



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:17 PM UTC

PDB ID : 3T6D / pdb_00003t6d
Title : Crystal Structure of the Reaction Centre from Blastochloris viridis strain DSM 133 (ATCC 19567) substrain-08
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2011-07-28
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

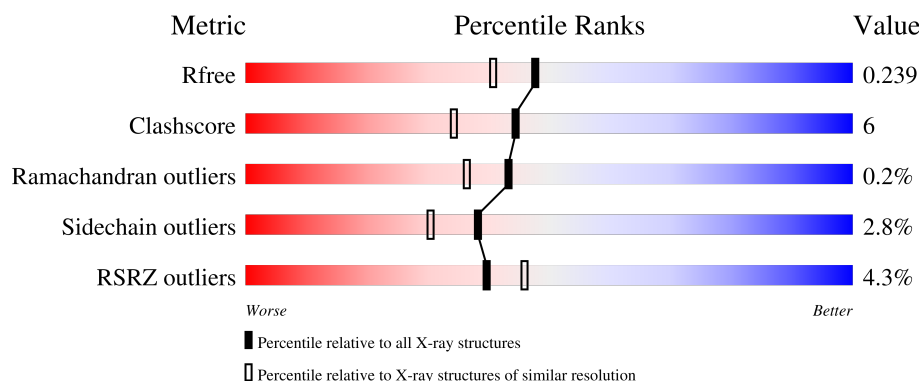
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	356	2% 85% 8% 6%
2	H	258	6% 88% 12%
3	L	273	3% 89% 11%
4	M	323	6% 91% 8%

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	GOL	C	370	-	-	-	X
10	GOL	C	373	-	-	-	X
10	GOL	C	377	-	-	X	-
11	BCB	L	400	X	-	-	-
11	BCB	L	401	X	-	-	-
11	BCB	M	400	X	-	-	-
11	BCB	M	401	X	-	-	-
17	HTH	M	332	-	-	-	X
6	LDA	H	718[B]	-	-	-	X
6	LDA	L	712	-	-	-	X
8	SO4	M	326	-	-	X	-
9	HTO	C	355	-	-	X	-
9	HTO	C	358[A]	-	X	-	-
9	HTO	H	274[A]	-	-	-	X
9	HTO	L	279	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 12156 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	334	Total	C	N	O	S	0	3	0
			2647	1667	474	486	20			

- Molecule 2 is a protein called Photosynthetic reaction center H-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	44	4	0
			2035	1300	353	379	3			

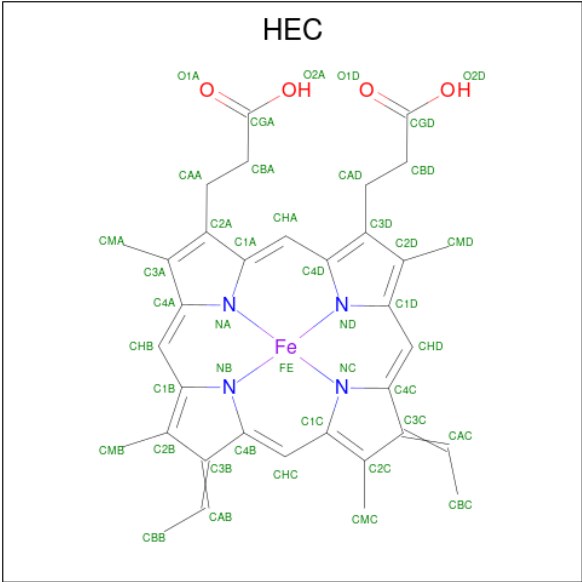
- Molecule 3 is a protein called Photosynthetic reaction center L-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	2	0
			2191	1474	352	358	7			

- Molecule 4 is a protein called Photosynthetic reaction center M-subunit.

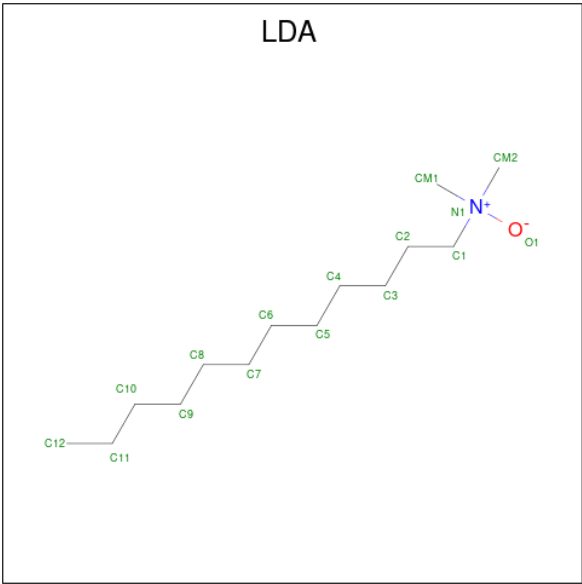
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2574	1716	424	423	11			

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



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

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



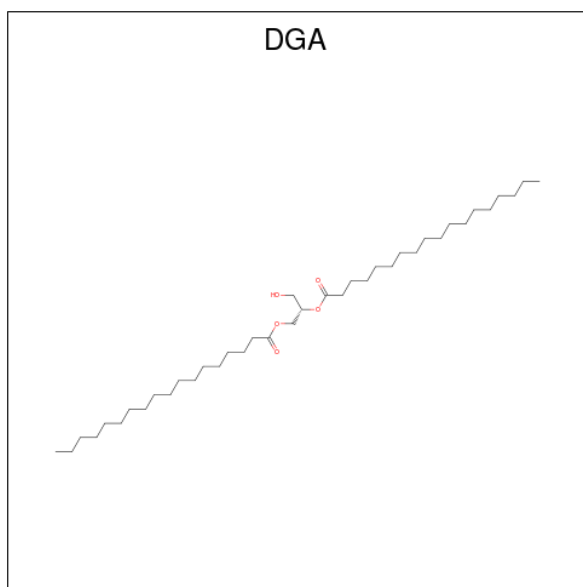
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total 16	C 14	N 1	O 1	0	0
6	C	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	1
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	H	1	Total 16	C 14	N 1	O 1	0	0
6	L	1	Total 16	C 14	N 1	O 1	0	0
6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

Continued on next page...

Continued from previous page...

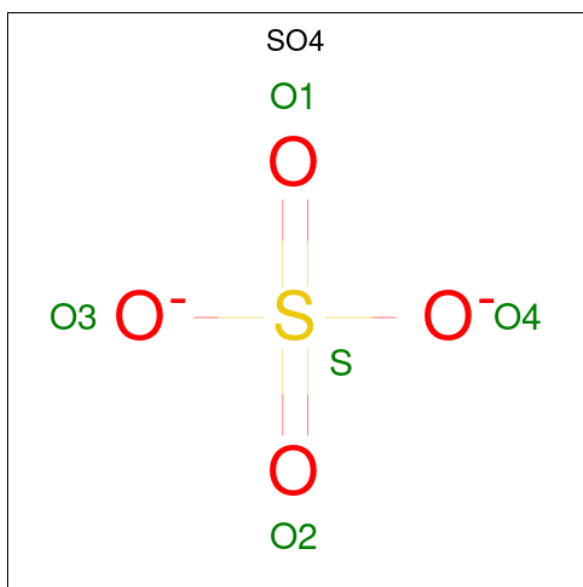
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	1
			10	8	2		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

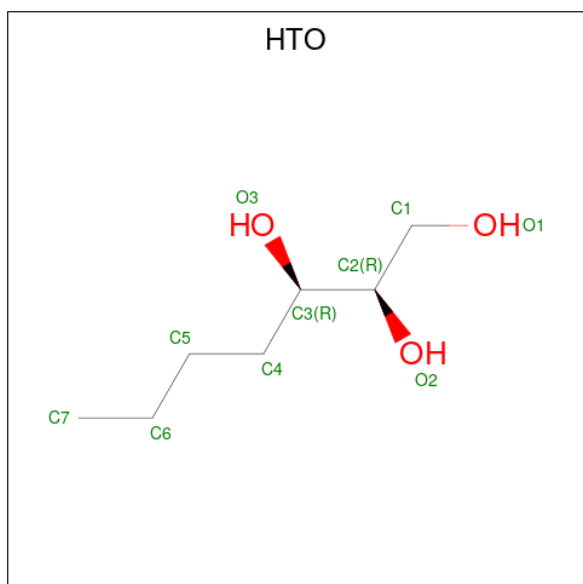
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	1
			10	8	2		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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

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



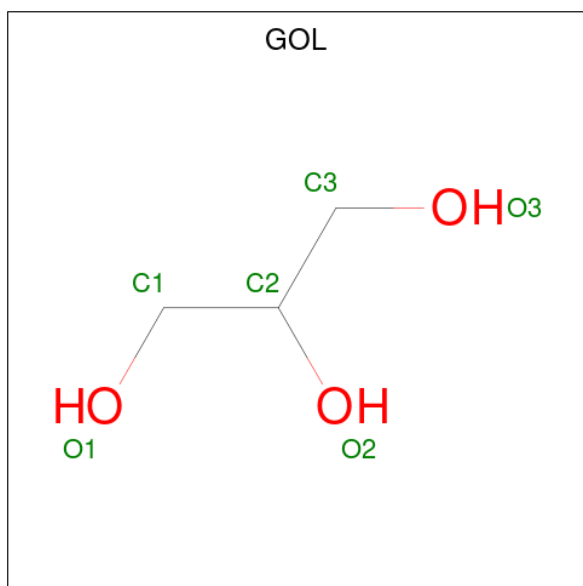
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	1
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		

Continued on next page...

Continued from previous page...

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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	1
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 8	C 4	O 4	0	1
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0

Continued on next page...

Continued from previous page...

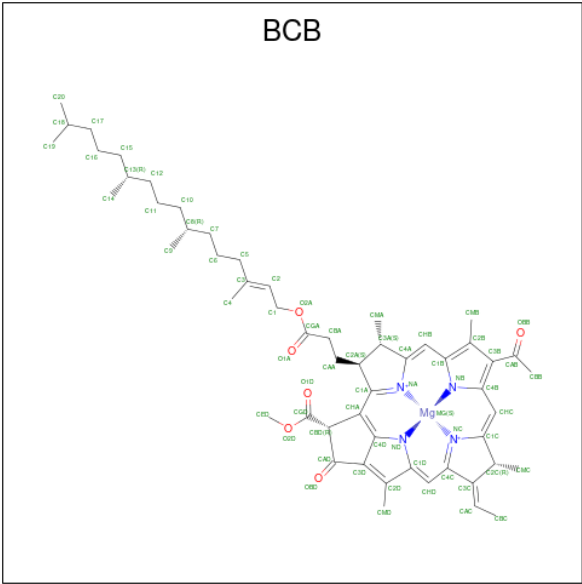
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		
10	L	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		
10	M	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆).



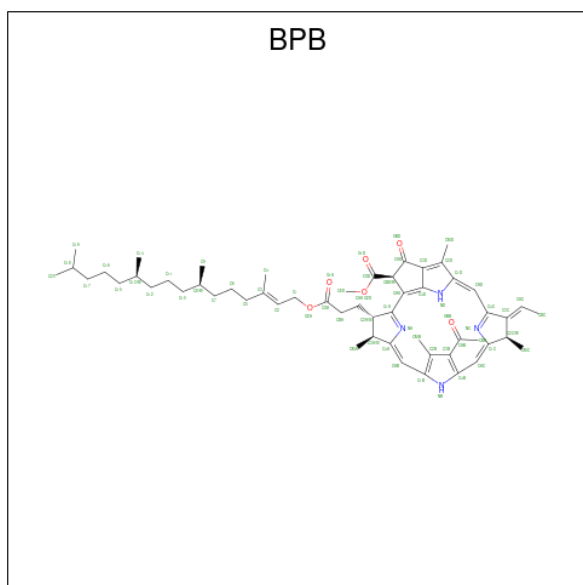
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

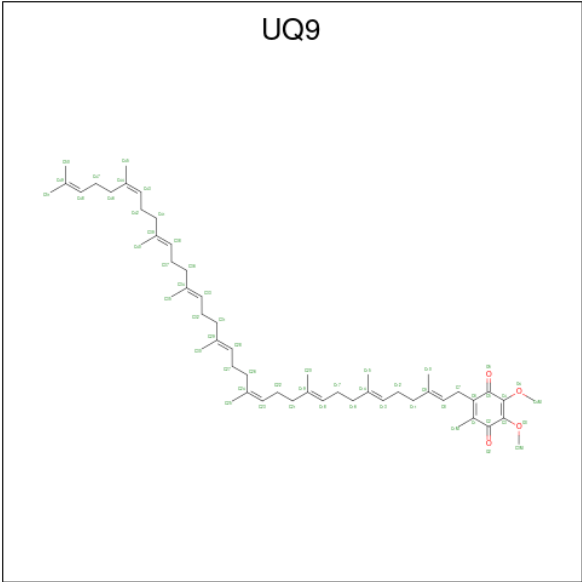
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 12 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$).



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

- Molecule 13 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).

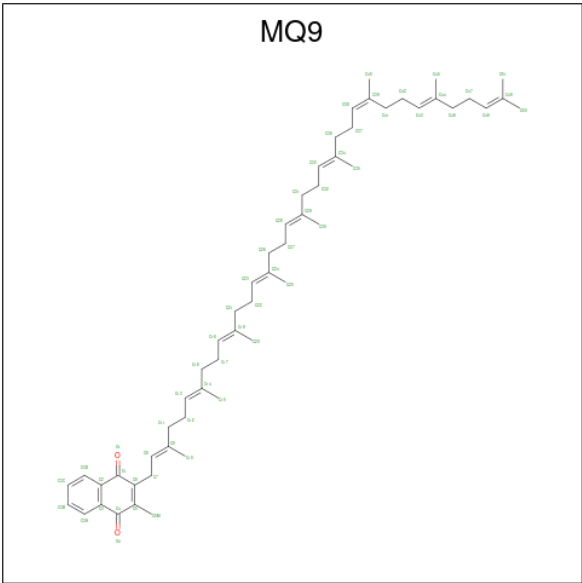


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	54	4		
13	L	1	Total	C	O	0	0
			23	19	4		

- Molecule 14 is FE (II) ION (CCD ID: FE2) (formula: Fe).

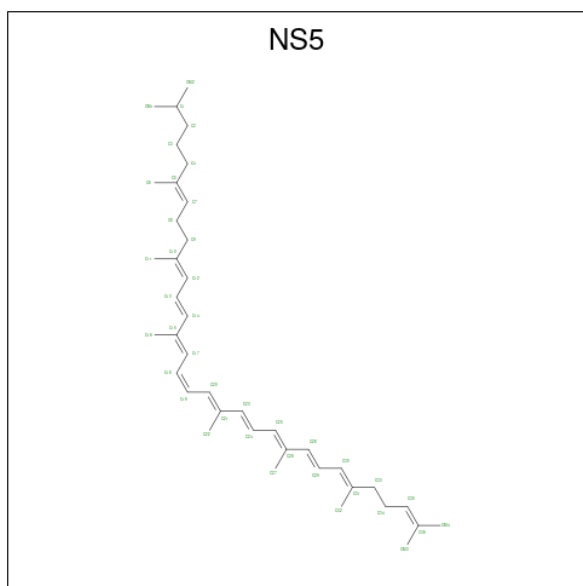
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total	Fe	0	0
			1	1		

- Molecule 15 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).



