



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:21 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

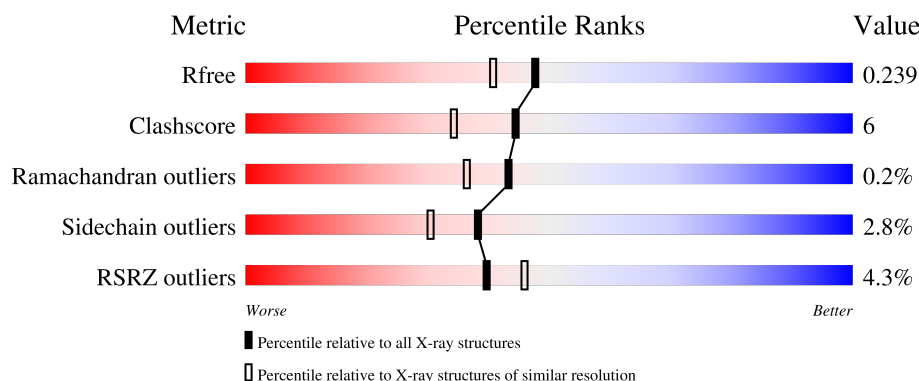
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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			

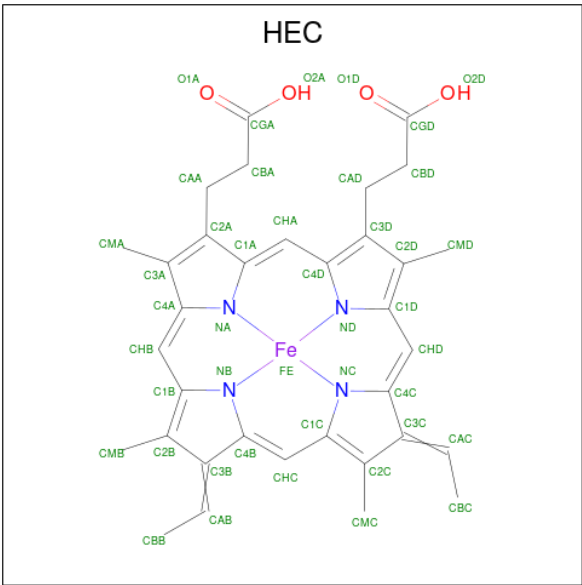
- Molecule 3 is a protein called Photosynthetic reaction center L-subunit.

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.

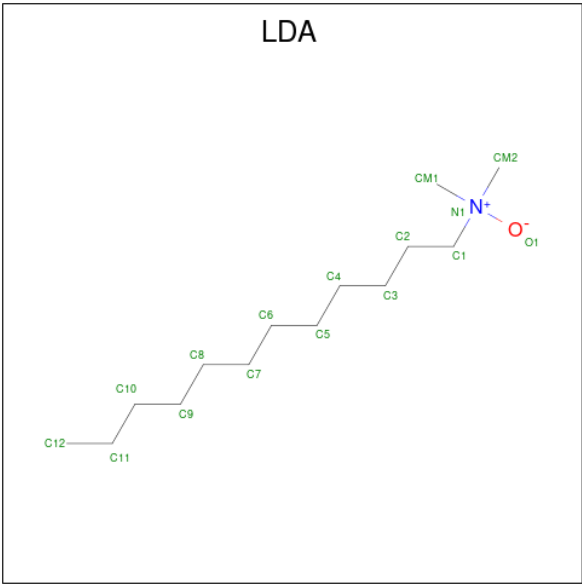
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2574	1716	424	423	11			

- 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).



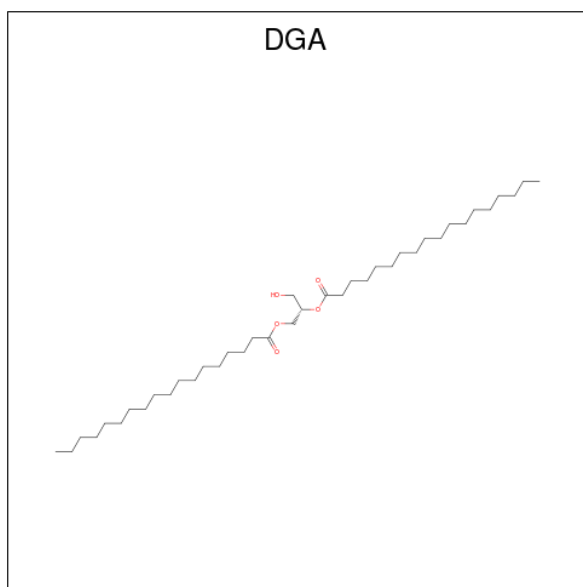
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	1
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1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

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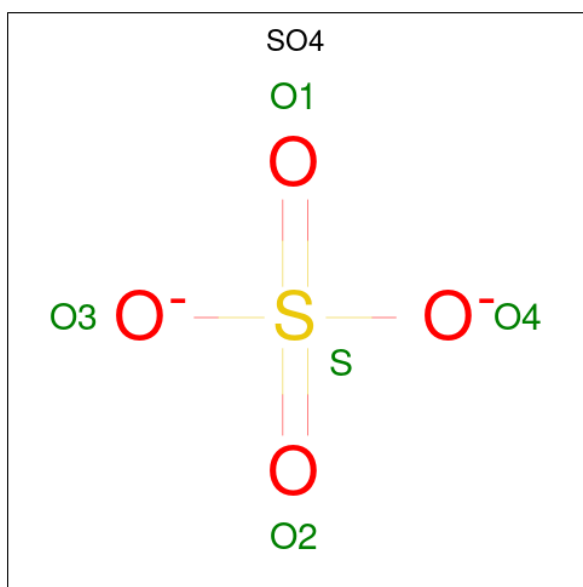
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- 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		

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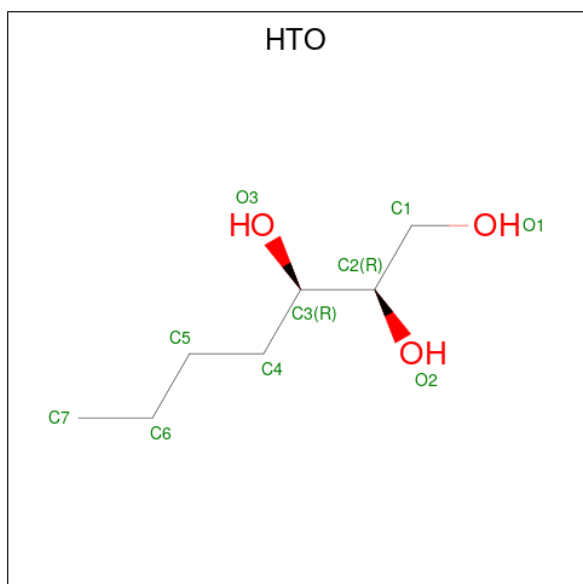
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	1
			10	8	2		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total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

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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: $C_7H_{16}O_3$).



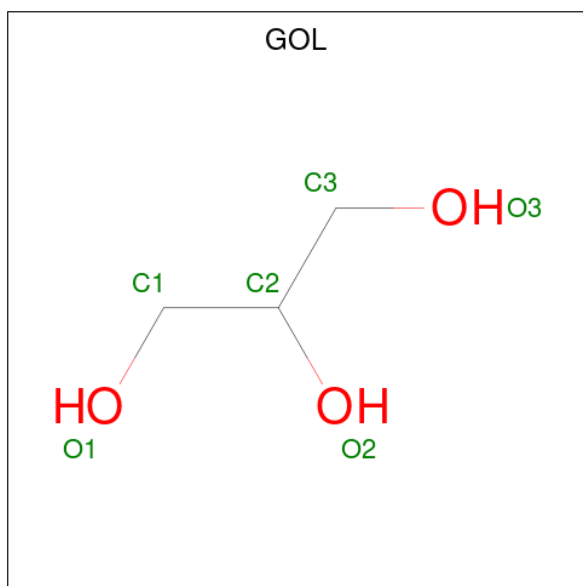
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	1
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		

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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		

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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

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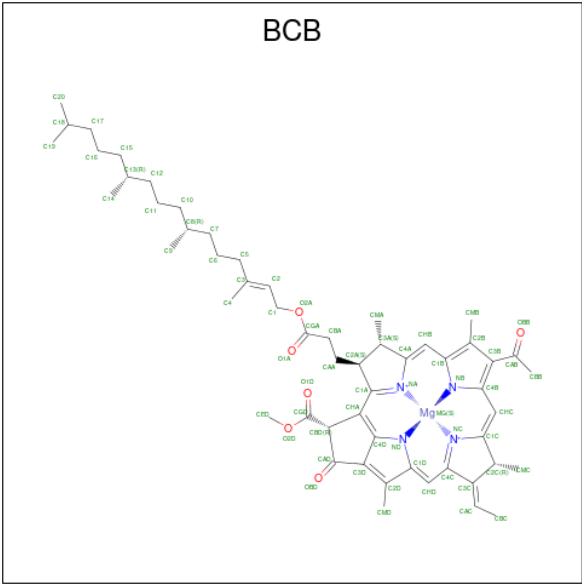
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10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

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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		

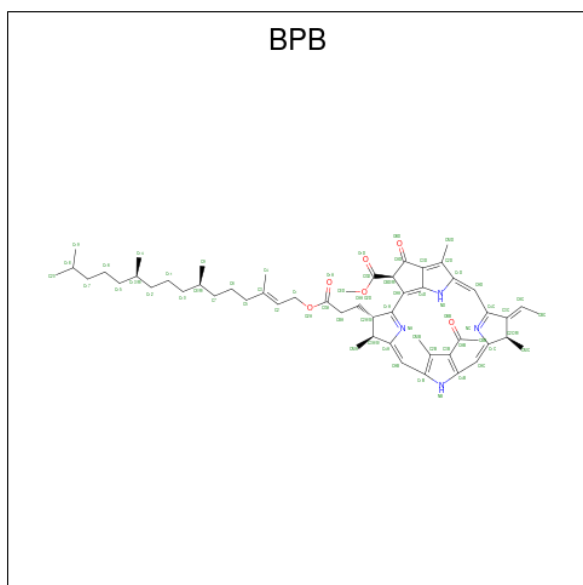
- Molecule 11 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆).



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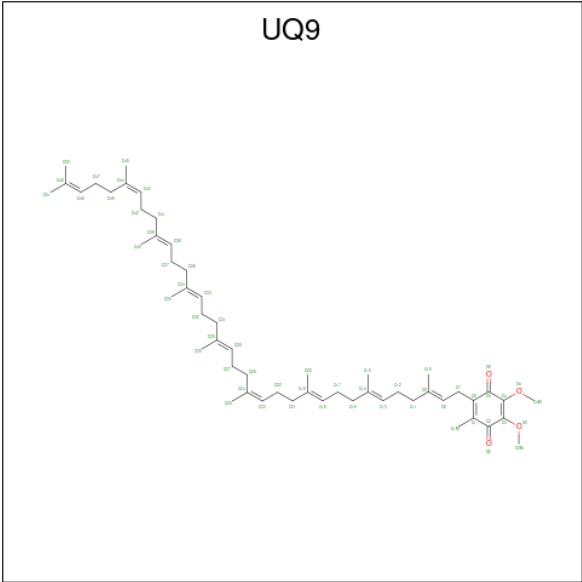
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- 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: $C_{54}H_{82}O_4$).

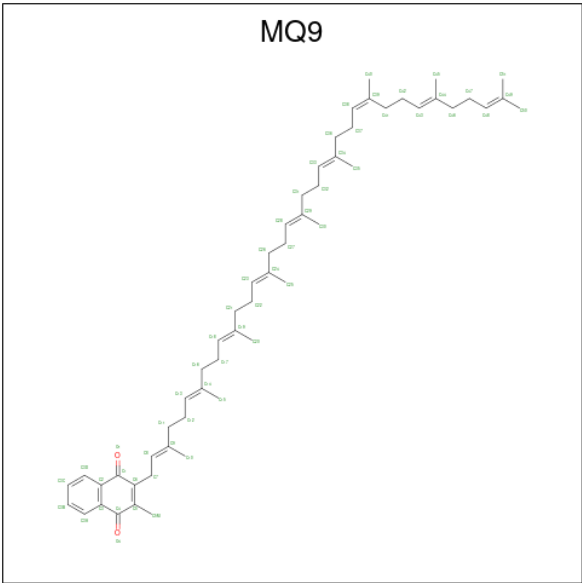


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	54	4		
13	L	1	Total	C	O	0	0
			23	19	4		

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

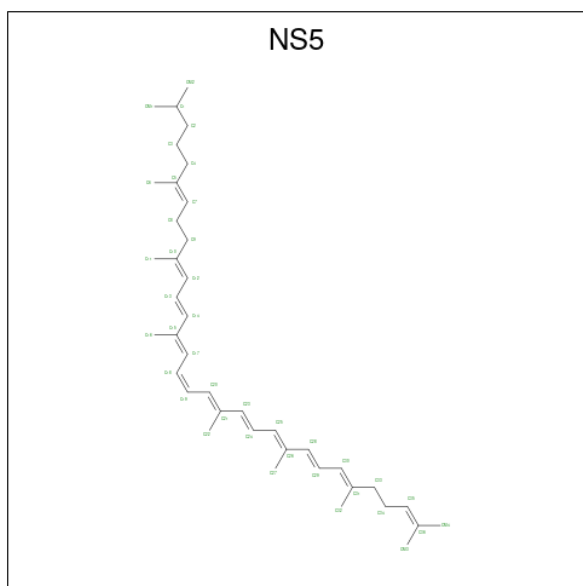
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total	Fe	0	0
			1	1		

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



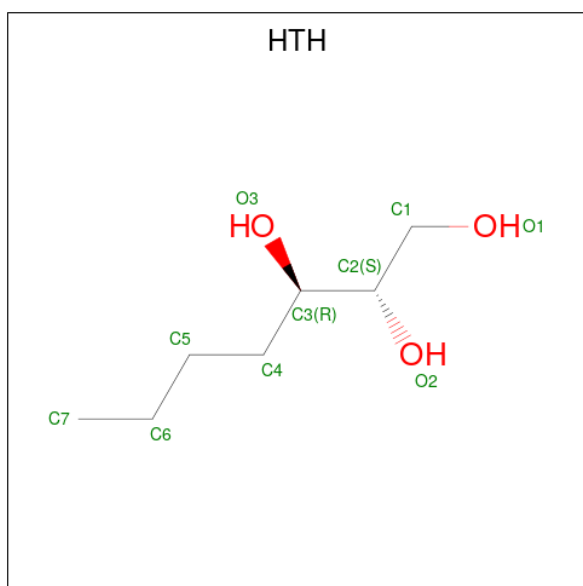
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			58	56	2		

- 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		

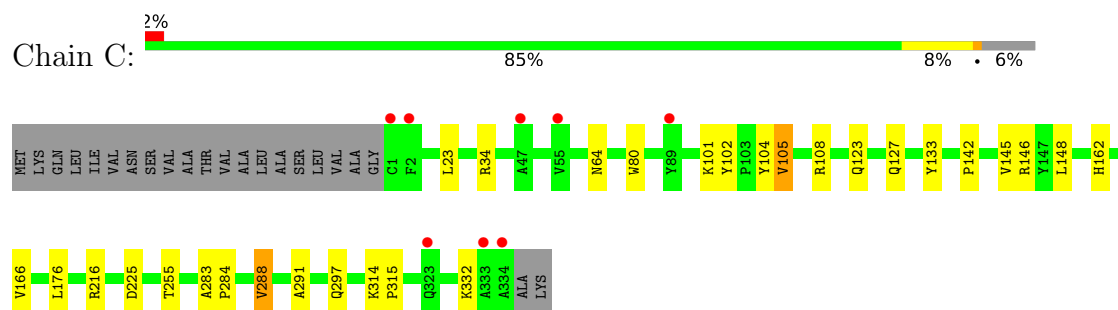
- Molecule 18 is water.

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		

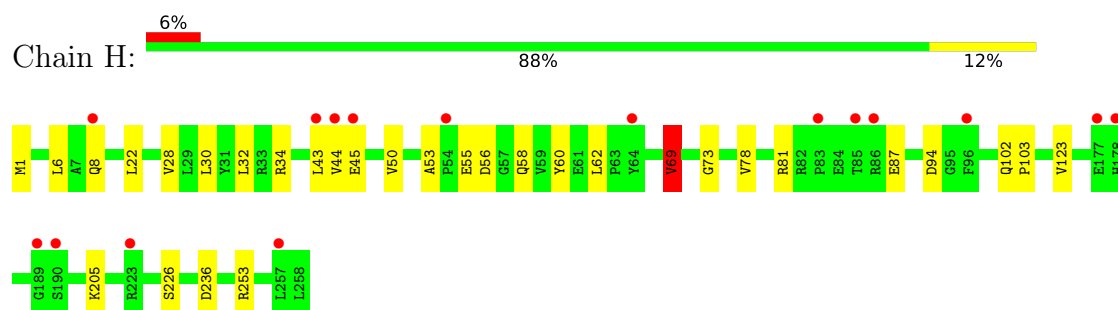
3 Residue-property plots [i](#)

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.

