Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2026 – 09:50 am BST

PDB ID	:	6ZI4 / pdb_00006zi4
Title	:	Ultrafast Structural Response to Charge Redistribution Within a Photosynthetic Reaction Centre - 5 ps (a) structure
Authors	:	Baath, P.; Dods, R.; Braenden, G.; Neutze, R.
Deposited on	:	2020-06-24
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

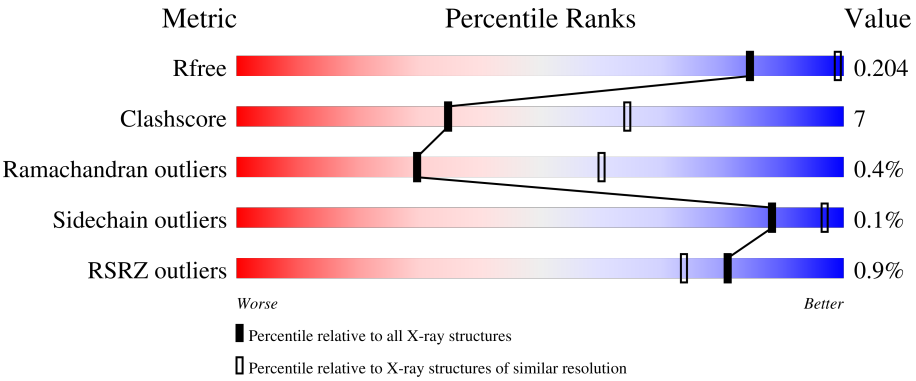
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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}	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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	336	84% 15%
2	H	258	85% 14%
3	L	273	79% 21%
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	-	-	-
5	HEC	C	401	X	-	-	-
5	HEC	C	402	X	-	-	-
5	HEC	C	403	X	-	-	-
5	HEC	C	404	X	-	-	-

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosynthetic reaction center cytochrome c subunit.

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

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

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

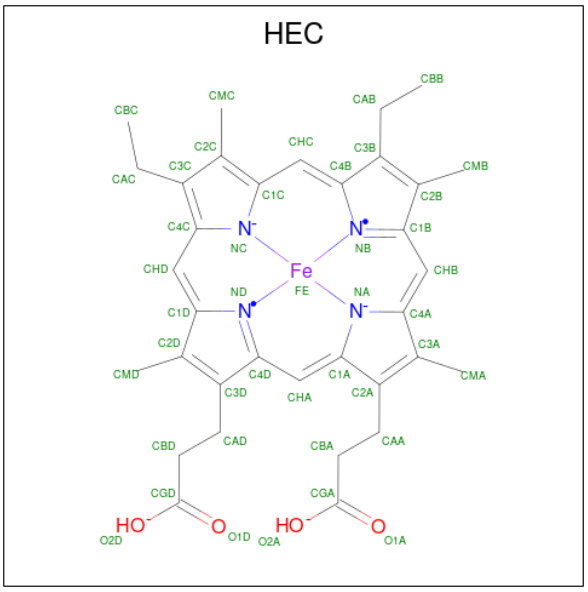
- Molecule 3 is a protein called Reaction center protein L chain.

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

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

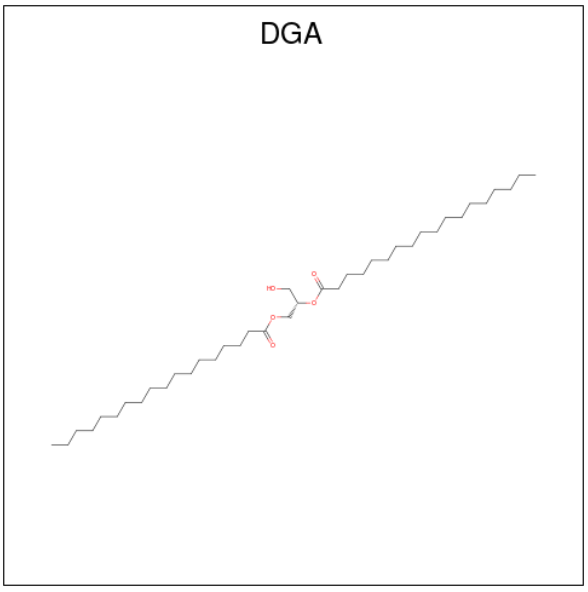
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	51	0
			2977	1983	491	490	13			

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



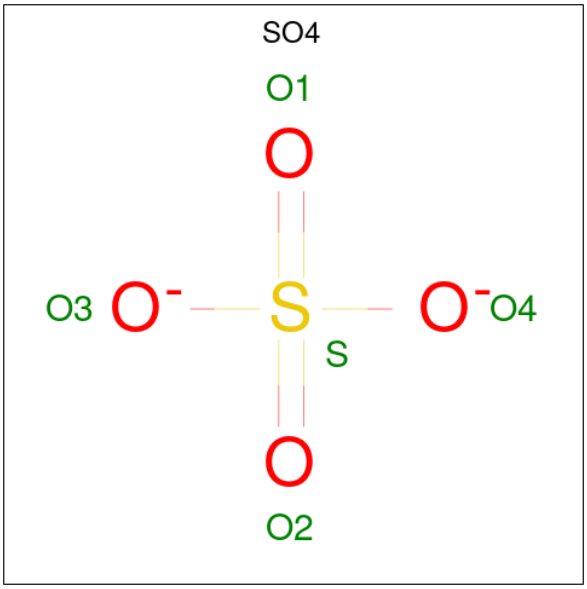
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 37 33 4	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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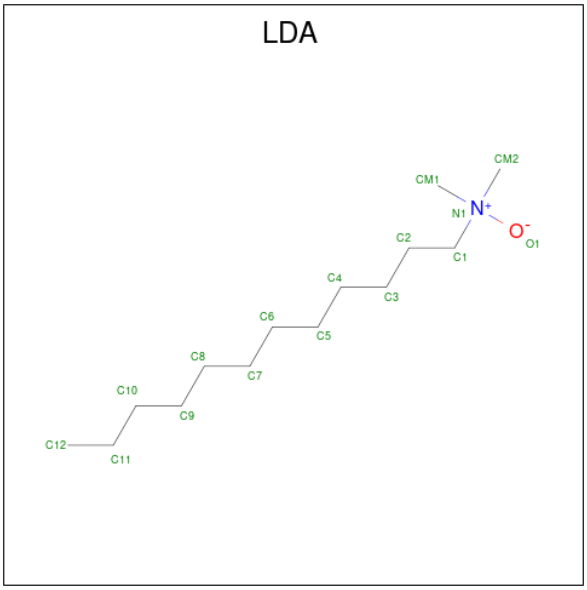
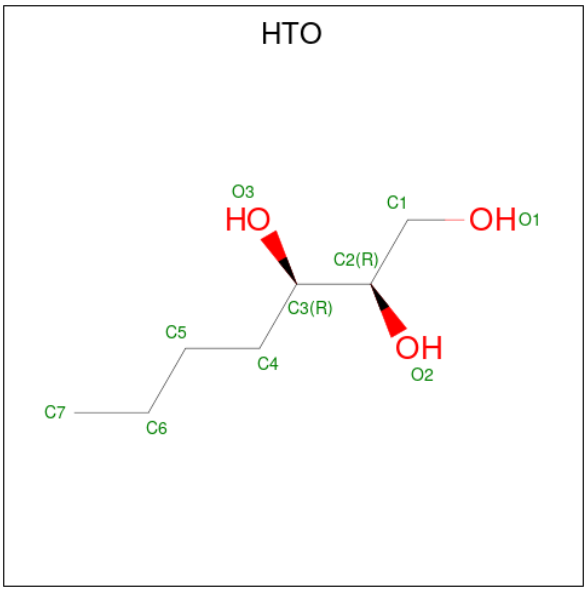
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total O S 5 4 1	0	0

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



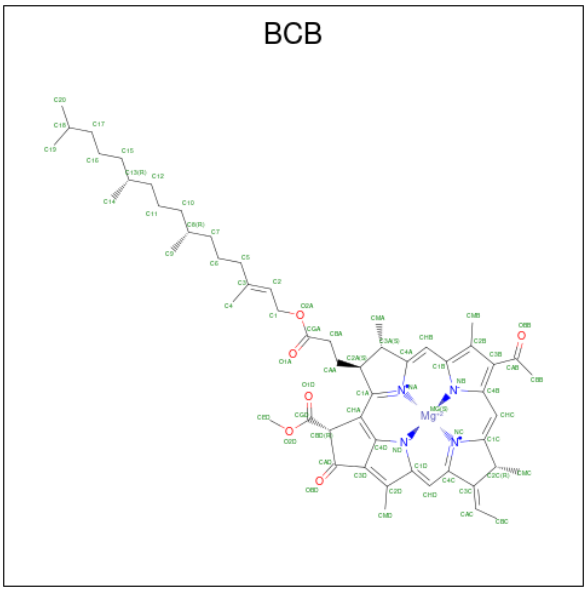
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C N O 16 14 1 1	0	0
8	H	1	Total C N O 16 14 1 1	0	0
8	H	1	Total C N O 16 14 1 1	0	0
8	L	1	Total C N O 16 14 1 1	0	0

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



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

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



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

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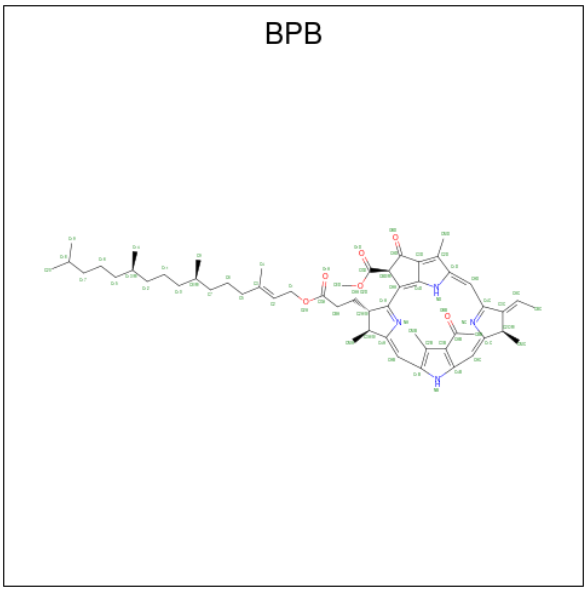
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C Mg N O 132 110 2 8 12	0	1
10	L	1	Total C Mg N O 66 55 1 4 6	0	0
10	M	1	Total C Mg N O 132 110 2 8 12	0	1

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

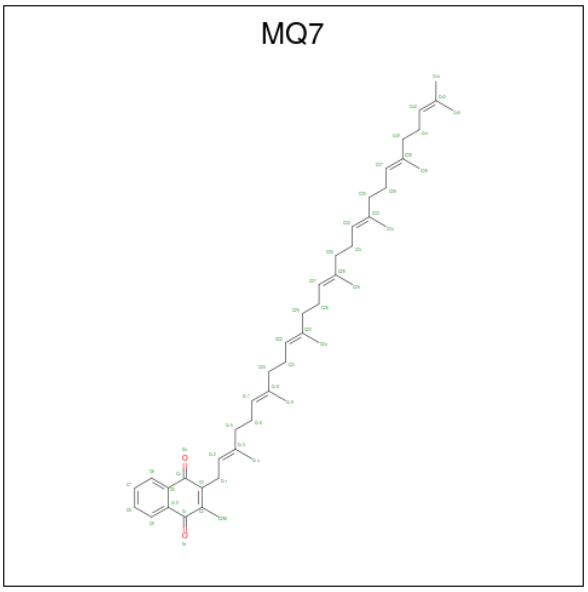


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C N O 130 110 8 12	0	1
11	M	1	Total C N O 65 55 4 6	0	0

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

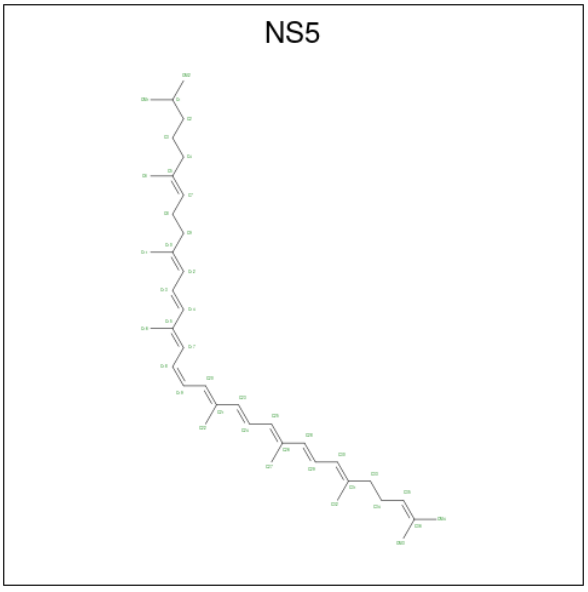
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total Fe 2 2	0	1

- 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 96 92 4	0	1

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



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

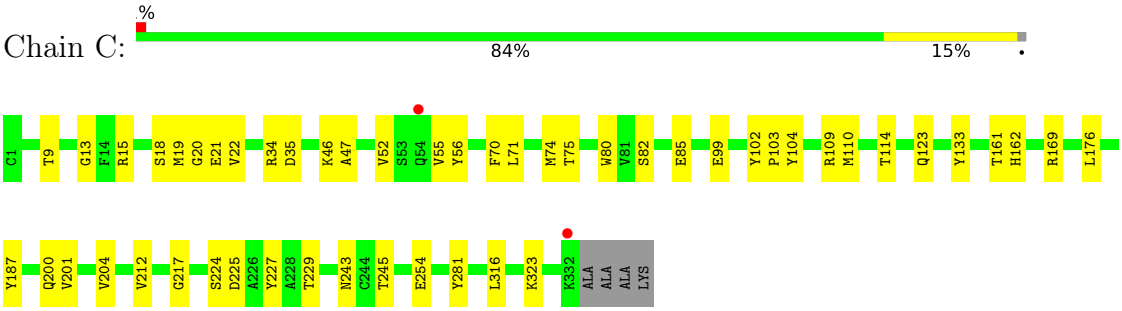
- Molecule 15 is water.

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

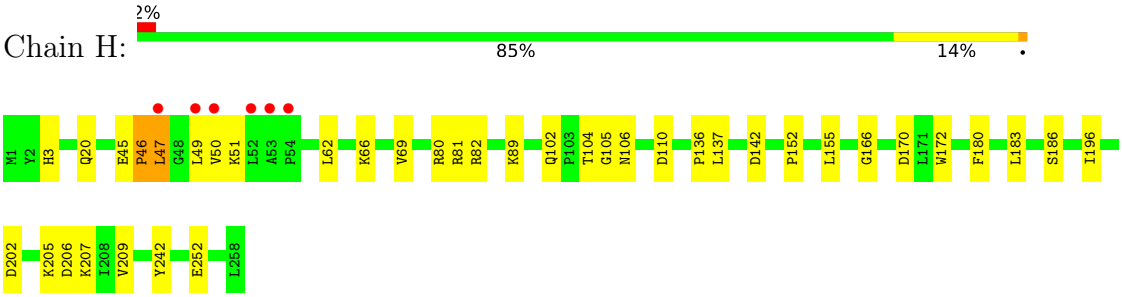
3 Residue-property plots (i)

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.

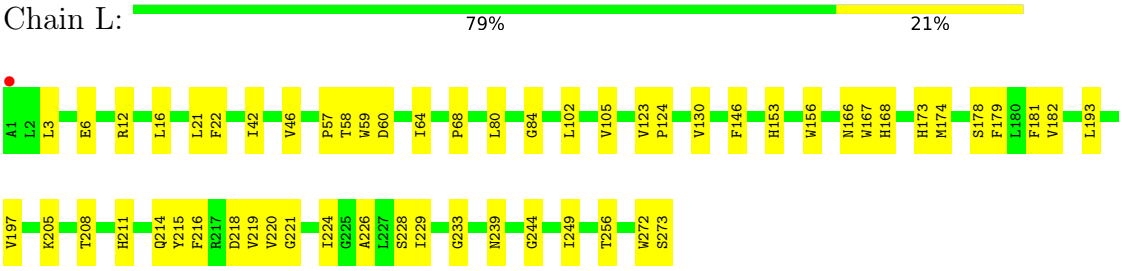
• Molecule 1: Photosynthetic reaction center cytochrome c subunit



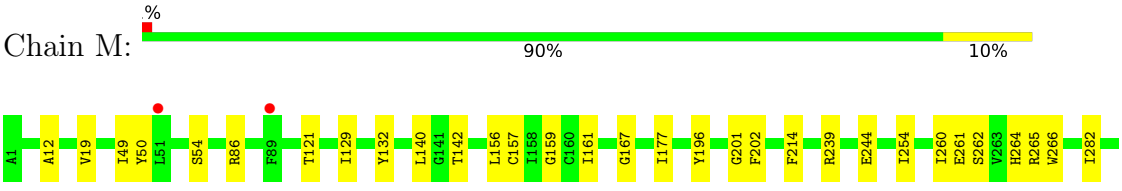
• Molecule 2: Reaction center protein H chain



• Molecule 3: Reaction center protein L chain



• Molecule 4: Reaction center protein M chain




W292
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	226.40Å 226.40Å 113.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.88 – 2.80 36.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.88-2.80) 99.9 (36.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0158, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.176 , 0.201 0.180 , 0.204	Depositor DCC
R_{free} test set	4562 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å^2)	75.4	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HTO, LDA, FME, HEC, MQ7, FE, BPB, SO4, NS5, 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	0.38	0/2669	0.59	0/3637
2	H	0.37	0/2055	0.58	0/2807
3	L	0.34	0/2612	0.54	0/3568
4	M	0.35	0/3101	0.51	0/4242
All	All	0.36	0/10437	0.55	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

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	53	0
2	H	2018	0	2020	40	0
3	L	2508	0	2390	51	0
4	M	2977	0	2832	28	0
5	C	172	0	120	3	0
6	C	37	0	58	0	0
7	C	5	0	0	0	0
7	H	20	0	0	0	0
7	M	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	48	0	93	2	0
8	L	16	0	31	1	0
9	H	10	0	16	0	0
9	L	10	0	16	0	0
10	L	330	0	360	13	0
10	M	132	0	144	4	0
11	L	130	0	148	8	0
11	M	65	0	74	5	0
12	M	2	0	0	0	0
13	M	96	0	128	2	0
14	M	40	0	60	3	0
15	C	3	0	0	0	0
15	H	2	0	0	0	0
15	L	4	0	0	0	0
15	M	4	0	0	0	0
All	All	11266	0	11068	167	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 7.

