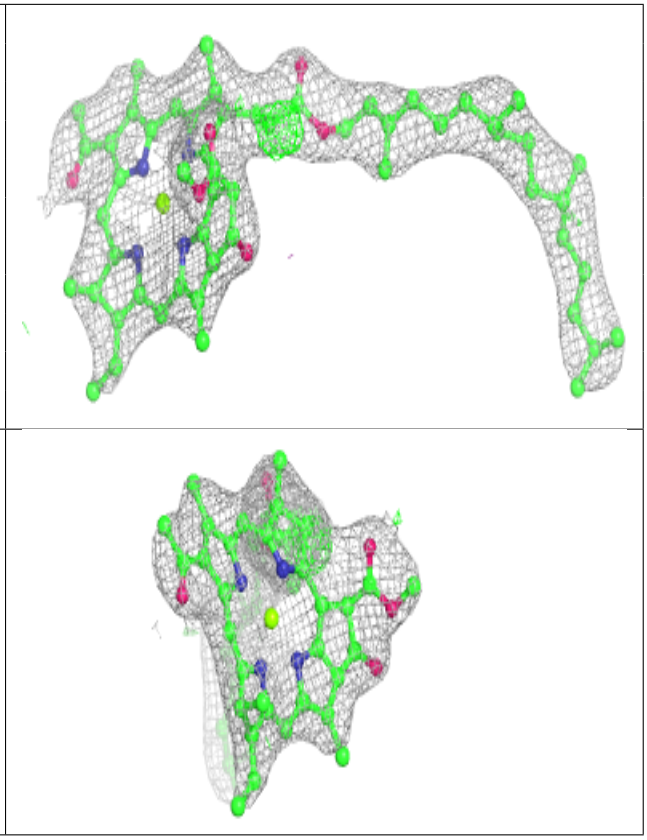


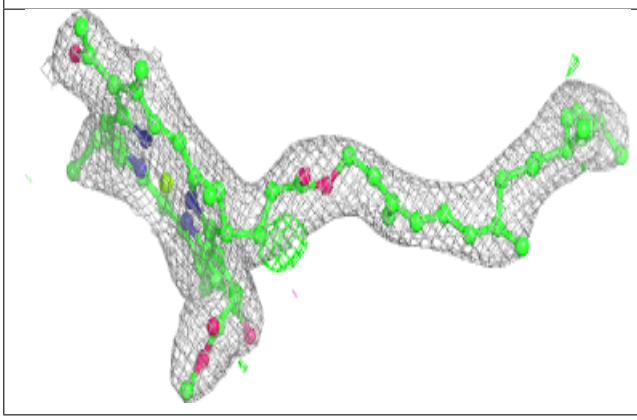




Electron density around BCB M 403 (B):

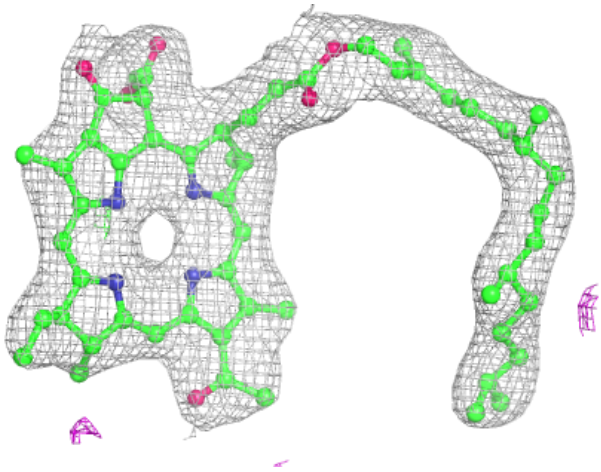
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

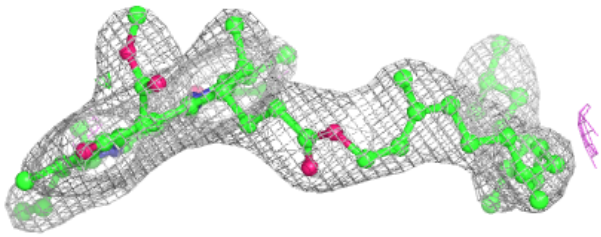


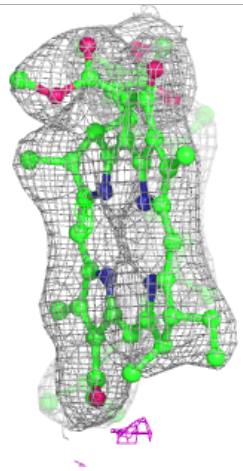


Electron density around BPB L 303 (A):