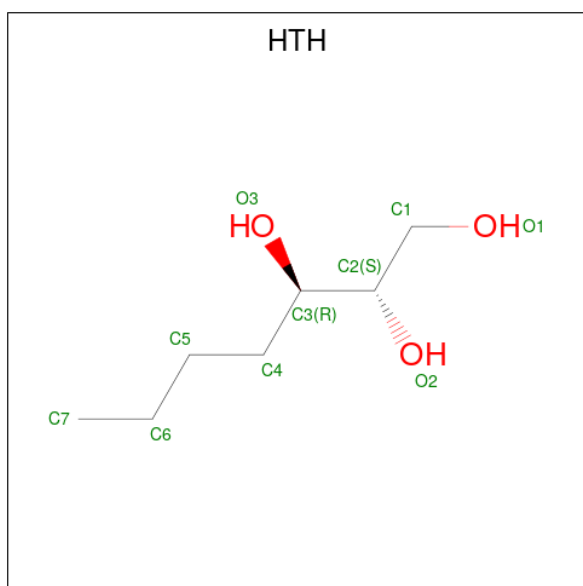
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 17 is (2S,3R)-heptane-1,2,3-triol (CCD ID: HTH) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	M	1	Total	C	O	0	0
			10	7	3		

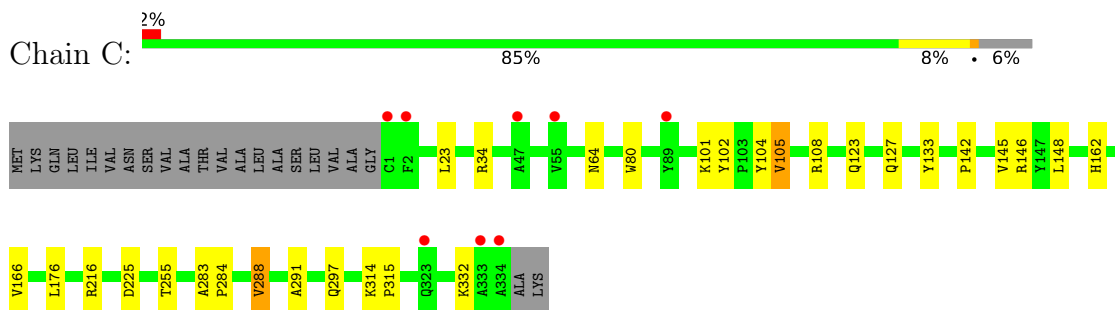
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	388	Total	O	0	0
			388	388		
18	H	211	Total	O	0	0
			211	211		
18	L	109	Total	O	0	0
			109	109		
18	M	153	Total	O	0	0
			153	153		

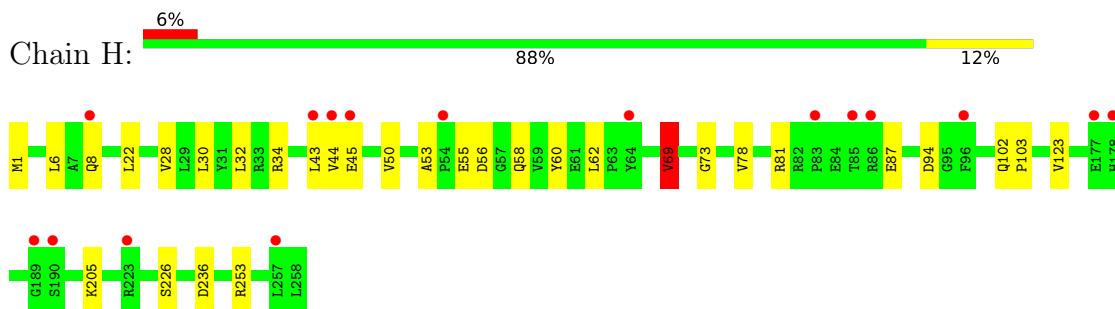
3 Residue-property plots [i](#)

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.

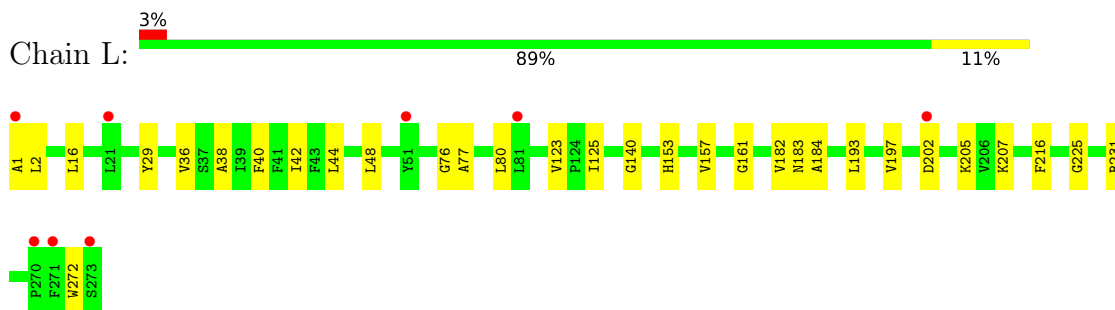
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



- Molecule 2: Photosynthetic reaction center H-subunit

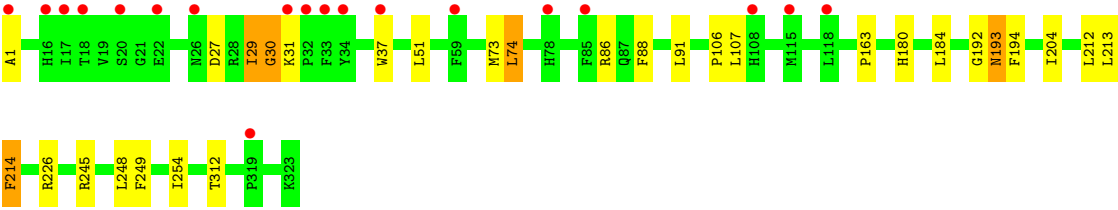


- Molecule 3: Photosynthetic reaction center L-subunit



- Molecule 4: Photosynthetic reaction center M-subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	220.44Å 220.44Å 113.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 1.95 48.34 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.34-1.95) 96.2 (48.34-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, R_{free}	0.182 , 0.216 (Not available) , 0.239	Depositor DCC
R_{free} test set	9677 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12156	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, DGA, UQ9, HEC, MQ9, SO4, BCB, BPB, LDA, HTH, HTO, NS5, FME, GOL

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	1.11	1/2716 (0.0%)	1.01	3/3701 (0.1%)
2	H	1.12	3/2069 (0.1%)	0.98	6/2827 (0.2%)
3	L	1.14	3/2280 (0.1%)	0.98	2/3113 (0.1%)
4	M	1.17	2/2679 (0.1%)	1.01	4/3662 (0.1%)
All	All	1.14	9/9744 (0.1%)	1.00	15/13303 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	142	PRO	CA-C	6.86	1.55	1.51
2	H	53	ALA	CA-C	-6.55	1.44	1.52
2	H	78	VAL	C-O	5.66	1.28	1.24
2	H	73	GLY	C-O	-5.61	1.17	1.24
4	M	312	THR	C-O	-5.58	1.20	1.25

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	VAL	CB-CA-C	-7.46	104.14	111.30
2	H	69	VAL	CB-CA-C	7.34	119.84	110.96
1	C	102	TYR	CA-C-N	-6.33	113.17	119.56
1	C	102	TYR	C-N-CA	-6.33	113.17	119.56
4	M	30	GLY	N-CA-C	-6.29	105.25	112.29

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	2647	0	2610	30	0
2	H	2035	0	2017	14	0
3	L	2191	0	2116	22	0
4	M	2574	0	2470	31	0
5	C	172	0	120	1	0
6	C	32	0	62	3	0
6	H	80	0	155	1	0
6	L	144	0	279	8	0
6	M	128	0	248	11	0
7	C	37	0	58	3	0
8	C	95	0	0	1	0
8	H	70	0	0	0	0
8	L	10	0	0	0	0
8	M	40	0	0	2	0
9	C	40	0	64	8	0
9	H	30	0	48	4	0
9	L	50	0	80	3	0
9	M	10	0	16	0	0
10	C	120	0	160	13	0
10	H	104	0	135	4	0
10	L	48	0	64	1	0
10	M	54	0	72	5	0
11	L	132	0	144	9	0
11	M	132	0	144	17	0
12	L	65	0	74	0	0
12	M	65	0	74	0	0
13	L	81	0	105	16	0
14	M	1	0	0	0	0
15	M	58	0	80	2	0
16	M	40	0	60	3	0
17	M	10	0	16	0	0
18	C	388	0	0	2	0
18	H	211	0	0	2	0
18	L	109	0	0	0	0
18	M	153	0	0	0	0
All	All	12156	0	11471	137	0

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

The worst 5 of 137 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)
13:L:502:UQ9:H15A	11:M:400:BCB:C9	1.75	1.15
13:L:502:UQ9:H15A	11:M:400:BCB:H93	1.46	0.98
13:L:502:UQ9:H15A	11:M:400:BCB:H91	1.49	0.94
6:C:716:LDA:H51	10:H:280:GOL:O1	1.75	0.85
3:L:272:TRP:CD1	4:M:86:ARG:HD3	2.13	0.83

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	335/356 (94%)	326 (97%)	9 (3%)	0	100	100
2	H	259/258 (100%)	247 (95%)	11 (4%)	1 (0%)	30	21
3	L	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	315 (98%)	7 (2%)	1 (0%)	36	28
All	All	1190/1210 (98%)	1156 (97%)	32 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	50	VAL
4	M	193	ASN

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	286/299 (96%)	281 (98%)	5 (2%)	53	49
2	H	209/211 (99%)	201 (96%)	8 (4%)	29	19
3	L	220/218 (101%)	214 (97%)	6 (3%)	39	32
4	M	249/247 (101%)	241 (97%)	8 (3%)	34	25
All	All	964/975 (99%)	937 (97%)	27 (3%)	38	30

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	16	LEU
3	L	80	LEU
4	M	194	PHE
3	L	48	LEU
3	L	202	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	220	ASN
3	L	183	ASN
3	L	239	ASN
3	L	213	ASN
2	H	102	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	H	1[A]	-	8,9,10	1.21	1 (12%)	8,9,11	2.94	2 (25%)
2	FME	H	1[B]	-	8,9,10	0.96	1 (12%)	8,9,11	2.95	2 (25%)

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[A]	-	-	3/7/9/11	-
2	FME	H	1[B]	-	-	4/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1[A]	FME	CN-N	2.29	1.40	1.33
2	H	1[B]	FME	CN-N	2.01	1.39	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1[B]	FME	CA-N-CN	-7.48	111.32	122.82
2	H	1[A]	FME	CA-N-CN	-7.16	111.81	122.82
2	H	1[A]	FME	CB-CA-N	2.97	115.93	110.52
2	H	1[B]	FME	CB-CA-N	-2.60	105.78	110.52

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1[A]	FME	O1-CN-N-CA
2	H	1[A]	FME	CB-CA-N-CN
2	H	1[B]	FME	O1-CN-N-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	1[A]	FME	CB-CG-SD-CE
2	H	1[B]	FME	CB-CA-N-CN