All (167) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLY:CA	1:C:19:MET:HE2	1.69	1.21
1:C:13:GLY:HA3	1:C:19:MET:HE2	1.17	1.08
2:H:89:LYS:HE2	2:H:110:ASP:CB	1.96	0.95
2:H:89:LYS:HE2	2:H:110:ASP:HB2	1.55	0.86
1:C:13:GLY:HA3	1:C:19:MET:CE	2.05	0.86
2:H:152:PRO:HA	2:H:155:LEU:HD13	1.60	0.80
1:C:13:GLY:CA	1:C:19:MET:CE	2.59	0.79
11:M:404:BPB:HHC	11:M:404:BPB:HBBB	1.66	0.78
4:M:54:SER:HB3	4:M:129:ILE:HD11	1.64	0.77
1:C:20:GLY:N	1:C:245:THR:HG21	1.99	0.77
1:C:200:GLN:HE21	1:C:201:VAL:H	1.31	0.77
2:H:205:LYS:HD3	2:H:205:LYS:H	1.48	0.76
1:C:52:VAL:HA	1:C:55:VAL:HG12	1.68	0.75
3:L:233:GLY:HA3	4:M:214[A]:PHE:CZ	2.23	0.74
3:L:208:THR:HG22	3:L:211:HIS:ND1	2.04	0.72
1:C:110:MET:O	1:C:114:THR:HG23	1.88	0.72
1:C:243:ASN:OD1	1:C:245:THR:HB	1.89	0.72
1:C:200:GLN:HE21	1:C:201:VAL:N	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:233:GLY:HA3	4:M:214[A]:PHE:CE1	2.27	0.69
1:C:20:GLY:H	1:C:245:THR:HG21	1.55	0.69
1:C:204:VAL:HG11	1:C:254:GLU:HB3	1.76	0.68
1:C:204:VAL:CG1	1:C:254:GLU:HB3	2.24	0.68
1:C:169:ARG:HG3	1:C:169:ARG:HH11	1.58	0.67
1:C:13:GLY:N	1:C:19:MET:HE2	2.09	0.67
1:C:46:LYS:HD3	1:C:47:ALA:H	1.59	0.66
2:H:47:LEU:C	2:H:47:LEU:HD13	2.21	0.65
1:C:46:LYS:HA	1:C:46:LYS:HE2	1.77	0.65
2:H:89:LYS:HE2	2:H:110:ASP:HB3	1.77	0.63
3:L:42:ILE:O	3:L:46:VAL:HG12	1.98	0.63
2:H:252:GLU:OE2	2:H:252:GLU:N	2.27	0.63
8:H:701:LDA:HM11	8:L:305:LDA:HM21	1.81	0.62
1:C:201:VAL:O	1:C:229:THR:HG21	2.01	0.60
2:H:205:LYS:H	2:H:205:LYS:CD	2.14	0.60
1:C:18:SER:HB2	3:L:156[B]:TRP:CD1	2.37	0.60
2:H:89:LYS:HZ3	2:H:106:ASN:C	2.11	0.59
2:H:45:GLU:HG3	2:H:46:PRO:HD2	1.85	0.58
3:L:166[B]:ASN:OD1	3:L:168[B]:HIS:HB2	2.04	0.58
1:C:52:VAL:HA	1:C:55:VAL:CG1	2.34	0.58
4:M:54:SER:HB3	4:M:129:ILE:CD1	2.33	0.58
1:C:19:MET:HB3	1:C:245:THR:HG23	1.86	0.57
3:L:197:VAL:HA	4:M:140:LEU:HD22	1.85	0.57
2:H:89:LYS:HZ2	2:H:105:GLY:C	2.12	0.56
1:C:161:THR:HG21	3:L:273:SER:O	2.05	0.56
3:L:60:ASP:O	3:L:64:ILE:HD12	2.06	0.56
3:L:224:ILE:HG12	3:L:228:SER:HB2	1.86	0.56
3:L:181:PHE:HB3	11:M:404:BPB:HBBA	1.87	0.56
1:C:34:ARG:HD2	1:C:35:ASP:OD1	2.06	0.54
1:C:323:LYS:HD3	1:C:323:LYS:H	1.72	0.54
1:C:82:SER:HB2	1:C:85:GLU:HB2	1.89	0.54
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.43	0.54
1:C:109:ARG:HH11	1:C:281:TYR:HA	1.73	0.54
1:C:169:ARG:HG3	1:C:169:ARG:NH1	2.21	0.54
2:H:136:PRO:HA	2:H:172:TRP:HA	1.89	0.53
4:M:196[B]:TYR:O	4:M:292:TRP:HB3	2.08	0.53
1:C:114:THR:HG21	5:C:402:HEC:HHC	1.90	0.53
1:C:225:ASP:O	1:C:229:THR:HG23	2.08	0.52
3:L:215:TYR:O	3:L:219:VAL:HG12	2.10	0.52
1:C:102:TYR:CG	1:C:103:PRO:HD3	2.45	0.51
3:L:16:LEU:HD11	3:L:105:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:168[B]:HIS:CE1	10:L:301[B]:BCB:HMC2	2.45	0.51
2:H:155:LEU:HD23	2:H:206:ASP:C	2.35	0.51
10:L:304:BCB:HHC	10:L:304:BCB:HBB2	1.92	0.51
2:H:196:ILE:HD12	2:H:242:TYR:CZ	2.45	0.51
2:H:202:ASP:HB3	2:H:209:VAL:HB	1.92	0.51
3:L:181:PHE:HB3	11:M:404:BPB:CBB	2.40	0.51
3:L:80:LEU:HA	3:L:84:GLY:HA3	1.93	0.51
2:H:142:ASP:OD1	2:H:142:ASP:N	2.36	0.51
4:M:159:GLY:HA3	14:M:405:NS5:H272	1.91	0.51
3:L:226:ALA:O	3:L:229:ILE:HG22	2.11	0.51
4:M:260[B]:ILE:O	4:M:264[B]:HIS:ND1	2.36	0.50
1:C:99:GLU:HG2	1:C:104:TYR:CE1	2.45	0.50
4:M:157:CYS:HA	4:M:161:ILE:HB	1.92	0.50
1:C:20:GLY:N	1:C:245:THR:CG2	2.72	0.50
4:M:121:THR:HG23	4:M:156:LEU:HD21	1.94	0.50
3:L:214:GLN:HG2	4:M:19:VAL:HB	1.94	0.49
5:C:402:HEC:HHA	5:C:402:HEC:O1D	2.13	0.49
2:H:89:LYS:HB2	2:H:104:THR:OG1	2.12	0.49
10:L:301[B]:BCB:H2C	10:M:403[B]:BCB:H2C	1.95	0.49
10:L:304:BCB:HBB3	10:M:403[A]:BCB:H62	1.95	0.49
3:L:178[A]:SER:O	3:L:182:VAL:HG12	2.13	0.48
1:C:46:LYS:HD3	1:C:47:ALA:N	2.25	0.48
2:H:166:GLY:HA3	2:H:186:SER:O	2.14	0.48
2:H:45:GLU:HG3	2:H:46:PRO:CD	2.43	0.48
2:H:66:LYS:NZ	4:M:261[B]:GLU:OE2	2.47	0.48
3:L:174[B]:MET:HA	10:L:304:BCB:OBD	2.14	0.48
10:L:301[B]:BCB:H143	11:L:303[B]:BPB:H5A	1.96	0.48
1:C:18:SER:HB2	3:L:156[A]:TRP:CD1	2.49	0.47
10:L:301[A]:BCB:H202	13:M:402[A]:MQ7:H261	1.96	0.47
3:L:179:PHE:CD2	3:L:239[B]:ASN:HB3	2.49	0.47
3:L:233:GLY:CA	4:M:214[A]:PHE:CZ	2.96	0.47
2:H:47:LEU:C	2:H:47:LEU:CD1	2.86	0.47
3:L:181:PHE:CD2	11:M:404:BPB:HBB	2.50	0.47
3:L:174[A]:MET:HE3	10:L:304:BCB:HED2	1.96	0.47
1:C:102:TYR:CD2	1:C:103:PRO:HD3	2.50	0.47
2:H:69:VAL:CG2	3:L:205:LYS:HA	2.45	0.47
4:M:132:TYR:CE2	4:M:142:THR:HG21	2.51	0.47
10:M:403[B]:BCB:HBD	10:M:403[B]:BCB:HAA1	1.97	0.46
10:L:302[B]:BCB:OBD	4:M:201[B]:GLY:HA2	2.15	0.46
2:H:62:LEU:O	8:H:707:LDA:HM21	2.16	0.46
2:H:80:ARG:NH2	2:H:82:ARG:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:303[A]:BPB:HEDB	4:M:254:ILE:HG21	1.96	0.46
2:H:49:LEU:O	2:H:51:LYS:N	2.50	0.45
1:C:109:ARG:NH1	1:C:281:TYR:HA	2.32	0.45
2:H:47:LEU:CD1	2:H:49:LEU:HB3	2.46	0.45
2:H:196:ILE:HD12	2:H:242:TYR:CE1	2.50	0.45
4:M:265[B]:ARG:NH1	7:M:408:SO4:O1	2.45	0.45
3:L:244[A]:GLY:O	10:L:301[A]:BCB:HED3	2.16	0.45
2:H:137:LEU:HB2	2:H:170:ASP:OD1	2.16	0.45
4:M:239:ARG:HD3	4:M:244[B]:GLU:HG2	1.99	0.45
2:H:80:ARG:CZ	2:H:82:ARG:HD2	2.47	0.44
2:H:89:LYS:CD	2:H:105:GLY:H	2.31	0.44
4:M:262[B]:SER:O	4:M:266[B]:TRP:HD1	2.00	0.44
1:C:71:LEU:O	1:C:75:THR:HG23	2.17	0.44
3:L:3:LEU:HB2	3:L:6:GLU:HB2	1.99	0.44
3:L:146:PHE:HB3	3:L:156[A]:TRP:CD2	2.53	0.44
1:C:22:VAL:HG22	3:L:256:THR:HG22	2.00	0.44
3:L:153[B]:HIS:HD2	10:L:302[B]:BCB:HMC3	1.82	0.44
3:L:146:PHE:HB3	3:L:156[B]:TRP:CE3	2.53	0.44
2:H:81:ARG:HD2	2:H:81:ARG:H	1.83	0.44
14:M:405:NS5:H18	14:M:405:NS5:H161	1.82	0.44
3:L:244[B]:GLY:O	10:L:301[B]:BCB:HED3	2.17	0.43
11:L:303[B]:BPB:OBB	11:L:303[B]:BPB:HHC	2.18	0.43
1:C:35:ASP:OD2	1:C:316:LEU:HA	2.19	0.43
11:L:303[A]:BPB:OBB	11:L:303[A]:BPB:HHC	2.18	0.43
3:L:130:VAL:HG13	3:L:249:ILE:HG12	2.01	0.43
1:C:176:LEU:HD11	1:C:187:TYR:O	2.19	0.43
4:M:254:ILE:HD11	13:M:402[A]:MQ7:H142	2.01	0.43
2:H:20:GLN:HG2	4:M:202[A]:PHE:CE2	2.53	0.43
3:L:221:GLY:N	4:M:49:ILE:HD13	2.34	0.43
14:M:405:NS5:H29	14:M:405:NS5:H271	1.86	0.43
1:C:19:MET:HA	1:C:245:THR:HG21	2.00	0.42
1:C:204:VAL:HG13	1:C:254:GLU:HB3	2.01	0.42
2:H:89:LYS:HD2	2:H:105:GLY:H	1.84	0.42
4:M:239:ARG:HD3	4:M:244[A]:GLU:HG2	1.99	0.42
1:C:161:THR:OG1	1:C:162:HIS:N	2.52	0.42
3:L:16:LEU:HD11	3:L:105:VAL:HG23	2.01	0.42
1:C:15:ARG:HD2	3:L:68:PRO:O	2.19	0.42
3:L:102:LEU:O	3:L:105:VAL:HG22	2.20	0.42
10:L:301[B]:BCB:H192	10:L:301[B]:BCB:H162	1.75	0.42
4:M:282:ILE:HD11	10:M:403[B]:BCB:OBD	2.20	0.42
2:H:183:LEU:HB2	2:H:196:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:124:PRO:HD3	11:L:303[A]:BPB:HAC	2.01	0.42
1:C:56:TYR:HB3	5:C:401:HEC:O2A	2.20	0.42
1:C:9:THR:HA	1:C:21:GLU:O	2.19	0.41
1:C:217:GLY:HA2	4:M:167:GLY:O	2.20	0.41
1:C:323:LYS:H	1:C:323:LYS:CD	2.32	0.41
1:C:224:SER:HA	1:C:227:TYR:HD1	1.85	0.41
3:L:21:LEU:HD12	3:L:22:PHE:CE2	2.55	0.41
2:H:180:PHE:CE2	4:M:12:ALA:HB2	2.56	0.41
1:C:18:SER:HB2	3:L:156[B]:TRP:NE1	2.35	0.41
3:L:58:THR:OG1	3:L:59:TRP:N	2.54	0.41
3:L:193:LEU:HD22	3:L:216:PHE:HE2	1.84	0.41
11:L:303[A]:BPB:HMBB	11:L:303[A]:BPB:HBBB	2.03	0.41
11:L:303[B]:BPB:H7A	11:L:303[B]:BPB:H11A	1.89	0.41
2:H:45:GLU:O	2:H:47:LEU:N	2.54	0.41
2:H:155:LEU:HD23	2:H:207:LYS:N	2.36	0.41
3:L:123:VAL:HG22	3:L:124:PRO:HD3	2.02	0.41
3:L:218:ASP:O	4:M:50:TYR:HB3	2.20	0.41
2:H:47:LEU:HD12	2:H:49:LEU:HB3	2.02	0.41
2:H:102:GLN:HE21	3:L:12:ARG:HD3	1.86	0.40
3:L:220:VAL:HG11	11:M:404:BPB:HEDA	2.04	0.40
1:C:212:VAL:HG22	2:H:3:HIS:CD2	2.56	0.40
3:L:146:PHE:HB3	3:L:156[B]:TRP:CD2	2.55	0.40
3:L:272:TRP:CE2	4:M:86:ARG:HG3	2.56	0.40
1:C:70:PHE:CZ	1:C:74:MET:HE3	2.56	0.40
3:L:42:ILE:HG12	11:L:303[B]:BPB:H6A	2.02	0.40
3:L:167[A]:TRP:HE1	3:L:173[A]:HIS:CD2	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	330/336 (98%)	319 (97%)	11 (3%)	0	100	100
2	H	256/258 (99%)	245 (96%)	8 (3%)	3 (1%)	10	34
3	L	312/273 (114%)	298 (96%)	13 (4%)	1 (0%)	36	66
4	M	372/323 (115%)	358 (96%)	13 (4%)	1 (0%)	36	66
All	All	1270/1190 (107%)	1220 (96%)	45 (4%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	47	LEU
2	H	50	VAL
2	H	46	PRO
4	M	177	ILE
3	L	57	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	281/282 (100%)	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 (9) such sidechains are listed below:

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

5.3.3 RNA (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	1.01	0	7,9,11	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	1/7/9/11	-

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	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	SO4	H	704	-	4,4,4	0.12	0	6,6,6	0.14	0
10	BCB	L	304	4	68,74,74	1.96	16 (23%)	79,115,115	3.28	25 (31%)
7	SO4	H	702	-	4,4,4	0.21	0	6,6,6	0.28	0
8	LDA	H	706	-	12,15,15	0.38	0	14,17,17	0.79	0
14	NS5	M	405	-	39,39,39	1.38	1 (2%)	44,46,46	2.04	12 (27%)
7	SO4	C	406	-	4,4,4	0.24	0	6,6,6	0.18	0
7	SO4	M	412	-	4,4,4	0.22	0	6,6,6	0.14	0
7	SO4	M	411	-	4,4,4	0.32	0	6,6,6	0.33	0
10	BCB	M	403[A]	4	68,74,74	2.04	16 (23%)	79,115,115	3.26	26 (32%)
7	SO4	M	407	-	4,4,4	0.11	0	6,6,6	0.14	0
10	BCB	L	301[B]	3	68,74,74	2.06	16 (23%)	79,115,115	3.19	29 (36%)
11	BPB	M	404	-	57,70,70	2.68	13 (22%)	56,101,101	2.83	20 (35%)
10	BCB	L	302[B]	3	68,74,74	2.02	17 (25%)	79,115,115	3.04	28 (35%)
9	HTO	L	306	-	9,9,9	0.75	0	10,10,10	0.89	1 (10%)
5	HEC	C	404	1	50,50,50	1.45	6 (12%)	68,82,82	1.57	14 (20%)
7	SO4	M	409	-	4,4,4	0.26	0	6,6,6	0.21	0
11	BPB	L	303[A]	-	57,70,70	2.65	14 (24%)	56,101,101	2.88	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SO4	M	410	-	4,4,4	0.27	0	6,6,6	0.24	0
10	BCB	M	403[B]	4	68,74,74	2.01	16 (23%)	79,115,115	3.28	30 (37%)
7	SO4	M	408	-	4,4,4	0.20	0	6,6,6	0.26	0
9	HTO	H	708	-	9,9,9	0.79	0	10,10,10	0.79	0
13	MQ7	M	402[A]	-	49,49,49	1.54	2 (4%)	60,63,63	1.49	10 (16%)
7	SO4	H	705	-	4,4,4	0.15	0	6,6,6	0.15	0
5	HEC	C	403	1	50,50,50	1.39	6 (12%)	68,82,82	1.74	13 (19%)
7	SO4	M	406	-	4,4,4	0.13	0	6,6,6	0.41	0
5	HEC	C	401	1	50,50,50	1.39	6 (12%)	68,82,82	1.64	15 (22%)
7	SO4	H	703	-	4,4,4	0.22	0	6,6,6	0.19	0
5	HEC	C	402	1	50,50,50	1.36	6 (12%)	68,82,82	1.59	10 (14%)
8	LDA	H	701	-	12,15,15	0.36	0	14,17,17	0.68	0
8	LDA	L	305	-	12,15,15	0.37	0	14,17,17	0.73	0
11	BPB	L	303[B]	-	57,70,70	2.70	14 (24%)	56,101,101	2.80	19 (33%)
10	BCB	L	301[A]	3	68,74,74	2.07	16 (23%)	79,115,115	3.26	28 (35%)
13	MQ7	M	402[B]	-	49,49,49	1.46	2 (4%)	60,63,63	1.38	10 (16%)
6	DGA	C	405	1	36,36,43	1.17	3 (8%)	38,38,45	1.22	4 (10%)
10	BCB	L	302[A]	3	68,74,74	1.95	16 (23%)	79,115,115	3.13	29 (36%)
8	LDA	H	707	-	12,15,15	0.31	0	14,17,17	1.17	1 (7%)

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
10	BCB	L	304	4	3/3/21/26	18/41/137/137	-
8	LDA	H	706	-	-	6/13/13/13	-
14	NS5	M	405	-	-	10/43/43/43	-
10	BCB	M	403[A]	4	3/3/21/26	13/41/137/137	-
11	BPB	M	404	-	-	8/37/105/105	0/5/6/6
10	BCB	L	301[B]	3	3/3/21/26	11/41/137/137	-
10	BCB	L	302[B]	3	2/2/21/26	11/41/137/137	-
9	HTO	L	306	-	-	4/10/10/10	-
5	HEC	C	404	1	1/1/3/7	7/14/54/54	-
11	BPB	L	303[A]	-	-	8/37/105/105	0/5/6/6
10	BCB	M	403[B]	4	3/3/21/26	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTO	H	708	-	-	1/10/10/10	-
13	MQ7	M	402[A]	-	-	0/41/61/61	0/2/2/2
5	HEC	C	403	1	1/1/3/7	4/14/54/54	-
5	HEC	C	401	1	1/1/3/7	7/14/54/54	-
5	HEC	C	402	1	1/1/3/7	7/14/54/54	-
8	LDA	H	701	-	-	4/13/13/13	-
8	LDA	L	305	-	-	6/13/13/13	-
11	BPB	L	303[B]	-	-	7/37/105/105	0/5/6/6
10	BCB	L	301[A]	3	3/3/21/26	7/41/137/137	-
13	MQ7	M	402[B]	-	-	2/41/61/61	0/2/2/2
10	BCB	L	302[A]	3	2/2/21/26	6/41/137/137	-
6	DGA	C	405	1	-	15/37/37/45	-
8	LDA	H	707	-	-	11/13/13/13	-

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	303[A]	BPB	C1B-C2B	9.26	1.49	1.39
11	L	303[B]	BPB	C1B-C2B	9.23	1.49	1.39
11	M	404	BPB	C1B-C2B	8.85	1.49	1.39
13	M	402[B]	MQ7	C3-C2	8.26	1.50	1.35
13	M	402[A]	MQ7	C3-C2	8.08	1.50	1.35
11	L	303[B]	BPB	C1D-C2D	7.68	1.48	1.39
11	M	404	BPB	CAC-C3C	7.34	1.52	1.33
14	M	405	NS5	C35-C36	7.33	1.53	1.32
11	L	303[A]	BPB	CAC-C3C	7.31	1.52	1.33
11	L	303[B]	BPB	CAC-C3C	7.30	1.52	1.33
11	L	303[A]	BPB	C1D-C2D	7.12	1.47	1.39
11	M	404	BPB	C1D-C2D	7.12	1.47	1.39
10	M	403[A]	BCB	CAC-C3C	6.25	1.50	1.33
10	L	301[A]	BCB	CAC-C3C	6.13	1.50	1.33
10	L	302[A]	BCB	CAC-C3C	6.07	1.50	1.33
10	M	403[B]	BCB	CAC-C3C	5.98	1.49	1.33
10	L	301[B]	BCB	CAC-C3C	5.97	1.49	1.33
10	L	302[B]	BCB	CAC-C3C	5.92	1.49	1.33
11	L	303[A]	BPB	C4D-CHA	5.77	1.48	1.39
11	M	404	BPB	C4D-CHA	5.73	1.48	1.39
10	L	304	BCB	CAC-C3C	5.70	1.49	1.33
11	L	303[B]	BPB	C3B-C2B	5.66	1.49	1.39
10	M	403[B]	BCB	O2D-CGD	5.55	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	403[A]	BCB	O2D-CGD	5.46	1.46	1.33
10	L	301[B]	BCB	O2D-CGD	5.46	1.46	1.33
10	L	301[A]	BCB	O2D-CGD	5.44	1.46	1.33
11	M	404	BPB	O2A-CGA	5.35	1.49	1.33
13	M	402[A]	MQ7	C10-C5	5.33	1.49	1.40
11	L	303[B]	BPB	C4D-CHA	5.21	1.47	1.39
11	L	303[B]	BPB	O2D-CGD	5.19	1.45	1.33
10	L	301[A]	BCB	CHC-C1C	5.17	1.49	1.37
11	L	303[A]	BPB	C3B-C2B	5.08	1.48	1.39
10	L	301[B]	BCB	CHC-C1C	5.08	1.49	1.37
11	L	303[A]	BPB	O2D-CGD	5.07	1.45	1.33
11	L	303[B]	BPB	C3D-C2D	5.04	1.48	1.39
11	M	404	BPB	C3D-C2D	5.03	1.48	1.39
11	L	303[B]	BPB	OBD-CAD	4.98	1.29	1.22
11	M	404	BPB	O2D-CGD	4.96	1.45	1.33
10	L	302[B]	BCB	O2D-CGD	4.90	1.45	1.33
11	L	303[A]	BPB	C3D-C2D	4.87	1.48	1.39
10	M	403[A]	BCB	C3B-C4B	4.86	1.50	1.41
10	L	301[B]	BCB	C3B-C4B	4.84	1.50	1.41
10	L	304	BCB	O2D-CGD	4.83	1.45	1.33
10	L	302[B]	BCB	C3B-C4B	4.80	1.50	1.41
10	L	301[A]	BCB	C3B-C4B	4.78	1.50	1.41
11	M	404	BPB	C3B-C2B	4.75	1.47	1.39
11	M	404	BPB	OBD-CAD	4.73	1.28	1.22
10	L	302[B]	BCB	CHC-C1C	4.73	1.48	1.37
10	L	302[A]	BCB	O2D-CGD	4.72	1.44	1.33
5	C	404	HEC	FE-ND	4.72	2.09	1.94
10	L	302[A]	BCB	C3B-C4B	4.67	1.49	1.41
13	M	402[B]	MQ7	C10-C5	4.62	1.48	1.40
10	M	403[B]	BCB	C3B-C4B	4.60	1.49	1.41
5	C	401	HEC	FE-ND	4.58	2.09	1.94
10	M	403[A]	BCB	CHC-C1C	4.54	1.47	1.37
10	L	301[B]	BCB	C2C-C3C	-4.50	1.45	1.51
10	L	301[A]	BCB	C2C-C3C	-4.45	1.46	1.51
10	L	304	BCB	CHC-C4B	4.39	1.49	1.39
10	L	302[B]	BCB	O2A-CGA	4.38	1.46	1.33
10	L	302[A]	BCB	CHC-C1C	4.36	1.47	1.37
10	L	304	BCB	C2C-C3C	-4.33	1.46	1.51
10	M	403[A]	BCB	O2A-CGA	4.33	1.46	1.33
10	L	301[A]	BCB	O2A-CGA	4.32	1.46	1.33
11	L	303[A]	BPB	OBD-CAD	4.31	1.28	1.22
10	L	304	BCB	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	301[A]	BCB	CHC-C4B	4.24	1.48	1.39
10	L	301[B]	BCB	O2A-CGA	4.23	1.45	1.33
10	L	304	BCB	CHC-C1C	4.19	1.47	1.37
11	L	303[A]	BPB	O2A-CGA	4.19	1.45	1.33
10	L	304	BCB	C3B-C4B	4.11	1.48	1.41
11	L	303[B]	BPB	O2A-CGA	4.11	1.45	1.33
10	L	302[B]	BCB	CHC-C4B	4.10	1.48	1.39
10	L	302[B]	BCB	OBD-CAD	4.09	1.29	1.22
10	M	403[B]	BCB	CHC-C1C	4.07	1.46	1.37
5	C	402	HEC	FE-ND	4.05	2.07	1.94
10	M	403[B]	BCB	O2A-CGA	4.05	1.45	1.33
10	M	403[B]	BCB	OBD-CAD	4.02	1.29	1.22
10	L	301[B]	BCB	OBD-CAD	4.01	1.29	1.22
10	L	302[B]	BCB	CHD-C1D	4.00	1.46	1.38
10	M	403[A]	BCB	CHC-C4B	3.99	1.48	1.39
10	L	302[A]	BCB	C2C-C3C	-3.98	1.46	1.51
10	L	301[B]	BCB	CHD-C1D	3.96	1.46	1.38
10	L	304	BCB	CHB-C1B	3.95	1.48	1.39
10	M	403[A]	BCB	C3D-C2D	3.95	1.49	1.39
10	L	302[A]	BCB	O2A-CGA	3.92	1.44	1.33
11	L	303[A]	BPB	C3B-C4B	3.92	1.48	1.41
10	L	301[B]	BCB	CHC-C4B	3.90	1.48	1.39
10	L	302[A]	BCB	CHC-C4B	3.88	1.48	1.39
10	L	302[A]	BCB	CHD-C1D	3.86	1.45	1.38
11	L	303[B]	BPB	C3B-C4B	3.86	1.48	1.41
10	L	301[A]	BCB	OBD-CAD	3.86	1.29	1.22
10	L	304	BCB	C3D-C2D	3.82	1.49	1.39
10	M	403[B]	BCB	CHD-C1D	3.81	1.45	1.38
10	L	301[A]	BCB	C3D-C2D	3.81	1.49	1.39
10	M	403[A]	BCB	CHD-C1D	3.80	1.45	1.38
10	M	403[B]	BCB	C2C-C3C	-3.79	1.46	1.51
10	M	403[A]	BCB	OBD-CAD	3.75	1.28	1.22
5	C	403	HEC	FE-ND	3.75	2.06	1.94
11	M	404	BPB	C3B-C4B	3.74	1.48	1.41
10	L	302[B]	BCB	C2C-C3C	-3.73	1.46	1.51
10	L	302[A]	BCB	OBD-CAD	3.72	1.28	1.22
10	M	403[B]	BCB	CHC-C4B	3.71	1.47	1.39
10	L	301[A]	BCB	CHD-C1D	3.70	1.45	1.38
10	L	304	BCB	CHD-C1D	3.68	1.45	1.38
10	M	403[B]	BCB	C3D-C2D	3.63	1.49	1.39
11	M	404	BPB	CHA-CBD	-3.61	1.47	1.51
10	M	403[A]	BCB	C2C-C3C	-3.58	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	301[B]	BCB	CHB-C1B	3.55	1.47	1.39
10	L	301[A]	BCB	C1D-ND	-3.53	1.33	1.37
10	L	302[B]	BCB	CHB-C1B	3.53	1.47	1.39
10	L	302[B]	BCB	CHD-C4C	3.52	1.47	1.39
10	L	302[A]	BCB	CHB-C1B	3.50	1.47	1.39
5	C	404	HEC	FE-NA	3.50	2.07	1.95
10	M	403[A]	BCB	CHB-C1B	3.50	1.47	1.39
10	L	301[A]	BCB	CHB-C1B	3.46	1.47	1.39
5	C	401	HEC	FE-NA	3.45	2.06	1.95
11	M	404	BPB	C4C-NC	-3.41	1.27	1.37
10	L	302[A]	BCB	C3D-C2D	3.41	1.48	1.39
10	M	403[B]	BCB	CHB-C1B	3.37	1.47	1.39
5	C	403	HEC	FE-NB	3.37	2.05	1.94
5	C	402	HEC	FE-NA	3.35	2.06	1.95
10	L	304	BCB	OBD-CAD	3.35	1.28	1.22
5	C	404	HEC	FE-NC	3.35	2.06	1.95
5	C	403	HEC	FE-NA	3.34	2.06	1.95
10	L	302[B]	BCB	C3D-C2D	3.32	1.48	1.39
5	C	402	HEC	FE-NC	3.27	2.06	1.95
10	L	301[B]	BCB	C3D-C2D	3.27	1.48	1.39
5	C	402	HEC	FE-NB	3.27	2.05	1.94
5	C	401	HEC	FE-NC	3.24	2.06	1.95
5	C	403	HEC	FE-NC	3.18	2.05	1.95
11	L	303[A]	BPB	C3A-C2A	-3.13	1.51	1.54
6	C	405	DGA	OG1-CA1	3.12	1.42	1.33
11	L	303[B]	BPB	C4C-NC	-3.10	1.28	1.37
10	L	301[B]	BCB	C1D-ND	-3.10	1.34	1.37
6	C	405	DGA	OG2-CB1	3.08	1.43	1.34
11	L	303[A]	BPB	C4C-NC	-3.07	1.28	1.37
10	L	304	BCB	CHD-C4C	3.02	1.46	1.39
10	L	302[A]	BCB	CHD-C4C	3.00	1.46	1.39
11	L	303[A]	BPB	CHA-CBD	-2.94	1.48	1.51
10	M	403[B]	BCB	CHD-C4C	2.93	1.45	1.39
10	L	302[A]	BCB	C1B-C2B	2.90	1.50	1.43
10	M	403[B]	BCB	C1D-ND	-2.89	1.34	1.37
5	C	401	HEC	FE-NB	2.89	2.03	1.94
10	M	403[A]	BCB	CHD-C4C	2.85	1.45	1.39
11	L	303[B]	BPB	CHA-CBD	-2.85	1.48	1.51
10	L	301[B]	BCB	CHD-C4C	2.84	1.45	1.39
10	L	304	BCB	C1D-ND	-2.83	1.34	1.37
10	L	302[A]	BCB	C1D-ND	-2.81	1.34	1.37
6	C	405	DGA	OG2-CG2	-2.76	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	301[B]	BCB	C1B-C2B	2.75	1.49	1.43
10	L	302[B]	BCB	C1B-C2B	2.69	1.49	1.43
5	C	404	HEC	FE-NB	2.64	2.03	1.94
10	L	302[B]	BCB	C1D-ND	-2.58	1.34	1.37
11	L	303[B]	BPB	C3A-C2A	-2.56	1.52	1.54
10	M	403[B]	BCB	C1B-C2B	2.50	1.49	1.43
10	M	403[A]	BCB	C1D-ND	-2.49	1.34	1.37
10	M	403[A]	BCB	C1B-C2B	2.49	1.49	1.43
5	C	404	HEC	CAC-C3C	2.45	1.57	1.51
10	L	301[A]	BCB	CHD-C4C	2.41	1.44	1.39
10	L	301[A]	BCB	MG-NA	-2.37	2.00	2.06
5	C	403	HEC	CBA-CGA	2.35	1.56	1.50
10	M	403[B]	BCB	C4D-CHA	2.35	1.46	1.38
5	C	403	HEC	CAC-C3C	2.34	1.57	1.51
5	C	404	HEC	C4B-NB	-2.34	1.36	1.40
10	L	304	BCB	C1B-C2B	2.33	1.48	1.43
10	M	403[A]	BCB	C4D-CHA	2.32	1.46	1.38
10	L	301[A]	BCB	C1B-C2B	2.32	1.48	1.43
10	L	302[B]	BCB	MG-NA	-2.30	2.00	2.06
10	L	301[B]	BCB	C4D-CHA	2.22	1.46	1.38
10	L	301[B]	BCB	MG-NA	-2.22	2.01	2.06
10	L	302[A]	BCB	MG-NA	-2.22	2.01	2.06
11	L	303[B]	BPB	C4D-ND	2.22	1.41	1.38
10	M	403[A]	BCB	MG-NA	-2.21	2.01	2.06
10	L	302[B]	BCB	C3D-C4D	-2.16	1.39	1.44
10	L	302[A]	BCB	C4D-CHA	2.15	1.46	1.38
10	L	301[A]	BCB	C4D-CHA	2.15	1.46	1.38
5	C	402	HEC	CAC-C3C	2.14	1.56	1.51
5	C	401	HEC	CBD-CGD	2.10	1.55	1.50
11	L	303[A]	BPB	C4D-ND	2.08	1.41	1.38
10	M	403[B]	BCB	MG-NA	-2.06	2.01	2.06
10	L	304	BCB	C4D-CHA	2.05	1.45	1.38
10	L	302[B]	BCB	C4D-CHA	2.04	1.45	1.38
5	C	401	HEC	CAC-C3C	2.03	1.56	1.51
10	L	304	BCB	MG-NA	-2.02	2.01	2.06
5	C	402	HEC	CBA-CGA	2.01	1.55	1.50
11	M	404	BPB	C3A-C2A	-2.01	1.52	1.54