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

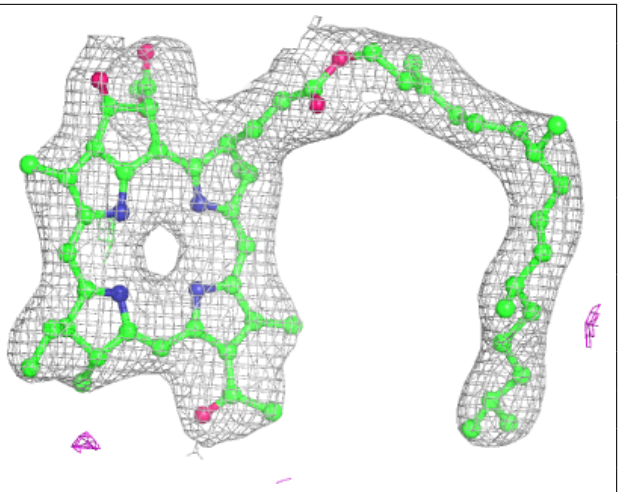


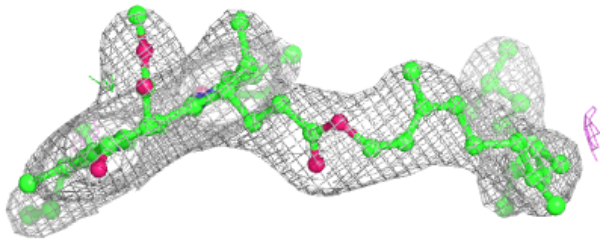


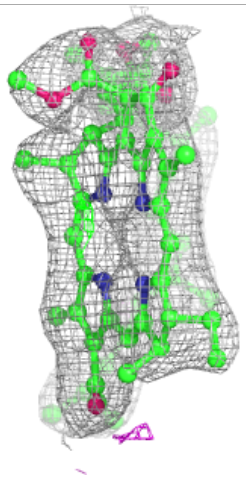


Electron density around BPB L 303 (B):

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

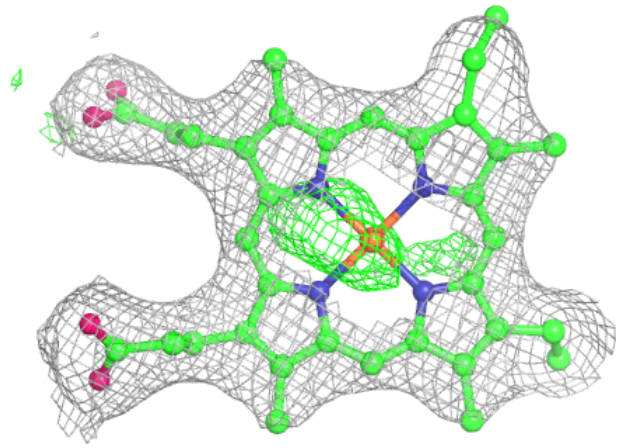


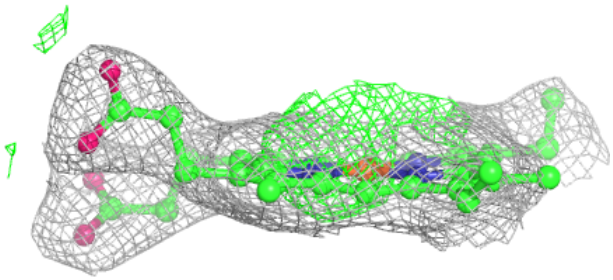


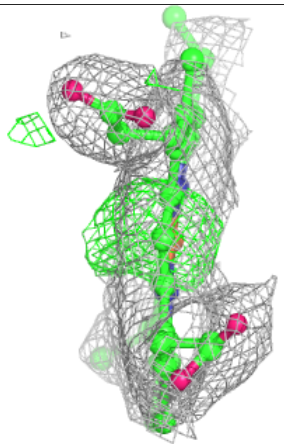


Electron density around HEC C 403:

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

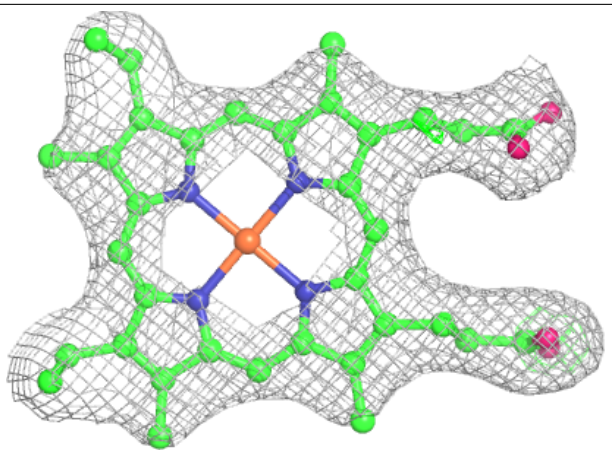


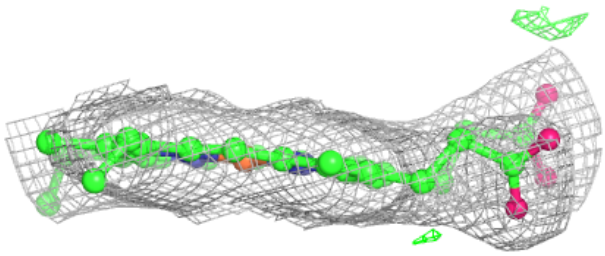


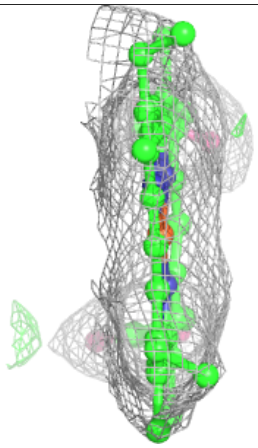


Electron density around HEC C 404:

