



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:29 PM UTC

PDB ID : 3T6E / pdb_00003t6e
Title : Crystal Structure of the Reaction Centre from Blastochloris viridis strain DSM 133 (ATCC 19567) substrain-94
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2011-07-28
Resolution : 1.92 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

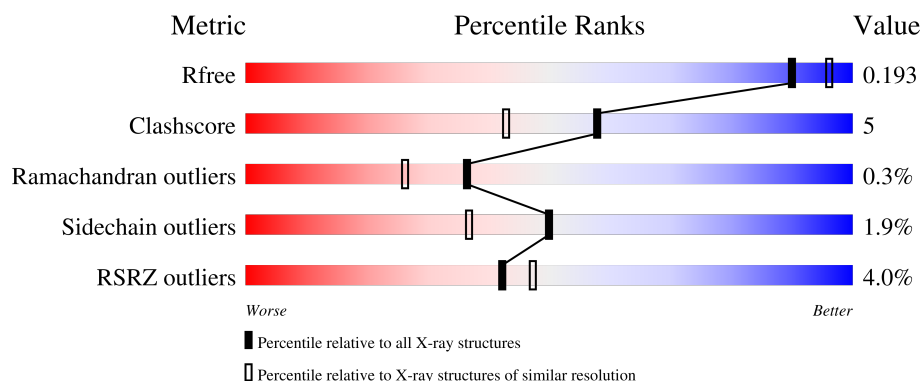
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	0.1% 86% 8% 6%
2	H	258	6% 90% 9% .
3	L	273	3% 93% 7% .
4	M	323	6% 93% 6% .

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	H	270	-	-	-	X
10	GOL	H	279	-	-	-	X
10	GOL	L	279	-	-	X	-
11	BCB	L	400	X	-	-	-
11	BCB	L	401	X	-	-	-
11	BCB	M	400	X	-	-	-
11	BCB	M	401	X	-	-	-
6	LDA	H	718	-	-	-	X
6	LDA	M	715	-	-	-	X
8	SO4	C	344	-	-	X	-
9	HTO	M	332	-	X	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 12066 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	4	0
			2651	1667	480	486	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	45	4	0
			2034	1298	349	384	3			

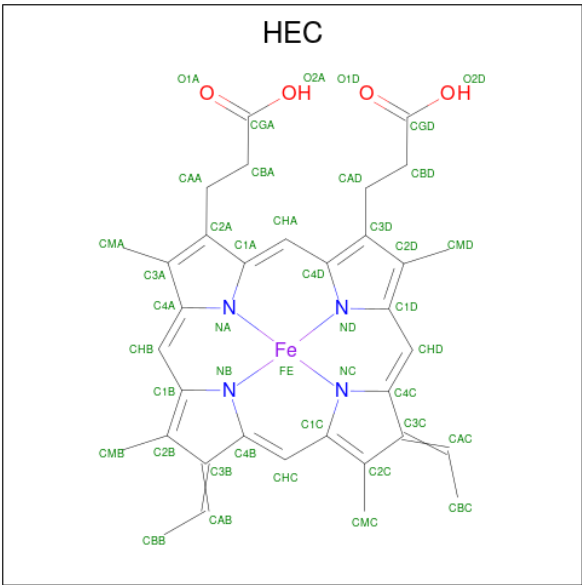
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	5	0
			2207	1482	354	361	10			

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

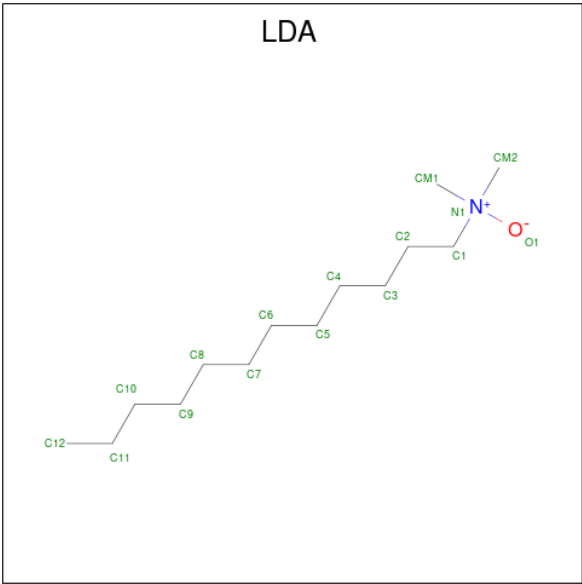
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	4	0
			2591	1725	425	429	12			

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



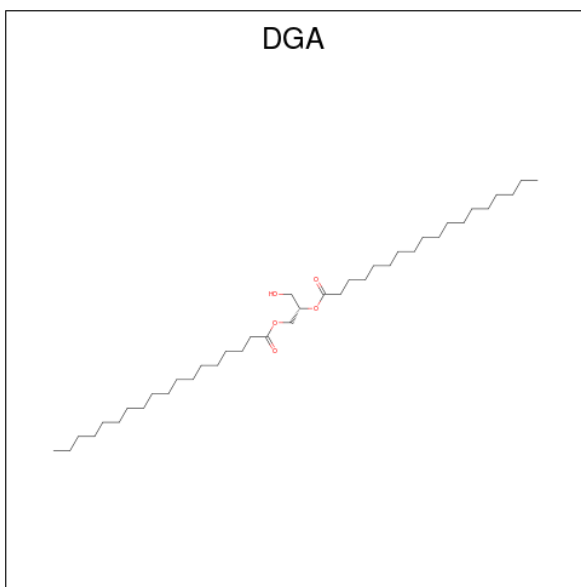
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 55	C 43	Fe 1	N 5	O 6	0	1

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



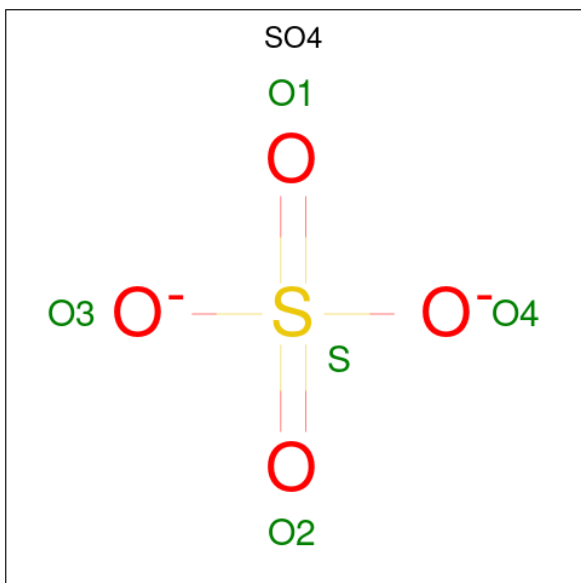
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			13	11	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
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	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		

- Molecule 7 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			37	33	4		
7	H	1	Total	C	O	0	0
			31	26	5		
7	L	1	Total	C	O	0	0
			33	28	5		
7	M	1	Total	C	O	0	0
			34	29	5		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



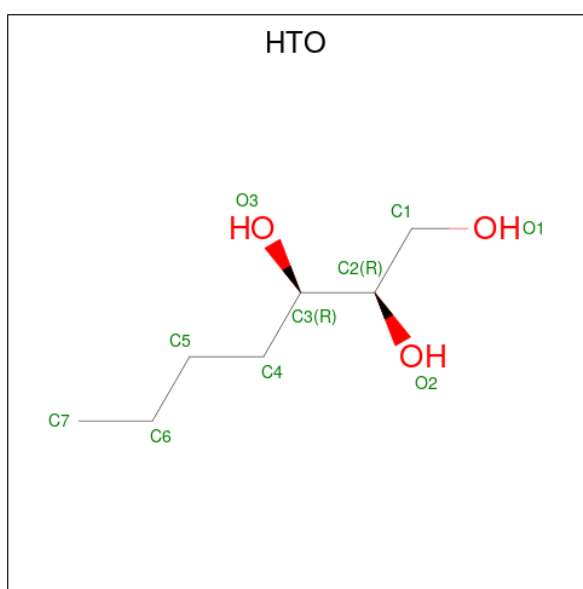
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0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

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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		

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



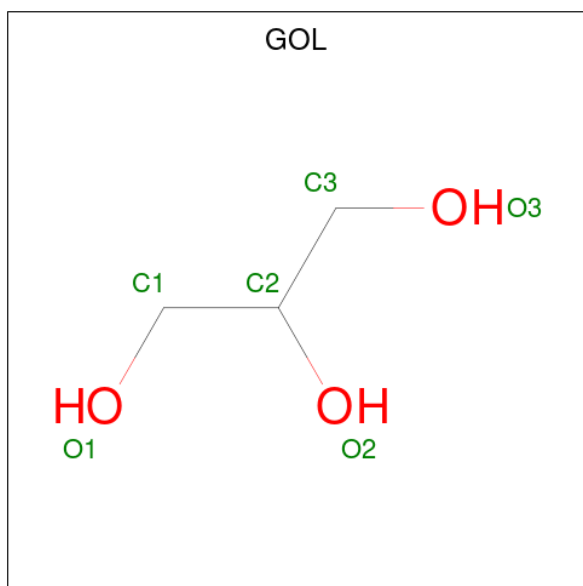
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		
10	C	1	Total	C	O	0	1
			12	6	6		
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		
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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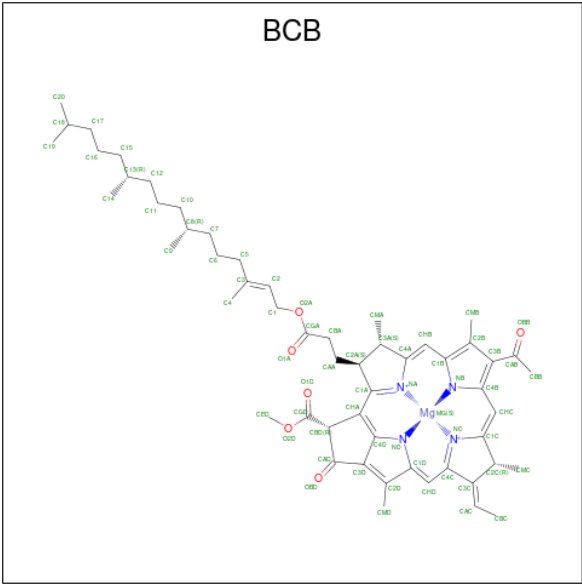
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	C	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	H	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0
10	L	1	Total 6	C 3	O 3	0	0

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

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



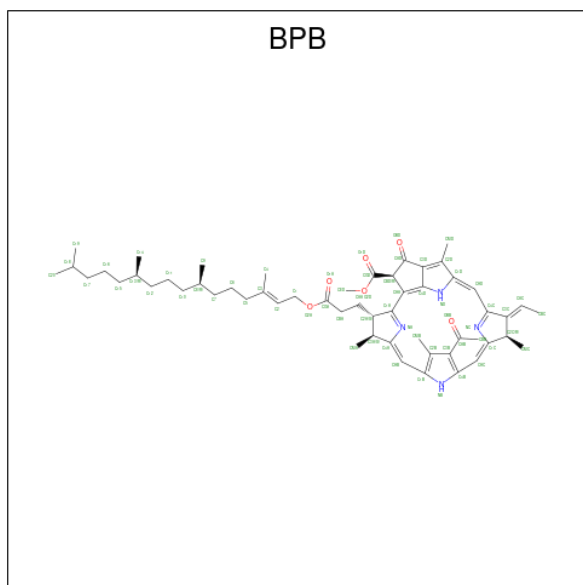
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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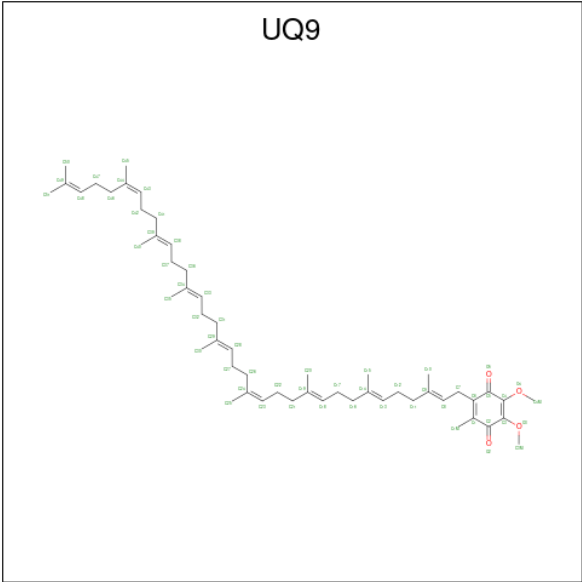
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



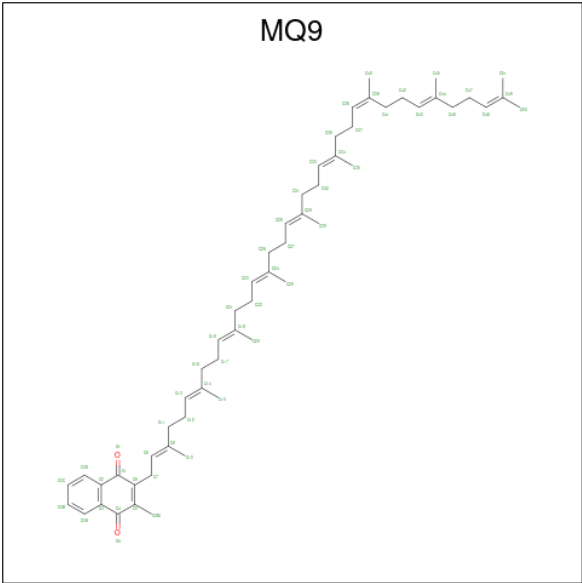
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- 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
			19	15	4		

- Molecule 14 is MENAQUINONE-9 (CCD ID: MQ9) (formula: $C_{56}H_{80}O_2$).

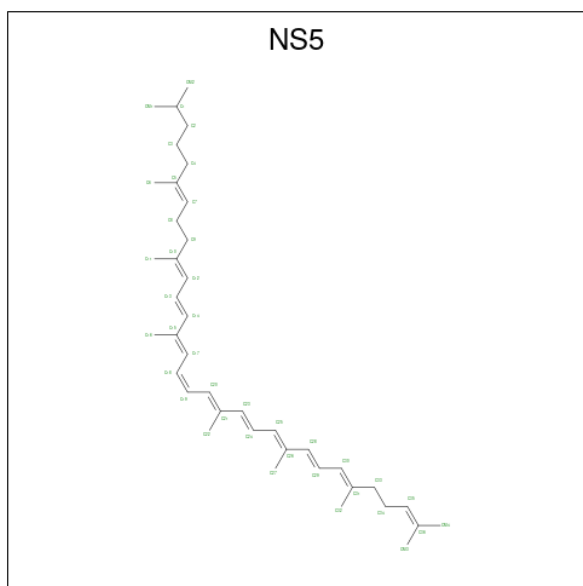


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 15 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



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

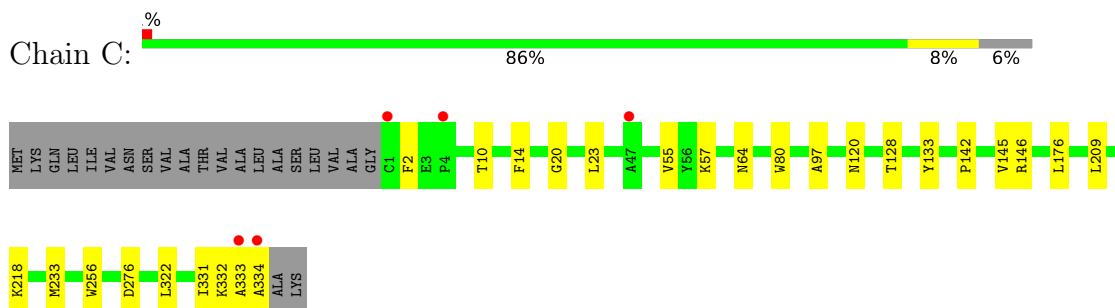
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	441	Total	O	0	0
			441	441		
17	H	233	Total	O	0	0
			233	233		
17	L	125	Total	O	0	0
			125	125		
17	M	175	Total	O	0	0
			175	175		

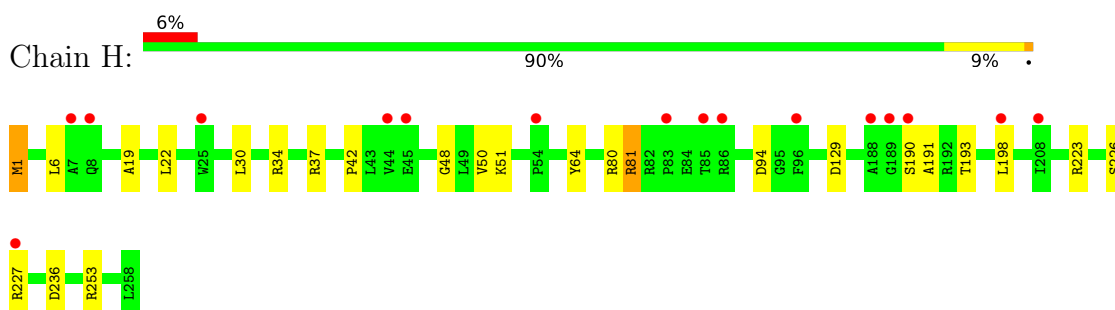
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

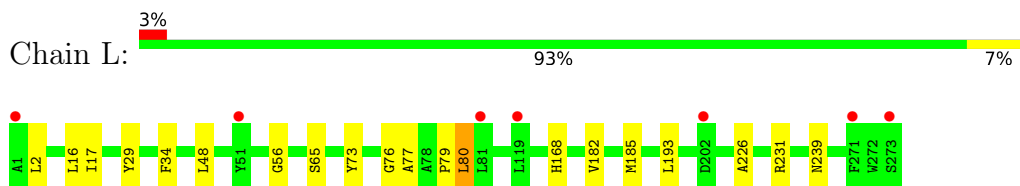
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



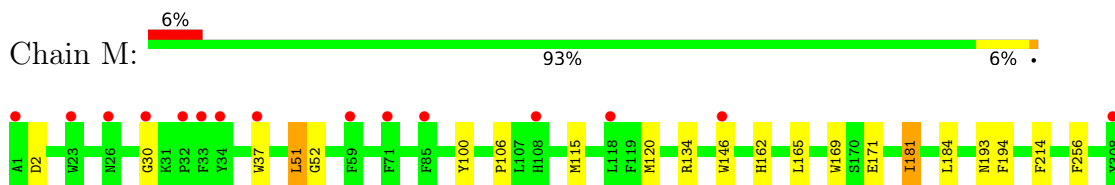
- Molecule 2: Reaction center protein H chain

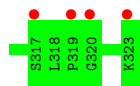


- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	221.58Å 221.58Å 113.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.46 – 1.92 43.46 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.46-1.92) 99.4 (43.46-1.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, R_{free}	0.155 , 0.178 (Not available) , 0.193	Depositor DCC
R_{free} test set	10655 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12066	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: MQ9, NS5, GOL, BPB, HTO, SO4, FME, BCB, HEC, FE2, LDA, DGA, CSO, UQ9

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	1.05	0/2718	0.94	3/3702 (0.1%)
2	H	1.03	0/2064	0.90	2/2820 (0.1%)
3	L	1.03	1/2298 (0.0%)	0.92	0/3135
4	M	1.03	1/2689 (0.0%)	0.92	2/3676 (0.1%)
All	All	1.04	2/9769 (0.0%)	0.92	7/13333 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	181	ILE	CA-CB	5.82	1.61	1.54
3	L	226	ALA	CA-CB	5.63	1.62	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	PRO	O-C-N	6.63	124.36	121.31
4	M	30	GLY	N-CA-C	-6.63	105.28	112.04
1	C	55	VAL	CB-CA-C	-5.27	105.30	111.94
2	H	190	SER	N-CA-C	-5.26	102.26	110.42
1	C	128	THR	N-CA-C	-5.21	105.65	111.27
2	H	191	ALA	N-CA-C	-5.15	101.79	109.11
4	M	100	TYR	N-CA-C	-5.04	106.55	113.30

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	2651	0	2624	19	0
2	H	2034	0	2011	18	0
3	L	2207	0	2134	22	0
4	M	2591	0	2478	14	0
5	C	184	0	108	1	0
6	C	32	0	62	2	0
6	H	77	0	146	11	0
6	L	64	0	124	5	0
6	M	80	0	155	7	0
7	C	37	0	58	1	0
7	H	31	0	44	2	0
7	L	33	0	48	2	0
7	M	34	0	50	2	0
8	C	55	0	0	2	0
8	H	40	0	0	1	0
8	M	40	0	0	0	0
9	C	20	0	32	4	0
9	H	30	0	48	2	0
9	L	20	0	32	0	0
9	M	10	0	16	0	0
10	C	102	0	136	4	0
10	H	66	0	88	3	0
10	L	42	0	56	6	0
10	M	42	0	56	1	0
11	L	132	0	144	7	0
11	M	132	0	144	11	0
12	L	65	0	74	2	0
12	M	65	0	74	3	0
13	L	77	0	99	8	0
14	M	58	0	80	0	0
15	M	1	0	0	0	0
16	M	40	0	60	3	0
17	C	441	0	0	1	0
17	H	233	0	0	3	0
17	L	125	0	0	0	0
17	M	175	0	0	2	0
All	All	12066	0	11181	101	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 5.