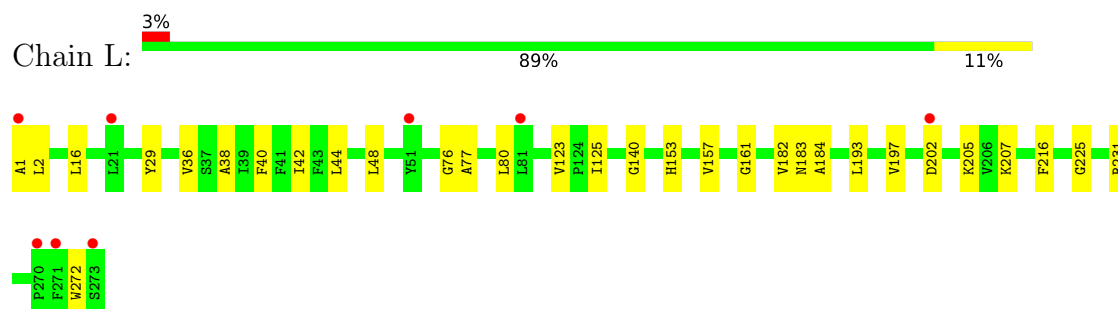
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



- 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%)

All (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
4	M	245	ARG	C-O	-5.58	1.17	1.24
3	L	184	ALA	CA-CB	5.47	1.61	1.53
3	L	40	PHE	N-CA	-5.37	1.40	1.46
3	L	123	VAL	CA-CB	-5.12	1.51	1.54

All (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
2	H	53	ALA	O-C-N	-6.06	114.35	121.32
2	H	32	LEU	N-CA-C	5.97	117.45	111.07
3	L	225	GLY	CA-C-N	5.65	127.79	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	225	GLY	C-N-CA	5.65	127.79	120.44
4	M	254	ILE	N-CA-C	5.58	118.36	112.83
2	H	28	VAL	N-CA-C	5.44	115.64	110.42
4	M	204	ILE	N-CA-C	5.39	116.12	110.62
2	H	45	GLU	CA-C-N	-5.18	113.20	118.85
2	H	45	GLU	C-N-CA	-5.18	113.20	118.85
4	M	31	LYS	N-CA-C	-5.08	101.72	109.64

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
4:M:73:MET:HE1	4:M:88:PHE:CE1	2.16	0.80
4:M:29:ILE:CD1	4:M:51:LEU:HD13	2.14	0.77
10:C:364:GOL:H11	6:M:715:LDA:HM11	1.68	0.76
1:C:34:ARG:HD3	9:C:357:HTO:H3	1.65	0.75
4:M:29:ILE:HD11	4:M:51:LEU:HD13	1.70	0.74
1:C:297:GLN:HE22	10:C:365:GOL:H31	1.53	0.73
11:M:400:BCB:HBB2	11:M:400:BCB:HMB3	1.68	0.73
1:C:255:THR:HG23	10:C:363:GOL:H32	1.72	0.72
1:C:64[A]:ASN:HD21	9:C:355:HTO:C2	2.03	0.71
2:H:226:SER:HB3	9:H:272:HTO:H42	1.72	0.71
4:M:73:MET:HE1	4:M:88:PHE:CD1	2.30	0.67
11:L:400:BCB:HMB1	11:L:400:BCB:HBB3	1.78	0.66
1:C:148:LEU:HD13	10:C:365:GOL:H12	1.78	0.66
13:L:502:UQ9:C15	11:M:400:BCB:H91	2.26	0.65
4:M:29:ILE:HD12	4:M:51:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:231:ARG:HG2	6:L:723:LDA:HM23	1.80	0.63
1:C:332:LYS:H	9:C:355:HTO:H71	1.63	0.63
10:C:364:GOL:C1	6:M:715:LDA:HM11	2.30	0.62
2:H:253:ARG:HE	10:H:278:GOL:H31	1.64	0.62
1:C:291:ALA:HB3	10:C:377:GOL:C3	2.29	0.62
13:L:503:UQ9:O5	13:L:503:UQ9:H4MA	2.01	0.61
13:L:502:UQ9:C15	11:M:400:BCB:H93	2.27	0.61
4:M:73:MET:HE3	4:M:91:LEU:HB2	1.83	0.61
6:L:710:LDA:H32	9:L:277:HTO:H73	1.83	0.59
2:H:253:ARG:HE	10:H:278:GOL:C3	2.16	0.59
13:L:503:UQ9:O5	13:L:503:UQ9:H8	2.03	0.59
4:M:30:GLY:HA3	10:M:342:GOL:H12	1.85	0.58
3:L:36:VAL:HG12	9:L:279:HTO:H3	1.85	0.58
11:L:401:BCB:HMB1	11:L:401:BCB:CBB	2.34	0.57
1:C:291:ALA:HB3	10:C:377:GOL:H31	1.86	0.57
11:L:400:BCB:H193	15:M:501:MQ9:H252	1.87	0.57
4:M:74:LEU:CD1	16:M:600:NS5:HM23	2.36	0.56
4:M:1:ALA:N	8:M:326:SO4:O3	2.31	0.56
8:C:338:SO4:O4	10:M:334:GOL:O1	2.21	0.56
2:H:205:LYS:O	10:H:279:GOL:O1	2.23	0.55
1:C:101:LYS:NZ	18:C:631:HOH:O	2.40	0.55
4:M:212:LEU:C	4:M:212:LEU:HD23	2.32	0.55
3:L:140:GLY:HA3	6:L:712:LDA:HM13	1.88	0.55
3:L:38:ALA:O	3:L:42:ILE:HG13	2.07	0.54
4:M:37:TRP:HD1	6:M:704:LDA:CM1	2.21	0.54
1:C:123:GLN:HE21	10:M:338:GOL:H11	1.72	0.54
2:H:81[A]:ARG:HG3	2:H:81[A]:ARG:HH11	1.72	0.54
3:L:76:GLY:HA3	6:L:711:LDA:HM13	1.89	0.54
4:M:37:TRP:CD1	6:M:704:LDA:HM12	2.44	0.53
2:H:6:LEU:HD23	9:H:274[A]:HTO:H2	1.90	0.53
7:C:730:DGA:HB22	7:C:730:DGA:HA22	1.91	0.53
2:H:43:LEU:HB3	3:L:1:ALA:HB1	1.90	0.53
13:L:502:UQ9:C15	11:M:400:BCB:C9	2.67	0.53
1:C:123:GLN:HE21	10:M:338:GOL:H31	1.74	0.52
2:H:62:LEU:O	6:H:721:LDA:HM21	2.08	0.52
1:C:162:HIS:HB2	10:C:368:GOL:H2	1.92	0.52
1:C:291:ALA:N	10:C:377:GOL:H32	2.25	0.52
3:L:193:LEU:HD22	3:L:216:PHE:CE2	2.44	0.52
3:L:272:TRP:CG	4:M:86:ARG:HD3	2.45	0.52
4:M:37:TRP:HD1	6:M:704:LDA:HM12	1.75	0.51
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:400:BCB:HBB2	11:M:400:BCB:CMB	2.39	0.51
1:C:314:LYS:HZ2	10:C:373:GOL:H2	1.75	0.51
1:C:225:ASP:OD1	10:C:369:GOL:O3	2.29	0.51
3:L:231:ARG:CG	6:L:723:LDA:HM23	2.40	0.50
11:L:400:BCB:HMB1	11:L:400:BCB:CBB	2.41	0.50
11:M:401:BCB:HMB3	11:M:401:BCB:CBB	2.42	0.50
13:L:503:UQ9:H3MB	13:L:503:UQ9:O4	2.11	0.50
4:M:37:TRP:H	6:M:704:LDA:HM13	1.77	0.50
1:C:145:VAL:O	1:C:146:ARG:HD2	2.11	0.50
11:L:400:BCB:OBB	11:L:400:BCB:HHC	2.11	0.49
1:C:291:ALA:HB3	10:C:377:GOL:H32	1.95	0.49
9:H:273:HTO:C1	18:H:499:HOH:O	2.60	0.49
1:C:64[A]:ASN:ND2	9:C:355:HTO:H3	2.27	0.49
3:L:193:LEU:HD22	3:L:216:PHE:HE2	1.77	0.49
13:L:503:UQ9:O5	13:L:503:UQ9:C8	2.60	0.49
13:L:502:UQ9:O2	13:L:502:UQ9:H3MB	2.13	0.49
4:M:192:GLY:O	4:M:193:ASN:HB3	2.13	0.49
1:C:105:VAL:CG2	1:C:288:VAL:HG11	2.43	0.48
9:H:273:HTO:H12	18:H:499:HOH:O	2.12	0.48
7:C:730:DGA:HB62	7:C:730:DGA:HA52	1.94	0.48
2:H:69:VAL:HG22	3:L:205:LYS:HA	1.94	0.47
1:C:64[A]:ASN:HD21	9:C:355:HTO:C3	2.27	0.47
1:C:123:GLN:NE2	10:M:338:GOL:H31	2.29	0.47
11:L:401:BCB:HMB1	11:L:401:BCB:HBB2	1.96	0.47
4:M:73:MET:HE1	4:M:88:PHE:HE1	1.75	0.47
3:L:161:GLY:HA3	11:L:400:BCB:HAC1	1.96	0.47
4:M:29:ILE:HD12	4:M:51:LEU:HD13	1.96	0.46
4:M:74:LEU:HD12	16:M:600:NS5:CM2	2.45	0.46
4:M:226:ARG:NH1	8:M:326:SO4:O1	2.44	0.46
3:L:272:TRP:CD1	4:M:86:ARG:CD	2.93	0.46
1:C:108:ARG:HD2	18:C:780:HOH:O	2.15	0.46
3:L:125:ILE:HG21	6:L:724:LDA:HM22	1.97	0.46
4:M:106:PRO:HB3	6:M:714:LDA:H31	1.98	0.46
1:C:64[A]:ASN:HD21	9:C:355:HTO:H3	1.80	0.46
4:M:184:LEU:HD21	11:M:400:BCB:CAC	2.47	0.45
11:M:401:BCB:HAA2	11:M:401:BCB:HBD	1.98	0.45
2:H:81[A]:ARG:HG3	2:H:81[A]:ARG:NH1	2.32	0.45
6:C:716:LDA:HM21	10:C:364:GOL:O3	2.17	0.45
4:M:107:LEU:H	6:M:714:LDA:H32	1.82	0.45
13:L:502:UQ9:H4MB	13:L:502:UQ9:O3	2.16	0.44
11:M:401:BCB:HAA2	11:M:401:BCB:CBD	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:502:UQ9:C51	11:M:400:BCB:H191	2.47	0.44
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.52	0.44
7:C:730:DGA:HB22	7:C:730:DGA:CA2	2.47	0.44
3:L:182:VAL:HA	11:M:400:BCB:H43	2.00	0.44
4:M:74:LEU:HD12	16:M:600:NS5:HM23	1.99	0.44
13:L:503:UQ9:O5	13:L:503:UQ9:C4M	2.65	0.44
4:M:37:TRP:CD1	6:M:704:LDA:CM1	3.01	0.43
2:H:30:LEU:O	2:H:34:ARG:HD2	2.18	0.43
3:L:29:TYR:OH	6:L:702:LDA:H12	2.19	0.43
3:L:153:HIS:O	3:L:157:VAL:HG23	2.18	0.43
4:M:212:LEU:HD23	4:M:212:LEU:O	2.17	0.43
3:L:77:ALA:HB1	9:L:277:HTO:O3	2.18	0.43
11:M:400:BCB:CMB	11:M:400:BCB:CBB	2.97	0.43
2:H:102:GLN:HA	2:H:103:PRO:HD3	1.94	0.42
4:M:37:TRP:H	6:M:704:LDA:CM1	2.32	0.42
15:M:501:MQ9:C38	15:M:501:MQ9:H33	2.49	0.42
11:M:401:BCB:OBB	11:M:401:BCB:HHC	2.20	0.42
1:C:104:TYR:C	1:C:104:TYR:CD1	2.98	0.42
11:L:401:BCB:OBB	11:L:401:BCB:HHC	2.20	0.42
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.80	0.42
9:C:357:HTO:H73	10:L:286:GOL:O1	2.20	0.42
3:L:125:ILE:CG2	6:L:724:LDA:HM22	2.51	0.41
1:C:64[A]:ASN:HD21	9:C:355:HTO:C1	2.33	0.41
2:H:55:GLU:H	2:H:58:GLN:HE21	1.67	0.41
11:L:401:BCB:O1A	11:L:401:BCB:H43	2.21	0.41
1:C:216:ARG:HG3	6:C:716:LDA:HM22	2.02	0.41
3:L:197:VAL:HG13	3:L:207:LYS:HB2	2.02	0.41
1:C:314:LYS:O	1:C:315:PRO:C	2.63	0.40
5:C:401:HEC:HBB3	5:C:401:HEC:CMB	2.51	0.40
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.56	0.40
3:L:183:ASN:HD21	4:M:214:PHE:HB3	1.85	0.40
13:L:502:UQ9:H32	13:L:502:UQ9:H35	1.95	0.40
4:M:248:LEU:O	4:M:249:PHE:C	2.62	0.40
6:M:707:LDA:HM13	6:M:707:LDA:H21	1.81	0.40
13:L:502:UQ9:H51A	11:M:400:BCB:H191	2.04	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	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

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	105	VAL
1	C	127	GLN
1	C	166	VAL
1	C	176	LEU
2	H	8	GLN
2	H	22	LEU
2	H	44	VAL
2	H	69	VAL
2	H	87	GLU
2	H	94	ASP
2	H	123	VAL
2	H	236	ASP
3	L	2	LEU
3	L	16	LEU
3	L	44	LEU
3	L	48	LEU
3	L	80	LEU
3	L	202	ASP
4	M	27	ASP
4	M	29	ILE
4	M	74	LEU
4	M	163	PRO
4	M	180	HIS
4	M	194	PHE
4	M	213	LEU
4	M	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	297	GLN
2	H	58	GLN
2	H	102	GLN
2	H	220	ASN
3	L	183	ASN
3	L	213	ASN
3	L	239	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

All (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
2	H	1[A]	FME	CB-CG-SD-CE
2	H	1[B]	FME	CB-CA-N-CN
2	H	1[B]	FME	CB-CG-SD-CE
2	H	1[B]	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	703	LDA	O1-N1	-6.94	1.25	1.42
6	L	710	LDA	O1-N1	-6.85	1.25	1.42
6	L	712	LDA	O1-N1	-6.85	1.25	1.42
6	L	702	LDA	O1-N1	-6.78	1.25	1.42
6	L	711	LDA	O1-N1	-6.77	1.25	1.42
6	L	723	LDA	O1-N1	-6.65	1.25	1.42
6	M	715	LDA	O1-N1	-6.65	1.25	1.42
6	H	718[B]	LDA	O1-N1	-6.53	1.26	1.42
6	H	719	LDA	O1-N1	-6.52	1.26	1.42
6	M	713	LDA	O1-N1	-6.51	1.26	1.42
6	C	716	LDA	O1-N1	-6.50	1.26	1.42
6	L	708	LDA	O1-N1	-6.46	1.26	1.42
6	C	722	LDA	O1-N1	-6.45	1.26	1.42
6	L	709	LDA	O1-N1	-6.41	1.26	1.42
6	M	717	LDA	O1-N1	-6.38	1.26	1.42
6	M	706	LDA	O1-N1	-6.33	1.26	1.42
6	H	721	LDA	O1-N1	-6.10	1.27	1.42
13	L	502	UQ9	C7-C8	-6.09	1.41	1.50
13	L	503	UQ9	C7-C8	-6.07	1.41	1.50
6	M	705	LDA	O1-N1	-6.07	1.27	1.42
5	C	402	HEC	CAB-C3B	5.45	1.52	1.35
6	L	723	LDA	C1-N1	-5.37	1.45	1.51
5	C	403	HEC	CAB-C3B	5.31	1.52	1.35
11	M	400	BCB	C1B-C2B	5.15	1.45	1.39
11	L	401	BCB	C3A-C2A	-5.14	1.50	1.54
5	C	404	HEC	CAC-C3C	5.14	1.51	1.35
6	L	703	LDA	C1-N1	-5.06	1.46	1.51
5	C	403	HEC	CAC-C3C	5.02	1.51	1.35
5	C	404	HEC	CAB-C3B	4.98	1.51	1.35
6	H	701	LDA	O1-N1	-4.94	1.30	1.42
12	M	402	BPB	C1B-C2B	4.89	1.44	1.39
12	L	402	BPB	C1B-C2B	4.76	1.44	1.39
5	C	402	HEC	CAC-C3C	4.75	1.50	1.35
5	C	401	HEC	CAC-C3C	4.71	1.50	1.35
15	M	501	MQ9	C7-C8	-4.62	1.43	1.50
15	M	501	MQ9	C6-C5	4.57	1.43	1.35
15	M	501	MQ9	C2-C1	-4.54	1.39	1.48
5	C	401	HEC	CAB-C3B	4.54	1.49	1.35
6	M	714	LDA	C1-N1	-4.50	1.46	1.51
6	C	722	LDA	C1-N1	-4.46	1.46	1.51
6	H	720	LDA	C1-N1	-4.38	1.47	1.51
11	M	400	BCB	CHB-C4A	4.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	401	BCB	CHA-CBD	-4.16	1.46	1.51
6	M	704	LDA	C1-N1	-4.08	1.47	1.51
11	M	401	BCB	CBD-CGD	4.04	1.57	1.52
5	C	403	HEC	C3B-C4B	-4.02	1.39	1.46
6	L	724	LDA	C1-N1	-3.87	1.47	1.51
15	M	501	MQ9	C43-C44	3.84	1.41	1.33
15	M	501	MQ9	C33-C34	3.78	1.41	1.33
11	L	400	BCB	C3A-C2A	-3.72	1.51	1.54
13	L	502	UQ9	C42-C43	-3.69	1.39	1.50
6	L	702	LDA	C1-N1	-3.69	1.47	1.51
6	H	719	LDA	C1-N1	-3.65	1.47	1.51
13	L	502	UQ9	C32-C33	-3.57	1.39	1.50
6	H	721	LDA	C1-N1	-3.57	1.47	1.51
15	M	501	MQ9	C8-C9	3.57	1.41	1.33
15	M	501	MQ9	C5M-C5	3.55	1.58	1.50
13	L	502	UQ9	C47-C48	-3.53	1.39	1.50
15	M	501	MQ9	C37-C38	-3.50	1.39	1.50
13	L	502	UQ9	C22-C23	-3.48	1.39	1.50
15	M	501	MQ9	C38-C39	3.48	1.41	1.33
6	H	718[B]	LDA	C1-N1	-3.47	1.47	1.51
11	L	401	BCB	C4A-C3A	3.45	1.57	1.51
13	L	502	UQ9	C8-C9	3.43	1.41	1.33
5	C	403	HEC	C2A-C3A	3.43	1.44	1.36
6	M	705	LDA	C1-N1	-3.43	1.48	1.51
13	L	502	UQ9	C27-C28	-3.42	1.40	1.50
5	C	401	HEC	C3B-C4B	-3.41	1.40	1.46
13	L	502	UQ9	C12-C13	-3.40	1.40	1.50
6	M	717	LDA	C1-N1	-3.38	1.48	1.51
15	M	501	MQ9	C5-C4	-3.37	1.39	1.47
15	M	501	MQ9	C28-C29	3.35	1.40	1.33
6	M	706	LDA	C1-N1	-3.35	1.48	1.51
11	M	401	BCB	O2D-CGD	3.33	1.41	1.33
12	M	402	BPB	C3A-C2A	3.30	1.57	1.54
15	M	501	MQ9	C27-C28	-3.28	1.40	1.50
15	M	501	MQ9	C47-C48	-3.27	1.40	1.50
13	L	503	UQ9	C8-C9	3.26	1.40	1.33
11	L	401	BCB	CMA-C3A	3.26	1.58	1.53
13	L	502	UQ9	C4-C5	-3.25	1.39	1.48
13	L	503	UQ9	C12-C13	-3.25	1.40	1.50
13	L	502	UQ9	C28-C29	3.24	1.40	1.33
13	L	502	UQ9	C38-C39	3.22	1.40	1.33
13	L	502	UQ9	C6-C1	3.20	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	501	MQ9	C32-C33	-3.20	1.40	1.50
13	L	502	UQ9	C18-C19	3.19	1.40	1.33
15	M	501	MQ9	C22-C23	-3.19	1.40	1.50
13	L	502	UQ9	C3-C2	-3.18	1.39	1.48
13	L	502	UQ9	C17-C18	-3.18	1.40	1.50
13	L	502	UQ9	C37-C38	-3.14	1.41	1.50
11	M	401	BCB	C1B-C2B	3.14	1.43	1.39
5	C	401	HEC	C1A-C2A	-3.13	1.39	1.45
12	M	402	BPB	C3D-C4D	-3.08	1.37	1.41
11	L	401	BCB	C1D-C2D	3.07	1.43	1.39
15	M	501	MQ9	C18-C19	3.05	1.40	1.33
13	L	503	UQ9	C6-C1	3.04	1.40	1.35
16	M	600	NS5	C24-C25	3.03	1.52	1.43
15	M	501	MQ9	C42-C43	-3.01	1.41	1.50
6	M	713	LDA	C1-N1	-3.01	1.48	1.51
13	L	502	UQ9	C13-C14	2.93	1.39	1.33
15	M	501	MQ9	C12-C13	-2.90	1.41	1.50
16	M	600	NS5	C23-C21	2.89	1.52	1.46
16	M	600	NS5	C29-C30	2.88	1.52	1.43
5	C	401	HEC	C4A-NA	-2.88	1.34	1.39
11	M	401	BCB	CAA-CBA	-2.88	1.44	1.52
13	L	503	UQ9	C3-C2	-2.84	1.40	1.48
15	M	501	MQ9	C6-C1	-2.84	1.40	1.47
13	L	502	UQ9	C23-C24	2.83	1.39	1.33
6	L	710	LDA	C1-N1	-2.83	1.48	1.51
6	L	711	LDA	C1-N1	-2.82	1.48	1.51
13	L	502	UQ9	C6-C5	-2.81	1.38	1.46
11	L	400	BCB	MG-ND	-2.80	2.00	2.05
5	C	402	HEC	C4A-C3A	-2.77	1.39	1.45
13	L	502	UQ9	C48-C49	2.76	1.40	1.32
11	L	400	BCB	CHA-CBD	-2.76	1.48	1.51
13	L	502	UQ9	C33-C34	2.72	1.39	1.33
11	L	400	BCB	O2D-CGD	2.72	1.39	1.33
13	L	503	UQ9	C4-C5	-2.71	1.41	1.48
6	M	707	LDA	C1-N1	-2.69	1.48	1.51
5	C	402	HEC	C3C-C4C	-2.69	1.41	1.46
5	C	403	HEC	C4A-C3A	-2.69	1.40	1.45
6	L	712	LDA	C1-N1	-2.69	1.48	1.51
7	C	730	DGA	CG1-CG2	2.65	1.56	1.50
12	L	402	BPB	C3D-CAD	-2.63	1.42	1.47
13	L	502	UQ9	C43-C44	2.63	1.39	1.33
15	M	501	MQ9	C17-C18	-2.62	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	503	UQ9	C13-C14	2.62	1.40	1.32
11	M	401	BCB	MG-NB	-2.61	2.00	2.05
5	C	403	HEC	C1D-ND	-2.60	1.34	1.39
5	C	404	HEC	C3C-C4C	-2.60	1.41	1.46
5	C	404	HEC	C4D-ND	-2.60	1.34	1.39
11	M	400	BCB	CMD-C2D	2.59	1.56	1.51
15	M	501	MQ9	C48-C49	2.59	1.40	1.32
11	M	401	BCB	OBD-CAD	2.58	1.25	1.22
5	C	403	HEC	C1A-C2A	-2.56	1.40	1.45
12	M	402	BPB	C3B-C4B	2.55	1.45	1.41
16	M	600	NS5	C28-C26	2.54	1.51	1.46
5	C	401	HEC	C1B-NB	-2.50	1.34	1.39
12	L	402	BPB	C1D-C2D	2.50	1.42	1.39
15	M	501	MQ9	C41-C39	2.49	1.56	1.51
5	C	402	HEC	C4A-NA	-2.49	1.34	1.39
16	M	600	NS5	C22-C21	2.47	1.55	1.50
15	M	501	MQ9	C23-C24	2.46	1.38	1.33
16	M	600	NS5	C16-C15	2.46	1.55	1.50
6	L	709	LDA	C1-N1	-2.45	1.49	1.51
5	C	404	HEC	C4A-C3A	-2.44	1.40	1.45
5	C	401	HEC	C1D-ND	-2.43	1.35	1.39
16	M	600	NS5	C19-C20	2.42	1.50	1.43
15	M	501	MQ9	C46-C44	2.40	1.56	1.51
11	L	401	BCB	C3D-CAD	-2.37	1.43	1.47
16	M	600	NS5	C20-C21	2.35	1.41	1.35
5	C	404	HEC	C1B-NB	-2.34	1.35	1.39
11	L	401	BCB	C3D-C4D	2.32	1.45	1.41
16	M	600	NS5	C13-C12	2.31	1.50	1.43
11	L	401	BCB	CBD-CGD	-2.31	1.49	1.52
11	L	400	BCB	C3D-CAD	-2.30	1.43	1.47
11	M	400	BCB	CBD-CGD	-2.29	1.49	1.52
12	L	402	BPB	C3B-C4B	2.29	1.45	1.41
6	H	701	LDA	C1-N1	-2.26	1.49	1.51
13	L	503	UQ9	C7-C6	2.24	1.55	1.51
15	M	501	MQ9	O4-C4	2.23	1.27	1.23
5	C	403	HEC	CHD-C4C	2.21	1.42	1.38
11	M	400	BCB	MG-NB	-2.19	2.01	2.05
16	M	600	NS5	C33-C31	2.17	1.55	1.51
5	C	401	HEC	O1D-CGD	2.16	1.29	1.22
5	C	401	HEC	C2A-C3A	2.14	1.41	1.36
13	L	502	UQ9	C7-C6	2.14	1.55	1.51
5	C	402	HEC	O2A-CGA	-2.13	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	M	600	NS5	C34-C35	2.12	1.56	1.50
5	C	404	HEC	CHC-C1C	-2.12	1.34	1.39
13	L	502	UQ9	C25-C24	2.10	1.55	1.50
5	C	401	HEC	C4C-NC	-2.07	1.35	1.39
5	C	403	HEC	C1A-NA	-2.07	1.35	1.39
12	M	402	BPB	C3D-CAD	-2.06	1.43	1.47
5	C	401	HEC	C3C-C4C	-2.05	1.42	1.46
5	C	401	HEC	CMB-C2B	2.05	1.55	1.50
13	L	503	UQ9	C1-C2	-2.04	1.40	1.47
7	C	730	DGA	CA2-CA1	2.04	1.56	1.50
11	M	401	BCB	MG-ND	-2.04	2.01	2.05
5	C	403	HEC	C3C-C4C	-2.04	1.42	1.46
5	C	402	HEC	C1D-ND	-2.03	1.35	1.39
5	C	401	HEC	C4A-C3A	-2.03	1.41	1.45
11	M	401	BCB	O2A-CGA	2.01	1.39	1.33
5	C	403	HEC	O2D-CGD	-2.01	1.24	1.30