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 152 ligands modelled in this entry, 1 is monoatomic - leaving 151 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	$\# Z > 2$
10	GOL	H	290	-	5,5,5	0.35	0	5,5,5	0.56	0
10	GOL	L	288	-	5,5,5	0.15	0	5,5,5	0.67	0
10	GOL	M	340	-	5,5,5	0.47	0	5,5,5	0.61	0
8	SO4	C	344	-	4,4,4	0.51	0	6,6,6	0.19	0
9	HTO	H	274[A]	-	9,9,9	0.33	0	10,10,10	0.78	0
8	SO4	C	349	-	4,4,4	0.55	0	6,6,6	0.20	0
8	SO4	C	353	-	4,4,4	0.57	0	6,6,6	0.28	0
6	LDA	L	711	-	13,15,15	2.06	2 (15%)	14,17,17	0.60	0
10	GOL	C	359	-	5,5,5	0.85	0	5,5,5	0.89	0
10	GOL	H	278	-	5,5,5	0.49	0	5,5,5	0.83	0
8	SO4	C	339	-	4,4,4	0.42	0	6,6,6	0.41	0
8	SO4	H	264	-	4,4,4	0.43	0	6,6,6	0.16	0
6	LDA	L	724	-	13,15,15	2.28	2 (15%)	14,17,17	0.59	0
8	SO4	M	325	-	4,4,4	0.25	0	6,6,6	0.60	0
10	GOL	H	282	-	5,5,5	0.39	0	5,5,5	0.22	0
8	SO4	H	262	-	4,4,4	0.43	0	6,6,6	0.42	0
6	LDA	C	716	-	13,15,15	1.91	1 (7%)	14,17,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	H	291	-	5,5,5	0.38	0	5,5,5	0.45	0
5	HEC	C	403	1	46,50,50	1.88	11 (23%)	58,82,82	1.79	8 (13%)
6	LDA	H	701	-	13,15,15	1.55	2 (15%)	14,17,17	0.93	0
8	SO4	C	354	-	4,4,4	0.37	0	6,6,6	0.38	0
6	LDA	L	710	-	13,15,15	2.07	2 (15%)	14,17,17	0.48	0
10	GOL	H	279	-	5,5,5	0.39	0	5,5,5	0.57	0
6	LDA	H	721	-	13,15,15	1.97	2 (15%)	14,17,17	0.59	0
10	GOL	L	283	-	5,5,5	0.44	0	5,5,5	0.58	0
11	BCB	M	401	4	60,74,74	1.41	9 (15%)	59,115,115	3.33	19 (32%)
6	LDA	M	714	-	13,15,15	2.38	2 (15%)	14,17,17	0.36	0
8	SO4	H	261[B]	-	4,4,4	0.36	0	6,6,6	0.43	0
8	SO4	C	351	-	4,4,4	0.42	0	6,6,6	0.17	0
10	GOL	C	378	-	5,5,5	0.34	0	5,5,5	0.18	0
9	HTO	H	273	-	9,9,9	0.45	0	10,10,10	1.23	1 (10%)
8	SO4	C	340	-	4,4,4	0.45	0	6,6,6	0.67	0
6	LDA	M	713	-	13,15,15	2.00	2 (15%)	14,17,17	0.71	0
13	UQ9	L	503	-	23,23,58	2.20	9 (39%)	30,31,73	1.52	5 (16%)
8	SO4	L	275	-	4,4,4	0.42	0	6,6,6	0.15	0
10	GOL	C	369	-	5,5,5	0.40	0	5,5,5	0.66	0
9	HTO	C	356	-	9,9,9	0.79	0	10,10,10	1.78	2 (20%)
10	GOL	C	367	-	5,5,5	0.25	0	5,5,5	1.16	0
8	SO4	M	324	-	4,4,4	0.40	0	6,6,6	0.88	0
10	GOL	C	372	-	5,5,5	0.29	0	5,5,5	0.67	0
10	GOL	M	336	-	5,5,5	0.18	0	5,5,5	1.09	0
6	LDA	L	712	-	13,15,15	2.07	2 (15%)	14,17,17	0.35	0
8	SO4	M	329	-	4,4,4	0.40	0	6,6,6	0.33	0
8	SO4	M	326	-	4,4,4	0.29	0	6,6,6	0.45	0
8	SO4	C	352	-	4,4,4	0.41	0	6,6,6	0.17	0
6	LDA	L	702	-	13,15,15	2.15	2 (15%)	14,17,17	0.63	0
10	GOL	L	287	-	5,5,5	0.36	0	5,5,5	0.64	0
6	LDA	L	723	-	13,15,15	2.38	2 (15%)	14,17,17	0.78	0
10	GOL	C	373	-	5,5,5	0.36	0	5,5,5	0.29	0
9	HTO	L	278	-	9,9,9	0.68	0	10,10,10	1.64	3 (30%)
8	SO4	H	270	-	4,4,4	0.44	0	6,6,6	0.18	0
5	HEC	C	402	1	46,50,50	1.68	7 (15%)	58,82,82	1.80	7 (12%)
8	SO4	H	263	-	4,4,4	0.47	0	6,6,6	0.28	0
8	SO4	M	327	-	4,4,4	0.51	0	6,6,6	0.21	0
10	GOL	C	375	-	5,5,5	0.29	0	5,5,5	0.21	0
9	HTO	L	277	-	9,9,9	0.46	0	10,10,10	1.32	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	M	335	-	5,5,5	0.46	0	5,5,5	0.38	0
7	DGA	C	730	1	36,36,43	0.87	2 (5%)	38,38,45	1.43	6 (15%)
11	BCB	M	400	4	60,74,74	1.33	5 (8%)	59,115,115	3.01	18 (30%)
10	GOL	M	337	-	5,5,5	0.34	0	5,5,5	0.38	0
8	SO4	C	337[A]	-	4,4,4	0.47	0	6,6,6	0.21	0
9	HTO	C	355	-	9,9,9	0.58	0	10,10,10	1.65	3 (30%)
8	SO4	C	342	-	4,4,4	0.48	0	6,6,6	0.22	0
12	BPB	L	402	-	57,70,70	1.22	4 (7%)	55,101,101	2.36	14 (25%)
6	LDA	H	719	-	13,15,15	2.09	2 (15%)	14,17,17	0.53	0
10	GOL	M	339	-	5,5,5	0.26	0	5,5,5	0.35	0
13	UQ9	L	502	-	58,58,58	2.28	24 (41%)	72,73,73	1.55	14 (19%)
10	GOL	H	283	-	5,5,5	0.19	0	5,5,5	1.05	0
6	LDA	M	705	-	13,15,15	1.96	2 (15%)	14,17,17	0.53	0
9	HTO	L	279	-	9,9,9	0.42	0	10,10,10	1.45	1 (10%)
6	LDA	L	703	-	13,15,15	2.40	2 (15%)	14,17,17	0.57	0
8	SO4	L	274	-	4,4,4	0.40	0	6,6,6	0.34	0
8	SO4	C	348	-	4,4,4	0.50	0	6,6,6	0.40	0
8	SO4	C	347	-	4,4,4	0.64	0	6,6,6	0.21	0
6	LDA	L	709	-	13,15,15	1.93	2 (15%)	14,17,17	0.46	0
10	GOL	H	280	-	5,5,5	0.75	0	5,5,5	1.15	1 (20%)
10	GOL	H	285	-	5,5,5	0.18	0	5,5,5	0.62	0
10	GOL	H	284	-	5,5,5	0.37	0	5,5,5	0.87	0
6	LDA	C	722	-	13,15,15	2.19	2 (15%)	14,17,17	0.58	0
5	HEC	C	401	1	46,50,50	1.80	13 (28%)	58,82,82	2.24	8 (13%)
8	SO4	H	267	-	4,4,4	0.37	0	6,6,6	0.20	0
10	GOL	H	276[B]	-	5,5,5	0.84	0	5,5,5	0.98	0
10	GOL	M	338	-	5,5,5	0.42	0	5,5,5	0.51	0
8	SO4	H	271	-	4,4,4	0.45	0	6,6,6	0.11	0
5	HEC	C	404	1	46,50,50	1.65	7 (15%)	58,82,82	1.88	12 (20%)
8	SO4	C	345	-	4,4,4	0.43	0	6,6,6	0.29	0
10	GOL	M	334	-	5,5,5	0.15	0	5,5,5	0.32	0
10	GOL	C	364	-	5,5,5	0.57	0	5,5,5	1.01	0
10	GOL	C	377	-	5,5,5	0.18	0	5,5,5	0.37	0
9	HTO	H	272	-	9,9,9	0.75	0	10,10,10	1.74	4 (40%)
10	GOL	C	371	-	5,5,5	0.35	0	5,5,5	0.83	0
10	GOL	L	284	-	5,5,5	0.38	0	5,5,5	0.53	0
9	HTO	L	280	-	9,9,9	0.44	0	10,10,10	1.00	1 (10%)
10	GOL	C	360	-	5,5,5	0.26	0	5,5,5	0.67	0
6	LDA	M	707	-	13,15,15	2.11	2 (15%)	14,17,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	H	277	-	5,5,5	0.42	0	5,5,5	0.58	0
9	HTO	C	358[A]	-	9,9,9	0.75	0	10,10,10	2.65	4 (40%)
10	GOL	M	342	-	5,5,5	0.41	0	5,5,5	0.71	0
8	SO4	M	330	-	4,4,4	0.52	0	6,6,6	0.18	0
6	LDA	M	715	-	13,15,15	1.96	1 (7%)	14,17,17	0.44	0
8	SO4	H	266	-	4,4,4	0.46	0	6,6,6	0.38	0
8	SO4	H	269	-	4,4,4	0.47	0	6,6,6	0.20	0
10	GOL	C	361	-	5,5,5	0.60	0	5,5,5	1.15	1 (20%)
8	SO4	C	338	-	4,4,4	0.51	0	6,6,6	0.44	0
8	SO4	H	268	-	4,4,4	0.40	0	6,6,6	0.15	0
10	GOL	M	341	-	5,5,5	0.39	0	5,5,5	0.25	0
6	LDA	M	717	-	13,15,15	2.01	2 (15%)	14,17,17	0.59	0
10	GOL	L	282	-	5,5,5	0.90	0	5,5,5	1.25	1 (20%)
8	SO4	H	261[A]	-	4,4,4	0.50	0	6,6,6	0.34	0
10	GOL	C	363	-	5,5,5	0.82	0	5,5,5	1.12	0
12	BPB	M	402	-	57,70,70	1.24	5 (8%)	55,101,101	1.71	10 (18%)
9	HTO	L	276	-	9,9,9	0.49	0	10,10,10	1.52	2 (20%)
9	HTO	C	357	-	9,9,9	0.61	0	10,10,10	0.77	0
10	GOL	H	276[A]	-	5,5,5	0.85	0	5,5,5	0.59	0
10	GOL	L	286	-	5,5,5	0.21	0	5,5,5	0.84	0
10	GOL	C	366	-	5,5,5	0.48	0	5,5,5	0.44	0
17	HTH	M	332	-	9,9,9	0.44	0	10,10,10	1.19	1 (10%)
10	GOL	C	370	-	5,5,5	0.27	0	5,5,5	0.25	0
11	BCB	L	400	3	60,74,74	1.10	5 (8%)	59,115,115	2.77	19 (32%)
10	GOL	C	365	-	5,5,5	0.36	0	5,5,5	0.38	0
10	GOL	H	275	-	5,5,5	0.68	0	5,5,5	0.40	0
8	SO4	H	260	-	4,4,4	0.43	0	6,6,6	0.22	0
8	SO4	C	341	-	4,4,4	0.45	0	6,6,6	0.27	0
10	GOL	H	286	-	5,5,5	0.26	0	5,5,5	0.61	0
8	SO4	H	259	-	4,4,4	0.36	0	6,6,6	0.43	0
10	GOL	L	281	-	5,5,5	0.19	0	5,5,5	0.48	0
8	SO4	C	343	-	4,4,4	0.24	0	6,6,6	0.80	0
8	SO4	C	337[B]	-	4,4,4	0.45	0	6,6,6	0.21	0
11	BCB	L	401	3	60,74,74	1.41	7 (11%)	59,115,115	3.05	18 (30%)
8	SO4	M	328	-	4,4,4	0.40	0	6,6,6	0.25	0
10	GOL	C	374[B]	-	5,5,5	0.35	0	5,5,5	0.42	0
10	GOL	H	281	-	5,5,5	0.57	0	5,5,5	0.38	0
15	MQ9	M	501	-	59,59,59	2.31	25 (42%)	73,75,75	1.20	8 (10%)
8	SO4	M	331	-	4,4,4	0.45	0	6,6,6	0.17	0
9	HTO	M	333	-	9,9,9	0.51	0	10,10,10	2.66	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	H	265	-	4,4,4	0.52	0	6,6,6	0.32	0
6	LDA	H	720	-	13,15,15	2.38	2 (15%)	14,17,17	0.76	0
10	GOL	H	288	-	5,5,5	0.39	0	5,5,5	0.38	0
10	GOL	H	287	-	5,5,5	0.32	0	5,5,5	0.12	0
10	GOL	L	285	-	5,5,5	0.57	0	5,5,5	0.78	0
6	LDA	M	704	-	13,15,15	2.45	2 (15%)	14,17,17	1.53	3 (21%)
6	LDA	H	718[B]	-	13,15,15	2.06	2 (15%)	14,17,17	0.61	0
6	LDA	L	708	-	13,15,15	1.82	1 (7%)	14,17,17	1.25	2 (14%)
10	GOL	C	362	-	5,5,5	0.72	0	5,5,5	0.89	0
8	SO4	C	350	-	4,4,4	0.47	0	6,6,6	0.14	0
10	GOL	C	376	-	5,5,5	0.34	0	5,5,5	0.32	0
6	LDA	M	706	-	13,15,15	2.00	2 (15%)	14,17,17	0.57	0
10	GOL	C	368	-	5,5,5	0.15	0	5,5,5	0.74	0
10	GOL	H	289	-	5,5,5	0.34	0	5,5,5	0.27	0
16	NS5	M	600	-	39,39,39	1.60	11 (28%)	46,46,46	2.79	15 (32%)
8	SO4	C	346	-	4,4,4	0.49	0	6,6,6	0.40	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
10	GOL	H	290	-	-	2/4/4/4	-
10	GOL	L	288	-	-	2/4/4/4	-
10	GOL	M	340	-	-	2/4/4/4	-
9	HTO	H	274[A]	-	-	4/10/10/10	-
10	GOL	H	278	-	-	2/4/4/4	-
6	LDA	L	711	-	-	4/13/13/13	-
10	GOL	C	359	-	-	1/4/4/4	-
6	LDA	L	724	-	-	6/13/13/13	-
10	GOL	H	282	-	-	2/4/4/4	-
6	LDA	C	716	-	-	10/13/13/13	-
10	GOL	H	291	-	-	2/4/4/4	-
5	HEC	C	403	1	-	4/14/54/54	-
6	LDA	H	701	-	-	4/13/13/13	-
6	LDA	L	710	-	-	8/13/13/13	-
10	GOL	H	279	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	H	721	-	-	10/13/13/13	-
10	GOL	L	283	-	-	2/4/4/4	-
11	BCB	M	401	4	3/3/21/26	10/37/137/137	-
6	LDA	M	714	-	-	8/13/13/13	-
10	GOL	C	378	-	-	2/4/4/4	-
9	HTO	H	273	-	-	4/10/10/10	-
6	LDA	M	713	-	-	4/13/13/13	-
13	UQ9	L	503	-	-	3/15/39/81	0/1/1/1
10	GOL	C	369	-	-	2/4/4/4	-
9	HTO	C	356	-	-	8/10/10/10	-
10	GOL	C	367	-	-	3/4/4/4	-
10	GOL	C	372	-	-	2/4/4/4	-
10	GOL	M	336	-	-	4/4/4/4	-
6	LDA	L	712	-	-	7/13/13/13	-
6	LDA	L	702	-	-	7/13/13/13	-
10	GOL	L	287	-	-	0/4/4/4	-
6	LDA	L	723	-	-	8/13/13/13	-
10	GOL	C	373	-	-	2/4/4/4	-
9	HTO	L	278	-	-	4/10/10/10	-
5	HEC	C	402	1	-	9/14/54/54	-
10	GOL	C	375	-	-	0/4/4/4	-
9	HTO	L	277	-	-	0/10/10/10	-
10	GOL	M	335	-	-	0/4/4/4	-
7	DGA	C	730	1	-	27/37/37/45	-
11	BCB	M	400	4	3/3/21/26	11/37/137/137	-
10	GOL	M	337	-	-	2/4/4/4	-
9	HTO	C	355	-	-	4/10/10/10	-
12	BPB	L	402	-	-	3/37/105/105	0/5/6/6
6	LDA	H	719	-	-	8/13/13/13	-
10	GOL	M	339	-	-	2/4/4/4	-
13	UQ9	L	502	-	-	17/57/81/81	0/1/1/1
10	GOL	H	283	-	-	4/4/4/4	-
6	LDA	M	705	-	-	6/13/13/13	-
9	HTO	L	279	-	-	3/10/10/10	-
6	LDA	L	703	-	-	6/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	L	709	-	-	6/13/13/13	-
10	GOL	H	280	-	-	2/4/4/4	-
10	GOL	H	285	-	-	3/4/4/4	-
10	GOL	H	284	-	-	2/4/4/4	-
6	LDA	C	722	-	-	9/13/13/13	-
5	HEC	C	401	1	-	7/14/54/54	-
10	GOL	H	276[B]	-	-	2/4/4/4	-
10	GOL	M	338	-	-	4/4/4/4	-
5	HEC	C	404	1	-	5/14/54/54	-
10	GOL	M	334	-	-	4/4/4/4	-
10	GOL	C	364	-	-	3/4/4/4	-
10	GOL	C	377	-	-	2/4/4/4	-
9	HTO	H	272	-	-	1/10/10/10	-
10	GOL	C	371	-	-	0/4/4/4	-
10	GOL	L	284	-	-	4/4/4/4	-
9	HTO	L	280	-	-	5/10/10/10	-
10	GOL	C	360	-	-	0/4/4/4	-
6	LDA	M	707	-	-	7/13/13/13	-
10	GOL	H	277	-	-	2/4/4/4	-
9	HTO	C	358[A]	-	-	10/10/10/10	-
10	GOL	M	342	-	-	4/4/4/4	-
6	LDA	M	715	-	-	5/13/13/13	-
10	GOL	C	361	-	-	0/4/4/4	-
10	GOL	M	341	-	-	0/4/4/4	-
6	LDA	M	717	-	-	2/13/13/13	-
10	GOL	L	282	-	-	2/4/4/4	-
10	GOL	C	363	-	-	0/4/4/4	-
12	BPB	M	402	-	-	8/37/105/105	0/5/6/6
9	HTO	L	276	-	-	6/10/10/10	-
9	HTO	C	357	-	-	6/10/10/10	-
10	GOL	H	276[A]	-	-	4/4/4/4	-
10	GOL	L	286	-	-	4/4/4/4	-
10	GOL	C	366	-	-	2/4/4/4	-
17	HTH	M	332	-	-	7/10/10/10	-
10	GOL	C	370	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCB	L	400	3	3/3/21/26	7/37/137/137	-
10	GOL	C	365	-	-	2/4/4/4	-
10	GOL	H	275	-	-	2/4/4/4	-
10	GOL	H	286	-	-	3/4/4/4	-
10	GOL	L	281	-	-	0/4/4/4	-
11	BCB	L	401	3	3/3/21/26	7/37/137/137	-
10	GOL	C	374[B]	-	-	4/4/4/4	-
10	GOL	H	281	-	-	3/4/4/4	-
15	MQ9	M	501	-	-	2/53/73/73	0/2/2/2
9	HTO	M	333	-	-	7/10/10/10	-
6	LDA	H	720	-	-	6/13/13/13	-
10	GOL	H	288	-	-	2/4/4/4	-
10	GOL	H	287	-	-	4/4/4/4	-
10	GOL	L	285	-	-	2/4/4/4	-
6	LDA	M	704	-	-	5/13/13/13	-
6	LDA	H	718[B]	-	-	8/13/13/13	-
6	LDA	L	708	-	-	8/13/13/13	-
10	GOL	C	362	-	-	2/4/4/4	-
10	GOL	C	376	-	-	2/4/4/4	-
6	LDA	M	706	-	-	8/13/13/13	-
10	GOL	C	368	-	-	4/4/4/4	-
10	GOL	H	289	-	-	4/4/4/4	-
16	NS5	M	600	-	-	8/43/43/43	-

The worst 5 of 189 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	704	LDA	O1-N1	-7.60	1.23	1.42
6	H	720	LDA	O1-N1	-7.31	1.24	1.42
6	M	714	LDA	O1-N1	-7.26	1.24	1.42
6	L	724	LDA	O1-N1	-7.18	1.24	1.42
6	M	707	LDA	O1-N1	-7.03	1.24	1.42

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	401	BCB	C4B-CHC-C1C	13.68	130.12	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	C4B-CHC-C1C	13.06	129.72	121.32
11	M	401	BCB	O2D-CGD-CBD	12.40	124.57	110.95
11	M	401	BCB	C4B-CHC-C1C	12.07	129.08	121.32
5	C	401	HEC	CBB-CAB-C3B	-11.00	105.45	127.43

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	L	400	BCB	ND
11	L	400	BCB	NA
11	L	400	BCB	NC
11	L	401	BCB	ND
11	L	401	BCB	NA

5 of 475 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	401	HEC	C4B-C3B-CAB-CBB
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	401	HEC	C4C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

45 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	H	274[A]	HTO	1	0
6	L	711	LDA	1	0
10	H	278	GOL	2	0
6	L	724	LDA	2	0
6	C	716	LDA	3	0
6	L	710	LDA	1	0
10	H	279	GOL	1	0
6	H	721	LDA	1	0
11	M	401	BCB	4	0
6	M	714	LDA	2	0
9	H	273	HTO	2	0
13	L	503	UQ9	5	0
10	C	369	GOL	1	0
6	L	712	LDA	1	0
8	M	326	SO4	2	0

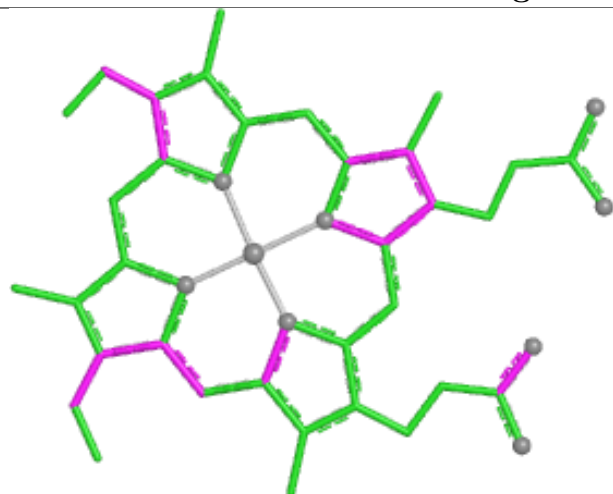
Continued on next page...