All (101) 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)
3:L:185[B]:MET:SD	11:M:400:BCB:H41	1.94	1.08
1:C:332:LYS:H	9:C:349:HTO:H71	1.27	0.96
7:H:733:DGA:HA42	17:M:960:HOH:O	1.78	0.82
6:H:701:LDA:CM2	6:M:702:LDA:HM11	2.11	0.80
1:C:333:ALA:HB1	1:C:334:ALA:HB2	1.65	0.76
4:M:106:PRO:HB3	7:M:732:DGA:HB52	1.67	0.76
4:M:115[B]:MET:HE2	4:M:115[B]:MET:HA	1.68	0.74
13:L:502:UQ9:H15	11:M:400:BCB:C14	2.18	0.73
13:L:502:UQ9:H15	11:M:400:BCB:H143	1.72	0.71
3:L:77:ALA:O	6:L:720:LDA:HM11	1.90	0.71
6:H:701:LDA:HM21	6:M:702:LDA:HM11	1.71	0.70
1:C:2:PHE:CD2	6:C:722:LDA:HM13	2.25	0.70
1:C:120:ASN:ND2	8:C:344:SO4:O2	2.22	0.70
3:L:76:GLY:HA3	7:L:731:DGA:HG32	1.75	0.69
11:L:401:BCB:HMB1	11:L:401:BCB:CBB	2.23	0.68
3:L:73:TYR:CE1	6:L:720:LDA:HM12	2.28	0.67
13:L:502:UQ9:C15	11:M:400:BCB:H143	2.25	0.67
2:H:81:ARG:HG3	6:H:721:LDA:H122	1.75	0.67
1:C:332:LYS:N	9:C:349:HTO:H71	2.05	0.65
3:L:239:ASN:HD21	13:L:502:UQ9:C43	2.10	0.64
3:L:65:SER:HB3	10:L:279:GOL:H12	1.81	0.62
6:H:701:LDA:HM23	6:M:702:LDA:HM11	1.81	0.62
4:M:106:PRO:CB	7:M:732:DGA:HB52	2.31	0.61
7:C:730:DGA:HB22	7:C:730:DGA:HA32	1.83	0.59
3:L:73:TYR:HE1	6:L:720:LDA:HM12	1.68	0.57
11:L:401:BCB:HMB1	11:L:401:BCB:HBB2	1.86	0.57
3:L:29:TYR:OH	6:M:702:LDA:H22	2.04	0.56
11:L:400:BCB:HMB1	11:L:400:BCB:HBB3	1.88	0.56
3:L:182:VAL:HA	11:M:400:BCB:H43	1.89	0.55
4:M:256:PHE:HB3	6:M:702:LDA:HM13	1.88	0.55
11:M:400:BCB:HMB1	11:M:400:BCB:CBB	2.37	0.54
3:L:17:ILE:HD12	3:L:34:PHE:CZ	2.43	0.54
10:L:276:GOL:O3	10:L:279:GOL:H31	2.08	0.53
1:C:331:ILE:HD12	9:C:349:HTO:H2	1.91	0.52
2:H:223:ARG:NH1	10:H:274:GOL:O3	2.39	0.51
3:L:231:ARG:CG	13:L:502:UQ9:H31A	2.41	0.51
2:H:6:LEU:HD22	6:H:718:LDA:H12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:HD12	10:C:352:GOL:H32	1.92	0.50
3:L:76:GLY:CA	7:L:731:DGA:HG32	2.41	0.50
7:H:733:DGA:HA52	4:M:165:LEU:HD22	1.91	0.50
4:M:162[B]:HIS:HE1	4:M:171:GLU:OE1	1.95	0.50
3:L:17:ILE:HD12	3:L:34:PHE:HZ	1.77	0.50
3:L:231:ARG:HG2	13:L:502:UQ9:H27A	1.93	0.50
2:H:42:PRO:HD2	6:H:721:LDA:H121	1.94	0.49
12:L:402:BPB:HMBB	12:L:402:BPB:HBBB	1.94	0.49
1:C:276:ASP:OD2	8:C:344:SO4:O1	2.30	0.49
4:M:120:MET:HE1	16:M:600:NS5:C24	2.43	0.49
12:M:402:BPB:H14A	12:M:402:BPB:HMAA	1.94	0.49
1:C:218:LYS:HG3	10:C:354:GOL:H2	1.94	0.49
1:C:57:LYS:HE2	1:C:97:ALA:CB	2.42	0.48
12:L:402:BPB:HMBB	12:L:402:BPB:CBB	2.43	0.48
4:M:184:LEU:HD21	11:M:400:BCB:CAC	2.44	0.48
2:H:227[A]:ARG:HG3	2:H:227[A]:ARG:HH11	1.79	0.47
2:H:1[B]:FME:HE2	17:H:690:HOH:O	2.14	0.47
11:L:400:BCB:HMB1	11:L:400:BCB:CBB	2.44	0.47
11:L:401:BCB:HMB1	11:L:401:BCB:HBB3	1.95	0.47
1:C:145:VAL:O	1:C:146:ARG:HD2	2.16	0.46
3:L:231:ARG:HD3	13:L:502:UQ9:H31A	1.97	0.46
1:C:256:TRP:HB2	10:C:353[B]:GOL:H2	1.99	0.45
3:L:56:GLY:CA	10:L:276:GOL:H32	2.47	0.45
3:L:79:PRO:HD3	6:L:720:LDA:HM13	1.99	0.44
4:M:51:LEU:HB3	4:M:52:GLY:H	1.61	0.44
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.53	0.44
11:M:400:BCB:HMB1	11:M:400:BCB:HBB2	1.99	0.44
11:M:400:BCB:H193	12:M:402:BPB:C20	2.47	0.44
1:C:64[A]:ASN:HD21	9:C:349:HTO:C2	2.29	0.44
10:C:358:GOL:C1	17:C:568:HOH:O	2.65	0.44
2:H:30:LEU:O	2:H:34:ARG:HD2	2.17	0.44
2:H:37:ARG:NH2	8:H:262[B]:SO4:O1	2.39	0.44
3:L:168:HIS:CE1	11:L:400:BCB:HMC2	2.54	0.43
1:C:2:PHE:CE2	6:C:722:LDA:HM13	2.53	0.43
3:L:65:SER:HB3	10:L:279:GOL:C1	2.47	0.43
2:H:223:ARG:NH2	17:H:558:HOH:O	2.48	0.43
2:H:253:ARG:HE	9:H:268:HTO:H11	1.84	0.43
6:H:701:LDA:HM21	6:M:702:LDA:CM1	2.47	0.43
1:C:14:PHE:CE2	10:L:279:GOL:H2	2.54	0.43
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.87	0.42
4:M:120:MET:CE	16:M:600:NS5:H273	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:146:TRP:CE3	4:M:146:TRP:HA	2.54	0.42
11:L:401:BCB:OBB	11:L:401:BCB:HHC	2.18	0.42
4:M:2:ASP:OD1	4:M:2:ASP:C	2.60	0.42
3:L:80:LEU:HD13	6:L:720:LDA:H72	2.02	0.42
4:M:37:TRP:CE3	6:M:704:LDA:HM22	2.55	0.42
1:C:10:THR:O	1:C:20:GLY:HA3	2.20	0.41
4:M:169:TRP:CH2	16:M:600:NS5:H342	2.55	0.41
2:H:64:TYR:CE2	6:H:721:LDA:HM22	2.55	0.41
2:H:81:ARG:HG3	6:H:721:LDA:C12	2.47	0.41
2:H:19:ALA:HB2	6:H:719:LDA:H122	2.01	0.41
2:H:223:ARG:CD	10:H:274:GOL:H11	2.50	0.41
3:L:185[B]:MET:HE1	12:M:402:BPB:HMAB	2.03	0.41
3:L:193:LEU:HD23	13:L:502:UQ9:C2	2.51	0.41
1:C:233:MET:HB3	5:C:403:HEC:C4B	2.51	0.41
2:H:193:THR:HG22	17:H:858:HOH:O	2.20	0.41
2:H:226:SER:HA	9:H:267:HTO:H73	2.03	0.41
10:M:333:GOL:C3	17:M:921:HOH:O	2.69	0.41
2:H:80:ARG:HH21	10:H:270:GOL:C2	2.34	0.40
10:L:276:GOL:O3	10:L:279:GOL:C3	2.69	0.40
2:H:1[A]:FME:H	2:H:1[A]:FME:HG3	1.58	0.40
11:M:401:BCB:CBB	11:M:401:BCB:HMB3	2.52	0.40
6:H:721:LDA:HM21	6:H:721:LDA:H21	1.91	0.40
11:M:401:BCB:OBB	11:M:401:BCB:HHC	2.21	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	336/356 (94%)	326 (97%)	10 (3%)	0	100	100
2	H	259/258 (100%)	249 (96%)	7 (3%)	3 (1%)	10	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	276/273 (101%)	272 (99%)	4 (1%)	0	100	100
4	M	324/323 (100%)	318 (98%)	5 (2%)	1 (0%)	36	26
All	All	1195/1210 (99%)	1165 (98%)	26 (2%)	4 (0%)	36	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	50	VAL
4	M	193	ASN
2	H	51	LYS
2	H	48	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	285/297 (96%)	282 (99%)	3 (1%)	65	60
2	H	210/212 (99%)	204 (97%)	6 (3%)	37	21
3	L	223/218 (102%)	219 (98%)	4 (2%)	51	39
4	M	252/248 (102%)	247 (98%)	5 (2%)	48	35
All	All	970/975 (100%)	952 (98%)	18 (2%)	50	37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	176	LEU
1	C	322	LEU
2	H	22	LEU
2	H	81	ARG
2	H	94	ASP
2	H	129	ASP
2	H	198	LEU

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Mol	Chain	Res	Type
2	H	236	ASP
3	L	2	LEU
3	L	16	LEU
3	L	48	LEU
3	L	80	LEU
4	M	51	LEU
4	M	134	ARG
4	M	181	ILE
4	M	194	PHE
4	M	214	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	302	GLN
2	H	58	GLN
2	H	220	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 ⓘ

3 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[B]	2	8,9,10	0.87	0	8,9,11	2.43	2 (25%)
4	CSO	M	160	4	3,6,7	0.67	0	1,6,8	0.23	0
2	FME	H	1[A]	2	8,9,10	0.78	0	8,9,11	2.13	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[B]	2	-	3/7/9/11	-
4	CSO	M	160	4	-	0/1/5/7	-
2	FME	H	1[A]	2	-	5/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1[B]	FME	CA-N-CN	-6.06	113.50	122.82
2	H	1[A]	FME	CA-N-CN	-5.04	115.06	122.82
2	H	1[A]	FME	O1-CN-N	-2.05	120.03	125.32
2	H	1[B]	FME	O-C-CA	-2.04	119.53	124.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1[B]	FME	1	0
2	H	1[A]	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 113 ligands modelled in this entry, 1 is monoatomic - leaving 112 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$
5	HEC	C	403	1	46,50,50	1.75	9 (19%)	58,82,82	1.78	9 (15%)
6	LDA	H	718	-	10,12,15	2.56	2 (20%)	11,14,17	0.60	0
8	SO4	H	261	-	4,4,4	0.43	0	6,6,6	1.06	1 (16%)
8	SO4	C	338	-	4,4,4	0.41	0	6,6,6	0.27	0
6	LDA	H	701	-	13,15,15	1.61	2 (15%)	14,17,17	1.12	1 (7%)
6	LDA	L	709	-	13,15,15	1.95	2 (15%)	14,17,17	0.28	0
9	HTO	H	268	-	9,9,9	0.34	0	10,10,10	1.85	3 (30%)
8	SO4	H	260	-	4,4,4	0.41	0	6,6,6	0.18	0
10	GOL	H	269	-	5,5,5	0.21	0	5,5,5	0.71	0
8	SO4	H	259	-	4,4,4	0.39	0	6,6,6	0.25	0
5	HEC	C	404[A]	-	46,50,50	1.74	9 (19%)	58,82,82	1.76	9 (15%)
8	SO4	M	325	-	4,4,4	0.34	0	6,6,6	0.26	0
10	GOL	M	336	-	5,5,5	0.18	0	5,5,5	0.69	0
6	LDA	H	707	-	13,15,15	2.16	2 (15%)	14,17,17	0.55	0
8	SO4	M	331	-	4,4,4	0.42	0	6,6,6	0.72	0
9	HTO	L	274	-	9,9,9	0.70	0	10,10,10	1.67	4 (40%)
10	GOL	M	338	-	5,5,5	0.31	0	5,5,5	1.57	1 (20%)
8	SO4	C	343	-	4,4,4	0.32	0	6,6,6	0.38	0
6	LDA	M	715	-	13,15,15	2.01	2 (15%)	14,17,17	0.47	0
10	GOL	C	350	-	5,5,5	1.06	1 (20%)	5,5,5	1.23	1 (20%)
10	GOL	H	272	-	5,5,5	0.25	0	5,5,5	0.69	0
13	UQ9	L	502	-	58,58,58	2.29	22 (37%)	72,73,73	1.46	14 (19%)
6	LDA	L	708	-	13,15,15	1.56	1 (7%)	14,17,17	0.84	1 (7%)
6	LDA	L	703	-	13,15,15	2.38	2 (15%)	14,17,17	0.61	0
10	GOL	H	270	-	5,5,5	0.35	0	5,5,5	0.64	0
11	BCB	M	401	4	60,74,74	1.13	4 (6%)	59,115,115	3.40	17 (28%)
10	GOL	C	358	-	5,5,5	0.52	0	5,5,5	0.57	0
9	HTO	H	266	-	9,9,9	0.39	0	10,10,10	1.41	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	C	337	-	4,4,4	0.44	0	6,6,6	0.15	0
8	SO4	M	327	-	4,4,4	0.42	0	6,6,6	0.12	0
8	SO4	M	330	-	4,4,4	0.50	0	6,6,6	0.42	0
11	BCB	L	401	3	60,74,74	1.34	9 (15%)	59,115,115	3.03	15 (25%)
5	HEC	C	404[B]	-	46,50,50	1.75	10 (21%)	58,82,82	1.64	6 (10%)
6	LDA	M	706	-	13,15,15	1.97	1 (7%)	14,17,17	0.57	0
6	LDA	M	704	-	13,15,15	2.09	2 (15%)	14,17,17	0.54	0
10	GOL	C	357	-	5,5,5	0.52	0	5,5,5	0.43	0
8	SO4	C	339	-	4,4,4	0.39	0	6,6,6	0.22	0
6	LDA	H	719	-	13,15,15	2.21	2 (15%)	14,17,17	0.68	0
8	SO4	H	265	-	4,4,4	0.45	0	6,6,6	0.11	0
10	GOL	C	365	-	5,5,5	0.22	0	5,5,5	0.52	0
10	GOL	C	360	-	5,5,5	0.21	0	5,5,5	0.35	0
10	GOL	L	280	-	5,5,5	0.28	0	5,5,5	0.22	0
10	GOL	L	279	-	5,5,5	0.81	0	5,5,5	1.14	0
12	BPB	M	402	-	57,70,70	1.47	8 (14%)	55,101,101	1.62	7 (12%)
10	GOL	L	277	-	5,5,5	0.27	0	5,5,5	1.13	0
6	LDA	M	705	-	13,15,15	1.95	2 (15%)	14,17,17	0.65	0
10	GOL	M	337	-	5,5,5	0.28	0	5,5,5	0.43	0
11	BCB	M	400	4	60,74,74	1.35	6 (10%)	59,115,115	2.61	16 (27%)
8	SO4	H	262[A]	-	4,4,4	0.51	0	6,6,6	0.48	0
13	UQ9	L	503	-	19,19,58	2.29	6 (31%)	24,26,73	1.75	5 (20%)
8	SO4	C	340	-	4,4,4	0.40	0	6,6,6	0.34	0
6	LDA	C	712	-	13,15,15	2.07	1 (7%)	14,17,17	0.52	0
10	GOL	C	363	-	5,5,5	0.33	0	5,5,5	0.55	0
10	GOL	H	278	-	5,5,5	0.18	0	5,5,5	0.75	0
6	LDA	L	720	-	13,15,15	1.83	1 (7%)	14,17,17	1.11	2 (14%)
10	GOL	C	364	-	5,5,5	0.69	0	5,5,5	2.37	2 (40%)
9	HTO	L	275	-	9,9,9	0.93	0	10,10,10	3.23	4 (40%)
10	GOL	C	354	-	5,5,5	0.75	0	5,5,5	0.56	0
10	GOL	L	276	-	5,5,5	0.38	0	5,5,5	0.57	0
9	HTO	C	348	-	9,9,9	0.44	0	10,10,10	1.88	2 (20%)
8	SO4	C	342	-	4,4,4	0.43	0	6,6,6	0.26	0
9	HTO	C	349	-	9,9,9	0.61	0	10,10,10	0.89	0
10	GOL	M	335	-	5,5,5	0.61	0	5,5,5	1.91	2 (40%)
10	GOL	L	281	-	5,5,5	0.26	0	5,5,5	0.39	0
9	HTO	H	267	-	9,9,9	0.56	0	10,10,10	1.02	0
10	GOL	C	359	-	5,5,5	0.44	0	5,5,5	0.39	0
10	GOL	C	352	-	5,5,5	0.35	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LDA	M	702	-	13,15,15	2.17	2 (15%)	14,17,17	0.80	0
10	GOL	H	274	-	5,5,5	0.22	0	5,5,5	0.46	0
10	GOL	C	356	-	5,5,5	0.87	0	5,5,5	1.64	1 (20%)
10	GOL	H	275	-	5,5,5	0.31	0	5,5,5	0.35	0
10	GOL	M	339	-	5,5,5	0.32	0	5,5,5	0.50	0
8	SO4	M	328	-	4,4,4	0.37	0	6,6,6	0.56	0
10	GOL	M	334	-	5,5,5	0.33	0	5,5,5	1.22	0
7	DGA	M	732	-	33,33,43	0.65	0	35,35,45	1.60	4 (11%)
10	GOL	H	273	-	5,5,5	0.25	0	5,5,5	0.73	0
8	SO4	H	262[B]	-	4,4,4	0.47	0	6,6,6	0.48	0
8	SO4	M	324	-	4,4,4	0.51	0	6,6,6	0.96	0
10	GOL	C	351	-	5,5,5	0.66	0	5,5,5	1.29	1 (20%)
8	SO4	M	329	-	4,4,4	0.31	0	6,6,6	0.36	0
8	SO4	C	341	-	4,4,4	0.46	0	6,6,6	0.28	0
14	MQ9	M	501	-	59,59,59	2.20	26 (44%)	73,75,75	1.26	10 (13%)
10	GOL	H	279	-	5,5,5	0.26	0	5,5,5	0.56	0
10	GOL	M	333	-	5,5,5	0.27	0	5,5,5	0.34	0
10	GOL	H	271	-	5,5,5	0.53	0	5,5,5	1.32	1 (20%)
8	SO4	C	347	-	4,4,4	0.42	0	6,6,6	0.10	0
7	DGA	C	730	1	36,36,43	0.84	2 (5%)	38,38,45	1.39	4 (10%)
10	GOL	L	278	-	5,5,5	0.91	0	5,5,5	1.49	1 (20%)
10	GOL	C	355	-	5,5,5	0.27	0	5,5,5	0.44	0
8	SO4	C	345	-	4,4,4	0.66	0	6,6,6	0.34	0
8	SO4	C	346	-	4,4,4	0.50	0	6,6,6	0.19	0
10	GOL	C	362	-	5,5,5	0.26	0	5,5,5	0.59	0
5	HEC	C	401	1	46,50,50	1.66	5 (10%)	58,82,82	1.98	12 (20%)
5	HEC	C	402	1	46,50,50	1.64	8 (17%)	58,82,82	1.82	10 (17%)
6	LDA	C	722	-	13,15,15	2.16	2 (15%)	14,17,17	0.50	0
11	BCB	L	400	3	60,74,74	1.41	9 (15%)	59,115,115	3.29	15 (25%)
8	SO4	C	344	-	4,4,4	0.38	0	6,6,6	0.26	0
7	DGA	L	731	-	32,32,43	0.67	0	34,34,45	1.61	6 (17%)
7	DGA	H	733	-	30,30,43	0.64	1 (3%)	32,32,45	1.83	8 (25%)
10	GOL	C	353[B]	-	5,5,5	0.53	0	5,5,5	0.41	0
10	GOL	H	277	-	5,5,5	0.34	0	5,5,5	0.34	0
10	GOL	H	276	-	5,5,5	0.19	0	5,5,5	0.49	0
8	SO4	H	263	-	4,4,4	0.45	0	6,6,6	0.36	0
10	GOL	C	361	-	5,5,5	0.25	0	5,5,5	0.40	0
8	SO4	M	326	-	4,4,4	0.25	0	6,6,6	0.29	0
8	SO4	H	264	-	4,4,4	0.50	0	6,6,6	0.23	0
10	GOL	L	282	-	5,5,5	0.34	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	C	353[A]	-	5,5,5	0.58	0	5,5,5	0.80	0
6	LDA	H	721	-	13,15,15	2.20	2 (15%)	14,17,17	1.05	1 (7%)
9	HTO	M	332	-	9,9,9	0.60	0	10,10,10	3.44	5 (50%)
16	NS5	M	600	-	39,39,39	1.82	13 (33%)	46,46,46	2.24	13 (28%)
12	BPB	L	402	-	57,70,70	1.45	7 (12%)	55,101,101	1.91	8 (14%)

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
5	HEC	C	403	1	-	4/14/54/54	-
6	LDA	H	718	-	-	6/10/10/13	-
6	LDA	H	701	-	-	5/13/13/13	-
6	LDA	L	709	-	-	4/13/13/13	-
9	HTO	H	268	-	-	8/10/10/10	-
10	GOL	H	269	-	-	4/4/4/4	-
5	HEC	C	404[A]	-	-	4/14/54/54	-
10	GOL	M	336	-	-	2/4/4/4	-
6	LDA	H	707	-	-	6/13/13/13	-
9	HTO	L	274	-	-	0/10/10/10	-
10	GOL	M	338	-	-	1/4/4/4	-
6	LDA	M	715	-	-	9/13/13/13	-
10	GOL	C	350	-	-	0/4/4/4	-
10	GOL	H	272	-	-	0/4/4/4	-
13	UQ9	L	502	-	-	24/57/81/81	0/1/1/1
6	LDA	L	708	-	-	1/13/13/13	-
6	LDA	L	703	-	-	7/13/13/13	-
10	GOL	H	270	-	-	4/4/4/4	-
11	BCB	M	401	4	3/3/21/26	8/37/137/137	-
10	GOL	C	358	-	-	2/4/4/4	-
9	HTO	H	266	-	-	7/10/10/10	-
11	BCB	L	401	3	3/3/21/26	6/37/137/137	-
5	HEC	C	404[B]	-	-	9/14/54/54	-
6	LDA	M	706	-	-	7/13/13/13	-
6	LDA	M	704	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	C	357	-	-	2/4/4/4	-
6	LDA	H	719	-	-	5/13/13/13	-
10	GOL	C	365	-	-	2/4/4/4	-
10	GOL	C	360	-	-	1/4/4/4	-
10	GOL	L	280	-	-	3/4/4/4	-
10	GOL	L	279	-	-	2/4/4/4	-
12	BPB	M	402	-	-	9/37/105/105	0/5/6/6
10	GOL	L	277	-	-	0/4/4/4	-
6	LDA	M	705	-	-	5/13/13/13	-
10	GOL	M	337	-	-	4/4/4/4	-
11	BCB	M	400	4	3/3/21/26	13/37/137/137	-
13	UQ9	L	503	-	-	6/11/35/81	0/1/1/1
6	LDA	C	712	-	-	9/13/13/13	-
10	GOL	C	363	-	-	2/4/4/4	-
10	GOL	H	278	-	-	4/4/4/4	-
6	LDA	L	720	-	-	6/13/13/13	-
10	GOL	C	364	-	-	1/4/4/4	-
9	HTO	L	275	-	-	7/10/10/10	-
10	GOL	C	354	-	-	2/4/4/4	-
10	GOL	L	276	-	-	2/4/4/4	-
9	HTO	C	348	-	-	7/10/10/10	-
9	HTO	C	349	-	-	7/10/10/10	-
10	GOL	M	335	-	-	2/4/4/4	-
10	GOL	L	281	-	-	3/4/4/4	-
9	HTO	H	267	-	-	5/10/10/10	-
10	GOL	C	359	-	-	2/4/4/4	-
10	GOL	C	352	-	-	2/4/4/4	-
6	LDA	M	702	-	-	10/13/13/13	-
10	GOL	H	274	-	-	2/4/4/4	-
10	GOL	C	356	-	-	0/4/4/4	-
10	GOL	H	275	-	-	2/4/4/4	-
10	GOL	M	339	-	-	2/4/4/4	-
10	GOL	M	334	-	-	2/4/4/4	-
7	DGA	M	732	-	-	16/35/35/45	-
10	GOL	H	273	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	C	351	-	-	2/4/4/4	-
14	MQ9	M	501	-	-	2/53/73/73	0/2/2/2
10	GOL	H	279	-	-	2/4/4/4	-
10	GOL	M	333	-	-	2/4/4/4	-
10	GOL	H	271	-	-	4/4/4/4	-
7	DGA	C	730	1	-	19/37/37/45	-
10	GOL	L	278	-	-	4/4/4/4	-
10	GOL	C	355	-	-	1/4/4/4	-
10	GOL	C	362	-	-	2/4/4/4	-
5	HEC	C	401	1	-	6/14/54/54	-
5	HEC	C	402	1	-	9/14/54/54	-
6	LDA	C	722	-	-	9/13/13/13	-
11	BCB	L	400	3	3/3/21/26	7/37/137/137	-
7	DGA	L	731	-	-	12/34/34/45	-
7	DGA	H	733	-	-	19/32/32/45	-
10	GOL	C	353[B]	-	-	4/4/4/4	-
10	GOL	H	277	-	-	4/4/4/4	-
10	GOL	H	276	-	-	2/4/4/4	-
10	GOL	C	361	-	-	3/4/4/4	-
10	GOL	L	282	-	-	2/4/4/4	-
10	GOL	C	353[A]	-	-	4/4/4/4	-
6	LDA	H	721	-	-	8/13/13/13	-
9	HTO	M	332	-	-	7/10/10/10	-
16	NS5	M	600	-	-	10/43/43/43	-
12	BPB	L	402	-	-	2/37/105/105	0/5/6/6