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

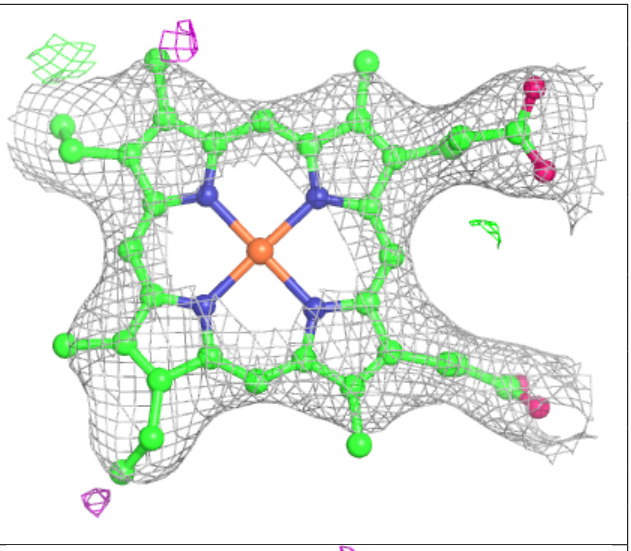


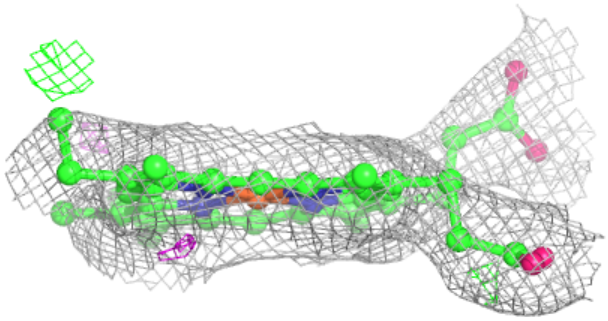


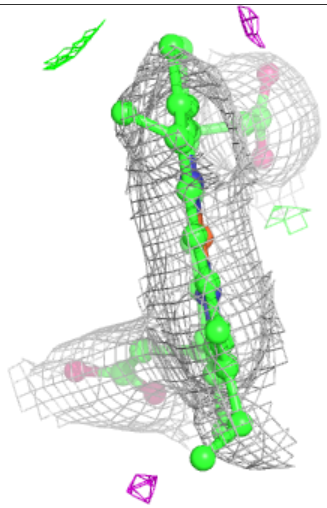


Electron density around HEC C 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

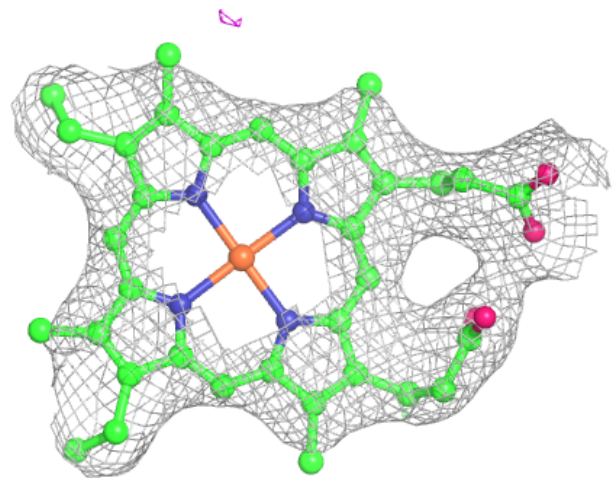


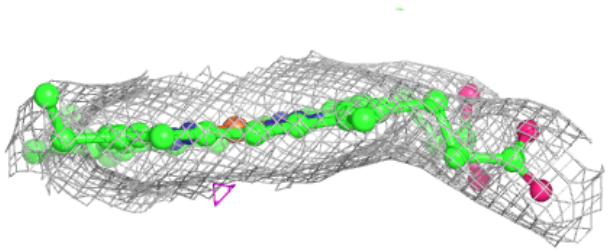


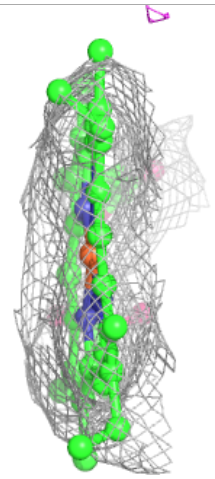


Electron density around HEC C 402:

$2mF_o$-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.