



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 11:10 AM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

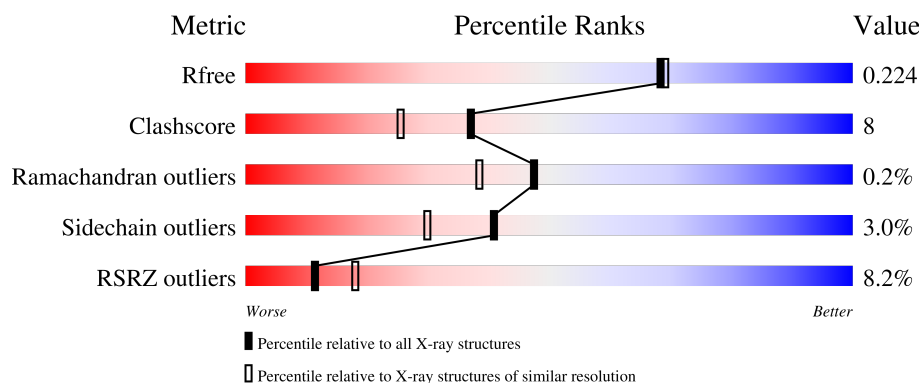
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>11%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
2	H	258	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>12%</div> </div> </div>
3	L	273	<div> <div>7%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
4	M	323	<div> <div>8%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	C	370	-	-	-	X
10	GOL	C	371	-	-	-	X
10	GOL	C	374[B]	-	-	-	X
10	GOL	C	377	-	-	X	-
10	GOL	C	378	-	-	-	X
10	GOL	H	283	-	-	X	-
10	GOL	L	288	-	-	-	X
10	GOL	M	341	-	-	-	X
6	LDA	H	718[B]	-	-	-	X
6	LDA	L	702	-	-	-	X
6	LDA	L	712	-	-	-	X
6	LDA	L	724	-	-	-	X
6	LDA	M	706	-	-	-	X
7	DGA	C	730	-	-	-	X
8	SO4	C	351	-	-	-	X
8	SO4	H	261[B]	-	-	X	-
8	SO4	L	275	-	-	-	X
8	SO4	M	326	-	-	X	-
8	SO4	M	329	-	-	-	X
8	SO4	M	330	-	-	-	X
9	HTO	C	355	-	-	X	-
9	HTO	C	356	-	X	-	-
9	HTO	C	357	-	-	-	X
9	HTO	C	358[A]	-	X	-	-
9	HTO	H	274[A]	-	-	-	X
9	HTO	M	333	-	-	-	X

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 12156 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	334	Total	C	N	O	S	0	3	0
			2647	1667	474	486	20			

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

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

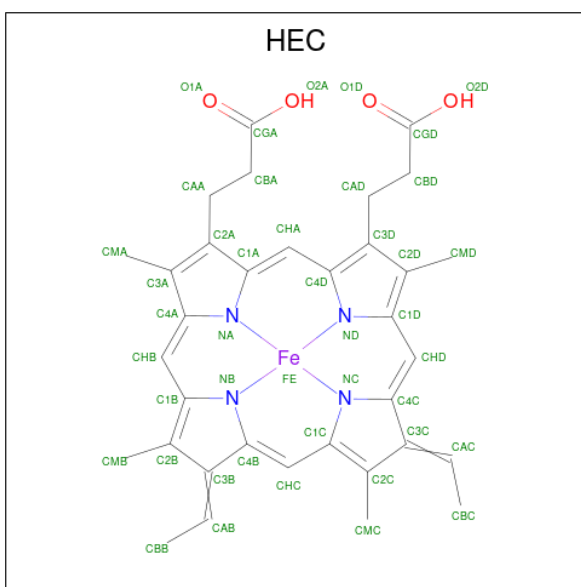
- Molecule 3 is a protein called Photosynthetic reaction center L-subunit.

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

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

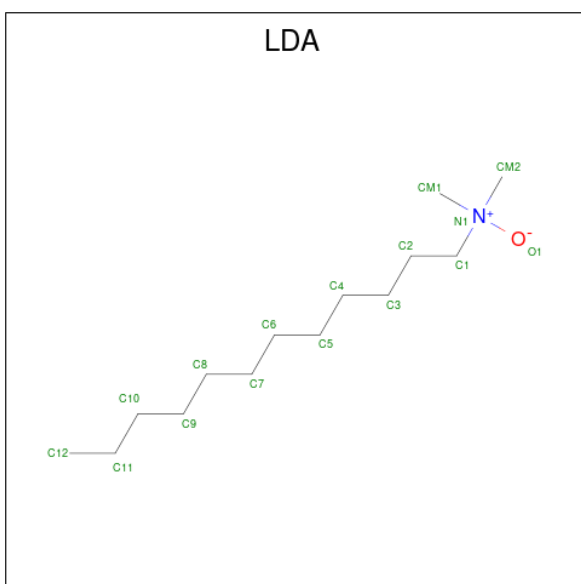
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2574	1716	424	423	11			

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



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

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



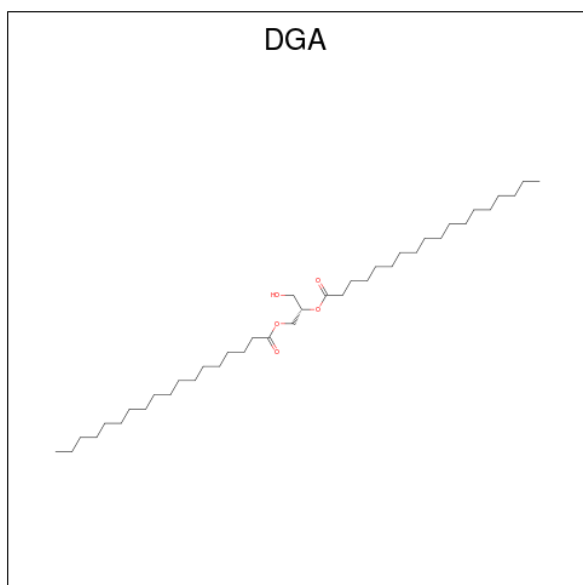
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	1
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1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

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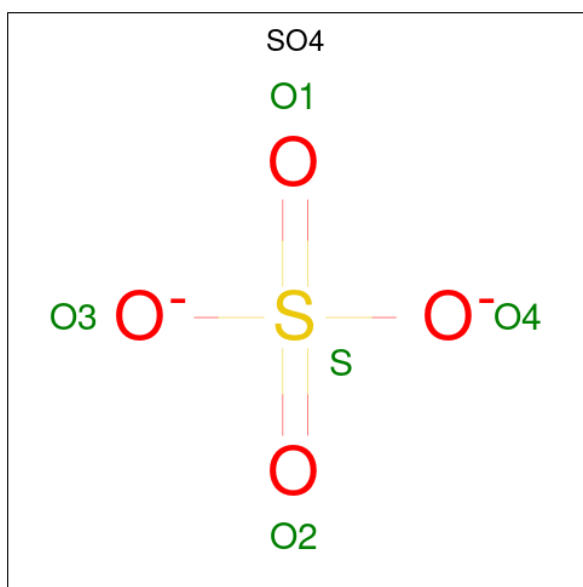
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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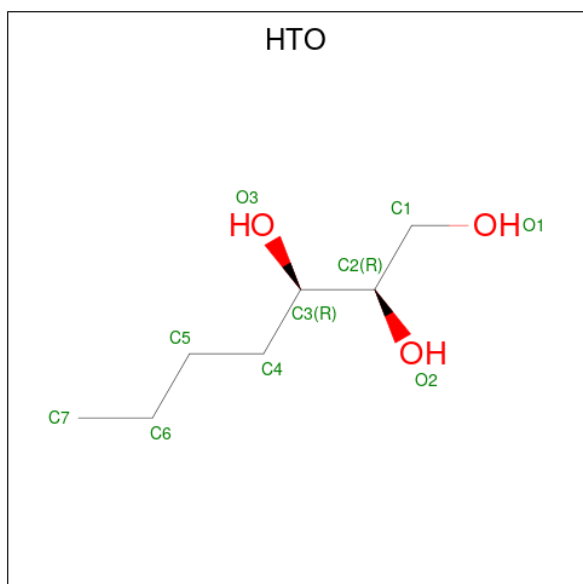
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	1
			10	8	2		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total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

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

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



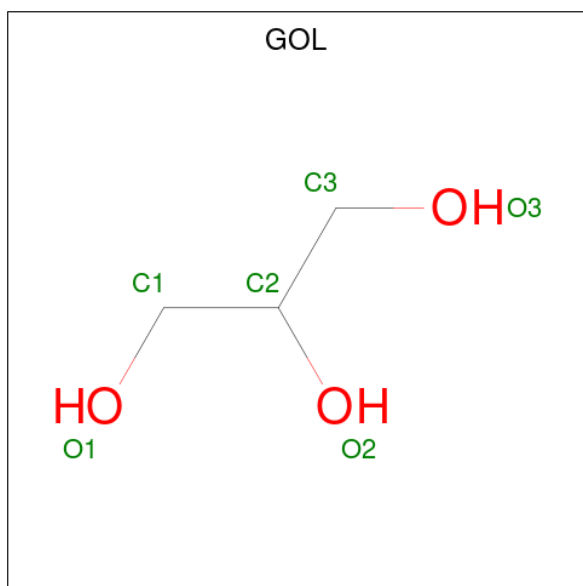
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	1
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		

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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

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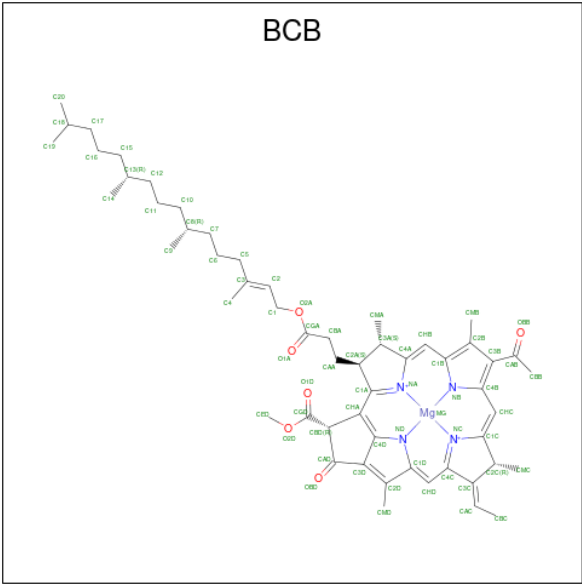
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10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

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

- Molecule 11 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



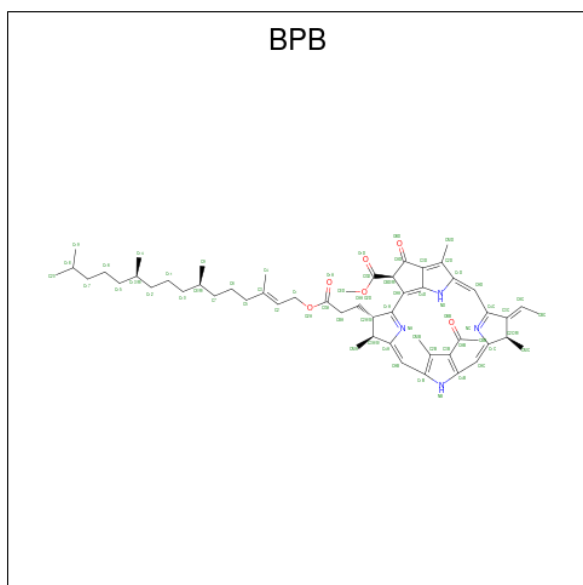
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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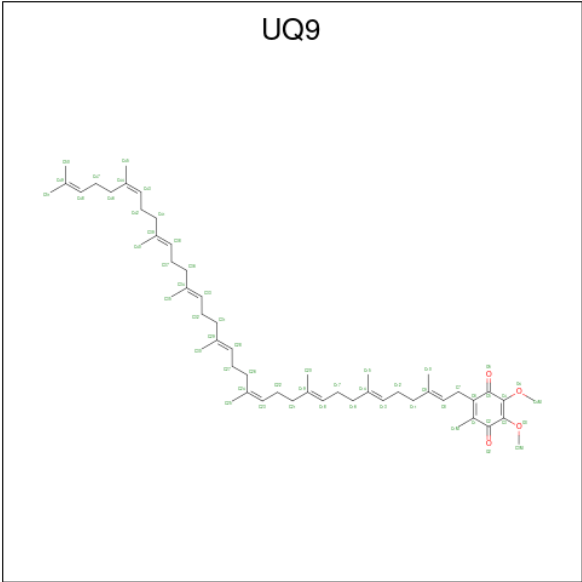
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 12 is BACTERIOPHEOPHYTIN B (three-letter code: 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 (three-letter code: UQ9) (formula:  $C_{54}H_{82}O_4$ ).

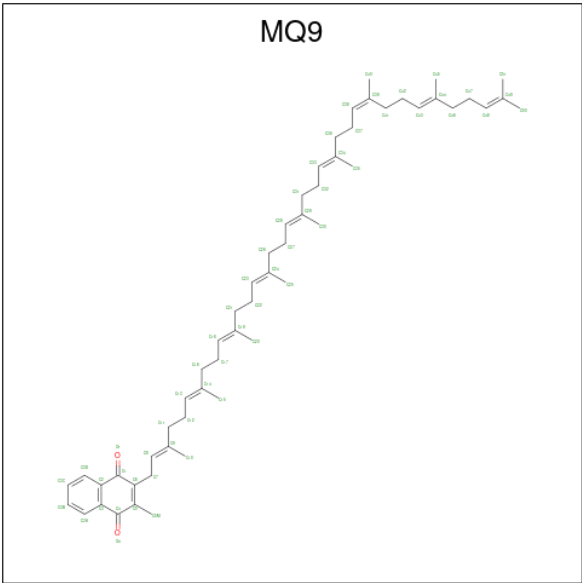


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	54	4		
13	L	1	Total	C	O	0	0
			23	19	4		

- Molecule 14 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

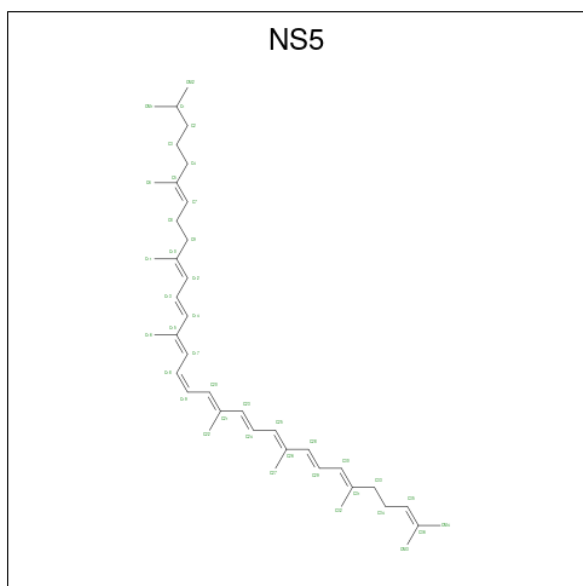
- Molecule 15 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C<sub>56</sub>H<sub>80</sub>O<sub>2</sub>).





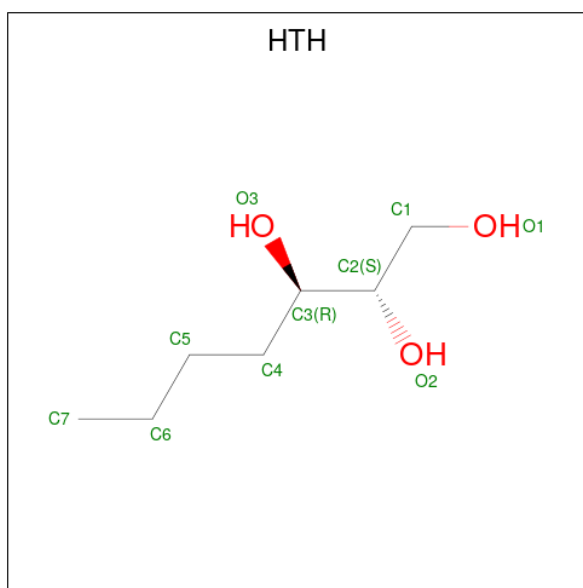
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			58	56	2		

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



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

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



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

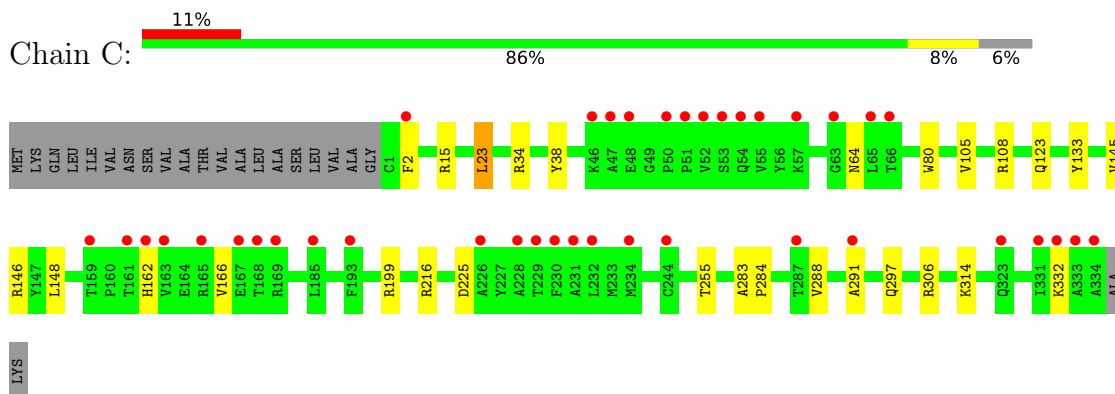
- Molecule 18 is water.

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

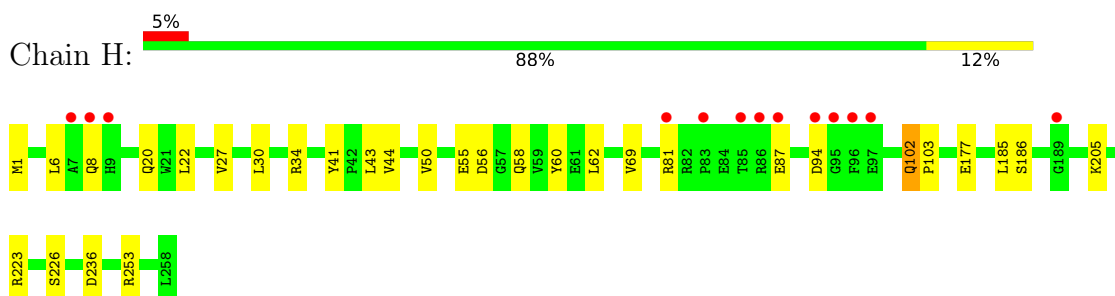
### 3 Residue-property plots

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

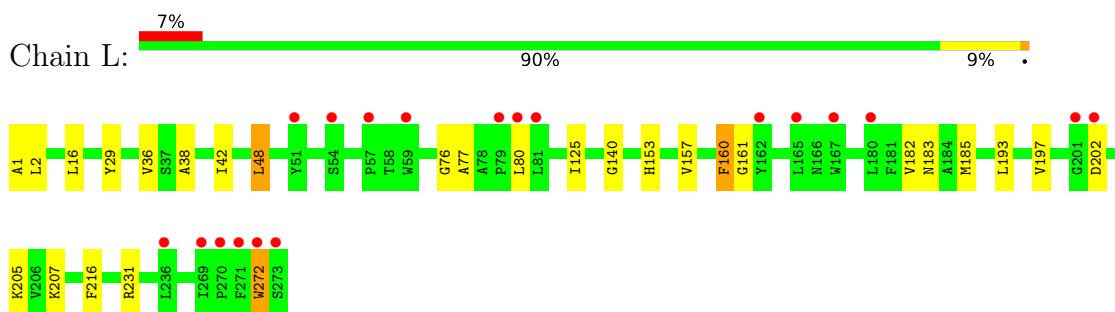
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



- Molecule 2: Photosynthetic reaction center H-subunit

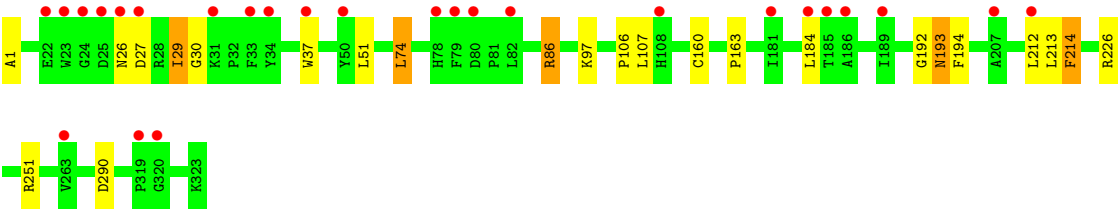


- Molecule 3: Photosynthetic reaction center L-subunit



- Molecule 4: Photosynthetic reaction center M-subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.44Å 220.44Å 113.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 1.95 48.34 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.34-1.95) 96.2 (48.34-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, $R_{free}$	0.182 , 0.216 0.192 , 0.224	Depositor DCC
$R_{free}$ test set	9677 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 75.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, LDA, BPB, HTO, BCB, HTH, UQ9, DGA, FE2, SO4, HEC, MQ9, FME, NS5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C	0.91	0/2716	0.82	3/3701 (0.1%)
2	H	0.91	2/2069 (0.1%)	0.84	0/2827
3	L	0.94	0/2280	0.81	2/3113 (0.1%)
4	M	0.94	1/2679 (0.0%)	0.79	2/3662 (0.1%)
All	All	0.93	3/9744 (0.0%)	0.81	7/13303 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	177	GLU	CD-OE1	5.52	1.31	1.25
2	H	27	VAL	CB-CG2	5.43	1.64	1.52
4	M	160	CYS	CB-SG	-5.19	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	251	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	23	LEU	CA-CB-CG	5.82	128.69	115.30
3	L	160	PHE	CB-CG-CD1	5.55	124.69	120.80
4	M	86	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	15	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	L	48	LEU	CA-CB-CG	5.21	127.29	115.30
1	C	306	ARG	NE-CZ-NH2	-5.19	117.71	120.30

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	2647	0	2610	33	0
2	H	2035	0	2017	19	0
3	L	2191	0	2116	22	0
4	M	2574	0	2470	28	0
5	C	172	0	120	4	0
6	C	32	0	62	7	0
6	H	80	0	155	9	0
6	L	144	0	279	19	0
6	M	128	0	248	12	0
7	C	37	0	58	3	0
8	C	95	0	0	3	0
8	H	70	0	0	5	0
8	L	10	0	0	0	0
8	M	40	0	0	2	0
9	C	40	0	64	8	0
9	H	30	0	48	5	0
9	L	50	0	80	3	0
9	M	10	0	16	2	0
10	C	120	0	160	15	0
10	H	104	0	135	10	0
10	L	48	0	64	1	0
10	M	54	0	72	6	0
11	L	132	0	144	9	0
11	M	132	0	144	17	0
12	L	65	0	74	2	0
12	M	65	0	74	1	0
13	L	81	0	105	16	0
14	M	1	0	0	0	0
15	M	58	0	80	2	0
16	M	40	0	60	3	0
17	M	10	0	16	0	0
18	C	388	0	0	4	0
18	H	211	0	0	4	0
18	L	109	0	0	0	0
18	M	153	0	0	1	0
All	All	12156	0	11471	178	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 8.