All (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
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
11	L	401	BCB	C4D-ND-C1D	10.42	113.13	105.22
12	L	402	BPB	C4D-CHA-CBD	-10.30	103.51	108.45
11	M	400	BCB	C4D-ND-C1D	10.10	112.89	105.22
11	L	400	BCB	C4D-ND-C1D	9.40	112.36	105.22
11	M	401	BCB	C1B-CHB-C4A	9.11	127.19	121.32
11	L	400	BCB	C4B-CHC-C1C	8.58	126.84	121.32
5	C	402	HEC	CBB-CAB-C3B	-8.43	110.58	127.43
11	L	400	BCB	C1B-CHB-C4A	7.99	126.46	121.32
5	C	403	HEC	CBB-CAB-C3B	-7.87	111.70	127.43
11	L	401	BCB	C1B-CHB-C4A	7.86	126.38	121.32
11	M	401	BCB	C4D-ND-C1D	7.41	110.84	105.22
5	C	404	HEC	CBC-CAC-C3C	-7.20	113.03	127.43
11	L	400	BCB	O2D-CGD-CBD	7.18	118.84	110.95
12	L	402	BPB	C2B-C1B-NB	-6.83	104.49	109.43
16	M	600	NS5	C19-C20-C21	-6.79	117.75	127.28
5	C	401	HEC	CBC-CAC-C3C	-6.76	113.93	127.43
11	M	401	BCB	O2D-CGD-O1D	-6.70	110.80	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	C1B-CHB-C4A	6.70	125.63	121.32
16	M	600	NS5	C14-C15-C17	-6.58	108.65	119.01
9	M	333	HTO	C5-C4-C3	-6.58	103.33	114.11
16	M	600	NS5	C11-C10-C9	6.52	126.55	115.23
16	M	600	NS5	C29-C30-C31	-5.94	119.34	127.69
11	M	400	BCB	O2D-CGD-CBD	5.90	117.43	110.95
9	C	358[A]	HTO	C5-C4-C3	-5.81	104.58	114.11
5	C	403	HEC	CBC-CAC-C3C	-5.75	115.93	127.43
5	C	404	HEC	CBB-CAB-C3B	-5.74	115.96	127.43
5	C	402	HEC	CBC-CAC-C3C	-5.29	116.85	127.43
16	M	600	NS5	C18-C19-C20	5.26	134.29	123.52
12	L	402	BPB	C4A-C3A-C2A	-5.25	97.84	102.84
12	M	402	BPB	C4D-CHA-CBD	-5.24	105.94	108.45
12	M	402	BPB	C4A-C3A-C2A	-5.15	97.94	102.84
16	M	600	NS5	C16-C15-C17	5.10	131.08	122.82
11	L	401	BCB	O2D-CGD-CBD	4.97	116.41	110.95
7	C	730	DGA	CG2-OG2-CB1	-4.60	111.15	117.78
16	M	600	NS5	C24-C25-C26	-4.58	120.85	127.28
11	L	401	BCB	C3D-C4D-ND	-4.40	105.88	112.94
13	L	503	UQ9	C7-C8-C9	4.34	134.30	126.83
11	M	400	BCB	C3D-CAD-CBD	4.32	113.29	107.61
13	L	502	UQ9	C25-C24-C26	4.18	122.49	115.23
9	C	356	HTO	O3-C3-C2	-4.18	100.80	109.57
5	C	401	HEC	CHD-C4C-NC	-4.16	119.92	124.45
6	M	704	LDA	CM1-N1-C1	-4.15	101.52	110.23
16	M	600	NS5	C12-C13-C14	-4.11	111.28	123.20
11	L	401	BCB	CMB-C2B-C3B	4.08	132.83	124.68
12	L	402	BPB	C4B-NB-C1B	4.03	114.69	108.82
7	C	730	DGA	OG2-CB1-CB2	4.00	120.13	111.48
12	L	402	BPB	OBD-CAD-CBD	-3.98	119.98	125.82
11	M	400	BCB	C3D-C4D-ND	-3.97	106.58	112.94
12	M	402	BPB	OBD-CAD-CBD	-3.95	120.03	125.82
11	M	400	BCB	C1-C2-C3	-3.94	119.73	126.20
16	M	600	NS5	C6-C5-C4	3.94	122.07	115.23
11	M	401	BCB	CHA-C1A-C2A	-3.85	124.26	133.31
12	M	402	BPB	CMB-C2B-C3B	3.85	132.37	124.68
11	M	400	BCB	CHA-C1A-C2A	-3.81	124.35	133.31
13	L	502	UQ9	C30-C29-C31	3.81	121.84	115.23
11	L	400	BCB	C3D-C4D-ND	-3.79	106.85	112.94
16	M	600	NS5	C8-C7-C5	-3.79	118.95	127.62
9	C	358[A]	HTO	O1-C1-C2	-3.78	103.22	111.16
11	M	401	BCB	C1-C2-C3	-3.76	120.04	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	400	BCB	C3D-C4D-CHA	3.73	114.22	108.54
11	M	400	BCB	CMA-C3A-C4A	-3.72	106.59	114.61
11	L	401	BCB	OBD-CAD-C3D	-3.71	122.10	127.89
5	C	403	HEC	CHD-C4C-NC	-3.68	120.45	124.45
11	L	401	BCB	CHA-C1A-C2A	-3.68	124.67	133.31
9	L	277	HTO	C5-C4-C3	-3.68	108.09	114.11
11	L	400	BCB	O2A-CGA-O1A	-3.68	114.43	123.63
5	C	401	HEC	CHC-C4B-NB	-3.63	120.50	124.45
11	L	400	BCB	C3D-CAD-CBD	3.61	112.36	107.61
11	M	401	BCB	C4C-CHD-C1D	3.61	128.99	116.07
9	C	358[A]	HTO	O3-C3-C4	-3.61	100.95	109.14
12	L	402	BPB	O1D-CGD-CBD	-3.59	119.27	124.72
11	L	401	BCB	C4-C3-C5	3.56	121.41	115.23
5	C	404	HEC	CHD-C4C-NC	-3.52	120.62	124.45
11	M	401	BCB	C3D-C4D-CHA	3.52	113.88	108.54
11	L	400	BCB	C4-C3-C5	3.51	121.33	115.23
16	M	600	NS5	C13-C12-C10	-3.51	122.76	127.69
11	M	401	BCB	OBD-CAD-CBD	-3.46	120.75	125.82
11	L	401	BCB	O1D-CGD-CBD	-3.45	119.49	124.72
13	L	502	UQ9	C35-C34-C36	3.42	121.16	115.23
9	M	333	HTO	O1-C1-C2	-3.42	103.98	111.16
11	M	400	BCB	OBD-CAD-CBD	-3.41	120.82	125.82
13	L	502	UQ9	C1M-C1-C6	-3.40	118.86	124.45
11	M	401	BCB	CED-O2D-CGD	3.37	123.55	115.92
12	M	402	BPB	C2D-C1D-ND	-3.30	107.04	109.43
11	M	400	BCB	C4-C3-C5	3.26	120.89	115.23
11	M	400	BCB	C4C-CHD-C1D	3.24	127.67	116.07
11	M	401	BCB	O2A-CGA-CBA	3.24	121.71	111.83
11	M	401	BCB	CMB-C2B-C3B	3.21	131.10	124.68
13	L	503	UQ9	C1-C6-C5	-3.16	116.55	119.62
15	M	501	MQ9	C40-C39-C38	-3.16	115.52	123.63
11	L	401	BCB	C3D-C4D-CHA	3.15	113.33	108.54
6	L	708	LDA	CM1-N1-C1	-3.13	103.65	110.23
11	L	400	BCB	CMB-C2B-C3B	3.12	130.92	124.68
6	M	704	LDA	CM2-N1-C1	3.12	116.78	110.23
7	C	730	DGA	OG1-CA1-CA2	3.11	121.33	111.83
15	M	501	MQ9	C5M-C5-C6	-3.11	119.34	124.45
11	L	400	BCB	C4C-CHD-C1D	3.10	127.17	116.07
5	C	404	HEC	CMD-C2D-C1D	3.10	130.14	125.42
9	H	272	HTO	C5-C4-C3	-3.09	109.05	114.11
12	L	402	BPB	CED-O2D-CGD	3.07	122.87	115.92
12	M	402	BPB	O2D-CGD-CBD	3.06	114.31	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	CBA-CAA-C2A	-3.04	104.82	113.78
5	C	402	HEC	CHD-C4C-NC	-3.04	121.14	124.45
16	M	600	NS5	C32-C31-C33	3.04	120.50	115.23
13	L	502	UQ9	C7-C8-C9	3.01	132.01	126.83
13	L	502	UQ9	C7-C6-C5	-3.01	115.02	118.52
11	M	401	BCB	C3D-C4D-ND	-3.00	108.12	112.94
11	L	401	BCB	C6-C5-C3	-2.99	106.18	113.47
11	L	400	BCB	C1-C2-C3	-2.99	121.30	126.20
5	C	402	HEC	CHC-C4B-NB	-2.98	121.20	124.45
15	M	501	MQ9	C15-C14-C16	2.95	120.35	115.23
9	L	278	HTO	O2-C2-C1	-2.93	102.35	109.03
11	L	400	BCB	CHA-C1A-C2A	-2.93	126.44	133.31
7	C	730	DGA	OG2-CG2-CG1	2.92	112.93	106.21
11	L	400	BCB	OBD-CAD-CBD	-2.91	121.55	125.82
12	L	402	BPB	C3B-C4B-NB	-2.87	103.88	108.05
9	L	278	HTO	O1-C1-C2	-2.86	105.16	111.16
12	M	402	BPB	C2B-C1B-NB	-2.86	107.37	109.43
9	H	272	HTO	O1-C1-C2	-2.85	105.16	111.16
12	L	402	BPB	OBD-CAD-C3D	2.84	132.32	127.89
12	L	402	BPB	O2D-CGD-CBD	2.81	114.04	110.95
11	M	400	BCB	O1D-CGD-CBD	-2.80	120.47	124.72
15	M	501	MQ9	C35-C34-C36	2.80	120.08	115.23
6	L	708	LDA	O1-N1-C1	2.76	116.04	109.27
12	M	402	BPB	CMD-C2D-C3D	2.75	130.19	124.68
13	L	502	UQ9	C6-C1-C2	2.75	121.34	119.17
5	C	404	HEC	O2A-CGA-CBA	2.75	122.69	114.00
17	M	332	HTH	O3-C3-C2	-2.74	103.81	109.57
5	C	401	HEC	CMA-C3A-C4A	2.73	129.53	124.73
5	C	404	HEC	CHA-C1A-NA	-2.70	121.51	124.45
11	L	401	BCB	C3D-CAD-CBD	2.68	111.13	107.61
12	L	402	BPB	CMD-C2D-C3D	2.66	130.00	124.68
11	L	400	BCB	O2A-CGA-CBA	2.66	119.93	111.83
9	C	358[A]	HTO	O2-C2-C1	-2.63	103.06	109.03
5	C	404	HEC	O1D-CGD-CBD	-2.60	114.85	123.09
11	M	400	BCB	C4D-CHA-CBD	2.60	111.58	108.97
11	M	401	BCB	C3D-CAD-CBD	2.56	110.97	107.61
13	L	502	UQ9	C45-C44-C46	2.55	119.66	115.23
13	L	502	UQ9	C1-C6-C5	-2.55	117.14	119.62
15	M	501	MQ9	C25-C24-C26	2.53	119.62	115.23
11	M	400	BCB	O2A-CGA-CBA	2.52	119.52	111.83
11	M	401	BCB	CAA-C2A-C3A	-2.52	106.20	113.00
11	M	400	BCB	C3D-C4D-CHA	2.51	112.36	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	401	BCB	CMA-C3A-C4A	-2.51	109.20	114.61
9	C	355	HTO	O2-C2-C1	2.46	114.61	109.03
13	L	503	UQ9	C8-C7-C6	-2.45	106.05	112.08
9	L	276	HTO	O2-C2-C3	-2.43	104.47	109.57
13	L	502	UQ9	O5-C5-C6	-2.41	117.12	121.79
12	L	402	BPB	CMB-C2B-C3B	2.41	129.51	124.68
9	L	278	HTO	O2-C2-C3	2.41	114.64	109.57
5	C	402	HEC	CAA-C2A-C1A	2.40	129.74	124.85
15	M	501	MQ9	C40-C39-C41	2.40	119.40	115.23
5	C	402	HEC	C1A-C2A-C3A	-2.40	103.95	107.11
11	L	401	BCB	C4C-CHD-C1D	2.39	124.62	116.07
5	C	404	HEC	CHC-C4B-NB	-2.37	121.87	124.45
16	M	600	NS5	C24-C23-C21	-2.35	119.92	126.36
16	M	600	NS5	C27-C26-C28	2.35	121.68	118.09
13	L	502	UQ9	O2-C2-C3	-2.33	116.10	121.03
5	C	404	HEC	C3D-C4D-ND	2.32	112.73	110.15
9	L	276	HTO	O3-C3-C4	2.32	114.41	109.14
9	H	272	HTO	O2-C2-C1	-2.32	103.76	109.03
15	M	501	MQ9	C3D-C2-C3	2.31	121.86	119.26
12	L	402	BPB	C1-C2-C3	-2.31	122.42	126.20
12	M	402	BPB	C1-O2A-CGA	2.31	122.24	116.65
11	M	400	BCB	CHD-C4C-C3C	-2.30	123.18	130.04
13	L	502	UQ9	C45-C44-C43	-2.27	117.79	123.63
11	M	401	BCB	C4-C3-C5	2.27	119.17	115.23
6	M	704	LDA	O1-N1-C1	2.25	114.80	109.27
12	M	402	BPB	C3D-CAD-CBD	2.24	110.56	107.61
13	L	503	UQ9	C3-C2-C1	2.24	122.53	118.10
9	H	273	HTO	O1-C1-C2	2.24	115.85	111.16
11	L	400	BCB	C5-C3-C2	-2.23	116.17	121.17
11	L	400	BCB	O2D-CGD-O1D	-2.22	119.53	123.85
5	C	401	HEC	CAD-C3D-C4D	2.21	129.26	124.94
9	L	280	HTO	C5-C4-C3	-2.21	110.49	114.11
9	C	356	HTO	C5-C4-C3	2.21	117.73	114.11
5	C	404	HEC	O2D-CGD-CBD	2.20	120.96	114.00
10	L	282	GOL	C3-C2-C1	2.20	119.86	111.80
5	C	403	HEC	C1D-CHD-C4C	2.18	131.39	124.66
11	L	400	BCB	CHD-C4C-C3C	-2.18	123.53	130.04
11	L	401	BCB	C1-C2-C3	-2.18	122.63	126.20
11	L	401	BCB	C5-C3-C2	-2.16	116.32	121.17
9	M	333	HTO	O3-C3-C2	2.16	114.11	109.57
5	C	404	HEC	C1D-C2D-C3D	-2.16	104.35	106.82
9	C	355	HTO	C4-C3-C2	-2.15	108.56	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	600	NS5	C28-C26-C25	-2.14	115.64	119.01
5	C	403	HEC	C3D-C4D-ND	2.14	112.52	110.15
5	C	404	HEC	O2A-CGA-O1A	-2.13	117.85	123.33
13	L	502	UQ9	C15-C14-C16	2.13	118.92	115.23
13	L	503	UQ9	C15-C14-C16	2.12	119.47	114.59
9	M	333	HTO	O3-C3-C4	-2.11	104.34	109.14
10	C	361	GOL	O1-C1-C2	-2.11	100.90	110.38
5	C	401	HEC	C4C-NC-C1C	-2.10	102.39	105.82
5	C	401	HEC	O2A-CGA-CBA	2.10	120.64	114.00
5	C	403	HEC	C4A-C3A-C2A	-2.10	103.86	106.97
11	M	401	BCB	CAA-CBA-CGA	-2.09	107.26	113.21
11	L	401	BCB	CHD-C4C-C3C	-2.08	123.82	130.04
7	C	730	DGA	OG1-CA1-OA1	-2.08	118.42	123.63
7	C	730	DGA	OG1-CG1-CG2	2.08	114.27	108.35
11	M	401	BCB	CHD-C4C-C3C	-2.07	123.87	130.04
5	C	403	HEC	C2C-C1C-NC	2.06	113.45	110.14
10	H	280	GOL	C3-C2-C1	2.06	119.34	111.80
9	L	279	HTO	C4-C3-C2	-2.05	108.81	113.73
11	L	400	BCB	O1D-CGD-CBD	-2.04	121.62	124.72
5	C	402	HEC	C2A-C1A-NA	2.04	112.29	110.32
15	M	501	MQ9	C51-C49-C50	2.03	119.27	114.59
5	C	403	HEC	O2A-CGA-O1A	-2.03	118.12	123.33
13	L	502	UQ9	C25-C24-C23	-2.01	118.46	123.63
12	L	402	BPB	O2A-CGA-O1A	-2.01	118.60	123.63
9	C	355	HTO	C1-C2-C3	-2.01	108.91	113.00
9	H	272	HTO	C1-C2-C3	2.01	117.09	113.00