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	712	LDA	O1-N1	-7.17	1.24	1.42
6	H	718	LDA	O1-N1	-6.98	1.25	1.42
12	M	402	BPB	C1B-C2B	6.92	1.47	1.39
6	L	703	LDA	O1-N1	-6.89	1.25	1.42
13	L	503	UQ9	C7-C8	-6.84	1.39	1.50
13	L	502	UQ9	C7-C8	-6.84	1.39	1.50
6	M	706	LDA	O1-N1	-6.74	1.25	1.42
6	H	719	LDA	O1-N1	-6.67	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	709	LDA	O1-N1	-6.60	1.26	1.42
6	M	704	LDA	O1-N1	-6.56	1.26	1.42
6	M	702	LDA	O1-N1	-6.53	1.26	1.42
6	H	707	LDA	O1-N1	-6.48	1.26	1.42
6	C	722	LDA	O1-N1	-6.46	1.26	1.42
6	M	715	LDA	O1-N1	-6.42	1.26	1.42
6	L	720	LDA	O1-N1	-6.33	1.26	1.42
12	L	402	BPB	C1B-C2B	6.07	1.46	1.39
6	H	721	LDA	O1-N1	-5.97	1.27	1.42
11	L	400	BCB	C3A-C2A	-5.85	1.49	1.54
6	M	705	LDA	O1-N1	-5.82	1.27	1.42
5	C	404[A]	HEC	CAB-C3B	5.78	1.53	1.35
5	C	404[B]	HEC	CAB-C3B	5.78	1.53	1.35
5	C	403	HEC	CAC-C3C	5.38	1.52	1.35
6	L	708	LDA	O1-N1	-5.34	1.29	1.42
14	M	501	MQ9	C6-C5	5.33	1.44	1.35
5	C	402	HEC	CAB-C3B	5.20	1.51	1.35
6	H	721	LDA	C1-N1	-5.16	1.46	1.51
6	L	703	LDA	C1-N1	-5.06	1.46	1.51
5	C	402	HEC	CAC-C3C	4.96	1.51	1.35
5	C	404[A]	HEC	CAC-C3C	4.92	1.51	1.35
5	C	404[B]	HEC	CAC-C3C	4.92	1.51	1.35
5	C	401	HEC	CAC-C3C	4.78	1.50	1.35
11	M	400	BCB	C3A-C2A	-4.78	1.50	1.54
5	C	401	HEC	CAB-C3B	4.69	1.50	1.35
6	H	701	LDA	O1-N1	-4.67	1.30	1.42
11	M	401	BCB	CHA-CBD	-4.67	1.46	1.51
12	M	402	BPB	C3B-C4B	4.50	1.48	1.41
12	L	402	BPB	C1D-C2D	4.40	1.44	1.39
5	C	403	HEC	CAB-C3B	4.34	1.49	1.35
6	H	719	LDA	C1-N1	-4.34	1.47	1.51
6	H	707	LDA	C1-N1	-4.24	1.47	1.51
6	M	702	LDA	C1-N1	-4.22	1.47	1.51
6	C	722	LDA	C1-N1	-4.21	1.47	1.51
6	H	718	LDA	C1-N1	-4.05	1.47	1.51
13	L	502	UQ9	C4-C5	-4.00	1.37	1.48
6	M	705	LDA	C1-N1	-3.86	1.47	1.51
14	M	501	MQ9	C43-C44	3.83	1.41	1.33
14	M	501	MQ9	C5M-C5	3.74	1.58	1.50
13	L	502	UQ9	C27-C28	-3.71	1.39	1.50
13	L	502	UQ9	C37-C38	-3.70	1.39	1.50
13	L	502	UQ9	C47-C48	-3.65	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	502	UQ9	C17-C18	-3.63	1.39	1.50
14	M	501	MQ9	C37-C38	-3.61	1.39	1.50
11	L	401	BCB	C3A-C2A	-3.61	1.51	1.54
13	L	502	UQ9	C22-C23	-3.57	1.39	1.50
6	M	704	LDA	C1-N1	-3.56	1.47	1.51
13	L	502	UQ9	C32-C33	-3.47	1.40	1.50
5	C	401	HEC	C3C-C4C	-3.45	1.40	1.46
13	L	502	UQ9	C12-C13	-3.44	1.40	1.50
14	M	501	MQ9	C38-C39	3.36	1.40	1.33
13	L	502	UQ9	C3-C2	-3.29	1.39	1.48
14	M	501	MQ9	C33-C34	3.24	1.40	1.33
6	M	715	LDA	C1-N1	-3.22	1.48	1.51
13	L	502	UQ9	C42-C43	-3.21	1.40	1.50
12	L	402	BPB	CHA-CBD	3.20	1.55	1.51
14	M	501	MQ9	C22-C23	-3.19	1.40	1.50
13	L	502	UQ9	C18-C19	3.18	1.40	1.33
14	M	501	MQ9	C28-C29	3.17	1.40	1.33
13	L	502	UQ9	C28-C29	3.15	1.40	1.33
13	L	502	UQ9	C38-C39	3.14	1.40	1.33
16	M	600	NS5	C13-C12	3.13	1.52	1.43
16	M	600	NS5	C29-C30	3.12	1.52	1.43
6	H	701	LDA	C1-N1	-3.12	1.48	1.51
16	M	600	NS5	C4-C5	3.11	1.57	1.51
14	M	501	MQ9	C3-C4	-3.10	1.42	1.48
14	M	501	MQ9	C47-C48	-3.08	1.41	1.50
13	L	503	UQ9	C6-C1	2.98	1.40	1.35
11	L	400	BCB	MG-ND	-2.98	1.99	2.05
11	L	401	BCB	C1A-CHA	2.97	1.43	1.40
14	M	501	MQ9	C42-C43	-2.97	1.41	1.50
16	M	600	NS5	C28-C26	2.94	1.52	1.46
5	C	403	HEC	C3C-C4C	-2.94	1.40	1.46
13	L	502	UQ9	C23-C24	2.92	1.39	1.33
13	L	502	UQ9	C43-C44	2.90	1.39	1.33
11	L	401	BCB	CMB-C2B	2.89	1.57	1.51
11	L	401	BCB	MG-NB	-2.88	2.00	2.05
14	M	501	MQ9	C2-C1	-2.88	1.42	1.48
13	L	502	UQ9	C13-C14	2.88	1.39	1.33
11	M	400	BCB	CHB-C4A	2.85	1.42	1.38
14	M	501	MQ9	C5-C4	-2.83	1.41	1.47
13	L	503	UQ9	C4-C5	-2.82	1.40	1.48
14	M	501	MQ9	C46-C44	2.80	1.57	1.51
13	L	502	UQ9	C33-C34	2.78	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	503	UQ9	C3-C2	-2.77	1.40	1.48
14	M	501	MQ9	C7-C8	-2.76	1.46	1.50
11	L	401	BCB	C3D-C2D	2.74	1.44	1.39
13	L	503	UQ9	C8-C9	2.74	1.39	1.33
12	L	402	BPB	C3D-CAD	-2.72	1.42	1.47
14	M	501	MQ9	C11-C9	2.69	1.56	1.51
13	L	502	UQ9	C8-C9	2.68	1.39	1.33
11	L	401	BCB	CBD-CGD	-2.65	1.49	1.52
12	M	402	BPB	CMB-C2B	2.64	1.56	1.51
13	L	502	UQ9	C6-C5	-2.63	1.39	1.46
14	M	501	MQ9	C41-C39	2.63	1.56	1.51
7	H	733	DGA	OG1-CG1	-2.63	1.39	1.45
11	M	401	BCB	CBD-CGD	2.61	1.55	1.52
14	M	501	MQ9	C27-C28	-2.61	1.42	1.50
14	M	501	MQ9	C48-C49	2.61	1.40	1.32
5	C	404[B]	HEC	O1D-CGD	2.60	1.30	1.22
11	L	400	BCB	C1A-C2A	2.59	1.56	1.51
16	M	600	NS5	C8-C7	2.56	1.58	1.50
14	M	501	MQ9	C32-C33	-2.55	1.42	1.50
5	C	404[A]	HEC	C1C-NC	-2.53	1.34	1.39
5	C	404[B]	HEC	C1C-NC	-2.53	1.34	1.39
16	M	600	NS5	C22-C21	2.52	1.55	1.50
14	M	501	MQ9	C8-C9	2.52	1.38	1.33
12	M	402	BPB	C3D-C2D	2.52	1.43	1.39
11	M	400	BCB	CHD-C4C	2.51	1.44	1.39
5	C	401	HEC	C1A-C2A	-2.50	1.40	1.45
5	C	403	HEC	C4A-C3A	-2.50	1.40	1.45
11	L	400	BCB	CHB-C1B	2.49	1.43	1.39
5	C	404[A]	HEC	C4B-NB	-2.48	1.34	1.39
5	C	404[B]	HEC	C4B-NB	-2.48	1.34	1.39
13	L	502	UQ9	C6-C1	2.48	1.39	1.35
11	L	401	BCB	OBD-CAD	2.46	1.25	1.22
11	L	401	BCB	CMA-C3A	2.46	1.57	1.53
5	C	403	HEC	C1C-NC	-2.45	1.35	1.39
14	M	501	MQ9	C23-C24	2.44	1.38	1.33
5	C	403	HEC	CBB-CAB	2.42	1.58	1.49
5	C	402	HEC	C4A-C3A	-2.41	1.40	1.45
7	C	730	DGA	CG1-CG2	2.41	1.56	1.50
14	M	501	MQ9	C18-C19	2.40	1.38	1.33
11	L	400	BCB	O2D-CGD	2.39	1.39	1.33
5	C	402	HEC	CBB-CAB	2.39	1.58	1.49
14	M	501	MQ9	C25-C24	2.39	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	400	BCB	C3D-C4D	2.38	1.45	1.41
5	C	404[A]	HEC	C3C-C4C	-2.38	1.41	1.46
5	C	404[B]	HEC	C3C-C4C	-2.38	1.41	1.46
5	C	402	HEC	C1A-C2A	-2.37	1.41	1.45
16	M	600	NS5	C24-C25	2.35	1.50	1.43
11	M	400	BCB	CHA-CBD	-2.33	1.48	1.51
12	M	402	BPB	C1D-C2D	2.33	1.42	1.39
5	C	404[A]	HEC	CMA-C3A	2.32	1.55	1.50
5	C	404[B]	HEC	CMA-C3A	2.32	1.55	1.50
6	L	709	LDA	C1-N1	-2.29	1.49	1.51
5	C	403	HEC	CMC-C2C	2.29	1.55	1.50
14	M	501	MQ9	C12-C13	-2.27	1.43	1.50
12	L	402	BPB	C1B-NB	-2.26	1.34	1.38
16	M	600	NS5	C34-C35	2.25	1.57	1.50
12	M	402	BPB	C1-C2	2.24	1.55	1.49
12	L	402	BPB	C1-C2	2.24	1.55	1.49
11	M	401	BCB	OBD-CAD	2.22	1.25	1.22
5	C	404[A]	HEC	CBC-CAC	2.22	1.57	1.49
5	C	404[B]	HEC	CBC-CAC	2.22	1.57	1.49
14	M	501	MQ9	C17-C18	-2.20	1.43	1.50
12	M	402	BPB	CHA-CBD	2.19	1.54	1.51
16	M	600	NS5	C19-C20	2.19	1.50	1.43
5	C	404[A]	HEC	O2A-CGA	-2.18	1.23	1.30
5	C	404[B]	HEC	O2A-CGA	-2.18	1.23	1.30
7	C	730	DGA	OG1-CG1	2.18	1.50	1.45
13	L	502	UQ9	C7-C6	2.17	1.55	1.51
11	M	400	BCB	CMB-C2B	2.16	1.55	1.51
5	C	404[A]	HEC	C3B-C4B	-2.16	1.42	1.46
5	C	404[B]	HEC	C3B-C4B	-2.16	1.42	1.46
16	M	600	NS5	C23-C21	2.16	1.50	1.46
11	M	401	BCB	O2D-CGD	2.16	1.38	1.33
11	L	400	BCB	CHA-CBD	-2.15	1.49	1.51
11	L	400	BCB	MG-NB	-2.14	2.01	2.05
13	L	503	UQ9	C1-C2	-2.13	1.40	1.47
5	C	403	HEC	CHB-C4A	2.12	1.42	1.38
5	C	402	HEC	CHD-C4C	2.11	1.42	1.38
16	M	600	NS5	C27-C26	2.11	1.55	1.50
5	C	401	HEC	CMB-C2B	2.09	1.55	1.50
5	C	402	HEC	CMB-C2B	2.09	1.55	1.50
11	L	401	BCB	CHA-CBD	-2.09	1.49	1.51
16	M	600	NS5	C7-C5	2.09	1.37	1.33
12	L	402	BPB	C3D-C4D	2.08	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	402	BPB	C3D-CAD	-2.06	1.43	1.47
5	C	402	HEC	O2D-CGD	-2.04	1.24	1.30
5	C	403	HEC	C1D-ND	-2.03	1.35	1.39
11	L	400	BCB	C1D-C2D	2.02	1.41	1.39
11	L	400	BCB	CMB-C2B	2.02	1.55	1.51
16	M	600	NS5	C35-C36	2.01	1.38	1.32
10	C	350	GOL	O3-C3	2.01	1.50	1.42

All (224) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	400	BCB	C1B-CHB-C4A	13.44	129.97	121.32
11	L	400	BCB	C4B-CHC-C1C	13.26	129.85	121.32
11	L	401	BCB	C4B-CHC-C1C	13.22	129.83	121.32
11	M	401	BCB	C4B-CHC-C1C	13.19	129.81	121.32
11	L	401	BCB	C1B-CHB-C4A	11.76	128.88	121.32
11	M	400	BCB	C4B-CHC-C1C	11.58	128.78	121.32
11	M	401	BCB	C1B-CHB-C4A	11.15	128.50	121.32
11	M	401	BCB	O2D-CGD-CBD	10.65	122.65	110.95
11	M	401	BCB	C4D-ND-C1D	9.91	112.74	105.22
5	C	401	HEC	CBB-CAB-C3B	-9.69	108.08	127.43
11	L	400	BCB	C4D-ND-C1D	9.21	112.21	105.22
11	L	401	BCB	C4D-ND-C1D	8.54	111.70	105.22
5	C	403	HEC	CBB-CAB-C3B	-8.37	110.70	127.43
12	L	402	BPB	C4D-CHA-CBD	-8.00	104.62	108.45
11	M	400	BCB	C1B-CHB-C4A	7.96	126.45	121.32
11	M	400	BCB	C4D-ND-C1D	7.77	111.11	105.22
5	C	402	HEC	CBB-CAB-C3B	-7.63	112.18	127.43
11	L	400	BCB	O2D-CGD-CBD	7.05	118.69	110.95
9	L	275	HTO	O2-C2-C3	-6.70	95.50	109.57
5	C	402	HEC	CBC-CAC-C3C	-6.56	114.32	127.43
16	M	600	NS5	C19-C20-C21	-6.39	118.32	127.28
5	C	404[A]	HEC	CBC-CAC-C3C	-6.08	115.28	127.43
5	C	404[B]	HEC	CBC-CAC-C3C	-6.08	115.28	127.43
9	M	332	HTO	O1-C1-C2	-6.08	98.39	111.16
11	M	401	BCB	O2D-CGD-O1D	-6.06	112.05	123.85
7	M	732	DGA	OG2-CB1-CB2	5.93	124.30	111.48
12	L	402	BPB	C2B-C1B-NB	-5.89	105.17	109.43
5	C	401	HEC	CBC-CAC-C3C	-5.82	115.81	127.43
9	M	332	HTO	C5-C4-C3	-5.78	104.64	114.11
16	M	600	NS5	C29-C30-C31	-5.75	119.61	127.69
5	C	404[A]	HEC	CBB-CAB-C3B	-5.66	116.12	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	404[B]	HEC	CBB-CAB-C3B	-5.66	116.12	127.43
16	M	600	NS5	C24-C25-C26	-5.61	119.41	127.28
12	M	402	BPB	C4A-C3A-C2A	-5.49	97.61	102.84
9	L	275	HTO	O3-C3-C2	-5.30	98.44	109.57
7	H	733	DGA	CG1-CG2-CG3	-5.20	99.80	111.80
12	M	402	BPB	C4D-CHA-CBD	-5.14	105.99	108.45
11	L	401	BCB	C4-C3-C5	4.91	123.74	115.23
7	C	730	DGA	OG2-CB1-CB2	4.84	121.95	111.48
9	C	348	HTO	C1-C2-C3	-4.69	103.45	113.00
7	L	731	DGA	OG2-CB1-CB2	4.69	121.63	111.48
16	M	600	NS5	C12-C13-C14	-4.68	109.65	123.20
9	L	275	HTO	C1-C2-C3	4.64	122.45	113.00
11	L	400	BCB	C1-C2-C3	-4.43	118.94	126.20
11	M	401	BCB	C3D-C4D-ND	-4.39	105.90	112.94
16	M	600	NS5	C11-C10-C9	4.31	122.71	115.23
9	H	268	HTO	C5-C4-C3	-4.23	107.18	114.11
7	H	733	DGA	OG2-CB1-CB2	4.21	120.60	111.48
9	M	332	HTO	O2-C2-C1	-4.21	99.45	109.03
11	M	400	BCB	O2D-CGD-CBD	4.14	115.49	110.95
7	C	730	DGA	CG2-OG2-CB1	-4.12	111.83	117.78
11	L	400	BCB	C3D-C4D-ND	-4.12	106.32	112.94
9	M	332	HTO	O3-C3-C4	-4.08	99.87	109.14
11	L	400	BCB	C3D-C4D-CHA	4.06	114.71	108.54
7	M	732	DGA	CB3-CB2-CB1	-4.01	99.01	113.69
12	L	402	BPB	C4A-C3A-C2A	-4.00	99.03	102.84
10	C	364	GOL	O3-C3-C2	-4.00	92.38	110.38
5	C	403	HEC	CBC-CAC-C3C	-3.99	119.46	127.43
13	L	502	UQ9	C1M-C1-C6	-3.97	117.92	124.45
11	L	401	BCB	C3D-C4D-ND	-3.95	106.60	112.94
11	M	400	BCB	C3D-C4D-ND	-3.91	106.67	112.94
13	L	503	UQ9	C10-C9-C11	3.88	120.70	116.13
12	M	402	BPB	O2D-CGD-CBD	3.78	115.10	110.95
11	M	401	BCB	C3D-C4D-CHA	3.78	114.28	108.54
11	L	401	BCB	CHA-C1A-C2A	-3.71	124.59	133.31
7	H	733	DGA	OG1-CG1-CG2	-3.66	97.84	108.40
5	C	403	HEC	CHC-C4B-NB	-3.60	120.53	124.45
12	M	402	BPB	CMB-C2B-C3B	3.59	131.86	124.68
14	M	501	MQ9	C25-C24-C26	3.59	121.46	115.23
7	L	731	DGA	OG2-CG2-CG3	3.57	121.01	108.30
11	M	400	BCB	C3D-C4D-CHA	3.56	113.96	108.54
11	M	401	BCB	CMB-C2B-C3B	3.55	131.77	124.68
13	L	502	UQ9	C35-C34-C36	3.53	121.36	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	501	MQ9	C35-C34-C36	3.52	121.33	115.23
14	M	501	MQ9	C40-C39-C38	-3.51	114.61	123.63
12	M	402	BPB	CMD-C2D-C3D	3.46	131.60	124.68
11	L	401	BCB	C3D-C4D-CHA	3.44	113.76	108.54
9	C	348	HTO	O3-C3-C2	-3.43	102.38	109.57
5	C	401	HEC	CHC-C4B-NB	-3.40	120.75	124.45
12	L	402	BPB	C4B-NB-C1B	3.39	113.75	108.82
12	L	402	BPB	OBD-CAD-CBD	-3.27	121.03	125.82
11	M	400	BCB	C4C-CHD-C1D	3.22	127.58	116.07
16	M	600	NS5	C14-C15-C17	-3.21	113.95	119.01
11	L	401	BCB	C4C-CHD-C1D	3.19	127.48	116.07
11	M	400	BCB	CHA-C1A-C2A	-3.19	125.82	133.31
5	C	404[A]	HEC	CHC-C4B-NB	-3.12	121.06	124.45
5	C	404[B]	HEC	CHC-C4B-NB	-3.12	121.06	124.45
13	L	502	UQ9	C30-C29-C31	3.10	120.61	115.23
14	M	501	MQ9	C5M-C5-C6	-3.09	119.37	124.45
11	L	400	BCB	C4C-CHD-C1D	3.09	127.11	116.07
5	C	404[A]	HEC	CMD-C2D-C1D	3.08	130.11	125.42
13	L	503	UQ9	C7-C6-C5	3.08	122.10	118.52
7	H	733	DGA	CG2-OG2-CB1	-3.07	110.44	117.80
7	M	732	DGA	OG1-CA1-CA2	3.07	121.19	111.83
9	H	266	HTO	C1-C2-C3	-3.07	106.76	113.00
11	M	400	BCB	C3D-CAD-CBD	3.06	111.64	107.61
7	L	731	DGA	CG2-OG2-CB1	-3.06	110.48	117.80
11	L	401	BCB	C5-C3-C2	-3.06	114.31	121.17
11	M	401	BCB	C4C-CHD-C1D	3.05	126.97	116.07
7	L	731	DGA	CG1-CG2-CG3	-3.04	104.77	111.80
16	M	600	NS5	C18-C19-C20	3.04	129.73	123.52
10	M	335	GOL	O2-C2-C3	-3.04	96.61	109.18
6	H	721	LDA	CM2-N1-C1	-3.00	103.93	110.23
11	L	401	BCB	O2D-CGD-CBD	2.98	114.22	110.95
11	L	401	BCB	C3D-CAD-CBD	2.95	111.49	107.61
13	L	502	UQ9	C1-C6-C5	-2.94	116.76	119.62
5	C	404[A]	HEC	CHD-C4C-NC	-2.93	121.26	124.45
5	C	403	HEC	CHD-C4C-NC	-2.93	121.26	124.45
13	L	502	UQ9	C10-C9-C11	2.87	120.21	115.23
9	H	266	HTO	O2-C2-C3	2.86	115.58	109.57
10	L	278	GOL	O2-C2-C1	-2.85	97.37	109.18
13	L	502	UQ9	C3M-O3-C3	2.84	126.47	116.47
7	C	730	DGA	OG1-CA1-CA2	2.82	120.44	111.83
12	M	402	BPB	C1-C2-C3	-2.77	121.66	126.20
9	M	332	HTO	C1-C2-C3	2.76	118.63	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	600	NS5	C16-C15-C17	2.76	127.29	122.82
13	L	503	UQ9	C7-C6-C1	-2.76	120.16	124.89
5	C	404[A]	HEC	O2D-CGD-CBD	2.75	122.70	114.00
6	L	720	LDA	CM2-N1-C1	2.75	116.01	110.23
5	C	401	HEC	CHD-C4C-NC	-2.75	121.46	124.45
9	L	275	HTO	O1-C1-C2	2.72	116.87	111.16
12	L	402	BPB	CMD-C2D-C3D	2.72	130.12	124.68
14	M	501	MQ9	C30-C29-C31	2.72	119.95	115.23
12	L	402	BPB	CMB-C2B-C3B	2.72	130.12	124.68
7	L	731	DGA	OG1-CA1-CA2	2.71	120.11	111.83
11	L	401	BCB	CMB-C2B-C3B	2.70	130.08	124.68
13	L	502	UQ9	C50-C49-C51	2.66	120.71	114.59
11	L	400	BCB	O2D-CGD-O1D	-2.65	118.69	123.85
9	L	274	HTO	C4-C3-C2	-2.65	107.36	113.73
11	L	400	BCB	CHA-C1A-C2A	-2.64	127.10	133.31
11	M	401	BCB	CED-O2D-CGD	2.62	121.87	115.92
11	M	401	BCB	OBD-CAD-CBD	-2.62	121.98	125.82
10	C	356	GOL	C3-C2-C1	2.62	121.40	111.80
7	M	732	DGA	OB1-CB1-CB2	-2.61	113.56	123.78
5	C	402	HEC	CAA-C2A-C1A	2.59	130.12	124.85
16	M	600	NS5	C24-C23-C21	-2.59	119.26	126.36
11	M	400	BCB	CMA-C3A-C4A	-2.59	109.04	114.61
11	L	400	BCB	C4-C3-C5	2.58	119.71	115.23
11	M	401	BCB	CMD-C2D-C3D	-2.58	119.52	124.68
11	L	400	BCB	C3D-CAD-CBD	2.58	111.00	107.61
5	C	404[B]	HEC	CHD-C4C-NC	-2.53	121.69	124.45
6	H	701	LDA	CM2-N1-C1	-2.53	104.91	110.23
6	L	720	LDA	CM1-N1-C1	-2.52	104.93	110.23
9	L	274	HTO	O2-C2-C1	-2.51	103.32	109.03
9	L	274	HTO	C1-C2-C3	2.50	118.10	113.00
5	C	404[A]	HEC	O1D-CGD-CBD	-2.50	115.15	123.09
11	M	400	BCB	O1D-CGD-CBD	-2.50	120.93	124.72
11	L	401	BCB	CHD-C4C-C3C	-2.50	122.58	130.04
5	C	403	HEC	CMC-C2C-C1C	2.47	129.18	125.42
11	L	400	BCB	CMB-C2B-C3B	2.47	129.61	124.68
5	C	402	HEC	CMA-C3A-C4A	2.44	129.03	124.73
16	M	600	NS5	C6-C5-C4	2.44	119.47	115.23
11	L	400	BCB	OBD-CAD-C3D	-2.42	124.12	127.89
5	C	401	HEC	O2A-CGA-CBA	2.40	121.60	114.00
11	M	400	BCB	CED-O2D-CGD	2.40	121.36	115.92
12	L	402	BPB	C3B-C4B-NB	-2.40	104.57	108.05
14	M	501	MQ9	C40-C39-C41	2.39	119.38	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	364	GOL	O2-C2-C3	-2.38	99.32	109.18
16	M	600	NS5	C25-C24-C23	-2.38	116.31	123.20
13	L	503	UQ9	C4M-O4-C4	-2.37	108.14	116.47
13	L	502	UQ9	C15-C14-C16	2.36	119.33	115.23
5	C	402	HEC	CAA-C2A-C3A	-2.36	123.45	127.87
7	H	733	DGA	OXT-CG3-CG2	-2.36	105.71	111.77
14	M	501	MQ9	C37-C38-C39	2.35	133.00	127.62
7	H	733	DGA	CG1-OG1-CA1	-2.34	108.55	117.12
11	L	400	BCB	CHD-C4C-C3C	-2.34	123.05	130.04
6	L	708	LDA	CM1-N1-C1	-2.33	105.34	110.23
13	L	502	UQ9	O3-C3-C2	2.33	124.49	116.64
5	C	404[A]	HEC	C1D-C2D-C3D	-2.33	104.15	106.82
11	M	401	BCB	C5-C3-C2	-2.33	115.95	121.17
5	C	402	HEC	CHD-C4C-NC	-2.32	121.93	124.45
7	L	731	DGA	CG1-OG1-CA1	-2.31	108.67	117.12
11	M	400	BCB	OBD-CAD-CBD	-2.31	122.44	125.82
13	L	502	UQ9	C25-C24-C26	2.30	119.23	115.23
14	M	501	MQ9	C7-C6-C5	-2.28	120.98	124.89
11	M	401	BCB	CHA-C1A-C2A	-2.27	127.97	133.31
12	M	402	BPB	C3B-C4B-NB	-2.27	104.75	108.05
5	C	403	HEC	O2D-CGD-O1D	-2.26	117.52	123.33
11	L	401	BCB	CMA-C3A-C4A	-2.26	109.74	114.61
10	M	338	GOL	O3-C3-C2	-2.25	100.25	110.38
13	L	502	UQ9	C4M-O4-C4	-2.25	108.58	116.47
9	H	268	HTO	C1-C2-C3	-2.24	108.44	113.00
13	L	503	UQ9	C1M-C1-C6	-2.24	120.77	124.45
11	M	400	BCB	C1-C2-C3	-2.24	122.53	126.20
16	M	600	NS5	C27-C26-C28	2.23	121.49	118.09
11	L	401	BCB	OBD-CAD-C3D	-2.23	124.42	127.89
13	L	502	UQ9	O2-C2-C3	-2.23	116.32	121.03
5	C	402	HEC	C3D-C4D-ND	2.22	112.62	110.15
5	C	404[B]	HEC	C3D-C4D-ND	2.18	112.58	110.15
10	M	335	GOL	O1-C1-C2	2.18	120.19	110.38
11	M	400	BCB	CHD-C4C-C3C	-2.18	123.53	130.04
11	M	400	BCB	O2A-CGA-CBA	2.18	118.47	111.83
10	C	350	GOL	O1-C1-C2	2.17	120.13	110.38
14	M	501	MQ9	C41-C39-C38	2.15	125.98	121.17
10	H	271	GOL	O2-C2-C3	-2.14	100.31	109.18
10	C	351	GOL	C3-C2-C1	-2.14	103.94	111.80
5	C	401	HEC	CMB-C2B-C3B	2.14	131.57	126.55
5	C	402	HEC	C2B-C1B-NB	2.13	113.56	110.14
5	C	401	HEC	CHB-C4A-NA	-2.13	122.14	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	600	NS5	C13-C12-C10	-2.12	124.70	127.69
5	C	403	HEC	C1C-CHC-C4B	2.12	131.21	124.66
9	L	274	HTO	O1-C1-C2	-2.12	106.70	111.16
7	H	733	DGA	OG1-CA1-CA2	2.12	118.30	111.83
5	C	402	HEC	CHC-C4B-NB	-2.12	122.15	124.45
5	C	401	HEC	CAA-C2A-C1A	2.11	129.14	124.85
8	H	261	SO4	O3-S-O1	2.10	120.54	109.56
9	H	268	HTO	O1-C1-C2	-2.10	106.75	111.16
5	C	402	HEC	C2D-C1D-ND	2.10	113.50	110.14
14	M	501	MQ9	C45-C44-C46	2.09	118.85	115.23
5	C	401	HEC	CHA-C1A-NA	-2.07	122.19	124.45
5	C	401	HEC	C2A-C1A-NA	2.07	112.32	110.32
5	C	401	HEC	CMA-C3A-C4A	2.07	128.38	124.73
5	C	403	HEC	O2D-CGD-CBD	2.06	120.52	114.00
7	H	733	DGA	CA3-CA2-CA1	-2.06	106.14	113.69
11	M	401	BCB	CGD-CBD-CAD	-2.05	104.22	110.85
13	L	502	UQ9	C35-C34-C33	-2.04	118.38	123.63
5	C	401	HEC	C1C-CHC-C4B	2.04	130.95	124.66
11	M	401	BCB	C11-C10-C8	-2.01	109.27	115.97
5	C	404[A]	HEC	C2C-C1C-NC	2.01	113.37	110.14
5	C	404[B]	HEC	C2C-C1C-NC	2.01	113.37	110.14
13	L	502	UQ9	C20-C19-C21	2.01	118.72	115.23
11	M	401	BCB	CHD-C4C-C3C	-2.01	124.04	130.04
7	C	730	DGA	OG2-CB1-OB1	-2.01	119.02	123.70
5	C	403	HEC	CMD-C2D-C1D	2.00	128.47	125.42