All (178) 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)
6:H:720:LDA:H72	6:H:720:LDA:C3	1.43	1.34
6:H:720:LDA:H32	6:H:720:LDA:C7	1.62	1.27
13:L:502:UQ9:H15A	11:M:400:BCB:C9	1.75	1.15
9:M:333:HTO:O3	9:M:333:HTO:H72	1.50	1.10
13:L:502:UQ9:H15A	11:M:400:BCB:H93	1.46	0.98
8:H:261[B]:SO4:O3	6:L:702:LDA:O1	1.81	0.96
13:L:502:UQ9:H15A	11:M:400:BCB:H91	1.49	0.94
11:M:400:BCB:HMB1	11:M:400:BCB:HBB2	1.50	0.91
9:M:333:HTO:O3	9:M:333:HTO:C7	2.23	0.85
6:C:716:LDA:H51	10:H:280:GOL:O1	1.75	0.85
3:L:272:TRP:CD1	4:M:86:ARG:HD3	2.13	0.83
6:H:720:LDA:C7	6:H:720:LDA:C3	2.21	0.81
8:H:261[B]:SO4:O3	6:L:702:LDA:HM23	1.82	0.79
4:M:29:ILE:CD1	4:M:51:LEU:HD13	2.14	0.77
1:C:199[B]:ARG:HH12	10:C:369:GOL:H12	1.48	0.77
10:C:364:GOL:H11	6:M:715:LDA:HM11	1.68	0.76
1:C:34:ARG:HD3	9:C:357:HTO:H3	1.65	0.75
8:H:261[B]:SO4:O3	6:L:702:LDA:CM2	2.34	0.75
4:M:29:ILE:HD11	4:M:51:LEU:HD13	1.70	0.74
1:C:297:GLN:HE22	10:C:365:GOL:H31	1.53	0.73
1:C:255:THR:HG23	10:C:363:GOL:H32	1.72	0.72
1:C:64[A]:ASN:HD21	9:C:355:HTO:C2	2.03	0.71
2:H:226:SER:HB3	9:H:272:HTO:H42	1.72	0.71
2:H:223[A]:ARG:HG3	10:H:283:GOL:O2	1.92	0.70
11:M:400:BCB:HMB1	11:M:400:BCB:CBB	2.22	0.69
6:C:722:LDA:H32	6:C:722:LDA:HM21	1.72	0.69
6:H:720:LDA:C7	6:H:720:LDA:H31	2.22	0.67
6:L:703:LDA:H32	6:L:703:LDA:HM21	1.76	0.67
11:L:400:BCB:HBB3	11:L:400:BCB:HMB1	1.78	0.66
1:C:148:LEU:HD13	10:C:365:GOL:H12	1.78	0.66
13:L:502:UQ9:C15	11:M:400:BCB:H91	2.26	0.65
4:M:29:ILE:HD12	4:M:51:LEU:HD22	1.78	0.65
6:C:722:LDA:C3	6:C:722:LDA:CM2	2.74	0.64
3:L:231:ARG:HG2	6:L:723:LDA:HM23	1.80	0.63
4:M:97:LYS:NZ	18:M:418:HOH:O	2.31	0.63
1:C:332:LYS:H	9:C:355:HTO:H71	1.63	0.63
10:C:364:GOL:C1	6:M:715:LDA:HM11	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:253:ARG:HE	10:H:278:GOL:H31	1.64	0.62
1:C:291:ALA:HB3	10:C:377:GOL:C3	2.29	0.62
8:H:261[B]:SO4:O3	6:L:702:LDA:N1	2.33	0.62
11:M:401:BCB:HMB1	11:M:401:BCB:HBB3	1.80	0.62
1:C:199[B]:ARG:NH1	10:C:369:GOL:H12	2.13	0.62
6:C:722:LDA:H32	6:C:722:LDA:CM2	2.30	0.62
13:L:503:UQ9:O5	13:L:503:UQ9:H4MA	2.01	0.61
1:C:199[A]:ARG:NH1	18:C:783:HOH:O	2.29	0.61
6:H:720:LDA:H32	6:H:720:LDA:H72	0.67	0.61
13:L:502:UQ9:C15	11:M:400:BCB:H93	2.27	0.61
6:L:710:LDA:H32	9:L:277:HTO:H73	1.83	0.59
2:H:253:ARG:HE	10:H:278:GOL:C3	2.16	0.59
13:L:503:UQ9:H8	13:L:503:UQ9:O5	2.03	0.59
4:M:30:GLY:HA3	10:M:342:GOL:H12	1.85	0.58
3:L:36:VAL:HG12	9:L:279:HTO:H3	1.85	0.58
12:L:402:BPB:HMB	12:L:402:BPB:HBBB	1.86	0.58
11:L:401:BCB:HMB1	11:L:401:BCB:CBB	2.34	0.57
1:C:291:ALA:HB3	10:C:377:GOL:H31	1.86	0.57
1:C:199[A]:ARG:NE	18:C:783:HOH:O	2.37	0.57
6:C:722:LDA:C3	6:C:722:LDA:HM21	2.31	0.57
11:M:401:BCB:CBB	11:M:401:BCB:HMB1	2.34	0.57
5:C:401:HEC:HMB1	5:C:401:HEC:HBB3	1.87	0.57
11:L:400:BCB:H193	15:M:501:MQ9:H252	1.87	0.57
4:M:74:LEU:CD1	16:M:600:NS5:HM23	2.36	0.56
4:M:1:ALA:N	8:M:326:SO4:O3	2.31	0.56
6:L:703:LDA:C3	6:L:703:LDA:HM21	2.33	0.56
2:H:205:LYS:O	10:H:279:GOL:O1	2.23	0.55
5:C:403:HEC:HBB3	5:C:403:HEC:HMB1	1.88	0.55
10:H:283:GOL:C1	18:H:537:HOH:O	2.55	0.55
3:L:140:GLY:HA3	6:L:712:LDA:HM13	1.88	0.55
3:L:38:ALA:O	3:L:42:ILE:HG13	2.07	0.54
4:M:37:TRP:HD1	6:M:704:LDA:CM1	2.21	0.54
1:C:123:GLN:HE21	10:M:338:GOL:H11	1.72	0.54
2:H:81[A]:ARG:HG3	2:H:81[A]:ARG:HH11	1.72	0.54
3:L:76:GLY:HA3	6:L:711:LDA:HM13	1.89	0.54
4:M:37:TRP:CD1	6:M:704:LDA:HM12	2.44	0.53
2:H:6:LEU:HD23	9:H:274[A]:HTO:H2	1.90	0.53
7:C:730:DGA:HB22	7:C:730:DGA:HA22	1.91	0.53
2:H:43:LEU:HB3	3:L:1:ALA:HB1	1.90	0.53
13:L:502:UQ9:C15	11:M:400:BCB:C9	2.67	0.53
2:H:62:LEU:O	6:H:721:LDA:HM21	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLN:HE21	10:M:338:GOL:H31	1.74	0.52
1:C:162:HIS:HB2	10:C:368:GOL:H2	1.92	0.52
1:C:291:ALA:N	10:C:377:GOL:H32	2.25	0.52
3:L:193:LEU:HD22	3:L:216:PHE:CE2	2.44	0.52
3:L:272:TRP:CG	4:M:86:ARG:HD3	2.45	0.52
4:M:37:TRP:HD1	6:M:704:LDA:HM12	1.75	0.51
1:C:283:ALA:HB3	1:C:284:PRO:HD3	1.92	0.51
1:C:225:ASP:OD1	10:C:369:GOL:O3	2.29	0.51
3:L:231:ARG:CG	6:L:723:LDA:HM23	2.40	0.50
11:L:400:BCB:CBB	11:L:400:BCB:HMB1	2.41	0.50
13:L:503:UQ9:O4	13:L:503:UQ9:H3MB	2.11	0.50
4:M:212:LEU:C	4:M:212:LEU:HD23	2.32	0.50
8:C:340:SO4:O3	8:C:354:SO4:O1	2.29	0.50
4:M:37:TRP:H	6:M:704:LDA:HM13	1.77	0.50
1:C:145:VAL:O	1:C:146:ARG:HD2	2.11	0.50
6:H:719:LDA:C9	6:H:720:LDA:H122	2.41	0.50
11:L:400:BCB:OBB	11:L:400:BCB:HHC	2.11	0.49
1:C:291:ALA:HB3	10:C:377:GOL:H32	1.95	0.49
9:H:273:HTO:C1	18:H:499:HOH:O	2.60	0.49
1:C:64[A]:ASN:ND2	9:C:355:HTO:H3	2.27	0.49
3:L:193:LEU:HD22	3:L:216:PHE:HE2	1.77	0.49
13:L:503:UQ9:C8	13:L:503:UQ9:O5	2.60	0.49
13:L:502:UQ9:H3MB	13:L:502:UQ9:O2	2.13	0.49
4:M:192:GLY:O	4:M:193:ASN:HB3	2.13	0.49
1:C:105:VAL:CG2	1:C:288:VAL:HG11	2.43	0.48
8:C:338:SO4:O4	10:M:334:GOL:O1	2.21	0.48
9:H:273:HTO:H12	18:H:499:HOH:O	2.12	0.48
7:C:730:DGA:HB62	7:C:730:DGA:HA52	1.94	0.48
2:H:223[B]:ARG:HG3	10:H:283:GOL:O2	2.14	0.47
2:H:69:VAL:HG22	3:L:205:LYS:HA	1.94	0.47
1:C:64[A]:ASN:HD21	9:C:355:HTO:C3	2.27	0.47
1:C:123:GLN:NE2	10:M:338:GOL:H31	2.29	0.47
11:L:401:BCB:HMB1	11:L:401:BCB:HBB2	1.96	0.47
3:L:161:GLY:HA3	11:L:400:BCB:HAC1	1.96	0.47
10:H:283:GOL:H11	18:H:537:HOH:O	2.14	0.47
4:M:29:ILE:HD12	4:M:51:LEU:HD13	1.96	0.46
4:M:74:LEU:HD12	16:M:600:NS5:CM2	2.45	0.46
1:C:199[A]:ARG:CZ	18:C:783:HOH:O	2.62	0.46
2:H:41:TYR:OH	8:H:261[A]:SO4:O3	2.25	0.46
2:H:223[A]:ARG:CG	10:H:283:GOL:O2	2.61	0.46
4:M:226:ARG:NH1	8:M:326:SO4:O1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:272:TRP:CD1	4:M:86:ARG:CD	2.93	0.46
1:C:108:ARG:HD2	18:C:780:HOH:O	2.15	0.46
6:L:703:LDA:CM2	6:L:703:LDA:C3	2.94	0.46
3:L:125:ILE:HG21	6:L:724:LDA:HM22	1.97	0.46
4:M:106:PRO:HB3	6:M:714:LDA:H31	1.98	0.46
1:C:64[A]:ASN:HD21	9:C:355:HTO:H3	1.80	0.46
4:M:184:LEU:HD21	11:M:400:BCB:CAC	2.47	0.45
9:H:273:HTO:H52	9:H:273:HTO:H2	1.69	0.45
11:M:401:BCB:HAA2	11:M:401:BCB:HBD	1.98	0.45
2:H:81[A]:ARG:HG3	2:H:81[A]:ARG:NH1	2.32	0.45
12:M:402:BPB:HBBB	12:M:402:BPB:HMB	1.98	0.45
6:C:716:LDA:HM21	10:C:364:GOL:O3	2.17	0.45
4:M:107:LEU:H	6:M:714:LDA:H32	1.82	0.45
13:L:502:UQ9:O3	13:L:502:UQ9:H4MB	2.16	0.44
11:M:401:BCB:HAA2	11:M:401:BCB:CBD	2.42	0.44
13:L:502:UQ9:C51	11:M:400:BCB:H191	2.47	0.44
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.52	0.44
1:C:2[B]:PHE:O	8:C:351:SO4:O2	2.36	0.44
7:C:730:DGA:CA2	7:C:730:DGA:HB22	2.47	0.44
3:L:182:VAL:HA	11:M:400:BCB:H43	2.00	0.44
4:M:74:LEU:HD12	16:M:600:NS5:HM23	1.99	0.44
6:H:719:LDA:H91	6:H:720:LDA:H122	2.00	0.44
13:L:503:UQ9:C4M	13:L:503:UQ9:O5	2.65	0.44
12:L:402:BPB:HMB	12:L:402:BPB:CBB	2.48	0.43
6:L:723:LDA:H22	6:L:723:LDA:HM21	1.45	0.43
6:L:702:LDA:H22	6:L:702:LDA:H52	1.83	0.43
4:M:37:TRP:CD1	6:M:704:LDA:CM1	3.01	0.43
2:H:30:LEU:O	2:H:34:ARG:HD2	2.18	0.43
3:L:153:HIS:O	3:L:157:VAL:HG23	2.18	0.43
3:L:29:TYR:OH	6:L:702:LDA:H12	2.19	0.43
6:L:703:LDA:H21	6:L:703:LDA:HM11	1.60	0.43
4:M:212:LEU:O	4:M:212:LEU:HD23	2.17	0.43
3:L:77:ALA:HB1	9:L:277:HTO:O3	2.18	0.43
2:H:102:GLN:HA	2:H:103:PRO:HD3	1.94	0.42
4:M:37:TRP:H	6:M:704:LDA:CM1	2.32	0.42
1:C:314:LYS:HZ2	10:C:373:GOL:H2	1.84	0.42
11:M:401:BCB:HHC	11:M:401:BCB:OBB	2.20	0.42
15:M:501:MQ9:H33	15:M:501:MQ9:C38	2.49	0.42
11:L:401:BCB:OBB	11:L:401:BCB:HHC	2.20	0.42
1:C:146:ARG:HD2	1:C:146:ARG:HA	1.80	0.42
5:C:403:HEC:HBC3	5:C:403:HEC:HMC1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:223[B]:ARG:CG	10:H:283:GOL:O2	2.66	0.42
9:C:357:HTO:H73	10:L:286:GOL:O1	2.20	0.42
6:L:723:LDA:H52	6:L:723:LDA:H81	1.82	0.41
3:L:125:ILE:CG2	6:L:724:LDA:HM22	2.51	0.41
1:C:64[A]:ASN:HD21	9:C:355:HTO:C1	2.33	0.41
2:H:55:GLU:H	2:H:58:GLN:HE21	1.67	0.41
11:L:401:BCB:O1A	11:L:401:BCB:H43	2.21	0.41
6:M:706:LDA:H62	6:M:706:LDA:H32	1.75	0.41
1:C:216:ARG:HG3	6:C:716:LDA:HM22	2.02	0.41
3:L:197:VAL:HG13	3:L:207:LYS:HB2	2.02	0.41
6:H:719:LDA:H92	6:H:720:LDA:H122	2.04	0.40
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.56	0.40
5:C:403:HEC:HBC1	5:C:404:HEC:HMA1	2.03	0.40
3:L:183:ASN:HD21	4:M:214:PHE:HB3	1.85	0.40
13:L:502:UQ9:H32	13:L:502:UQ9:H35	1.95	0.40
6:M:707:LDA:H21	6:M:707:LDA:HM13	1.81	0.40
13:L:502:UQ9:H51A	11:M:400:BCB:H191	2.04	0.40
4:M:26:ASN:H	10:M:336:GOL:HO3	1.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	335/356 (94%)	326 (97%)	9 (3%)	0	100	100
2	H	259/258 (100%)	247 (95%)	11 (4%)	1 (0%)	34	22
3	L	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	315 (98%)	7 (2%)	1 (0%)	41	30
All	All	1190/1210 (98%)	1156 (97%)	32 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	286/299 (96%)	283 (99%)	3 (1%)	76	74
2	H	209/211 (99%)	199 (95%)	10 (5%)	25	12
3	L	220/218 (101%)	212 (96%)	8 (4%)	35	23
4	M	249/247 (101%)	241 (97%)	8 (3%)	39	27
All	All	964/975 (99%)	935 (97%)	29 (3%)	41	30

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	23	LEU
1	C	38	TYR
1	C	166	VAL
2	H	8	GLN
2	H	20	GLN
2	H	22	LEU
2	H	44	VAL
2	H	87	GLU
2	H	94	ASP
2	H	102	GLN
2	H	185	LEU
2	H	186	SER
2	H	236	ASP
3	L	2	LEU
3	L	16	LEU
3	L	48	LEU
3	L	80	LEU
3	L	160	PHE
3	L	185	MET
3	L	202	ASP