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	304	BCB	C1C-NC-C4C	-20.38	97.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403[A]	BCB	C1C-NC-C4C	-19.33	98.01	106.71
10	L	301[A]	BCB	C1C-NC-C4C	-19.17	98.09	106.71
10	L	301[B]	BCB	C1C-NC-C4C	-18.59	98.35	106.71
10	M	403[B]	BCB	C1C-NC-C4C	-18.47	98.40	106.71
10	L	302[A]	BCB	C1C-NC-C4C	-16.80	99.15	106.71
10	L	302[B]	BCB	C1C-NC-C4C	-15.13	99.90	106.71
10	L	301[A]	BCB	C2B-C1B-NB	10.37	117.19	110.23
10	L	302[B]	BCB	C2B-C1B-NB	9.82	116.82	110.23
10	L	301[B]	BCB	C2B-C1B-NB	9.76	116.78	110.23
10	L	302[A]	BCB	C2B-C1B-NB	9.53	116.62	110.23
11	M	404	BPB	O2D-CGD-CBD	9.05	122.46	111.00
11	L	303[A]	BPB	C2B-C1B-NB	8.78	115.59	109.53
10	M	403[B]	BCB	C2B-C1B-NB	8.77	116.11	110.23
10	L	304	BCB	C2B-C1B-NB	8.59	115.99	110.23
11	L	303[B]	BPB	C3D-C4D-ND	8.38	119.15	107.72
10	M	403[A]	BCB	C2B-C1B-NB	8.35	115.83	110.23
11	M	404	BPB	C3D-C4D-ND	8.22	118.92	107.72
11	L	303[A]	BPB	O2D-CGD-CBD	8.11	121.28	111.00
11	L	303[B]	BPB	C2B-C1B-NB	7.99	115.04	109.53
11	L	303[A]	BPB	C3D-C4D-ND	7.72	118.25	107.72
5	C	403	HEC	CBC-CAC-C3C	6.95	131.59	112.43
11	M	404	BPB	C2B-C1B-NB	6.90	114.29	109.53
10	M	403[B]	BCB	C4D-C3D-CAD	-6.87	100.00	108.10
11	L	303[B]	BPB	C4D-ND-C1D	-6.76	101.95	108.83
10	M	403[A]	BCB	C4D-C3D-CAD	-6.74	100.15	108.10
11	L	303[B]	BPB	O2D-CGD-CBD	6.66	119.44	111.00
11	L	303[A]	BPB	C4D-ND-C1D	-6.65	102.07	108.83
10	M	403[B]	BCB	O2D-CGD-CBD	6.62	123.02	111.27
11	M	404	BPB	C4D-ND-C1D	-6.60	102.12	108.83
10	M	403[A]	BCB	O2D-CGD-CBD	6.46	122.74	111.27
10	L	302[B]	BCB	CMD-C2D-C1D	6.44	136.07	124.71
10	L	304	BCB	C4D-C3D-CAD	-6.40	100.56	108.10
11	L	303[B]	BPB	CBC-CAC-C3C	-6.26	110.09	126.70
11	L	303[A]	BPB	CBC-CAC-C3C	-6.20	110.26	126.70
11	M	404	BPB	CBC-CAC-C3C	-6.09	110.53	126.70
10	L	302[A]	BCB	O2D-CGD-CBD	6.06	122.03	111.27
10	L	302[A]	BCB	C4D-C3D-CAD	-6.06	100.96	108.10
10	L	301[A]	BCB	C4D-C3D-CAD	-6.02	101.00	108.10
10	L	302[B]	BCB	O2D-CGD-CBD	5.88	121.71	111.27
10	L	302[A]	BCB	CMD-C2D-C1D	5.86	135.04	124.71
10	L	301[B]	BCB	C4D-C3D-CAD	-5.83	101.23	108.10
10	M	403[B]	BCB	CMD-C2D-C1D	5.58	134.55	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	302[B]	BCB	C4D-C3D-CAD	-5.58	101.52	108.10
10	L	302[B]	BCB	C3D-C4D-ND	5.55	119.22	110.24
14	M	405	NS5	C19-C20-C21	-5.52	119.44	127.31
10	L	301[B]	BCB	CMD-C2D-C1D	5.49	134.39	124.71
10	L	302[A]	BCB	C3D-C4D-ND	5.34	118.88	110.24
10	L	304	BCB	C3D-C4D-ND	5.34	118.87	110.24
10	L	302[B]	BCB	C1D-ND-C4D	-5.33	102.55	106.33
10	L	301[B]	BCB	C3D-C4D-ND	5.15	118.57	110.24
10	L	301[A]	BCB	C3D-C4D-ND	5.14	118.55	110.24
10	L	304	BCB	C1D-ND-C4D	-5.02	102.77	106.33
10	L	304	BCB	CMD-C2D-C1D	4.98	133.49	124.71
10	M	403[A]	BCB	C3D-C4D-ND	4.98	118.30	110.24
10	L	304	BCB	O2D-CGD-CBD	4.96	120.08	111.27
10	L	302[A]	BCB	C1D-ND-C4D	-4.95	102.82	106.33
10	L	301[B]	BCB	C1D-ND-C4D	-4.93	102.83	106.33
10	M	403[A]	BCB	CMD-C2D-C1D	4.87	133.29	124.71
10	M	403[B]	BCB	O2D-CGD-O1D	-4.87	114.33	123.84
10	M	403[B]	BCB	C3D-C4D-ND	4.83	118.05	110.24
10	L	301[A]	BCB	O2D-CGD-CBD	4.77	119.74	111.27
10	L	302[A]	BCB	C1-C2-C3	-4.64	118.02	126.04
10	L	301[B]	BCB	O2D-CGD-CBD	4.64	119.51	111.27
10	L	301[A]	BCB	C1D-ND-C4D	-4.57	103.09	106.33
10	M	403[B]	BCB	C4A-NA-C1A	4.50	108.73	106.71
10	L	301[A]	BCB	CMD-C2D-C1D	4.46	132.58	124.71
11	L	303[B]	BPB	OBD-CAD-C3D	-4.41	120.67	127.98
10	L	304	BCB	CHC-C1C-NC	-4.39	118.44	124.51
10	L	302[B]	BCB	C2C-C1C-CHC	-4.38	113.34	123.64
10	L	302[B]	BCB	CMD-C2D-C3D	-4.35	117.61	127.61
10	M	403[A]	BCB	C1D-ND-C4D	-4.33	103.26	106.33
5	C	402	HEC	C4A-NA-C1A	4.33	109.59	105.35
6	C	405	DGA	OG2-CB1-CB2	4.33	120.84	111.50
14	M	405	NS5	CM4-C36-C35	-4.26	110.32	122.65
11	L	303[B]	BPB	CMB-C2B-C3B	4.26	132.65	124.68
10	M	403[A]	BCB	O2D-CGD-O1D	-4.25	115.53	123.84
10	L	302[A]	BCB	C2C-C1C-CHC	-4.23	113.67	123.64
5	C	404	HEC	CAD-CBD-CGD	-4.16	104.65	113.60
10	L	304	BCB	C2C-C1C-CHC	-4.14	113.89	123.64
11	M	404	BPB	C2D-C1D-ND	4.13	112.38	109.53
10	M	403[B]	BCB	C2C-C1C-CHC	-4.12	113.95	123.64
11	L	303[A]	BPB	C2D-C1D-ND	4.12	112.37	109.53
10	L	302[B]	BCB	C1-C2-C3	-4.08	118.98	126.04
10	M	403[B]	BCB	C1D-ND-C4D	-4.07	103.44	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	405	NS5	C18-C17-C15	-4.06	121.52	127.31
10	M	403[A]	BCB	C2C-C1C-CHC	-4.06	114.09	123.64
5	C	402	HEC	C2A-C1A-NA	-4.03	106.40	110.32
10	L	301[A]	BCB	C4-C3-C5	4.00	122.01	115.27
5	C	401	HEC	CBC-CAC-C3C	3.96	123.34	112.43
10	L	301[A]	BCB	CHC-C1C-NC	-3.94	119.07	124.51
11	M	404	BPB	C1A-C2A-C3A	-3.93	99.10	102.84
14	M	405	NS5	C34-C35-C36	-3.92	114.34	127.75
5	C	404	HEC	C4B-NB-C1B	3.92	109.12	105.07
10	L	304	BCB	OBD-CAD-C3D	-3.90	119.13	128.52
11	L	303[A]	BPB	OBD-CAD-C3D	-3.90	121.51	127.98
10	L	301[B]	BCB	C2C-C1C-CHC	-3.88	114.50	123.64
10	L	301[A]	BCB	C2D-C1D-ND	3.88	112.96	110.10
10	M	403[A]	BCB	CAD-C3D-C2D	3.87	159.48	140.80
11	M	404	BPB	OBD-CAD-C3D	-3.86	121.57	127.98
14	M	405	NS5	CM3-C36-C35	-3.86	111.49	122.65
10	M	403[B]	BCB	CAD-C3D-C2D	3.81	159.18	140.80
10	L	304	BCB	CAD-C3D-C2D	3.80	159.13	140.80
10	L	302[A]	BCB	CAD-C3D-C2D	3.77	158.97	140.80
11	L	303[A]	BPB	CMB-C2B-C3B	3.76	131.71	124.68
5	C	401	HEC	C4A-NA-C1A	3.76	109.03	105.35
5	C	403	HEC	CBB-CAB-C3B	-3.75	102.09	112.43
10	L	302[A]	BCB	CMD-C2D-C3D	-3.74	119.02	127.61
5	C	401	HEC	C2A-C1A-NA	-3.72	106.70	110.32
10	L	301[A]	BCB	CAD-C3D-C2D	3.72	158.74	140.80
5	C	402	HEC	C1D-ND-C4D	3.71	108.90	105.07
11	L	303[B]	BPB	C2D-C1D-ND	3.70	112.08	109.53
5	C	403	HEC	C1D-ND-C4D	3.68	108.87	105.07
11	M	404	BPB	O2A-CGA-CBA	3.68	123.45	111.91
10	L	302[B]	BCB	CAD-C3D-C2D	3.67	158.52	140.80
10	M	403[B]	BCB	OBD-CAD-C3D	-3.65	119.73	128.52
10	L	301[B]	BCB	CAD-C3D-C2D	3.64	158.35	140.80
10	L	301[B]	BCB	C4-C3-C5	3.62	121.37	115.27
5	C	401	HEC	C1D-ND-C4D	3.62	108.81	105.07
14	M	405	NS5	C11-C10-C9	3.61	121.35	115.27
10	M	403[B]	BCB	CHC-C1C-NC	-3.60	119.54	124.51
10	M	403[B]	BCB	C1-C2-C3	-3.60	119.83	126.04
10	L	302[A]	BCB	O1D-CGD-CBD	-3.56	117.20	124.48
10	L	304	BCB	C2D-C1D-ND	3.53	112.71	110.10
10	L	301[A]	BCB	O2A-CGA-CBA	3.52	122.94	111.91
10	M	403[A]	BCB	C4A-NA-C1A	3.49	108.28	106.71
10	L	302[A]	BCB	OBD-CAD-C3D	-3.49	120.12	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	403[A]	BCB	CHC-C1C-NC	-3.49	119.69	124.51
5	C	404	HEC	C4A-NA-C1A	3.49	108.76	105.35
10	L	302[B]	BCB	OBD-CAD-C3D	-3.46	120.20	128.52
11	M	404	BPB	O1D-CGD-CBD	-3.44	119.00	124.74
10	L	301[A]	BCB	C2C-C1C-CHC	-3.44	115.55	123.64
11	M	404	BPB	CMC-C2C-C1C	-3.43	108.60	114.36
11	L	303[B]	BPB	CMD-C2D-C3D	-3.42	118.28	124.68
5	C	403	HEC	C4C-NC-C1C	3.40	108.68	105.35
5	C	401	HEC	C4C-NC-C1C	3.39	108.67	105.35
11	L	303[A]	BPB	C3D-CAD-CBD	3.39	112.06	107.61
10	M	403[A]	BCB	C1D-CHD-C4C	-3.36	118.81	126.06
11	L	303[A]	BPB	C3B-C4B-NB	3.35	113.05	108.04
11	L	303[B]	BPB	C3B-C4B-NB	3.35	113.05	108.04
10	M	403[A]	BCB	C2D-C1D-ND	3.33	112.56	110.10
10	L	301[B]	BCB	CMD-C2D-C3D	-3.33	119.95	127.61
10	L	301[B]	BCB	OBD-CAD-C3D	-3.33	120.51	128.52
10	L	301[B]	BCB	CHC-C1C-NC	-3.32	119.92	124.51
5	C	403	HEC	C4A-NA-C1A	3.30	108.58	105.35
10	M	403[B]	BCB	CMD-C2D-C3D	-3.30	120.03	127.61
10	L	302[B]	BCB	C6-C5-C3	-3.29	104.82	113.45
11	L	303[A]	BPB	C4A-C3A-C2A	-3.29	99.71	102.84
10	L	301[B]	BCB	C2D-C1D-ND	3.28	112.52	110.10
5	C	402	HEC	C4C-NC-C1C	3.27	108.55	105.35
5	C	402	HEC	C4B-NB-C1B	3.27	108.45	105.07
11	L	303[B]	BPB	CMC-C2C-C1C	-3.24	108.92	114.36
13	M	402[A]	MQ7	C39-C38-C40	3.24	120.72	115.27
10	M	403[B]	BCB	C1D-CHD-C4C	-3.24	119.08	126.06
5	C	401	HEC	CBA-CAA-C2A	-3.23	103.66	112.63
13	M	402[A]	MQ7	C29-C28-C30	3.17	120.61	115.27
10	L	301[A]	BCB	OBD-CAD-C3D	-3.14	120.95	128.52
5	C	402	HEC	C3D-C4D-ND	-3.14	107.31	110.36
11	M	404	BPB	C1-O2A-CGA	3.14	124.67	116.44
10	M	403[B]	BCB	CGD-CBD-CAD	-3.13	100.61	110.73
13	M	402[B]	MQ7	C39-C38-C40	3.12	120.52	115.27
5	C	402	HEC	CAD-CBD-CGD	-3.11	106.91	113.60
10	L	301[A]	BCB	CHD-C4C-C3C	-3.10	122.01	125.89
10	L	302[A]	BCB	CHB-C1B-NB	-3.05	121.02	124.26
11	M	404	BPB	C3B-C4B-NB	3.05	112.61	108.04
5	C	401	HEC	C4B-NB-C1B	3.05	108.23	105.07
10	L	302[B]	BCB	O2A-CGA-CBA	3.04	121.46	111.91
11	L	303[B]	BPB	O1D-CGD-CBD	-3.04	119.68	124.74
10	L	304	BCB	C1-C2-C3	-3.03	120.80	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	404	BPB	CMD-C2D-C3D	-3.01	119.05	124.68
5	C	401	HEC	CBD-CAD-C3D	-3.00	104.29	112.63
10	L	302[A]	BCB	C2D-C1D-ND	3.00	112.31	110.10
10	L	302[A]	BCB	C6-C5-C3	-3.00	105.60	113.45
10	L	301[A]	BCB	CMB-C2B-C3B	2.99	134.01	125.93
11	L	303[A]	BPB	CMD-C2D-C3D	-2.99	119.08	124.68
5	C	403	HEC	C4B-NB-C1B	2.98	108.15	105.07
10	L	301[B]	BCB	O2A-CGA-CBA	2.98	121.25	111.91
6	C	405	DGA	OG1-CA1-CA2	2.97	121.24	111.91
10	L	301[A]	BCB	O2D-CGD-O1D	-2.97	118.04	123.84
10	M	403[B]	BCB	C2D-C1D-ND	2.97	112.29	110.10
10	M	403[A]	BCB	OBD-CAD-C3D	-2.95	121.43	128.52
5	C	404	HEC	C4C-NC-C1C	2.95	108.23	105.35
14	M	405	NS5	C32-C31-C33	2.92	120.18	115.27
10	L	301[B]	BCB	O2D-CGD-O1D	-2.92	118.14	123.84
5	C	404	HEC	CBB-CAB-C3B	-2.90	104.42	112.43
10	L	301[B]	BCB	CHD-C4C-C3C	-2.90	122.26	125.89
10	L	302[B]	BCB	CHD-C1D-ND	-2.90	121.79	124.45
10	L	304	BCB	O2A-CGA-CBA	2.89	120.99	111.91
13	M	402[A]	MQ7	C34-C33-C35	2.89	120.14	115.27
5	C	401	HEC	C3D-C4D-ND	-2.89	107.56	110.36
10	L	304	BCB	C4-C3-C5	2.88	120.12	115.27
11	L	303[B]	BPB	CED-O2D-CGD	2.83	122.33	115.94
11	L	303[A]	BPB	O1D-CGD-CBD	-2.83	120.03	124.74
10	L	302[A]	BCB	C1D-CHD-C4C	-2.81	119.99	126.06
10	L	301[B]	BCB	CMB-C2B-C3B	2.81	133.51	125.93
13	M	402[B]	MQ7	C29-C28-C30	2.81	120.00	115.27
10	L	304	BCB	CMD-C2D-C3D	-2.80	121.16	127.61
5	C	402	HEC	CBA-CAA-C2A	-2.80	104.84	112.63
10	L	301[B]	BCB	C1-C2-C3	-2.80	121.20	126.04
10	M	403[A]	BCB	CMD-C2D-C3D	-2.80	121.17	127.61
11	L	303[A]	BPB	CMC-C2C-C1C	-2.80	109.66	114.36
10	L	301[A]	BCB	CHB-C4A-NA	2.78	128.35	124.51
6	C	405	DGA	OG2-CG2-CG1	2.76	112.52	106.13
11	L	303[A]	BPB	O2A-CGA-CBA	2.75	120.54	111.91
10	M	403[B]	BCB	CHB-C1B-NB	-2.75	121.35	124.26
5	C	403	HEC	C3D-C4D-ND	-2.75	107.69	110.36
10	M	403[A]	BCB	O2A-CGA-O1A	-2.74	116.67	123.59
5	C	403	HEC	CAA-CBA-CGA	-2.74	107.71	113.60
5	C	404	HEC	C1D-ND-C4D	2.74	107.90	105.07
13	M	402[A]	MQ7	C16-C17-C18	-2.73	121.09	127.66
10	L	301[B]	BCB	CHB-C1B-NB	-2.73	121.37	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	302[B]	BCB	CHB-C1B-NB	-2.72	121.37	124.26
13	M	402[B]	MQ7	C31-C32-C33	-2.72	121.11	127.66
11	M	404	BPB	O2D-CGD-O1D	-2.71	118.54	123.84
10	L	302[B]	BCB	O1D-CGD-CBD	-2.71	118.94	124.48
10	M	403[B]	BCB	CHB-C4A-NA	2.70	128.24	124.51
13	M	402[A]	MQ7	C19-C18-C20	2.70	119.81	115.27
11	L	303[A]	BPB	CMA-C3A-C4A	-2.69	108.47	114.38
10	L	302[A]	BCB	CHC-C1C-NC	-2.68	120.81	124.51
10	M	403[B]	BCB	C4B-C3B-C2B	-2.68	104.05	108.36
10	M	403[A]	BCB	C4B-C3B-C2B	-2.67	104.06	108.36
5	C	403	HEC	C2A-C1A-NA	-2.65	107.74	110.32
10	L	302[B]	BCB	C4B-C3B-C2B	-2.65	104.10	108.36
10	M	403[A]	BCB	CHB-C4A-NA	2.64	128.17	124.51
10	M	403[A]	BCB	O2A-CGA-CBA	2.64	120.20	111.91
10	L	304	BCB	CHA-C4D-ND	-2.64	126.98	132.50
11	M	404	BPB	C3D-CAD-CBD	2.64	111.08	107.61
11	L	303[A]	BPB	O2D-CGD-O1D	-2.63	118.69	123.84
5	C	402	HEC	CAC-C3C-C2C	2.62	131.06	126.86
5	C	404	HEC	C3D-C4D-ND	-2.62	107.82	110.36
10	L	302[A]	BCB	O2A-CGA-O1A	-2.60	117.03	123.59
13	M	402[A]	MQ7	C12-C11-C3	-2.59	105.05	112.05
10	L	304	BCB	C2A-C1A-CHA	-2.59	119.33	123.86
5	C	404	HEC	C2A-C1A-NA	-2.58	107.81	110.32
10	M	403[B]	BCB	CHA-C4D-ND	-2.58	127.11	132.50
13	M	402[B]	MQ7	C16-C17-C18	-2.57	121.46	127.66
5	C	402	HEC	CHA-C4D-C3D	2.57	128.62	124.84
10	L	302[A]	BCB	C4-C3-C5	2.57	119.60	115.27
11	L	303[B]	BPB	C4-C3-C5	2.56	119.58	115.27
10	L	301[A]	BCB	C1D-CHD-C4C	-2.56	120.54	126.06
10	L	302[A]	BCB	CHC-C4B-C3B	-2.56	123.25	132.35
10	M	403[A]	BCB	CAA-C2A-C1A	2.56	120.35	111.97
10	L	304	BCB	CHC-C4B-C3B	-2.55	123.28	132.35
10	M	403[A]	BCB	CHA-C4D-ND	-2.55	127.16	132.50
11	L	303[B]	BPB	C4A-C3A-C2A	-2.55	100.42	102.84
10	L	301[B]	BCB	C1D-CHD-C4C	-2.55	120.57	126.06
10	L	301[A]	BCB	C4A-NA-C1A	2.54	107.85	106.71
11	M	404	BPB	CMA-C3A-C4A	-2.54	108.82	114.38
10	L	302[B]	BCB	C2D-C1D-ND	2.53	111.97	110.10
10	L	302[A]	BCB	CHA-C4D-ND	-2.52	127.22	132.50
10	L	302[A]	BCB	O2A-CGA-CBA	2.52	119.81	111.91
10	L	301[A]	BCB	O2A-CGA-O1A	-2.52	117.24	123.59
11	L	303[B]	BPB	O2A-CGA-CBA	2.51	119.80	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	402[B]	MQ7	C24-C23-C25	2.51	119.49	115.27
10	L	301[A]	BCB	CHA-C4D-ND	-2.50	127.28	132.50
11	L	303[A]	BPB	C4B-NB-C1B	-2.49	104.97	108.83
10	L	302[B]	BCB	CHA-C4D-ND	-2.49	127.28	132.50
11	M	404	BPB	O2A-C1-C2	2.49	115.17	108.64
10	M	403[B]	BCB	CMB-C2B-C3B	2.48	132.64	125.93
13	M	402[A]	MQ7	C45-C43-C44	2.48	120.07	114.60
10	L	301[A]	BCB	CED-O2D-CGD	2.47	121.52	115.94
10	L	302[B]	BCB	CHC-C4B-C3B	-2.47	123.58	132.35
10	M	403[A]	BCB	CHC-C4B-C3B	-2.46	123.59	132.35
13	M	402[B]	MQ7	C21-C22-C23	-2.45	121.75	127.66
10	M	403[B]	BCB	CHC-C4B-C3B	-2.45	123.63	132.35
14	M	405	NS5	C6-C5-C4	2.45	119.39	115.27
10	L	301[B]	BCB	O2A-CGA-O1A	-2.45	117.42	123.59
10	L	304	BCB	O2D-CGD-O1D	-2.45	119.05	123.84
5	C	404	HEC	CAD-C3D-C2D	-2.45	123.32	127.88
13	M	402[B]	MQ7	C14-C13-C15	2.44	119.38	115.27
14	M	405	NS5	C18-C19-C20	2.43	128.46	123.47
10	L	304	BCB	CMB-C2B-C1B	2.43	129.07	125.37
10	L	301[B]	BCB	CHA-C4D-ND	-2.43	127.42	132.50
5	C	403	HEC	CHB-C4A-NA	2.41	127.05	124.44
10	L	302[B]	BCB	C1D-CHD-C4C	-2.41	120.86	126.06
10	L	302[A]	BCB	CHD-C1D-ND	-2.41	122.24	124.45
10	L	302[B]	BCB	CHB-C4A-NA	2.41	127.84	124.51
5	C	404	HEC	CAD-C3D-C4D	2.39	128.83	124.66
13	M	402[B]	MQ7	C26-C27-C28	-2.37	121.95	127.66
10	L	301[B]	BCB	C4B-C3B-C2B	-2.37	104.55	108.36
10	L	301[B]	BCB	CHB-C4A-NA	2.36	127.78	124.51
5	C	403	HEC	CBD-CAD-C3D	-2.36	106.06	112.63
10	L	301[A]	BCB	CHB-C1B-C2B	-2.36	120.58	127.24
10	M	403[B]	BCB	O2A-CGA-O1A	-2.35	117.65	123.59
11	L	303[A]	BPB	C4-C3-C5	2.35	119.23	115.27
10	L	301[A]	BCB	CAA-CBA-CGA	-2.34	106.41	113.25
10	L	304	BCB	C1D-CHD-C4C	-2.33	121.02	126.06
13	M	402[A]	MQ7	C24-C23-C25	2.33	119.20	115.27
10	M	403[B]	BCB	C4D-CHA-C1A	2.33	124.08	121.25
14	M	405	NS5	C12-C13-C14	-2.32	115.98	123.22
10	L	301[A]	BCB	CMD-C2D-C3D	-2.32	122.28	127.61
9	L	306	HTO	C5-C4-C3	-2.32	110.37	114.18
10	L	302[B]	BCB	CMB-C2B-C3B	2.30	132.14	125.93
10	L	302[B]	BCB	O2D-CGD-O1D	-2.30	119.35	123.84
10	L	301[B]	BCB	CHC-C4B-C3B	-2.28	124.24	132.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	401	HEC	CBB-CAB-C3B	-2.28	106.15	112.43
10	L	302[B]	BCB	C4-C3-C5	2.27	119.09	115.27
8	H	707	LDA	CM2-N1-C1	-2.26	105.49	110.23
10	L	302[A]	BCB	CHB-C4A-NA	2.26	127.63	124.51
10	L	302[B]	BCB	C2A-C1A-CHA	-2.23	119.96	123.86
14	M	405	NS5	C8-C9-C10	-2.22	105.66	112.98
13	M	402[A]	MQ7	C14-C13-C15	2.22	119.01	115.27
13	M	402[A]	MQ7	C26-C27-C28	-2.22	122.31	127.66
11	L	303[A]	BPB	CBA-CAA-C2A	-2.21	107.36	113.81
5	C	401	HEC	CAC-C3C-C2C	2.20	130.39	126.86
10	L	301[A]	BCB	CHC-C4B-C3B	-2.19	124.56	132.35
10	M	403[B]	BCB	CHD-C1D-ND	-2.18	122.45	124.45
10	M	403[A]	BCB	CHD-C4C-C3C	-2.18	123.16	125.89
13	M	402[B]	MQ7	C34-C33-C35	2.18	118.94	115.27
10	M	403[A]	BCB	CMB-C2B-C3B	2.17	131.80	125.93
10	L	302[A]	BCB	C4B-C3B-C2B	-2.17	104.87	108.36
5	C	404	HEC	CHB-C4A-NA	2.17	126.78	124.44
10	L	301[B]	BCB	CAA-C2A-C1A	2.15	119.02	111.97
10	L	302[A]	BCB	CED-O2D-CGD	2.15	120.79	115.94
10	M	403[B]	BCB	C4-C3-C5	2.14	118.87	115.27
11	L	303[B]	BPB	C16-C15-C13	-2.13	109.03	115.92
5	C	403	HEC	O2D-CGD-CBD	2.13	120.88	114.03
5	C	404	HEC	CBD-CAD-C3D	2.13	118.54	112.63
10	L	304	BCB	CHB-C4A-NA	2.12	127.44	124.51
11	L	303[B]	BPB	CMA-C3A-C4A	-2.11	109.75	114.38
10	L	304	BCB	CHD-C4C-C3C	-2.11	123.25	125.89
10	M	403[B]	BCB	CHD-C4C-C3C	-2.10	123.26	125.89
14	M	405	NS5	C22-C21-C20	-2.10	119.98	122.92
10	L	301[B]	BCB	CHC-C4B-NB	-2.09	122.04	124.26
13	M	402[B]	MQ7	C45-C43-C44	2.09	119.22	114.60
10	M	403[A]	BCB	CHB-C1B-NB	-2.09	122.05	124.26
11	M	404	BPB	C4A-C3A-C2A	-2.09	100.85	102.84
5	C	401	HEC	CMC-C2C-C1C	-2.08	122.19	125.37
10	L	301[B]	BCB	C4A-NA-C1A	2.07	107.64	106.71
5	C	401	HEC	O2D-CGD-CBD	2.07	120.68	114.03
5	C	401	HEC	CMC-C2C-C3C	2.07	130.09	125.61
5	C	404	HEC	CBA-CAA-C2A	-2.07	106.89	112.63
10	L	304	BCB	CHB-C1B-NB	-2.06	122.08	124.26
5	C	401	HEC	CHB-C4A-NA	2.05	126.66	124.44
10	L	302[A]	BCB	CMB-C2B-C3B	2.04	131.44	125.93
10	L	302[B]	BCB	CED-O2D-CGD	2.03	120.53	115.94
5	C	403	HEC	O2A-CGA-CBA	2.02	120.53	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	405	DGA	OG1-CA1-OA1	-2.02	118.48	123.59
11	L	303[B]	BPB	C3D-CAD-CBD	2.02	110.26	107.61
5	C	404	HEC	C2B-C1B-NB	-2.01	107.47	109.88
10	M	403[B]	BCB	O2A-CGA-CBA	2.01	118.22	111.91
10	L	301[A]	BCB	C1-C2-C3	-2.01	122.56	126.04
11	M	404	BPB	CMB-C2B-C3B	2.01	128.44	124.68
11	L	303[A]	BPB	CAA-C2A-C3A	-2.01	107.28	112.78
10	L	302[A]	BCB	CHD-C4C-C3C	-2.00	123.39	125.89