All (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
11	L	401	BCB	NC
11	M	400	BCB	ND
11	M	400	BCB	NA
11	M	400	BCB	NC
11	M	401	BCB	ND
11	M	401	BCB	NA
11	M	401	BCB	NC

All (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
5	C	402	HEC	C4B-C3B-CAB-CBB
5	C	402	HEC	C2C-C3C-CAC-CBC
5	C	402	HEC	C4C-C3C-CAC-CBC
5	C	403	HEC	C2B-C3B-CAB-CBB
5	C	403	HEC	C4B-C3B-CAB-CBB
5	C	403	HEC	C2C-C3C-CAC-CBC
5	C	403	HEC	C4C-C3C-CAC-CBC
5	C	404	HEC	C2B-C3B-CAB-CBB
5	C	404	HEC	C4B-C3B-CAB-CBB
5	C	404	HEC	C2C-C3C-CAC-CBC
5	C	404	HEC	C4C-C3C-CAC-CBC
6	C	716	LDA	C2-C1-N1-CM1
6	C	716	LDA	N1-C1-C2-C3
6	C	722	LDA	C2-C1-N1-O1
6	C	722	LDA	N1-C1-C2-C3
6	H	718[B]	LDA	C2-C1-N1-O1
6	H	718[B]	LDA	C2-C1-N1-CM1
6	H	718[B]	LDA	C2-C1-N1-CM2
6	H	721	LDA	C2-C1-N1-CM1
6	H	721	LDA	C2-C1-N1-CM2
6	L	702	LDA	C2-C1-N1-CM1
6	L	703	LDA	N1-C1-C2-C3
6	L	710	LDA	C2-C1-N1-CM1
6	L	710	LDA	C2-C1-N1-CM2
6	L	712	LDA	N1-C1-C2-C3
6	L	723	LDA	C2-C1-N1-O1
6	L	723	LDA	C2-C1-N1-CM2
6	L	724	LDA	C2-C1-N1-CM1
6	M	706	LDA	C2-C1-N1-CM1
6	M	706	LDA	C2-C1-N1-CM2
6	M	707	LDA	C2-C1-N1-CM1
6	M	707	LDA	C2-C1-N1-CM2
6	M	707	LDA	N1-C1-C2-C3
6	M	714	LDA	N1-C1-C2-C3
7	C	730	DGA	CB2-CB1-OG2-CG2
7	C	730	DGA	OB1-CB1-OG2-CG2
7	C	730	DGA	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
7	C	730	DGA	CG1-CG2-OG2-CB1
9	C	355	HTO	O3-C3-C4-C5
9	C	356	HTO	C1-C2-C3-O3
9	C	356	HTO	C1-C2-C3-C4
9	C	356	HTO	O2-C2-C3-O3
9	C	356	HTO	O2-C2-C3-C4
9	C	356	HTO	O3-C3-C4-C5
9	C	357	HTO	C1-C2-C3-C4
9	C	357	HTO	O2-C2-C3-C4
9	C	358[A]	HTO	C1-C2-C3-O3
9	C	358[A]	HTO	C1-C2-C3-C4
9	C	358[A]	HTO	O2-C2-C3-O3
9	C	358[A]	HTO	O2-C2-C3-C4
9	C	358[A]	HTO	O3-C3-C4-C5
9	H	274[A]	HTO	O1-C1-C2-O2
9	H	274[A]	HTO	O1-C1-C2-C3
9	H	274[A]	HTO	C2-C3-C4-C5
9	H	274[A]	HTO	O3-C3-C4-C5
9	L	276	HTO	C1-C2-C3-O3
9	L	276	HTO	C1-C2-C3-C4
9	L	276	HTO	O2-C2-C3-O3
9	L	276	HTO	O2-C2-C3-C4
9	L	278	HTO	C1-C2-C3-O3
9	L	278	HTO	O2-C2-C3-O3
9	L	278	HTO	O2-C2-C3-C4
9	L	279	HTO	O3-C3-C4-C5
9	M	333	HTO	C1-C2-C3-O3
9	M	333	HTO	C1-C2-C3-C4
9	M	333	HTO	O2-C2-C3-O3
9	M	333	HTO	O2-C2-C3-C4
9	M	333	HTO	O3-C3-C4-C5
10	C	362	GOL	C1-C2-C3-O3
10	C	362	GOL	O2-C2-C3-O3
10	C	364	GOL	O1-C1-C2-C3
10	C	365	GOL	C1-C2-C3-O3
10	C	366	GOL	O1-C1-C2-C3
10	C	367	GOL	C1-C2-C3-O3
10	C	368	GOL	O1-C1-C2-C3
10	C	368	GOL	C1-C2-C3-O3
10	C	373	GOL	O1-C1-C2-O2
10	C	373	GOL	O1-C1-C2-C3
10	C	374[B]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	C	374[B]	GOL	C1-C2-C3-O3
10	H	275	GOL	C1-C2-C3-O3
10	H	276[A]	GOL	C1-C2-C3-O3
10	H	278	GOL	C1-C2-C3-O3
10	H	278	GOL	O2-C2-C3-O3
10	H	280	GOL	C1-C2-C3-O3
10	H	282	GOL	O1-C1-C2-C3
10	H	283	GOL	O1-C1-C2-C3
10	H	283	GOL	C1-C2-C3-O3
10	H	284	GOL	O1-C1-C2-C3
10	H	285	GOL	C1-C2-C3-O3
10	H	286	GOL	C1-C2-C3-O3
10	H	287	GOL	O1-C1-C2-C3
10	H	287	GOL	C1-C2-C3-O3
10	H	288	GOL	O1-C1-C2-C3
10	H	289	GOL	O1-C1-C2-C3
10	H	289	GOL	C1-C2-C3-O3
10	H	290	GOL	C1-C2-C3-O3
10	H	291	GOL	C1-C2-C3-O3
10	L	282	GOL	O1-C1-C2-C3
10	L	284	GOL	O1-C1-C2-C3
10	L	284	GOL	C1-C2-C3-O3
10	L	285	GOL	O1-C1-C2-C3
10	L	286	GOL	O1-C1-C2-C3
10	L	286	GOL	C1-C2-C3-O3
10	L	288	GOL	C1-C2-C3-O3
10	L	288	GOL	O2-C2-C3-O3
10	M	334	GOL	C1-C2-C3-O3
10	M	336	GOL	O1-C1-C2-C3
10	M	336	GOL	C1-C2-C3-O3
10	M	338	GOL	O1-C1-C2-C3
10	M	338	GOL	C1-C2-C3-O3
10	M	340	GOL	C1-C2-C3-O3
10	M	342	GOL	O1-C1-C2-C3
10	M	342	GOL	C1-C2-C3-O3
11	L	400	BCB	C2C-C3C-CAC-CBC
11	M	400	BCB	C2C-C3C-CAC-CBC
11	M	401	BCB	C2C-C3C-CAC-CBC
11	M	401	BCB	CAD-CBD-CGD-O1D
11	M	401	BCB	CAD-CBD-CGD-O2D
12	L	402	BPB	C2C-C3C-CAC-CBC
16	M	600	NS5	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
17	M	332	HTH	C1-C2-C3-O3
17	M	332	HTH	O2-C2-C3-C4
16	M	600	NS5	C3-C4-C5-C7
6	H	720	LDA	C1-C2-C3-C4
9	C	357	HTO	O1-C1-C2-O2
9	C	358[A]	HTO	O1-C1-C2-O2
9	H	273	HTO	O1-C1-C2-O2
9	C	357	HTO	O1-C1-C2-C3
9	H	273	HTO	O1-C1-C2-C3
6	L	723	LDA	C3-C4-C5-C6
11	L	400	BCB	C4-C3-C5-C6
12	M	402	BPB	C4-C3-C5-C6
11	L	400	BCB	C2-C3-C5-C6
12	M	402	BPB	C2-C3-C5-C6
16	M	600	NS5	C12-C10-C9-C8
6	H	720	LDA	C3-C4-C5-C6
13	L	502	UQ9	C39-C41-C42-C43
13	L	502	UQ9	C34-C36-C37-C38
11	M	401	BCB	C2A-CAA-CBA-CGA
6	M	706	LDA	C3-C4-C5-C6
16	M	600	NS5	C11-C10-C9-C8
6	C	722	LDA	C3-C4-C5-C6
10	C	368	GOL	O2-C2-C3-O3
10	H	275	GOL	O2-C2-C3-O3
10	H	287	GOL	O2-C2-C3-O3
10	H	289	GOL	O2-C2-C3-O3
10	L	285	GOL	O1-C1-C2-O2
12	M	402	BPB	C11-C12-C13-C15
13	L	502	UQ9	C24-C26-C27-C28
7	C	730	DGA	CB1-CB2-CB3-CB4
11	M	400	BCB	C8-C10-C11-C12
7	C	730	DGA	CA1-CA2-CA3-CA4
11	L	400	BCB	C15-C16-C17-C18
7	C	730	DGA	CA2-CA1-OG1-CG1
9	H	273	HTO	C2-C3-C4-C5
13	L	502	UQ9	C29-C31-C32-C33
6	L	702	LDA	C2-C3-C4-C5
10	C	369	GOL	C1-C2-C3-O3
10	C	372	GOL	O1-C1-C2-C3
10	C	376	GOL	O1-C1-C2-C3
10	C	377	GOL	O1-C1-C2-C3
10	C	378	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	H	276[A]	GOL	O1-C1-C2-C3
10	H	276[B]	GOL	O1-C1-C2-C3
10	H	277	GOL	O1-C1-C2-C3
10	L	283	GOL	C1-C2-C3-O3
10	M	334	GOL	O1-C1-C2-C3
10	M	337	GOL	O1-C1-C2-C3
10	M	339	GOL	C1-C2-C3-O3
6	L	703	LDA	C5-C6-C7-C8
9	C	355	HTO	O1-C1-C2-O2
11	L	401	BCB	C16-C17-C18-C19
6	C	722	LDA	C6-C7-C8-C9
6	M	714	LDA	C5-C6-C7-C8
7	C	730	DGA	CB5-CB6-CB7-CB8
6	L	710	LDA	C6-C7-C8-C9
6	M	704	LDA	C2-C3-C4-C5
10	C	364	GOL	O1-C1-C2-O2
10	C	365	GOL	O2-C2-C3-O3
10	C	366	GOL	O1-C1-C2-O2
10	C	368	GOL	O1-C1-C2-O2
10	C	372	GOL	O1-C1-C2-O2
10	C	374[B]	GOL	O1-C1-C2-O2
10	C	374[B]	GOL	O2-C2-C3-O3
10	H	276[A]	GOL	O1-C1-C2-O2
10	H	276[A]	GOL	O2-C2-C3-O3
10	H	276[B]	GOL	O1-C1-C2-O2
10	H	282	GOL	O1-C1-C2-O2
10	H	284	GOL	O1-C1-C2-O2
10	H	285	GOL	O2-C2-C3-O3
10	H	286	GOL	O2-C2-C3-O3
10	H	287	GOL	O1-C1-C2-O2
10	H	289	GOL	O1-C1-C2-O2
10	H	290	GOL	O2-C2-C3-O3
10	L	282	GOL	O1-C1-C2-O2
10	L	284	GOL	O1-C1-C2-O2
10	L	284	GOL	O2-C2-C3-O3
10	M	334	GOL	O2-C2-C3-O3
10	M	336	GOL	O2-C2-C3-O3
10	M	340	GOL	O2-C2-C3-O3
10	M	342	GOL	O2-C2-C3-O3
6	H	721	LDA	C3-C4-C5-C6
6	L	702	LDA	C4-C5-C6-C7
6	M	704	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	C	730	DGA	CA5-CA6-CA7-CA8
6	L	712	LDA	C4-C5-C6-C7
6	C	716	LDA	C3-C4-C5-C6
6	M	705	LDA	C6-C7-C8-C9
6	H	718[B]	LDA	C4-C5-C6-C7
6	L	724	LDA	C3-C4-C5-C6
7	C	730	DGA	CB4-CB5-CB6-CB7
11	M	401	BCB	C3A-C2A-CAA-CBA
7	C	730	DGA	CA4-CA5-CA6-CA7
6	L	710	LDA	C4-C5-C6-C7
7	C	730	DGA	OA1-CA1-OG1-CG1
6	C	716	LDA	C6-C7-C8-C9
6	H	721	LDA	C2-C3-C4-C5
6	L	712	LDA	C2-C3-C4-C5
6	L	712	LDA	C5-C6-C7-C8
6	H	718[B]	LDA	C3-C4-C5-C6
6	L	703	LDA	C4-C5-C6-C7
6	M	704	LDA	C5-C6-C7-C8
6	M	713	LDA	C2-C3-C4-C5
6	M	707	LDA	C4-C5-C6-C7
6	M	705	LDA	C7-C8-C9-C10
7	C	730	DGA	CB2-CB3-CB4-CB5
11	M	400	BCB	C6-C7-C8-C9
6	H	720	LDA	C4-C5-C6-C7
6	L	710	LDA	C3-C4-C5-C6
6	H	719	LDA	C2-C3-C4-C5
6	L	702	LDA	C3-C4-C5-C6
6	M	706	LDA	C5-C6-C7-C8
6	M	714	LDA	C2-C3-C4-C5
6	M	705	LDA	C11-C10-C9-C8
9	C	355	HTO	C4-C5-C6-C7
6	H	721	LDA	C4-C5-C6-C7
6	H	718[B]	LDA	C6-C7-C8-C9
13	L	502	UQ9	C30-C29-C31-C32
6	L	723	LDA	C1-C2-C3-C4
7	C	730	DGA	CA2-CA3-CA4-CA5
13	L	503	UQ9	C5-C6-C7-C8
6	L	712	LDA	C7-C8-C9-C10
9	C	356	HTO	O1-C1-C2-O2
6	M	713	LDA	C11-C10-C9-C8
6	M	715	LDA	C7-C8-C9-C10
13	L	502	UQ9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
6	M	707	LDA	C1-C2-C3-C4
6	L	708	LDA	C3-C4-C5-C6
10	C	367	GOL	O2-C2-C3-O3
10	C	376	GOL	O1-C1-C2-O2
10	C	377	GOL	O1-C1-C2-O2
10	H	280	GOL	O2-C2-C3-O3
10	H	283	GOL	O1-C1-C2-O2
10	H	288	GOL	O1-C1-C2-O2
10	H	291	GOL	O2-C2-C3-O3
10	L	286	GOL	O1-C1-C2-O2
10	L	286	GOL	O2-C2-C3-O3
10	M	338	GOL	O1-C1-C2-O2
10	M	338	GOL	O2-C2-C3-O3
10	M	342	GOL	O1-C1-C2-O2
6	L	703	LDA	C7-C8-C9-C10
11	M	401	BCB	C11-C12-C13-C15
12	M	402	BPB	C11-C10-C8-C7
13	L	502	UQ9	C28-C29-C31-C32
6	H	721	LDA	C7-C8-C9-C10
6	H	701	LDA	C4-C5-C6-C7
6	M	705	LDA	C4-C5-C6-C7
6	H	718[B]	LDA	C7-C8-C9-C10
6	L	724	LDA	C2-C3-C4-C5
6	M	717	LDA	C4-C5-C6-C7
6	L	724	LDA	C1-C2-C3-C4
9	C	357	HTO	O2-C2-C3-O3
17	M	332	HTH	O2-C2-C3-O3
6	L	702	LDA	C11-C10-C9-C8
13	L	502	UQ9	C15-C14-C16-C17
7	C	730	DGA	CA7-CA8-CA9-CAA
12	L	402	BPB	C8-C10-C11-C12
6	L	711	LDA	C2-C3-C4-C5
12	L	402	BPB	O2A-C1-C2-C3
6	L	703	LDA	C6-C7-C8-C9
9	M	333	HTO	C4-C5-C6-C7
6	M	715	LDA	C5-C6-C7-C8
7	C	730	DGA	CB6-CB7-CB8-CB9
6	L	708	LDA	N1-C1-C2-C3
6	L	723	LDA	N1-C1-C2-C3
6	M	715	LDA	N1-C1-C2-C3
7	C	730	DGA	CDB-CEB-CFB-CGB
6	L	724	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
9	C	358[A]	HTO	C4-C5-C6-C7
7	C	730	DGA	CB7-CB8-CB9-CAB
6	C	716	LDA	C9-C10-C11-C12
6	L	710	LDA	C9-C10-C11-C12
6	M	714	LDA	C3-C4-C5-C6
6	L	724	LDA	C11-C10-C9-C8
10	C	364	GOL	O2-C2-C3-O3
10	C	369	GOL	O2-C2-C3-O3
10	C	378	GOL	O1-C1-C2-O2
10	H	281	GOL	O1-C1-C2-O2
10	H	283	GOL	O2-C2-C3-O3
10	M	339	GOL	O2-C2-C3-O3
12	M	402	BPB	C11-C10-C8-C9
11	L	401	BCB	C12-C13-C15-C16
11	M	400	BCB	C11-C10-C8-C7
9	L	279	HTO	C4-C5-C6-C7
6	L	712	LDA	C9-C10-C11-C12
6	M	714	LDA	C9-C10-C11-C12
17	M	332	HTH	O3-C3-C4-C5
17	M	332	HTH	C4-C5-C6-C7
6	L	709	LDA	C1-C2-C3-C4
7	C	730	DGA	OG1-CG1-CG2-CG3
9	C	358[A]	HTO	O1-C1-C2-C3
6	L	709	LDA	C7-C8-C9-C10
6	M	705	LDA	C3-C4-C5-C6
6	L	702	LDA	C5-C6-C7-C8
6	H	701	LDA	C6-C7-C8-C9
6	M	717	LDA	C7-C8-C9-C10
6	H	719	LDA	C1-C2-C3-C4
6	M	705	LDA	C2-C3-C4-C5
7	C	730	DGA	CA3-CA4-CA5-CA6
7	C	730	DGA	CEB-CFB-CGB-CHB
9	L	280	HTO	C2-C3-C4-C5
9	L	280	HTO	C4-C5-C6-C7
6	M	706	LDA	C9-C10-C11-C12
11	M	400	BCB	C11-C10-C8-C9
6	H	701	LDA	C7-C8-C9-C10
11	L	401	BCB	C16-C17-C18-C20
10	C	359	GOL	O1-C1-C2-O2
10	C	370	GOL	O2-C2-C3-O3
10	H	285	GOL	O1-C1-C2-O2
10	M	334	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	M	336	GOL	O1-C1-C2-O2
11	M	400	BCB	C10-C11-C12-C13
6	M	714	LDA	C7-C8-C9-C10
6	H	721	LDA	C11-C10-C9-C8
6	M	706	LDA	C6-C7-C8-C9
7	C	730	DGA	CAB-CBB-CCB-CDB
5	C	402	HEC	C3D-CAD-CBD-CGD
13	L	503	UQ9	C1-C6-C7-C8
12	M	402	BPB	C16-C17-C18-C20
15	M	501	MQ9	C35-C34-C36-C37
6	L	709	LDA	C5-C6-C7-C8
11	M	400	BCB	C4-C3-C5-C6
15	M	501	MQ9	C33-C34-C36-C37
6	L	711	LDA	C7-C8-C9-C10
6	C	716	LDA	C1-C2-C3-C4
11	M	401	BCB	C11-C12-C13-C14
12	M	402	BPB	C11-C12-C13-C14
6	L	712	LDA	C3-C4-C5-C6
7	C	730	DGA	CB3-CB4-CB5-CB6
6	L	703	LDA	C1-C2-C3-C4
6	H	720	LDA	C6-C7-C8-C9
6	C	716	LDA	C2-C1-N1-CM2
6	C	722	LDA	C2-C1-N1-CM2
6	H	719	LDA	C2-C1-N1-CM1
6	H	719	LDA	C2-C1-N1-CM2
6	L	708	LDA	C2-C1-N1-CM1
6	L	708	LDA	C2-C1-N1-CM2
6	M	704	LDA	C2-C1-N1-CM2
9	L	280	HTO	O3-C3-C4-C5
6	H	721	LDA	C9-C10-C11-C12
6	L	723	LDA	C5-C6-C7-C8
16	M	600	NS5	C31-C33-C34-C35
17	M	332	HTH	C3-C4-C5-C6
6	C	722	LDA	C2-C3-C4-C5
11	M	400	BCB	C16-C17-C18-C19
11	M	400	BCB	C16-C17-C18-C20
6	M	713	LDA	C1-C2-C3-C4
16	M	600	NS5	C17-C18-C19-C20
11	L	401	BCB	C14-C13-C15-C16
6	M	714	LDA	C6-C7-C8-C9
6	C	716	LDA	C2-C1-N1-O1
6	H	719	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
6	L	708	LDA	C2-C1-N1-O1
6	L	710	LDA	C2-C1-N1-O1
11	M	400	BCB	C15-C16-C17-C18
6	H	720	LDA	C7-C8-C9-C10
11	M	400	BCB	C2-C3-C5-C6
11	L	400	BCB	CAD-CBD-CGD-O2D
6	L	709	LDA	C4-C5-C6-C7
11	L	400	BCB	CAD-CBD-CGD-O1D
6	L	710	LDA	C7-C8-C9-C10
6	H	701	LDA	C9-C10-C11-C12
6	C	722	LDA	C1-C2-C3-C4
11	L	400	BCB	C16-C17-C18-C20
6	H	720	LDA	C5-C6-C7-C8
6	H	719	LDA	C3-C4-C5-C6
12	M	402	BPB	C16-C17-C18-C19
11	M	401	BCB	C3-C5-C6-C7
6	M	704	LDA	C11-C10-C9-C8
13	L	502	UQ9	C5-C4-O4-C4M
16	M	600	NS5	C33-C34-C35-C36
6	H	718[B]	LDA	C11-C10-C9-C8
6	L	709	LDA	N1-C1-C2-C3
6	L	711	LDA	N1-C1-C2-C3
6	M	707	LDA	C6-C7-C8-C9
6	L	711	LDA	C5-C6-C7-C8
6	L	708	LDA	C11-C10-C9-C8
9	C	358[A]	HTO	C2-C3-C4-C5
10	H	286	GOL	O1-C1-C2-O2
9	C	356	HTO	C3-C4-C5-C6
9	H	272	HTO	C3-C4-C5-C6
9	L	278	HTO	C4-C5-C6-C7
6	C	716	LDA	C4-C5-C6-C7
6	M	706	LDA	C7-C8-C9-C10
9	L	280	HTO	C3-C4-C5-C6
13	L	503	UQ9	C2-C3-O3-C3M
6	C	722	LDA	C4-C5-C6-C7
10	C	370	GOL	C1-C2-C3-O3
6	H	719	LDA	C9-C10-C11-C12
6	C	716	LDA	C2-C3-C4-C5
5	C	402	HEC	CAA-CBA-CGA-O1A
5	C	402	HEC	CAA-CBA-CGA-O2A
7	C	730	DGA	CA6-CA7-CA8-CA9
9	L	280	HTO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
13	L	502	UQ9	C3-C4-O4-C4M
6	L	723	LDA	C4-C5-C6-C7
6	L	702	LDA	C6-C7-C8-C9
13	L	502	UQ9	C40-C39-C41-C42
16	M	600	NS5	C32-C31-C33-C34
7	C	730	DGA	CA8-CA9-CAA-CBA
6	L	708	LDA	C2-C3-C4-C5
10	C	367	GOL	O1-C1-C2-O2
10	H	277	GOL	O1-C1-C2-O2
10	L	283	GOL	O2-C2-C3-O3
10	M	337	GOL	O1-C1-C2-O2
6	M	706	LDA	C4-C5-C6-C7
9	H	273	HTO	O3-C3-C4-C5
11	L	401	BCB	CHA-CBD-CGD-O1D
13	L	502	UQ9	C4-C3-O3-C3M
6	L	708	LDA	C5-C6-C7-C8
6	L	723	LDA	C11-C10-C9-C8
5	C	401	HEC	CAA-CBA-CGA-O2A
9	C	356	HTO	O1-C1-C2-C3
13	L	502	UQ9	C46-C47-C48-C49
6	M	715	LDA	C1-C2-C3-C4
5	C	401	HEC	CAA-CBA-CGA-O1A
7	C	730	DGA	CA9-CAA-CBA-CCA
9	L	276	HTO	C3-C4-C5-C6
10	H	281	GOL	O2-C2-C3-O3
17	M	332	HTH	C2-C3-C4-C5
6	L	709	LDA	C11-C10-C9-C8
13	L	502	UQ9	C20-C19-C21-C22
5	C	402	HEC	CAD-CBD-CGD-O1D
9	C	358[A]	HTO	C3-C4-C5-C6
9	L	276	HTO	C4-C5-C6-C7
6	C	722	LDA	C5-C6-C7-C8
6	M	707	LDA	C3-C4-C5-C6
6	M	714	LDA	C4-C5-C6-C7
9	C	355	HTO	C1-C2-C3-O3
9	C	357	HTO	C1-C2-C3-O3
9	L	279	HTO	C1-C2-C3-O3
11	L	401	BCB	C2C-C3C-CAC-CBC
13	L	502	UQ9	C18-C19-C21-C22
5	C	402	HEC	CAD-CBD-CGD-O2D
6	M	715	LDA	C3-C4-C5-C6
7	C	730	DGA	CB9-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
10	H	281	GOL	O1-C1-C2-C3
5	C	404	HEC	CAD-CBD-CGD-O1D
9	M	333	HTO	C2-C3-C4-C5
13	L	502	UQ9	C35-C34-C36-C37
6	M	713	LDA	C9-C10-C11-C12
11	M	401	BCB	C14-C13-C15-C16
6	H	721	LDA	C2-C1-N1-O1
13	L	502	UQ9	C38-C39-C41-C42
11	L	401	BCB	CAD-CBD-CGD-O2D
6	H	721	LDA	C1-C2-C3-C4
6	H	719	LDA	C7-C8-C9-C10
11	M	401	BCB	C1A-C2A-CAA-CBA
5	C	401	HEC	CAD-CBD-CGD-O2D