Continued from previous page...

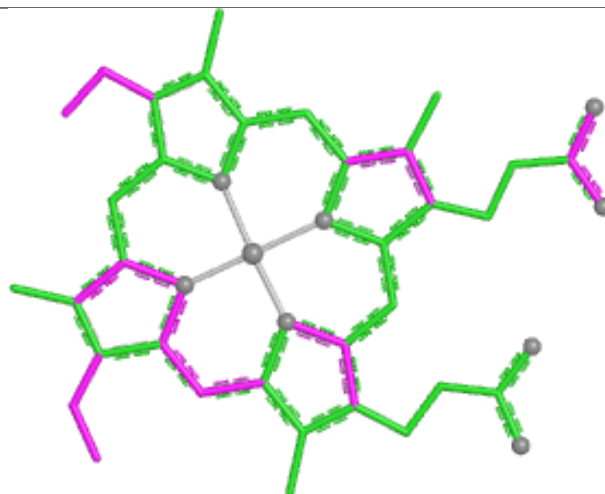
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	702	LDA	1	0
6	L	723	LDA	2	0
10	C	373	GOL	1	0
9	L	277	HTO	2	0
7	C	730	DGA	3	0
11	M	400	BCB	13	0
9	C	355	HTO	6	0
13	L	502	UQ9	11	0
9	L	279	HTO	1	0
10	H	280	GOL	1	0
5	C	401	HEC	1	0
10	M	338	GOL	3	0
10	M	334	GOL	1	0
10	C	364	GOL	3	0
10	C	377	GOL	4	0
9	H	272	HTO	1	0
6	M	707	LDA	1	0
10	M	342	GOL	1	0
6	M	715	LDA	2	0
8	C	338	SO4	1	0
10	C	363	GOL	1	0
9	C	357	HTO	2	0
10	L	286	GOL	1	0
11	L	400	BCB	5	0
10	C	365	GOL	2	0
11	L	401	BCB	4	0
15	M	501	MQ9	2	0
6	M	704	LDA	6	0
10	C	368	GOL	1	0
16	M	600	NS5	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