All (23) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	401	HEC	NA
5	C	402	HEC	NA
5	C	403	HEC	NA
5	C	404	HEC	NA
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[A]	BCB	ND
10	M	403[B]	BCB	NA
10	M	403[B]	BCB	NC
10	M	403[B]	BCB	ND

All (181) 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	706	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
8	H	706	LDA	C2-C1-N1-CM1
8	H	706	LDA	C2-C1-N1-CM2
8	H	706	LDA	N1-C1-C2-C3
8	H	707	LDA	C2-C1-N1-O1
8	H	707	LDA	C2-C1-N1-CM1
8	H	707	LDA	N1-C1-C2-C3
9	L	306	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	C4-C3-C5-C6
10	L	302[A]	BCB	C2C-C3C-CAC-CBC
10	L	302[B]	BCB	C2C-C3C-CAC-CBC
10	L	304	BCB	C2B-C3B-CAB-OBB
10	L	304	BCB	C2B-C3B-CAB-CBB
10	L	304	BCB	C4B-C3B-CAB-OBB
10	L	304	BCB	C4B-C3B-CAB-CBB
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
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
14	M	405	NS5	C13-C14-C15-C16
14	M	405	NS5	C13-C14-C15-C17
14	M	405	NS5	C34-C35-C36-CM3
10	L	304	BCB	CBD-CGD-O2D-CED
10	L	301[B]	BCB	C2-C3-C5-C6
10	M	403[A]	BCB	C2A-CAA-CBA-CGA
14	M	405	NS5	C34-C35-C36-CM4
11	M	404	BPB	CBA-CGA-O2A-C1
5	C	402	HEC	C2C-C3C-CAC-CBC
11	M	404	BPB	O1A-CGA-O2A-C1
10	L	304	BCB	O1D-CGD-O2D-CED
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB
6	C	405	DGA	CA2-CA1-OG1-CG1
6	C	405	DGA	OA1-CA1-OG1-CG1
10	L	302[B]	BCB	C13-C15-C16-C17
10	L	304	BCB	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
10	L	301[B]	BCB	C15-C16-C17-C18
5	C	402	HEC	C4C-C3C-CAC-CBC
5	C	403	HEC	C2C-C3C-CAC-CBC
10	M	403[A]	BCB	C15-C16-C17-C18
10	M	403[B]	BCB	C8-C10-C11-C12
14	M	405	NS5	C7-C8-C9-C10
5	C	401	HEC	C4C-C3C-CAC-CBC
10	L	301[A]	BCB	C13-C15-C16-C17
10	L	304	BCB	C3-C5-C6-C7
8	H	707	LDA	C2-C3-C4-C5
8	H	707	LDA	C4-C5-C6-C7
8	L	305	LDA	C2-C3-C4-C5
6	C	405	DGA	CCB-CDB-CEB-CFB
11	L	303[A]	BPB	C4-C3-C5-C6
10	L	302[A]	BCB	C14-C13-C15-C16
8	H	707	LDA	C6-C7-C8-C9
14	M	405	NS5	C31-C33-C34-C35
6	C	405	DGA	CBB-CAB-CB9-CB8
5	C	403	HEC	C4C-C3C-CAC-CBC
11	L	303[A]	BPB	O2A-C1-C2-C3
11	L	303[B]	BPB	C8-C10-C11-C12
11	L	303[A]	BPB	C2-C3-C5-C6
11	L	303[A]	BPB	C8-C10-C11-C12
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	404	HEC	C2B-C3B-CAB-CBB
5	C	402	HEC	C4B-C3B-CAB-CBB
10	M	403[A]	BCB	C8-C10-C11-C12
6	C	405	DGA	CAB-CBB-CCB-CDB
10	M	403[A]	BCB	C13-C15-C16-C17
8	L	305	LDA	C1-C2-C3-C4
10	L	302[A]	BCB	C12-C13-C15-C16
11	L	303[A]	BPB	CBD-CGD-O2D-CED
8	H	706	LDA	C3-C4-C5-C6
10	L	302[B]	BCB	C8-C10-C11-C12
14	M	405	NS5	C3-C4-C5-C6
8	H	701	LDA	C6-C7-C8-C9
8	L	305	LDA	C5-C6-C7-C8
9	H	708	HTO	O1-C1-C2-O2
5	C	401	HEC	C2A-CAA-CBA-CGA
10	L	301[A]	BCB	C15-C16-C17-C18
10	M	403[A]	BCB	C12-C13-C15-C16
10	M	403[A]	BCB	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
8	H	706	LDA	C6-C7-C8-C9
9	L	306	HTO	C4-C5-C6-C7
14	M	405	NS5	C10-C12-C13-C14
5	C	402	HEC	C3D-CAD-CBD-CGD
8	H	707	LDA	C11-C10-C9-C8
11	L	303[B]	BPB	O2A-C1-C2-C3
8	L	305	LDA	C4-C5-C6-C7
9	L	306	HTO	O1-C1-C2-O2
11	M	404	BPB	C10-C11-C12-C13
11	L	303[B]	BPB	C4-C3-C5-C6
10	L	302[A]	BCB	C13-C15-C16-C17
10	L	301[B]	BCB	C13-C15-C16-C17
11	M	404	BPB	C15-C16-C17-C18
11	L	303[A]	BPB	O1D-CGD-O2D-CED
5	C	404	HEC	C4B-C3B-CAB-CBB
10	L	301[B]	BCB	C11-C12-C13-C15
10	L	302[B]	BCB	C11-C10-C8-C7
10	L	304	BCB	C11-C10-C8-C7
11	L	303[B]	BPB	C2-C3-C5-C6
10	M	403[B]	BCB	CBA-CGA-O2A-C1
11	M	404	BPB	C16-C17-C18-C20
10	L	304	BCB	CAD-CBD-CGD-O2D
6	C	405	DGA	CBB-CCB-CDB-CEB
8	H	707	LDA	C2-C1-N1-CM2
10	L	302[B]	BCB	CHA-CBD-CGD-O1D
10	L	302[B]	BCB	CHA-CBD-CGD-O2D
6	C	405	DGA	CB9-CAB-CBB-CCB
5	C	404	HEC	C2D-C3D-CAD-CBD
10	L	304	BCB	C8-C10-C11-C12
10	M	403[B]	BCB	O1A-CGA-O2A-C1
10	L	301[B]	BCB	CBA-CGA-O2A-C1
8	H	707	LDA	C5-C6-C7-C8
10	L	301[A]	BCB	C2C-C3C-CAC-CBC
10	L	301[A]	BCB	CAD-CBD-CGD-O1D
10	L	301[B]	BCB	CAD-CBD-CGD-O1D
10	L	304	BCB	C2C-C3C-CAC-CBC
5	C	401	HEC	C4B-C3B-CAB-CBB
10	M	403[B]	BCB	C12-C13-C15-C16
10	L	301[B]	BCB	O1A-CGA-O2A-C1
8	H	701	LDA	C2-C3-C4-C5
10	L	301[B]	BCB	C16-C17-C18-C19
10	L	304	BCB	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	M	405	NS5	C3-C4-C5-C7
9	L	306	HTO	O2-C2-C3-O3
10	L	304	BCB	C11-C10-C8-C9
10	M	403[B]	BCB	C14-C13-C15-C16
6	C	405	DGA	CA6-CA7-CA8-CA9
5	C	403	HEC	C2B-C3B-CAB-CBB
6	C	405	DGA	CA7-CA8-CA9-CAA
5	C	403	HEC	C4B-C3B-CAB-CBB
11	M	404	BPB	C16-C17-C18-C19
8	H	701	LDA	C9-C10-C11-C12
5	C	404	HEC	C3D-CAD-CBD-CGD
5	C	404	HEC	C4D-C3D-CAD-CBD
14	M	405	NS5	C23-C24-C25-C26
6	C	405	DGA	CB2-CB3-CB4-CB5
8	L	305	LDA	C3-C4-C5-C6
11	M	404	BPB	C14-C13-C15-C16
11	L	303[B]	BPB	C5-C6-C7-C8
6	C	405	DGA	CB6-CB7-CB8-CB9
10	L	304	BCB	C2-C3-C5-C6
10	L	302[A]	BCB	CBD-CGD-O2D-CED
5	C	401	HEC	CAA-CBA-CGA-O2A
10	M	403[A]	BCB	C5-C6-C7-C8
10	L	301[B]	BCB	C11-C12-C13-C14
10	L	302[B]	BCB	C11-C10-C8-C9
8	H	707	LDA	C3-C4-C5-C6
11	L	303[A]	BPB	CAD-CBD-CGD-O2D
8	H	701	LDA	C5-C6-C7-C8
13	M	402[B]	MQ7	C39-C38-C40-C41
10	M	403[B]	BCB	C16-C17-C18-C20
6	C	405	DGA	CB4-CB5-CB6-CB7
10	M	403[A]	BCB	O2A-C1-C2-C3
10	M	403[B]	BCB	O2A-C1-C2-C3
10	L	304	BCB	CHA-CBD-CGD-O1D
10	L	304	BCB	CHA-CBD-CGD-O2D
13	M	402[B]	MQ7	C37-C38-C40-C41
5	C	401	HEC	CAA-CBA-CGA-O1A
5	C	404	HEC	CAD-CBD-CGD-O2D
11	L	303[B]	BPB	CHA-CBD-CGD-O1D
10	L	302[A]	BCB	C1A-C2A-CAA-CBA
10	L	302[B]	BCB	C16-C17-C18-C19
5	C	402	HEC	CAA-CBA-CGA-O1A
8	L	305	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
10	L	302[B]	BCB	C14-C13-C15-C16
10	L	304	BCB	C11-C12-C13-C14
6	C	405	DGA	CA3-CA4-CA5-CA6
10	L	301[B]	BCB	CAA-CBA-CGA-O2A
10	L	301[A]	BCB	C6-C7-C8-C10
10	L	302[B]	BCB	C12-C13-C15-C16
5	C	404	HEC	CAD-CBD-CGD-O1D
5	C	402	HEC	CAA-CBA-CGA-O2A
10	L	302[B]	BCB	C2A-CAA-CBA-CGA
8	H	707	LDA	C9-C10-C11-C12

There are no ring outliers.