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
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

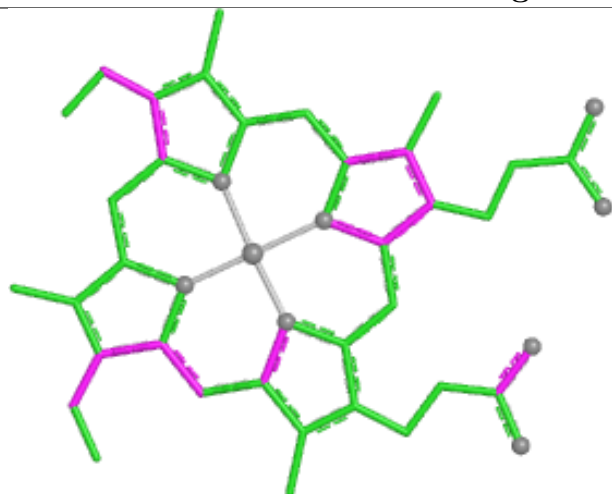
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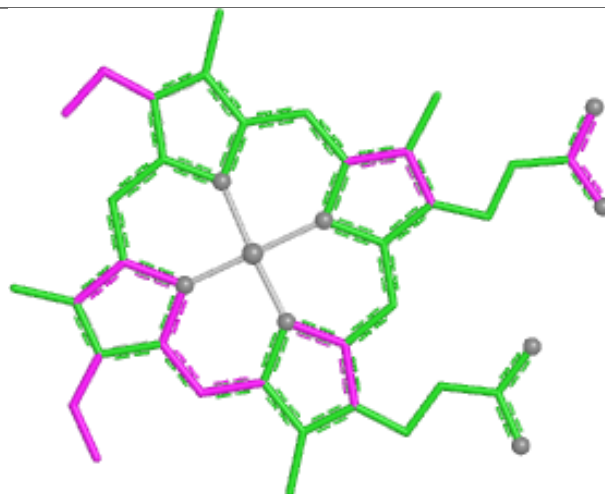
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	280	GOL	1	0
5	C	401	HEC	1	0
10	M	338	GOL	3	0
10	M	334	GOL	1	0
10	C	364	GOL	3	0
10	C	377	GOL	4	0
9	H	272	HTO	1	0
6	M	707	LDA	1	0
10	M	342	GOL	1	0
6	M	715	LDA	2	0
8	C	338	SO4	1	0
10	C	363	GOL	1	0
9	C	357	HTO	2	0
10	L	286	GOL	1	0
11	L	400	BCB	5	0
10	C	365	GOL	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.