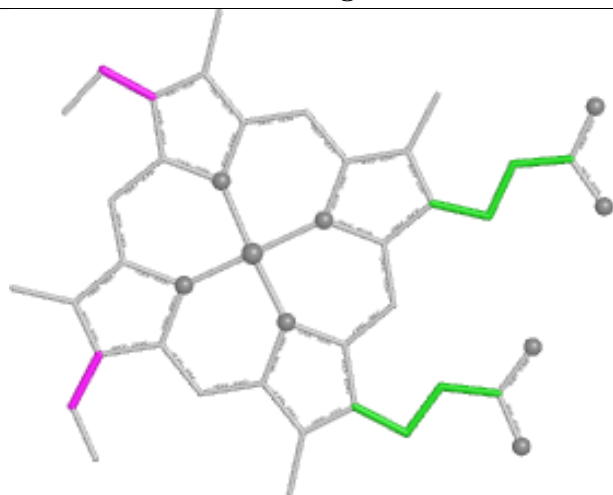
Ligand HEC C 403



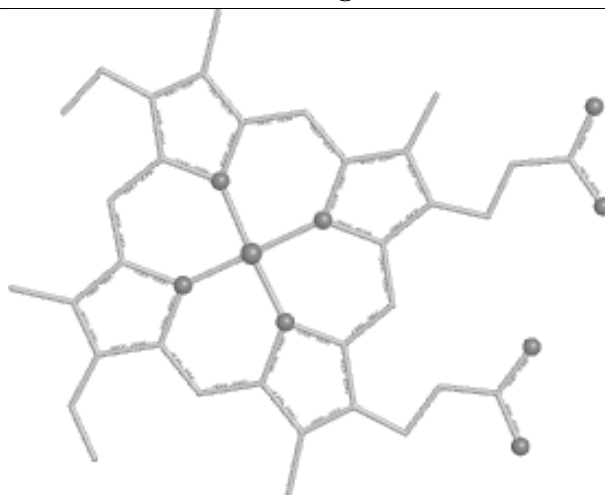
Bond lengths



Bond angles

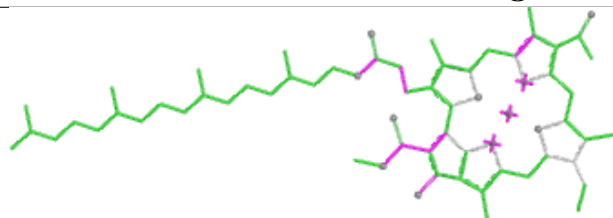


Torsions

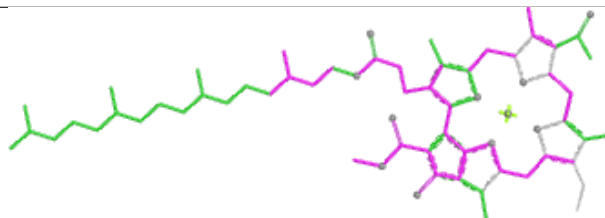


Rings

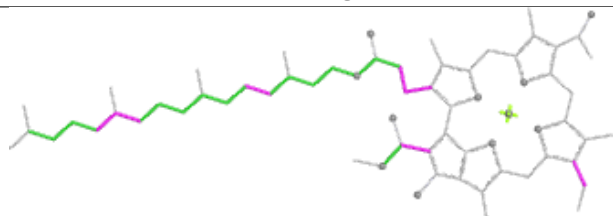
Ligand BCB M 401



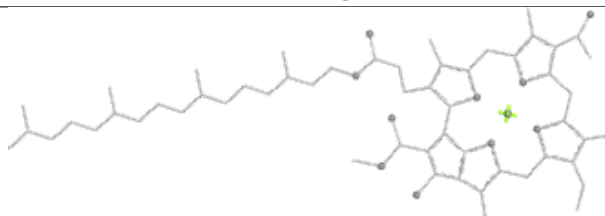
Bond lengths



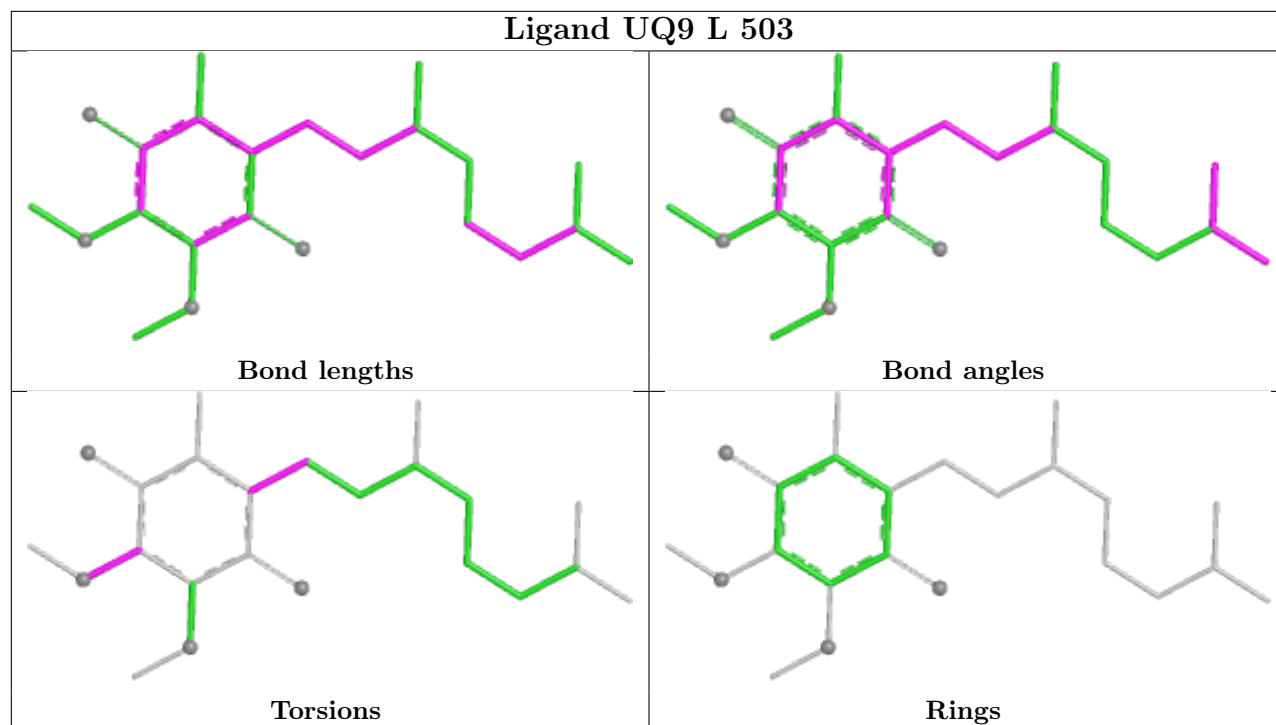
Bond angles



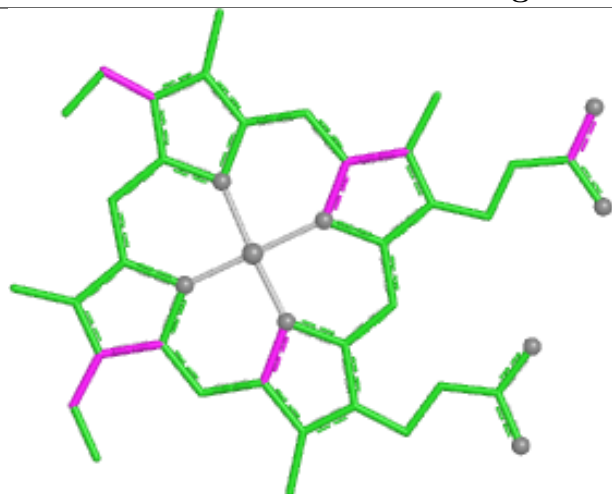
Torsions



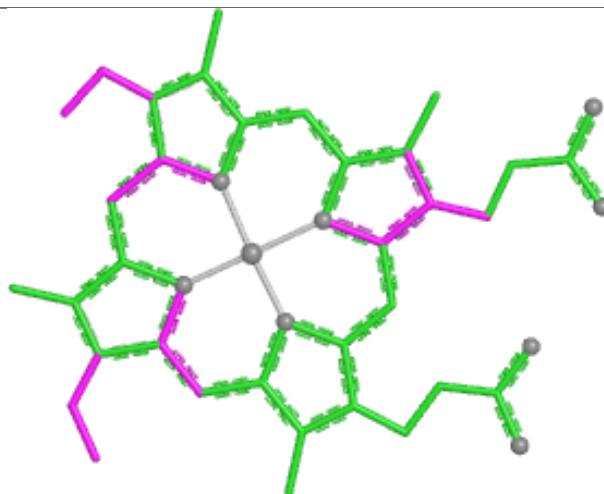
Rings



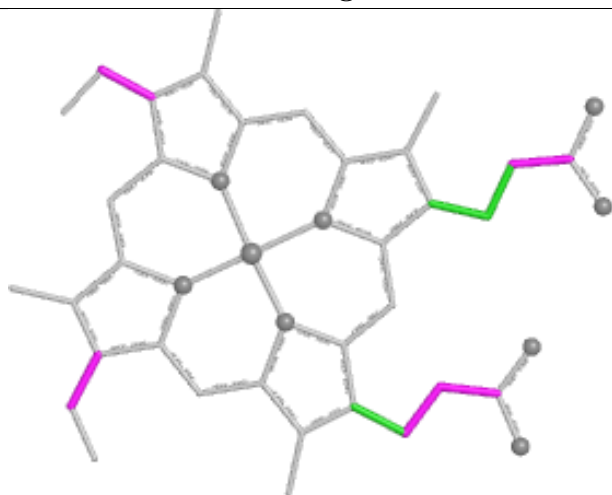
Ligand HEC C 402



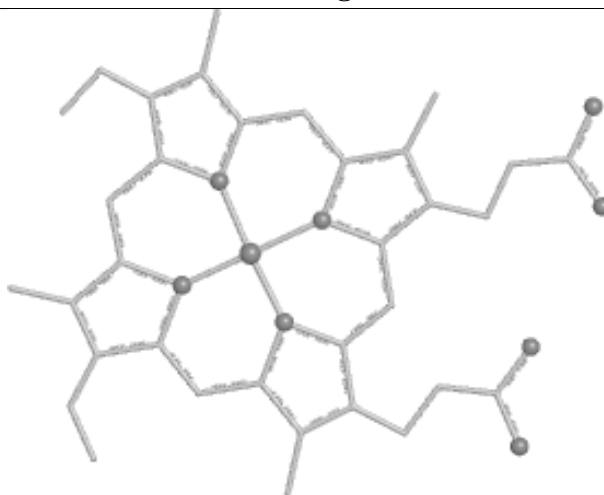
Bond lengths



Bond angles

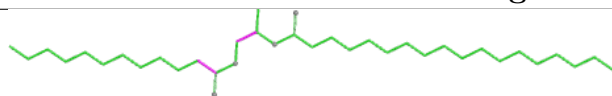


Torsions

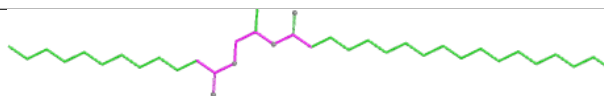


Rings

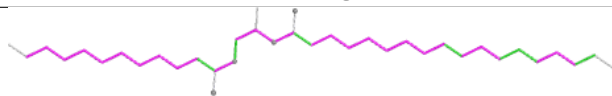
Ligand DGA C 730



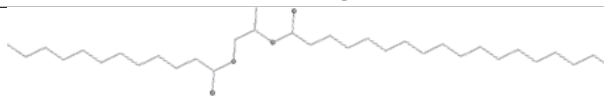
Bond lengths



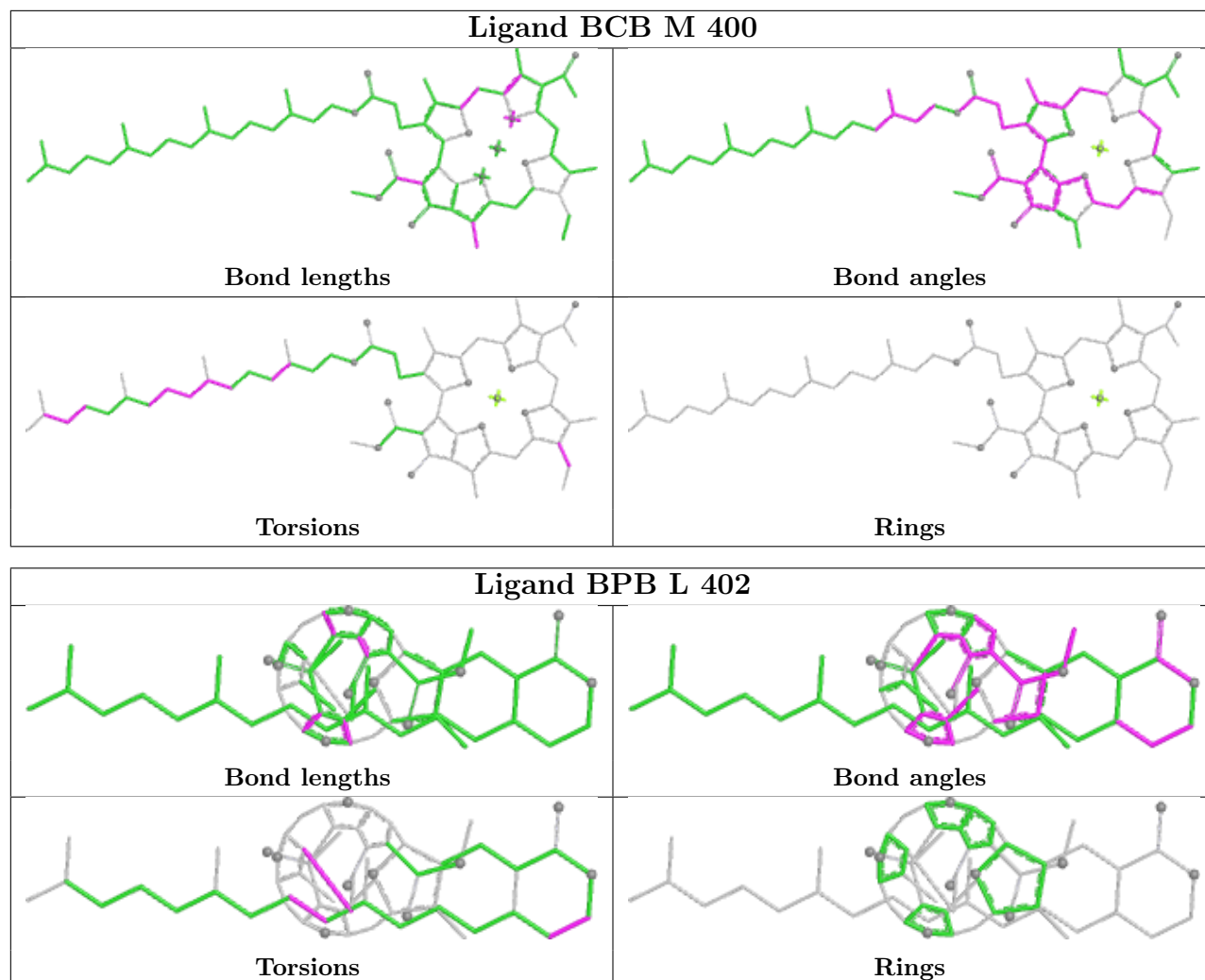
Bond angles

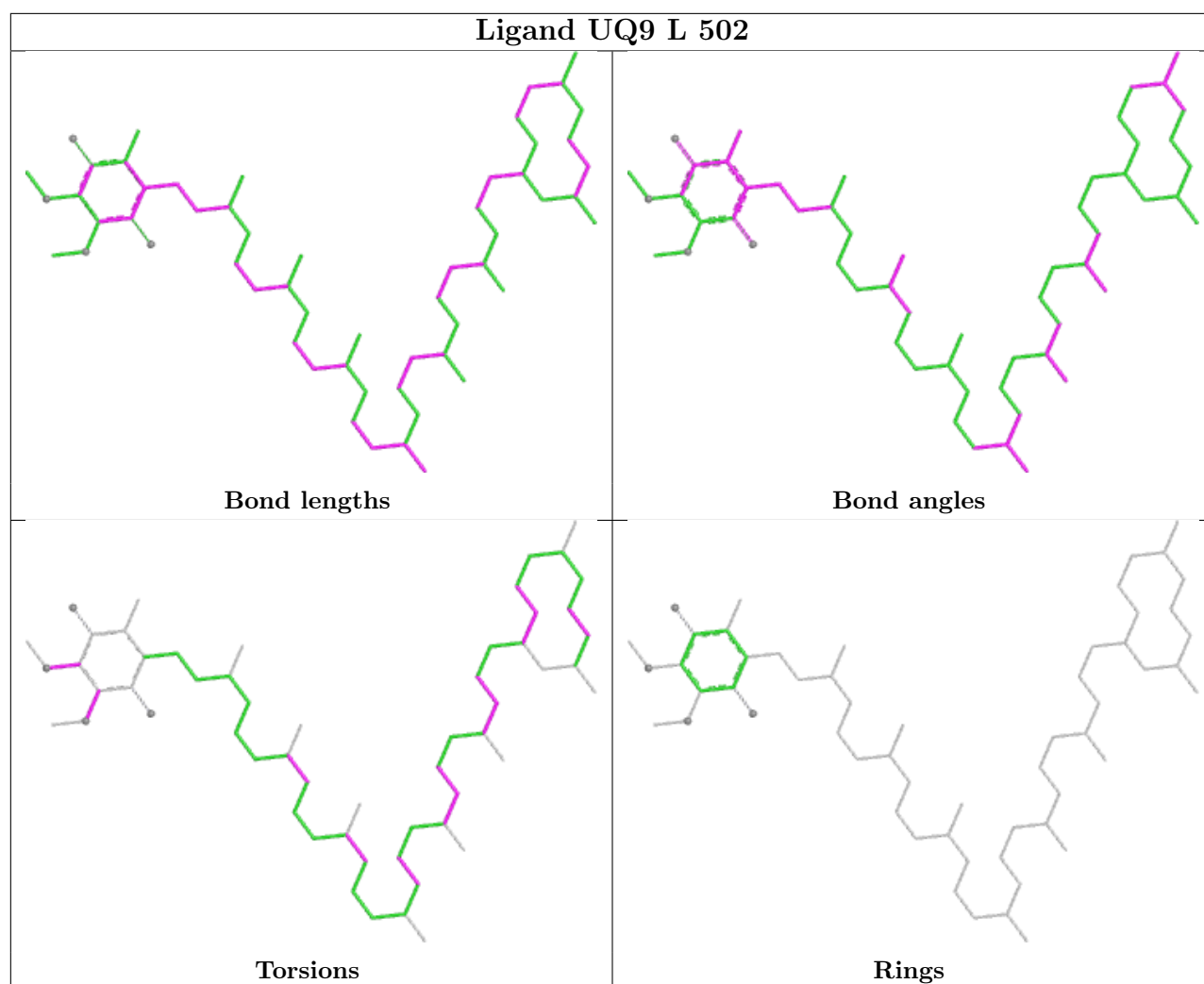


Torsions

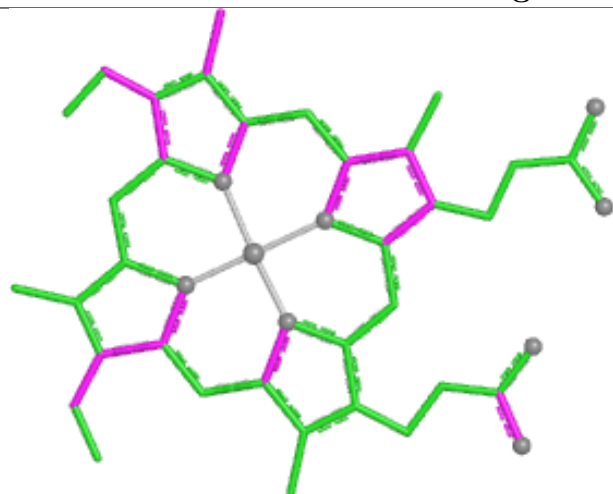


Rings

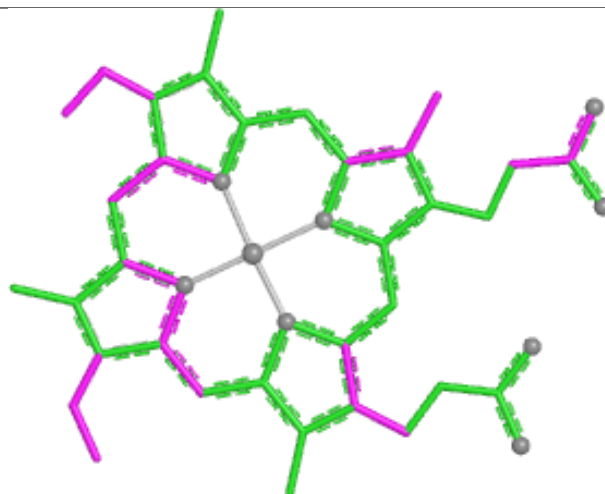




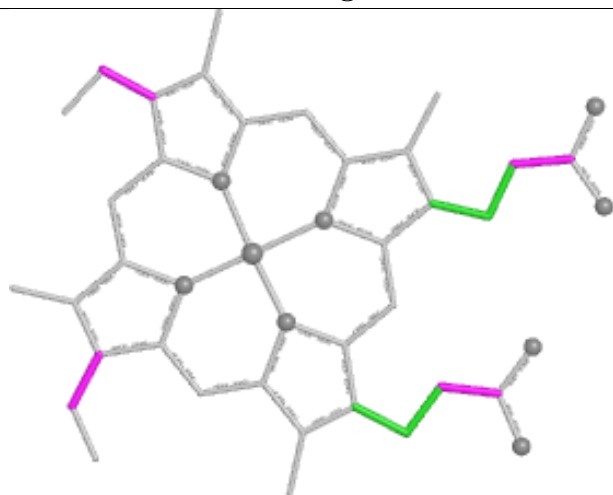
Ligand HEC C 401



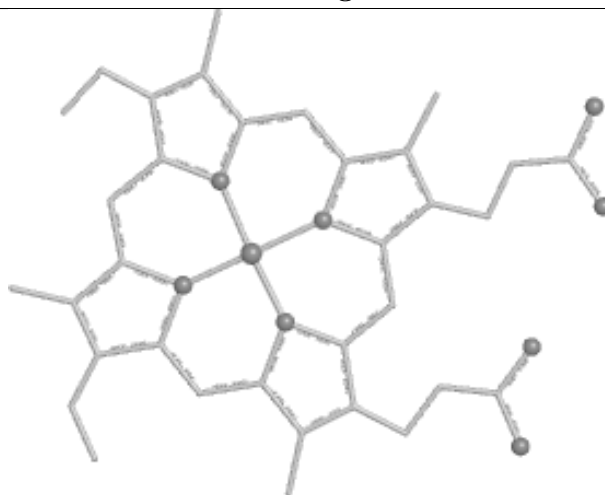
Bond lengths



Bond angles

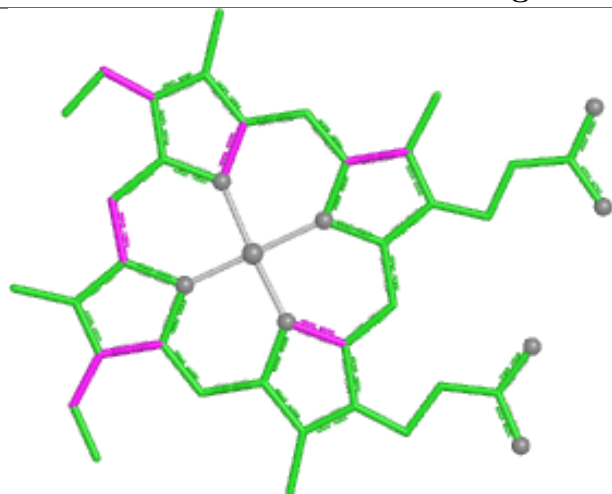


Torsions

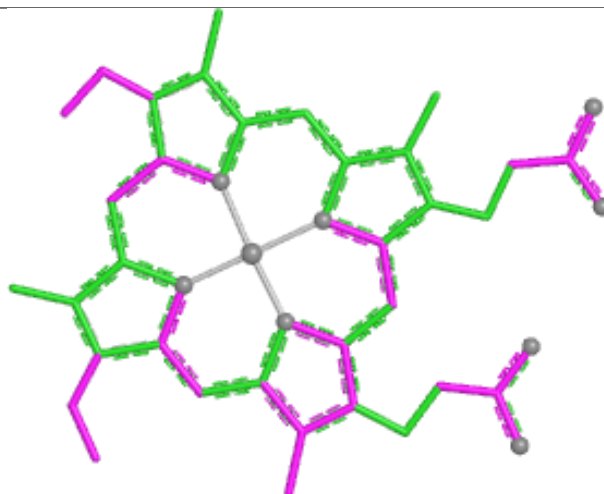


Rings

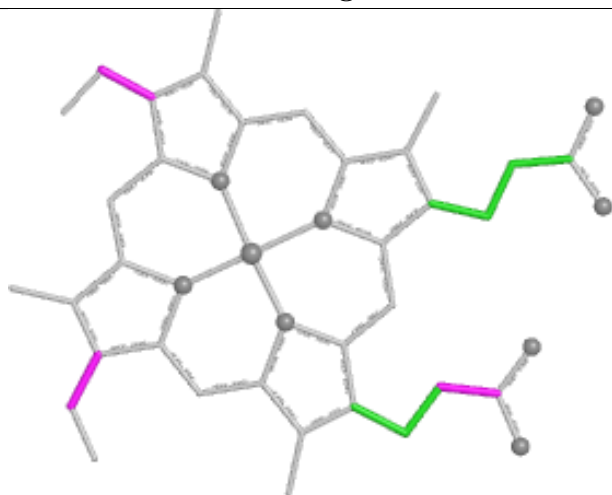
Ligand HEC C 404



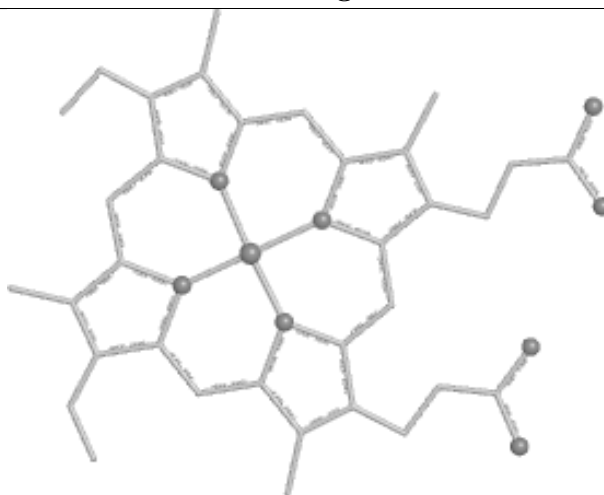
Bond lengths



Bond angles

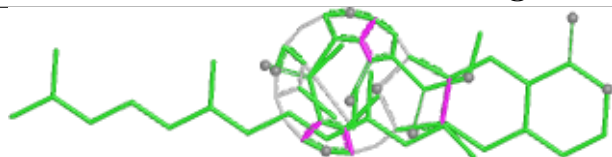


Torsions

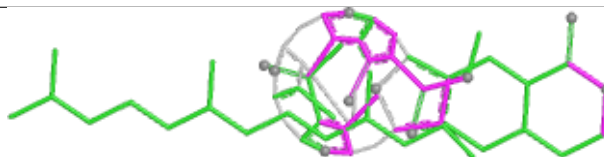


Rings

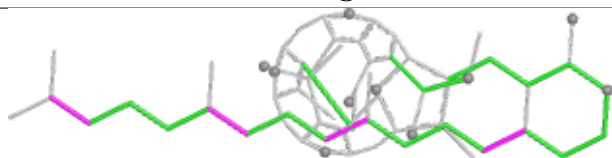
Ligand BPB M 402



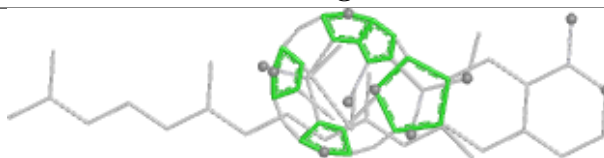
Bond lengths



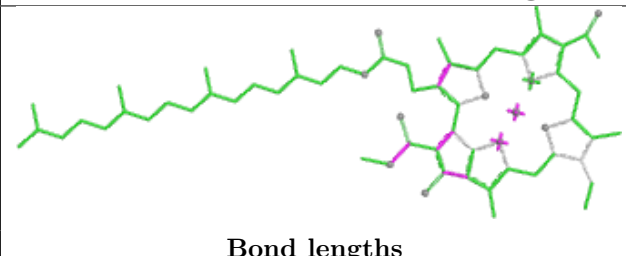
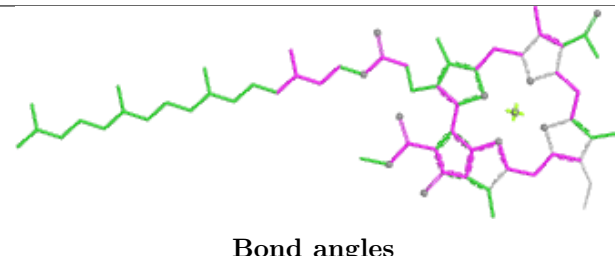
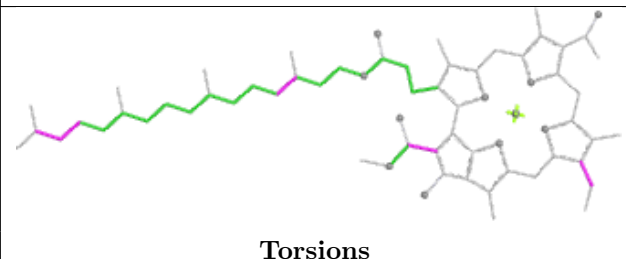
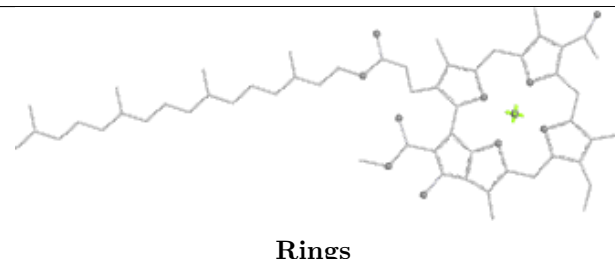
Bond angles