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Mol	Chain	Res	Type
3	L	272	TRP
4	M	27	ASP
4	M	29	ILE
4	M	74	LEU
4	M	163	PRO
4	M	194	PHE
4	M	213	LEU
4	M	214	PHE
4	M	290	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	297	GLN
1	C	302	GLN
2	H	58	GLN
2	H	102	GLN
2	H	220	ASN
3	L	183	ASN
3	L	213	ASN
3	L	239	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FME	H	1[B]	-	8,9,10	0.97	0	7,9,11	3.00	1 (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
2	FME	H	1[B]	-	-	4/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1[B]	FME	CA-N-CN	-7.48	111.32	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 152 ligands modelled in this entry, 1 is monoatomic - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	H	265	-	4,4,4	0.43	0	6,6,6	0.29	0
10	GOL	H	290	-	5,5,5	0.34	0	5,5,5	0.52	0
6	LDA	L	703	-	12,15,15	2.12	1 (8%)	14,17,17	0.57	0
17	HTH	M	332	-	9,9,9	0.43	0	10,10,10	1.20	1 (10%)
10	GOL	M	335	-	5,5,5	0.45	0	5,5,5	0.37	0
8	SO4	H	269	-	4,4,4	0.38	0	6,6,6	0.16	0
9	HTO	L	278	-	9,9,9	0.67	0	10,10,10	1.63	3 (30%)
10	GOL	C	377	-	5,5,5	0.18	0	5,5,5	0.34	0
8	SO4	C	348	-	4,4,4	0.40	0	6,6,6	0.41	0
10	GOL	C	364	-	5,5,5	0.57	0	5,5,5	0.96	0
5	HEC	C	401	1	26,50,50	1.10	1 (3%)	18,82,82	2.26	7 (38%)
10	GOL	M	342	-	5,5,5	0.40	0	5,5,5	0.66	0
8	SO4	H	259	-	4,4,4	0.26	0	6,6,6	0.43	0
9	HTO	H	274[A]	-	9,9,9	0.32	0	10,10,10	0.75	0
10	GOL	H	276[B]	-	5,5,5	0.82	0	5,5,5	0.94	0
9	HTO	M	333	-	9,9,9	0.48	0	10,10,10	2.65	4 (40%)
10	GOL	H	287	-	5,5,5	0.32	0	5,5,5	0.11	0
10	GOL	C	361	-	5,5,5	0.58	0	5,5,5	1.05	0
6	LDA	L	710	-	12,15,15	2.09	1 (8%)	14,17,17	0.49	0
8	SO4	C	345	-	4,4,4	0.33	0	6,6,6	0.32	0
10	GOL	L	284	-	5,5,5	0.37	0	5,5,5	0.48	0
11	BCB	L	400	3	60,74,74	3.86	18 (30%)	48,115,115	2.33	17 (35%)
8	SO4	C	338	-	4,4,4	0.46	0	6,6,6	0.42	0
10	GOL	L	286	-	5,5,5	0.20	0	5,5,5	0.77	0
10	GOL	C	373	-	5,5,5	0.35	0	5,5,5	0.27	0
10	GOL	C	378	-	5,5,5	0.33	0	5,5,5	0.17	0
9	HTO	H	273	-	9,9,9	0.44	0	10,10,10	1.21	1 (10%)
6	LDA	M	705	-	12,15,15	1.86	1 (8%)	14,17,17	0.53	0
6	LDA	H	718[B]	-	12,15,15	1.99	1 (8%)	14,17,17	0.61	0
9	HTO	C	357	-	9,9,9	0.58	0	10,10,10	0.76	0
9	HTO	C	358[A]	-	9,9,9	0.73	0	10,10,10	2.66	4 (40%)
6	LDA	L	708	-	12,15,15	1.98	1 (8%)	14,17,17	1.25	2 (14%)
8	SO4	H	262	-	4,4,4	0.34	0	6,6,6	0.39	0
10	GOL	C	376	-	5,5,5	0.33	0	5,5,5	0.31	0
8	SO4	H	266	-	4,4,4	0.36	0	6,6,6	0.40	0
10	GOL	M	341	-	5,5,5	0.39	0	5,5,5	0.24	0
6	LDA	M	713	-	12,15,15	1.98	1 (8%)	14,17,17	0.71	0
10	GOL	H	279	-	5,5,5	0.37	0	5,5,5	0.53	0
10	GOL	H	288	-	5,5,5	0.38	0	5,5,5	0.34	0
5	HEC	C	404	1	26,50,50	1.01	2 (7%)	18,82,82	1.76	4 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	C	350	-	4,4,4	0.37	0	6,6,6	0.14	0
8	SO4	L	274	-	4,4,4	0.29	0	6,6,6	0.34	0
9	HTO	H	272	-	9,9,9	0.74	0	10,10,10	1.68	3 (30%)
8	SO4	L	275	-	4,4,4	0.32	0	6,6,6	0.13	0
8	SO4	C	354	-	4,4,4	0.27	0	6,6,6	0.38	0
9	HTO	C	355	-	9,9,9	0.55	0	10,10,10	1.61	2 (20%)
6	LDA	L	723	-	12,15,15	2.02	1 (8%)	14,17,17	0.78	0
8	SO4	M	329	-	4,4,4	0.30	0	6,6,6	0.34	0
5	HEC	C	403	1	26,50,50	1.09	3 (11%)	18,82,82	1.03	1 (5%)
10	GOL	C	367	-	5,5,5	0.25	0	5,5,5	1.07	0
10	GOL	L	282	-	5,5,5	0.88	0	5,5,5	1.20	1 (20%)
12	BPB	M	402	-	64,70,70	1.04	4 (6%)	64,101,101	1.28	8 (12%)
10	GOL	C	368	-	5,5,5	0.15	0	5,5,5	0.68	0
8	SO4	M	325	-	4,4,4	0.17	0	6,6,6	0.60	0
6	LDA	M	707	-	12,15,15	2.15	1 (8%)	14,17,17	0.89	0
15	MQ9	M	501	-	59,59,59	2.28	25 (42%)	72,75,75	1.24	9 (12%)
10	GOL	H	291	-	5,5,5	0.38	0	5,5,5	0.42	0
10	GOL	C	360	-	5,5,5	0.26	0	5,5,5	0.62	0
10	GOL	M	334	-	5,5,5	0.15	0	5,5,5	0.30	0
13	UQ9	L	502	-	58,58,58	2.24	24 (41%)	70,73,73	1.58	14 (20%)
10	GOL	H	289	-	5,5,5	0.34	0	5,5,5	0.24	0
8	SO4	C	340	-	4,4,4	0.36	0	6,6,6	0.65	0
9	HTO	C	356	-	9,9,9	0.75	0	10,10,10	1.85	3 (30%)
10	GOL	L	281	-	5,5,5	0.19	0	5,5,5	0.44	0
8	SO4	C	353	-	4,4,4	0.48	0	6,6,6	0.27	0
11	BCB	M	401	4	60,74,74	3.70	24 (40%)	48,115,115	2.62	16 (33%)
6	LDA	H	719	-	12,15,15	1.99	1 (8%)	14,17,17	0.54	0
9	HTO	L	277	-	9,9,9	0.45	0	10,10,10	1.35	1 (10%)
6	LDA	M	704	-	12,15,15	2.36	1 (8%)	14,17,17	1.53	3 (21%)
6	LDA	M	714	-	12,15,15	2.21	1 (8%)	14,17,17	0.37	0
6	LDA	L	712	-	12,15,15	2.10	1 (8%)	14,17,17	0.36	0
10	GOL	H	286	-	5,5,5	0.26	0	5,5,5	0.57	0
10	GOL	H	281	-	5,5,5	0.55	0	5,5,5	0.36	0
6	LDA	L	711	-	12,15,15	2.07	1 (8%)	14,17,17	0.61	0
6	LDA	L	709	-	12,15,15	1.97	1 (8%)	14,17,17	0.48	0
11	BCB	M	400	4	60,74,74	3.47	18 (30%)	48,115,115	2.33	14 (29%)
8	SO4	C	337[A]	-	4,4,4	0.36	0	6,6,6	0.23	0
8	SO4	M	328	-	4,4,4	0.30	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	SO4	C	337[B]	-	4,4,4	0.36	0	6,6,6	0.21	0
10	GOL	L	287	-	5,5,5	0.35	0	5,5,5	0.60	0
6	LDA	C	722	-	12,15,15	1.98	1 (8%)	14,17,17	0.58	0
10	GOL	C	371	-	5,5,5	0.34	0	5,5,5	0.78	0
10	GOL	H	280	-	5,5,5	0.73	0	5,5,5	1.09	0
6	LDA	L	724	-	12,15,15	2.20	1 (8%)	14,17,17	0.59	0
8	SO4	C	346	-	4,4,4	0.40	0	6,6,6	0.41	0
8	SO4	C	351	-	4,4,4	0.32	0	6,6,6	0.17	0
6	LDA	M	706	-	12,15,15	1.93	1 (8%)	14,17,17	0.57	0
10	GOL	H	282	-	5,5,5	0.38	0	5,5,5	0.22	0
8	SO4	H	271	-	4,4,4	0.35	0	6,6,6	0.08	0
8	SO4	C	349	-	4,4,4	0.47	0	6,6,6	0.26	0
10	GOL	C	362	-	5,5,5	0.70	0	5,5,5	0.85	0
6	LDA	M	717	-	12,15,15	1.94	1 (8%)	14,17,17	0.58	0
8	SO4	M	326	-	4,4,4	0.19	0	6,6,6	0.45	0
10	GOL	H	275	-	5,5,5	0.67	0	5,5,5	0.38	0
10	GOL	C	375	-	5,5,5	0.28	0	5,5,5	0.19	0
6	LDA	H	720	-	12,15,15	2.23	1 (8%)	14,17,17	0.76	0
8	SO4	C	339	-	4,4,4	0.32	0	6,6,6	0.43	0
10	GOL	H	285	-	5,5,5	0.18	0	5,5,5	0.56	0
8	SO4	C	343	-	4,4,4	0.16	0	6,6,6	0.83	0
9	HTO	L	280	-	9,9,9	0.43	0	10,10,10	1.04	1 (10%)
10	GOL	M	340	-	5,5,5	0.47	0	5,5,5	0.57	0
8	SO4	H	261[B]	-	4,4,4	0.30	0	6,6,6	0.42	0
8	SO4	H	261[A]	-	4,4,4	0.41	0	6,6,6	0.33	0
10	GOL	L	283	-	5,5,5	0.41	0	5,5,5	0.54	0
8	SO4	C	347	-	4,4,4	0.56	0	6,6,6	0.18	0
8	SO4	C	341	-	4,4,4	0.35	0	6,6,6	0.31	0
8	SO4	M	330	-	4,4,4	0.42	0	6,6,6	0.15	0
10	GOL	L	285	-	5,5,5	0.55	0	5,5,5	0.74	0
10	GOL	H	278	-	5,5,5	0.47	0	5,5,5	0.79	0
6	LDA	M	715	-	12,15,15	2.08	1 (8%)	14,17,17	0.46	0
10	GOL	M	337	-	5,5,5	0.34	0	5,5,5	0.36	0
9	HTO	L	279	-	9,9,9	0.39	0	10,10,10	1.46	1 (10%)
10	GOL	H	283	-	5,5,5	0.18	0	5,5,5	0.96	0
8	SO4	H	268	-	4,4,4	0.29	0	6,6,6	0.19	0
10	GOL	C	372	-	5,5,5	0.29	0	5,5,5	0.61	0
6	LDA	C	716	-	12,15,15	2.00	1 (8%)	14,17,17	0.68	0
10	GOL	C	369	-	5,5,5	0.39	0	5,5,5	0.63	0
6	LDA	H	701	-	12,15,15	1.54	1 (8%)	14,17,17	0.93	0
10	GOL	C	359	-	5,5,5	0.83	0	5,5,5	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEC	C	402	1	26,50,50	0.74	0	18,82,82	1.73	5 (27%)
8	SO4	C	344	-	4,4,4	0.41	0	6,6,6	0.17	0
12	BPB	L	402	-	64,70,70	0.95	2 (3%)	64,101,101	1.52	13 (20%)
13	UQ9	L	503	-	23,23,58	2.27	8 (34%)	28,31,73	1.52	4 (14%)
8	SO4	H	267	-	4,4,4	0.27	0	6,6,6	0.16	0
10	GOL	H	284	-	5,5,5	0.36	0	5,5,5	0.80	0
8	SO4	C	352	-	4,4,4	0.31	0	6,6,6	0.15	0
10	GOL	H	276[A]	-	5,5,5	0.83	0	5,5,5	0.58	0
10	GOL	C	363	-	5,5,5	0.79	0	5,5,5	1.07	0
8	SO4	H	270	-	4,4,4	0.34	0	6,6,6	0.14	0
8	SO4	M	324	-	4,4,4	0.35	0	6,6,6	0.87	0
6	LDA	H	721	-	12,15,15	1.86	1 (8%)	14,17,17	0.59	0
16	NS5	M	600	-	39,39,39	1.82	12 (30%)	44,46,46	2.72	14 (31%)
9	HTO	L	276	-	9,9,9	0.47	0	10,10,10	1.55	2 (20%)
10	GOL	C	374[B]	-	5,5,5	0.35	0	5,5,5	0.39	0
10	GOL	M	336	-	5,5,5	0.16	0	5,5,5	1.01	0
8	SO4	M	327	-	4,4,4	0.42	0	6,6,6	0.25	0
10	GOL	C	365	-	5,5,5	0.35	0	5,5,5	0.36	0
10	GOL	M	338	-	5,5,5	0.41	0	5,5,5	0.47	0
6	LDA	L	702	-	12,15,15	2.07	1 (8%)	14,17,17	0.64	0
10	GOL	H	277	-	5,5,5	0.41	0	5,5,5	0.54	0
11	BCB	L	401	3	60,74,74	3.57	20 (33%)	48,115,115	2.16	13 (27%)
8	SO4	M	331	-	4,4,4	0.35	0	6,6,6	0.13	0
10	GOL	C	366	-	5,5,5	0.47	0	5,5,5	0.41	0
7	DGA	C	730	1	36,36,43	0.85	2 (5%)	38,38,45	1.48	6 (15%)
10	GOL	M	339	-	5,5,5	0.25	0	5,5,5	0.31	0
8	SO4	H	260	-	4,4,4	0.35	0	6,6,6	0.28	0
10	GOL	L	288	-	5,5,5	0.15	0	5,5,5	0.61	0
8	SO4	H	264	-	4,4,4	0.33	0	6,6,6	0.16	0
8	SO4	H	263	-	4,4,4	0.38	0	6,6,6	0.31	0
8	SO4	C	342	-	4,4,4	0.39	0	6,6,6	0.27	0
10	GOL	C	370	-	5,5,5	0.27	0	5,5,5	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	H	290	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	L	703	-	-	6/13/13/13	-
17	HTH	M	332	-	-	7/10/10/10	-
10	GOL	M	335	-	-	0/4/4/4	-
10	GOL	C	377	-	-	2/4/4/4	-
15	MQ9	M	501	-	-	2/53/73/73	0/2/2/2
5	HEC	C	401	1	-	0/6/54/54	-
10	GOL	M	342	-	-	4/4/4/4	-
9	HTO	H	274[A]	-	-	4/10/10/10	-
10	GOL	L	285	-	-	2/4/4/4	-
9	HTO	M	333	-	-	7/10/10/10	-
10	GOL	H	287	-	-	4/4/4/4	-
10	GOL	C	361	-	-	0/4/4/4	-
6	LDA	L	710	-	-	8/13/13/13	-
10	GOL	L	284	-	-	4/4/4/4	-
11	BCB	L	400	3	-	9/41/177/177	-
10	GOL	L	286	-	-	4/4/4/4	-
10	GOL	C	373	-	-	2/4/4/4	-
10	GOL	C	378	-	-	2/4/4/4	-
9	HTO	H	273	-	-	4/10/10/10	-
6	LDA	M	705	-	-	6/13/13/13	-
6	LDA	H	718[B]	-	-	8/13/13/13	-
9	HTO	C	357	-	-	6/10/10/10	-
9	HTO	C	358[A]	-	-	10/10/10/10	-
6	LDA	L	708	-	-	8/13/13/13	-
10	GOL	C	376	-	-	2/4/4/4	-
10	GOL	M	341	-	-	0/4/4/4	-
6	LDA	M	713	-	-	4/13/13/13	-
10	GOL	H	279	-	-	1/4/4/4	-
10	GOL	H	288	-	-	2/4/4/4	-
5	HEC	C	404	1	-	0/6/54/54	-
9	HTO	H	272	-	-	1/10/10/10	-
9	HTO	C	355	-	-	4/10/10/10	-
6	LDA	L	723	-	-	8/13/13/13	-
10	GOL	H	276[B]	-	-	2/4/4/4	-
5	HEC	C	403	1	-	0/6/54/54	-
10	GOL	C	367	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	L	282	-	-	2/4/4/4	-
12	BPB	M	402	-	-	10/47/105/105	0/5/6/6
10	GOL	C	368	-	-	4/4/4/4	-
6	LDA	M	707	-	-	7/13/13/13	-
10	GOL	C	364	-	-	4/4/4/4	-
10	GOL	H	291	-	-	2/4/4/4	-
10	GOL	C	360	-	-	0/4/4/4	-
10	GOL	M	334	-	-	4/4/4/4	-
13	UQ9	L	502	-	-	15/57/81/81	0/1/1/1
10	GOL	H	289	-	-	4/4/4/4	-
9	HTO	C	356	-	-	9/10/10/10	-
10	GOL	L	281	-	-	0/4/4/4	-
11	BCB	M	401	4	-	12/41/177/177	-
6	LDA	H	719	-	-	8/13/13/13	-
9	HTO	L	277	-	-	0/10/10/10	-
6	LDA	M	704	-	-	5/13/13/13	-
6	LDA	M	714	-	-	8/13/13/13	-
6	LDA	L	712	-	-	7/13/13/13	-
10	GOL	H	286	-	-	3/4/4/4	-
10	GOL	H	281	-	-	3/4/4/4	-
6	LDA	L	711	-	-	4/13/13/13	-
6	LDA	L	709	-	-	6/13/13/13	-
11	BCB	M	400	4	-	16/41/177/177	-
10	GOL	L	287	-	-	0/4/4/4	-
6	LDA	C	722	-	-	9/13/13/13	-
10	GOL	C	371	-	-	1/4/4/4	-
10	GOL	H	280	-	-	2/4/4/4	-
6	LDA	L	724	-	-	6/13/13/13	-
10	GOL	H	275	-	-	2/4/4/4	-
6	LDA	M	706	-	-	8/13/13/13	-
10	GOL	H	282	-	-	2/4/4/4	-
10	GOL	C	374[B]	-	-	4/4/4/4	-
10	GOL	C	362	-	-	2/4/4/4	-
6	LDA	M	717	-	-	2/13/13/13	-
6	LDA	H	720	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTO	L	278	-	-	4/10/10/10	-
10	GOL	H	285	-	-	4/4/4/4	-
9	HTO	L	280	-	-	5/10/10/10	-
10	GOL	M	340	-	-	3/4/4/4	-
10	GOL	L	283	-	-	2/4/4/4	-
10	GOL	H	278	-	-	2/4/4/4	-
6	LDA	M	715	-	-	5/13/13/13	-
10	GOL	M	337	-	-	2/4/4/4	-
9	HTO	L	279	-	-	3/10/10/10	-
10	GOL	H	283	-	-	4/4/4/4	-
10	GOL	C	375	-	-	0/4/4/4	-
10	GOL	C	372	-	-	2/4/4/4	-
6	LDA	C	716	-	-	10/13/13/13	-
10	GOL	C	369	-	-	2/4/4/4	-
6	LDA	H	701	-	-	4/13/13/13	-
10	GOL	C	359	-	-	2/4/4/4	-
5	HEC	C	402	1	-	1/6/54/54	-
10	GOL	H	277	-	-	2/4/4/4	-
12	BPB	L	402	-	-	5/47/105/105	0/5/6/6
13	UQ9	L	503	-	-	3/15/39/81	0/1/1/1
10	GOL	H	284	-	-	2/4/4/4	-
10	GOL	H	276[A]	-	-	4/4/4/4	-
10	GOL	C	363	-	-	0/4/4/4	-
6	LDA	H	721	-	-	10/13/13/13	-
16	NS5	M	600	-	-	8/43/43/43	-
9	HTO	L	276	-	-	6/10/10/10	-
10	GOL	M	336	-	-	4/4/4/4	-
10	GOL	C	365	-	-	2/4/4/4	-
10	GOL	M	338	-	-	4/4/4/4	-
6	LDA	L	702	-	-	7/13/13/13	-
11	BCB	L	401	3	-	9/41/177/177	-
10	GOL	C	366	-	-	3/4/4/4	-
7	DGA	C	730	1	-	26/37/37/45	-
10	GOL	M	339	-	-	2/4/4/4	-
10	GOL	L	288	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	C	370	-	-	2/4/4/4	-