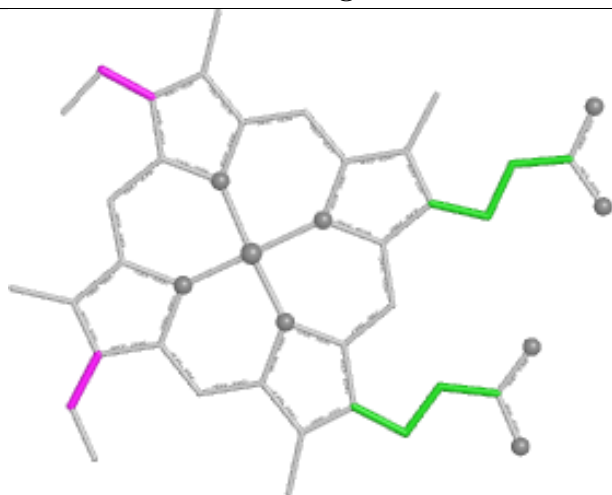
Ligand HEC C 403



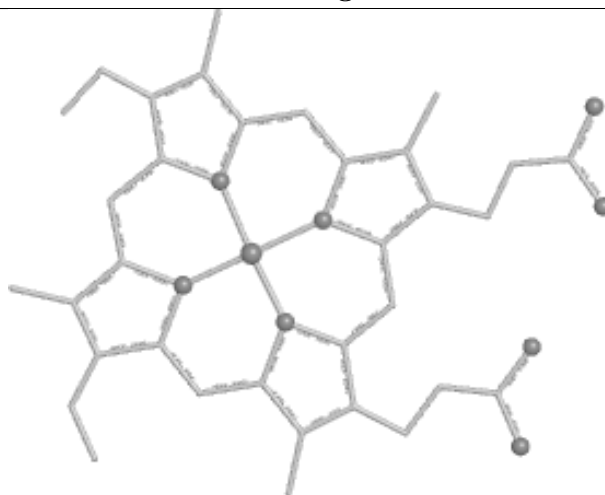
Bond lengths



Bond angles

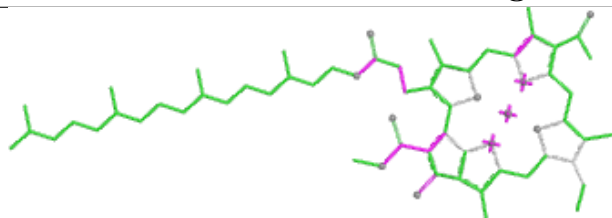


Torsions

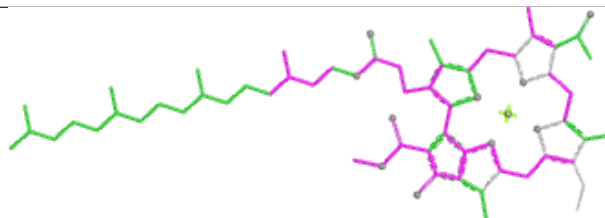


Rings

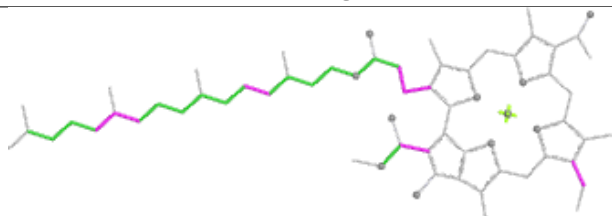
Ligand BCB M 401



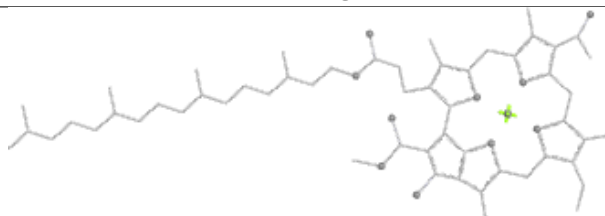
Bond lengths



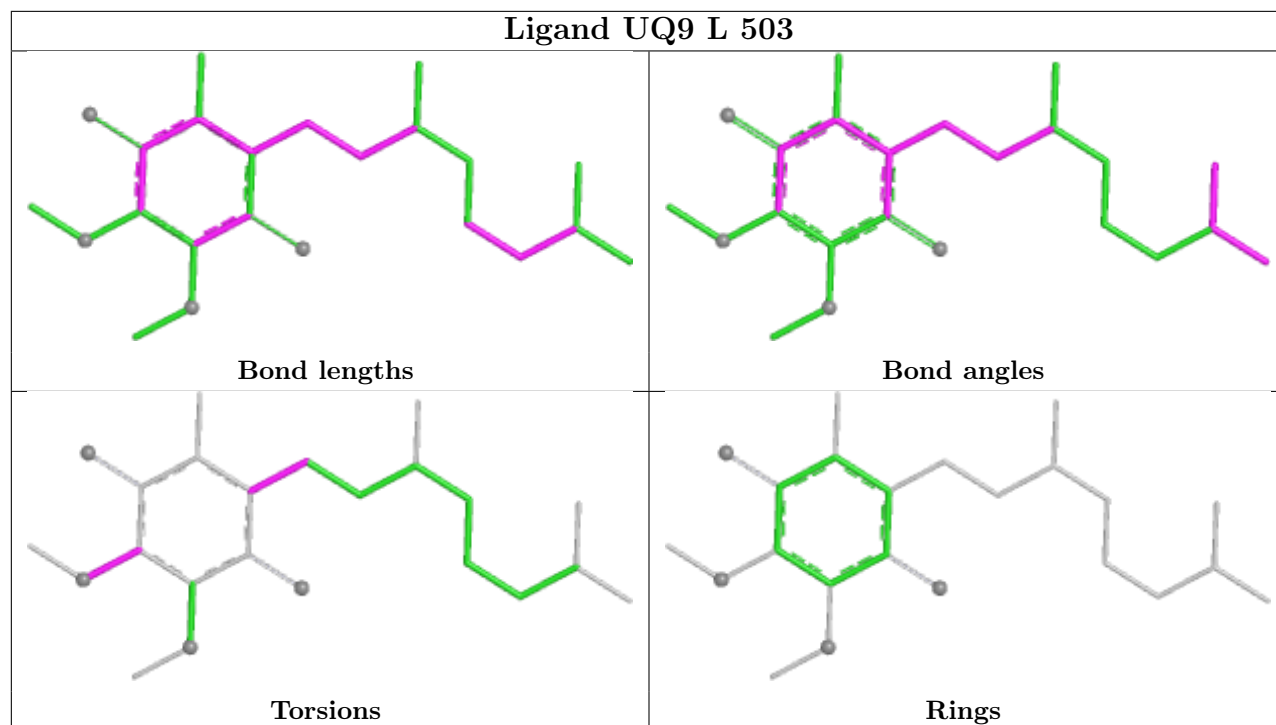
Bond angles



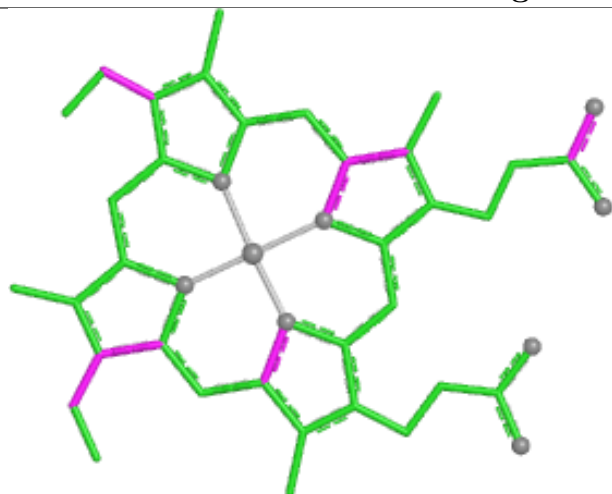
Torsions



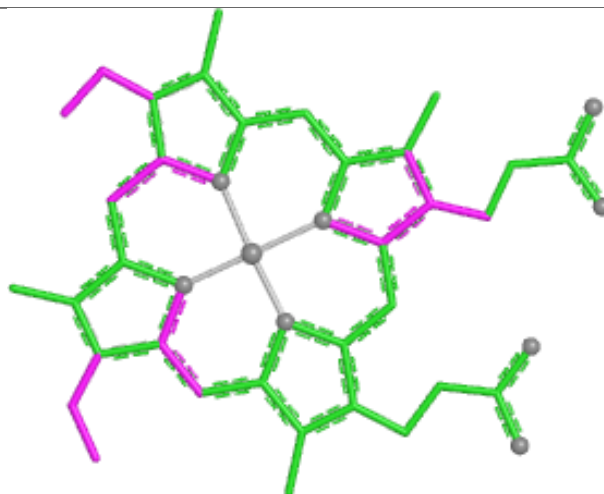
Rings



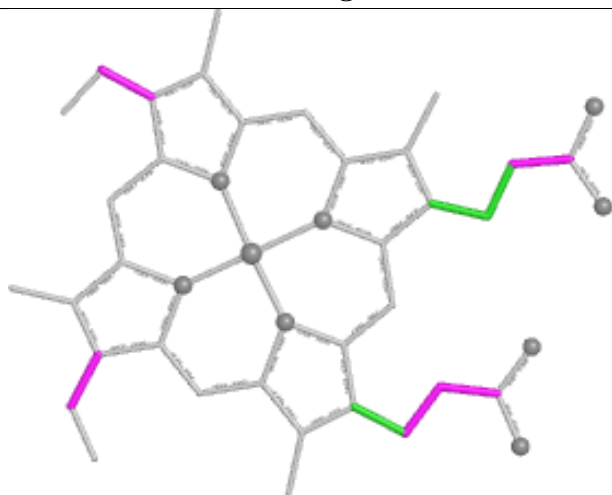
Ligand HEC C 402



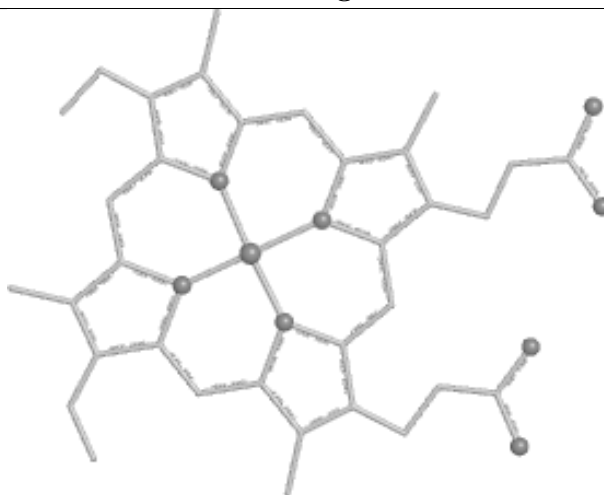
Bond lengths



Bond angles

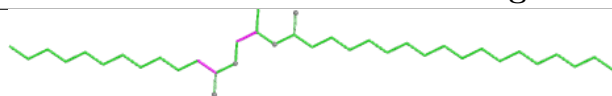


Torsions

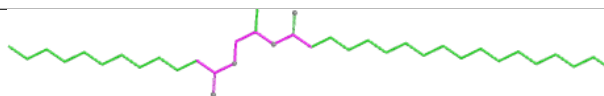


Rings

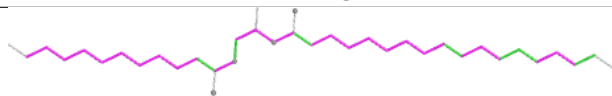
Ligand DGA C 730



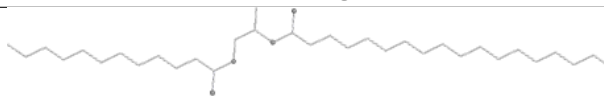
Bond lengths



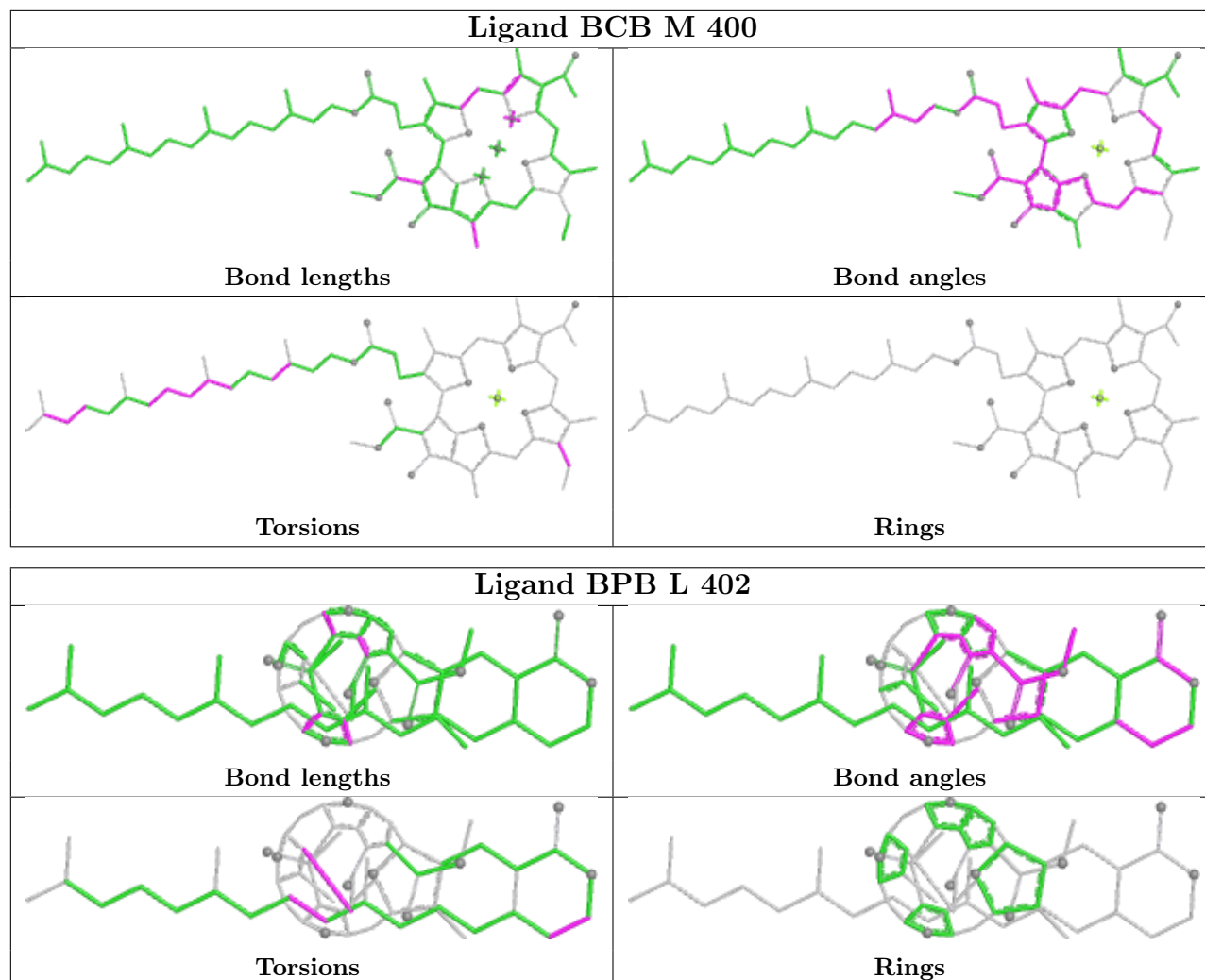
Bond angles

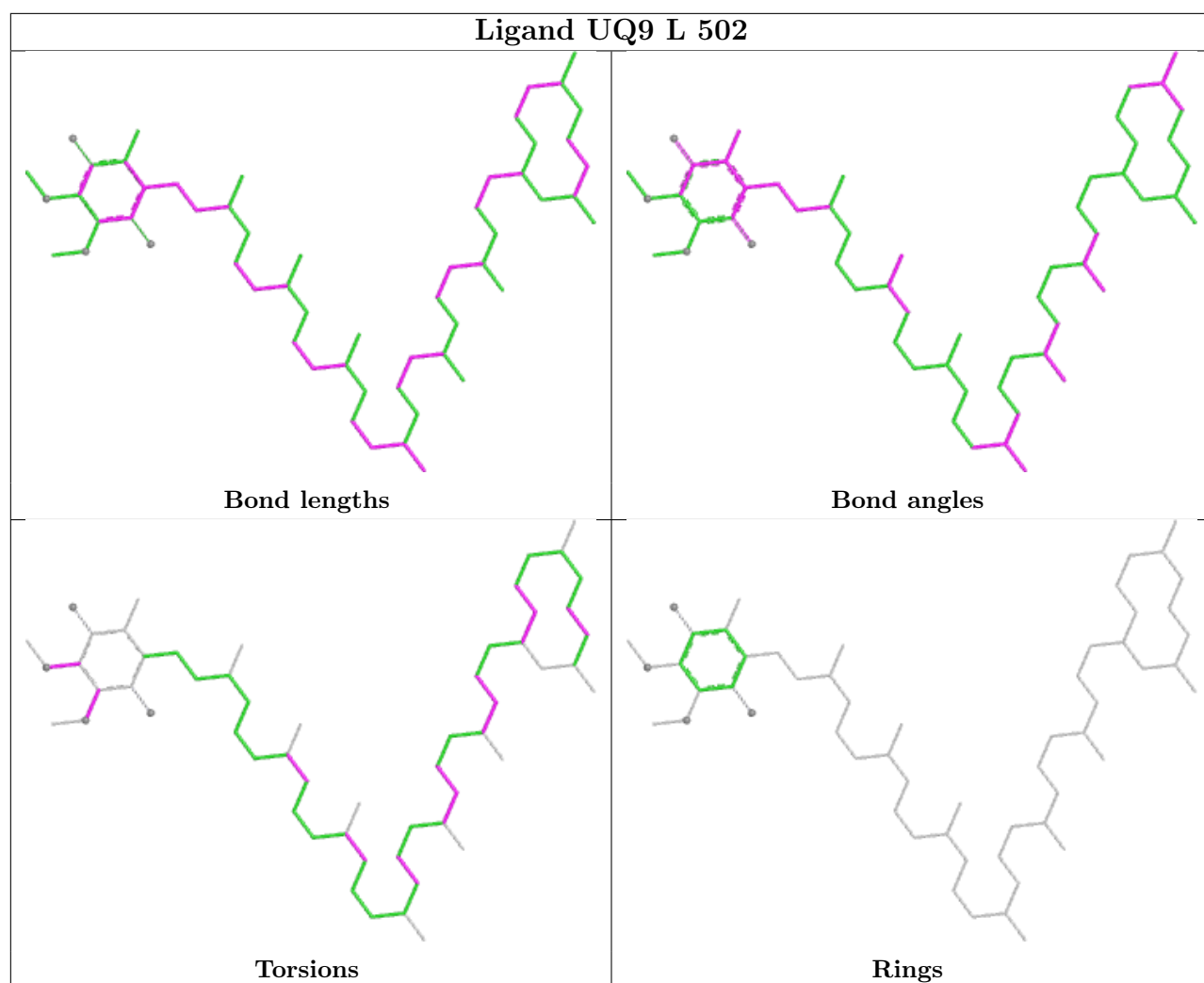


Torsions

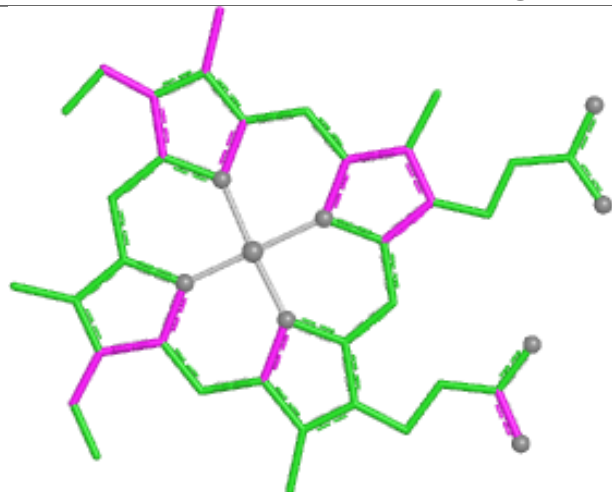


Rings

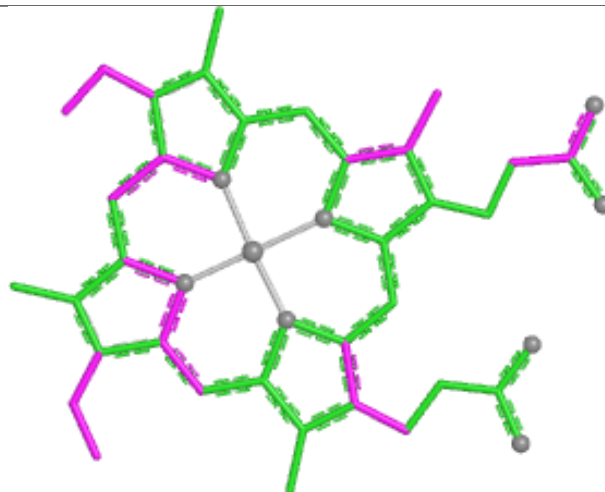




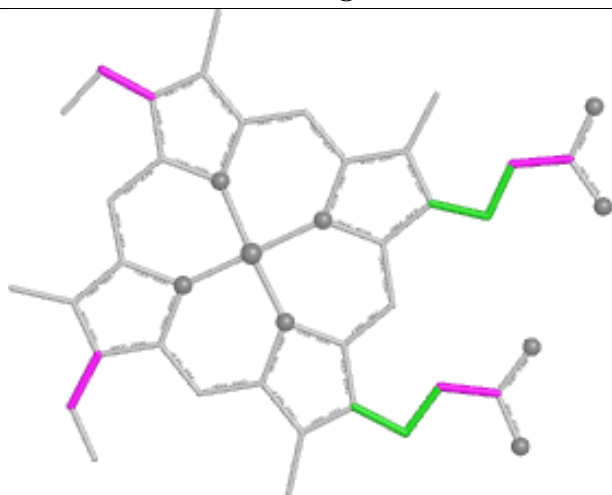
Ligand HEC C 401



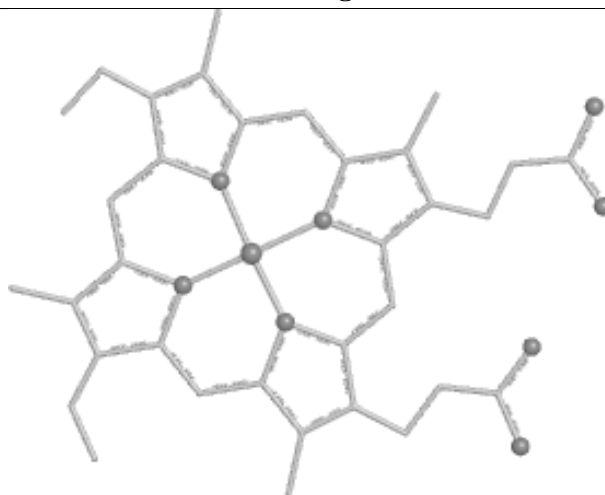
Bond lengths



Bond angles

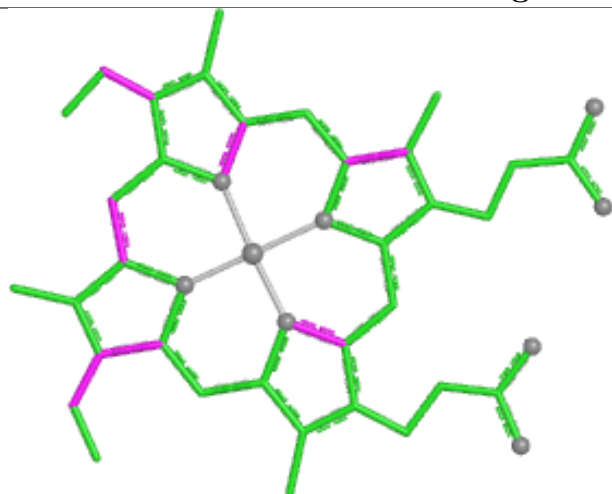


Torsions

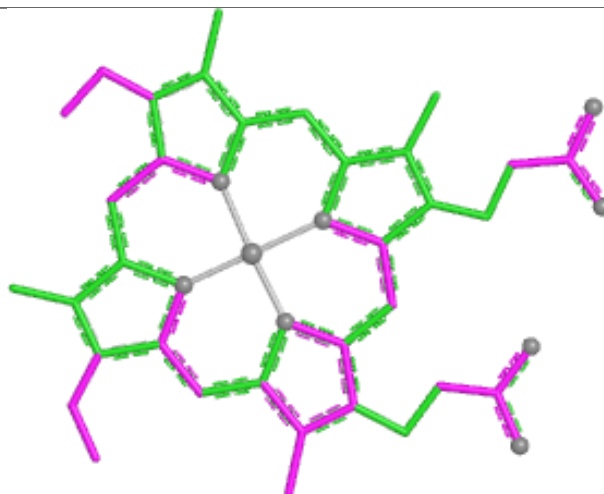


Rings

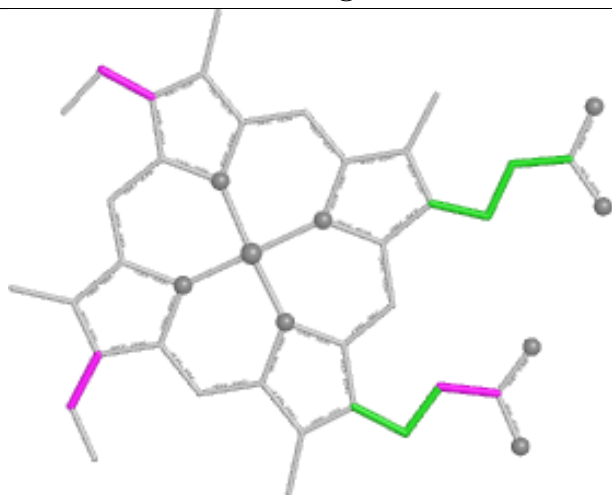
Ligand HEC C 404



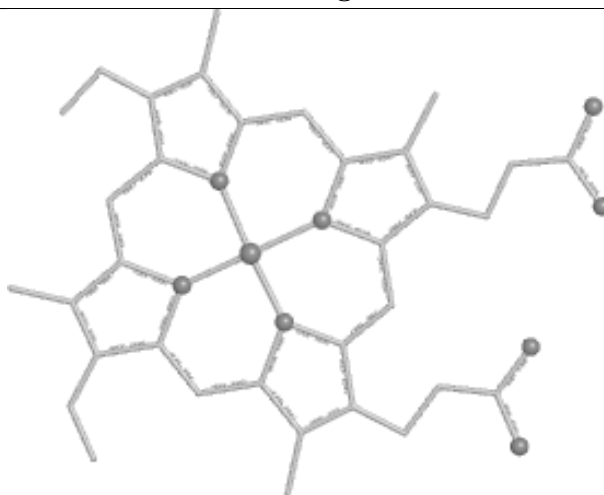
Bond lengths



Bond angles

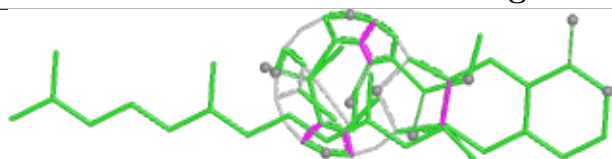


Torsions

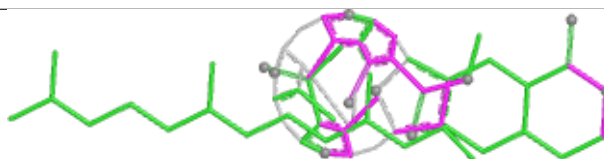


Rings

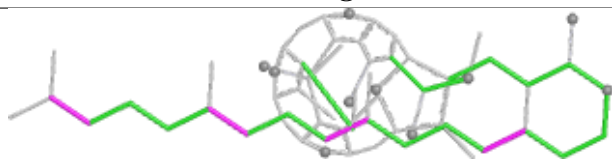
Ligand BPB M 402



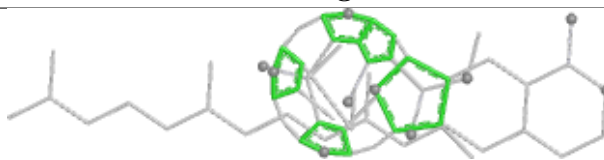
Bond lengths



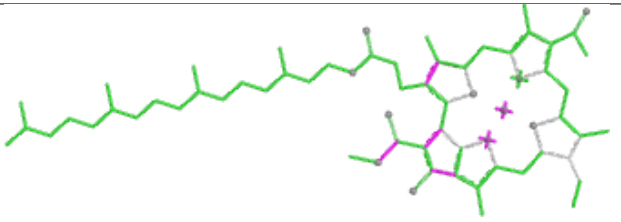
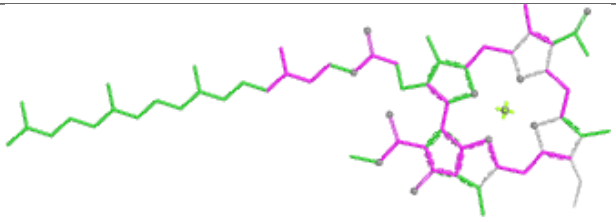
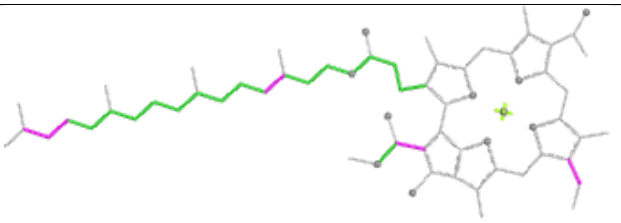
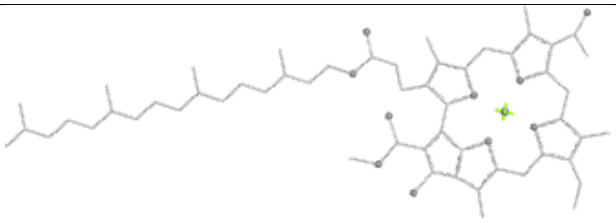
Bond angles

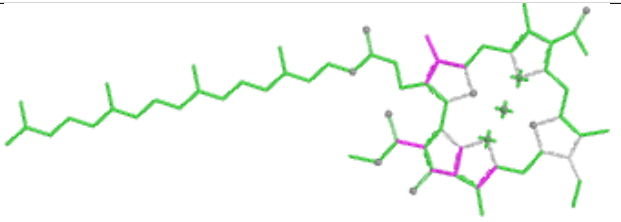
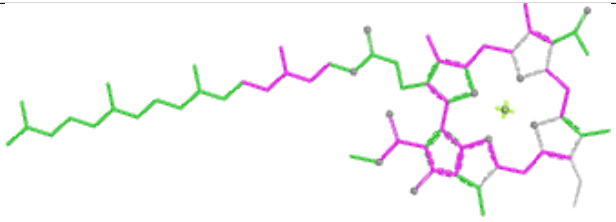
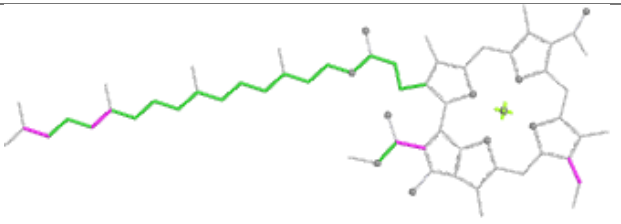
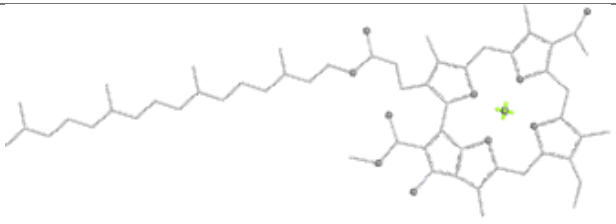


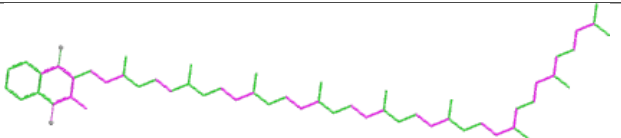
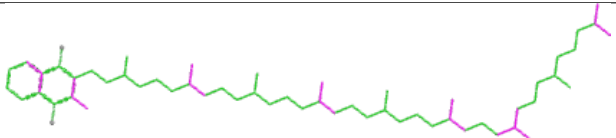
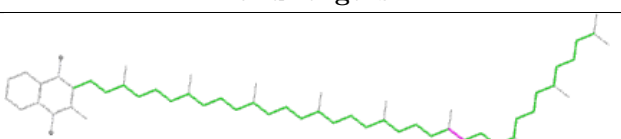
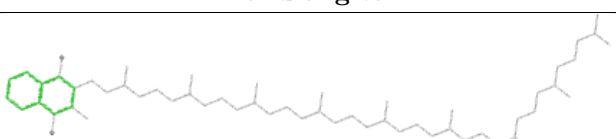
Torsions

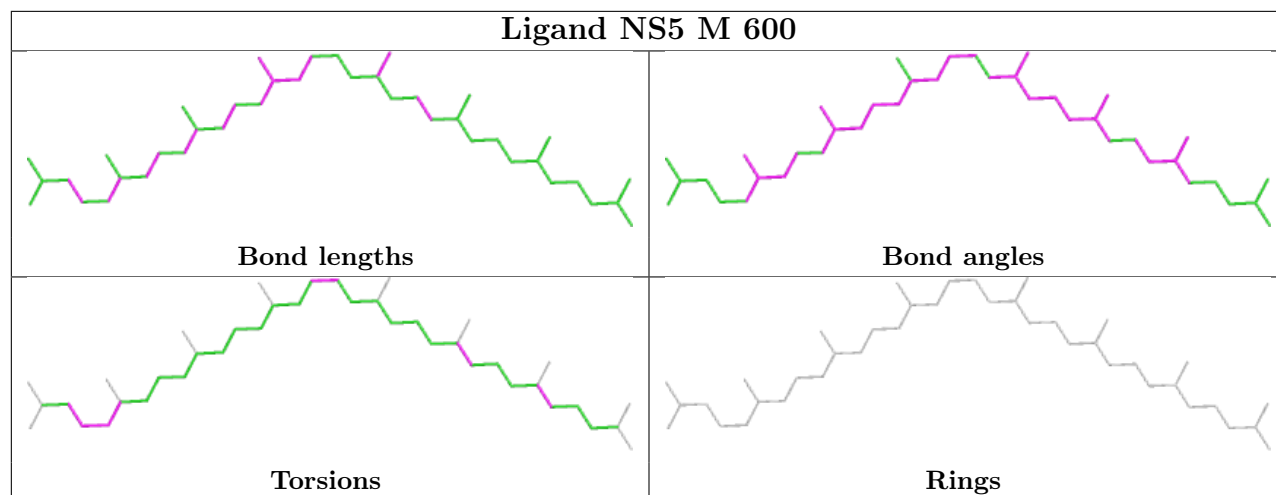


Rings

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 ⓘ