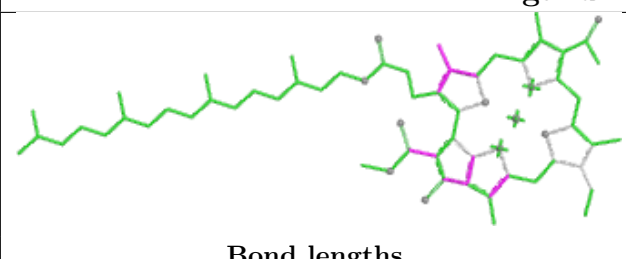
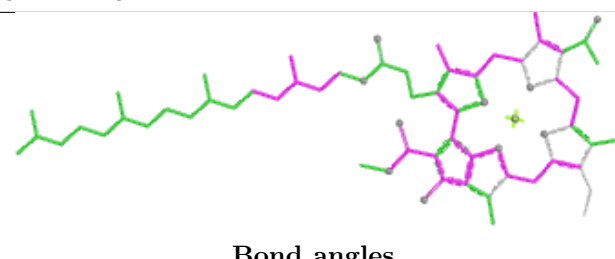
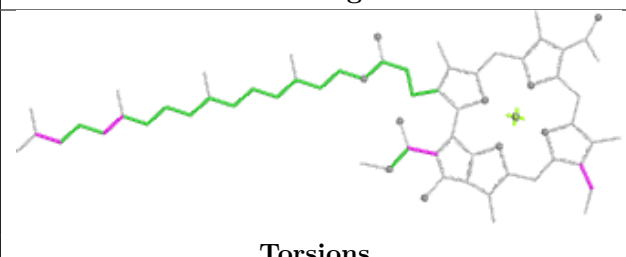
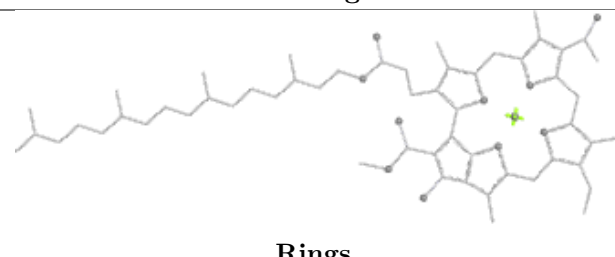


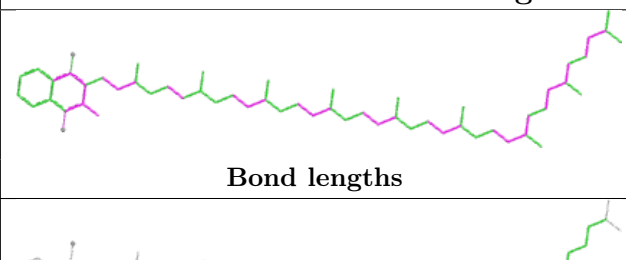
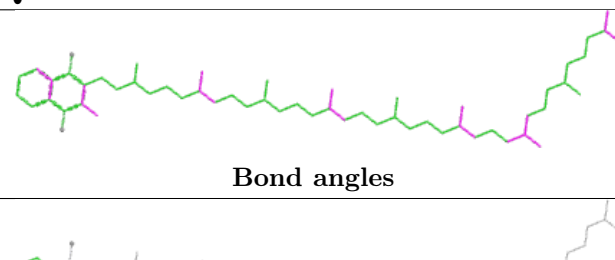
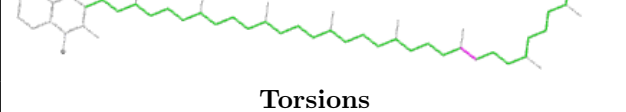
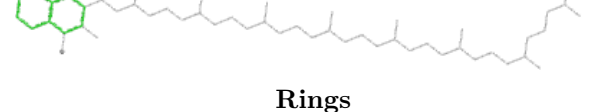
Torsions

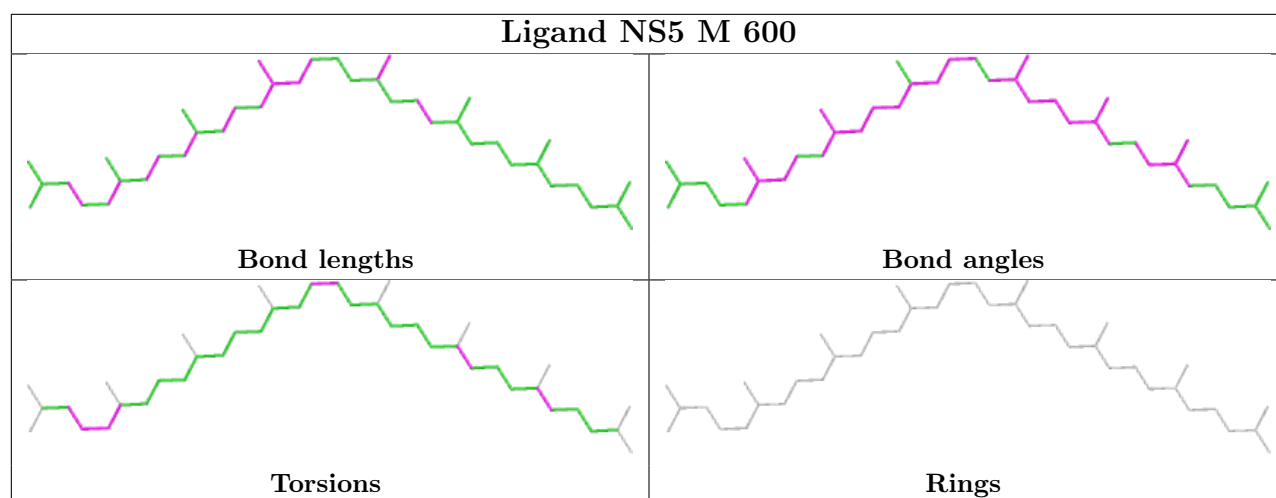


Rings

Ligand BCB L 400	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCB L 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand MQ9 M 501	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	334/356 (93%)	0.34	8 (2%) 59 66	26, 45, 68, 125	3 (0%)
2	H	249/258 (96%)	0.56	16 (6%) 25 29	27, 50, 80, 119	3 (1%)
3	L	273/273 (100%)	0.28	8 (2%) 53 60	21, 42, 58, 82	2 (0%)
4	M	323/323 (100%)	0.40	19 (5%) 28 32	26, 43, 65, 83	2 (0%)
All	All	1179/1210 (97%)	0.39	51 (4%) 40 46	21, 45, 69, 125	10 (0%)

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	334	ALA	4.4
3	L	273	SER	4.4
1	C	1	CYS	4.3
1	C	333	ALA	4.2
2	H	85	THR	3.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FME	H	1[A]	10/11	0.94	0.11	47,50,54,56	7
2	FME	H	1[B]	10/11	0.94	0.11	47,53,59,61	7

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
9	HTO	H	274[A]	10/10	0.58	0.43	53,69,72,75	10
9	HTO	L	279	10/10	0.71	0.44	65,66,69,75	10
6	LDA	H	718[B]	16/16	0.72	0.56	50,80,89,90	16
10	GOL	H	279	6/6	0.72	0.27	63,68,71,72	6
10	GOL	M	342	6/6	0.73	0.34	66,67,69,70	6
10	GOL	C	372	6/6	0.74	0.35	56,62,65,65	6
8	SO4	C	344	5/5	0.75	0.17	74,76,79,82	5
6	LDA	L	711	16/16	0.76	0.35	60,68,76,77	16
8	SO4	C	342	5/5	0.76	0.15	63,68,71,75	5
6	LDA	C	716	16/16	0.77	0.36	50,65,72,74	16
10	GOL	C	376	6/6	0.77	0.22	63,74,77,83	6
17	HTH	M	332	10/10	0.77	0.40	58,68,76,77	10
10	GOL	H	287	6/6	0.78	0.32	65,71,72,73	6
9	HTO	L	280	10/10	0.78	0.38	63,69,71,72	10
9	HTO	C	355	10/10	0.78	0.27	62,66,71,72	10
10	GOL	H	280	6/6	0.79	0.27	52,60,65,66	6
6	LDA	M	706	16/16	0.80	0.42	49,55,65,68	16
8	SO4	C	348	5/5	0.80	0.25	70,73,77,80	5
8	SO4	M	331	5/5	0.80	0.16	60,60,61,62	5
10	GOL	H	283	6/6	0.80	0.34	59,60,61,61	6
10	GOL	C	370	6/6	0.80	0.42	64,66,68,68	6
10	GOL	L	286	6/6	0.80	0.30	58,63,64,68	6
6	LDA	L	712	16/16	0.80	0.40	51,64,70,71	16
13	UQ9	L	503	23/58	0.80	0.30	59,73,85,87	23
10	GOL	C	373	6/6	0.80	0.41	60,63,64,65	6
9	HTO	L	278	10/10	0.81	0.30	57,65,67,69	10
6	LDA	L	702	16/16	0.81	0.34	51,53,57,57	16
10	GOL	L	288	6/6	0.81	0.49	54,57,58,60	6
10	GOL	M	341	6/6	0.81	0.43	68,71,74,75	6
6	LDA	M	717	16/16	0.81	0.35	50,59,89,91	16
10	GOL	C	374[B]	6/6	0.81	0.42	66,67,68,68	6
10	GOL	H	285	6/6	0.81	0.36	68,70,71,71	6
7	DGA	C	730	37/44	0.82	0.28	112,125,144,151	0
8	SO4	H	270	5/5	0.82	0.35	60,61,63,63	5
10	GOL	H	288	6/6	0.82	0.39	60,68,68,73	6
10	GOL	H	291	6/6	0.82	0.19	74,78,80,81	6
9	HTO	C	357	10/10	0.82	0.36	59,65,73,80	10

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	HTO	C	358[A]	10/10	0.82	0.43	58,62,67,68	10
10	GOL	C	363	6/6	0.82	0.26	46,59,65,69	6
10	GOL	C	368	6/6	0.82	0.30	62,63,68,70	6
10	GOL	H	281	6/6	0.82	0.28	64,67,72,76	6
9	HTO	H	272	10/10	0.82	0.23	61,67,75,80	10
10	GOL	C	371	6/6	0.83	0.39	55,62,62,63	6
8	SO4	H	271	5/5	0.83	0.34	64,64,65,68	5
8	SO4	C	340	5/5	0.83	0.19	57,71,76,82	5
10	GOL	C	360	6/6	0.83	0.19	44,56,62,71	6
10	GOL	C	375	6/6	0.83	0.42	66,69,70,72	6
10	GOL	L	285	6/6	0.84	0.27	51,67,70,71	6
6	LDA	C	722	16/16	0.84	0.31	53,63,66,66	16
8	SO4	C	343	5/5	0.84	0.18	52,62,65,66	5
8	SO4	M	327	5/5	0.84	0.15	53,58,68,75	5
8	SO4	C	339	5/5	0.84	0.15	69,71,75,80	5
8	SO4	C	347	5/5	0.84	0.20	78,82,83,90	5
6	LDA	L	710	16/16	0.84	0.32	52,60,81,82	16
8	SO4	C	346	5/5	0.85	0.26	57,65,71,72	5
10	GOL	M	336	6/6	0.85	0.34	68,69,70,71	6
10	GOL	M	340	6/6	0.85	0.26	60,64,65,66	6
10	GOL	H	277	6/6	0.85	0.23	55,59,62,62	6
10	GOL	L	282	6/6	0.85	0.24	53,59,59,63	6
6	LDA	M	704	16/16	0.85	0.31	49,80,87,87	16
8	SO4	M	330	5/5	0.85	0.20	67,68,68,69	5
10	GOL	C	364	6/6	0.86	0.22	52,67,67,68	6
10	GOL	H	276[A]	6/6	0.86	0.17	50,60,62,62	2
10	GOL	L	284	6/6	0.86	0.21	52,65,67,67	6
10	GOL	H	276[B]	6/6	0.86	0.17	50,59,60,62	2
10	GOL	C	366	6/6	0.86	0.28	56,62,63,71	6
10	GOL	L	287	6/6	0.86	0.23	54,55,57,57	6
6	LDA	L	723	16/16	0.86	0.44	55,58,64,68	16
6	LDA	M	715	16/16	0.86	0.33	58,71,77,79	16
10	GOL	M	338	6/6	0.86	0.33	57,60,62,63	6
9	HTO	C	356	10/10	0.86	0.30	59,72,76,77	10
6	LDA	H	720	16/16	0.86	0.27	55,69,73,73	16
8	SO4	M	328	5/5	0.86	0.23	61,62,64,69	5
10	GOL	C	361	6/6	0.86	0.26	60,64,72,75	6
8	SO4	C	349	5/5	0.86	0.20	63,64,71,71	5
10	GOL	L	283	6/6	0.87	0.20	59,63,68,70	6
8	SO4	C	350	5/5	0.87	0.25	64,67,69,72	5
10	GOL	C	367	6/6	0.87	0.34	50,58,59,60	6
8	SO4	C	353	5/5	0.87	0.18	66,69,72,76	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	H	263	5/5	0.87	0.20	75,76,78,79	5
8	SO4	H	265	5/5	0.87	0.15	69,74,75,81	5
9	HTO	M	333	10/10	0.87	0.30	44,51,55,55	10
10	GOL	H	284	6/6	0.87	0.34	58,63,65,68	6
10	GOL	M	339	6/6	0.87	0.32	60,65,66,66	6
8	SO4	H	268	5/5	0.87	0.39	63,66,70,72	5
6	LDA	M	714	16/16	0.87	0.35	70,75,81,82	16
8	SO4	C	337[A]	5/5	0.87	0.21	59,62,67,67	5
13	UQ9	L	502	58/58	0.87	0.25	44,80,97,99	58
8	SO4	C	337[B]	5/5	0.87	0.21	59,64,69,70	5
10	GOL	C	365	6/6	0.87	0.17	60,67,69,72	6
6	LDA	H	719	16/16	0.88	0.27	58,63,71,72	16
10	GOL	C	377	6/6	0.88	0.20	63,65,67,67	6
10	GOL	C	369	6/6	0.88	0.29	49,56,61,61	6
9	HTO	H	273	10/10	0.88	0.32	48,51,60,62	10
10	GOL	H	289	6/6	0.88	0.31	62,66,66,67	6
6	LDA	L	724	16/16	0.88	0.33	53,63,68,69	16
10	GOL	H	278	6/6	0.88	0.17	63,67,68,71	6
8	SO4	C	345	5/5	0.88	0.13	66,68,72,72	5
8	SO4	C	341	5/5	0.88	0.12	67,74,80,81	5
8	SO4	C	338	5/5	0.88	0.13	53,57,60,64	5
8	SO4	H	264	5/5	0.88	0.25	61,67,72,73	5
6	LDA	L	703	16/16	0.89	0.25	52,57,61,63	16
6	LDA	M	707	16/16	0.89	0.26	42,58,72,81	16
8	SO4	H	269	5/5	0.89	0.25	71,72,75,76	5
9	HTO	L	276	10/10	0.89	0.25	50,67,70,71	10
8	SO4	M	329	5/5	0.89	0.25	57,58,63,67	5
10	GOL	M	337	6/6	0.89	0.30	68,69,69,70	6
6	LDA	M	705	16/16	0.89	0.25	61,69,87,87	16
8	SO4	C	354	5/5	0.90	0.29	66,69,70,71	5
10	GOL	H	282	6/6	0.90	0.26	59,66,68,69	6
6	LDA	L	709	16/16	0.90	0.23	39,63,93,97	16
10	GOL	C	378	6/6	0.90	0.27	78,80,81,81	6
10	GOL	M	334	6/6	0.90	0.17	40,56,66,69	6
10	GOL	H	290	6/6	0.91	0.26	49,59,63,67	6
8	SO4	H	260	5/5	0.91	0.09	59,63,68,71	5
10	GOL	C	362	6/6	0.91	0.19	51,57,63,63	6
8	SO4	H	259	5/5	0.91	0.10	60,62,67,69	5
16	NS5	M	600	40/40	0.91	0.16	42,54,95,96	0
8	SO4	M	326	5/5	0.91	0.13	56,61,62,62	5
10	GOL	L	281	6/6	0.92	0.20	54,58,66,68	6
10	GOL	H	286	6/6	0.92	0.25	67,67,69,70	6

Continued on next page...