All (12) chirality outliers are listed below:

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

All (429) 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[A]	HEC	C2B-C3B-CAB-CBB
5	C	404[A]	HEC	C4B-C3B-CAB-CBB
5	C	404[A]	HEC	C2C-C3C-CAC-CBC
5	C	404[A]	HEC	C4C-C3C-CAC-CBC
5	C	404[B]	HEC	C2B-C3B-CAB-CBB
5	C	404[B]	HEC	C4B-C3B-CAB-CBB
5	C	404[B]	HEC	C2C-C3C-CAC-CBC
5	C	404[B]	HEC	C4C-C3C-CAC-CBC
6	C	712	LDA	C2-C1-N1-O1
6	C	712	LDA	C2-C1-N1-CM1
6	C	712	LDA	C2-C1-N1-CM2
6	C	712	LDA	N1-C1-C2-C3
6	C	722	LDA	C2-C1-N1-O1
6	C	722	LDA	C2-C1-N1-CM1
6	C	722	LDA	C2-C1-N1-CM2
6	C	722	LDA	N1-C1-C2-C3
6	H	707	LDA	C2-C1-N1-O1
6	H	707	LDA	C2-C1-N1-CM1
6	H	707	LDA	C2-C1-N1-CM2
6	H	718	LDA	N1-C1-C2-C3
6	H	721	LDA	C2-C1-N1-O1
6	H	721	LDA	C2-C1-N1-CM1
6	L	703	LDA	C2-C1-N1-CM1
6	L	703	LDA	C2-C1-N1-CM2
6	L	703	LDA	N1-C1-C2-C3
6	L	720	LDA	C2-C1-N1-O1
6	L	720	LDA	C2-C1-N1-CM1
6	L	720	LDA	C2-C1-N1-CM2
6	M	706	LDA	C2-C1-N1-O1
6	M	706	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
6	M	706	LDA	C2-C1-N1-CM2
6	M	715	LDA	C2-C1-N1-O1
6	M	715	LDA	C2-C1-N1-CM1
6	M	715	LDA	C2-C1-N1-CM2
7	C	730	DGA	OG1-CG1-CG2-OG2
7	C	730	DGA	CG1-CG2-OG2-CB1
7	H	733	DGA	CA2-CA1-OG1-CG1
7	H	733	DGA	OA1-CA1-OG1-CG1
7	L	731	DGA	CA2-CA1-OG1-CG1
7	L	731	DGA	OA1-CA1-OG1-CG1
7	M	732	DGA	CB2-CB1-OG2-CG2
7	M	732	DGA	OB1-CB1-OG2-CG2
9	C	348	HTO	C1-C2-C3-O3
9	C	348	HTO	C1-C2-C3-C4
9	C	348	HTO	O2-C2-C3-O3
9	C	348	HTO	O2-C2-C3-C4
9	C	349	HTO	C1-C2-C3-O3
9	C	349	HTO	C1-C2-C3-C4
9	C	349	HTO	O2-C2-C3-O3
9	C	349	HTO	O2-C2-C3-C4
9	C	349	HTO	C2-C3-C4-C5
9	C	349	HTO	O3-C3-C4-C5
9	H	266	HTO	C1-C2-C3-O3
9	H	266	HTO	C1-C2-C3-C4
9	H	266	HTO	O2-C2-C3-O3
9	H	266	HTO	O2-C2-C3-C4
9	H	268	HTO	C1-C2-C3-O3
9	H	268	HTO	O2-C2-C3-O3
9	H	268	HTO	O2-C2-C3-C4
9	L	275	HTO	O1-C1-C2-O2
9	L	275	HTO	O1-C1-C2-C3
9	L	275	HTO	C1-C2-C3-O3
9	L	275	HTO	O2-C2-C3-O3
9	L	275	HTO	O2-C2-C3-C4
9	M	332	HTO	O3-C3-C4-C5
10	C	351	GOL	C1-C2-C3-O3
10	C	352	GOL	C1-C2-C3-O3
10	C	353[A]	GOL	O1-C1-C2-C3
10	C	354	GOL	O1-C1-C2-C3
10	C	357	GOL	C1-C2-C3-O3
10	C	361	GOL	C1-C2-C3-O3
10	C	362	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
10	C	363	GOL	O1-C1-C2-C3
10	C	365	GOL	O1-C1-C2-C3
10	H	269	GOL	O1-C1-C2-C3
10	H	271	GOL	C1-C2-C3-O3
10	H	273	GOL	C1-C2-C3-O3
10	H	274	GOL	C1-C2-C3-O3
10	H	274	GOL	O2-C2-C3-O3
10	H	275	GOL	C1-C2-C3-O3
10	H	276	GOL	C1-C2-C3-O3
10	H	276	GOL	O2-C2-C3-O3
10	H	277	GOL	C1-C2-C3-O3
10	H	278	GOL	C1-C2-C3-O3
10	H	279	GOL	C1-C2-C3-O3
10	L	278	GOL	O1-C1-C2-C3
10	L	278	GOL	C1-C2-C3-O3
10	L	279	GOL	C1-C2-C3-O3
10	L	281	GOL	C1-C2-C3-O3
10	L	282	GOL	O1-C1-C2-C3
10	M	333	GOL	C1-C2-C3-O3
10	M	334	GOL	O1-C1-C2-C3
10	M	335	GOL	C1-C2-C3-O3
10	M	336	GOL	C1-C2-C3-O3
10	M	337	GOL	O1-C1-C2-O2
10	M	337	GOL	O1-C1-C2-C3
10	M	337	GOL	C1-C2-C3-O3
10	M	339	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
13	L	502	UQ9	C46-C47-C48-C49
13	L	502	UQ9	C31-C32-C33-C34
13	L	502	UQ9	C16-C17-C18-C19
13	L	503	UQ9	C12-C11-C9-C10
13	L	503	UQ9	C12-C11-C9-C8
7	M	732	DGA	OA1-CA1-OG1-CG1
7	M	732	DGA	CA2-CA1-OG1-CG1
13	L	502	UQ9	C30-C29-C31-C32
13	L	502	UQ9	C25-C24-C26-C27
13	L	502	UQ9	C28-C29-C31-C32
13	L	502	UQ9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
6	M	702	LDA	C1-C2-C3-C4
11	L	400	BCB	C4-C3-C5-C6
13	L	502	UQ9	C12-C11-C9-C10
11	L	400	BCB	C2-C3-C5-C6
13	L	502	UQ9	C38-C39-C41-C42
13	L	502	UQ9	C12-C11-C9-C8
13	L	502	UQ9	C44-C46-C47-C48
13	L	502	UQ9	C29-C31-C32-C33
5	C	404[B]	HEC	C3D-CAD-CBD-CGD
7	H	733	DGA	CA3-CA4-CA5-CA6
6	C	712	LDA	C3-C4-C5-C6
7	H	733	DGA	CA5-CA6-CA7-CA8
13	L	502	UQ9	C40-C39-C41-C42
11	M	400	BCB	C11-C10-C8-C9
11	M	400	BCB	C11-C12-C13-C14
12	M	402	BPB	C14-C13-C15-C16
6	L	703	LDA	C5-C6-C7-C8
7	L	731	DGA	CB7-CB8-CB9-CAB
6	M	704	LDA	C11-C10-C9-C8
11	L	400	BCB	C15-C16-C17-C18
10	C	353[B]	GOL	O1-C1-C2-O2
10	C	354	GOL	O1-C1-C2-O2
10	C	357	GOL	O2-C2-C3-O3
10	C	363	GOL	O1-C1-C2-O2
10	L	278	GOL	O1-C1-C2-O2
10	M	335	GOL	O2-C2-C3-O3
10	M	336	GOL	O2-C2-C3-O3
9	H	268	HTO	O1-C1-C2-C3
16	M	600	NS5	C2-C3-C4-C5
13	L	502	UQ9	C4-C3-O3-C3M
13	L	503	UQ9	C3-C4-O4-C4M
7	M	732	DGA	CA1-CA2-CA3-CA4
11	M	401	BCB	C2A-CAA-CBA-CGA
16	M	600	NS5	C1-C2-C3-C4
11	M	400	BCB	C8-C10-C11-C12
16	M	600	NS5	C13-C14-C15-C16
16	M	600	NS5	C22-C21-C23-C24
7	M	732	DGA	CB4-CB5-CB6-CB7
10	C	353[A]	GOL	C1-C2-C3-O3
10	C	353[B]	GOL	O1-C1-C2-C3
10	C	358	GOL	O1-C1-C2-C3
10	C	359	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	H	269	GOL	C1-C2-C3-O3
10	H	270	GOL	O1-C1-C2-C3
10	H	270	GOL	C1-C2-C3-O3
10	H	271	GOL	O1-C1-C2-C3
10	H	278	GOL	O1-C1-C2-C3
10	L	280	GOL	O1-C1-C2-C3
7	L	731	DGA	CG1-CG2-OG2-CB1
12	M	402	BPB	C5-C6-C7-C8
9	H	267	HTO	O1-C1-C2-O2
9	M	332	HTO	O1-C1-C2-O2
11	L	401	BCB	C16-C17-C18-C19
16	M	600	NS5	CM2-C1-C2-C3
6	L	703	LDA	C2-C3-C4-C5
7	C	730	DGA	CA6-CA7-CA8-CA9
6	M	704	LDA	C4-C5-C6-C7
6	H	719	LDA	C2-C3-C4-C5
10	C	351	GOL	O2-C2-C3-O3
10	C	353[A]	GOL	O1-C1-C2-O2
10	C	362	GOL	O2-C2-C3-O3
10	C	365	GOL	O1-C1-C2-O2
10	H	269	GOL	O1-C1-C2-O2
10	H	270	GOL	O1-C1-C2-O2
10	H	270	GOL	O2-C2-C3-O3
10	H	271	GOL	O1-C1-C2-O2
10	H	275	GOL	O2-C2-C3-O3
10	H	277	GOL	O2-C2-C3-O3
10	H	278	GOL	O2-C2-C3-O3
10	H	279	GOL	O2-C2-C3-O3
10	L	279	GOL	O2-C2-C3-O3
10	L	281	GOL	O2-C2-C3-O3
10	L	282	GOL	O1-C1-C2-O2
10	M	339	GOL	O2-C2-C3-O3
16	M	600	NS5	CM1-C1-C2-C3
7	M	732	DGA	CB3-CB4-CB5-CB6
11	M	400	BCB	C13-C15-C16-C17
11	M	400	BCB	C15-C16-C17-C18
7	C	730	DGA	CA5-CA6-CA7-CA8
7	H	733	DGA	CB6-CB7-CB8-CB9
6	H	721	LDA	C3-C4-C5-C6
6	M	702	LDA	C5-C6-C7-C8
7	H	733	DGA	CA2-CA3-CA4-CA5
6	M	705	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	M	715	LDA	C2-C3-C4-C5
6	L	703	LDA	C6-C7-C8-C9
6	H	721	LDA	C2-C3-C4-C5
7	M	732	DGA	CB6-CB7-CB8-CB9
6	C	712	LDA	C5-C6-C7-C8
6	M	702	LDA	C6-C7-C8-C9
11	L	401	BCB	C16-C17-C18-C20
6	C	712	LDA	C6-C7-C8-C9
7	M	732	DGA	CB5-CB6-CB7-CB8
7	C	730	DGA	CA7-CA8-CA9-CAA
7	H	733	DGA	CBB-CAB-CB9-CB8
6	M	704	LDA	C2-C3-C4-C5
7	C	730	DGA	CB2-CB1-OG2-CG2
7	L	731	DGA	CA1-CA2-CA3-CA4
9	C	348	HTO	O3-C3-C4-C5
7	C	730	DGA	OB1-CB1-OG2-CG2
6	M	705	LDA	C4-C5-C6-C7
6	M	705	LDA	C11-C10-C9-C8
7	H	733	DGA	CB2-CB3-CB4-CB5
6	H	719	LDA	C1-C2-C3-C4
6	H	718	LDA	C6-C7-C8-C9
9	H	268	HTO	C4-C5-C6-C7
7	M	732	DGA	CBB-CAB-CB9-CB8
6	H	721	LDA	C4-C5-C6-C7
13	L	503	UQ9	C5-C4-O4-C4M
6	H	701	LDA	C4-C5-C6-C7
6	M	706	LDA	C6-C7-C8-C9
6	H	718	LDA	C1-C2-C3-C4
7	C	730	DGA	CBB-CAB-CB9-CB8
6	M	706	LDA	C3-C4-C5-C6
7	L	731	DGA	CA3-CA4-CA5-CA6
6	L	709	LDA	C3-C4-C5-C6
6	H	707	LDA	C3-C4-C5-C6
7	C	730	DGA	CB7-CB8-CB9-CAB
10	C	352	GOL	O2-C2-C3-O3
10	C	361	GOL	O2-C2-C3-O3
10	H	269	GOL	O2-C2-C3-O3
10	H	271	GOL	O2-C2-C3-O3
10	H	273	GOL	O2-C2-C3-O3
10	M	334	GOL	O1-C1-C2-O2
10	M	337	GOL	O2-C2-C3-O3
7	H	733	DGA	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
7	C	730	DGA	CA8-CA9-CAA-CBA
9	C	348	HTO	C2-C3-C4-C5
9	H	266	HTO	C2-C3-C4-C5
9	M	332	HTO	C2-C3-C4-C5
13	L	502	UQ9	C45-C44-C46-C47
13	L	502	UQ9	C43-C44-C46-C47
6	M	702	LDA	C7-C8-C9-C10
12	M	402	BPB	C15-C16-C17-C18
13	L	502	UQ9	C2-C3-O3-C3M
6	L	720	LDA	C6-C7-C8-C9
7	H	733	DGA	CB5-CB6-CB7-CB8
7	M	732	DGA	CA3-CA4-CA5-CA6
10	H	277	GOL	O1-C1-C2-C3
6	L	709	LDA	C7-C8-C9-C10
7	C	730	DGA	CB4-CB5-CB6-CB7
7	C	730	DGA	CB9-CAB-CBB-CCB
6	C	722	LDA	C1-C2-C3-C4
9	H	267	HTO	C4-C5-C6-C7
7	L	731	DGA	OG1-CG1-CG2-OG2
7	M	732	DGA	OG1-CG1-CG2-OG2
6	M	702	LDA	C9-C10-C11-C12
6	H	718	LDA	C3-C4-C5-C6
7	L	731	DGA	CA5-CA6-CA7-CA8
7	C	730	DGA	CA9-CAA-CBA-CCA
11	M	400	BCB	C4-C3-C5-C6
6	C	722	LDA	C11-C10-C9-C8
10	C	355	GOL	O1-C1-C2-O2
10	C	358	GOL	O1-C1-C2-O2
10	L	280	GOL	O2-C2-C3-O3
10	M	333	GOL	O2-C2-C3-O3
6	C	712	LDA	C2-C3-C4-C5
6	H	718	LDA	C2-C3-C4-C5
6	H	719	LDA	C3-C4-C5-C6
7	H	733	DGA	OG2-CB1-CB2-CB3
11	M	400	BCB	C11-C10-C8-C7
7	H	733	DGA	CAB-CBB-CCB-CDB
6	C	722	LDA	C6-C7-C8-C9
6	M	706	LDA	C5-C6-C7-C8
9	H	266	HTO	O3-C3-C4-C5
7	C	730	DGA	OG1-CG1-CG2-CG3
9	L	275	HTO	C1-C2-C3-C4
9	M	332	HTO	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	C	722	LDA	C2-C3-C4-C5
12	L	402	BPB	C8-C10-C11-C12
11	M	400	BCB	C2-C3-C5-C6
6	H	719	LDA	C11-C10-C9-C8
6	M	715	LDA	C6-C7-C8-C9
9	H	268	HTO	C2-C3-C4-C5
6	M	702	LDA	C3-C4-C5-C6
7	L	731	DGA	CB9-CAB-CBB-CCB
7	M	732	DGA	CAB-CBB-CCB-CDB
6	M	706	LDA	C2-C3-C4-C5
7	C	730	DGA	CBB-CCB-CDB-CEB
13	L	502	UQ9	C34-C36-C37-C38
7	C	730	DGA	CA2-CA3-CA4-CA5
9	M	332	HTO	C4-C5-C6-C7
7	H	733	DGA	CB1-CB2-CB3-CB4
10	C	353[B]	GOL	O2-C2-C3-O3
10	C	361	GOL	O1-C1-C2-O2
6	L	709	LDA	C1-C2-C3-C4
9	H	267	HTO	O3-C3-C4-C5
9	H	268	HTO	O3-C3-C4-C5
7	H	733	DGA	CA1-CA2-CA3-CA4
6	H	707	LDA	C6-C7-C8-C9
12	L	402	BPB	O2A-C1-C2-C3
6	H	701	LDA	C7-C8-C9-C10
11	L	400	BCB	C16-C17-C18-C20
6	M	715	LDA	C5-C6-C7-C8
7	M	732	DGA	CB9-CAB-CBB-CCB
7	C	730	DGA	CA1-CA2-CA3-CA4
6	M	702	LDA	C2-C1-N1-CM1
6	M	702	LDA	C2-C1-N1-CM2
9	M	332	HTO	C1-C2-C3-O3
9	H	268	HTO	O1-C1-C2-O2
10	C	359	GOL	O1-C1-C2-O2
10	H	278	GOL	O1-C1-C2-O2
10	L	281	GOL	O1-C1-C2-O2
11	L	401	BCB	C12-C13-C15-C16
11	M	400	BCB	C11-C12-C13-C15
6	H	721	LDA	C11-C10-C9-C8
16	M	600	NS5	C17-C18-C19-C20
7	H	733	DGA	OG1-CG1-CG2-OG2
7	L	731	DGA	CB6-CB7-CB8-CB9
7	H	733	DGA	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
7	L	731	DGA	OG1-CG1-CG2-CG3
6	M	705	LDA	C7-C8-C9-C10
11	L	400	BCB	CAD-CBD-CGD-O2D
9	M	332	HTO	O1-C1-C2-C3
11	L	400	BCB	CAD-CBD-CGD-O1D
5	C	404[B]	HEC	C4D-C3D-CAD-CBD
5	C	402	HEC	C3D-CAD-CBD-CGD
6	L	709	LDA	C2-C3-C4-C5
6	L	703	LDA	C4-C5-C6-C7
10	L	276	GOL	O1-C1-C2-C3
9	C	349	HTO	C3-C4-C5-C6
11	L	401	BCB	C14-C13-C15-C16
6	C	722	LDA	C5-C6-C7-C8
6	H	701	LDA	C9-C10-C11-C12
7	C	730	DGA	CEB-CFB-CGB-CHB
7	M	732	DGA	CB7-CB8-CB9-CAB
13	L	502	UQ9	C35-C34-C36-C37
6	M	702	LDA	C4-C5-C6-C7
6	M	704	LDA	C7-C8-C9-C10
12	M	402	BPB	C4-C3-C5-C6
6	C	712	LDA	C9-C10-C11-C12
6	M	715	LDA	C7-C8-C9-C10
6	M	705	LDA	C3-C4-C5-C6
11	M	401	BCB	C11-C12-C13-C15
12	M	402	BPB	C12-C13-C15-C16
6	H	718	LDA	C5-C6-C7-C8
6	M	715	LDA	C1-C2-C3-C4
6	H	701	LDA	C3-C4-C5-C6
5	C	401	HEC	CAA-CBA-CGA-O1A
14	M	501	MQ9	C35-C34-C36-C37
6	H	707	LDA	C5-C6-C7-C8
11	M	400	BCB	C5-C6-C7-C8
13	L	503	UQ9	C2-C3-O3-C3M
6	H	721	LDA	C7-C8-C9-C10
7	H	733	DGA	OB1-CB1-CB2-CB3
5	C	402	HEC	CAA-CBA-CGA-O1A
11	M	401	BCB	C16-C17-C18-C19
6	M	715	LDA	C11-C10-C9-C8
7	H	733	DGA	CG1-CG2-OG2-CB1
7	H	733	DGA	CB9-CAB-CBB-CCB
12	M	402	BPB	C2-C3-C5-C6
14	M	501	MQ9	C33-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
10	C	353[A]	GOL	O2-C2-C3-O3
10	C	360	GOL	O2-C2-C3-O3
10	L	280	GOL	O1-C1-C2-O2
5	C	402	HEC	CAA-CBA-CGA-O2A
6	H	719	LDA	C5-C6-C7-C8
9	L	275	HTO	C4-C5-C6-C7
5	C	401	HEC	CAA-CBA-CGA-O2A
5	C	404[B]	HEC	CAD-CBD-CGD-O1D
13	L	502	UQ9	C33-C34-C36-C37
11	M	400	BCB	C6-C7-C8-C10
13	L	502	UQ9	C5-C4-O4-C4M
9	H	267	HTO	C2-C3-C4-C5
16	M	600	NS5	C20-C21-C23-C24
6	H	701	LDA	C6-C7-C8-C9
11	M	401	BCB	C11-C12-C13-C14
13	L	502	UQ9	C15-C14-C16-C17
5	C	404[B]	HEC	CAD-CBD-CGD-O2D
6	H	721	LDA	C5-C6-C7-C8
13	L	502	UQ9	C13-C14-C16-C17
11	L	401	BCB	CHA-CBD-CGD-O1D
11	M	400	BCB	CHA-CBD-CGD-O1D
7	C	730	DGA	CB3-CB4-CB5-CB6
12	M	402	BPB	C11-C12-C13-C14
5	C	402	HEC	CAD-CBD-CGD-O2D
6	M	704	LDA	C1-C2-C3-C4
10	C	353[B]	GOL	C1-C2-C3-O3
12	M	402	BPB	O2A-C1-C2-C3
7	M	732	DGA	OG1-CG1-CG2-CG3
13	L	502	UQ9	C39-C41-C42-C43
10	C	364	GOL	O1-C1-C2-O2
10	L	278	GOL	O2-C2-C3-O3
10	M	338	GOL	O2-C2-C3-O3
5	C	402	HEC	CAD-CBD-CGD-O1D
12	M	402	BPB	C11-C12-C13-C15
16	M	600	NS5	C7-C8-C9-C10
6	L	708	LDA	C2-C1-N1-CM2
11	L	401	BCB	C2C-C3C-CAC-CBC
6	M	704	LDA	C6-C7-C8-C9
16	M	600	NS5	C3-C4-C5-C6
7	L	731	DGA	CA9-CAA-CBA-CCA
10	L	276	GOL	O1-C1-C2-O2
9	H	266	HTO	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
13	L	503	UQ9	C4-C3-O3-C3M
9	C	348	HTO	C3-C4-C5-C6
6	L	720	LDA	C5-C6-C7-C8
6	M	702	LDA	C2-C1-N1-O1
10	H	277	GOL	O1-C1-C2-O2
6	L	720	LDA	C7-C8-C9-C10
5	C	404[B]	HEC	C2D-C3D-CAD-CBD
9	H	267	HTO	O1-C1-C2-C3
11	M	401	BCB	C15-C16-C17-C18