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	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%)

All (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
4	M	85[A]	PHE	3.8
4	M	34	TYR	3.7
1	C	2[A]	PHE	3.6
3	L	271	PHE	3.6
3	L	1	ALA	3.6
2	H	86	ARG	3.4
4	M	1	ALA	3.4
3	L	202	ASP	3.3
2	H	96	PHE	3.3
2	H	44	VAL	3.2
2	H	189	GLY	3.2
4	M	37	TRP	3.2
2	H	45	GLU	3.2
4	M	108	HIS	3.1
2	H	54	PRO	3.1
3	L	81	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	177	GLU	3.0
3	L	270	PRO	2.9
4	M	26	ASN	2.9
3	L	51[A]	TYR	2.8
1	C	47	ALA	2.8
4	M	33	PHE	2.8
4	M	16	HIS	2.7
2	H	178[A]	HIS	2.7
2	H	43	LEU	2.6
3	L	21	LEU	2.6
2	H	64	TYR	2.5
4	M	118	LEU	2.5
4	M	18	THR	2.5
1	C	89	TYR	2.5
4	M	31	LYS	2.4
2	H	190	SER	2.4
1	C	323	GLN	2.3
1	C	55	VAL	2.3
4	M	20	SER	2.3
2	H	8	GLN	2.3
4	M	115	MET	2.3
4	M	78	HIS	2.2
4	M	319	PRO	2.2
4	M	59	PHE	2.2
2	H	257	LEU	2.2
4	M	17	ILE	2.1
4	M	22	GLU	2.1
2	H	223[A]	ARG	2.1
4	M	32	PRO	2.0
2	H	83	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(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 ⓘ

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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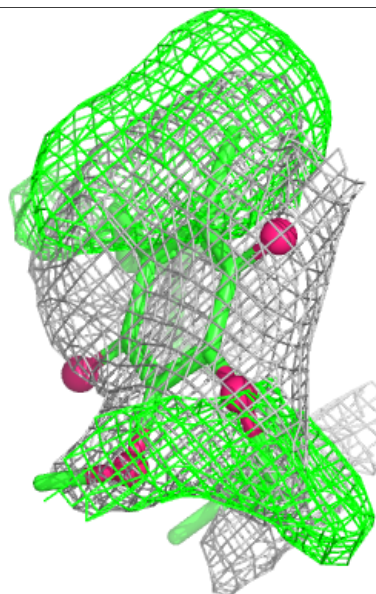
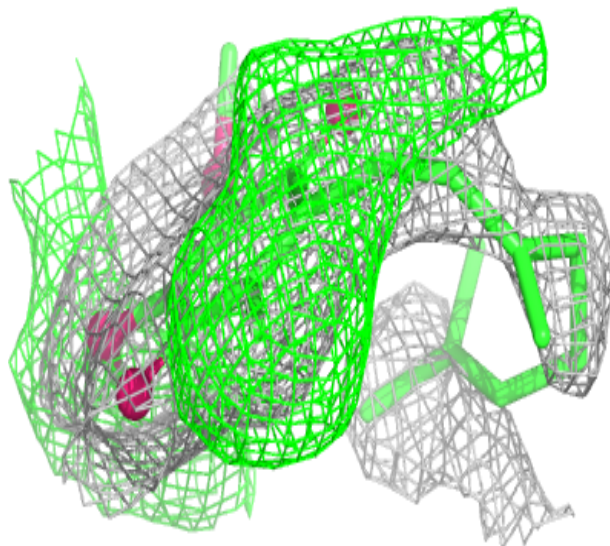
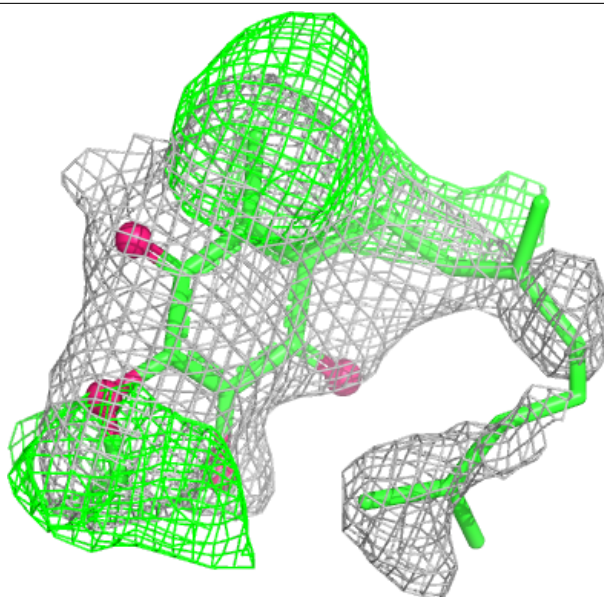
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	H	259	5/5	0.91	0.10	60,62,67,69	5
16	NS5	M	600	40/40	0.91	0.16	42,54,95,96	0
8	SO4	M	326	5/5	0.91	0.13	56,61,62,62	5
10	GOL	L	281	6/6	0.92	0.20	54,58,66,68	6
10	GOL	H	286	6/6	0.92	0.25	67,67,69,70	6
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.

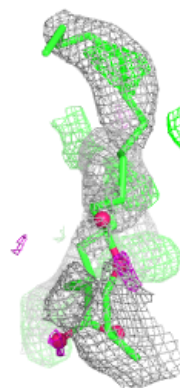
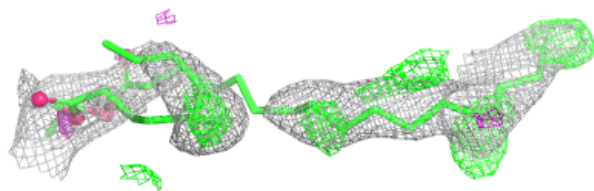
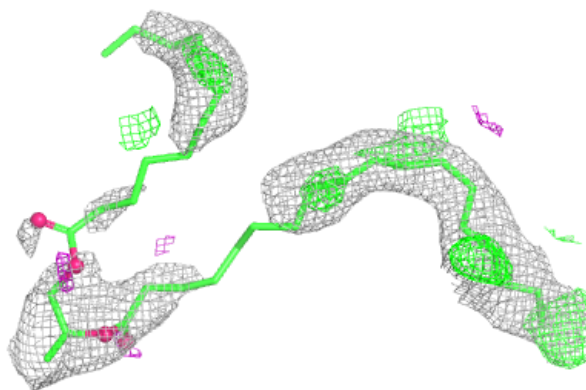
Electron density around UQ9 L 503:

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



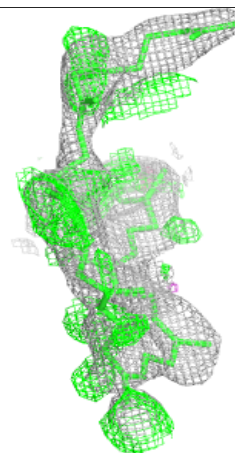
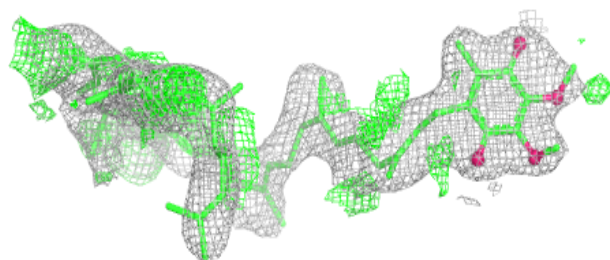
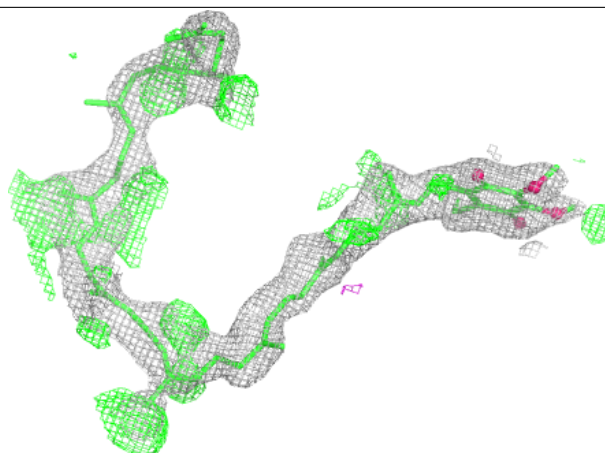
Electron density around DGA C 730:

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

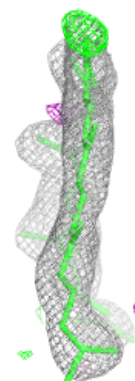
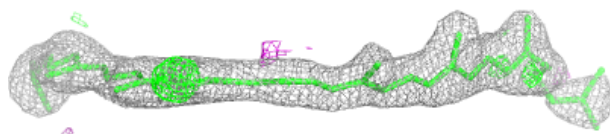
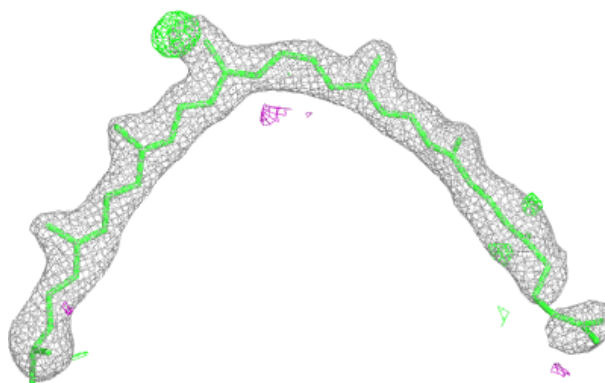


Electron density around UQ9 L 502:

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

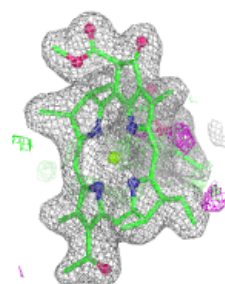
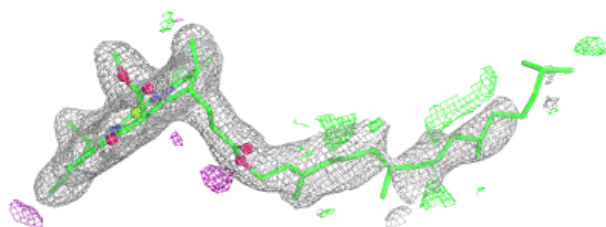
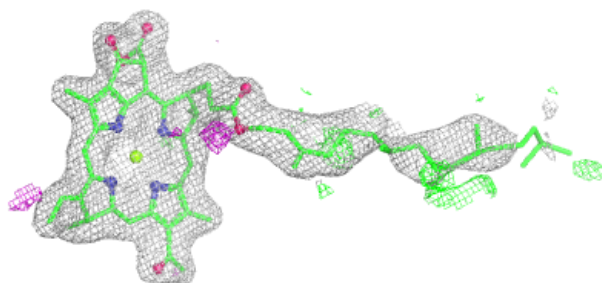
**Electron density around NS5 M 600:**