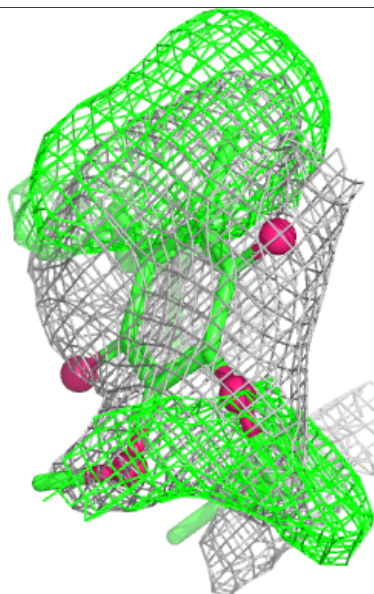
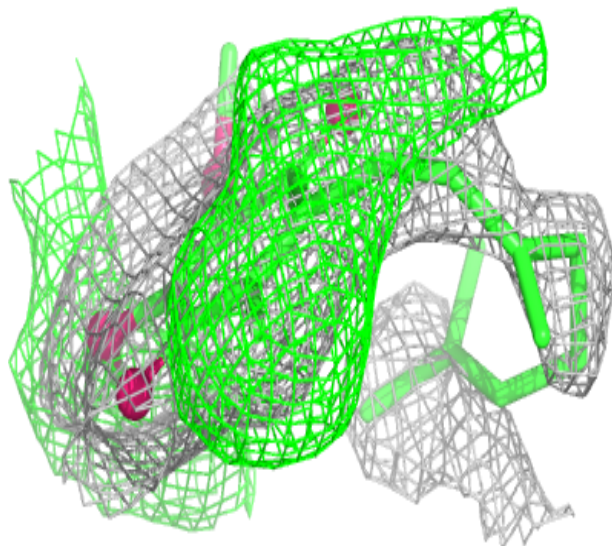
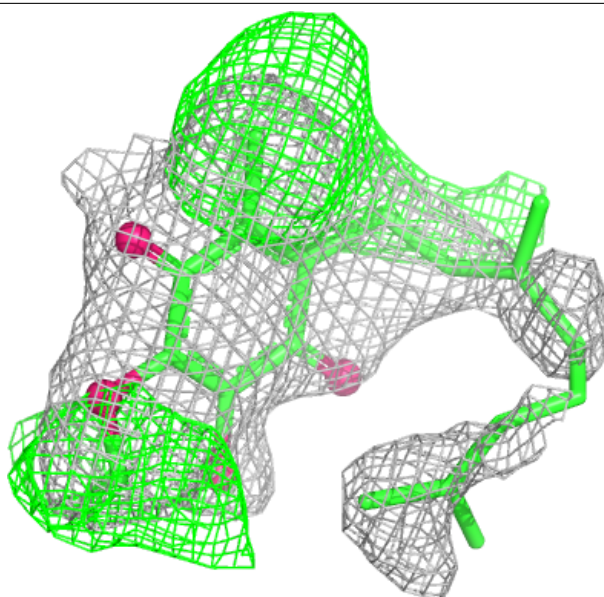
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	C	352	5/5	0.92	0.15	78,78,81,82	5
8	SO4	H	266	5/5	0.92	0.19	65,66,68,71	5
6	LDA	L	708	16/16	0.93	0.13	40,56,68,76	0
6	LDA	M	713	16/16	0.93	0.24	63,69,84,86	16
10	GOL	H	275	6/6	0.93	0.15	59,62,64,67	0
9	HTO	L	277	10/10	0.93	0.27	57,64,69,76	10
8	SO4	L	274	5/5	0.93	0.15	62,62,65,68	5
6	LDA	H	701	16/16	0.94	0.12	43,57,71,73	0
8	SO4	H	261[A]	5/5	0.94	0.14	52,58,64,65	5
8	SO4	H	261[B]	5/5	0.94	0.14	47,54,61,61	5
8	SO4	C	351	5/5	0.94	0.15	60,60,63,67	5
11	BCB	M	400	66/66	0.95	0.11	34,40,109,121	0
10	GOL	M	335	6/6	0.95	0.15	44,54,60,68	6
6	LDA	H	721	16/16	0.95	0.15	50,66,69,69	0
10	GOL	C	359	6/6	0.95	0.12	44,50,54,55	6
8	SO4	L	275	5/5	0.95	0.27	66,66,67,68	5
8	SO4	M	324	5/5	0.96	0.09	47,52,61,63	0
12	BPB	M	402	65/65	0.96	0.10	33,41,124,132	0
11	BCB	L	400	66/66	0.97	0.07	28,36,48,52	0
8	SO4	H	267	5/5	0.97	0.17	56,64,65,65	5
15	MQ9	M	501	58/58	0.97	0.10	31,41,92,98	0
11	BCB	M	401	66/66	0.97	0.08	28,34,58,66	0
8	SO4	M	325	5/5	0.97	0.09	64,67,78,79	0
5	HEC	C	404	43/43	0.98	0.07	32,38,51,64	0
11	BCB	L	401	66/66	0.98	0.07	27,35,64,75	0
12	BPB	L	402	65/65	0.98	0.06	32,39,48,51	0
5	HEC	C	401	43/43	0.99	0.06	41,46,55,58	0
8	SO4	H	262	5/5	0.99	0.06	41,43,45,47	5
5	HEC	C	402	43/43	0.99	0.07	39,44,52,60	0
5	HEC	C	403	43/43	0.99	0.06	32,36,41,42	0
14	FE2	M	500	1/1	1.00	0.04	37,37,37,37	0

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.

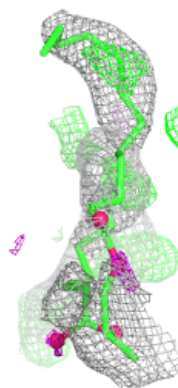
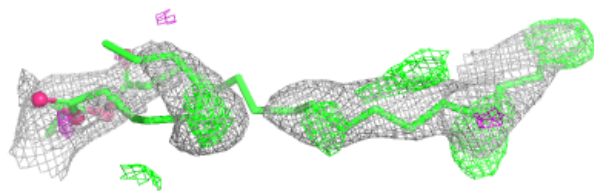
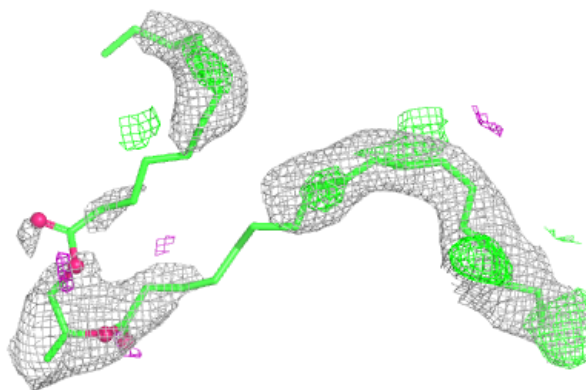
Electron density around UQ9 L 503:

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



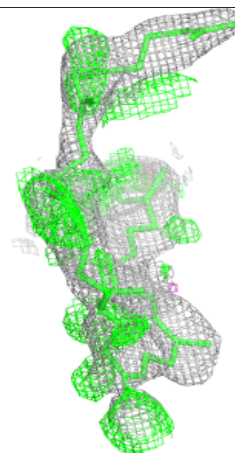
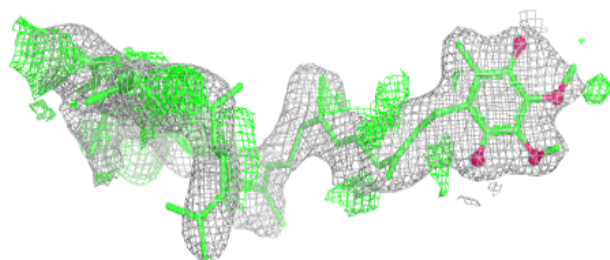
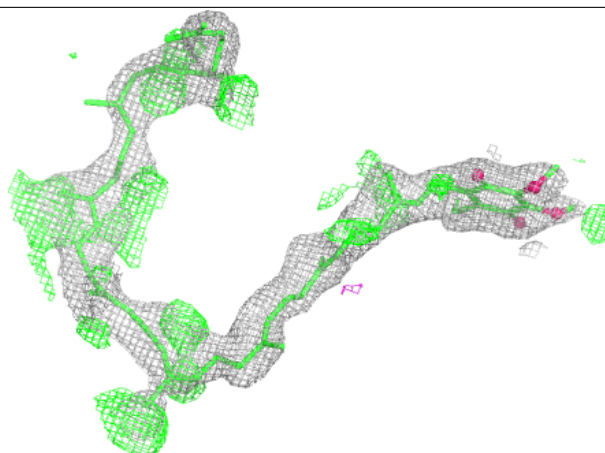
Electron density around DGA C 730:

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

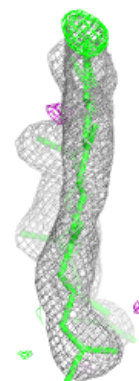
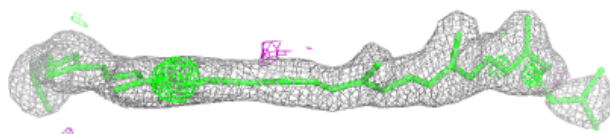
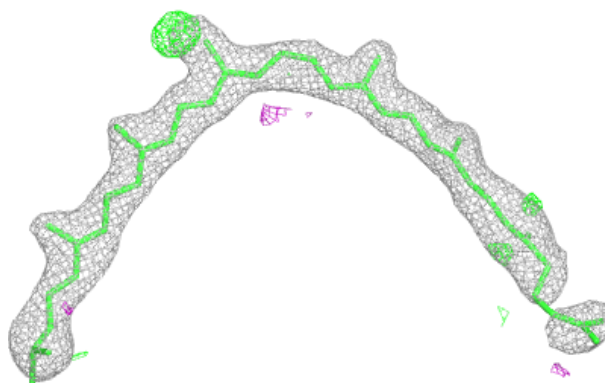


Electron density around UQ9 L 502:

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

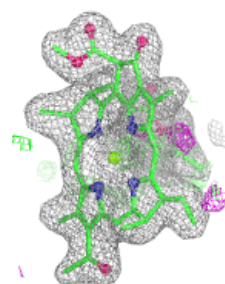
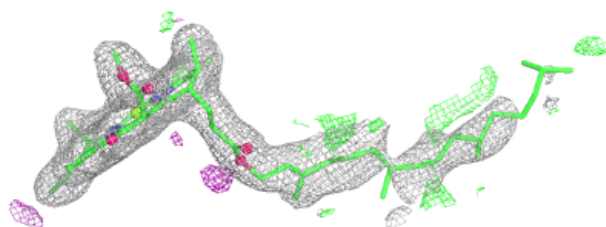
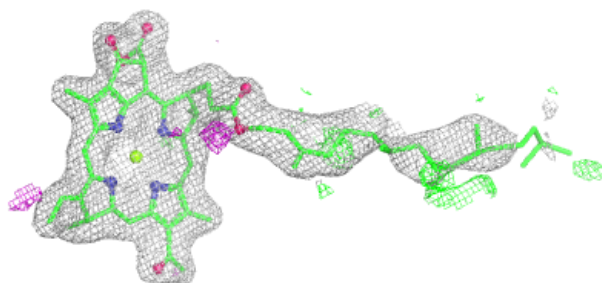
**Electron density around NS5 M 600:**

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

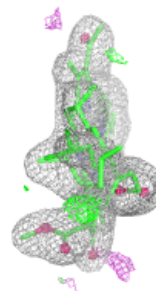
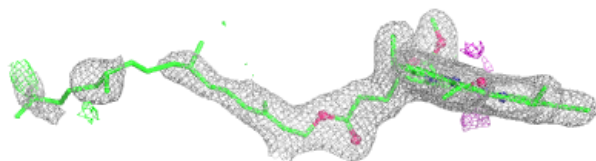
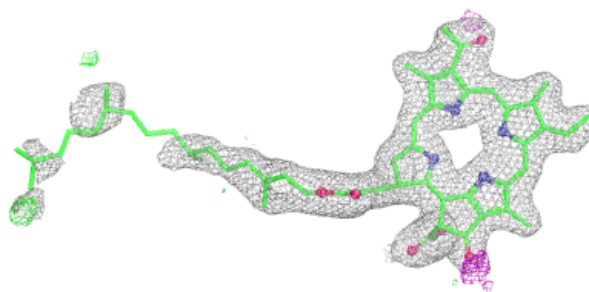


Electron density around BCB M 400:

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

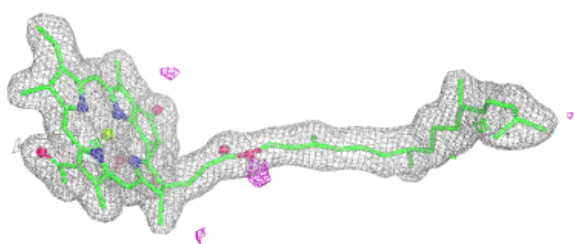
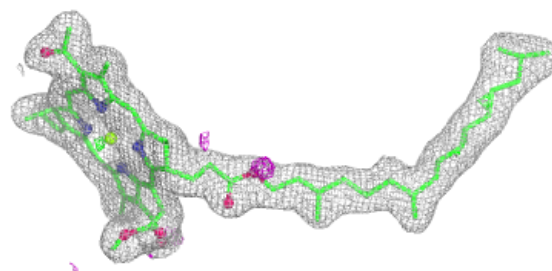
**Electron density around BPB M 402:**

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

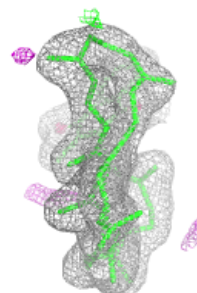
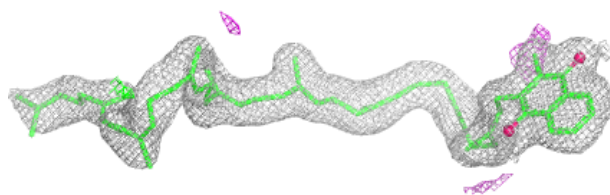
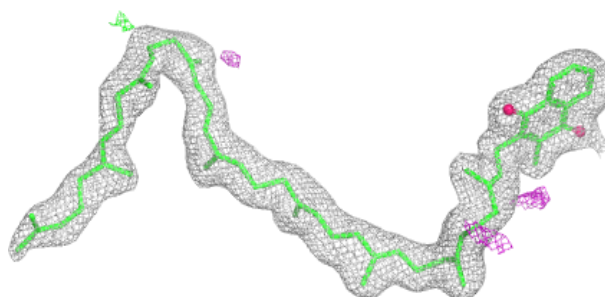