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	L	401	BCB	CHD-C1D	-10.08	1.37	1.53
11	L	400	BCB	CHD-C1D	-9.85	1.38	1.53
11	M	400	BCB	C1A-CHA	-9.82	1.38	1.54
11	L	400	BCB	C4D-ND	-9.81	1.29	1.50
11	M	401	BCB	CHD-C1D	-9.67	1.38	1.53
11	L	400	BCB	C1A-CHA	-9.12	1.39	1.54
11	L	400	BCB	CHC-C4B	-9.06	1.39	1.53
11	L	400	BCB	CHB-C1B	-9.04	1.39	1.53
11	M	401	BCB	CHC-C4B	-8.68	1.39	1.53
11	M	401	BCB	C1A-CHA	-8.65	1.40	1.54
11	M	400	BCB	C4D-ND	-8.60	1.32	1.50
11	M	400	BCB	CHB-C1B	-8.36	1.40	1.53
11	M	401	BCB	CHD-C4C	-8.33	1.39	1.53
11	M	401	BCB	CHB-C1B	-8.24	1.40	1.53
11	L	401	BCB	C1A-CHA	-8.14	1.41	1.54
6	M	704	LDA	O1-N1	-7.97	1.23	1.42
11	L	401	BCB	CHB-C1B	-7.72	1.41	1.53
11	L	400	BCB	C2B-C1B	-7.71	1.39	1.53
6	H	720	LDA	O1-N1	-7.66	1.24	1.42
11	M	401	BCB	C4D-ND	-7.61	1.34	1.50
6	M	714	LDA	O1-N1	-7.61	1.24	1.42
11	L	400	BCB	CHD-C4C	-7.59	1.40	1.53
6	L	724	LDA	O1-N1	-7.52	1.24	1.42
11	M	400	BCB	CHC-C4B	-7.49	1.41	1.53
11	L	401	BCB	C4D-ND	-7.48	1.34	1.50
11	M	400	BCB	CHD-C1D	-7.47	1.41	1.53
6	M	707	LDA	O1-N1	-7.37	1.24	1.42
11	M	401	BCB	C2D-C1D	-7.36	1.40	1.53
6	L	703	LDA	O1-N1	-7.27	1.25	1.42
11	L	401	BCB	CHC-C4B	-7.23	1.42	1.53
6	L	710	LDA	O1-N1	-7.19	1.25	1.42
6	L	712	LDA	O1-N1	-7.18	1.25	1.42
11	L	400	BCB	C2D-C1D	-7.13	1.40	1.53
6	L	702	LDA	O1-N1	-7.11	1.25	1.42
6	L	711	LDA	O1-N1	-7.10	1.25	1.42
11	M	400	BCB	C2D-C1D	-7.10	1.40	1.53
6	L	723	LDA	O1-N1	-6.97	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	715	LDA	O1-N1	-6.97	1.25	1.42
11	M	400	BCB	CHD-C4C	-6.87	1.41	1.53
6	H	718[B]	LDA	O1-N1	-6.85	1.26	1.42
6	H	719	LDA	O1-N1	-6.84	1.26	1.42
11	L	401	BCB	C2B-C1B	-6.83	1.41	1.53
11	M	401	BCB	C1D-ND	-6.82	1.35	1.50
6	M	713	LDA	O1-N1	-6.82	1.26	1.42
6	C	716	LDA	O1-N1	-6.81	1.26	1.42
6	L	708	LDA	O1-N1	-6.77	1.26	1.42
6	C	722	LDA	O1-N1	-6.77	1.26	1.42
6	L	709	LDA	O1-N1	-6.72	1.26	1.42
6	M	717	LDA	O1-N1	-6.69	1.26	1.42
13	L	502	UQ9	C7-C8	-6.68	1.41	1.50
13	L	503	UQ9	C7-C8	-6.66	1.41	1.50
6	M	706	LDA	O1-N1	-6.64	1.26	1.42
11	L	401	BCB	CHC-C1C	-6.60	1.37	1.52
11	M	400	BCB	C1D-ND	-6.57	1.36	1.50
11	M	400	BCB	CHC-C1C	-6.43	1.38	1.52
6	H	721	LDA	O1-N1	-6.40	1.27	1.42
11	L	400	BCB	CHC-C1C	-6.38	1.38	1.52
6	M	705	LDA	O1-N1	-6.37	1.27	1.42
11	M	401	BCB	CHC-C1C	-6.06	1.39	1.52
11	L	401	BCB	CHD-C4C	-6.04	1.43	1.53
11	M	400	BCB	C3B-C2B	-6.03	1.39	1.55
11	L	400	BCB	C1D-ND	-5.97	1.37	1.50
11	L	400	BCB	C4B-NB	-5.95	1.37	1.50
11	L	401	BCB	CHB-C4A	-5.85	1.39	1.52
11	L	401	BCB	C1D-ND	-5.84	1.37	1.50
11	L	400	BCB	C3B-C2B	-5.80	1.40	1.55
11	L	401	BCB	C2D-C1D	-5.72	1.43	1.53
11	M	401	BCB	C2B-C1B	-5.68	1.43	1.53
11	L	401	BCB	C1B-NB	-5.51	1.38	1.50
11	L	401	BCB	C3D-C2D	-5.42	1.41	1.55
11	L	400	BCB	C3D-C2D	-5.34	1.41	1.55
11	L	401	BCB	C4B-NB	-5.25	1.39	1.50
11	L	400	BCB	CHB-C4A	-5.21	1.40	1.52
6	H	701	LDA	O1-N1	-5.19	1.30	1.42
11	M	401	BCB	CHB-C4A	-5.14	1.41	1.52
11	L	400	BCB	C1B-NB	-5.13	1.39	1.50
15	M	501	MQ9	C7-C8	-5.09	1.43	1.50
11	M	400	BCB	C3D-C2D	-5.08	1.42	1.55
11	L	401	BCB	C3B-C2B	-5.06	1.42	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	401	BCB	C4B-NB	-5.00	1.39	1.50
11	M	401	BCB	C3D-C2D	-4.98	1.42	1.55
11	M	401	BCB	C3B-C2B	-4.96	1.42	1.55
15	M	501	MQ9	C2-C1	-4.65	1.39	1.48
15	M	501	MQ9	C6-C5	4.49	1.43	1.35
11	L	401	BCB	C3D-CAD	-4.40	1.43	1.51
11	M	400	BCB	C2B-C1B	-4.38	1.45	1.53
11	L	400	BCB	C3D-CAD	-4.33	1.43	1.51
11	M	400	BCB	C1B-NB	-4.28	1.41	1.50
11	M	401	BCB	C1B-NB	-4.21	1.41	1.50
16	M	600	NS5	C20-C21	4.12	1.41	1.35
12	M	402	BPB	C1C-NC	-3.90	1.31	1.38
11	M	400	BCB	CHB-C4A	-3.88	1.43	1.52
16	M	600	NS5	C30-C31	3.82	1.38	1.34
11	L	401	BCB	C4A-C3A	3.80	1.57	1.53
15	M	501	MQ9	C5-C4	-3.78	1.39	1.48
15	M	501	MQ9	C43-C44	3.72	1.41	1.33
15	M	501	MQ9	C33-C34	3.66	1.41	1.33
11	M	400	BCB	C4B-NB	-3.59	1.42	1.50
15	M	501	MQ9	C8-C9	3.46	1.41	1.33
15	M	501	MQ9	C5M-C5	3.43	1.58	1.50
13	L	502	UQ9	C42-C43	-3.41	1.39	1.50
15	M	501	MQ9	C38-C39	3.37	1.41	1.33
11	M	401	BCB	O2D-CGD	3.37	1.41	1.33
11	M	401	BCB	CBD-CGD	3.36	1.57	1.52
12	M	402	BPB	C3B-C4B	3.35	1.45	1.41
13	L	502	UQ9	C8-C9	3.33	1.41	1.33
13	L	502	UQ9	C32-C33	-3.30	1.39	1.50
13	L	502	UQ9	C4-C5	-3.27	1.39	1.48
13	L	502	UQ9	C47-C48	-3.26	1.39	1.50
11	M	401	BCB	C3D-CAD	-3.25	1.45	1.51
15	M	501	MQ9	C28-C29	3.25	1.40	1.33
15	M	501	MQ9	C37-C38	-3.23	1.39	1.50
13	L	502	UQ9	C22-C23	-3.22	1.39	1.50
13	L	502	UQ9	C3-C2	-3.20	1.39	1.48
13	L	502	UQ9	C27-C28	-3.16	1.40	1.50
13	L	503	UQ9	C8-C9	3.16	1.40	1.33
13	L	502	UQ9	C6-C1	3.14	1.40	1.35
13	L	502	UQ9	C28-C29	3.14	1.40	1.33
13	L	502	UQ9	C12-C13	-3.14	1.40	1.50
11	M	400	BCB	CBD-CAD	-3.13	1.48	1.53
13	L	502	UQ9	C38-C39	3.13	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	502	UQ9	C18-C19	3.10	1.40	1.33
15	M	501	MQ9	C27-C28	-3.04	1.40	1.50
15	M	501	MQ9	C47-C48	-3.02	1.40	1.50
12	L	402	BPB	C3B-C4B	3.02	1.45	1.41
13	L	503	UQ9	C12-C13	-3.00	1.40	1.50
11	M	401	BCB	CBD-CAD	-2.98	1.48	1.53
13	L	503	UQ9	C6-C1	2.98	1.40	1.35
15	M	501	MQ9	C18-C19	2.96	1.40	1.33
15	M	501	MQ9	C32-C33	-2.95	1.40	1.50
16	M	600	NS5	C24-C25	2.95	1.52	1.43
15	M	501	MQ9	C22-C23	-2.94	1.40	1.50
13	L	502	UQ9	C17-C18	-2.94	1.40	1.50
13	L	502	UQ9	C48-C49	2.91	1.40	1.32
13	L	502	UQ9	C37-C38	-2.90	1.41	1.50
13	L	502	UQ9	C6-C5	-2.88	1.38	1.46
16	M	600	NS5	C23-C21	2.88	1.52	1.45
13	L	503	UQ9	C3-C2	-2.86	1.40	1.48
13	L	502	UQ9	C13-C14	2.85	1.39	1.33
15	M	501	MQ9	C6-C1	-2.84	1.40	1.47
11	M	400	BCB	C4C-C3C	-2.83	1.42	1.50
16	M	600	NS5	C29-C30	2.80	1.52	1.43
5	C	401	HEC	CAD-C3D	-2.79	1.47	1.52
15	M	501	MQ9	C42-C43	-2.78	1.41	1.50
13	L	503	UQ9	C13-C14	2.76	1.40	1.32
13	L	502	UQ9	C23-C24	2.75	1.39	1.33
11	L	400	BCB	O2D-CGD	2.75	1.39	1.33
11	M	401	BCB	CAA-CBA	-2.74	1.44	1.52
11	L	401	BCB	C4C-C3C	-2.73	1.42	1.50
13	L	503	UQ9	C4-C5	-2.73	1.41	1.48
15	M	501	MQ9	C48-C49	2.73	1.40	1.32
15	M	501	MQ9	C12-C13	-2.68	1.41	1.50
13	L	502	UQ9	C33-C34	2.64	1.39	1.33
11	L	401	BCB	CMA-C3A	2.64	1.58	1.53
16	M	600	NS5	C17-C15	2.63	1.39	1.35
7	C	730	DGA	CG1-CG2	2.58	1.56	1.50
12	M	402	BPB	C1D-C2D	-2.58	1.40	1.45
13	L	502	UQ9	C43-C44	2.56	1.39	1.33
13	L	503	UQ9	C7-C6	2.55	1.55	1.51
16	M	600	NS5	C28-C26	2.54	1.51	1.45
5	C	403	HEC	CAA-C2A	-2.53	1.47	1.52
11	L	401	BCB	C2A-C3A	-2.52	1.50	1.54
11	M	401	BCB	OBD-CAD	2.52	1.25	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	M	501	MQ9	C41-C39	2.48	1.56	1.51
11	L	400	BCB	C4C-C3C	-2.44	1.43	1.50
13	L	502	UQ9	C7-C6	2.43	1.55	1.51
15	M	501	MQ9	C17-C18	-2.42	1.42	1.50
12	L	402	BPB	C2C-C3C	2.40	1.55	1.51
16	M	600	NS5	C22-C21	2.40	1.55	1.50
15	M	501	MQ9	C23-C24	2.40	1.38	1.33
16	M	600	NS5	C16-C15	2.39	1.55	1.50
15	M	501	MQ9	C46-C44	2.38	1.56	1.51
16	M	600	NS5	C19-C20	2.34	1.50	1.43
11	M	400	BCB	C3B-CAB	-2.33	1.49	1.52
5	C	404	HEC	C1C-CHC	-2.28	1.34	1.41
16	M	600	NS5	C13-C12	2.23	1.50	1.43
5	C	403	HEC	C3B-C4B	-2.22	1.39	1.43
11	M	401	BCB	C4C-C3C	-2.21	1.44	1.50
15	M	501	MQ9	O4-C4	2.21	1.27	1.23
5	C	403	HEC	C2A-C3A	2.19	1.44	1.37
11	M	401	BCB	CHA-CBD	-2.18	1.46	1.53
16	M	600	NS5	C33-C31	2.16	1.55	1.51
12	M	402	BPB	C3D-C4D	-2.05	1.37	1.43
7	C	730	DGA	CA2-CA1	2.02	1.56	1.50
11	M	401	BCB	O2A-CGA	2.01	1.39	1.33
5	C	404	HEC	CAD-C3D	-2.01	1.49	1.52
13	L	502	UQ9	C25-C24	2.00	1.55	1.50

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	CBA-CAA-C2A	-8.01	104.82	115.72
11	M	401	BCB	C1D-CHD-C4C	7.80	128.99	112.37
11	L	401	BCB	CMB-C2B-C3B	7.47	132.83	114.29
11	M	400	BCB	C1D-CHD-C4C	7.18	127.67	112.37
11	L	400	BCB	C1D-CHD-C4C	6.94	127.17	112.37
11	M	401	BCB	CMB-C2B-C3B	6.77	131.10	114.29
16	M	600	NS5	C11-C10-C9	6.71	126.55	115.27
16	M	600	NS5	C14-C15-C17	-6.70	108.65	118.94
16	M	600	NS5	C19-C20-C21	-6.70	117.75	127.31
11	L	400	BCB	CMB-C2B-C3B	6.70	130.92	114.29
11	M	401	BCB	O2D-CGD-O1D	-6.67	110.80	123.84
9	M	333	HTO	C5-C4-C3	-6.60	103.33	114.18
9	C	358[A]	HTO	C5-C4-C3	-5.84	104.58	114.18
16	M	600	NS5	C16-C15-C17	5.82	131.08	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	CMB-C2B-C3B	5.75	128.57	114.29
11	L	401	BCB	C1D-CHD-C4C	5.75	124.62	112.37
11	M	401	BCB	O2D-CGD-CBD	5.73	124.57	111.11
16	M	600	NS5	C18-C19-C20	5.28	134.29	123.47
7	C	730	DGA	CG2-OG2-CB1	-5.23	111.15	117.88
11	M	401	BCB	CHA-CBD-CGD	-4.88	103.98	115.02
11	L	401	BCB	CBA-CAA-C2A	-4.88	109.09	115.72
16	M	600	NS5	C24-C25-C26	-4.52	120.85	127.31
13	L	503	UQ9	C7-C8-C9	4.51	134.30	126.79
12	L	402	BPB	CBD-CHA-C4D	-4.46	103.51	108.54
5	C	401	HEC	CMC-C2C-C3C	4.38	130.97	125.82
9	C	356	HTO	O3-C3-C2	-4.35	100.80	109.72
13	L	502	UQ9	C25-C24-C26	4.29	122.49	115.27
12	L	402	BPB	C4B-CHC-C1C	4.17	133.95	128.57
6	M	704	LDA	CM1-N1-C1	-4.15	101.52	110.23
12	M	402	BPB	CMB-C2B-C3B	4.11	132.37	124.68
16	M	600	NS5	C6-C5-C4	4.04	122.07	115.27
7	C	730	DGA	OG2-CB1-CB2	4.00	120.13	111.50
11	L	400	BCB	C3B-C4B-NB	3.94	110.93	103.75
12	M	402	BPB	C4B-C3B-CAB	-3.92	118.69	127.19
13	L	502	UQ9	C30-C29-C31	3.91	121.84	115.27
16	M	600	NS5	C12-C13-C14	-3.82	111.28	123.22
5	C	401	HEC	CMB-C2B-C3B	3.82	130.31	125.82
5	C	401	HEC	CMC-C2C-C1C	-3.81	122.61	128.46
5	C	404	HEC	C1D-C2D-C3D	-3.81	104.35	107.00
11	L	401	BCB	CMD-C2D-C3D	3.80	123.73	114.29
5	C	402	HEC	CMC-C2C-C3C	3.80	130.28	125.82
9	C	358[A]	HTO	O3-C3-C4	-3.77	100.95	109.15
9	L	277	HTO	C5-C4-C3	-3.71	108.09	114.18
11	M	401	BCB	C3B-C4B-NB	3.65	110.41	103.75
11	M	400	BCB	C1-C2-C3	-3.65	119.73	126.04
11	L	401	BCB	C4-C3-C5	3.65	121.41	115.27
11	L	400	BCB	O2A-CGA-O1A	-3.63	114.43	123.59
11	L	400	BCB	CHA-CBD-CGD	-3.62	106.82	115.02
16	M	600	NS5	C8-C7-C5	-3.62	118.95	127.66
9	C	358[A]	HTO	O1-C1-C2	-3.60	103.22	111.07
11	L	400	BCB	C4-C3-C5	3.60	121.33	115.27
11	M	400	BCB	CMD-C2D-C3D	3.57	123.15	114.29
11	L	400	BCB	OBB-CAB-C3B	-3.55	117.78	121.52
13	L	502	UQ9	C35-C34-C36	3.50	121.16	115.27
11	M	401	BCB	C1-C2-C3	-3.47	120.04	126.04
11	M	401	BCB	CHC-C4B-C3B	3.43	126.58	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	502	UQ9	C1M-C1-C6	-3.39	118.86	124.40
11	M	401	BCB	CED-O2D-CGD	3.37	123.55	115.94
11	M	401	BCB	CHC-C1C-C2C	3.36	127.33	117.19
11	M	400	BCB	C4-C3-C5	3.34	120.89	115.27
11	M	400	BCB	CHC-C4B-C3B	3.29	126.25	118.17
11	L	400	BCB	O2D-CGD-CBD	3.29	118.84	111.11
11	M	400	BCB	C3B-C4B-NB	3.29	109.75	103.75
9	M	333	HTO	O1-C1-C2	-3.25	103.98	111.07
13	L	503	UQ9	C1-C6-C5	-3.23	116.55	119.58
11	L	401	BCB	CHC-C4B-C3B	3.21	126.03	118.17
15	M	501	MQ9	C40-C39-C38	-3.18	115.52	123.68
13	L	502	UQ9	C7-C8-C9	3.14	132.01	126.79
6	L	708	LDA	CM1-N1-C1	-3.13	103.65	110.23
11	M	401	BCB	O2A-CGA-CBA	3.12	121.71	111.91
9	H	272	HTO	C5-C4-C3	-3.12	109.05	114.18
6	M	704	LDA	CM2-N1-C1	3.12	116.78	110.23
16	M	600	NS5	C32-C31-C33	3.11	120.50	115.27
15	M	501	MQ9	C5M-C5-C6	-3.10	119.34	124.40
12	L	402	BPB	CED-O2D-CGD	3.07	122.87	115.94
11	L	401	BCB	C3B-C4B-NB	3.07	109.34	103.75
15	M	501	MQ9	C15-C14-C16	3.02	120.35	115.27
7	C	730	DGA	OG1-CA1-CA2	3.00	121.33	111.91
5	C	401	HEC	CMB-C2B-C1B	-2.99	123.87	128.46
11	L	400	BCB	CMD-C2D-C3D	2.99	121.70	114.29
5	C	402	HEC	CMC-C2C-C1C	-2.98	123.88	128.46
5	C	401	HEC	CAD-CBD-CGD	2.97	117.66	112.67
7	C	730	DGA	OG2-CG2-CG1	2.93	112.93	106.13
5	C	404	HEC	CMB-C2B-C1B	-2.92	123.98	128.46
9	L	278	HTO	O2-C2-C1	-2.89	102.35	109.14
11	L	400	BCB	CHC-C4B-C3B	2.89	125.26	118.17
17	M	332	HTH	O3-C3-C2	-2.88	103.81	109.72
13	L	502	UQ9	C7-C6-C5	-2.87	115.02	118.48
12	L	402	BPB	CHB-C4A-NA	-2.86	121.80	125.20
15	M	501	MQ9	C35-C34-C36	2.86	120.08	115.27
11	M	401	BCB	CMD-C2D-C3D	2.84	121.34	114.29
11	M	401	BCB	OBD-CAD-CBD	-2.81	120.75	127.49
5	C	402	HEC	CMB-C2B-C1B	-2.79	124.17	128.46
11	M	400	BCB	OBD-CAD-CBD	-2.78	120.82	127.49
11	L	401	BCB	C6-C5-C3	-2.78	106.18	113.45
6	L	708	LDA	O1-N1-C1	2.76	116.04	109.27
11	L	400	BCB	C1-C2-C3	-2.74	121.30	126.04
5	C	404	HEC	C4B-C3B-C2B	-2.73	103.40	106.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	502	UQ9	C6-C1-C2	2.73	121.34	119.18
9	L	278	HTO	O1-C1-C2	-2.72	105.16	111.07
9	H	272	HTO	O1-C1-C2	-2.71	105.16	111.07
5	C	404	HEC	CMB-C2B-C3B	2.70	128.99	125.82
11	M	400	BCB	O2D-CGD-CBD	2.69	117.43	111.11
5	C	401	HEC	C4C-C3C-C2C	-2.68	103.46	106.35
16	M	600	NS5	C9-C10-C12	-2.66	113.94	121.98
12	L	402	BPB	C3D-C4D-CHA	2.65	116.65	109.49
12	M	402	BPB	C3D-C4D-CHA	2.63	116.59	109.49
11	L	401	BCB	OBD-CAD-C3D	-2.63	122.10	126.73
13	L	502	UQ9	C45-C44-C46	2.61	119.66	115.27
13	L	502	UQ9	C1-C6-C5	-2.60	117.14	119.58
9	C	358[A]	HTO	O2-C2-C1	-2.60	103.06	109.14
15	M	501	MQ9	C25-C24-C26	2.59	119.62	115.27
12	L	402	BPB	CMB-C2B-C3B	2.58	129.51	124.68
9	L	276	HTO	O2-C2-C3	-2.56	104.47	109.72
11	L	400	BCB	O2A-CGA-CBA	2.56	119.93	111.91
11	L	401	BCB	O1D-CGD-CBD	-2.55	119.49	124.54
12	L	402	BPB	O1D-CGD-CBD	-2.55	119.27	124.48
5	C	403	HEC	CMA-C3A-C2A	2.54	129.72	124.94
13	L	502	UQ9	O5-C5-C6	-2.53	117.12	121.55
12	L	402	BPB	C2A-C3A-C4A	-2.49	97.84	101.87
11	L	400	BCB	OBD-CAD-CBD	-2.47	121.55	127.49
11	L	401	BCB	CHC-C1C-C2C	2.47	124.66	117.19
15	M	501	MQ9	C40-C39-C41	2.45	119.40	115.27
11	L	400	BCB	C5-C3-C2	-2.44	116.17	121.12
12	M	402	BPB	C2A-C3A-C4A	-2.43	97.94	101.87
11	M	400	BCB	O2A-CGA-CBA	2.43	119.52	111.91
9	L	276	HTO	O3-C3-C4	2.42	114.41	109.15
9	L	278	HTO	O2-C2-C3	2.39	114.64	109.72
5	C	401	HEC	CBD-CAD-C3D	-2.38	108.11	112.49
11	L	401	BCB	C5-C3-C2	-2.37	116.32	121.12
15	M	501	MQ9	C3D-C2-C3	2.34	121.86	119.26
9	C	355	HTO	O2-C2-C1	2.33	114.61	109.14
11	M	401	BCB	C4-C3-C5	2.32	119.17	115.27
16	M	600	NS5	C24-C23-C21	-2.31	119.92	126.42
12	L	402	BPB	CBC-CAC-C3C	-2.31	119.97	126.72
12	M	402	BPB	CBD-CHA-C4D	-2.31	105.94	108.54
11	M	400	BCB	CHC-C1C-C2C	2.30	124.13	117.19
9	H	272	HTO	O2-C2-C1	-2.30	103.76	109.14
13	L	502	UQ9	C45-C44-C43	-2.29	117.79	123.68
16	M	600	NS5	C27-C26-C28	2.29	121.68	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	502	UQ9	O2-C2-C3	-2.28	116.10	120.93
11	L	401	BCB	O2D-CGD-CBD	2.26	116.41	111.11
6	M	704	LDA	O1-N1-C1	2.25	114.80	109.27
9	L	280	HTO	C5-C4-C3	-2.25	110.49	114.18
13	L	503	UQ9	C8-C7-C6	-2.22	106.05	112.05
9	M	333	HTO	O3-C3-C4	-2.21	104.34	109.15
12	M	402	BPB	C1-O2A-CGA	2.21	122.24	116.44
13	L	503	UQ9	C15-C14-C16	2.20	119.47	114.60
11	L	400	BCB	O2D-CGD-O1D	-2.20	119.53	123.84
12	M	402	BPB	C4D-ND-C1D	2.20	110.72	106.76
9	H	273	HTO	O1-C1-C2	2.19	115.85	111.07
12	L	402	BPB	C4B-C3B-CAB	-2.19	122.44	127.19
11	L	400	BCB	CBB-CAB-C3B	2.19	119.03	116.80
5	C	402	HEC	CAD-CBD-CGD	2.18	116.32	112.67
11	L	400	BCB	CHC-C1C-C2C	2.17	123.75	117.19
13	L	502	UQ9	C15-C14-C16	2.17	118.92	115.27
5	C	402	HEC	CMB-C2B-C3B	2.17	128.37	125.82
9	C	356	HTO	C5-C4-C3	2.16	117.73	114.18
16	M	600	NS5	C28-C26-C25	-2.15	115.64	118.94
12	M	402	BPB	CHD-C1D-C2D	2.14	131.12	125.73
9	M	333	HTO	O3-C3-C2	2.13	114.11	109.72
12	L	402	BPB	C3C-C4C-NC	2.13	112.99	109.58
15	M	501	MQ9	C51-C49-C50	2.11	119.27	114.60
10	L	282	GOL	C3-C2-C1	2.10	119.86	111.70
12	L	402	BPB	C1-C2-C3	-2.10	122.42	126.04
12	L	402	BPB	CHD-C1D-C2D	2.09	131.00	125.73
9	L	279	HTO	O3-C3-C4	2.06	113.63	109.15
11	M	400	BCB	O1D-CGD-CBD	-2.05	120.47	124.54
11	M	401	BCB	CAA-CBA-CGA	-2.05	107.26	113.25
7	C	730	DGA	OG1-CA1-OA1	-2.05	118.42	123.59
7	C	730	DGA	OG1-CG1-CG2	2.04	114.27	108.38
11	M	401	BCB	CBA-CAA-C2A	2.04	118.50	115.72
13	L	502	UQ9	C25-C24-C23	-2.03	118.46	123.68
11	M	400	BCB	OBB-CAB-C3B	-2.03	119.37	121.52
9	C	356	HTO	O3-C3-C4	2.03	113.57	109.15
15	M	501	MQ9	C5M-C5-C4	2.03	119.63	116.27
9	C	355	HTO	C4-C3-C2	-2.02	108.56	113.35