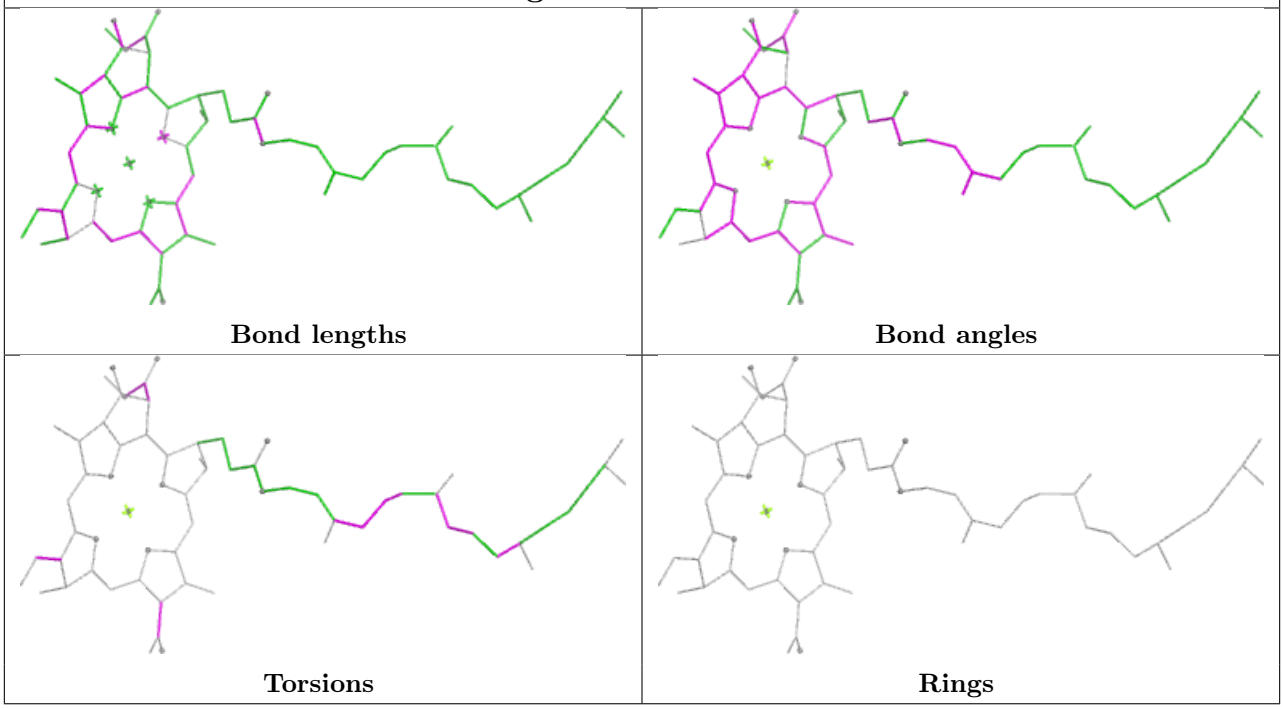
17 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	304	BCB	4	0
14	M	405	NS5	3	0
10	M	403[A]	BCB	1	0
10	L	301[B]	BCB	5	0
11	M	404	BPB	5	0
10	L	302[B]	BCB	2	0
11	L	303[A]	BPB	4	0
10	M	403[B]	BCB	3	0
7	M	408	SO4	1	0
13	M	402[A]	MQ7	2	0
5	C	401	HEC	1	0
5	C	402	HEC	2	0
8	H	701	LDA	1	0
8	L	305	LDA	1	0
11	L	303[B]	BPB	4	0
10	L	301[A]	BCB	2	0
8	H	707	LDA	1	0

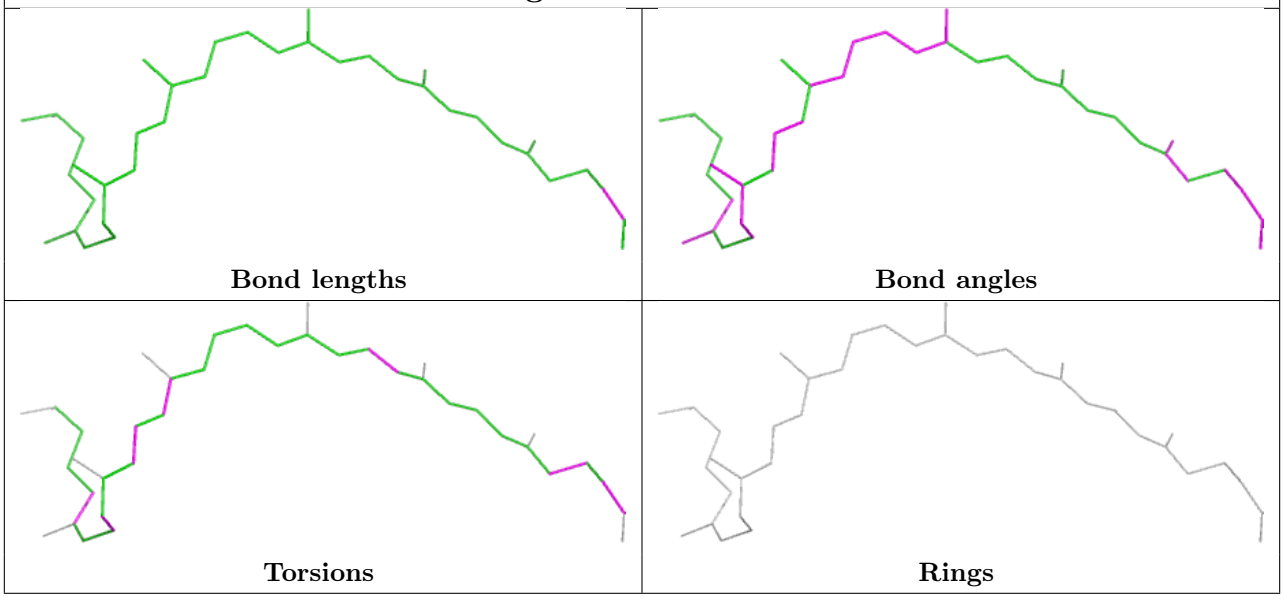
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

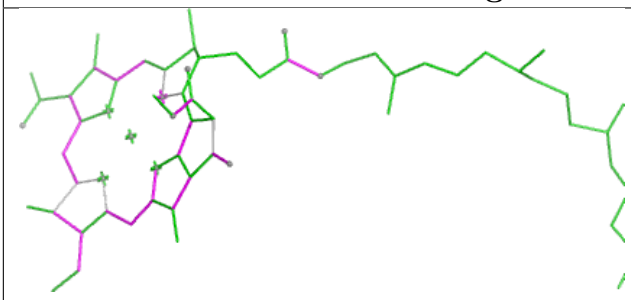
Ligand BCB L 304



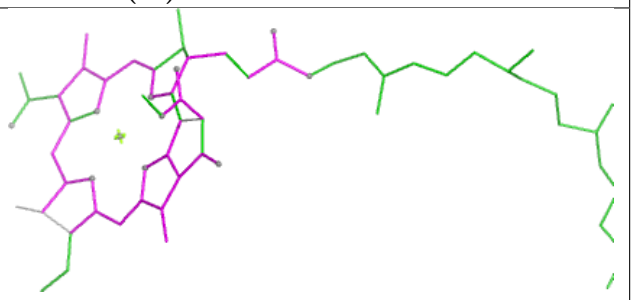
Ligand NS5 M 405



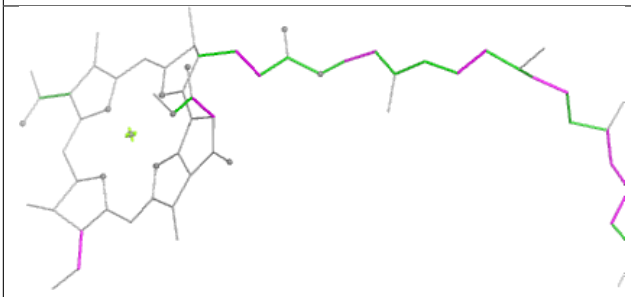
Ligand BCB M 403 (A)



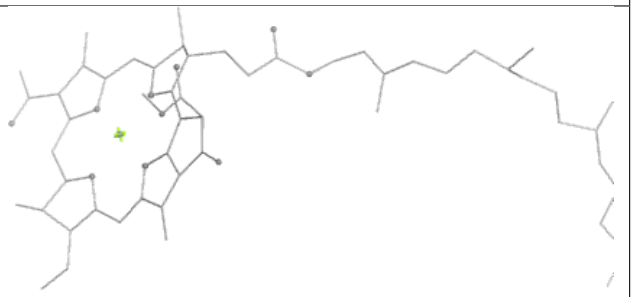
Bond lengths



Bond angles

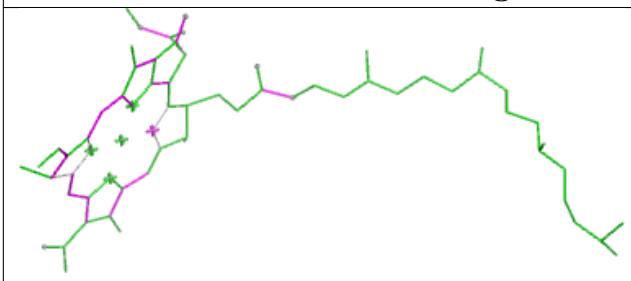


Torsions

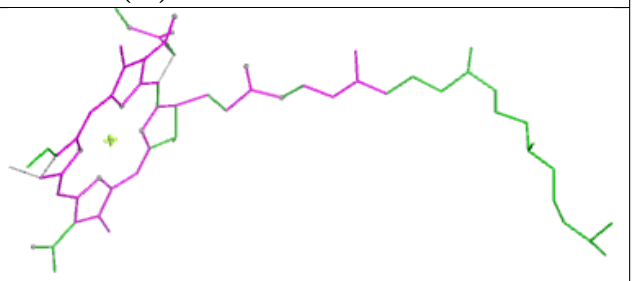


Rings

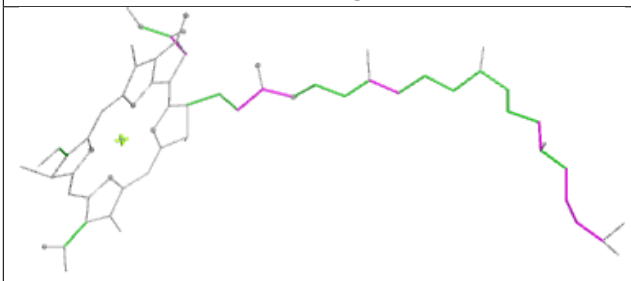
Ligand BCB L 301 (B)



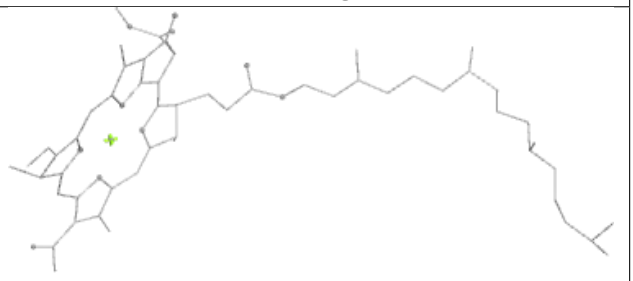
Bond lengths



Bond angles

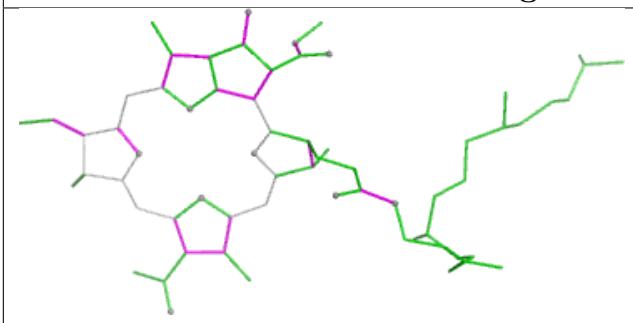


Torsions



Rings

Ligand BPB M 404



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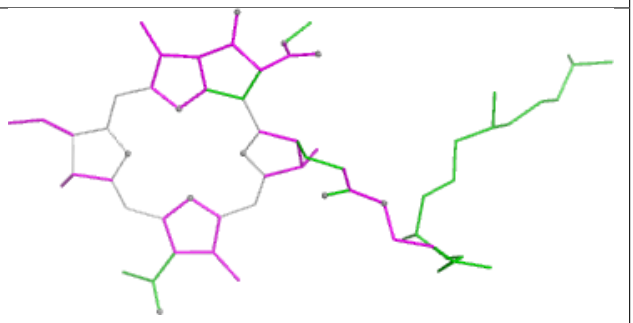

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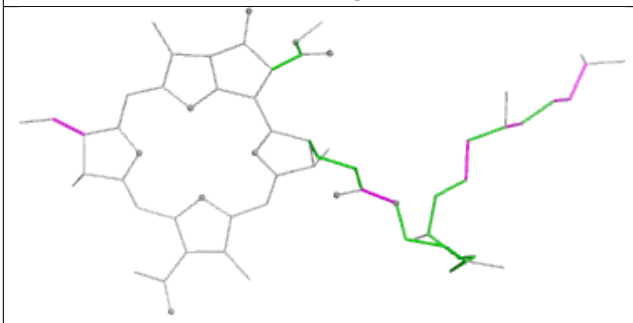

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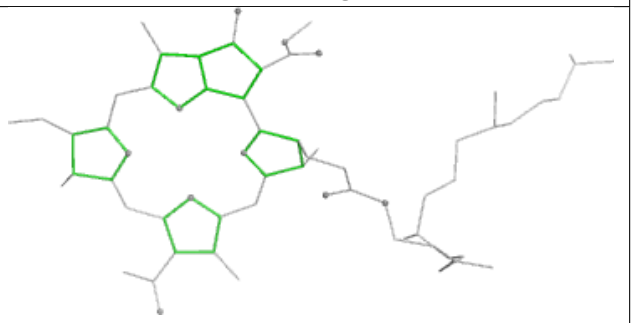
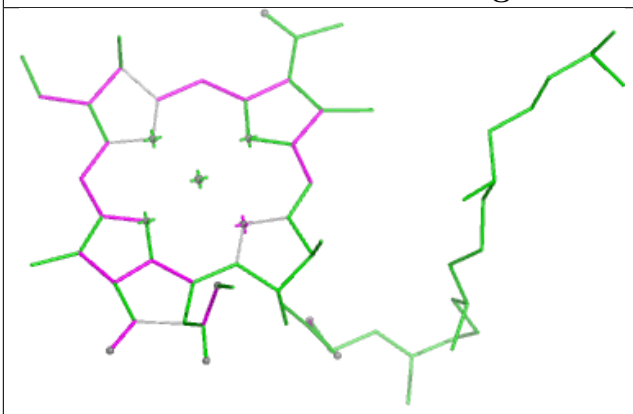


Rings

Ligand BCB L 302 (B)



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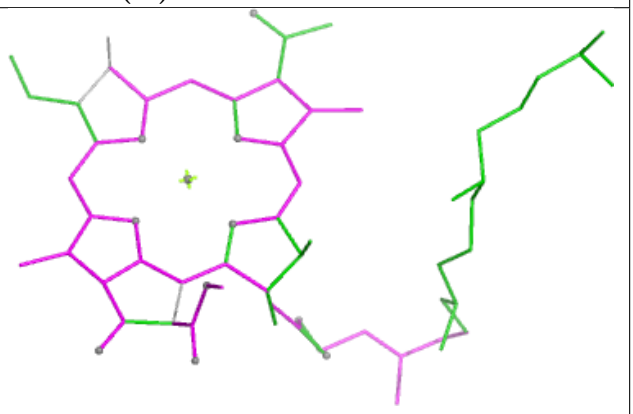
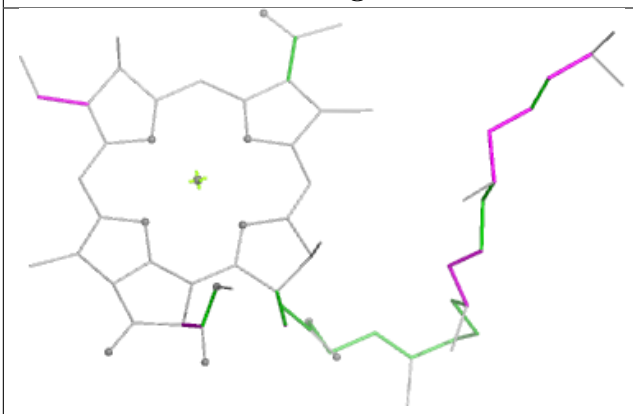


Bond angles

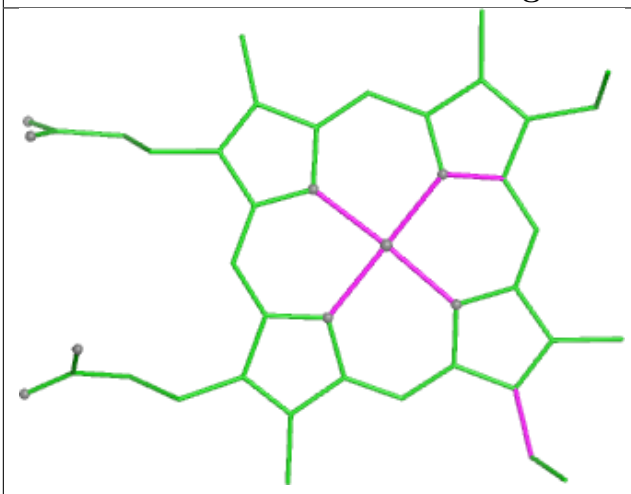


Torsions



Rings

Ligand HEC C 404



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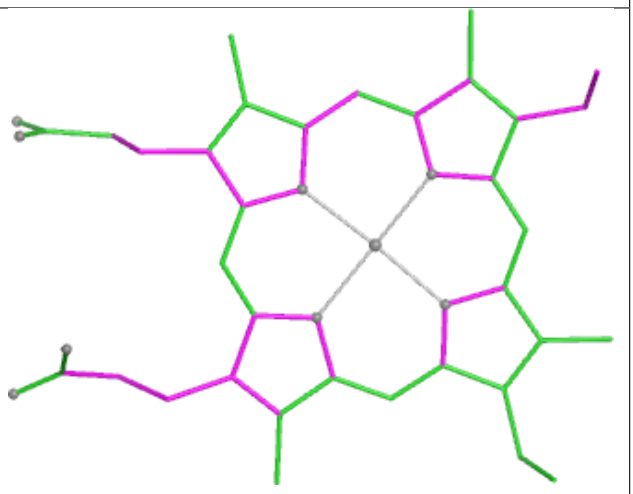
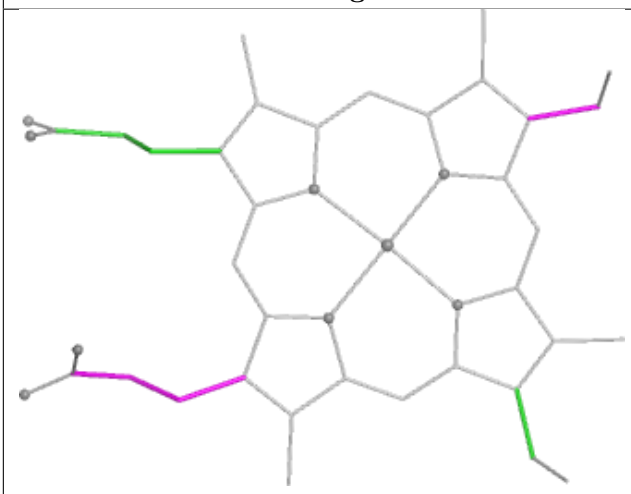


Bond angles



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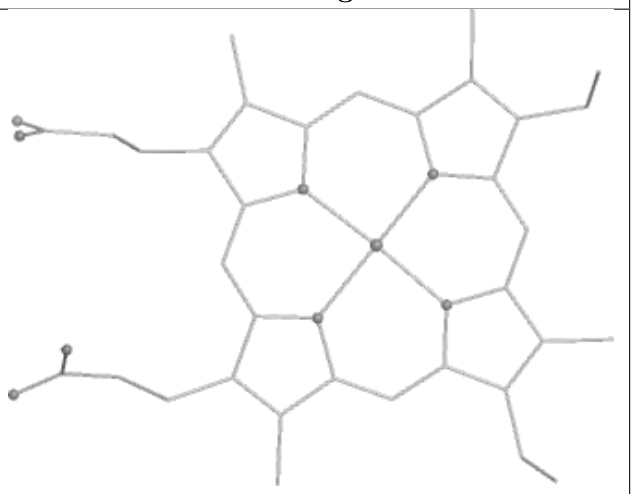
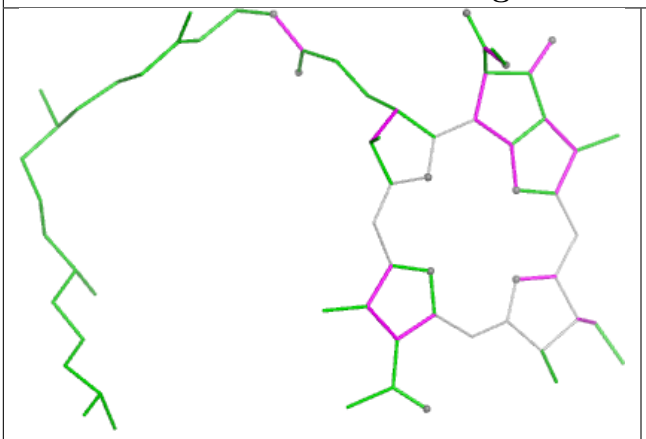


Rings

Ligand BPB L 303 (A)



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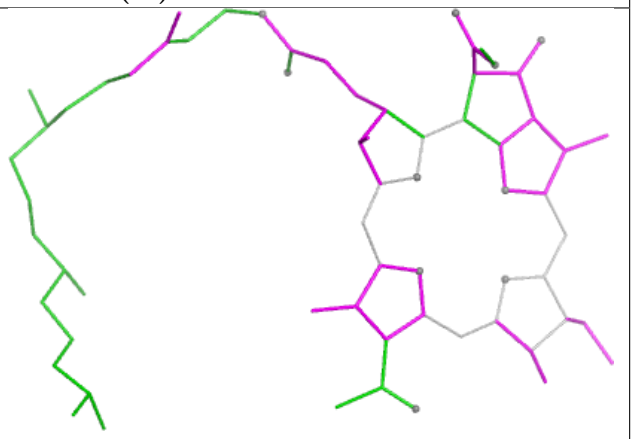
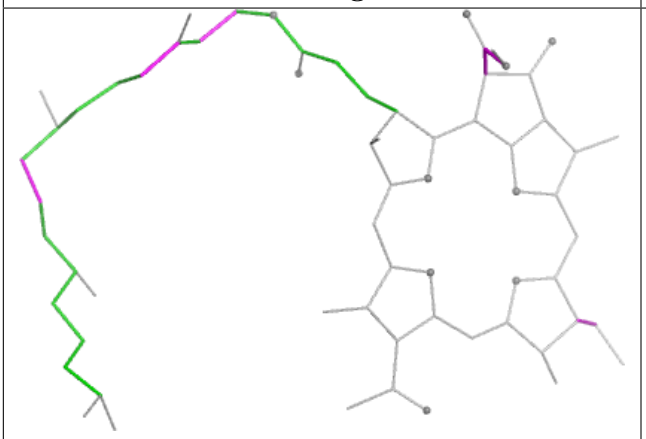


Bond angles



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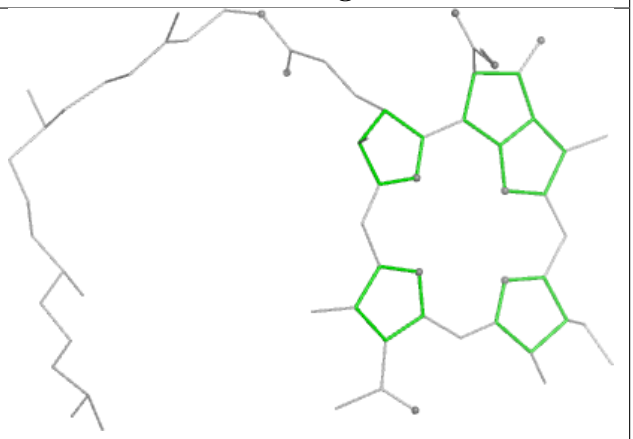
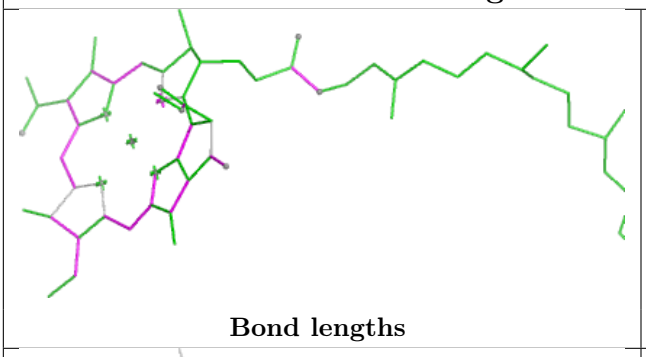


Rings

Ligand BCB M 403 (B)