Electron density around BCB L 400:

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

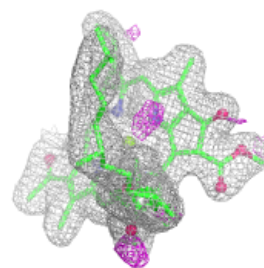
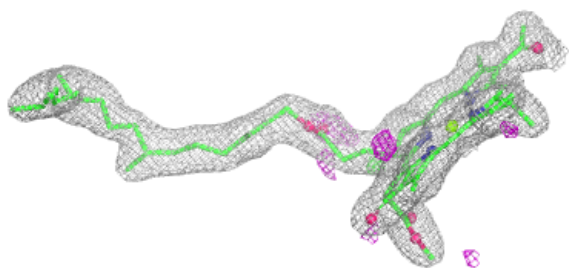
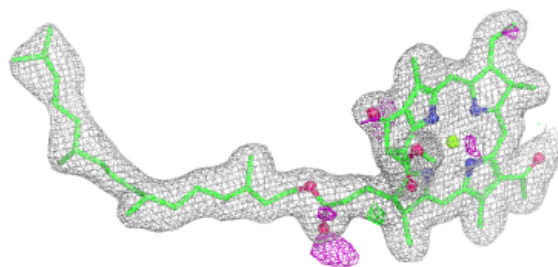
**Electron density around MQ9 M 501:**

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



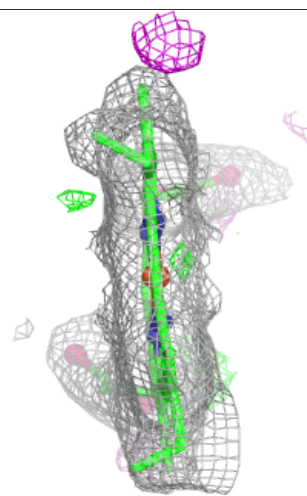
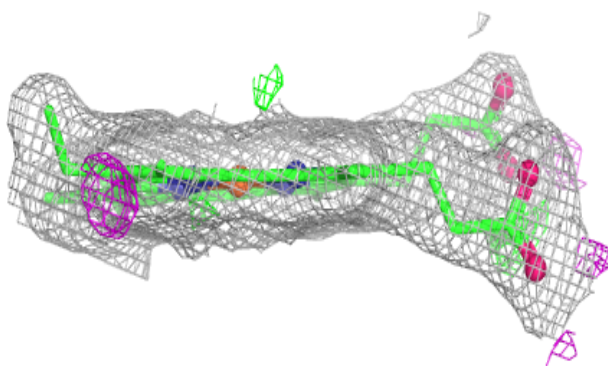
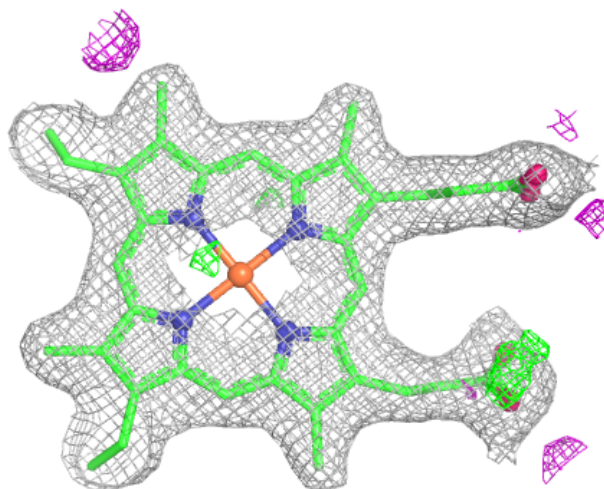
Electron density around BCB M 401:

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



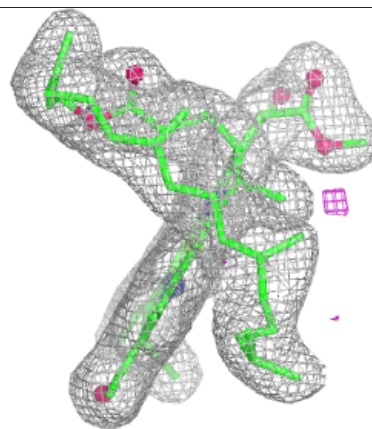
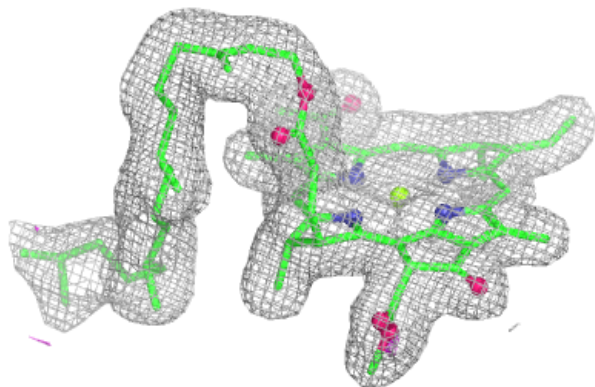
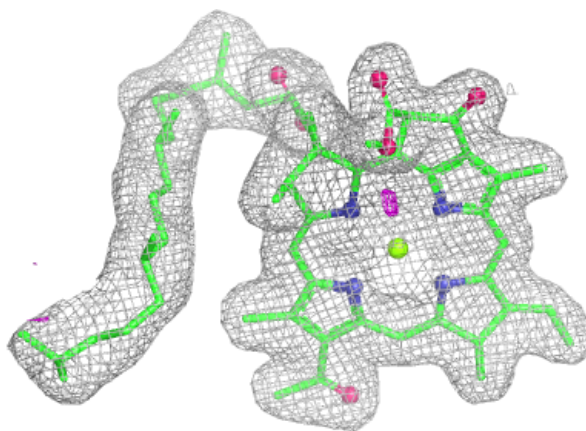
Electron density around HEC C 404:

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



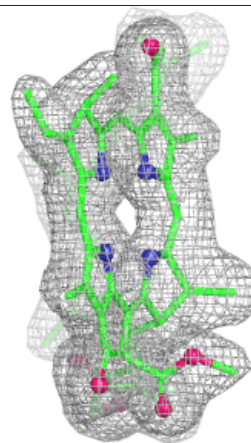
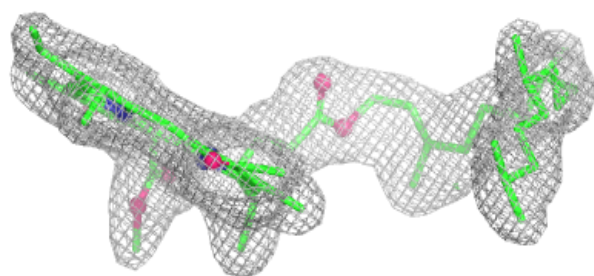
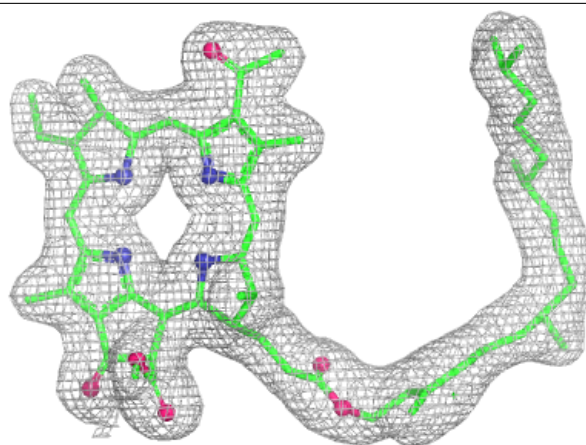
Electron density around BCB L 401:

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



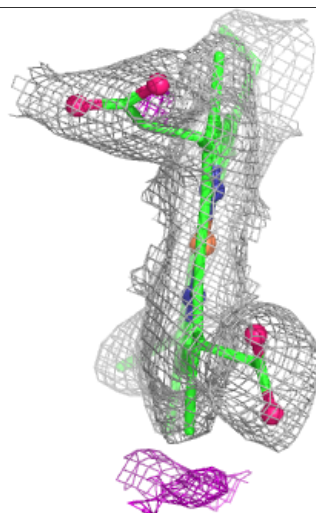
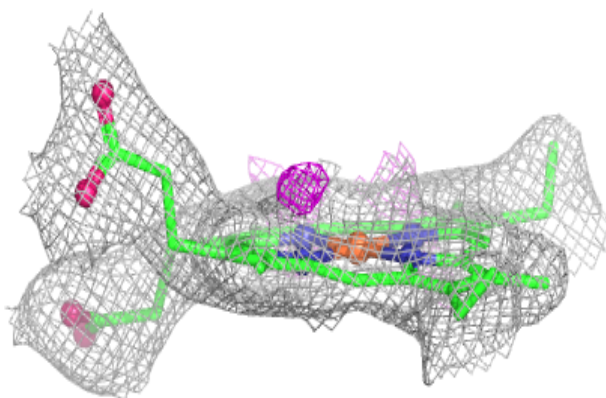
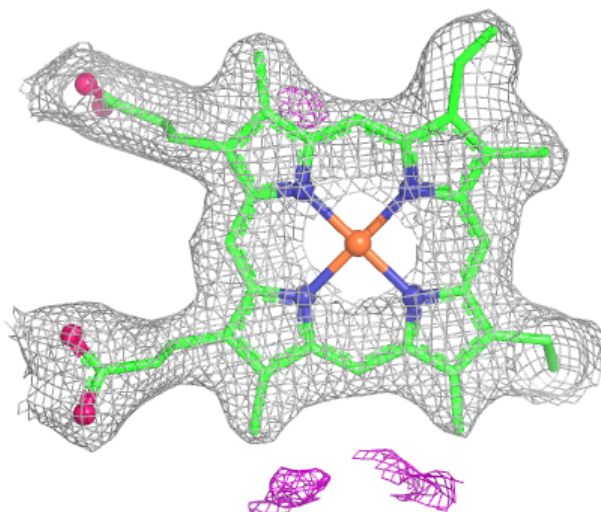
Electron density around BPB L 402:

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



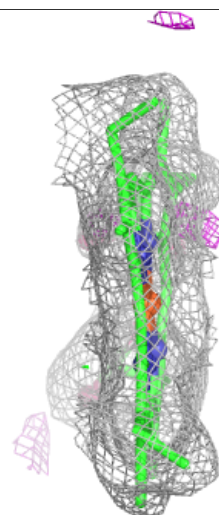
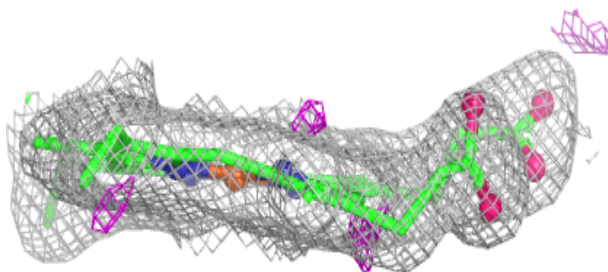
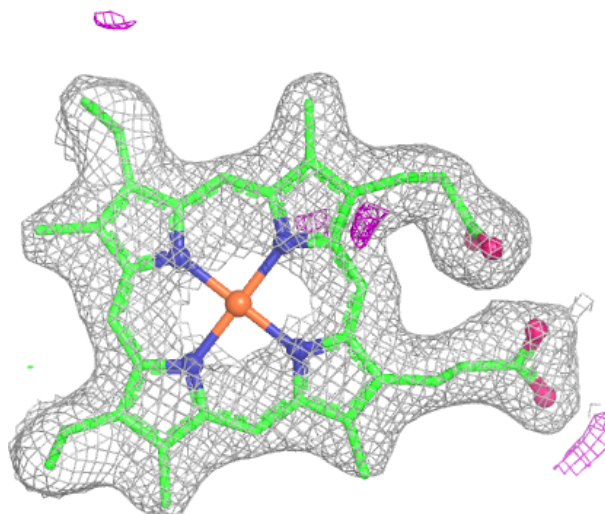
Electron density around HEC C 401:

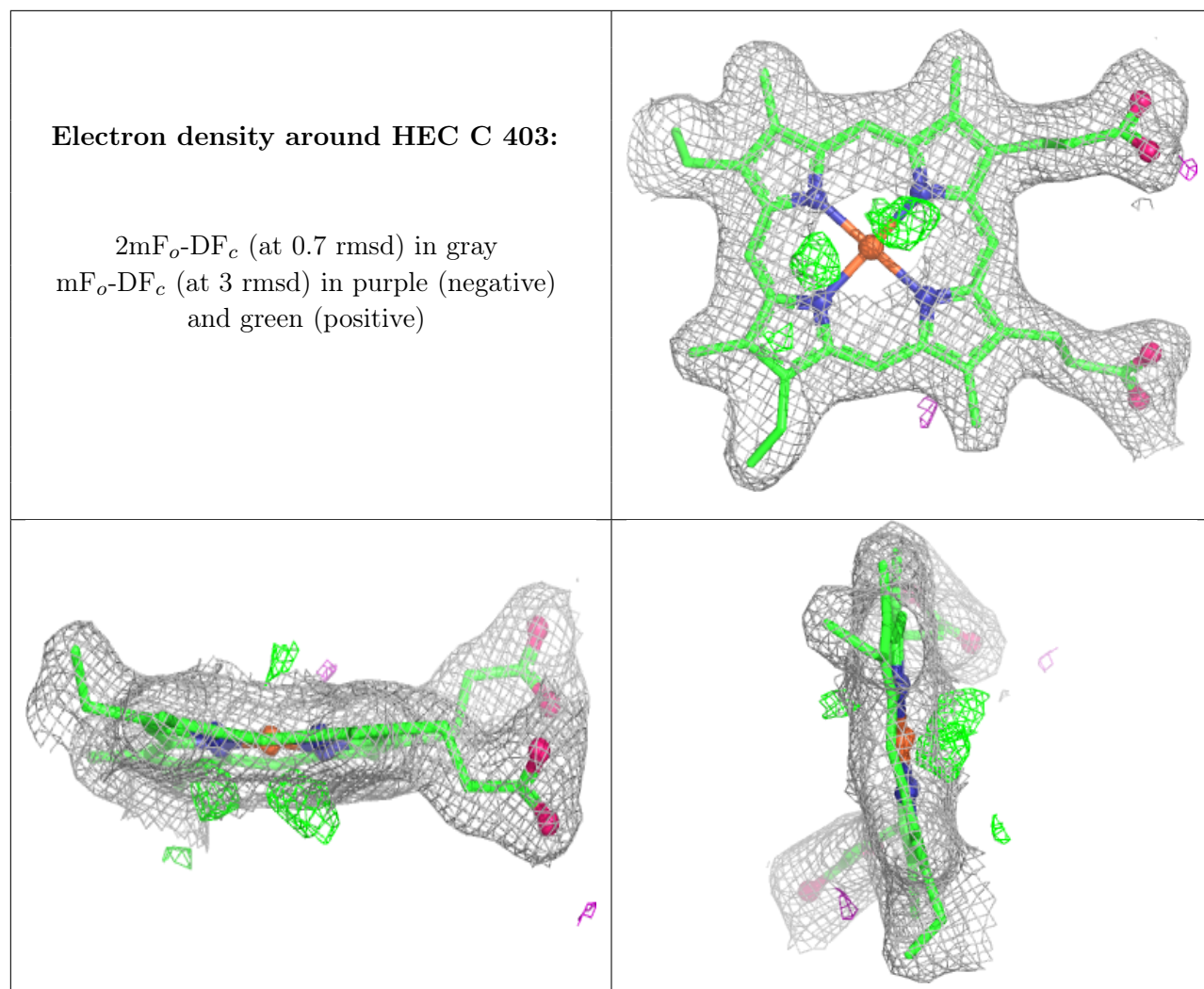
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 402:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.