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

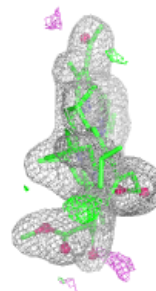
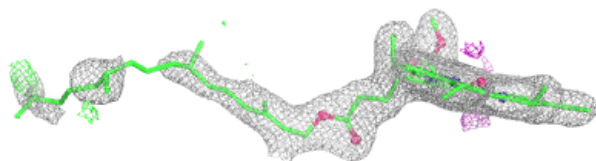
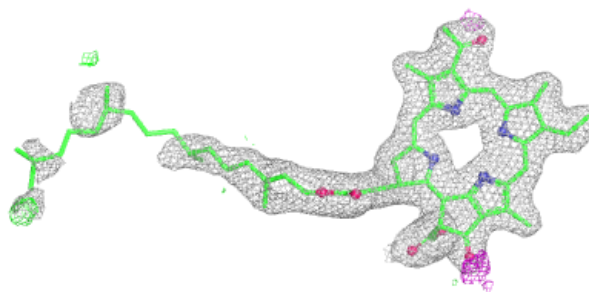


Electron density around BCB M 400:

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

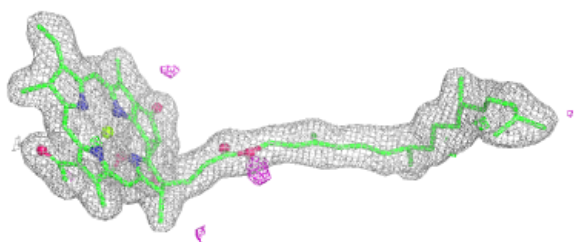
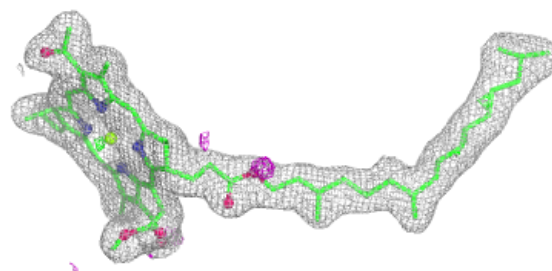
**Electron density around BPB M 402:**

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

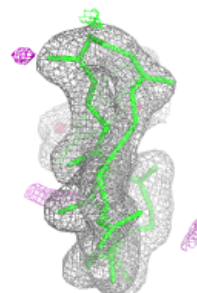
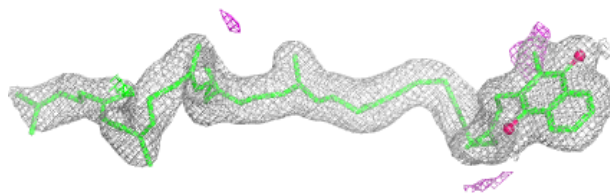
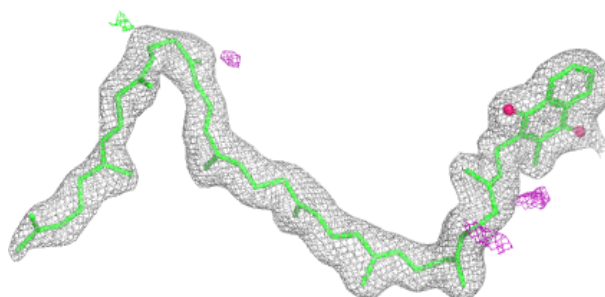


Electron density around BCB L 400:

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

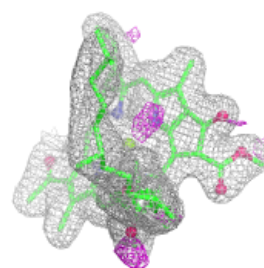
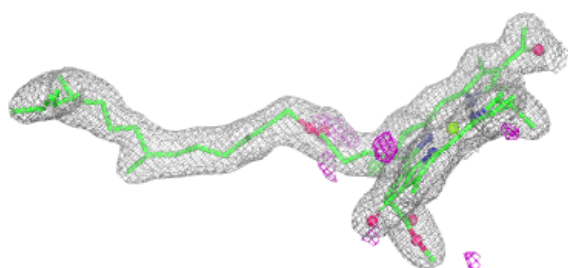
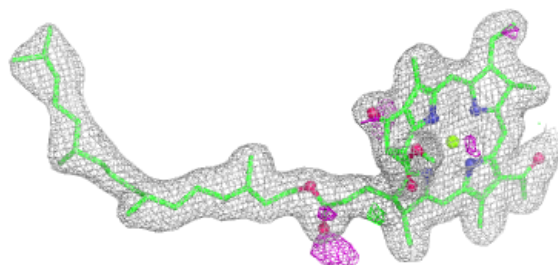
**Electron density around MQ9 M 501:**

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



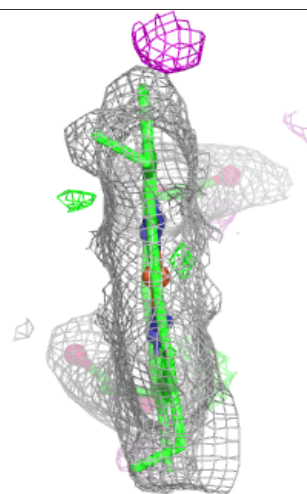
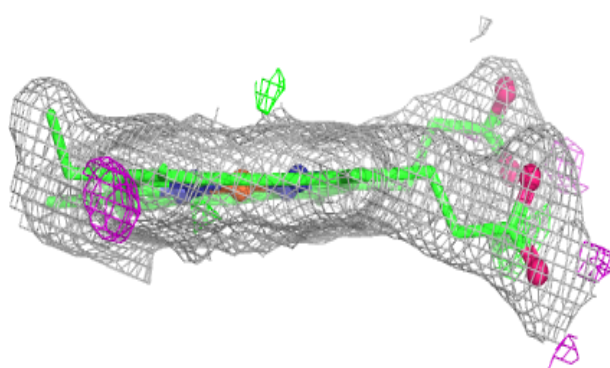
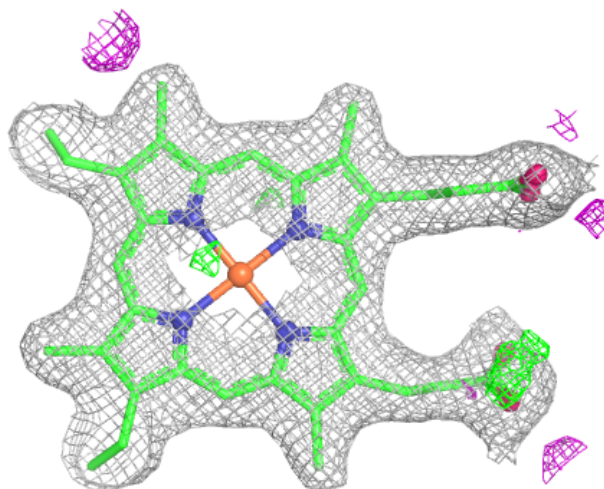
Electron density around BCB M 401:

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



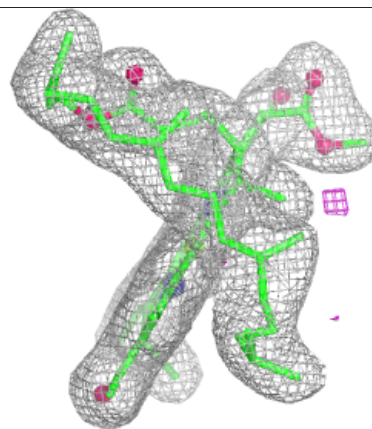
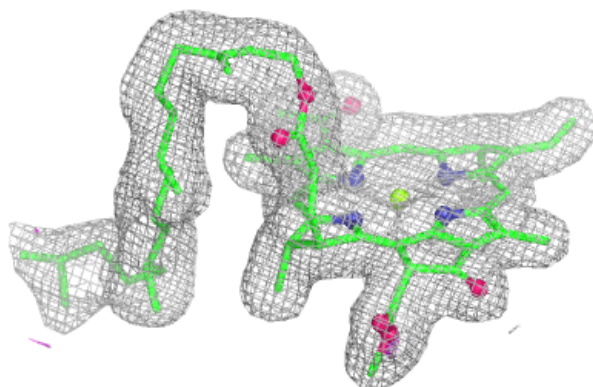
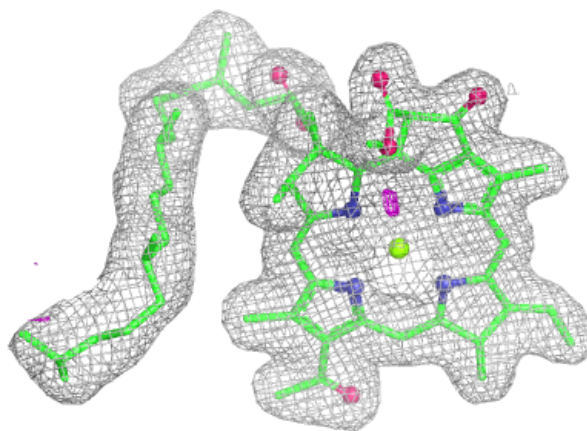
Electron density around HEC C 404:

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



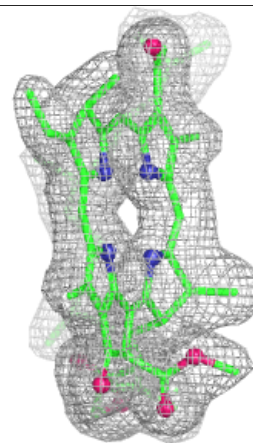
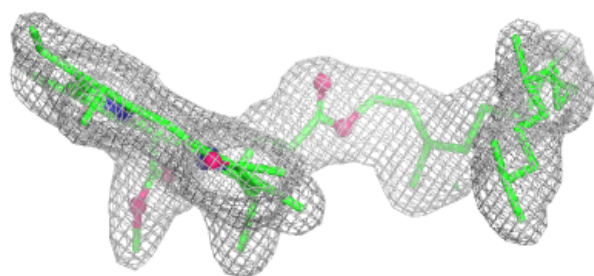
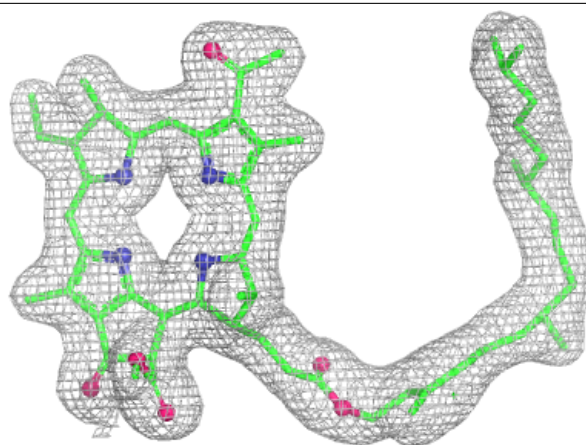
Electron density around BCB L 401:

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



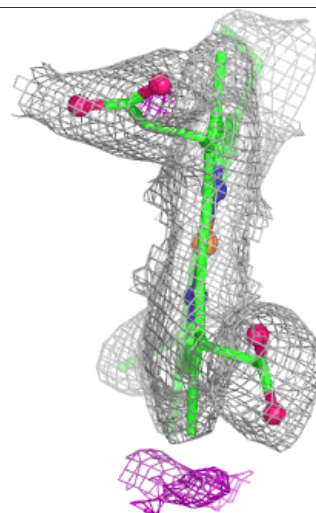
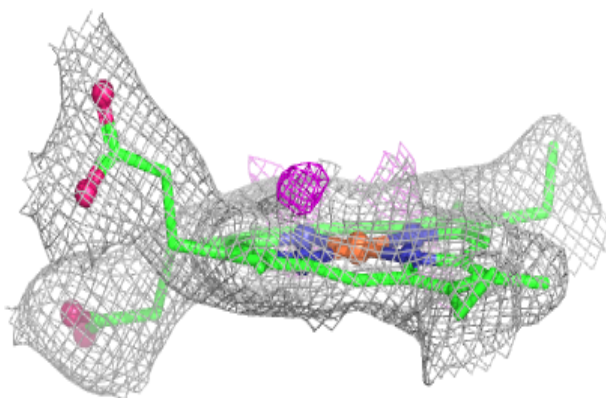
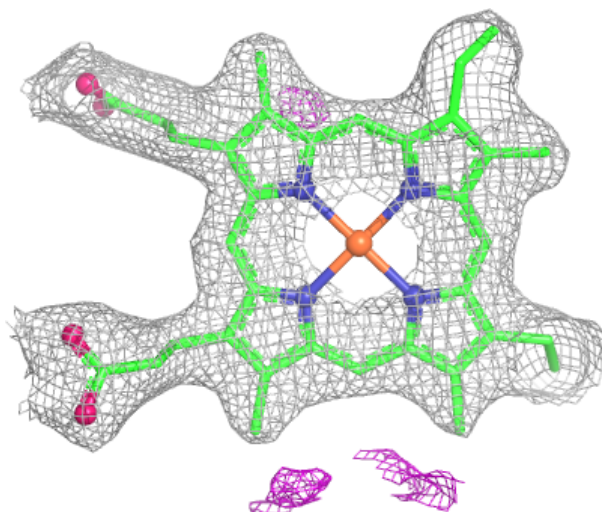
Electron density around BPB L 402:

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



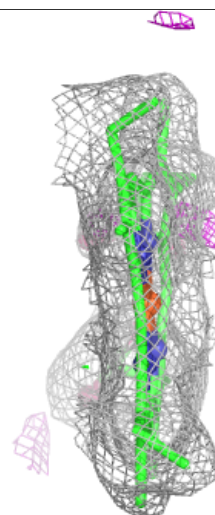
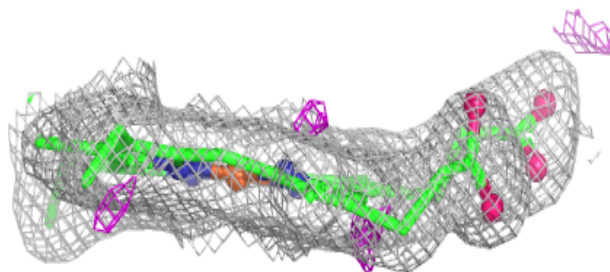
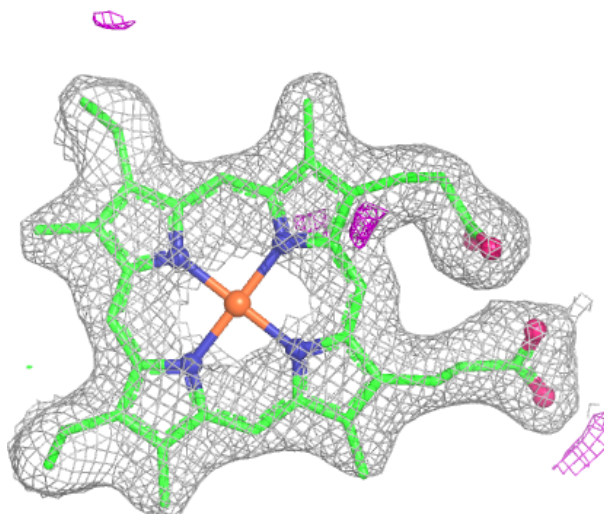
Electron density around HEC C 401:

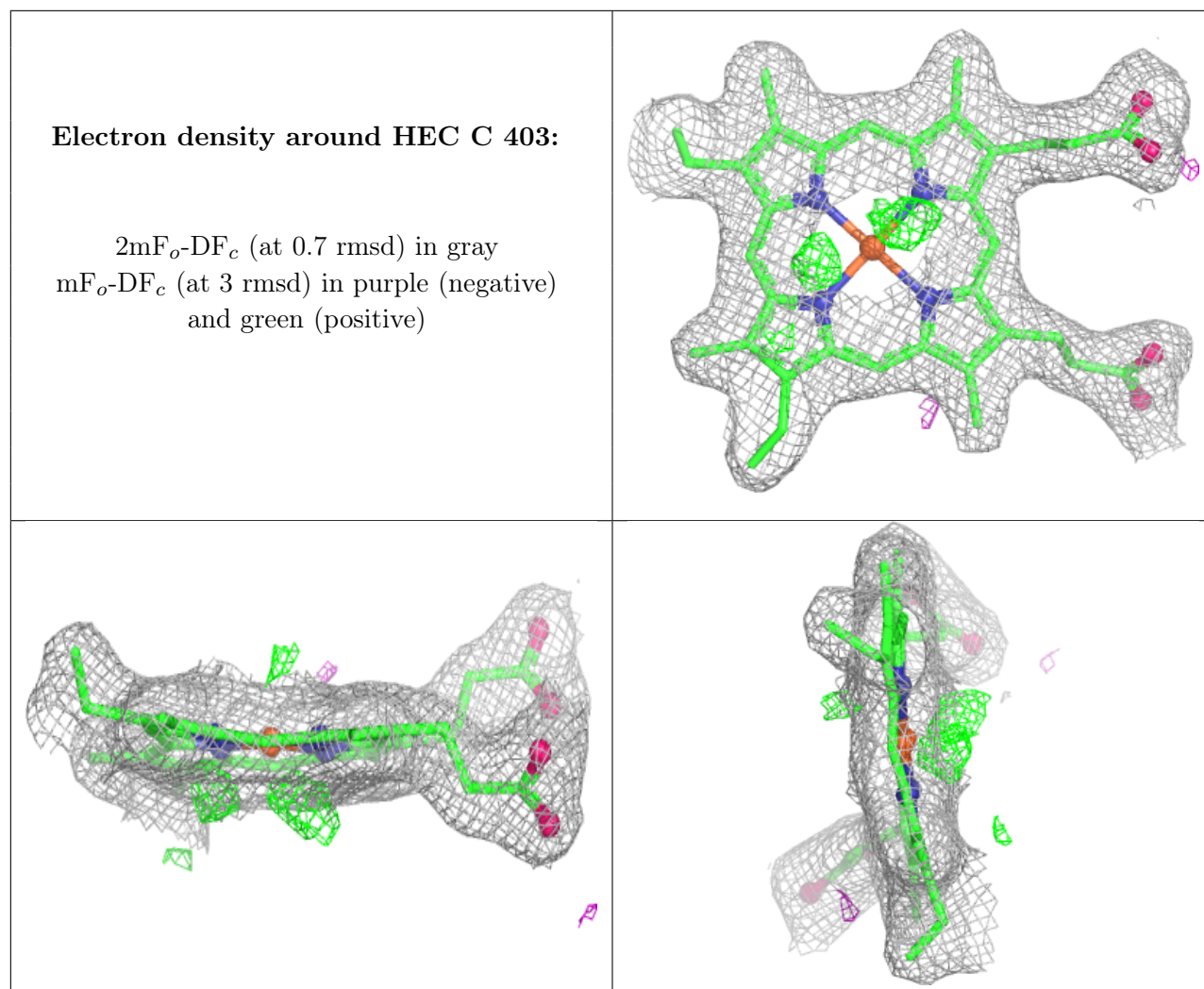
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.