There are no ring outliers.

35 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	HEC	1	0
6	H	718	LDA	1	0
6	H	701	LDA	4	0
9	H	268	HTO	1	0
13	L	502	UQ9	8	0
10	H	270	GOL	1	0
11	M	401	BCB	2	0
10	C	358	GOL	1	0
11	L	401	BCB	4	0
6	M	704	LDA	1	0
6	H	719	LDA	1	0
10	L	279	GOL	5	0
12	M	402	BPB	3	0
11	M	400	BCB	9	0
6	L	720	LDA	5	0
10	C	354	GOL	1	0
10	L	276	GOL	3	0
9	C	349	HTO	4	0
9	H	267	HTO	1	0
10	C	352	GOL	1	0
6	M	702	LDA	6	0
10	H	274	GOL	2	0
7	M	732	DGA	2	0
8	H	262[B]	SO4	1	0
10	M	333	GOL	1	0
7	C	730	DGA	1	0
6	C	722	LDA	2	0
11	L	400	BCB	3	0

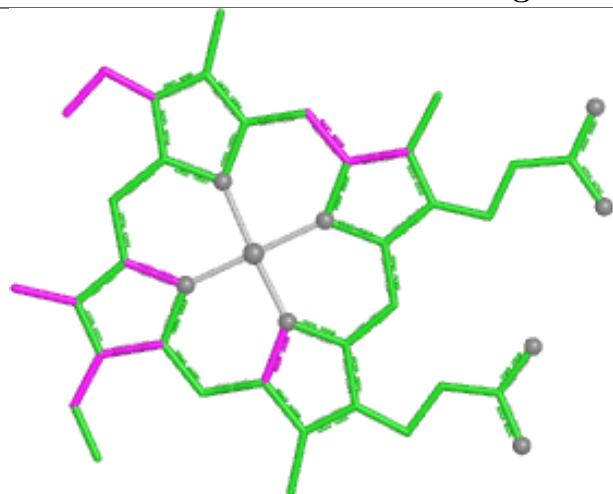
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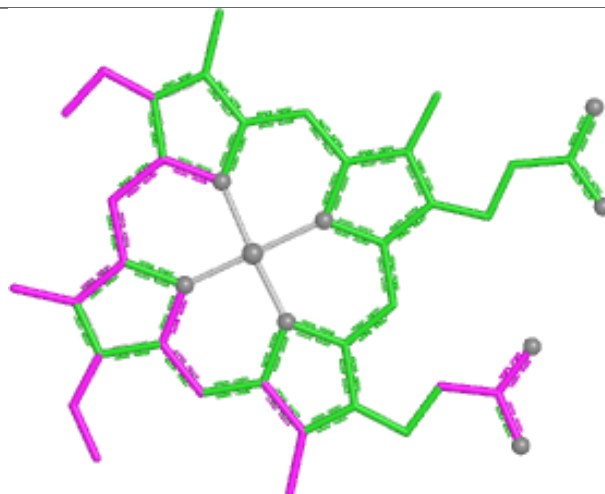
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	344	SO4	2	0
7	L	731	DGA	2	0
7	H	733	DGA	2	0
10	C	353[B]	GOL	1	0
6	H	721	LDA	5	0
16	M	600	NS5	3	0
12	L	402	BPB	2	0

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.

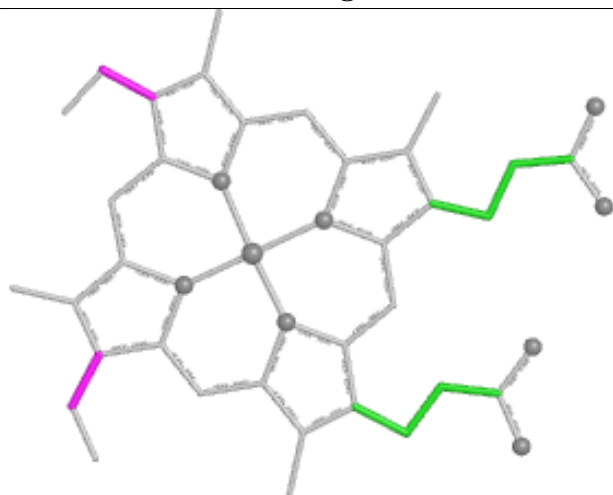
Ligand HEC C 403



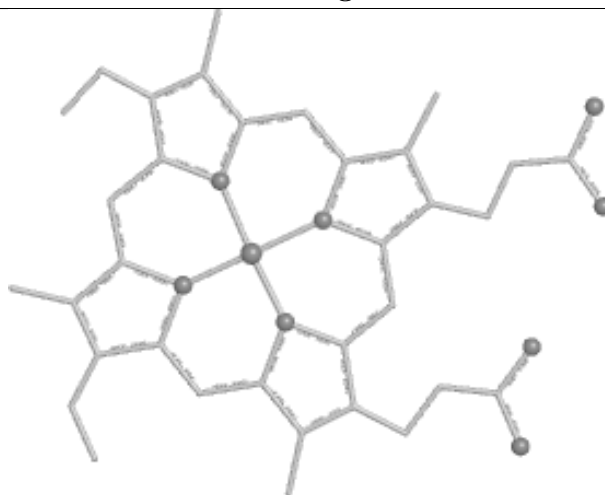
Bond lengths



Bond angles

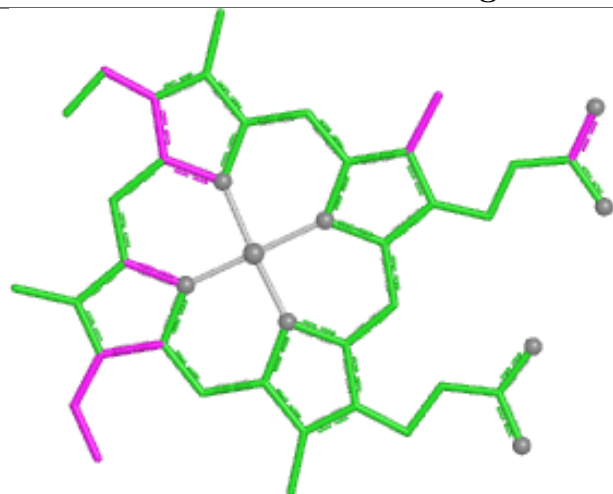


Torsions

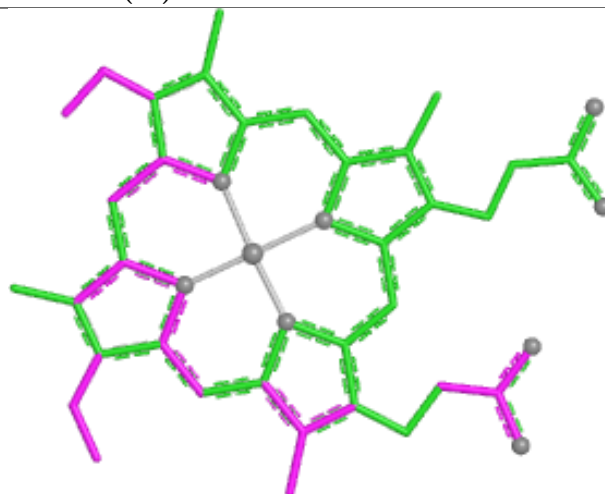


Rings

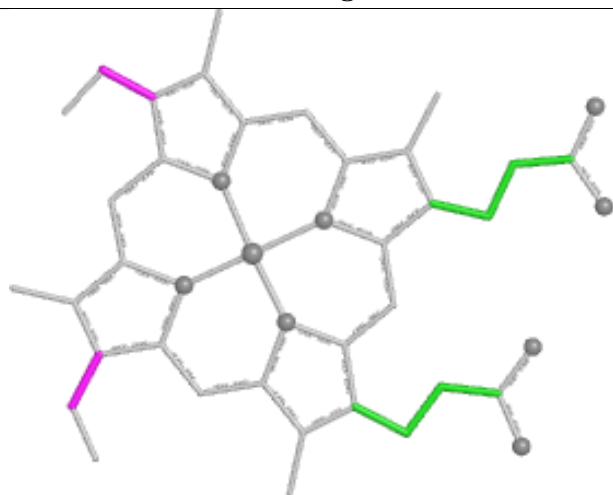
Ligand HEC C 404 (A)



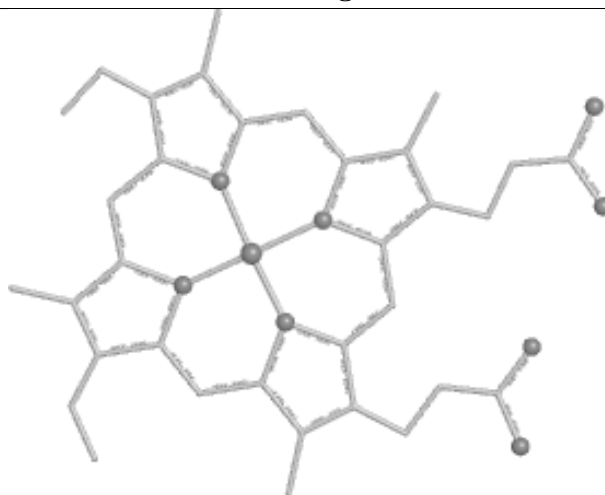
Bond lengths



Bond angles

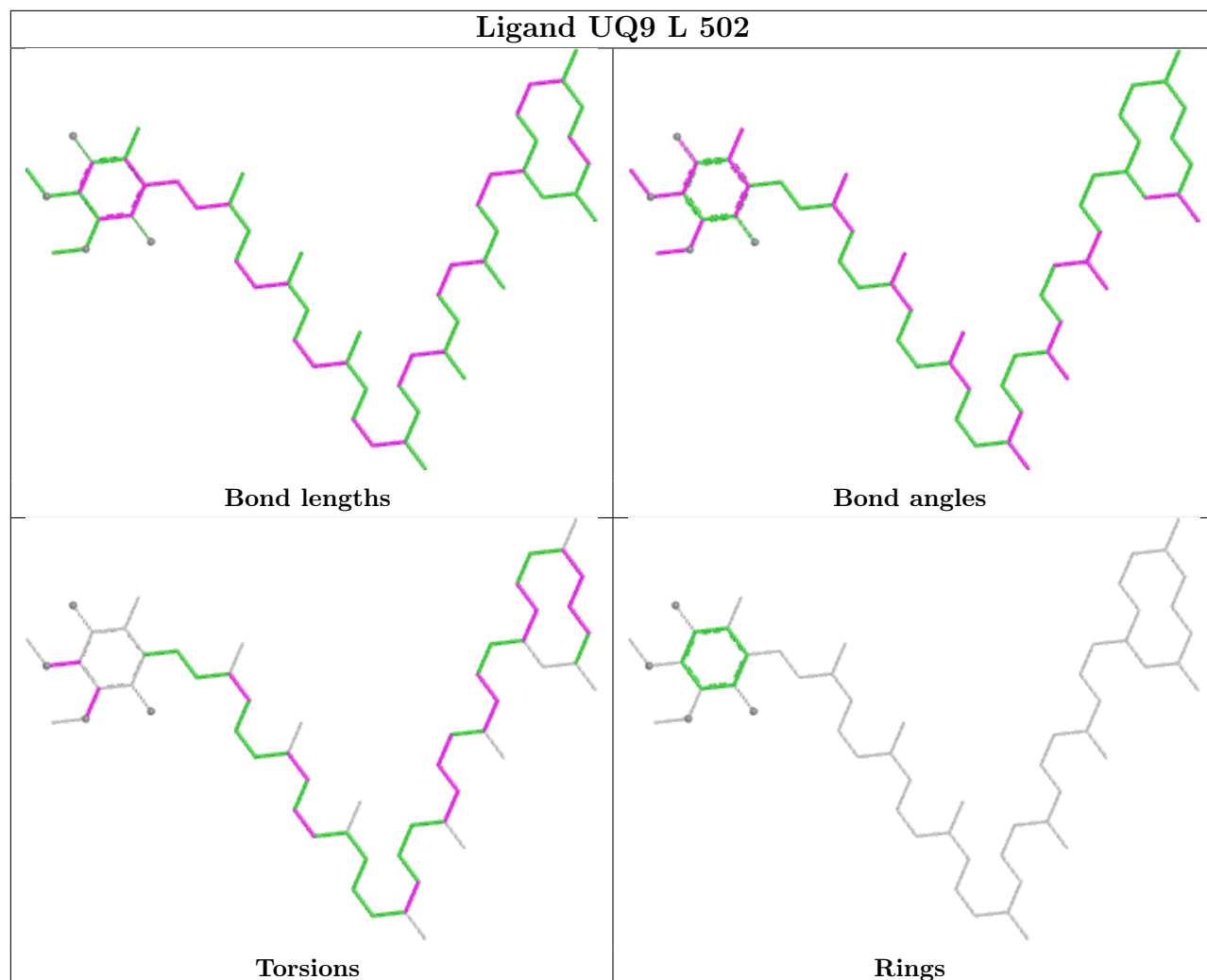


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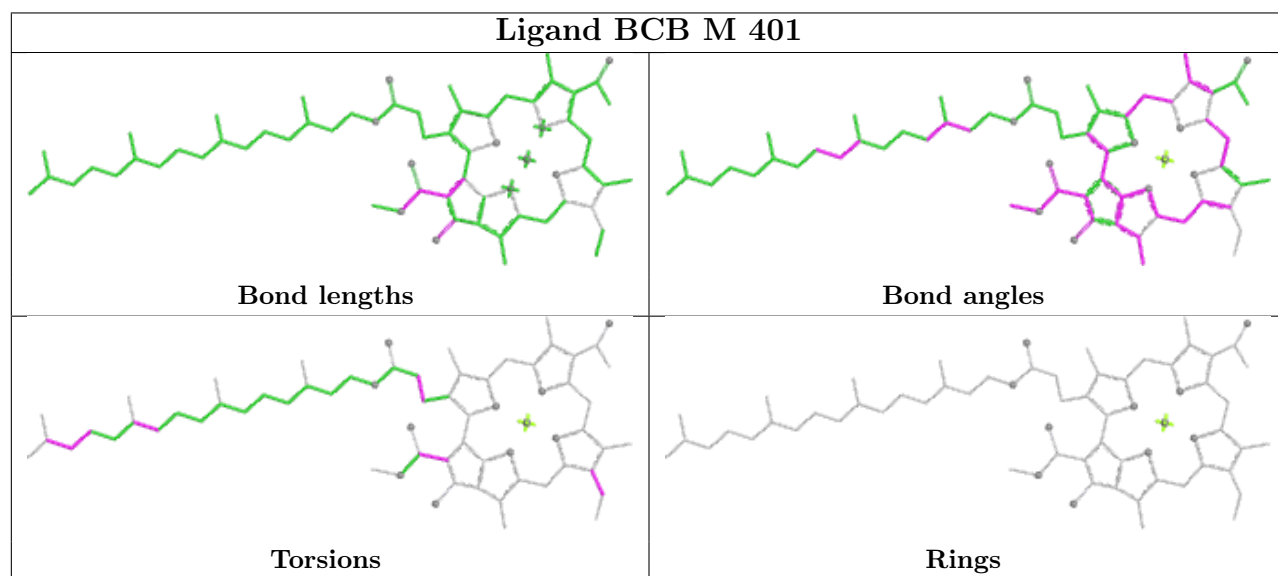