There are no chirality outliers.

All (472) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
10	H	290	GOL	C1-C2-C3-O3
6	L	703	LDA	N1-C1-C2-C3
17	M	332	HTH	C1-C2-C3-O3
17	M	332	HTH	O2-C2-C3-C4
9	L	278	HTO	C1-C2-C3-O3
9	L	278	HTO	O2-C2-C3-O3
9	L	278	HTO	O2-C2-C3-C4
10	C	364	GOL	O1-C1-C2-C3
10	M	342	GOL	O1-C1-C2-C3
10	M	342	GOL	C1-C2-C3-O3
9	H	274[A]	HTO	O1-C1-C2-O2
9	H	274[A]	HTO	O1-C1-C2-C3
9	H	274[A]	HTO	C2-C3-C4-C5
9	H	274[A]	HTO	O3-C3-C4-C5
9	M	333	HTO	C1-C2-C3-O3
9	M	333	HTO	C1-C2-C3-C4
9	M	333	HTO	O2-C2-C3-O3
9	M	333	HTO	O2-C2-C3-C4
9	M	333	HTO	O3-C3-C4-C5
10	H	287	GOL	O1-C1-C2-C3
10	H	287	GOL	C1-C2-C3-O3
6	L	710	LDA	C2-C1-N1-CM1
6	L	710	LDA	C2-C1-N1-CM2
10	L	284	GOL	O1-C1-C2-C3
10	L	284	GOL	C1-C2-C3-O3
11	L	400	BCB	C2B-C3B-CAB-OBB
11	L	400	BCB	C2B-C3B-CAB-CBB
10	L	286	GOL	O1-C1-C2-C3
10	L	286	GOL	C1-C2-C3-O3
10	C	373	GOL	O1-C1-C2-O2
10	C	373	GOL	O1-C1-C2-C3
10	C	378	GOL	O1-C1-C2-C3
9	H	273	HTO	C2-C3-C4-C5
6	H	718[B]	LDA	C2-C1-N1-O1
6	H	718[B]	LDA	C2-C1-N1-CM1
6	H	718[B]	LDA	C2-C1-N1-CM2
9	C	357	HTO	C1-C2-C3-C4
9	C	357	HTO	O2-C2-C3-C4
9	C	358[A]	HTO	C1-C2-C3-O3
9	C	358[A]	HTO	C1-C2-C3-C4
9	C	358[A]	HTO	O2-C2-C3-O3
9	C	358[A]	HTO	O2-C2-C3-C4
9	C	358[A]	HTO	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
10	H	288	GOL	O1-C1-C2-C3
9	C	355	HTO	O3-C3-C4-C5
6	L	723	LDA	C2-C1-N1-O1
6	L	723	LDA	C2-C1-N1-CM2
10	C	367	GOL	C1-C2-C3-O3
10	L	282	GOL	O1-C1-C2-C3
10	C	368	GOL	O1-C1-C2-C3
10	C	368	GOL	C1-C2-C3-O3
6	M	707	LDA	C2-C1-N1-CM1
6	M	707	LDA	C2-C1-N1-CM2
6	M	707	LDA	N1-C1-C2-C3
10	H	291	GOL	C1-C2-C3-O3
10	M	334	GOL	C1-C2-C3-O3
13	L	502	UQ9	C39-C41-C42-C43
10	H	289	GOL	O1-C1-C2-C3
10	H	289	GOL	C1-C2-C3-O3
9	C	356	HTO	C1-C2-C3-O3
9	C	356	HTO	C1-C2-C3-C4
9	C	356	HTO	O2-C2-C3-O3
9	C	356	HTO	O2-C2-C3-C4
9	C	356	HTO	O3-C3-C4-C5
11	M	401	BCB	C2A-CAA-CBA-CGA
11	M	401	BCB	C2B-C3B-CAB-OBB
11	M	401	BCB	C2B-C3B-CAB-CBB
11	M	401	BCB	CAD-CBD-CGD-O1D
11	M	401	BCB	CAD-CBD-CGD-O2D
6	M	714	LDA	N1-C1-C2-C3
6	L	712	LDA	N1-C1-C2-C3
10	H	286	GOL	C1-C2-C3-O3
6	C	722	LDA	C2-C1-N1-O1
6	C	722	LDA	N1-C1-C2-C3
10	H	280	GOL	C1-C2-C3-O3
6	L	724	LDA	C2-C1-N1-CM1
6	M	706	LDA	C2-C1-N1-CM1
6	M	706	LDA	C2-C1-N1-CM2
10	H	282	GOL	O1-C1-C2-C3
10	C	362	GOL	C1-C2-C3-O3
10	C	362	GOL	O2-C2-C3-O3
10	H	275	GOL	C1-C2-C3-O3
10	H	285	GOL	C1-C2-C3-O3
10	M	340	GOL	C1-C2-C3-O3
10	L	285	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	H	278	GOL	C1-C2-C3-O3
10	H	278	GOL	O2-C2-C3-O3
9	L	279	HTO	O3-C3-C4-C5
10	H	283	GOL	O1-C1-C2-C3
10	H	283	GOL	C1-C2-C3-O3
6	C	716	LDA	C2-C1-N1-CM1
6	C	716	LDA	N1-C1-C2-C3
12	L	402	BPB	O2A-C1-C2-C3
12	L	402	BPB	C2C-C3C-CAC-CBC
13	L	503	UQ9	C5-C6-C7-C8
10	H	284	GOL	O1-C1-C2-C3
10	H	276[A]	GOL	C1-C2-C3-O3
6	H	721	LDA	C2-C1-N1-CM1
6	H	721	LDA	C2-C1-N1-CM2
16	M	600	NS5	C3-C4-C5-C6
16	M	600	NS5	C3-C4-C5-C7
9	L	276	HTO	C1-C2-C3-O3
9	L	276	HTO	C1-C2-C3-C4
9	L	276	HTO	O2-C2-C3-O3
9	L	276	HTO	O2-C2-C3-C4
10	C	374[B]	GOL	O1-C1-C2-C3
10	C	374[B]	GOL	C1-C2-C3-O3
10	M	336	GOL	O1-C1-C2-C3
10	M	336	GOL	C1-C2-C3-O3
10	C	365	GOL	C1-C2-C3-O3
10	M	338	GOL	O1-C1-C2-C3
10	M	338	GOL	C1-C2-C3-O3
6	L	702	LDA	C2-C1-N1-CM1
11	L	401	BCB	C2B-C3B-CAB-OBB
11	L	401	BCB	C2B-C3B-CAB-CBB
10	C	366	GOL	O1-C1-C2-C3
7	C	730	DGA	CB2-CB1-OG2-CG2
7	C	730	DGA	OB1-CB1-OG2-CG2
7	C	730	DGA	OG1-CG1-CG2-OG2
7	C	730	DGA	OG1-CG1-CG2-CG3
10	L	288	GOL	C1-C2-C3-O3
10	L	288	GOL	O2-C2-C3-O3
6	H	720	LDA	C1-C2-C3-C4
9	H	273	HTO	O1-C1-C2-O2
9	C	357	HTO	O1-C1-C2-O2
9	C	358[A]	HTO	O1-C1-C2-O2
6	L	723	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	H	720	LDA	C3-C4-C5-C6
9	H	273	HTO	O1-C1-C2-C3
9	C	357	HTO	O1-C1-C2-C3
6	M	706	LDA	C3-C4-C5-C6
11	L	400	BCB	C4-C3-C5-C6
12	M	402	BPB	C4-C3-C5-C6
16	M	600	NS5	C11-C10-C9-C8
11	L	400	BCB	C2-C3-C5-C6
12	M	402	BPB	C2-C3-C5-C6
16	M	600	NS5	C12-C10-C9-C8
13	L	502	UQ9	C34-C36-C37-C38
6	C	722	LDA	C3-C4-C5-C6
11	M	400	BCB	C8-C10-C11-C12
10	H	287	GOL	O2-C2-C3-O3
10	C	368	GOL	O2-C2-C3-O3
10	H	289	GOL	O2-C2-C3-O3
10	H	275	GOL	O2-C2-C3-O3
10	L	285	GOL	O1-C1-C2-O2
7	C	730	DGA	CB1-CB2-CB3-CB4
7	C	730	DGA	CA1-CA2-CA3-CA4
11	L	400	BCB	C15-C16-C17-C18
12	M	402	BPB	C11-C12-C13-C15
13	L	502	UQ9	C29-C31-C32-C33
13	L	502	UQ9	C24-C26-C27-C28
6	L	702	LDA	C2-C3-C4-C5
6	L	703	LDA	C5-C6-C7-C8
7	C	730	DGA	CA2-CA1-OG1-CG1
6	M	714	LDA	C5-C6-C7-C8
6	C	722	LDA	C6-C7-C8-C9
7	C	730	DGA	CB5-CB6-CB7-CB8
6	L	710	LDA	C6-C7-C8-C9
6	L	712	LDA	C4-C5-C6-C7
6	H	721	LDA	C3-C4-C5-C6
6	L	702	LDA	C4-C5-C6-C7
6	H	718[B]	LDA	C4-C5-C6-C7
6	C	716	LDA	C3-C4-C5-C6
7	C	730	DGA	CB4-CB5-CB6-CB7
6	M	704	LDA	C2-C3-C4-C5
7	C	730	DGA	CA4-CA5-CA6-CA7
6	H	718[B]	LDA	C3-C4-C5-C6
6	M	704	LDA	C6-C7-C8-C9
7	C	730	DGA	CA5-CA6-CA7-CA8