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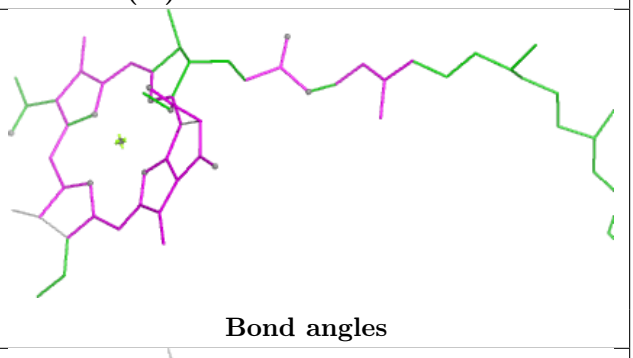
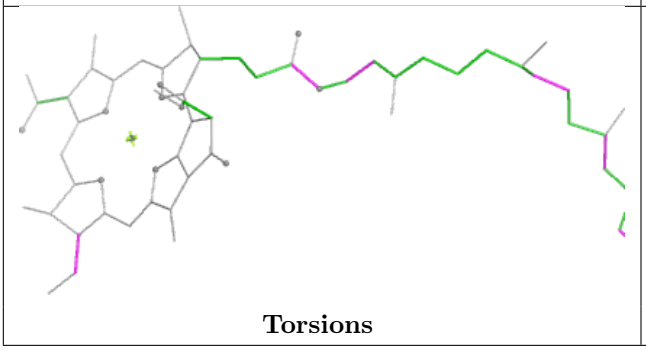
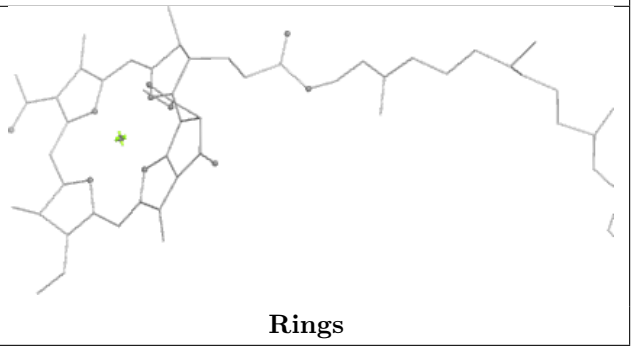


Bond angles

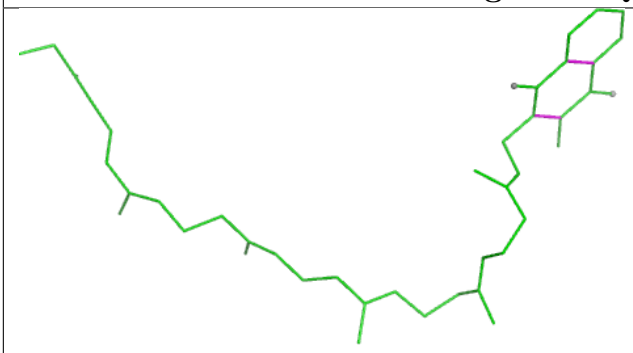


Torsions



Rings

Ligand MQ7 M 402 (A)



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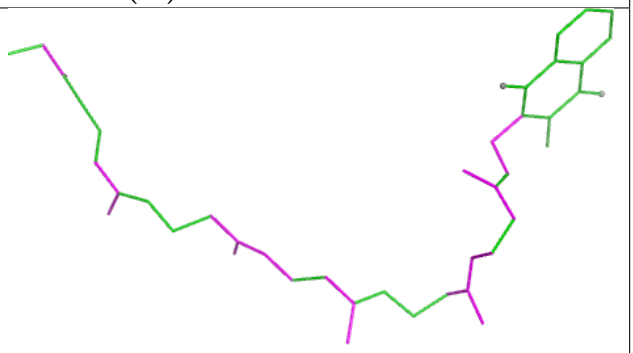
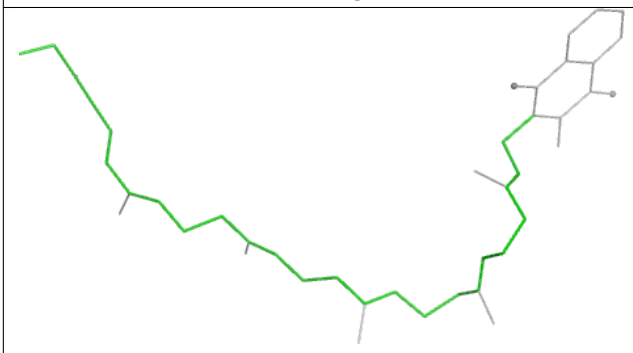


Bond angles

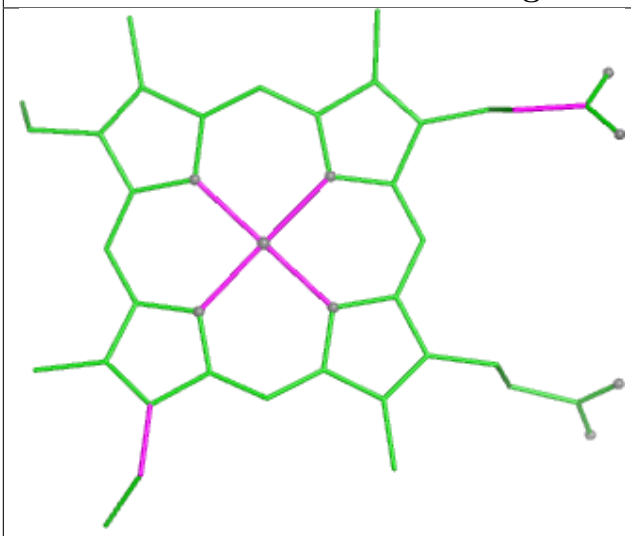


Torsions



Rings

Ligand HEC C 403



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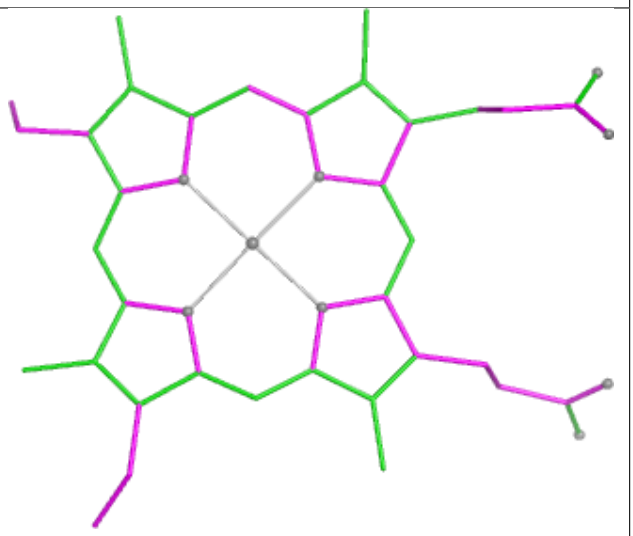
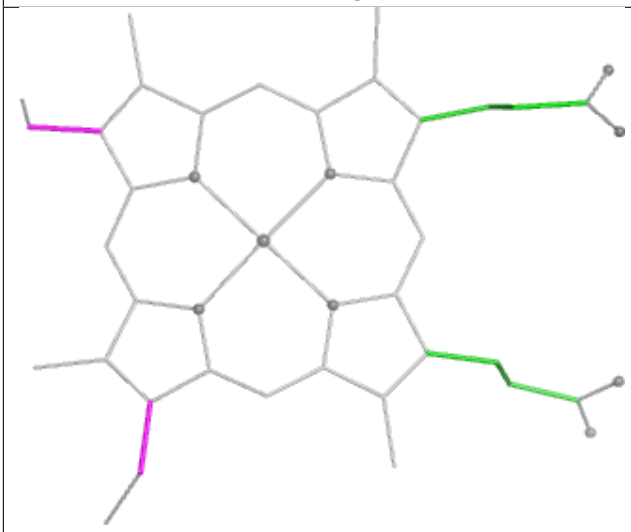


Bond angles



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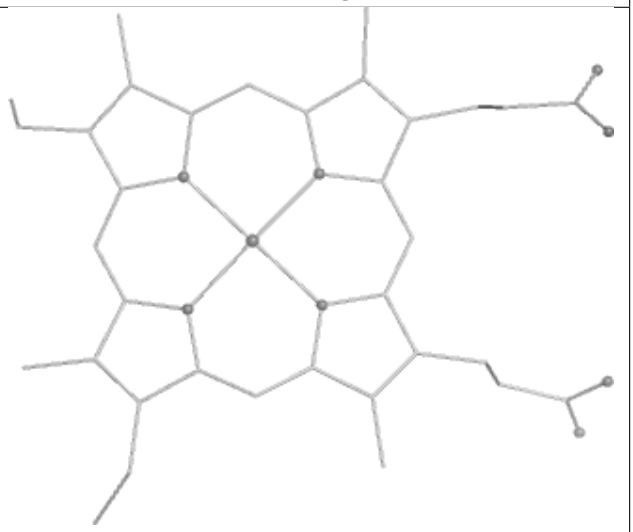
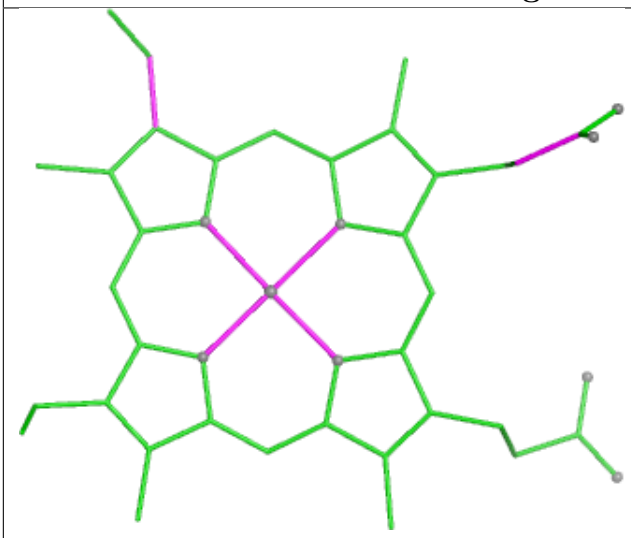


Rings

Ligand HEC C 401



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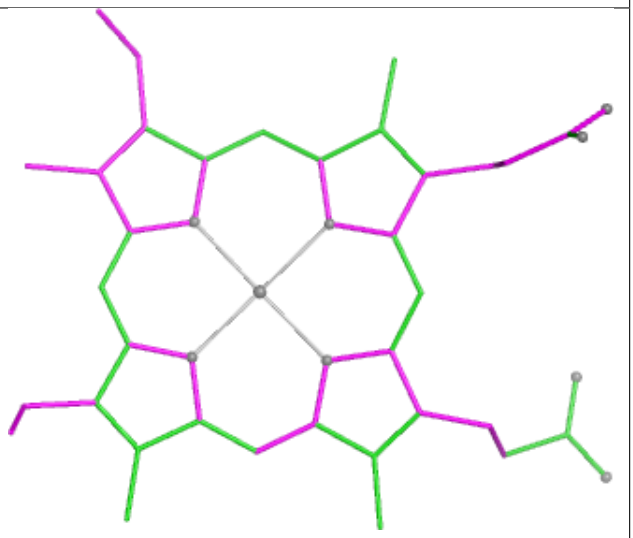
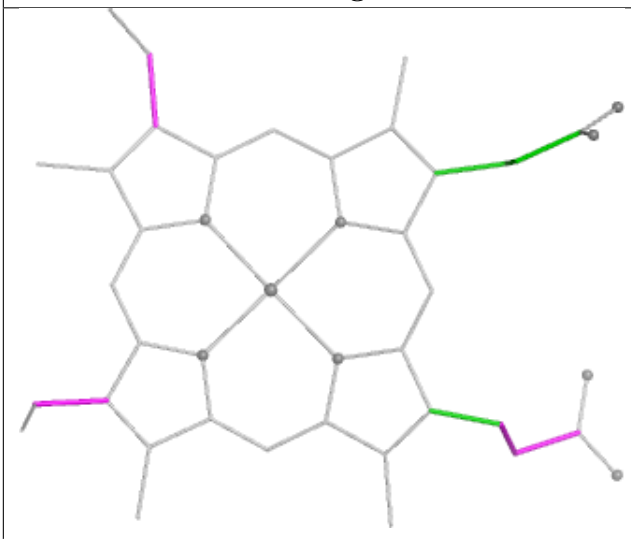


Bond angles



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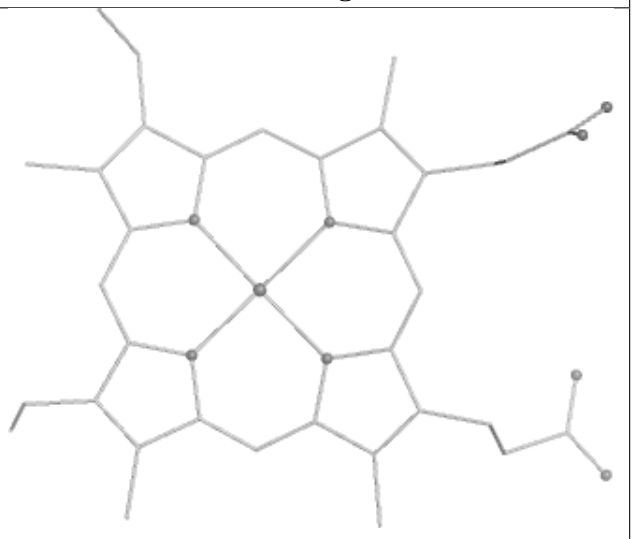
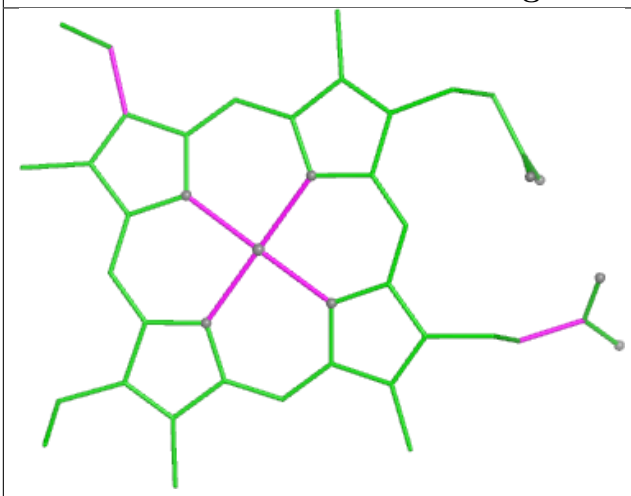
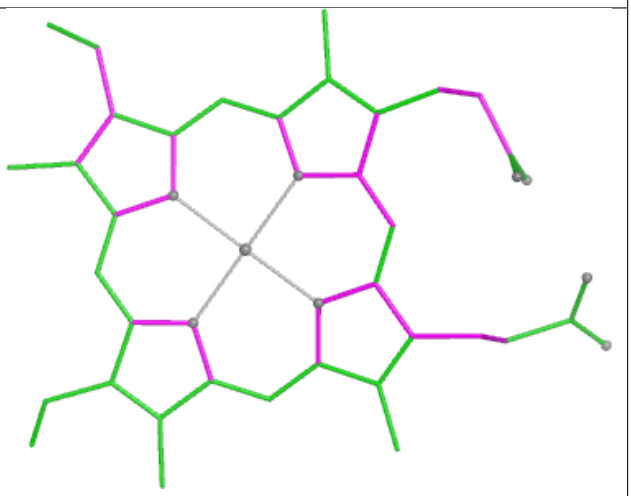


Rings

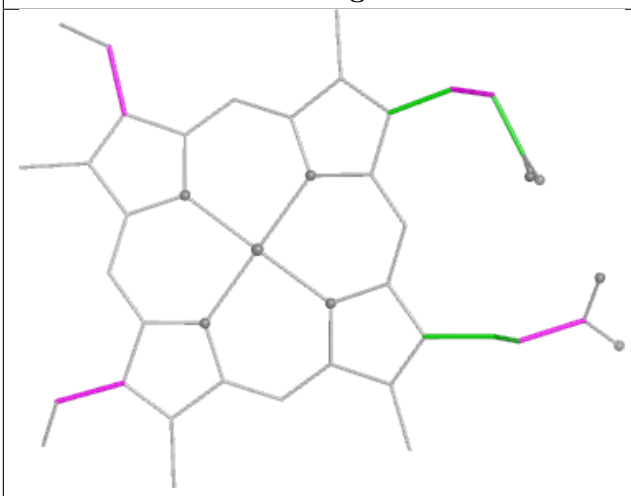
Ligand HEC C 402



Bond lengths



Bond angles



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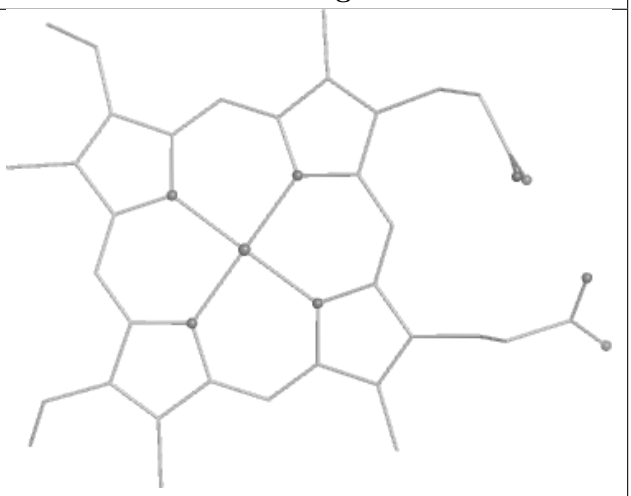
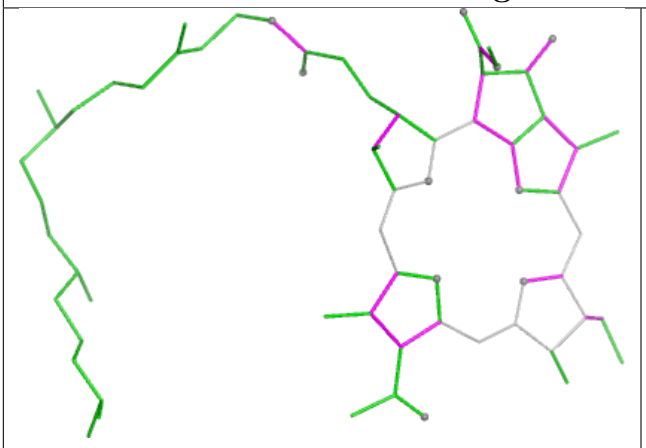


Rings

Ligand BPB L 303 (B)



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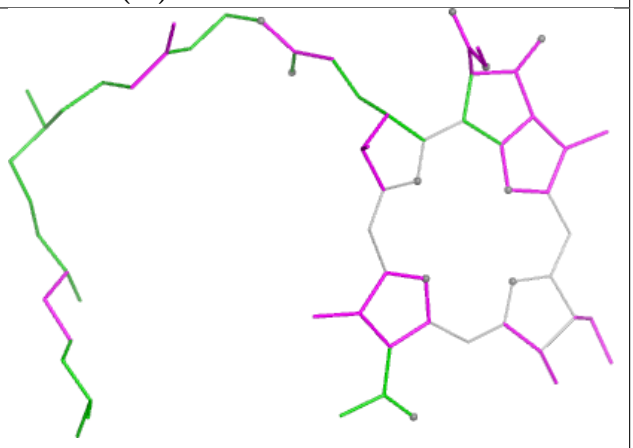
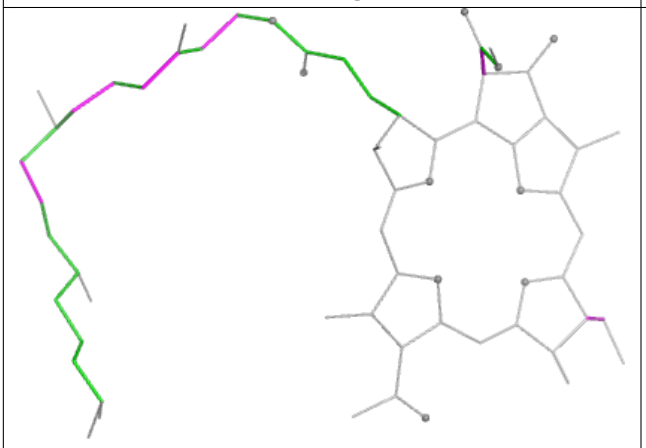


Bond angles



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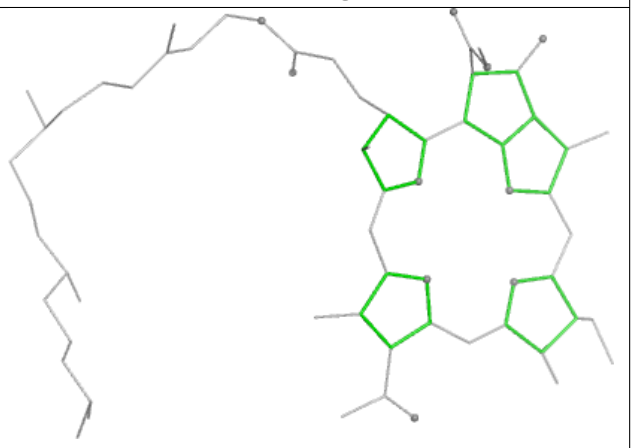
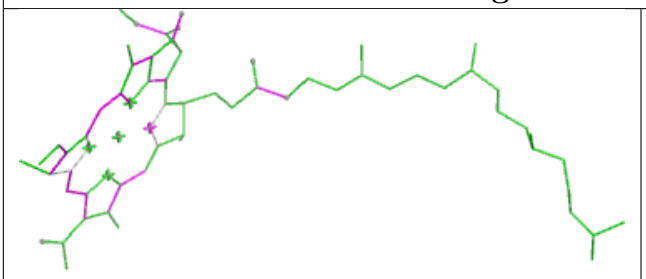
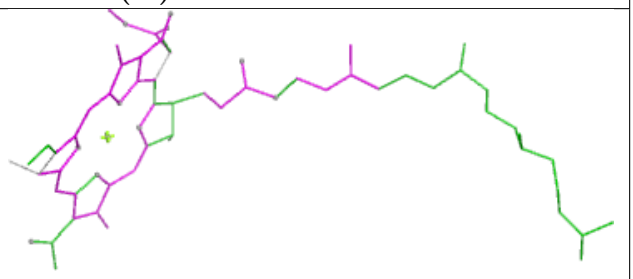


Rings

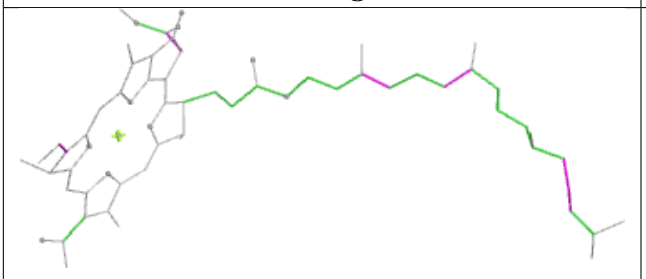
Ligand BCB L 301 (A)



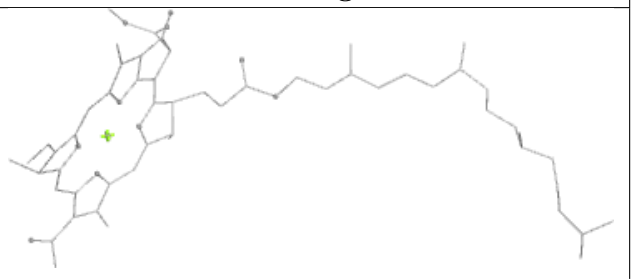
Bond lengths



Bond angles

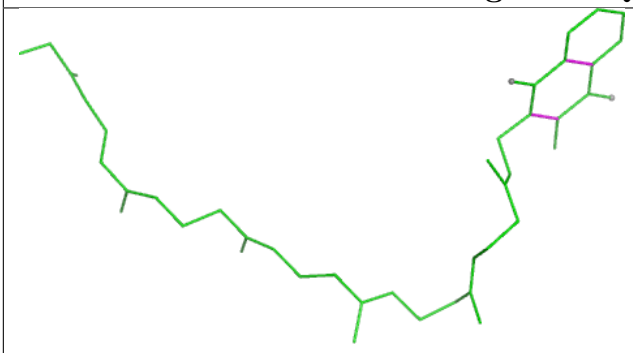


Torsions

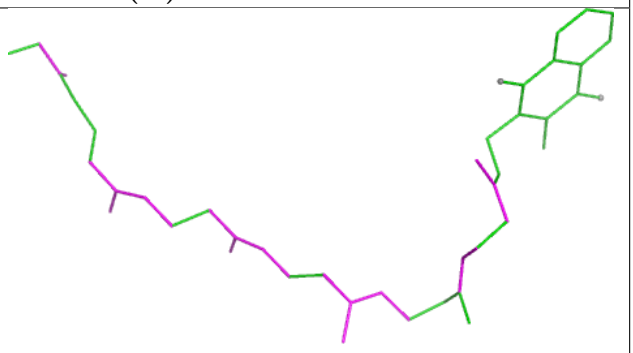


Rings

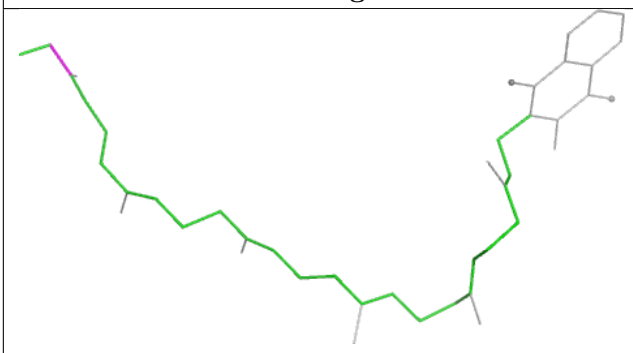
Ligand MQ7 M 402 (B)