Rings

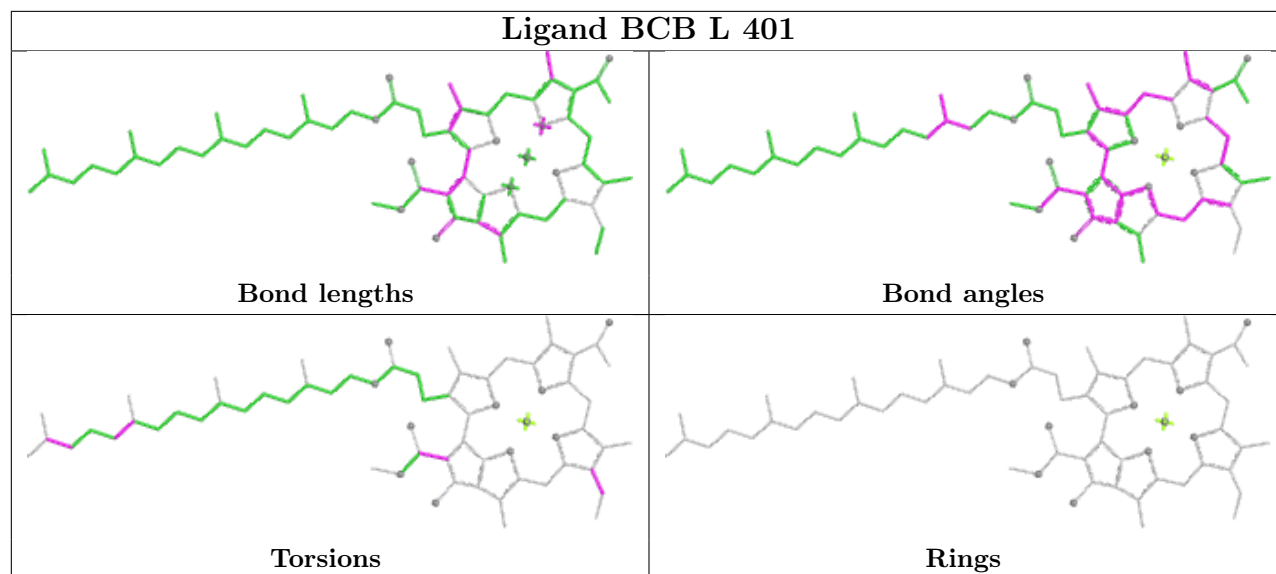
Ligand UQ9 L 502



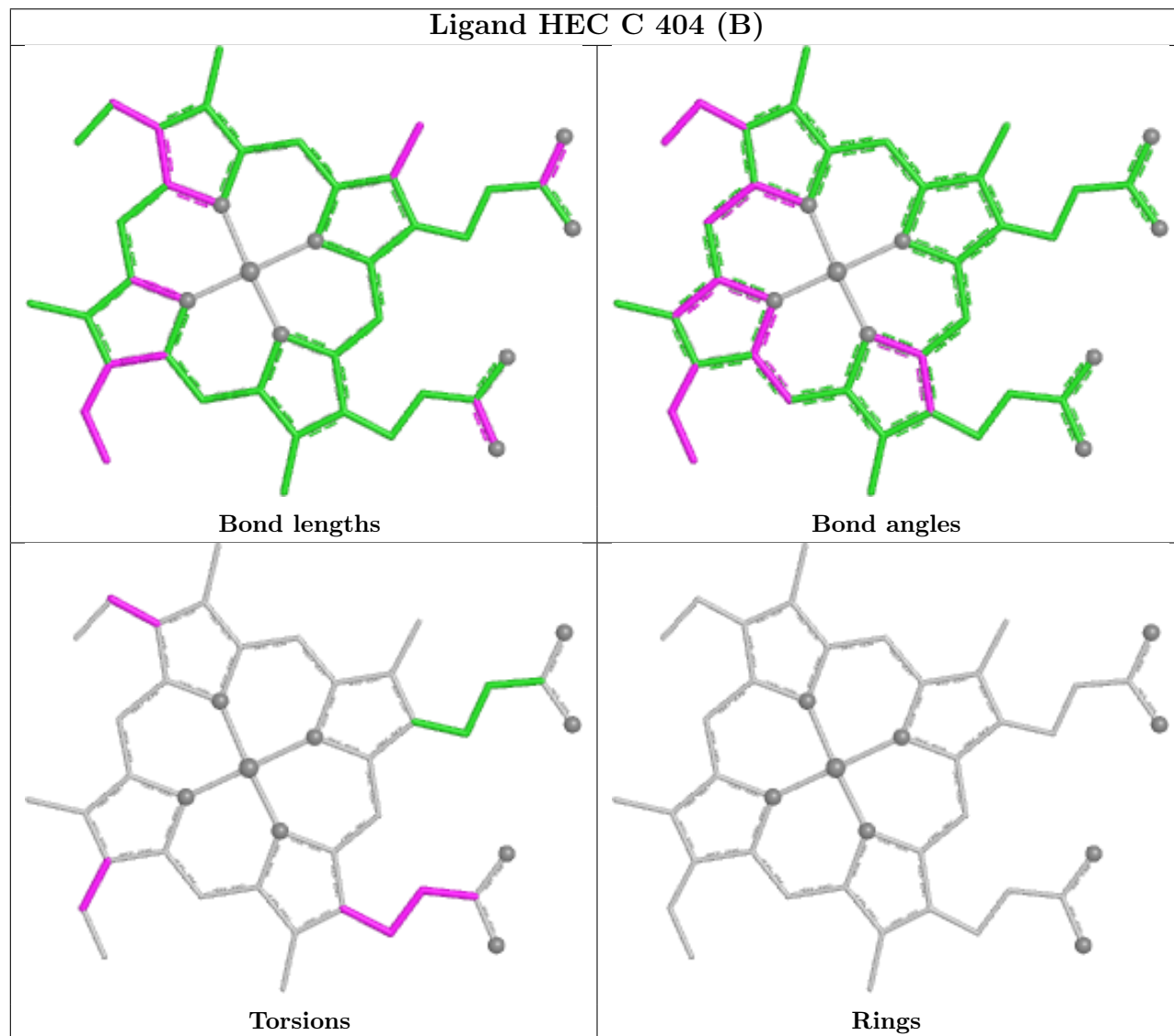
Ligand BCB M 401

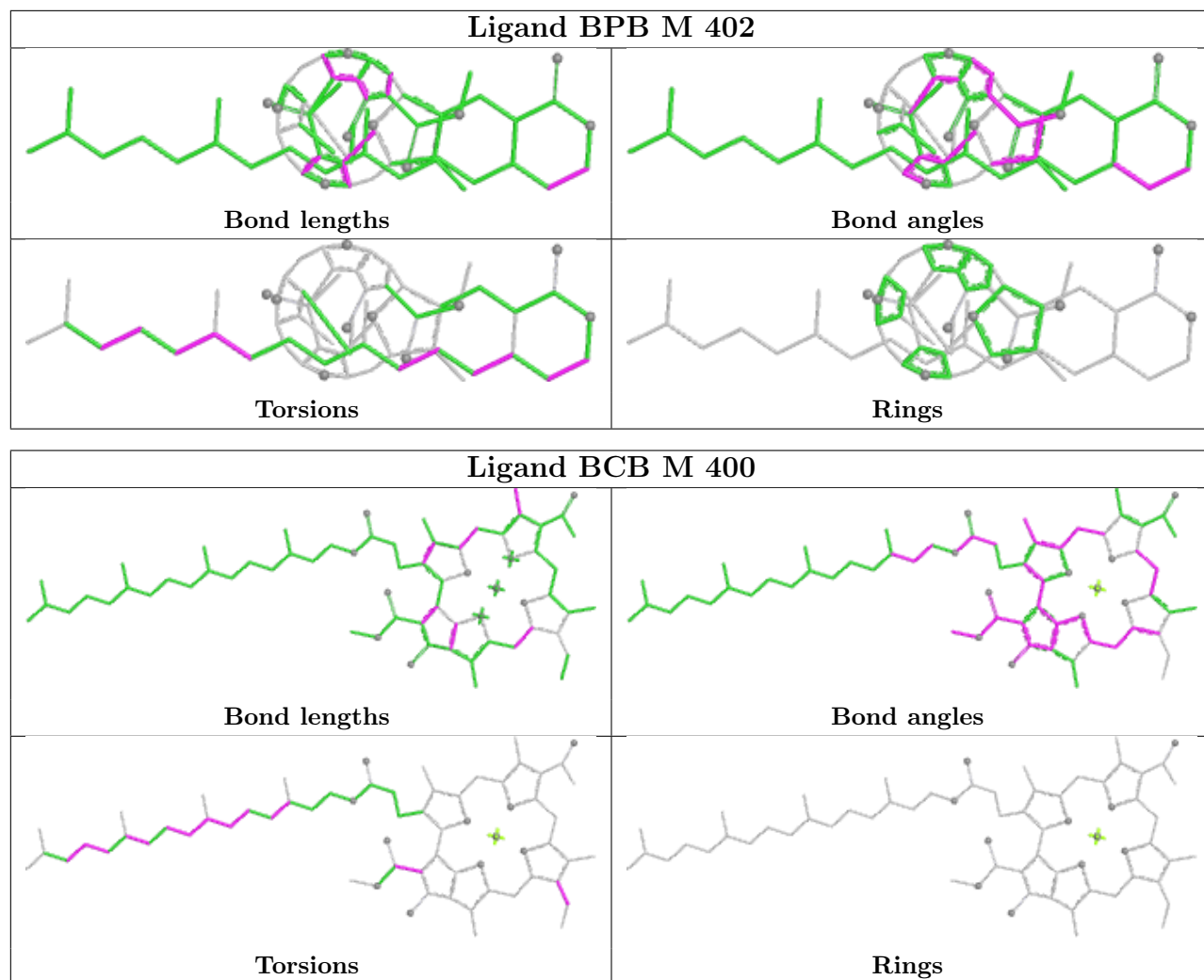


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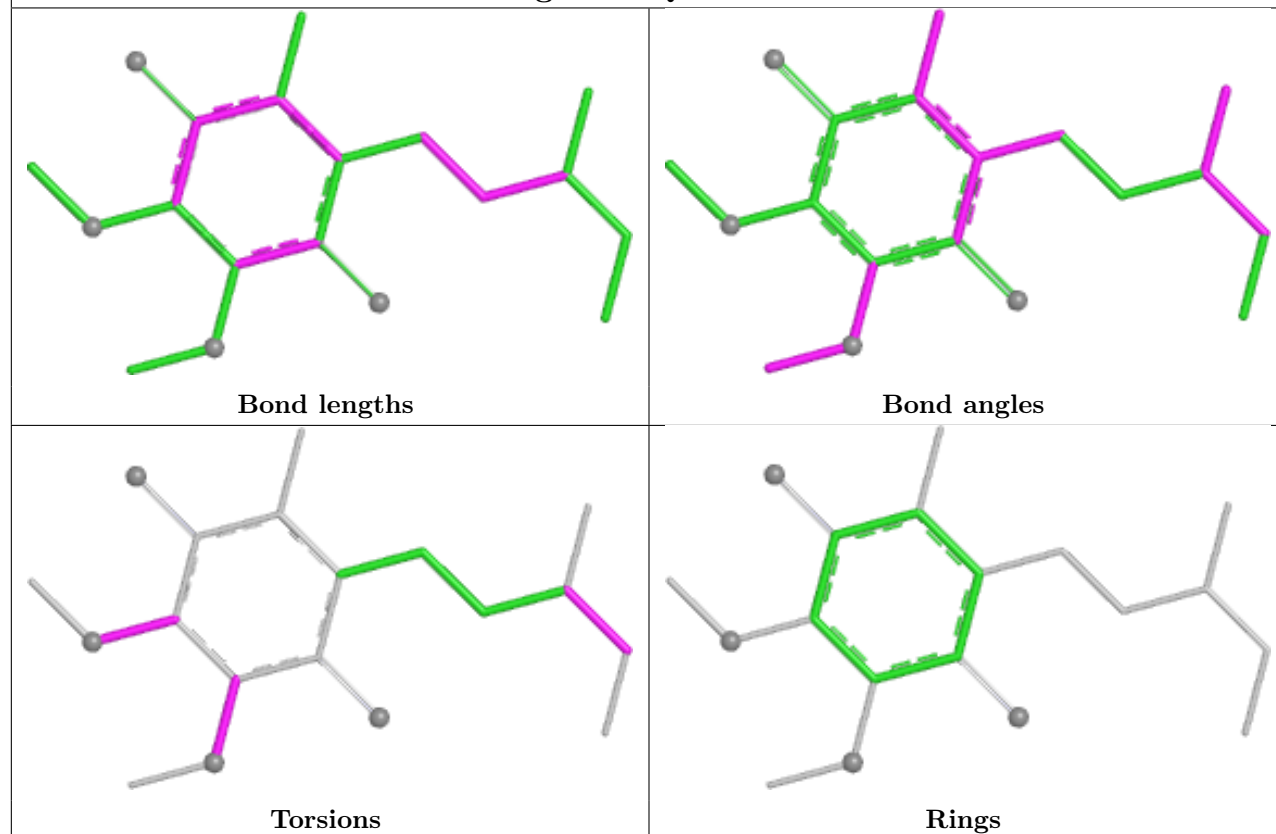


Ligand HEC C 404 (B)

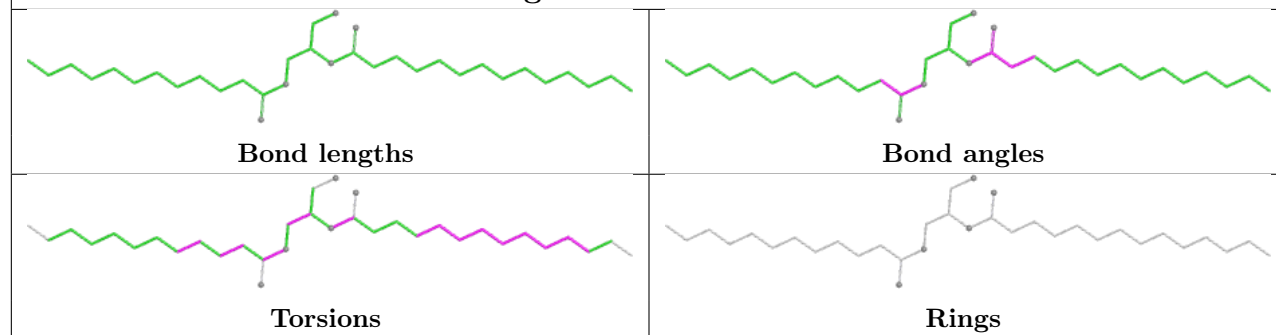




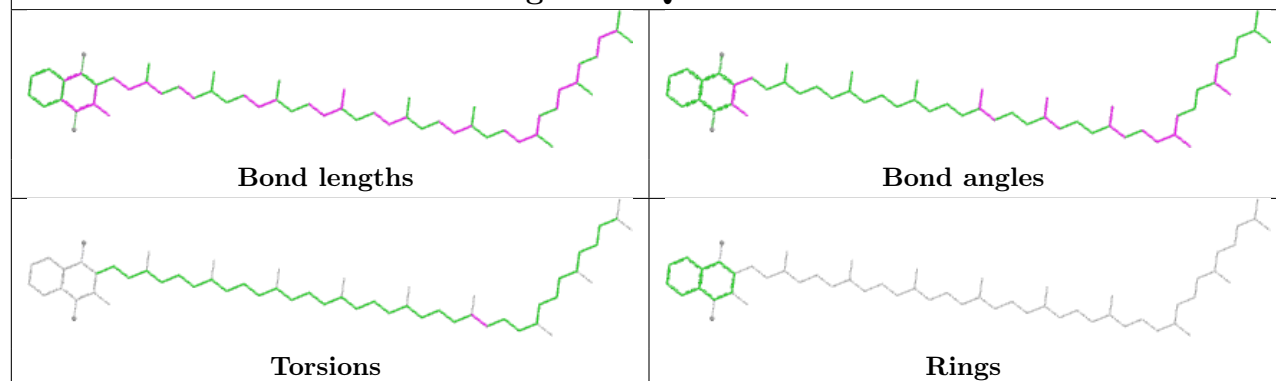
Ligand UQ9 L 503

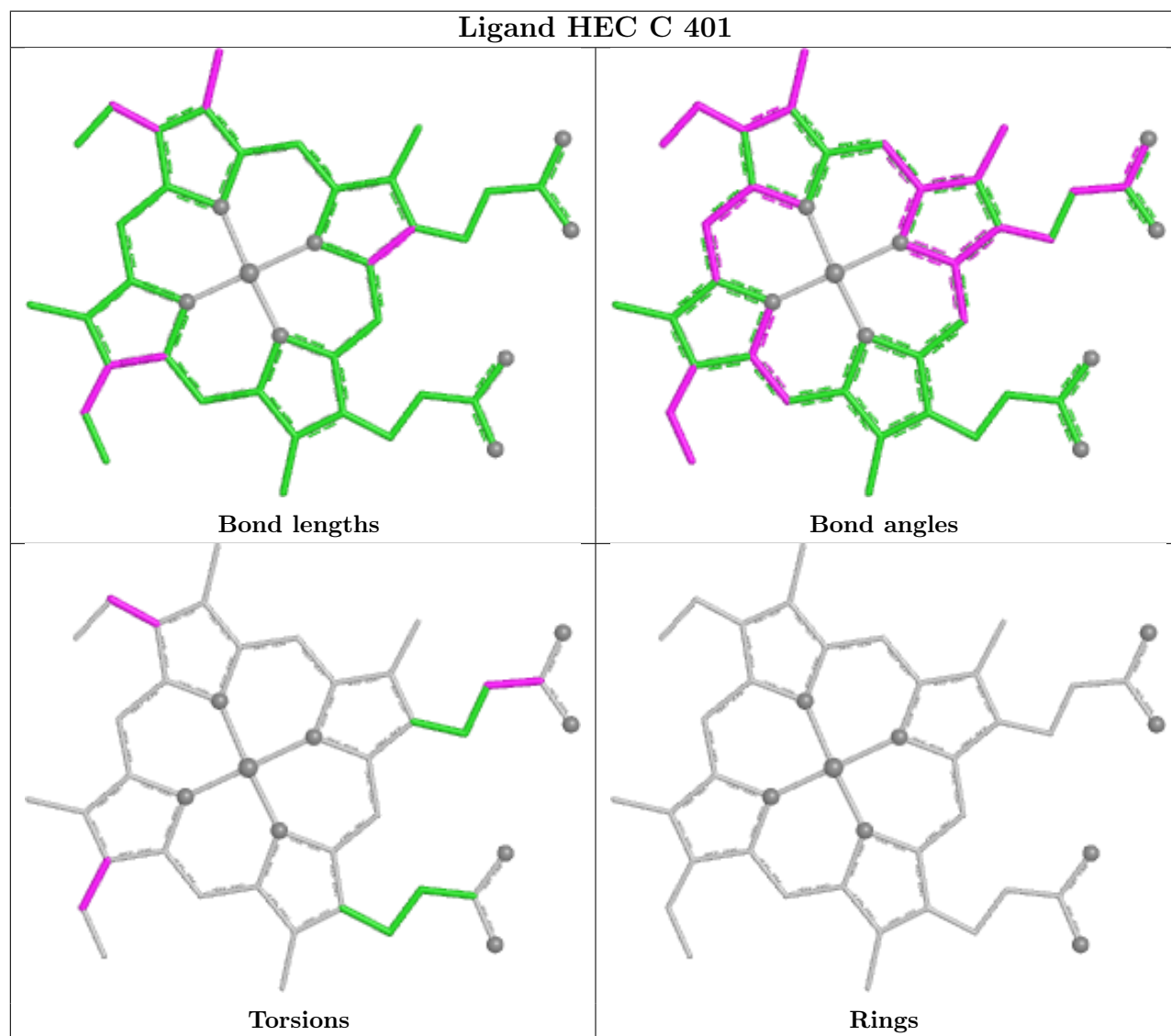
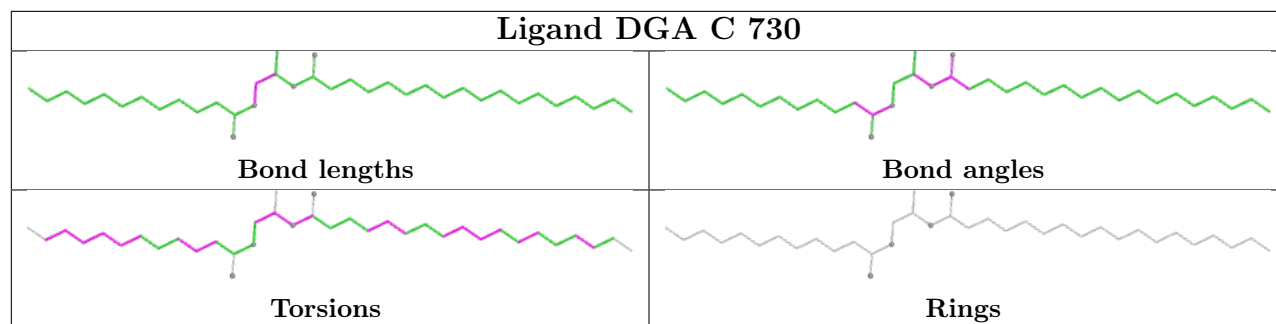


Ligand DGA M 732

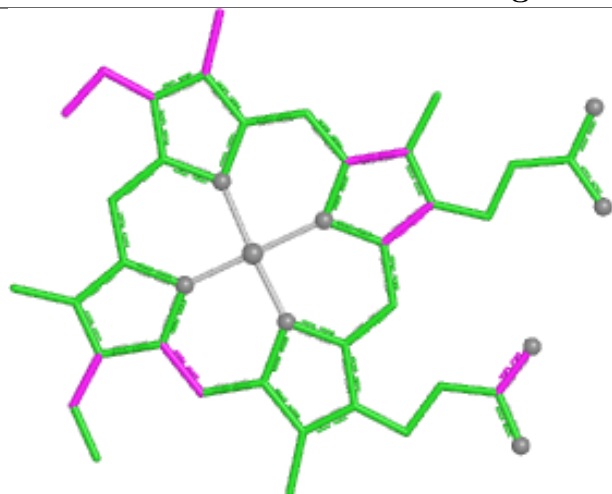


Ligand MQ9 M 501

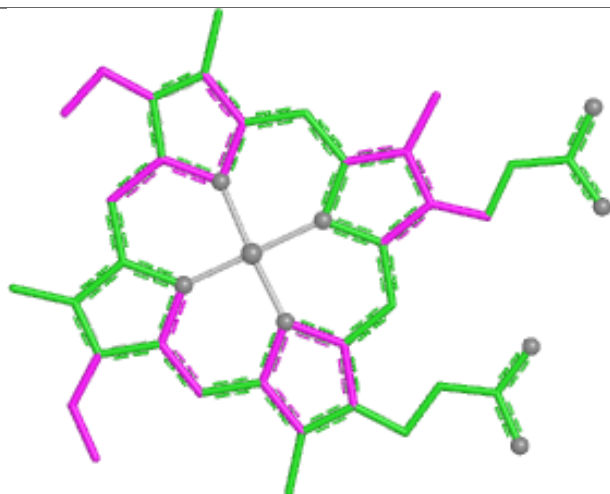




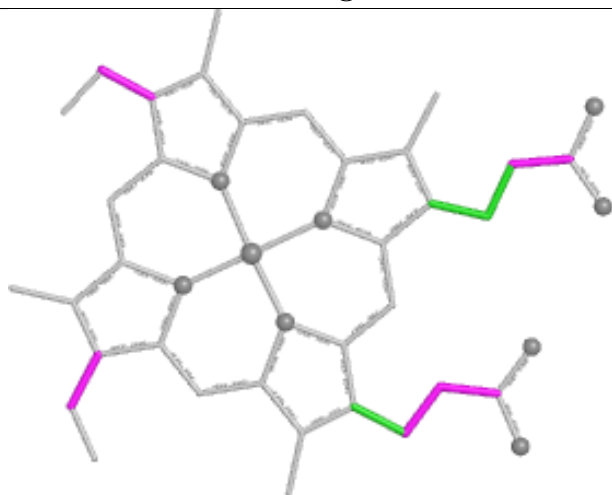
Ligand HEC C 402



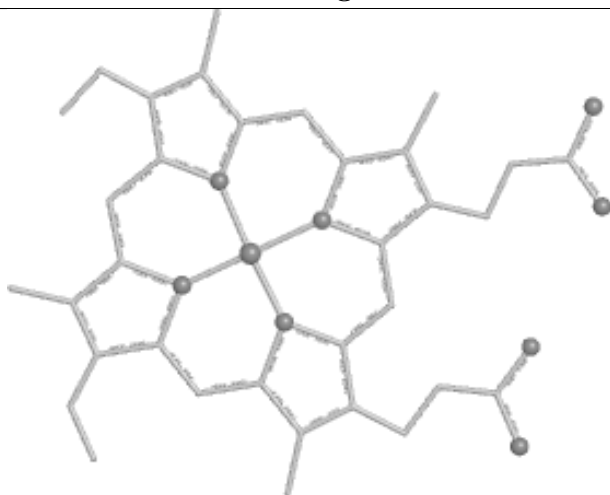
Bond lengths



Bond angles

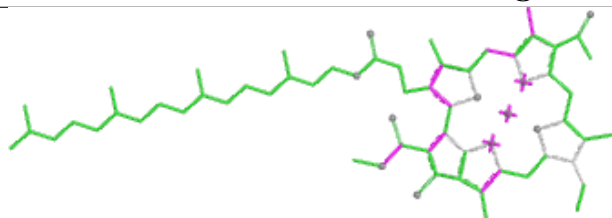


Torsions

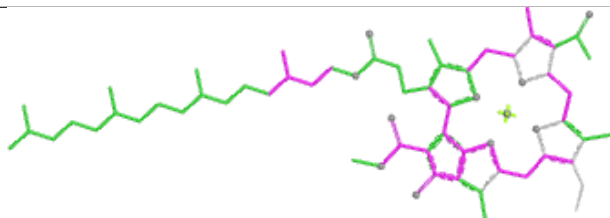


Rings

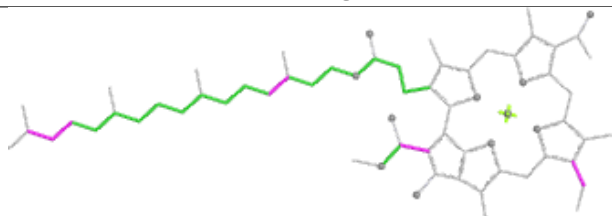
Ligand BCB L 400



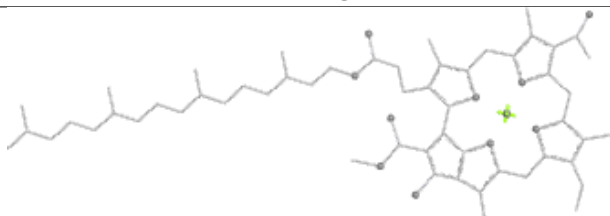
Bond lengths



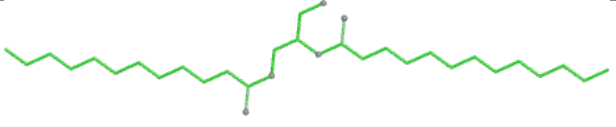
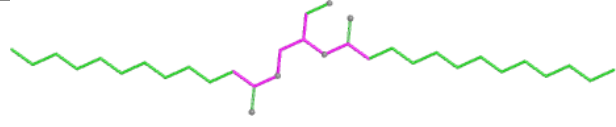
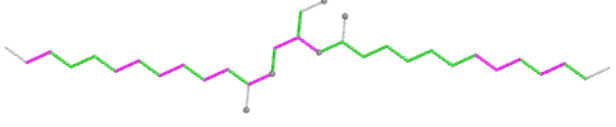
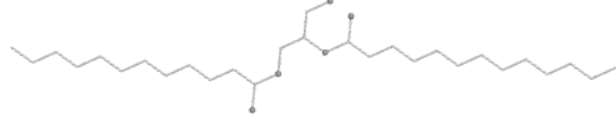
Bond angles