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Mol	Chain	Res	Type	Atoms
9	C	355	HTO	O1-C1-C2-O2
6	M	705	LDA	C6-C7-C8-C9
6	L	703	LDA	C4-C5-C6-C7
6	L	712	LDA	C2-C3-C4-C5
6	L	712	LDA	C5-C6-C7-C8
6	C	716	LDA	C6-C7-C8-C9
11	M	400	BCB	C6-C7-C8-C9
6	L	710	LDA	C4-C5-C6-C7
6	L	724	LDA	C3-C4-C5-C6
10	C	377	GOL	O1-C1-C2-C3
10	H	276[B]	GOL	O1-C1-C2-C3
10	C	376	GOL	O1-C1-C2-C3
10	M	334	GOL	O1-C1-C2-C3
10	L	283	GOL	C1-C2-C3-O3
10	M	337	GOL	O1-C1-C2-C3
10	C	372	GOL	O1-C1-C2-C3
10	C	369	GOL	C1-C2-C3-O3
10	H	276[A]	GOL	O1-C1-C2-C3
10	H	277	GOL	O1-C1-C2-C3
10	M	339	GOL	C1-C2-C3-O3
7	C	730	DGA	CB2-CB3-CB4-CB5
6	M	705	LDA	C11-C10-C9-C8
6	M	714	LDA	C2-C3-C4-C5
6	M	706	LDA	C5-C6-C7-C8
6	H	721	LDA	C2-C3-C4-C5
6	L	702	LDA	C3-C4-C5-C6
11	L	401	BCB	C16-C17-C18-C19
6	H	719	LDA	C2-C3-C4-C5
6	H	718[B]	LDA	C6-C7-C8-C9
6	M	704	LDA	C5-C6-C7-C8
6	M	713	LDA	C2-C3-C4-C5
7	C	730	DGA	CA2-CA3-CA4-CA5
6	M	707	LDA	C4-C5-C6-C7
6	L	712	LDA	C7-C8-C9-C10
13	L	502	UQ9	C15-C14-C16-C17
13	L	502	UQ9	C13-C14-C16-C17
6	H	720	LDA	C4-C5-C6-C7
10	H	290	GOL	O2-C2-C3-O3
10	C	364	GOL	O1-C1-C2-O2
10	M	342	GOL	O2-C2-C3-O3
10	H	276[B]	GOL	O1-C1-C2-O2
10	H	287	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
10	L	284	GOL	O1-C1-C2-O2
10	L	284	GOL	O2-C2-C3-O3
10	L	282	GOL	O1-C1-C2-O2
10	C	368	GOL	O1-C1-C2-O2
10	M	334	GOL	O2-C2-C3-O3
10	H	289	GOL	O1-C1-C2-O2
10	H	286	GOL	O2-C2-C3-O3
10	H	282	GOL	O1-C1-C2-O2
10	H	285	GOL	O2-C2-C3-O3
10	M	340	GOL	O2-C2-C3-O3
10	C	372	GOL	O1-C1-C2-O2
10	H	284	GOL	O1-C1-C2-O2
10	H	276[A]	GOL	O1-C1-C2-O2
10	H	276[A]	GOL	O2-C2-C3-O3
10	C	374[B]	GOL	O1-C1-C2-O2
10	C	374[B]	GOL	O2-C2-C3-O3
10	M	336	GOL	O2-C2-C3-O3
10	C	365	GOL	O2-C2-C3-O3
10	C	366	GOL	O1-C1-C2-O2
6	M	705	LDA	C7-C8-C9-C10
6	M	713	LDA	C11-C10-C9-C8
6	M	715	LDA	C7-C8-C9-C10
6	L	710	LDA	C3-C4-C5-C6
7	C	730	DGA	OA1-CA1-OG1-CG1
6	L	723	LDA	C1-C2-C3-C4
6	H	721	LDA	C4-C5-C6-C7
6	L	703	LDA	C7-C8-C9-C10
9	C	355	HTO	C4-C5-C6-C7
6	M	705	LDA	C4-C5-C6-C7
6	H	701	LDA	C4-C5-C6-C7
6	H	718[B]	LDA	C7-C8-C9-C10
6	L	708	LDA	C3-C4-C5-C6
6	M	717	LDA	C4-C5-C6-C7
6	M	707	LDA	C1-C2-C3-C4
6	L	702	LDA	C11-C10-C9-C8
6	L	711	LDA	C2-C3-C4-C5
13	L	502	UQ9	C30-C29-C31-C32
6	L	703	LDA	C6-C7-C8-C9
6	H	721	LDA	C7-C8-C9-C10
9	C	356	HTO	O1-C1-C2-O2
6	L	724	LDA	C1-C2-C3-C4
6	M	715	LDA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
7	C	730	DGA	CB6-CB7-CB8-CB9
17	M	332	HTH	O3-C3-C4-C5
9	L	280	HTO	O3-C3-C4-C5
7	C	730	DGA	CDB-CEB-CFB-CGB
6	L	724	LDA	C2-C3-C4-C5
13	L	503	UQ9	C1-C6-C7-C8
9	C	358[A]	HTO	C4-C5-C6-C7
7	C	730	DGA	CA7-CA8-CA9-CAA
6	L	710	LDA	C9-C10-C11-C12
10	C	377	GOL	O1-C1-C2-O2
10	M	342	GOL	O1-C1-C2-O2
10	L	286	GOL	O1-C1-C2-O2
10	L	286	GOL	O2-C2-C3-O3
10	C	376	GOL	O1-C1-C2-O2
10	H	288	GOL	O1-C1-C2-O2
10	C	367	GOL	O2-C2-C3-O3
10	H	291	GOL	O2-C2-C3-O3
10	H	280	GOL	O2-C2-C3-O3
10	H	283	GOL	O1-C1-C2-O2
10	M	338	GOL	O1-C1-C2-O2
10	M	338	GOL	O2-C2-C3-O3
7	C	730	DGA	CB7-CB8-CB9-CAB
9	M	333	HTO	C4-C5-C6-C7
6	C	716	LDA	C9-C10-C11-C12
6	M	714	LDA	C3-C4-C5-C6
6	L	724	LDA	C11-C10-C9-C8
12	L	402	BPB	C8-C10-C11-C12
6	L	724	LDA	C9-C10-C11-C12
17	M	332	HTH	O2-C2-C3-O3
9	C	357	HTO	O2-C2-C3-O3
11	L	400	BCB	CAD-CBD-CGD-O2D
6	L	709	LDA	C1-C2-C3-C4
12	M	402	BPB	C11-C10-C8-C7
13	L	502	UQ9	C28-C29-C31-C32
11	M	401	BCB	C11-C12-C13-C15
11	L	401	BCB	C12-C13-C15-C16
9	L	279	HTO	C4-C5-C6-C7
12	M	402	BPB	C11-C10-C8-C9
11	M	401	BCB	C11-C12-C13-C14
9	C	358[A]	HTO	C2-C3-C4-C5
6	M	705	LDA	C3-C4-C5-C6
6	L	712	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	L	708	LDA	N1-C1-C2-C3
6	L	723	LDA	N1-C1-C2-C3
6	L	711	LDA	N1-C1-C2-C3
6	L	709	LDA	N1-C1-C2-C3
6	M	715	LDA	N1-C1-C2-C3
6	L	709	LDA	C7-C8-C9-C10
6	L	702	LDA	C5-C6-C7-C8
6	H	719	LDA	C1-C2-C3-C4
6	M	714	LDA	C9-C10-C11-C12
6	H	701	LDA	C6-C7-C8-C9
17	M	332	HTH	C4-C5-C6-C7
6	M	705	LDA	C2-C3-C4-C5
6	M	717	LDA	C7-C8-C9-C10
7	C	730	DGA	CEB-CFB-CGB-CHB
7	C	730	DGA	CA3-CA4-CA5-CA6
9	C	358[A]	HTO	O1-C1-C2-C3
10	C	364	GOL	O2-C2-C3-O3
10	C	378	GOL	O1-C1-C2-O2
10	H	281	GOL	O1-C1-C2-O2
10	H	283	GOL	O2-C2-C3-O3
10	C	369	GOL	O2-C2-C3-O3
10	M	339	GOL	O2-C2-C3-O3
6	H	701	LDA	C7-C8-C9-C10
11	M	400	BCB	C2B-C3B-CAB-OBB
11	M	400	BCB	C2B-C3B-CAB-CBB
9	L	280	HTO	C4-C5-C6-C7
6	M	714	LDA	C7-C8-C9-C10
6	H	721	LDA	C11-C10-C9-C8
6	M	706	LDA	C6-C7-C8-C9
6	M	706	LDA	C9-C10-C11-C12
7	C	730	DGA	CAB-CBB-CCB-CDB
6	C	716	LDA	C1-C2-C3-C4
11	L	401	BCB	C16-C17-C18-C20
6	L	703	LDA	C1-C2-C3-C4
11	M	400	BCB	C11-C10-C8-C7
6	L	709	LDA	C5-C6-C7-C8
11	M	400	BCB	C10-C11-C12-C13
6	L	711	LDA	C7-C8-C9-C10
11	L	400	BCB	C2C-C3C-CAC-CBC
12	M	402	BPB	CAD-CBD-CGD-O2D
11	M	401	BCB	C2C-C3C-CAC-CBC
11	M	400	BCB	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	L	712	LDA	C3-C4-C5-C6
7	C	730	DGA	CB3-CB4-CB5-CB6
15	M	501	MQ9	C35-C34-C36-C37
15	M	501	MQ9	C33-C34-C36-C37
16	M	600	NS5	C31-C33-C34-C35
11	M	401	BCB	C3A-C2A-CAA-CBA
6	H	721	LDA	C9-C10-C11-C12
6	L	708	LDA	C2-C1-N1-CM1
6	L	708	LDA	C2-C1-N1-CM2
6	H	719	LDA	C2-C1-N1-CM1
6	H	719	LDA	C2-C1-N1-CM2
6	M	704	LDA	C2-C1-N1-CM2
6	C	722	LDA	C2-C1-N1-CM2
6	C	716	LDA	C2-C1-N1-CM2
6	H	720	LDA	C6-C7-C8-C9
12	M	402	BPB	C16-C17-C18-C20
10	M	334	GOL	O1-C1-C2-O2
10	H	285	GOL	O1-C1-C2-O2
10	C	359	GOL	O1-C1-C2-O2
10	M	336	GOL	O1-C1-C2-O2
10	C	370	GOL	O2-C2-C3-O3
11	M	400	BCB	C4-C3-C5-C6
6	L	723	LDA	C5-C6-C7-C8
11	M	400	BCB	C11-C10-C8-C9
9	L	280	HTO	C2-C3-C4-C5
10	C	370	GOL	C1-C2-C3-O3
6	C	722	LDA	C2-C3-C4-C5
11	M	400	BCB	C16-C17-C18-C19
6	M	713	LDA	C1-C2-C3-C4
17	M	332	HTH	C3-C4-C5-C6
6	M	714	LDA	C6-C7-C8-C9
6	L	710	LDA	C2-C1-N1-O1
6	L	708	LDA	C2-C1-N1-O1
6	H	719	LDA	C2-C1-N1-O1
6	C	716	LDA	C2-C1-N1-O1
12	M	402	BPB	NA-C4A-CHB-C1B
6	H	720	LDA	C7-C8-C9-C10
6	C	722	LDA	C1-C2-C3-C4
6	L	709	LDA	C4-C5-C6-C7
6	H	701	LDA	C9-C10-C11-C12
6	L	710	LDA	C7-C8-C9-C10
11	L	400	BCB	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	M	402	BPB	C11-C12-C13-C14
11	L	401	BCB	C14-C13-C15-C16
11	M	400	BCB	C16-C17-C18-C20
11	M	400	BCB	C15-C16-C17-C18
6	H	720	LDA	C5-C6-C7-C8
6	H	719	LDA	C3-C4-C5-C6
13	L	502	UQ9	C5-C4-O4-C4M
11	M	400	BCB	C2-C3-C5-C6
6	H	718[B]	LDA	C11-C10-C9-C8
6	M	704	LDA	C11-C10-C9-C8
6	M	707	LDA	C6-C7-C8-C9
16	M	600	NS5	C17-C18-C19-C20
6	L	708	LDA	C11-C10-C9-C8
11	M	401	BCB	C3-C5-C6-C7
6	L	711	LDA	C5-C6-C7-C8
11	L	400	BCB	CAD-CBD-CGD-O1D
9	H	273	HTO	O3-C3-C4-C5
13	L	502	UQ9	C4-C3-O3-C3M
17	M	332	HTH	C2-C3-C4-C5
12	M	402	BPB	C16-C17-C18-C19
10	H	281	GOL	O1-C1-C2-C3
6	M	706	LDA	C7-C8-C9-C10
13	L	502	UQ9	C20-C19-C21-C22
16	M	600	NS5	C33-C34-C35-C36
13	L	502	UQ9	C18-C19-C21-C22
9	L	278	HTO	C4-C5-C6-C7
6	C	716	LDA	C4-C5-C6-C7
6	C	722	LDA	C4-C5-C6-C7
6	H	719	LDA	C9-C10-C11-C12
6	C	716	LDA	C2-C3-C4-C5
7	C	730	DGA	CA6-CA7-CA8-CA9
9	L	280	HTO	O1-C1-C2-O2
6	L	723	LDA	C4-C5-C6-C7
9	C	357	HTO	C1-C2-C3-O3
9	L	279	HTO	C1-C2-C3-O3
6	L	702	LDA	C6-C7-C8-C9
11	M	400	BCB	C1A-C2A-CAA-CBA
9	H	272	HTO	C3-C4-C5-C6
13	L	502	UQ9	C3-C4-O4-C4M
10	H	286	GOL	O1-C1-C2-O2
9	C	356	HTO	C3-C4-C5-C6
11	L	401	BCB	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	L	503	UQ9	C2-C3-O3-C3M
9	L	280	HTO	C3-C4-C5-C6
7	C	730	DGA	CA8-CA9-CAA-CBA
6	M	706	LDA	C4-C5-C6-C7
6	L	708	LDA	C2-C3-C4-C5
6	L	708	LDA	C5-C6-C7-C8
9	M	333	HTO	C2-C3-C4-C5
6	L	723	LDA	C11-C10-C9-C8
10	C	371	GOL	O1-C1-C2-C3
5	C	402	HEC	C3D-CAD-CBD-CGD
6	M	715	LDA	C1-C2-C3-C4
13	L	502	UQ9	C40-C39-C41-C42
16	M	600	NS5	C32-C31-C33-C34
7	C	730	DGA	CA9-CAA-CBA-CCA
12	L	402	BPB	CAD-CBD-CGD-O2D
11	L	401	BCB	C2C-C3C-CAC-CBC
6	L	709	LDA	C11-C10-C9-C8
13	L	502	UQ9	C46-C47-C48-C49
9	L	276	HTO	C4-C5-C6-C7
6	C	722	LDA	C5-C6-C7-C8
11	M	401	BCB	CHA-CBD-CGD-O2D
11	M	400	BCB	CHA-CBD-CGD-O1D
11	M	400	BCB	CHA-CBD-CGD-O2D
11	L	401	BCB	CHA-CBD-CGD-O1D
6	M	707	LDA	C3-C4-C5-C6
6	M	714	LDA	C4-C5-C6-C7
9	L	276	HTO	C3-C4-C5-C6
10	C	367	GOL	O1-C1-C2-O2
10	L	283	GOL	O2-C2-C3-O3
10	M	337	GOL	O1-C1-C2-O2
10	H	277	GOL	O1-C1-C2-O2
12	L	402	BPB	C2-C3-C5-C6
11	M	401	BCB	C14-C13-C15-C16
9	C	355	HTO	C2-C3-C4-C5
9	C	356	HTO	C2-C3-C4-C5
9	C	356	HTO	O1-C1-C2-C3
10	C	364	GOL	C1-C2-C3-O3
10	H	279	GOL	C1-C2-C3-O3
10	C	367	GOL	O1-C1-C2-C3
10	H	285	GOL	O1-C1-C2-C3
10	M	340	GOL	O1-C1-C2-C3
10	C	359	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	C	366	GOL	C1-C2-C3-O3
9	C	358[A]	HTO	C3-C4-C5-C6
7	C	730	DGA	CB9-CAB-CBB-CCB
6	M	715	LDA	C3-C4-C5-C6
6	M	713	LDA	C9-C10-C11-C12
6	H	721	LDA	C2-C1-N1-O1
10	H	281	GOL	O2-C2-C3-O3
6	H	719	LDA	C7-C8-C9-C10
6	H	721	LDA	C1-C2-C3-C4

There are no ring outliers.

62 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	703	LDA	4	0
10	C	377	GOL	4	0
10	C	364	GOL	3	0
5	C	401	HEC	1	0
10	M	342	GOL	1	0
9	H	274[A]	HTO	1	0
9	M	333	HTO	2	0
6	L	710	LDA	1	0
11	L	400	BCB	5	0
8	C	338	SO4	1	0
10	L	286	GOL	1	0
10	C	373	GOL	1	0
9	H	273	HTO	3	0
9	C	357	HTO	2	0
10	H	279	GOL	1	0
5	C	404	HEC	1	0
9	H	272	HTO	1	0
8	C	354	SO4	1	0
9	C	355	HTO	6	0
6	L	723	LDA	4	0
5	C	403	HEC	3	0
12	M	402	BPB	1	0
10	C	368	GOL	1	0
6	M	707	LDA	1	0
15	M	501	MQ9	2	0
10	M	334	GOL	1	0
13	L	502	UQ9	11	0
8	C	340	SO4	1	0

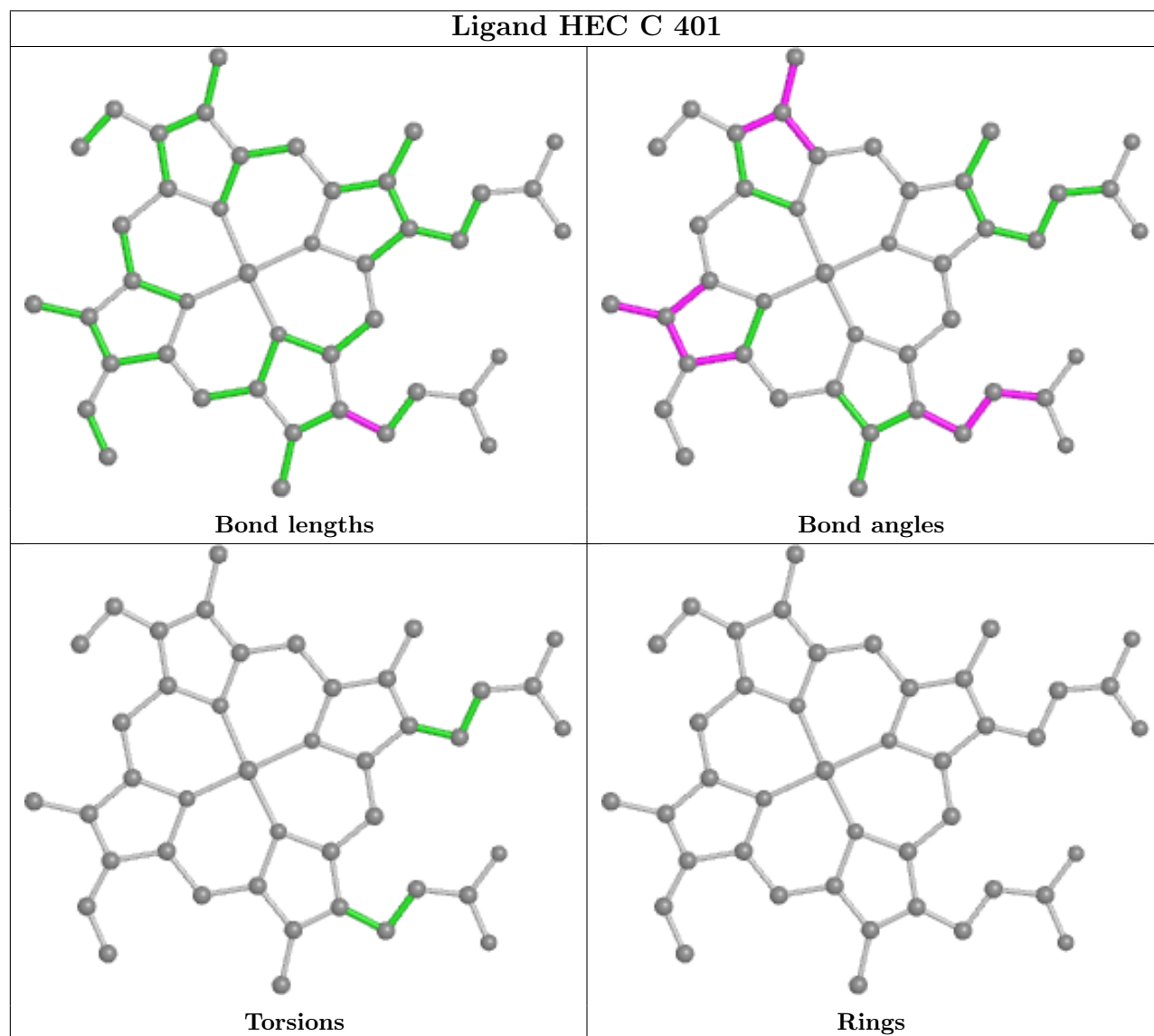
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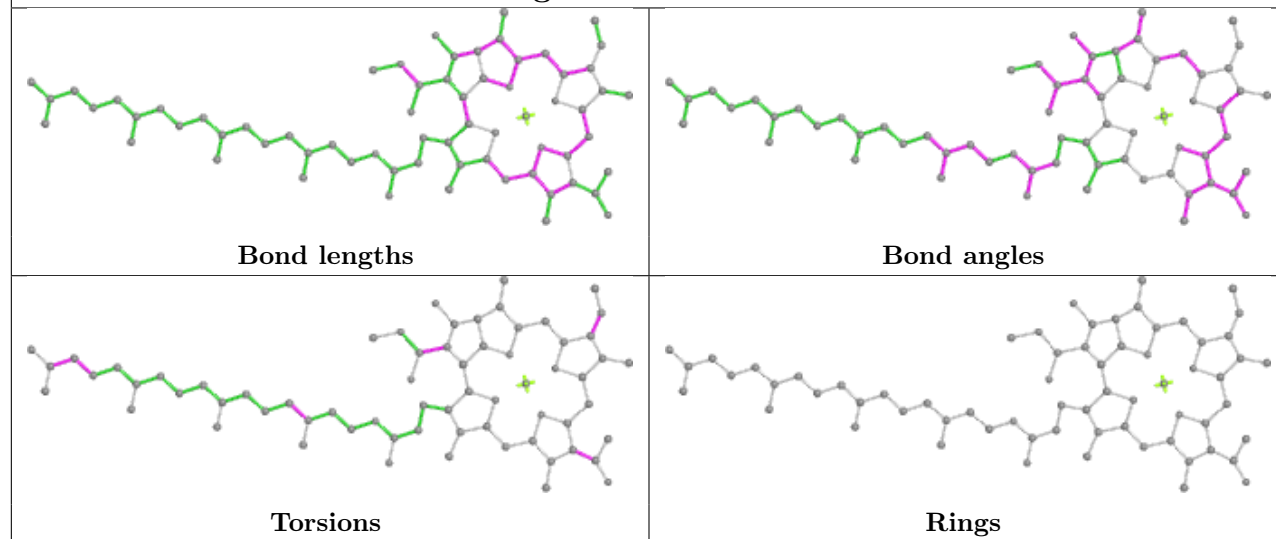
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	401	BCB	5	0
6	H	719	LDA	3	0
9	L	277	HTO	2	0
6	M	704	LDA	6	0
6	M	714	LDA	2	0
6	L	712	LDA	1	0
6	L	711	LDA	1	0
11	M	400	BCB	12	0
6	C	722	LDA	4	0
10	H	280	GOL	1	0
6	L	724	LDA	2	0
8	C	351	SO4	1	0
6	M	706	LDA	1	0
8	M	326	SO4	2	0
6	H	720	LDA	8	0
8	H	261[B]	SO4	4	0
8	H	261[A]	SO4	1	0
10	H	278	GOL	2	0
6	M	715	LDA	2	0
9	L	279	HTO	1	0
10	H	283	GOL	6	0
6	C	716	LDA	3	0
10	C	369	GOL	3	0
12	L	402	BPB	2	0
13	L	503	UQ9	5	0
10	C	363	GOL	1	0
6	H	721	LDA	1	0
16	M	600	NS5	3	0
10	M	336	GOL	1	0
10	C	365	GOL	2	0
10	M	338	GOL	3	0
6	L	702	LDA	6	0
11	L	401	BCB	4	0
7	C	730	DGA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