Bond lengths



Bond angles



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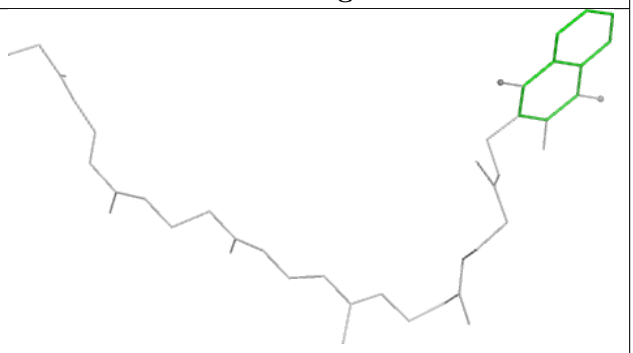
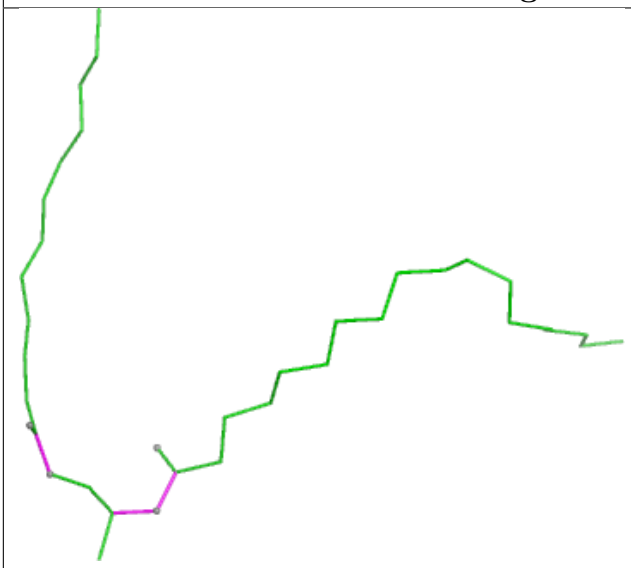
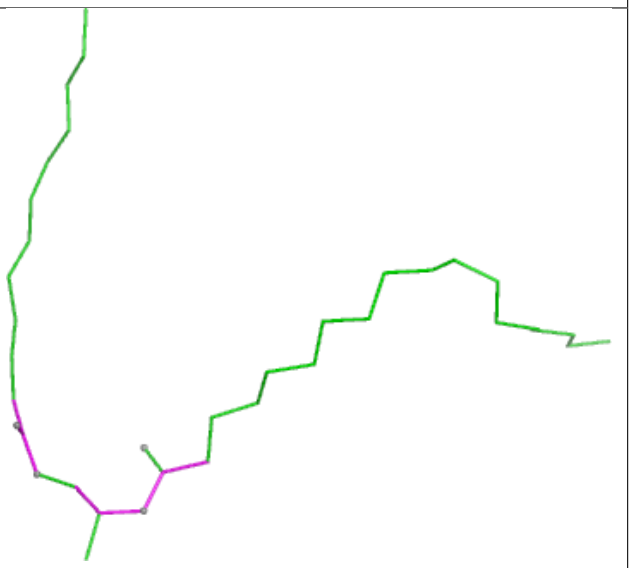


Rings

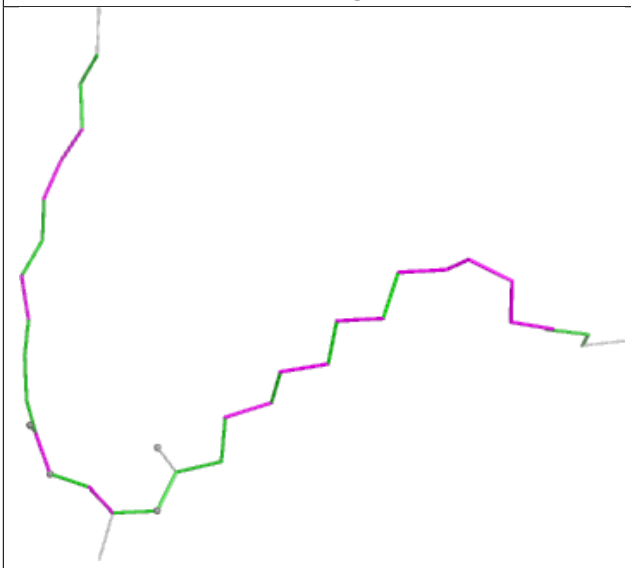
Ligand DGA C 405



Bond lengths



Bond angles

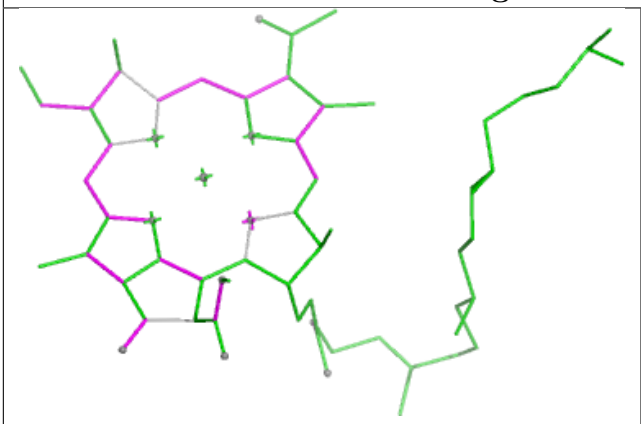


Torsions

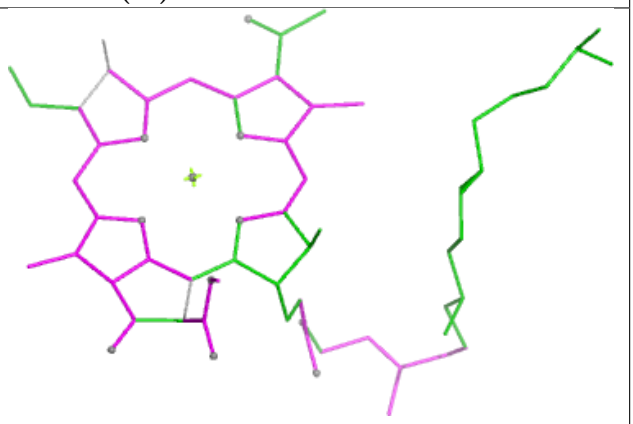


Rings

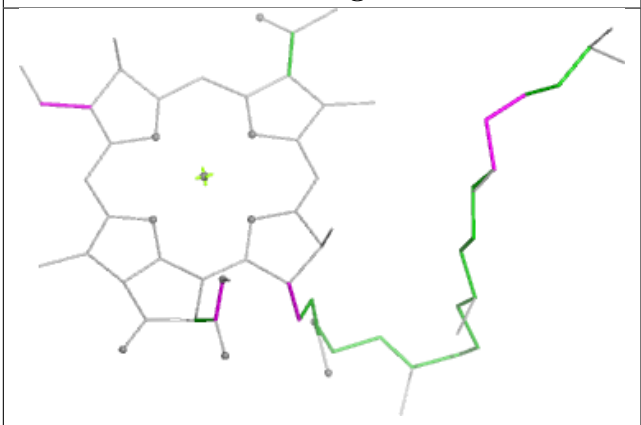
Ligand BCB L 302 (A)



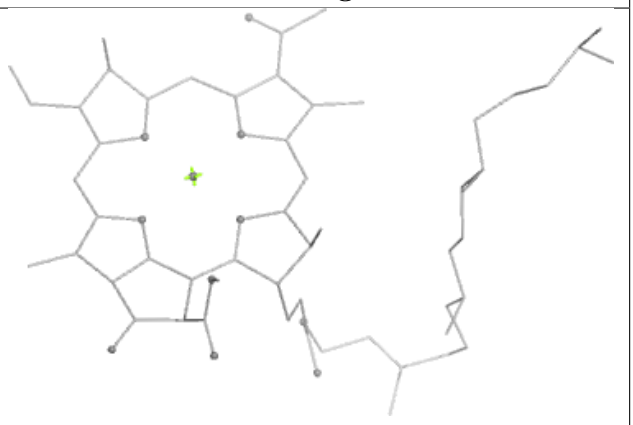
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.47	2 (0%)	85	80	64, 83, 110, 135	0
2	H	257/258 (99%)	-0.07	6 (2%)	61	51	71, 93, 133, 185	0
3	L	273/273 (100%)	-0.44	1 (0%)	88	84	33, 80, 105, 122	41 (15%)
4	M	323/323 (100%)	-0.37	2 (0%)	85	80	33, 79, 106, 134	51 (15%)
All	All	1185/1190 (99%)	-0.35	11 (0%)	81	74	33, 84, 114, 185	92 (7%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	52	LEU	4.3
2	H	50	VAL	4.1
2	H	53	ALA	4.0
3	L	1	ALA	3.5
4	M	89	PHE	3.3
2	H	54	PRO	3.1
1	C	332	LYS	2.9
1	C	54	GLN	2.7
2	H	49	LEU	2.4
4	M	51	LEU	2.4
2	H	47	LEU	2.1

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(Å^2)	Q<0.9
2	FME	H	1	10/11	0.94	0.12	81,93,103,118	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(Å^2)	Q<0.9
7	SO4	M	412	5/5	0.44	0.14	140,155,161,174	0
7	SO4	M	410	5/5	0.62	0.11	122,148,161,167	0
9	HTO	L	306	10/10	0.63	0.29	86,109,119,121	0
7	SO4	M	409	5/5	0.67	0.10	122,128,141,155	0
7	SO4	M	411	5/5	0.71	0.13	119,121,146,173	0
7	SO4	H	703	5/5	0.72	0.10	143,146,151,163	0
7	SO4	C	406	5/5	0.74	0.10	121,135,142,155	0
7	SO4	M	407	5/5	0.83	0.11	106,107,116,138	0
9	HTO	H	708	10/10	0.84	0.25	95,107,121,123	0
6	DGA	C	405	37/44	0.85	0.21	88,122,155,160	0
8	LDA	L	305	16/16	0.87	0.28	94,116,141,145	0
8	LDA	H	706	16/16	0.93	0.18	75,91,159,160	0
7	SO4	H	702	5/5	0.94	0.09	94,104,112,115	0
11	BPB	M	404	65/65	0.94	0.15	69,82,163,171	0
14	NS5	M	405	40/40	0.95	0.16	69,84,125,127	0
8	LDA	H	707	16/16	0.96	0.14	89,107,124,127	0
7	SO4	H	705	5/5	0.96	0.06	97,98,110,110	5
13	MQ7	M	402[A]	48/48	0.96	0.13	67,75,113,135	48
13	MQ7	M	402[B]	48/48	0.96	0.13	67,75,112,135	48
7	SO4	M	406	5/5	0.96	0.06	90,104,114,115	0
7	SO4	H	704	5/5	0.97	0.14	89,93,107,107	5
10	BCB	L	304	66/66	0.97	0.11	65,74,156,167	0
10	BCB	M	403[A]	66/66	0.97	0.11	52,66,97,103	66
10	BCB	M	403[B]	66/66	0.97	0.11	52,66,97,103	66
7	SO4	M	408	5/5	0.98	0.04	78,86,92,93	0
10	BCB	L	301[A]	66/66	0.98	0.10	56,66,82,99	66
11	BPB	L	303[A]	65/65	0.98	0.09	67,73,82,87	65
11	BPB	L	303[B]	65/65	0.98	0.09	67,73,82,87	65
10	BCB	L	301[B]	66/66	0.98	0.10	56,66,82,99	66
10	BCB	L	302[A]	66/66	0.98	0.10	62,70,102,105	66
10	BCB	L	302[B]	66/66	0.98	0.10	62,70,102,105	66
8	LDA	H	701	16/16	0.98	0.11	72,86,101,101	0

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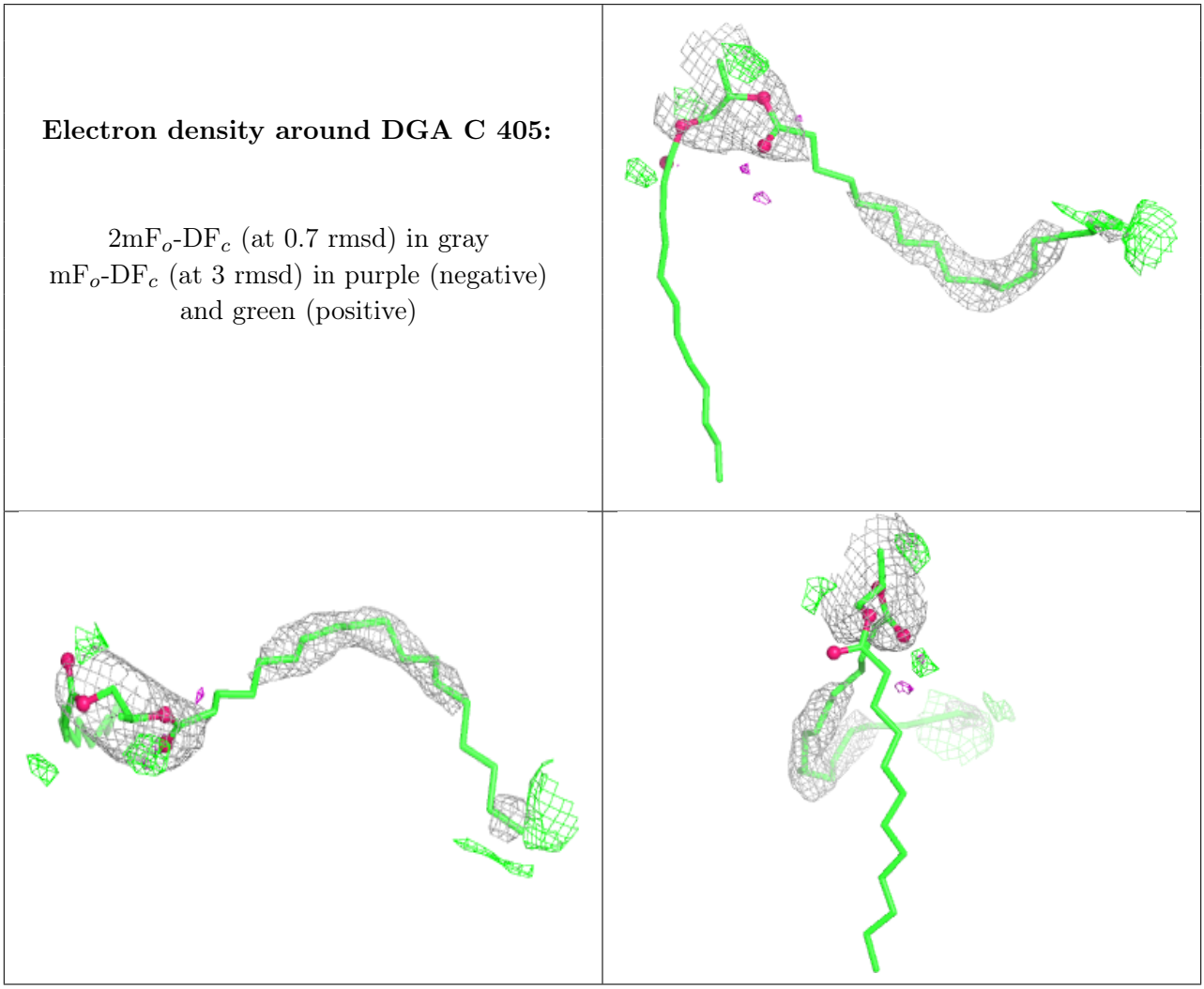
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	HEC	C	401	43/43	0.99	0.07	80,88,103,117	0
5	HEC	C	402	43/43	0.99	0.07	71,82,93,119	0
5	HEC	C	403	43/43	0.99	0.07	63,73,83,87	0
5	HEC	C	404	43/43	0.99	0.06	65,74,91,113	0
12	FE	M	401[B]	1/1	1.00	0.02	78,78,78,78	1
12	FE	M	401[A]	1/1	1.00	0.02	78,78,78,78	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.

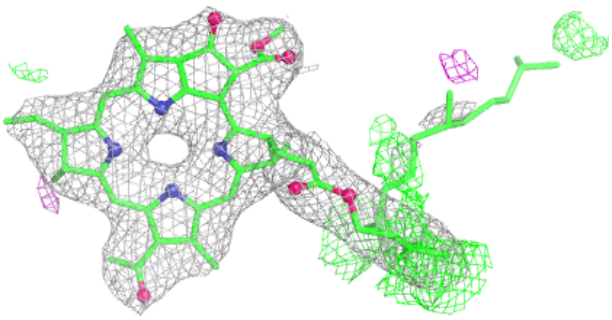
Electron density around DGA C 405:

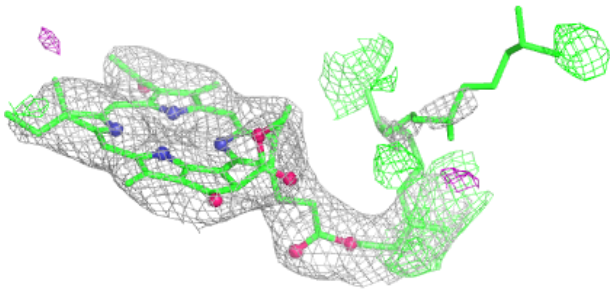
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

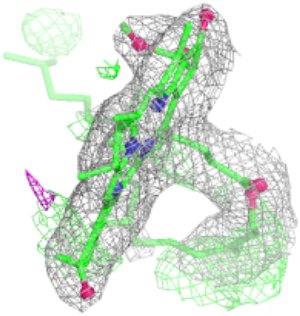


Electron density around BPB M 404:

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

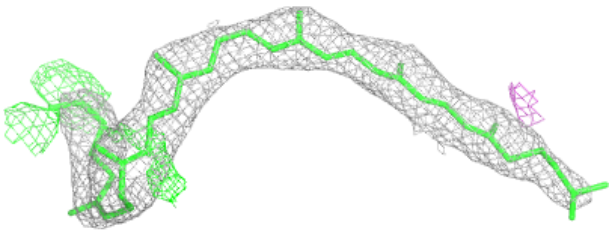


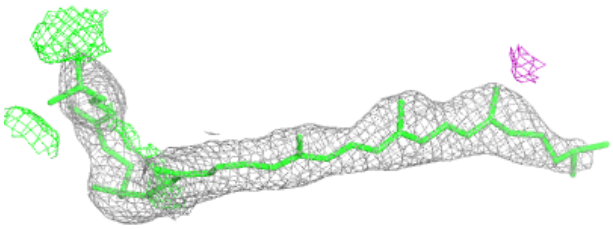


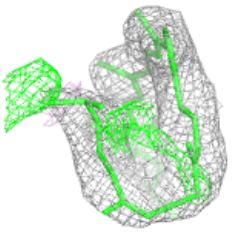


Electron density around NS5 M 405:

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

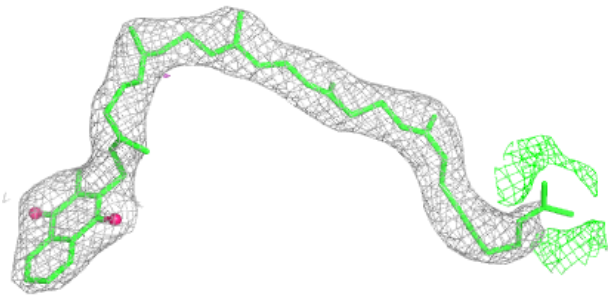


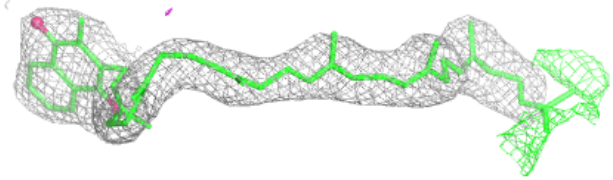


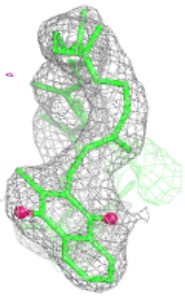


Electron density around MQ7 M 402 (A):

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

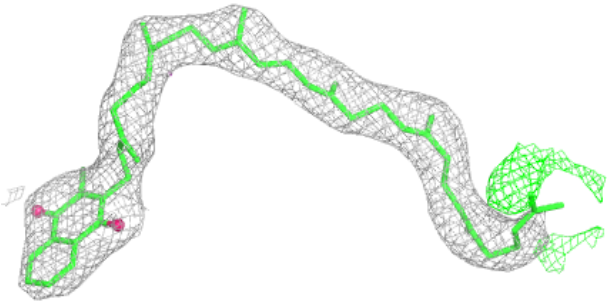


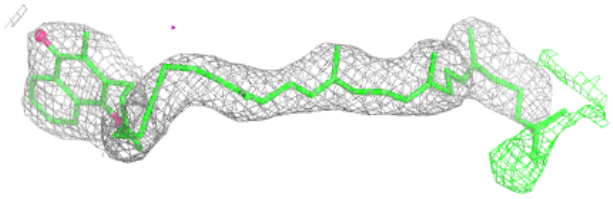


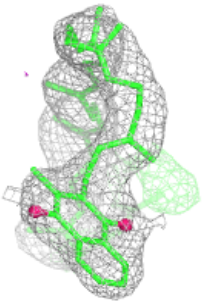


Electron density around MQ7 M 402 (B):

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

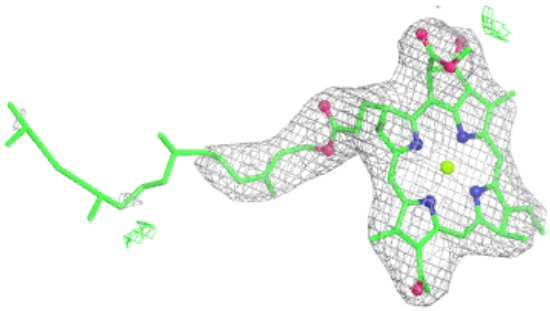


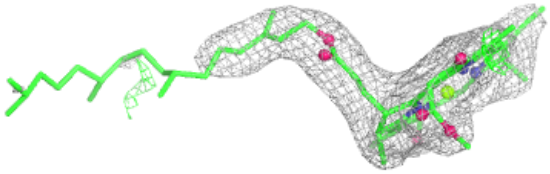


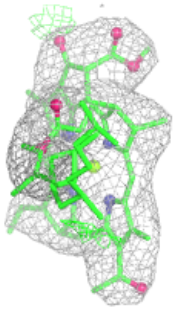


Electron density around BCB L 304:

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

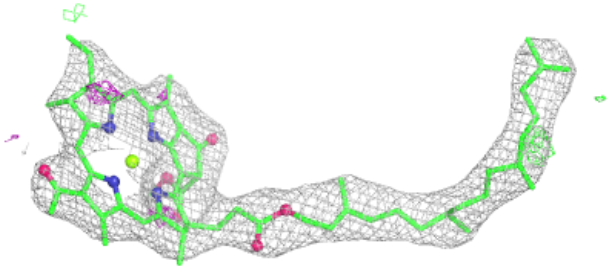


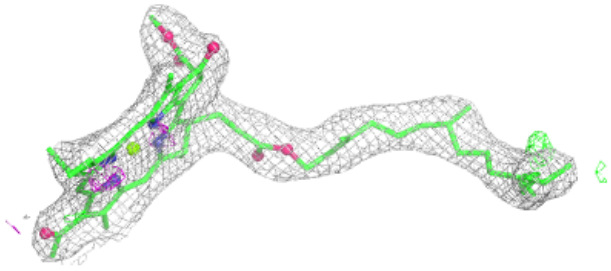


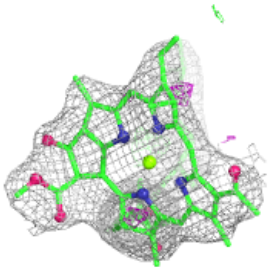


Electron density around BCB M 403 (A):

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

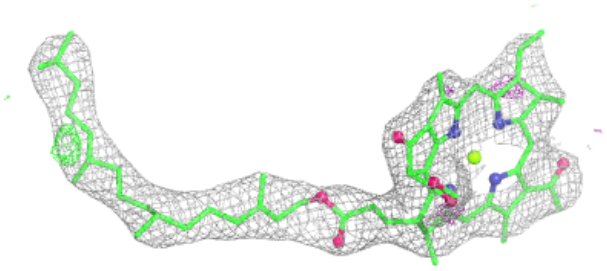


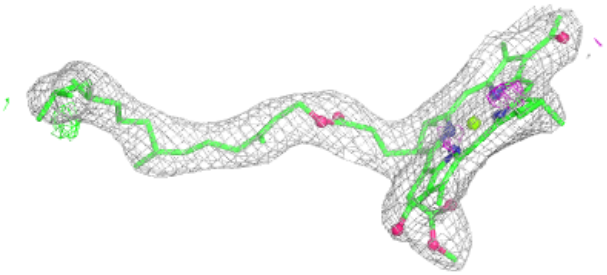


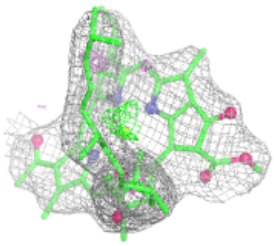


Electron density around BCB M 403 (B):

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

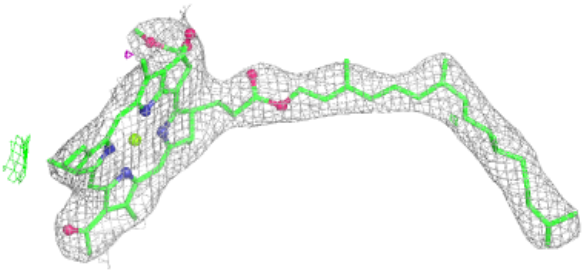


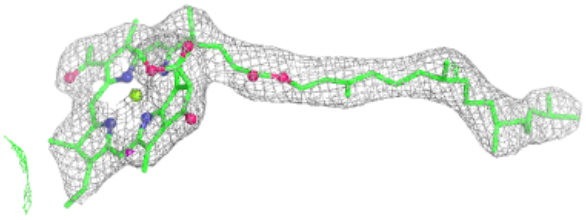


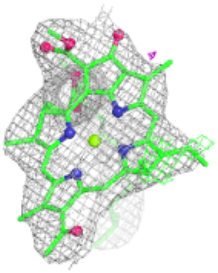


Electron density around BCB L 301 (A):

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

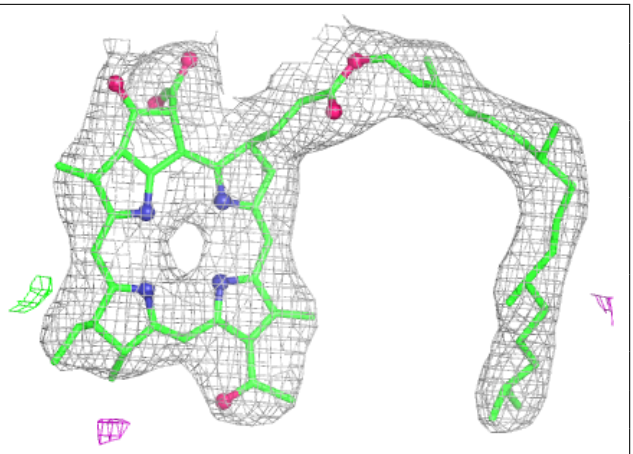


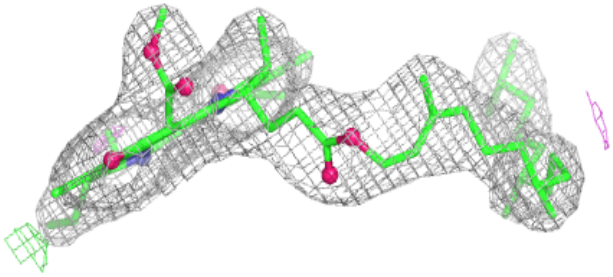


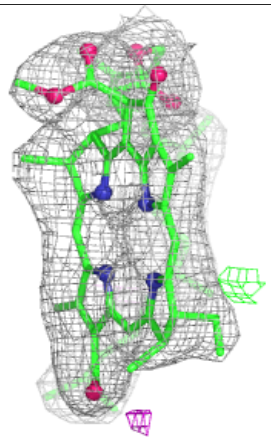


Electron density around BPB L 303 (A):

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

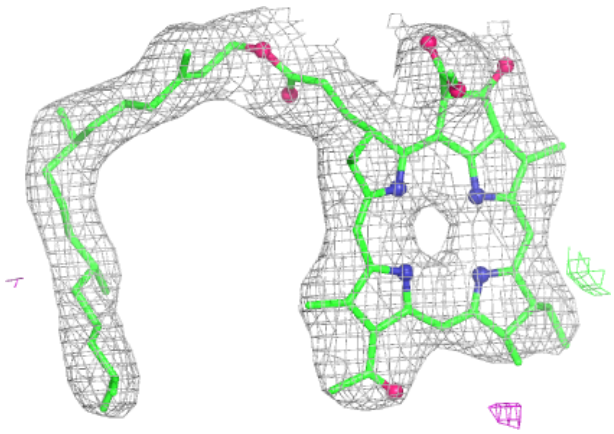


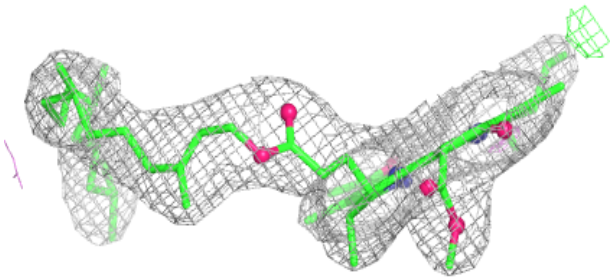


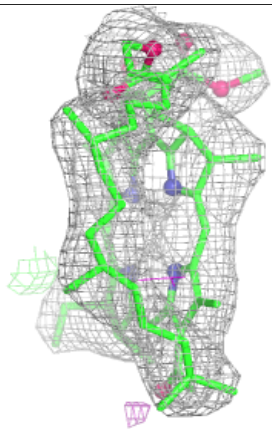


Electron density around BPB L 303 (B):

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

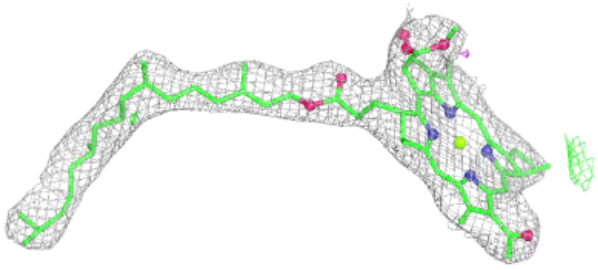


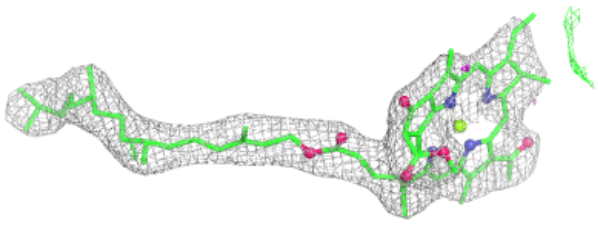


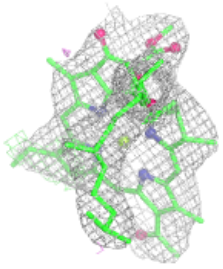


Electron density around BCB L 301 (B):

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

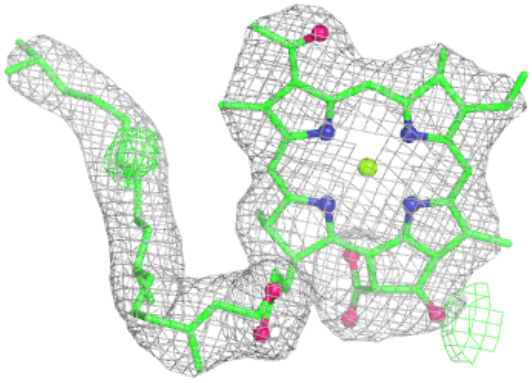


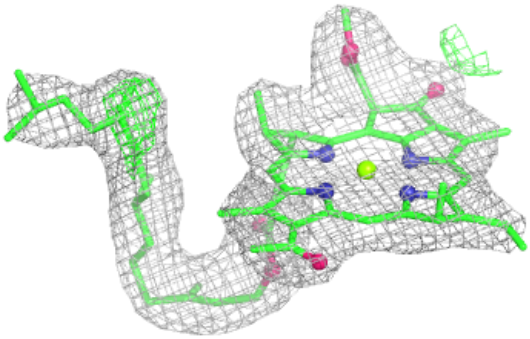


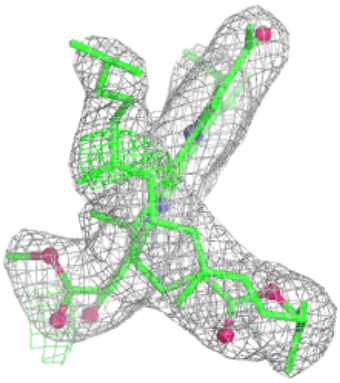


Electron density around BCB L 302 (A):

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

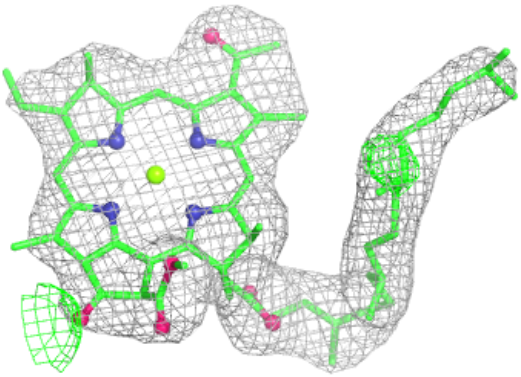


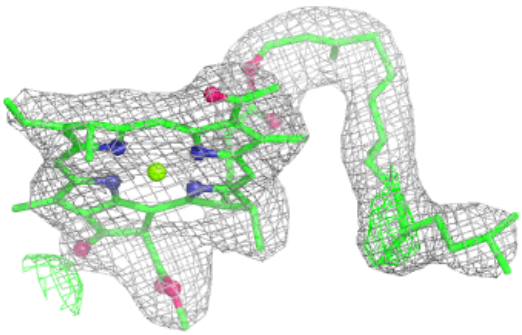


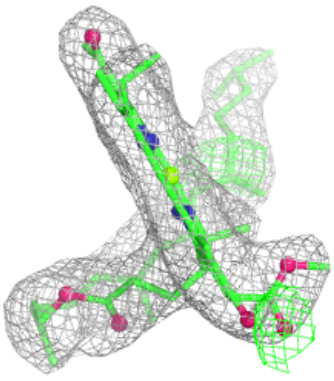


Electron density around BCB L 302 (B):

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

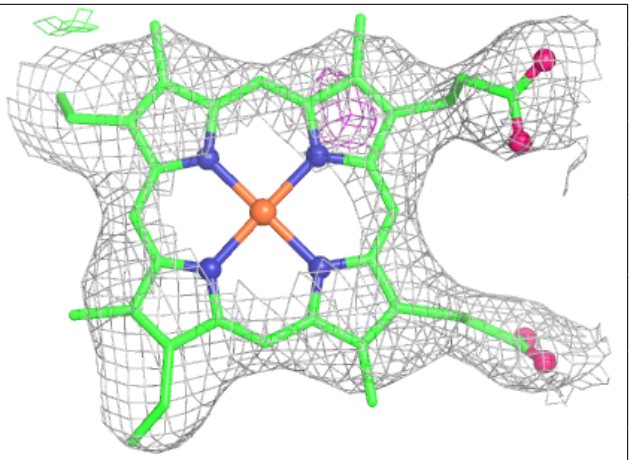


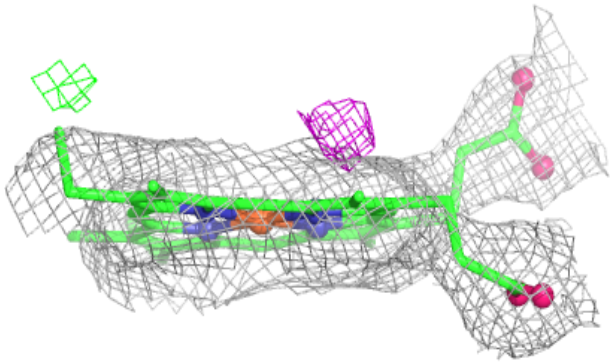


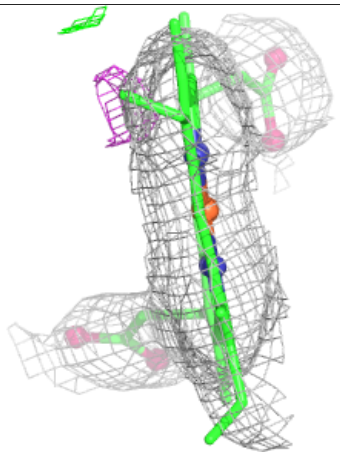


Electron density around HEC C 401:

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

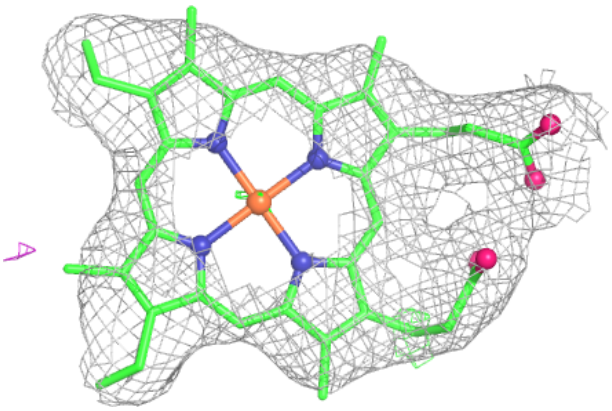


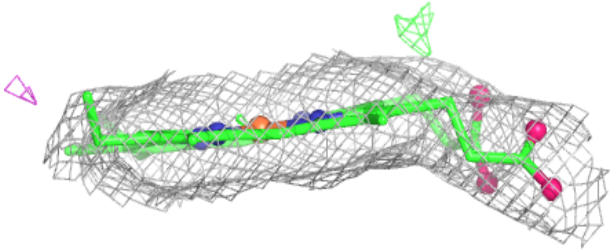


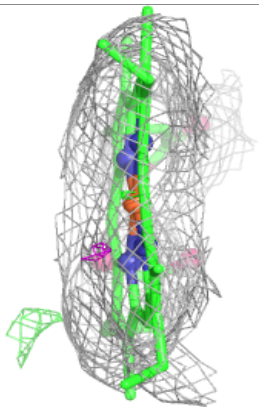


Electron density around HEC C 402:

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

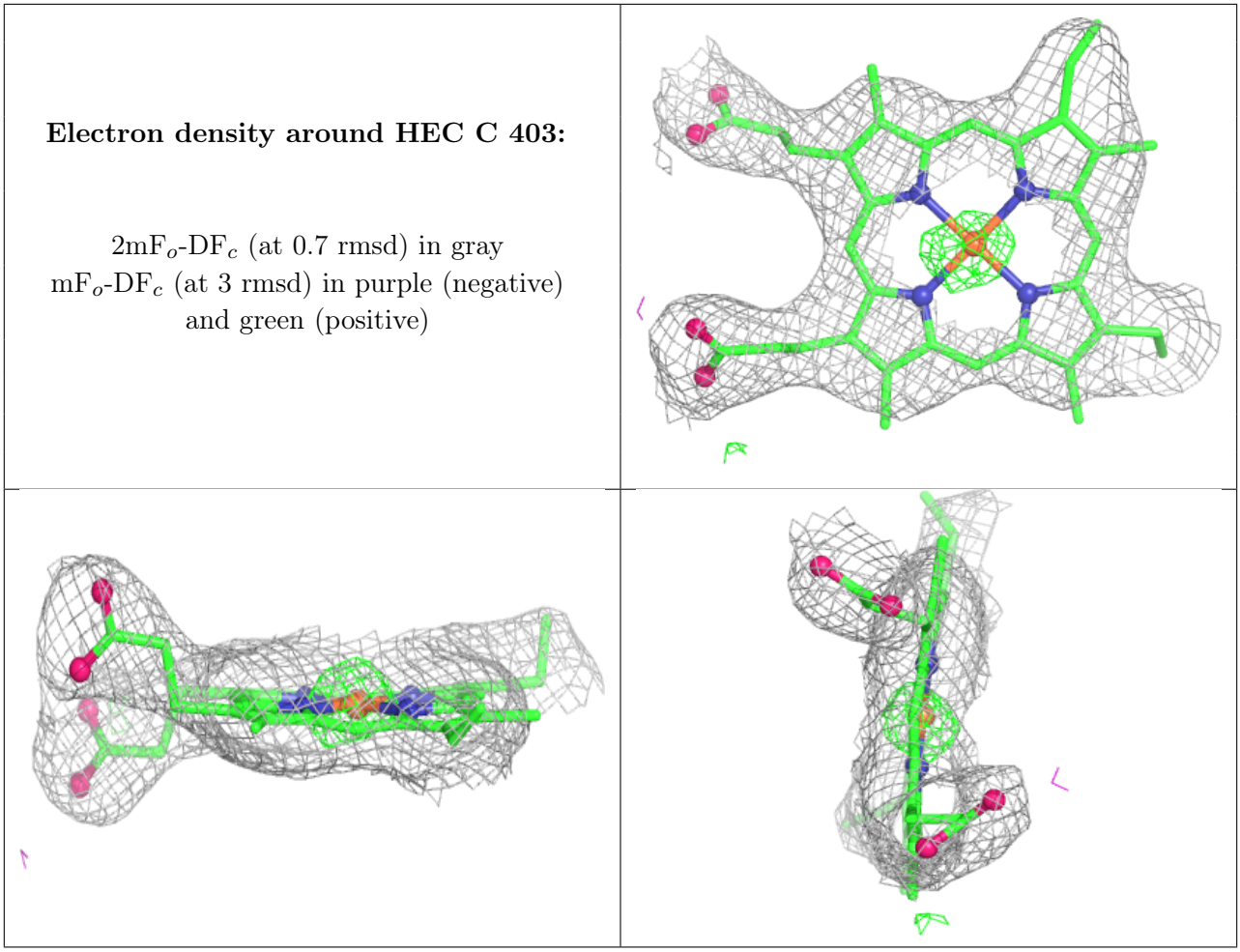






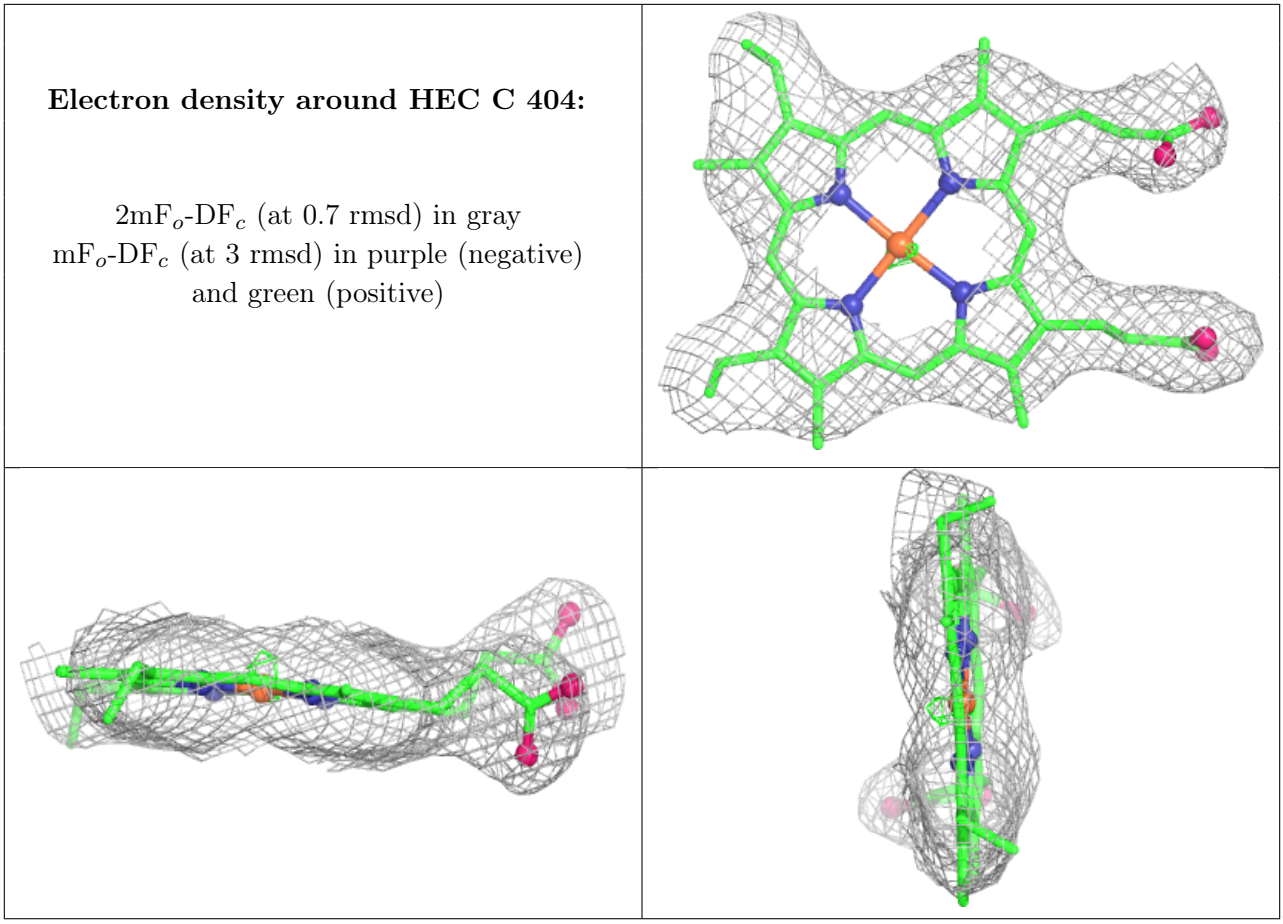
Electron density around HEC C 403:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.