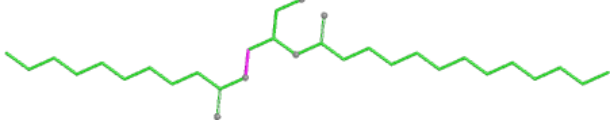
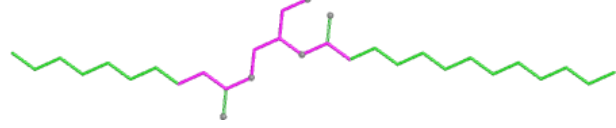
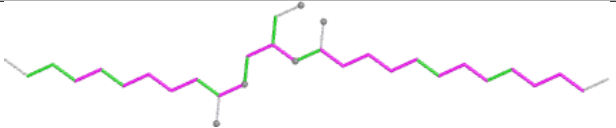
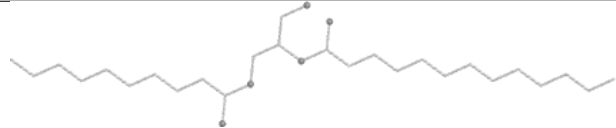


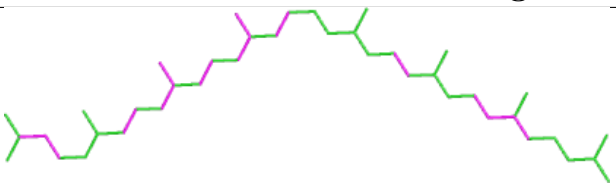
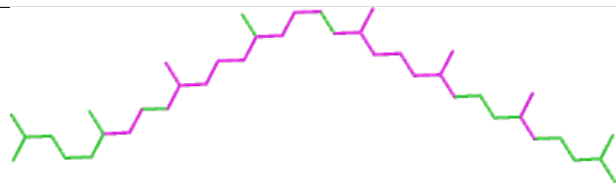
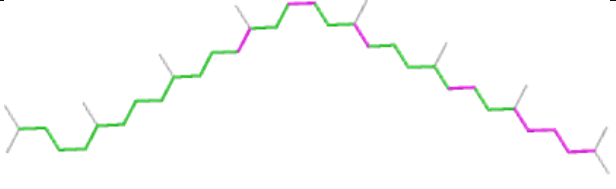
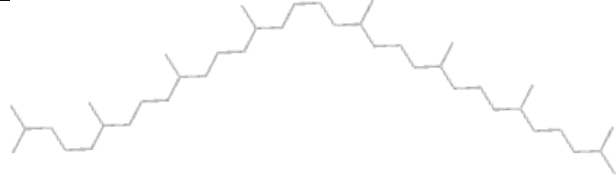
Torsions

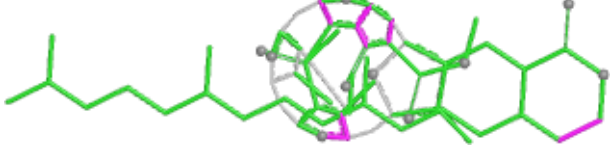
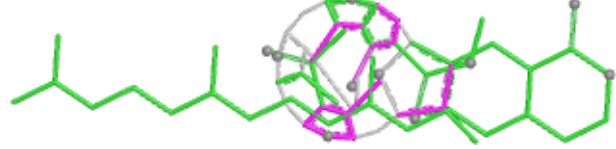
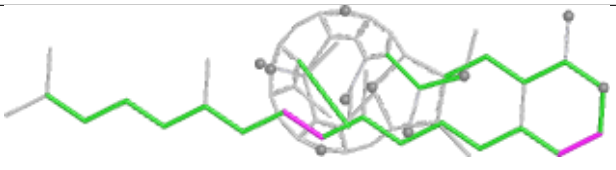


Rings

Ligand DGA L 731	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA H 733	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NS5 M 600	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BPB L 402	
	
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%)	0.26	5 (1%) 72 79	22, 49, 70, 122	4 (1%)
2	H	249/258 (96%)	0.71	16 (6%) 25 29	28, 58, 85, 120	4 (1%)
3	L	273/273 (100%)	0.24	7 (2%) 57 63	22, 47, 62, 88	5 (1%)
4	M	322/323 (99%)	0.41	19 (5%) 28 32	21, 49, 70, 91	4 (1%)
All	All	1178/1210 (97%)	0.39	47 (3%) 42 47	21, 50, 73, 122	17 (1%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	37	TRP	6.6
2	H	54	PRO	6.1
2	H	83	PRO	5.6
2	H	227[A]	ARG	5.1
1	C	334	ALA	4.4
4	M	71[A]	PHE	4.2
2	H	45	GLU	4.2
3	L	51	TYR	4.1
2	H	85	THR	4.1
2	H	96	PHE	3.8
3	L	202	ASP	3.7
1	C	333	ALA	3.6
4	M	146	TRP	3.4
3	L	81	LEU	3.4
3	L	1	ALA	3.2
2	H	8	GLN	3.2
1	C	47	ALA	3.2
4	M	108	HIS	3.2
3	L	271	PHE	3.2
4	M	320	GLY	3.1
4	M	33	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
4	M	1	ALA	2.9
2	H	44	VAL	2.9
4	M	26	ASN	2.7
2	H	86	ARG	2.7
2	H	198	LEU	2.7
4	M	323	LYS	2.7
2	H	25	TRP	2.6
3	L	119	LEU	2.6
2	H	7	ALA	2.5
1	C	1	CYS	2.5
2	H	189	GLY	2.4
4	M	34	TYR	2.3
2	H	188	ALA	2.3
2	H	208	ILE	2.3
3	L	273	SER	2.3
4	M	30	GLY	2.2
4	M	317	SER	2.2
4	M	308	TYR	2.2
4	M	85	PHE	2.1
4	M	23	TRP	2.1
1	C	4	PRO	2.0
4	M	32	PRO	2.0
4	M	319	PRO	2.0
4	M	118	LEU	2.0
2	H	190	SER	2.0
4	M	59	PHE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FME	H	1[A]	10/11	0.86	0.19	50,54,59,61	10
2	FME	H	1[B]	10/11	0.86	0.19	49,52,54,64	10
4	CSO	M	160	7/8	0.90	0.13	46,49,73,77	0

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
10	GOL	H	279	6/6	0.58	0.46	80,86,88,91	6
10	GOL	H	270	6/6	0.69	0.40	63,69,69,71	6
8	SO4	H	265	5/5	0.69	0.35	71,74,75,76	5
13	UQ9	L	503	19/58	0.72	0.39	49,70,84,86	19
6	LDA	H	718	13/16	0.76	0.45	55,61,79,84	13
8	SO4	H	264	5/5	0.77	0.35	63,65,67,73	5
8	SO4	C	345	5/5	0.78	0.27	71,79,83,86	5
6	LDA	M	715	16/16	0.78	0.58	63,77,84,85	16
10	GOL	C	361	6/6	0.79	0.35	66,71,76,80	6
10	GOL	M	334	6/6	0.80	0.53	63,65,67,68	6
9	HTO	H	267	10/10	0.80	0.28	74,77,89,91	10
8	SO4	C	347	5/5	0.81	0.32	71,73,76,77	5
10	GOL	H	273	6/6	0.81	0.48	71,75,79,80	6
10	GOL	H	277	6/6	0.81	0.27	65,69,71,72	6
6	LDA	H	707	16/16	0.82	0.39	53,67,77,85	16
8	SO4	C	340	5/5	0.82	0.23	72,73,77,79	5
8	SO4	C	343	5/5	0.82	0.23	66,66,70,74	5
10	GOL	M	333	6/6	0.83	0.47	70,70,73,78	6
9	HTO	C	348	10/10	0.83	0.35	52,62,68,74	10
10	GOL	C	364	6/6	0.83	0.34	53,55,61,62	6
6	LDA	M	702	16/16	0.84	0.38	52,56,62,65	16
10	GOL	H	276	6/6	0.84	0.34	71,79,85,85	6
6	LDA	M	704	16/16	0.84	0.44	64,67,86,88	16
6	LDA	C	712	16/16	0.84	0.42	56,62,74,74	16
10	GOL	C	363	6/6	0.84	0.27	72,75,78,78	6
7	DGA	C	730	37/44	0.84	0.28	58,76,94,99	37
10	GOL	M	337	6/6	0.84	0.34	56,64,66,69	6
13	UQ9	L	502	58/58	0.84	0.47	38,58,69,73	58
6	LDA	L	720	16/16	0.84	0.37	58,70,76,78	16
6	LDA	M	706	16/16	0.85	0.39	61,65,73,73	16
10	GOL	C	365	6/6	0.85	0.31	59,60,61,65	6
10	GOL	H	269	6/6	0.85	0.27	68,76,79,83	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	C	346	5/5	0.85	0.18	73,73,82,82	5
7	DGA	L	731	33/44	0.85	0.36	47,69,78,82	33
9	HTO	C	349	10/10	0.85	0.30	59,68,74,75	10
8	SO4	H	261	5/5	0.85	0.23	46,55,72,75	5
10	GOL	C	351	6/6	0.85	0.24	51,58,65,67	6
10	GOL	C	353[A]	6/6	0.85	0.26	44,55,59,61	6
10	GOL	C	353[B]	6/6	0.85	0.26	42,56,71,73	6
10	GOL	M	335	6/6	0.85	0.30	50,57,62,64	6
10	GOL	M	336	6/6	0.85	0.40	81,82,84,87	6
10	GOL	C	354	6/6	0.85	0.26	57,68,78,86	6
10	GOL	M	338	6/6	0.85	0.30	67,71,72,73	6
8	SO4	H	262[A]	5/5	0.85	0.13	55,56,67,71	5
8	SO4	H	262[B]	5/5	0.85	0.13	58,63,71,72	5
7	DGA	M	732	34/44	0.86	0.37	58,72,80,84	34
10	GOL	H	272	6/6	0.86	0.40	66,72,75,76	6
8	SO4	C	339	5/5	0.87	0.15	62,67,67,69	5
6	LDA	L	703	16/16	0.87	0.38	56,61,69,72	16
9	HTO	H	268	10/10	0.87	0.38	71,76,80,80	10
10	GOL	H	274	6/6	0.87	0.30	59,71,78,81	6
7	DGA	H	733	31/44	0.87	0.36	45,62,78,79	31
16	NS5	M	600	40/40	0.87	0.23	53,76,118,126	0
8	SO4	M	330	5/5	0.88	0.36	58,64,67,70	5
10	GOL	H	271	6/6	0.88	0.39	54,63,65,75	6
10	GOL	L	281	6/6	0.88	0.35	60,62,66,67	6
6	LDA	H	719	16/16	0.89	0.30	55,61,81,83	16
6	LDA	C	722	16/16	0.89	0.41	54,61,65,65	16
9	HTO	L	275	10/10	0.89	0.32	64,69,72,74	10
10	GOL	C	358	6/6	0.89	0.17	48,64,67,68	6
10	GOL	H	278	6/6	0.89	0.39	75,77,78,79	6
9	HTO	M	332	10/10	0.89	0.33	52,59,68,70	10
10	GOL	L	279	6/6	0.89	0.33	48,50,60,61	6
8	SO4	M	327	5/5	0.89	0.18	79,82,83,86	5
10	GOL	L	282	6/6	0.89	0.25	60,67,75,75	6
10	GOL	C	356	6/6	0.90	0.20	60,69,74,75	0
8	SO4	C	342	5/5	0.91	0.22	47,56,60,62	5
10	GOL	C	357	6/6	0.91	0.26	69,69,76,78	6
8	SO4	C	337	5/5	0.91	0.16	70,73,78,84	5
10	GOL	C	355	6/6	0.91	0.24	67,70,71,71	6
10	GOL	C	362	6/6	0.91	0.39	70,75,75,75	6
10	GOL	C	360	6/6	0.92	0.27	71,73,75,78	6
6	LDA	M	705	16/16	0.92	0.27	63,70,77,78	16
9	HTO	L	274	10/10	0.92	0.18	58,67,76,80	10

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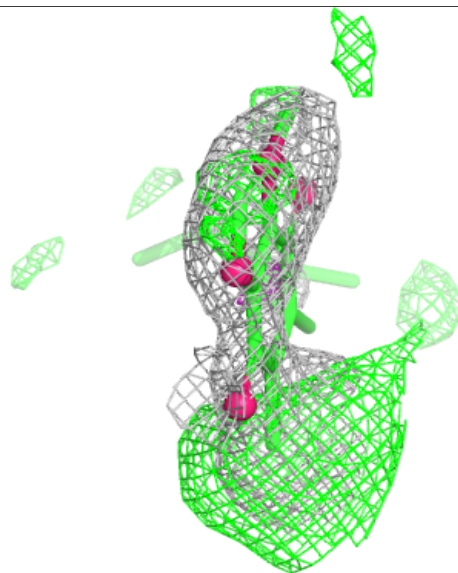
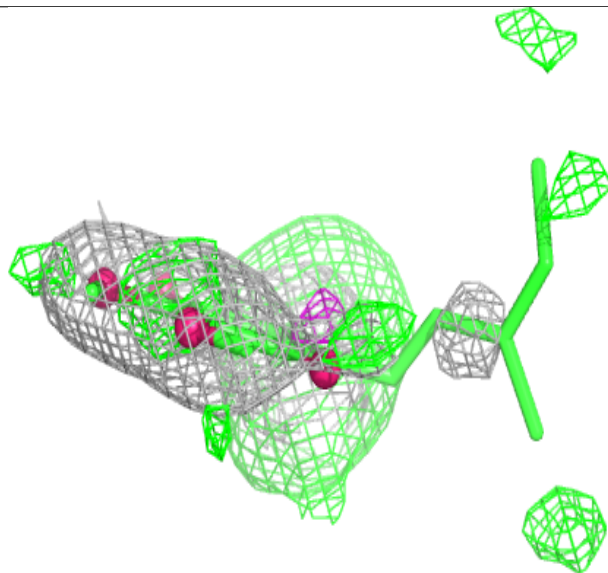
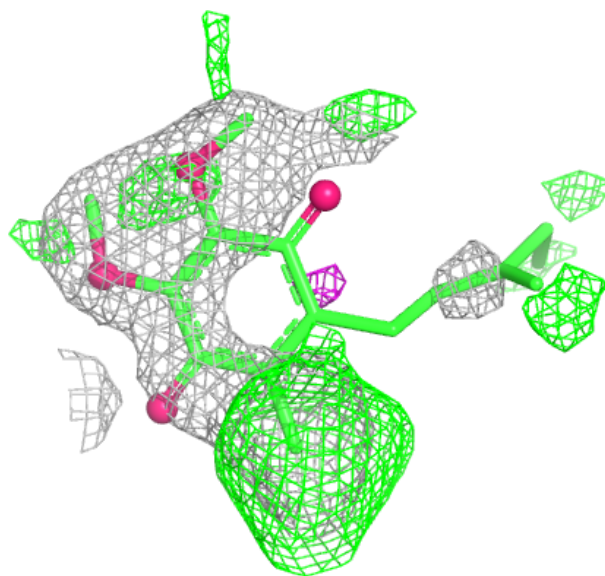
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	M	331	5/5	0.92	0.13	75,77,81,85	5
10	GOL	M	339	6/6	0.92	0.21	37,53,62,67	6
6	LDA	L	709	16/16	0.92	0.25	49,67,91,92	16
8	SO4	C	344	5/5	0.92	0.18	61,69,77,79	5
8	SO4	C	341	5/5	0.92	0.13	62,70,77,79	5
10	GOL	L	276	6/6	0.93	0.15	55,56,58,60	0
10	GOL	L	277	6/6	0.93	0.18	55,61,63,65	6
10	GOL	L	278	6/6	0.93	0.28	46,54,56,58	6
8	SO4	C	338	5/5	0.93	0.17	66,66,73,74	5
8	SO4	M	329	5/5	0.93	0.16	62,73,75,76	5
9	HTO	H	266	10/10	0.93	0.16	60,68,76,78	0
10	GOL	C	359	6/6	0.93	0.21	47,54,60,68	6
10	GOL	C	352	6/6	0.93	0.22	37,56,61,61	6
10	GOL	H	275	6/6	0.94	0.22	51,66,74,75	6
8	SO4	H	260	5/5	0.94	0.10	82,82,83,88	5
6	LDA	H	701	16/16	0.94	0.12	47,57,69,70	0
8	SO4	M	326	5/5	0.95	0.18	57,65,67,67	5
10	GOL	C	350	6/6	0.95	0.12	49,56,58,60	0
6	LDA	H	721	16/16	0.95	0.19	53,63,80,87	16
10	GOL	L	280	6/6	0.95	0.27	60,65,70,74	6
11	BCB	M	400	66/66	0.96	0.11	37,46,109,115	0
12	BPB	M	402	65/65	0.96	0.10	39,46,101,105	0
8	SO4	M	328	5/5	0.96	0.09	59,65,67,71	5
6	LDA	L	708	16/16	0.96	0.11	47,58,66,76	0
8	SO4	H	259	5/5	0.96	0.10	64,65,69,71	5
14	MQ9	M	501	58/58	0.97	0.10	38,46,92,98	0
11	BCB	M	401	66/66	0.97	0.08	33,39,62,67	0
11	BCB	L	400	66/66	0.98	0.07	34,39,49,57	0
11	BCB	L	401	66/66	0.98	0.07	35,39,69,79	0
8	SO4	M	324	5/5	0.98	0.08	54,54,60,71	0
8	SO4	M	325	5/5	0.98	0.07	69,70,77,82	0
12	BPB	L	402	65/65	0.98	0.06	37,41,51,53	0
5	HEC	C	401	43/43	0.99	0.07	46,52,61,67	0
8	SO4	H	263	5/5	0.99	0.10	47,50,52,52	5
5	HEC	C	402	43/43	0.99	0.07	41,46,55,61	0
5	HEC	C	403	43/43	0.99	0.06	36,40,43,49	0
5	HEC	C	404[A]	43/43	0.99	0.07	38,41,49,51	12
5	HEC	C	404[B]	43/43	0.99	0.07	38,41,46,49	12
15	FE2	M	500	1/1	1.00	0.02	42,42,42,42	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.

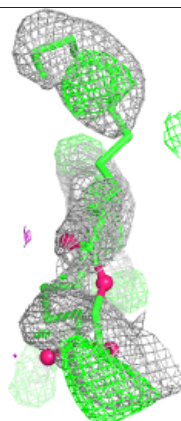
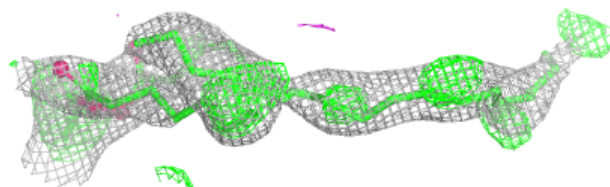
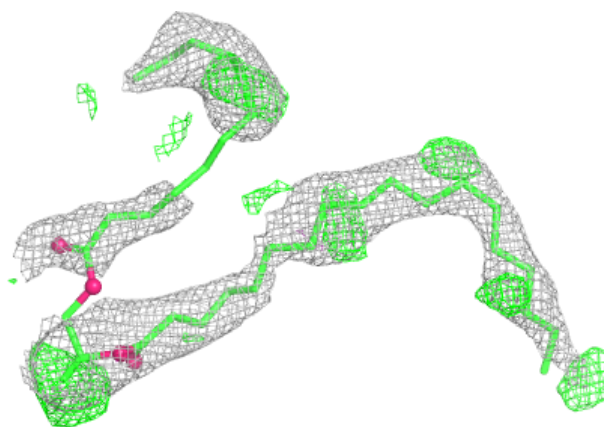
Electron density around UQ9 L 503:

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

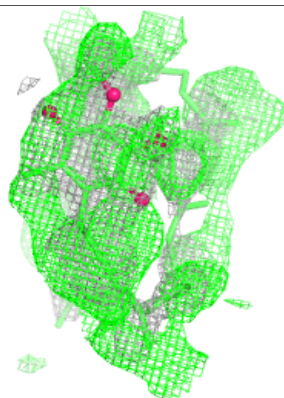
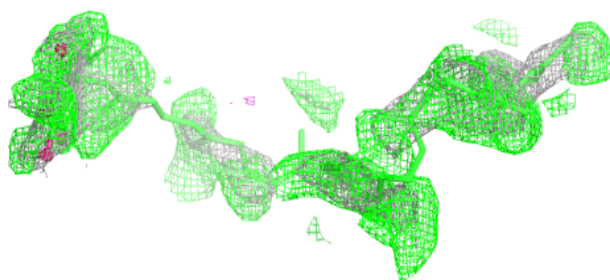
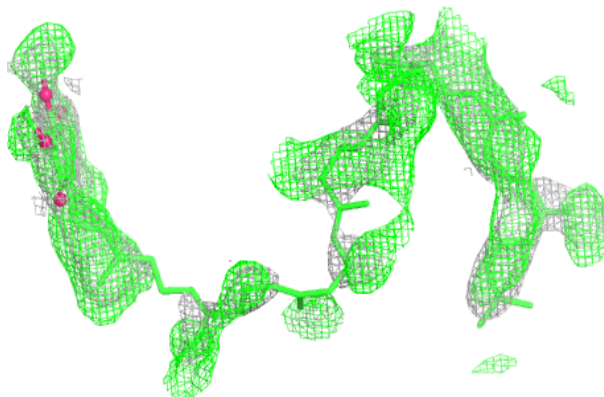


Electron density around DGA C 730:

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

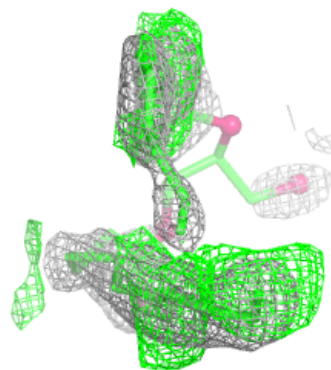
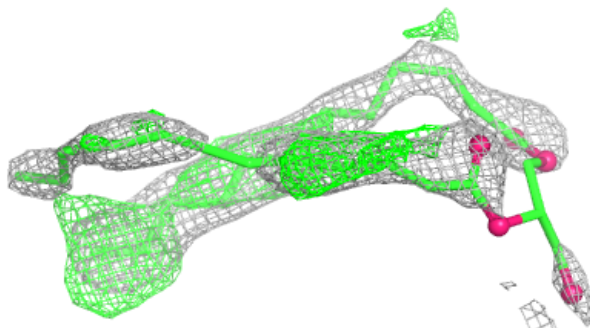
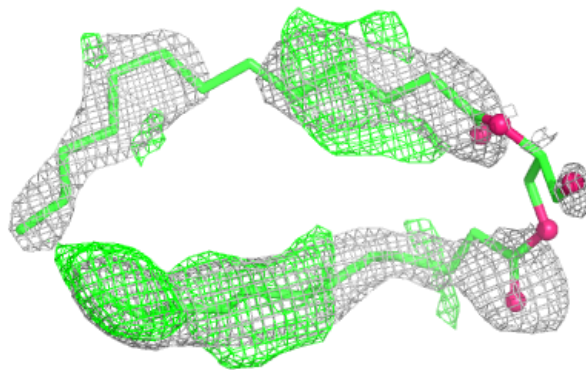
**Electron density around UQ9 L 502:**

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and green (positive)



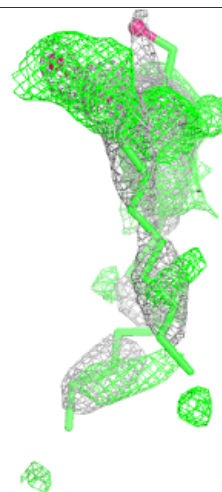
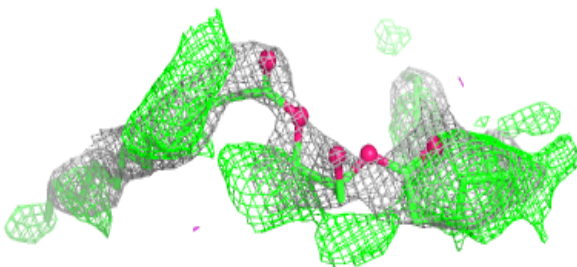
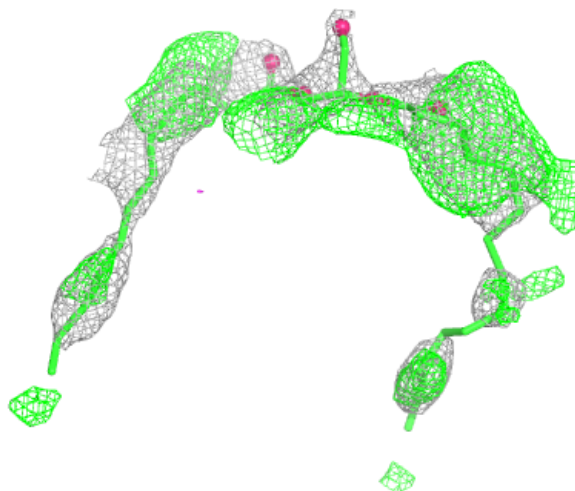
Electron density around DGA L 731:

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



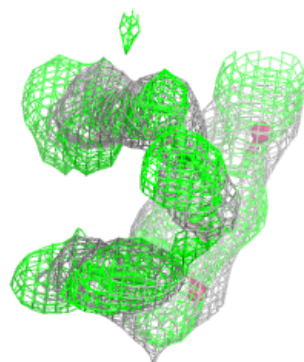
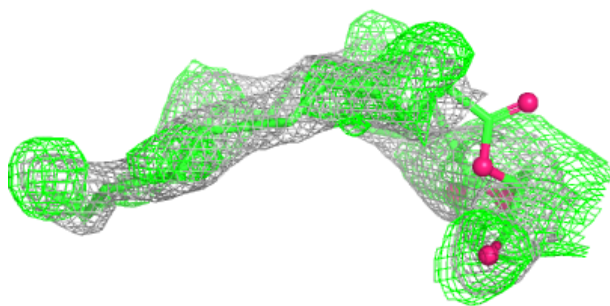
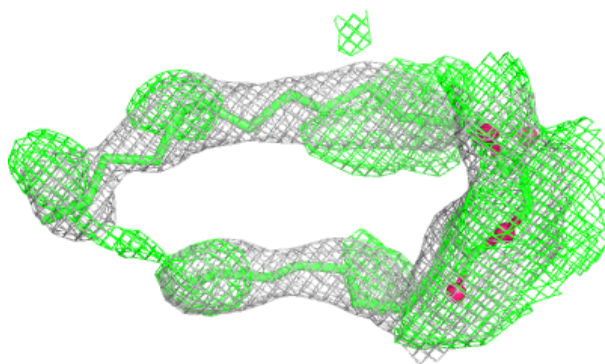
Electron density around DGA M 732:

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

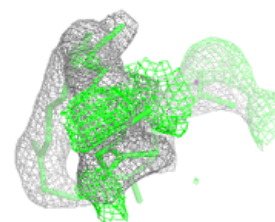
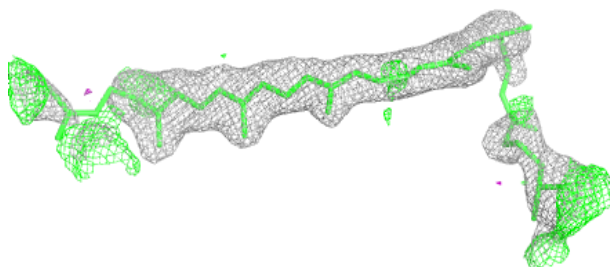
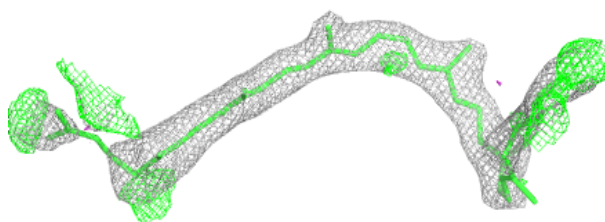


Electron density around DGA H 733:

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

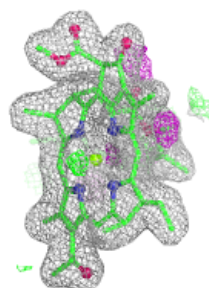
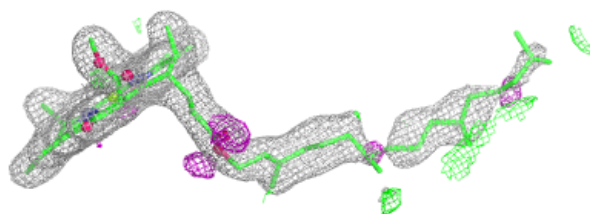
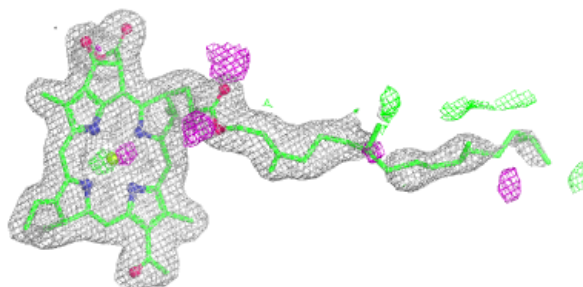
**Electron density around NS5 M 600:**

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

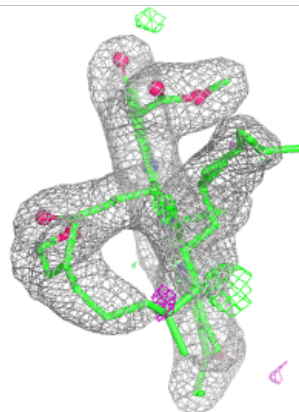
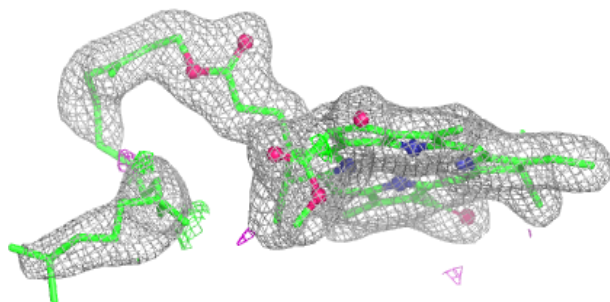
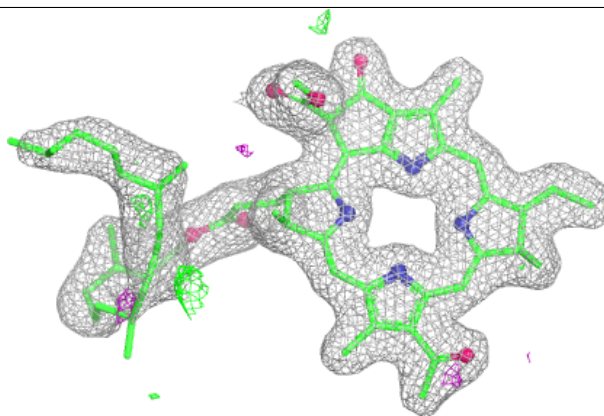


Electron density around BCB M 400:

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

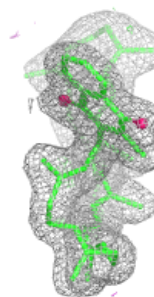
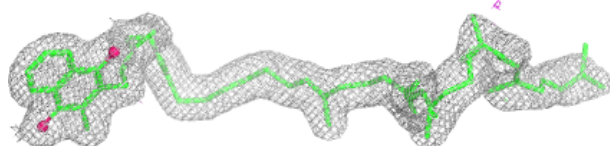
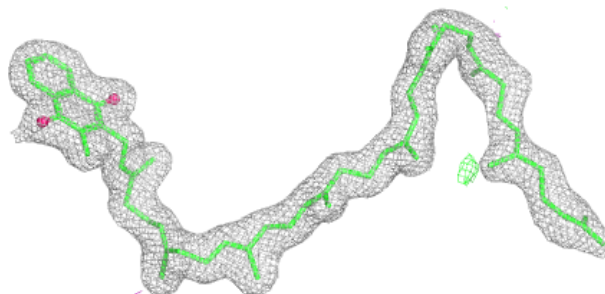
**Electron density around BPB M 402:**

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

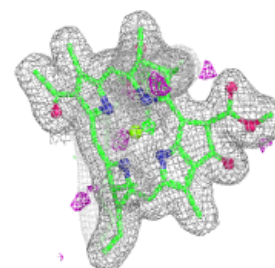
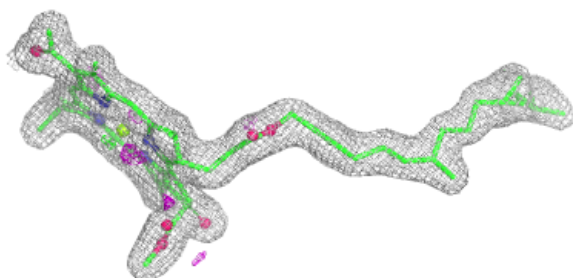
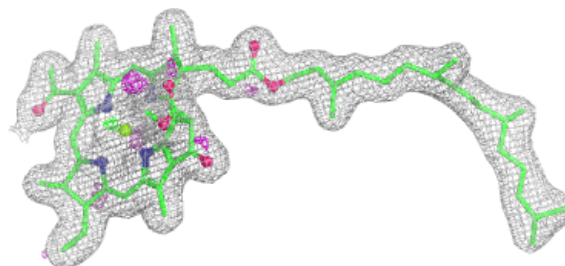


Electron density around MQ9 M 501:

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

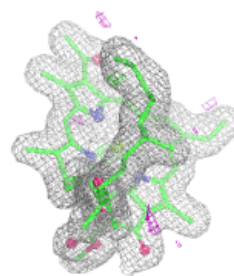
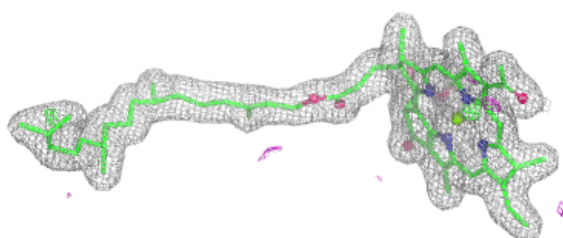
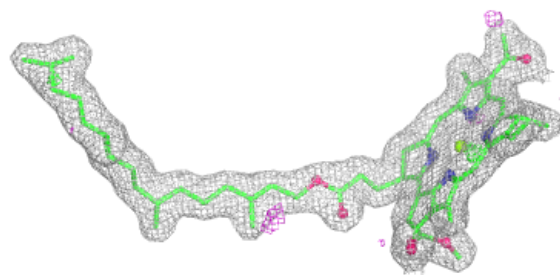
**Electron density around BCB M 401:**

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

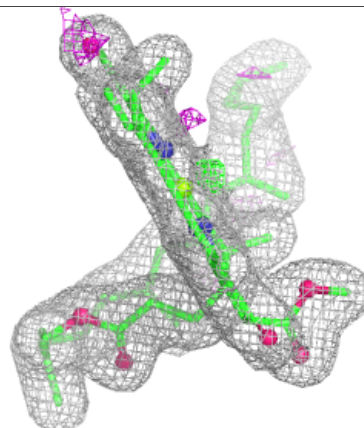
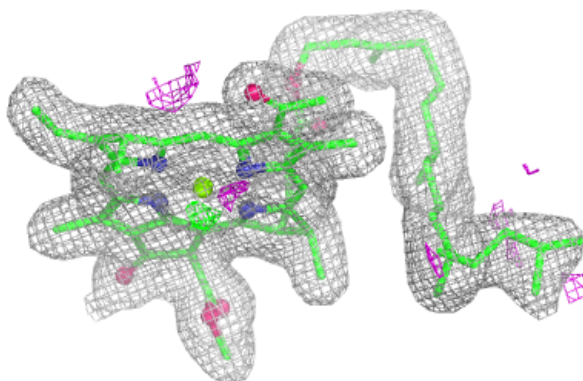
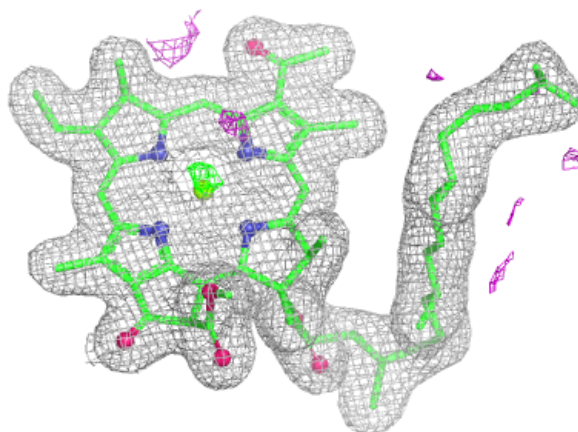


Electron density around BCB L 400:

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

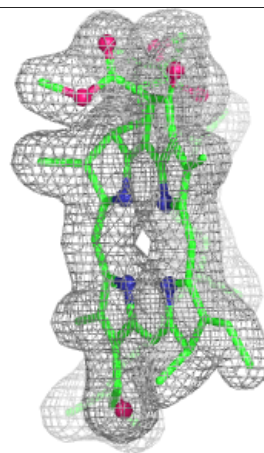
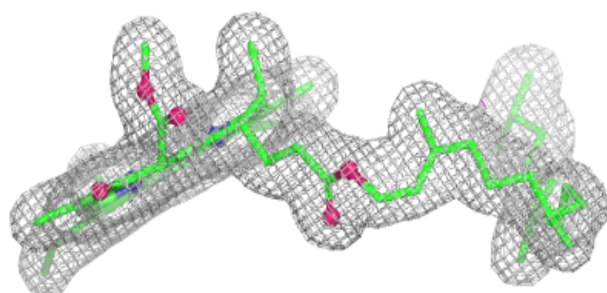
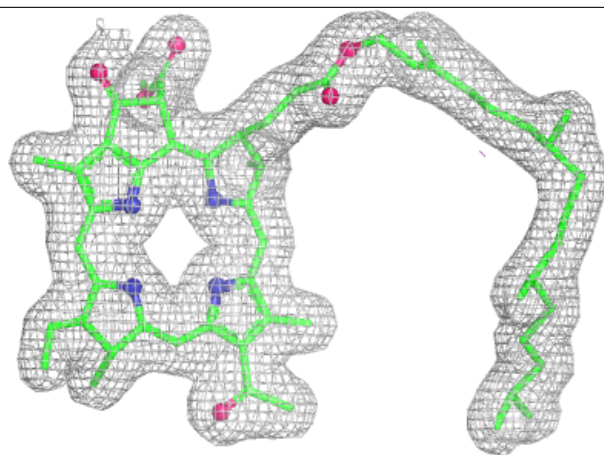
**Electron density around BCB L 401:**

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



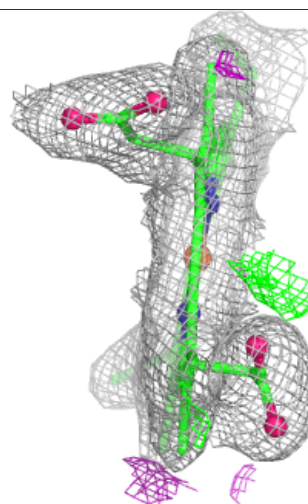
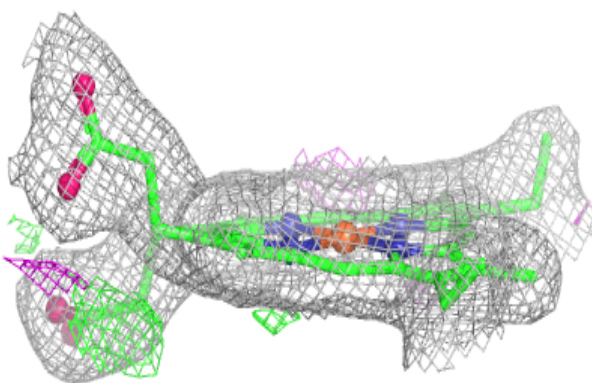
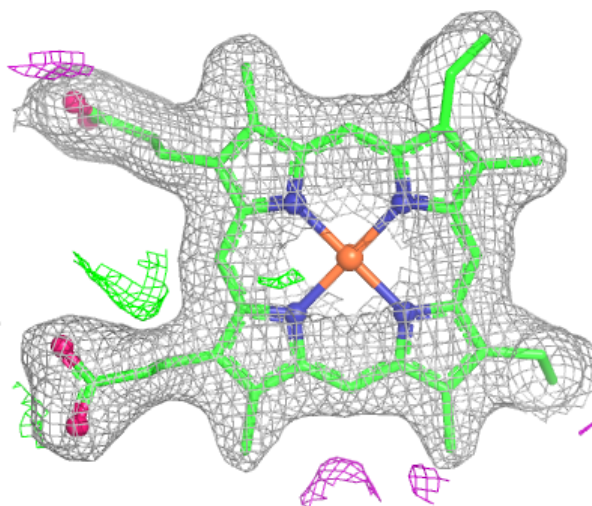
Electron density around BPB L 402:

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



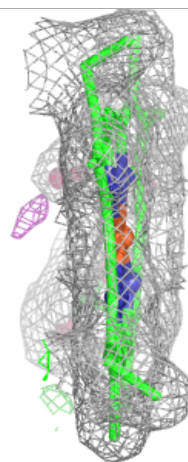
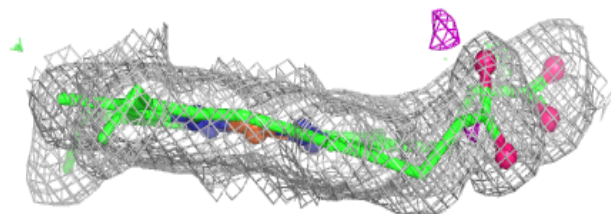
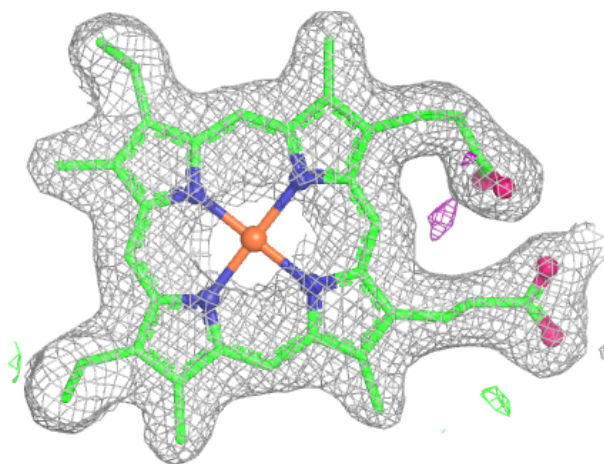
Electron density around HEC C 401:

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



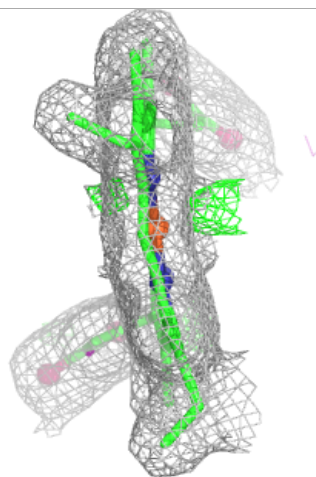
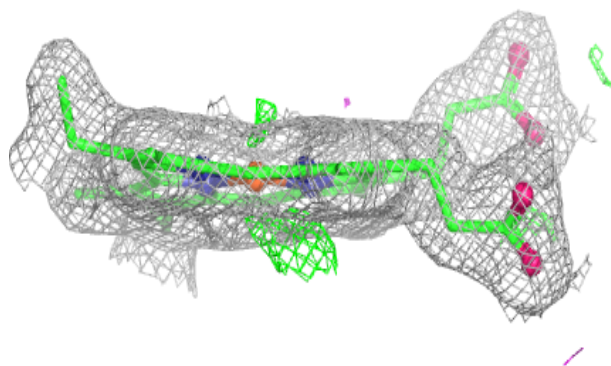
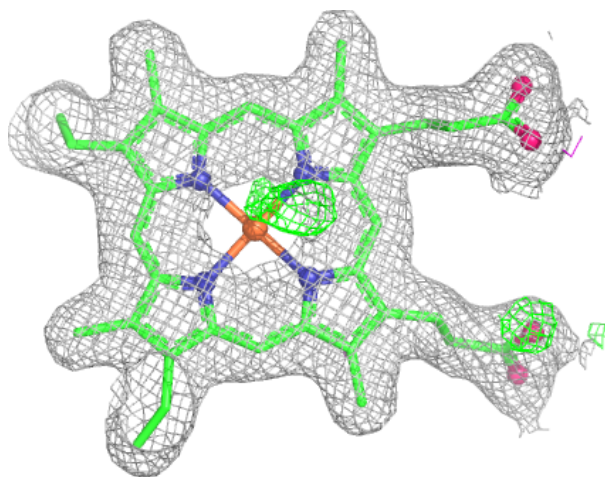
Electron density around HEC C 402:

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



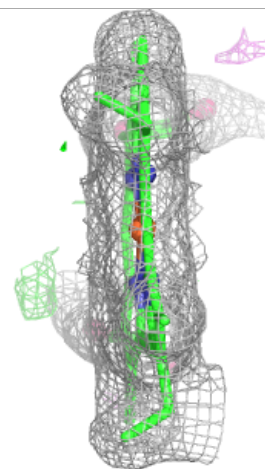
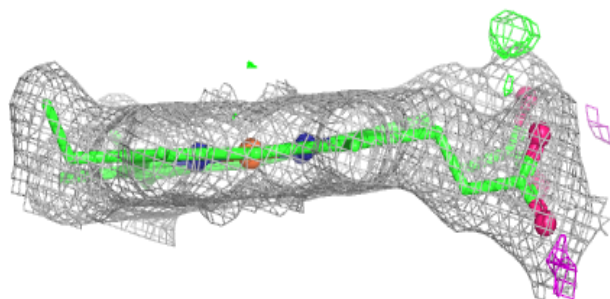
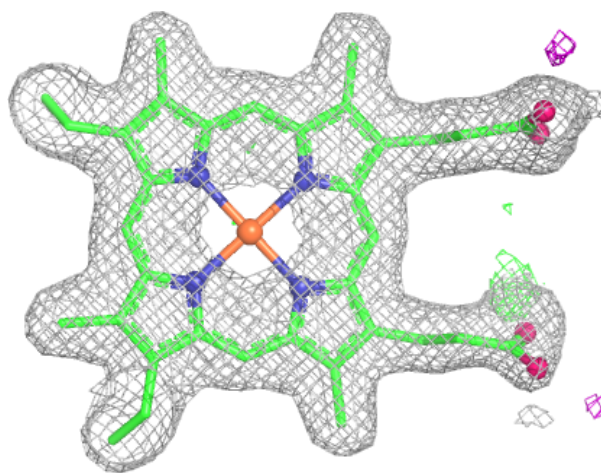
Electron density around HEC C 403:

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



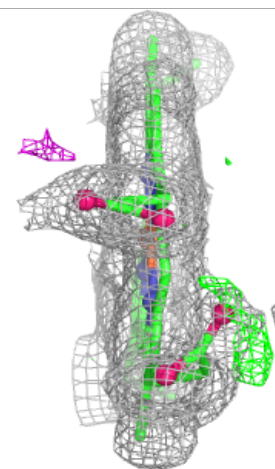
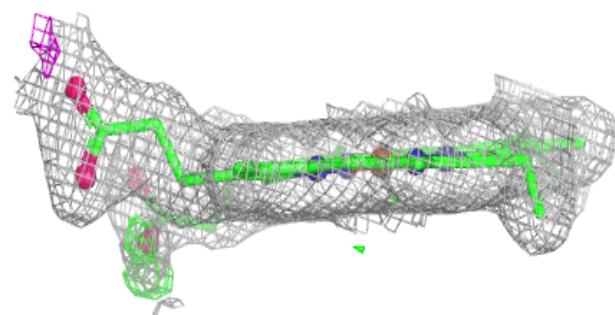
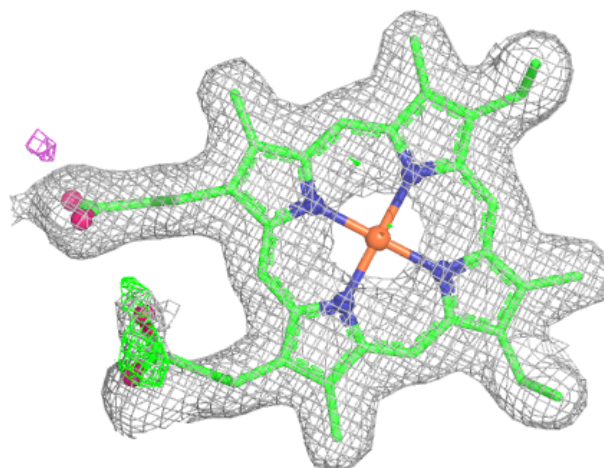
Electron density around HEC C 404 (A):

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



Electron density around HEC C 404 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.