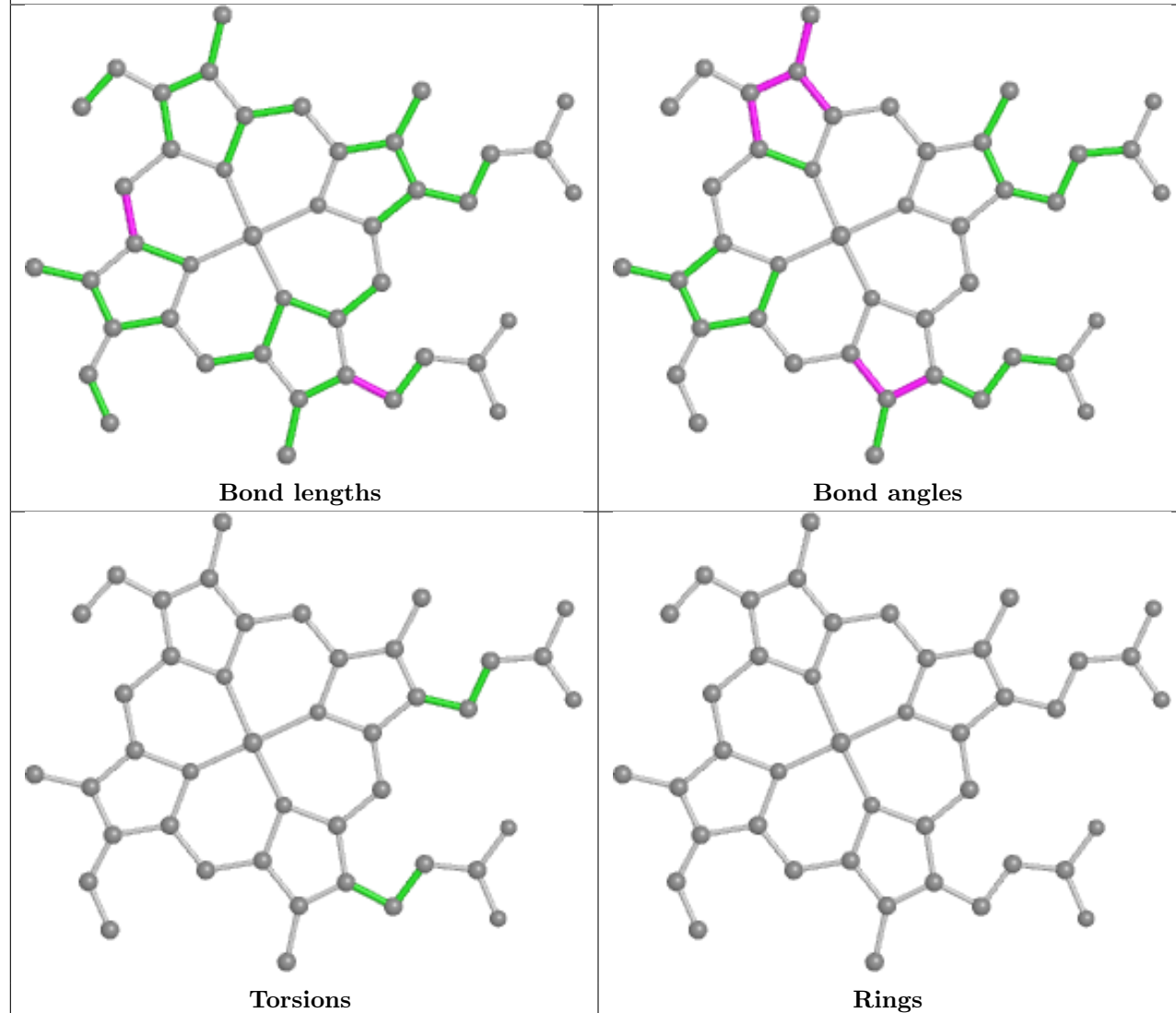
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



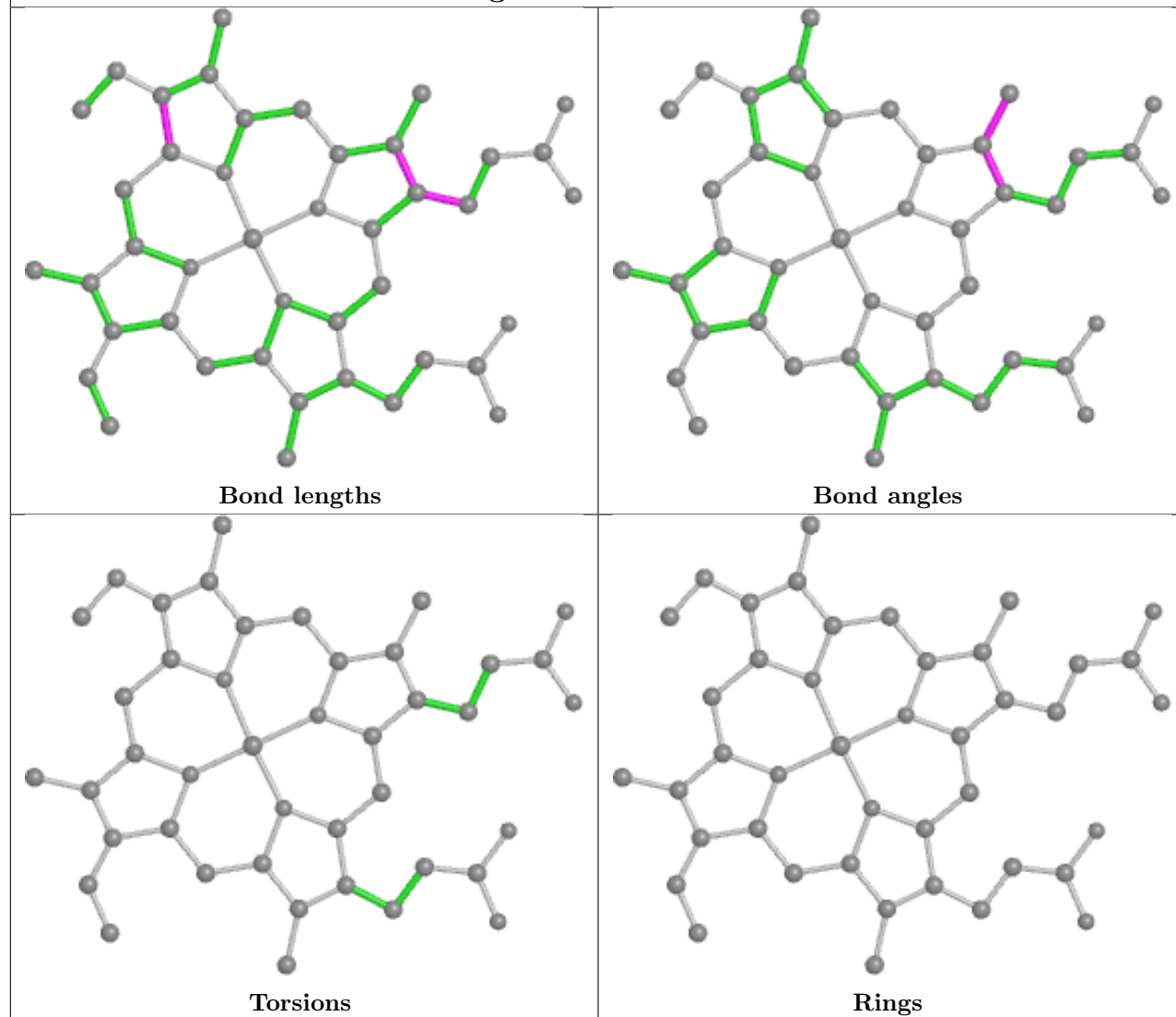
## Ligand BCB L 400



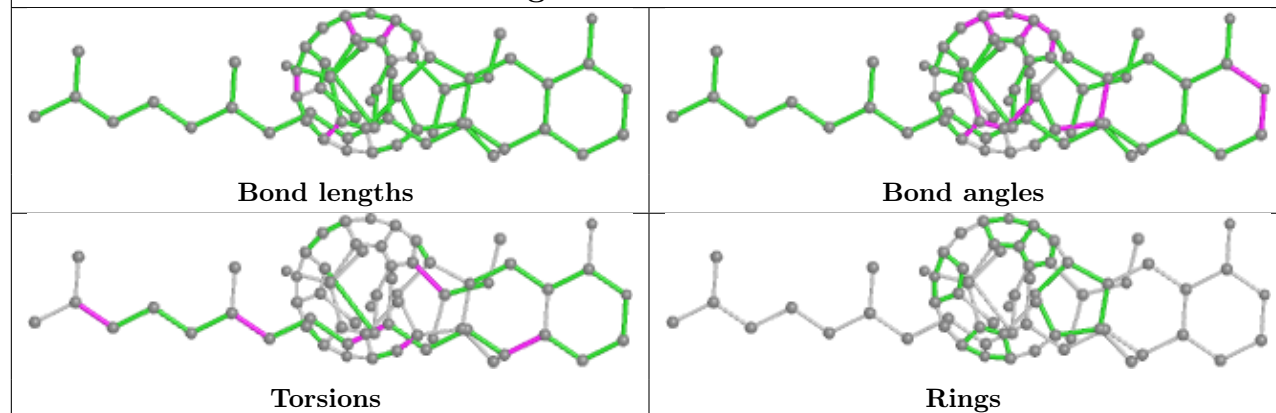
## Ligand HEC C 404

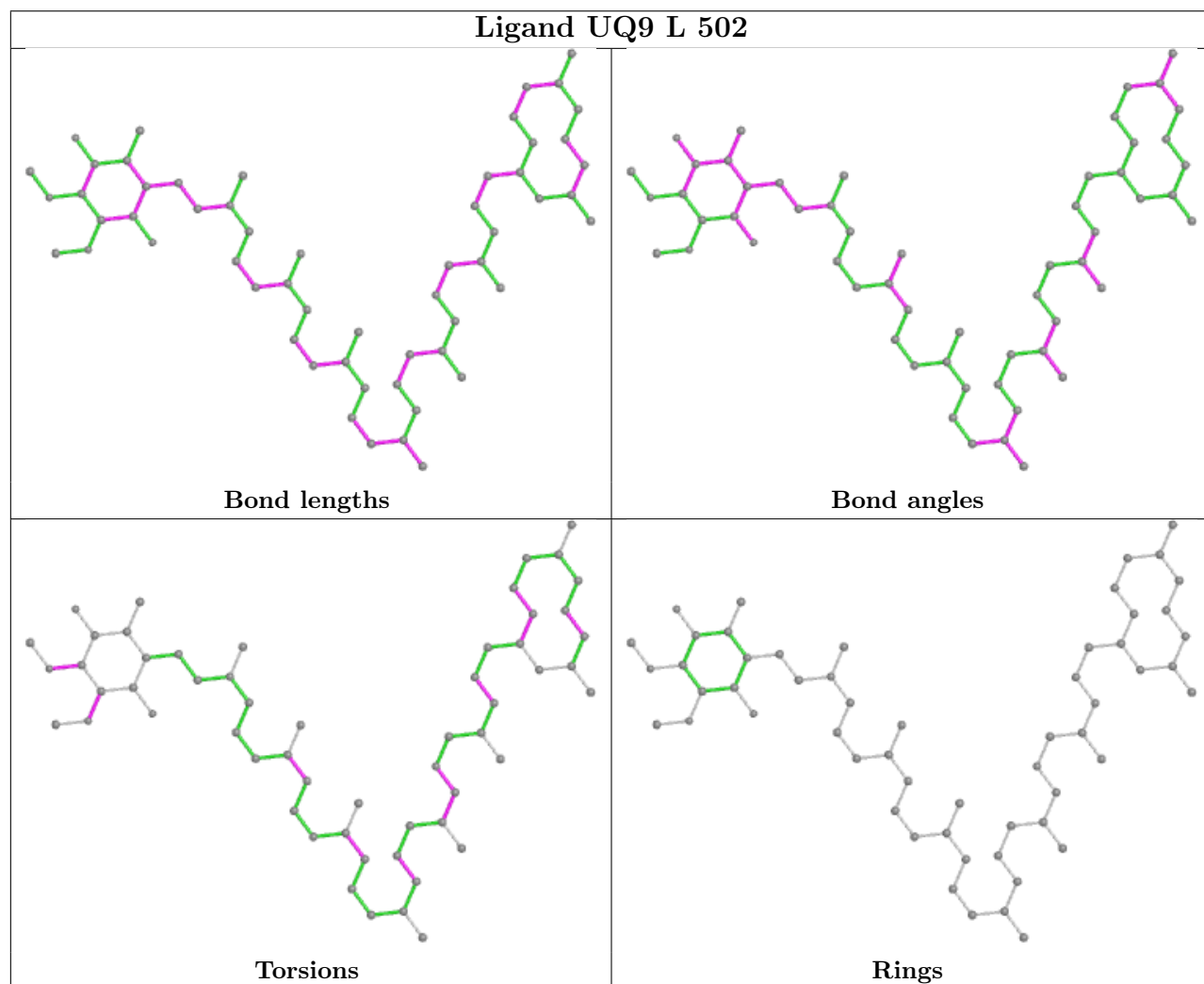
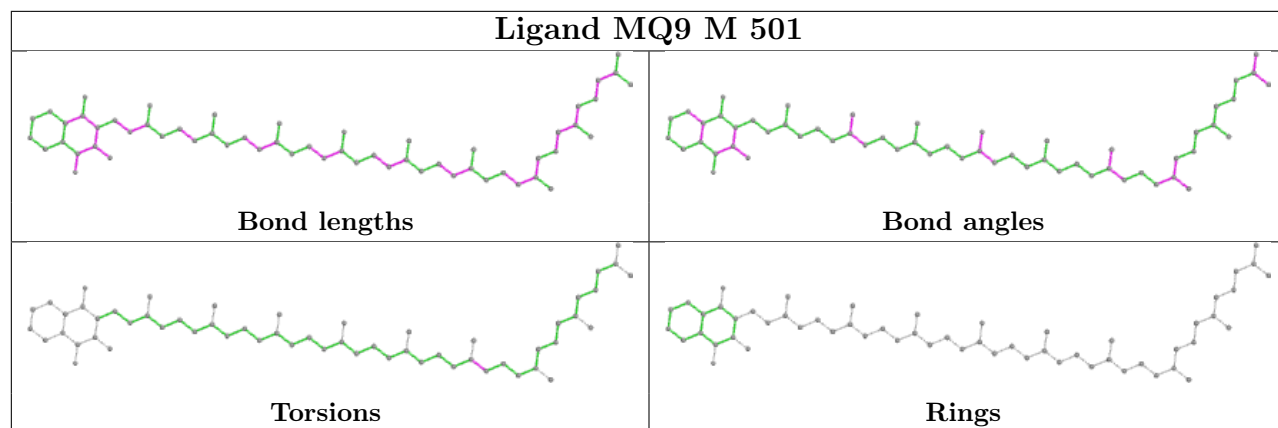


## Ligand HEC C 403

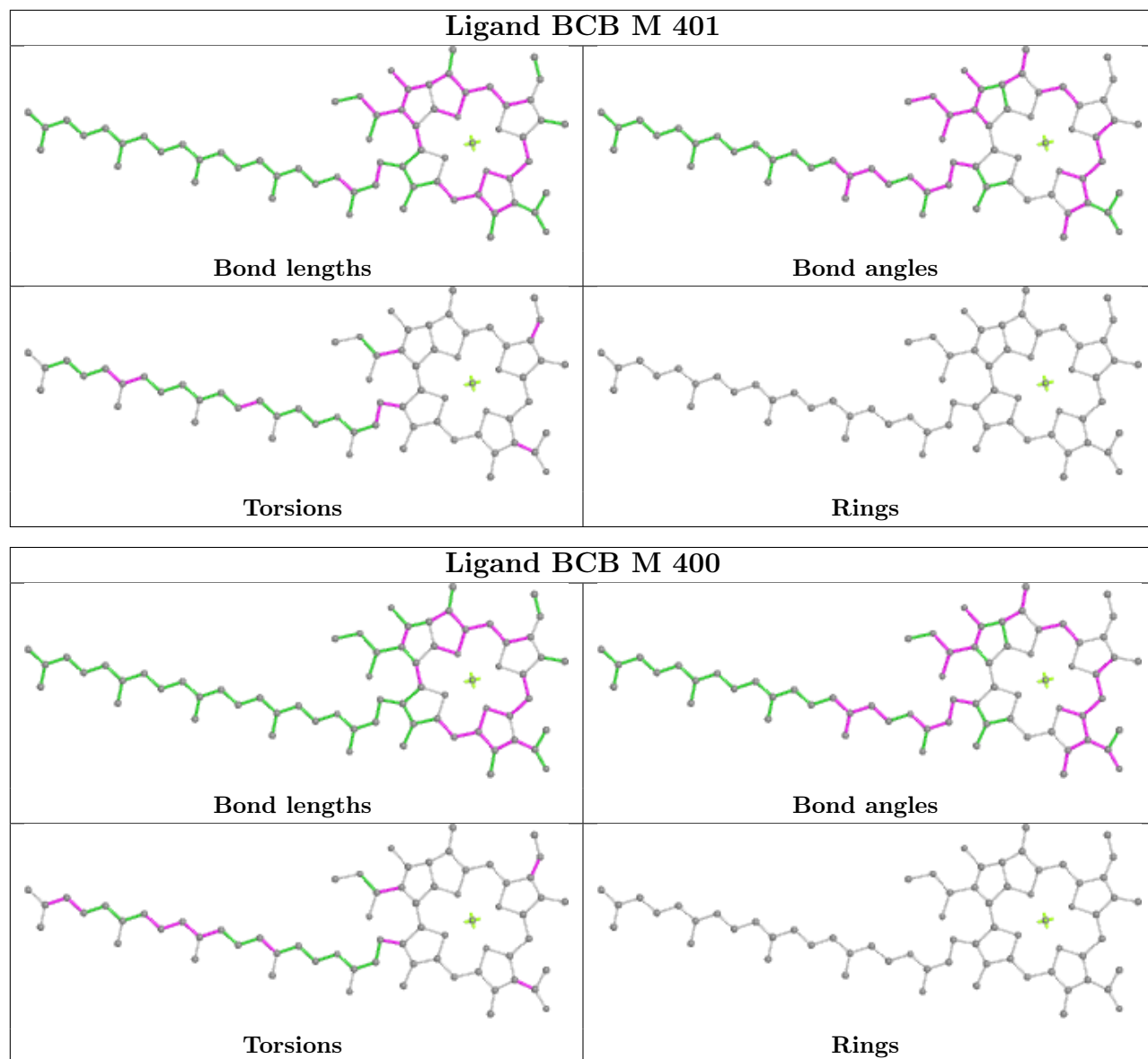


## Ligand BPB M 402

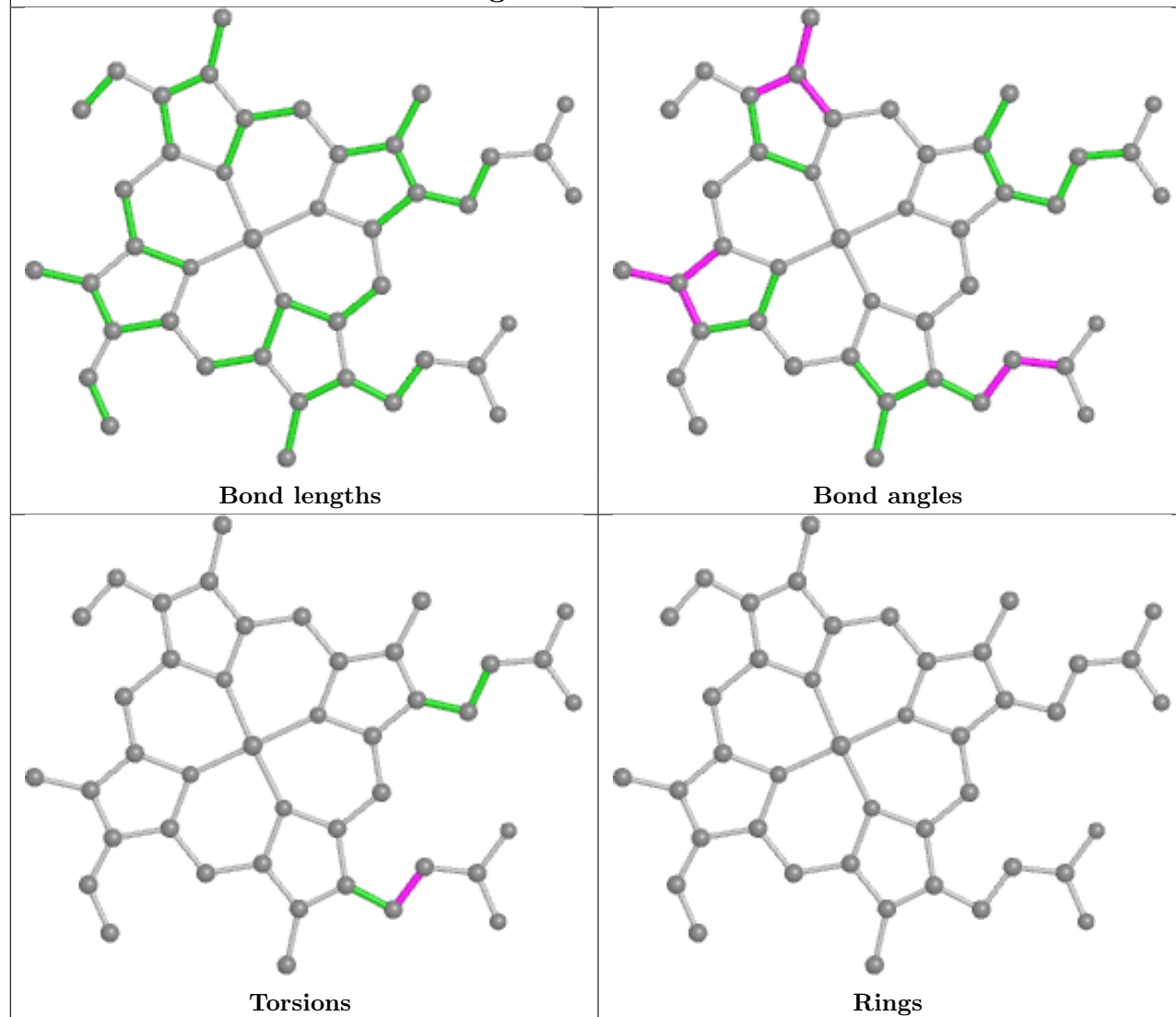




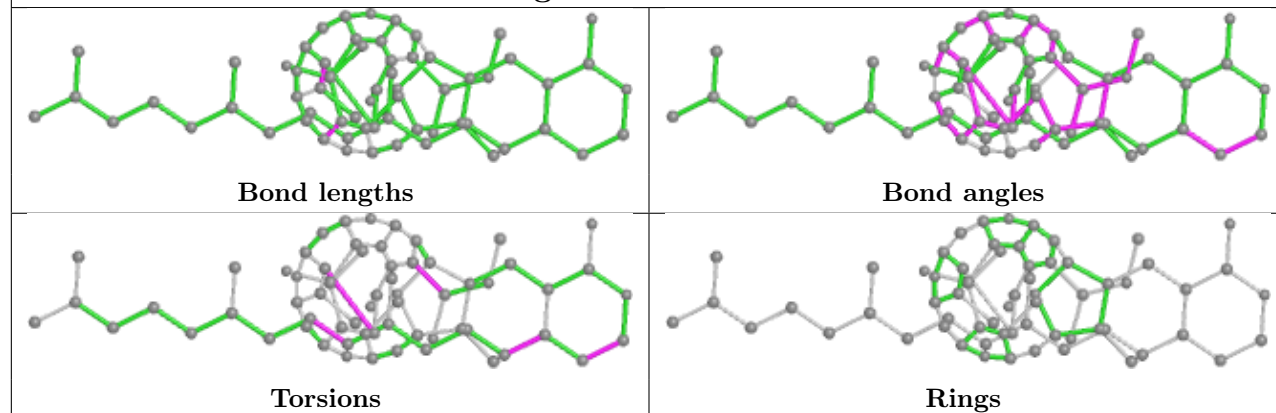




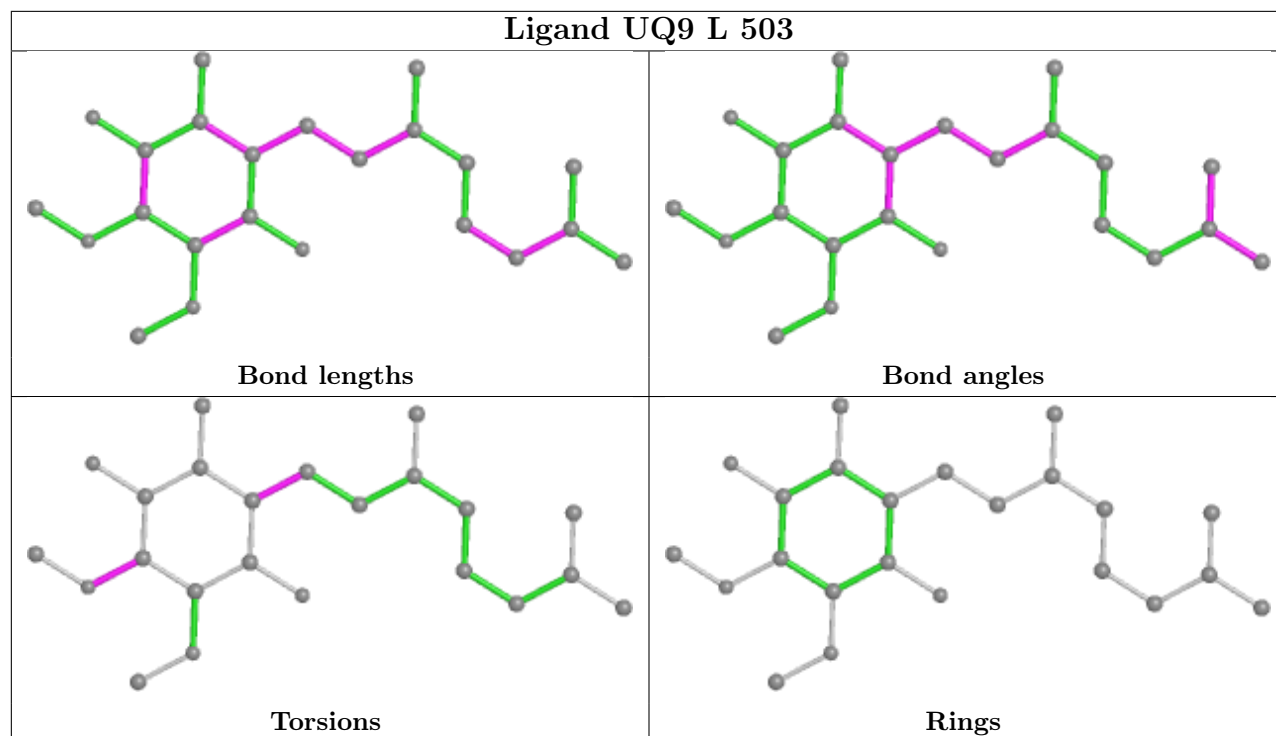
## Ligand HEC C 402



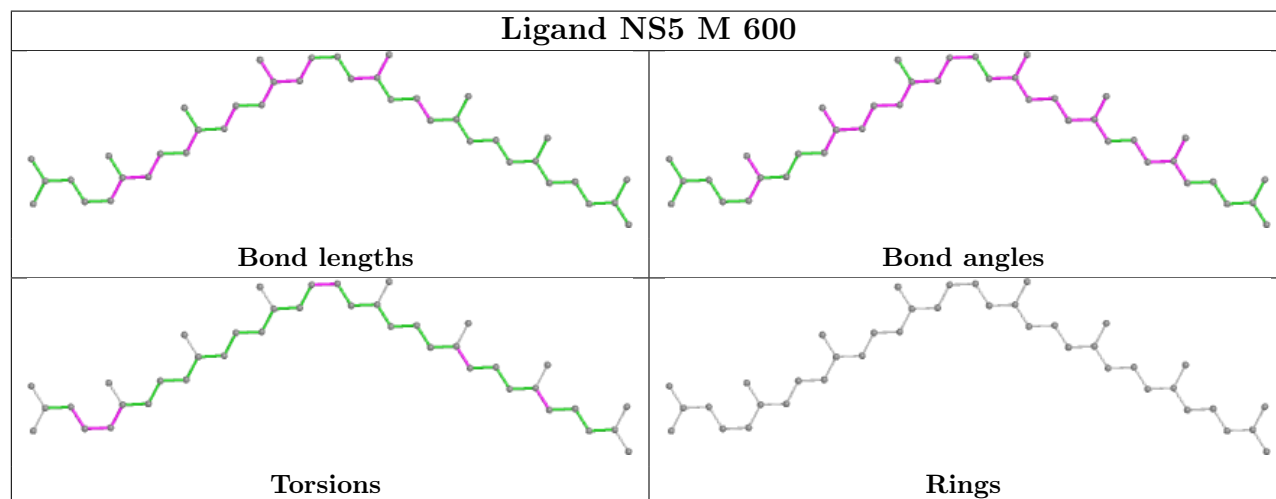
## Ligand BPB L 402

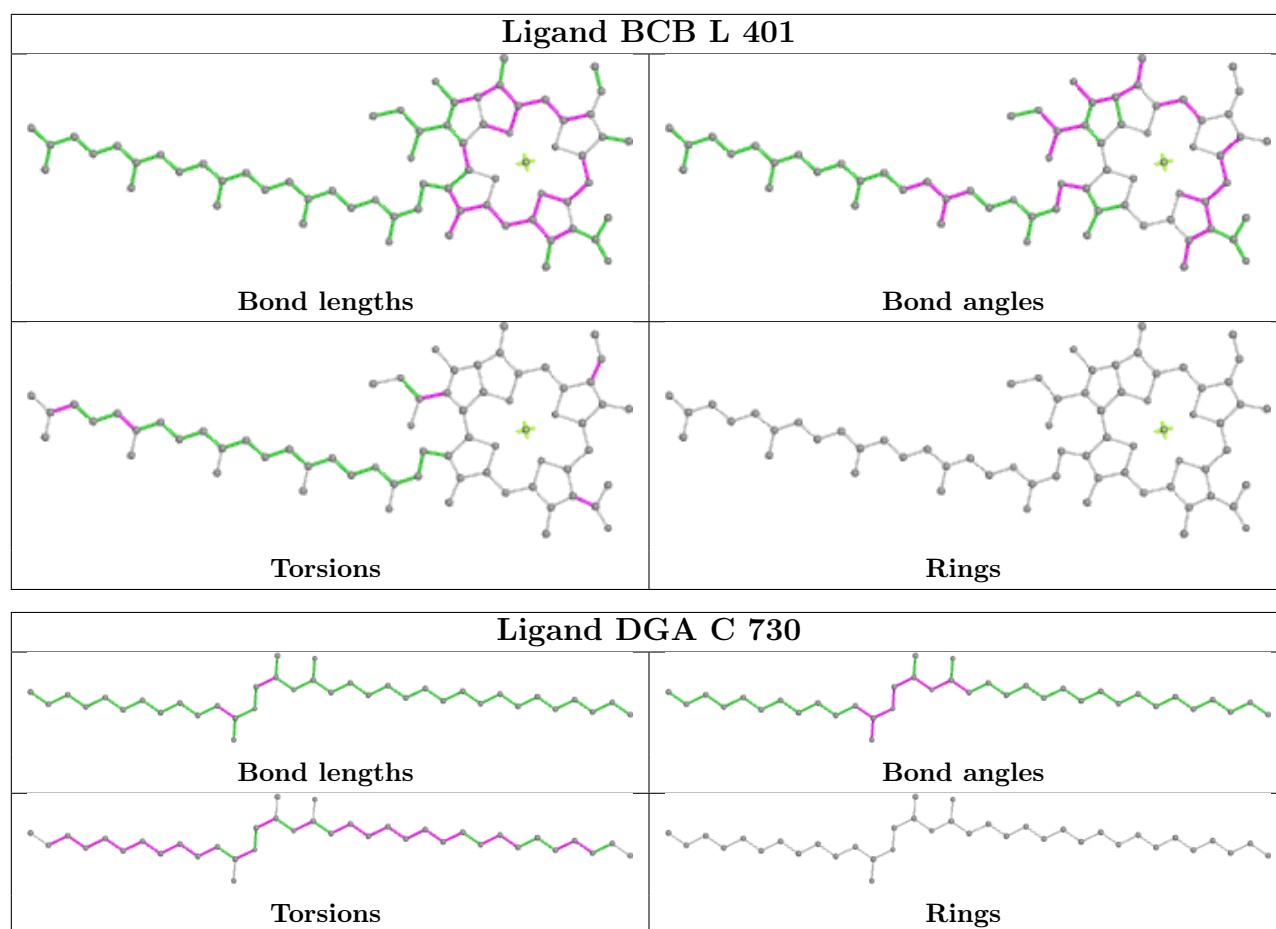


## Ligand UQ9 L 503



## Ligand NS5 M 600





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	334/356 (93%)	0.38	39 (11%) 4 7	34, 46, 68, 125	0
2	H	249/258 (96%)	-0.02	13 (5%) 27 37	35, 51, 81, 119	0
3	L	273/273 (100%)	0.08	19 (6%) 16 24	33, 42, 58, 82	0
4	M	323/323 (100%)	0.27	26 (8%) 12 19	32, 43, 65, 83	0
All	All	1179/1210 (97%)	0.19	97 (8%) 11 18	32, 45, 69, 125	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ALA	9.1
1	C	334	ALA	8.5
1	C	47	ALA	5.6
3	L	273	SER	5.1
1	C	332	LYS	4.9
2	H	85	THR	4.5
3	L	51[A]	TYR	4.3
3	L	271	PHE	4.2
2	H	8	GLN	4.1
3	L	202	ASP	4.1
4	M	78	HIS	4.1
1	C	230	PHE	4.0
4	M	26	ASN	4.0
1	C	48	GLU	3.9
3	L	81	LEU	3.9
3	L	270	PRO	3.9
4	M	23	TRP	3.8
2	H	7	ALA	3.8
4	M	319	PRO	3.8
4	M	37	TRP	3.7
4	M	31	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	168	THR	3.6
2	H	9	HIS	3.5
3	L	165	LEU	3.5
4	M	189	ILE	3.5
1	C	52	VAL	3.5
1	C	162	HIS	3.4
3	L	59	TRP	3.3
3	L	201	GLY	3.3
4	M	181	ILE	3.3
1	C	232	LEU	3.1
1	C	46	LYS	3.1
4	M	184	LEU	3.0
1	C	54	GLN	3.0
4	M	186	ALA	2.9
1	C	51	PRO	2.9
4	M	185	THR	2.9
3	L	162	TYR	2.8
1	C	185	LEU	2.8
1	C	66	THR	2.8
1	C	231	ALA	2.8
4	M	33	PHE	2.7
1	C	228	ALA	2.7
1	C	2[A]	PHE	2.7
1	C	244	CYS	2.7
2	H	83	PRO	2.7
4	M	80	ASP	2.6
1	C	159	THR	2.6
2	H	94	ASP	2.6
1	C	63	GLY	2.6
1	C	229	THR	2.5
2	H	95	GLY	2.5
1	C	331	ILE	2.5
1	C	167	GLU	2.5
1	C	163	VAL	2.5
1	C	291	ALA	2.5
2	H	96	PHE	2.5
4	M	82	LEU	2.5
1	C	169	ARG	2.5
2	H	81[A]	ARG	2.5
3	L	272	TRP	2.5
4	M	22	GLU	2.5
4	M	108	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	65	LEU	2.4
4	M	27	ASP	2.4
1	C	287	THR	2.3
3	L	269	ILE	2.3
4	M	212	LEU	2.3
3	L	167	TRP	2.3
2	H	189	GLY	2.3
3	L	79	PRO	2.3
4	M	25	ASP	2.3
1	C	161	THR	2.3
3	L	236	LEU	2.3
1	C	165	ARG	2.3
1	C	234	MET	2.2
4	M	207	ALA	2.2
3	L	80	LEU	2.2
4	M	24	GLY	2.2
1	C	226	ALA	2.2
1	C	50	PRO	2.2
4	M	320	GLY	2.2
1	C	53	SER	2.1
3	L	57	PRO	2.1
1	C	193	PHE	2.1
4	M	79	PHE	2.1
4	M	263	VAL	2.1
2	H	97	GLU	2.1
3	L	54	SER	2.1
3	L	180	LEU	2.1
1	C	55	VAL	2.0
2	H	87	GLU	2.0
4	M	34	TYR	2.0
4	M	50	TYR	2.0
2	H	86	ARG	2.0
1	C	323	GLN	2.0
1	C	57	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	FME	H	1[A]	10/11	0.97	0.10	47,50,54,56	7
2	FME	H	1[B]	10/11	0.97	0.10	47,53,59,61	7

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	LDA	H	718[B]	16/16	0.29	0.54	50,80,89,90	16
7	DGA	C	730	37/44	0.33	0.41	112,125,144,151	0
6	LDA	M	706	16/16	0.34	0.59	49,55,65,68	16
10	GOL	M	341	6/6	0.36	0.44	68,71,74,75	6
17	HTH	M	332	10/10	0.37	0.31	58,68,76,77	10
8	SO4	H	271	5/5	0.44	0.34	64,64,65,68	5
9	HTO	L	280	10/10	0.47	0.39	63,69,71,72	10
6	LDA	L	712	16/16	0.54	0.43	51,64,70,71	16
6	LDA	L	709	16/16	0.54	0.28	39,63,93,97	16
9	HTO	H	274[A]	10/10	0.54	0.57	53,69,72,75	10
6	LDA	L	711	16/16	0.55	0.31	60,68,76,77	16
6	LDA	L	702	16/16	0.56	0.80	51,53,57,57	16
10	GOL	M	338	6/6	0.56	0.36	57,60,62,63	6
6	LDA	M	717	16/16	0.59	0.39	50,59,89,91	16
10	GOL	C	374[B]	6/6	0.60	0.49	66,67,68,68	6
9	HTO	L	279	10/10	0.60	0.32	65,66,69,75	10
10	GOL	H	288	6/6	0.61	0.19	60,68,68,73	6
6	LDA	C	716	16/16	0.61	0.34	50,65,72,74	16
9	HTO	C	357	10/10	0.65	0.61	59,65,73,80	10
10	GOL	C	371	6/6	0.65	0.43	55,62,62,63	6
10	GOL	C	376	6/6	0.65	0.33	63,74,77,83	6
9	HTO	C	358[A]	10/10	0.66	0.30	58,62,67,68	10
8	SO4	M	330	5/5	0.66	0.46	67,68,68,69	5
8	SO4	C	351	5/5	0.67	0.40	60,60,63,67	5
10	GOL	M	342	6/6	0.67	0.24	66,67,69,70	6
10	GOL	C	370	6/6	0.67	0.42	64,66,68,68	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	GOL	C	363	6/6	0.68	0.29	46,59,65,69	6
8	SO4	L	275	5/5	0.69	0.44	66,66,67,68	5
6	LDA	M	707	16/16	0.69	0.31	42,58,72,81	16
10	GOL	L	288	6/6	0.70	0.52	54,57,58,60	6
6	LDA	C	722	16/16	0.70	0.24	53,63,66,66	16
6	LDA	M	715	16/16	0.71	0.39	58,71,77,79	16
10	GOL	H	281	6/6	0.71	0.39	64,67,72,76	6
8	SO4	H	270	5/5	0.71	0.33	60,61,63,63	5
10	GOL	H	287	6/6	0.72	0.17	65,71,72,73	6
8	SO4	M	329	5/5	0.73	0.41	57,58,63,67	5
6	LDA	L	710	16/16	0.73	0.28	52,60,81,82	16
10	GOL	H	277	6/6	0.73	0.31	55,59,62,62	6
8	SO4	C	354	5/5	0.74	0.37	66,69,70,71	5
10	GOL	C	378	6/6	0.74	0.43	78,80,81,81	6
10	GOL	H	279	6/6	0.74	0.28	63,68,71,72	6
10	GOL	H	289	6/6	0.74	0.35	62,66,66,67	6
10	GOL	H	283	6/6	0.75	0.21	59,60,61,61	6
10	GOL	C	372	6/6	0.75	0.22	56,62,65,65	6
8	SO4	C	347	5/5	0.75	0.40	78,82,83,90	5
6	LDA	H	719	16/16	0.75	0.22	58,63,71,72	16
9	HTO	C	355	10/10	0.75	0.24	62,66,71,72	10
10	GOL	M	340	6/6	0.75	0.29	60,64,65,66	6
6	LDA	M	705	16/16	0.76	0.25	61,69,87,87	16
10	GOL	C	375	6/6	0.76	0.38	66,69,70,72	6
9	HTO	H	273	10/10	0.76	0.34	48,51,60,62	10
10	GOL	L	287	6/6	0.76	0.25	54,55,57,57	6
8	SO4	C	350	5/5	0.76	0.39	64,67,69,72	5
13	UQ9	L	503	23/58	0.77	0.30	59,73,85,87	23
6	LDA	L	724	16/16	0.77	0.47	53,63,68,69	16
9	HTO	M	333	10/10	0.78	0.72	44,51,55,55	10
10	GOL	H	276[A]	6/6	0.79	0.26	50,60,62,62	2
9	HTO	L	278	10/10	0.79	0.20	57,65,67,69	10
10	GOL	H	276[B]	6/6	0.79	0.26	50,59,60,62	2
10	GOL	M	339	6/6	0.79	0.39	60,65,66,66	6
8	SO4	H	265	5/5	0.79	0.21	69,74,75,81	5
10	GOL	H	280	6/6	0.79	0.23	52,60,65,66	6
8	SO4	H	269	5/5	0.80	0.30	71,72,75,76	5
10	GOL	C	367	6/6	0.81	1.39	50,58,59,60	6
8	SO4	L	274	5/5	0.81	0.26	62,62,65,68	5
10	GOL	C	369	6/6	0.81	1.19	49,56,61,61	6
9	HTO	L	277	10/10	0.81	0.17	57,64,69,76	10
13	UQ9	L	502	58/58	0.81	0.52	44,80,97,99	58

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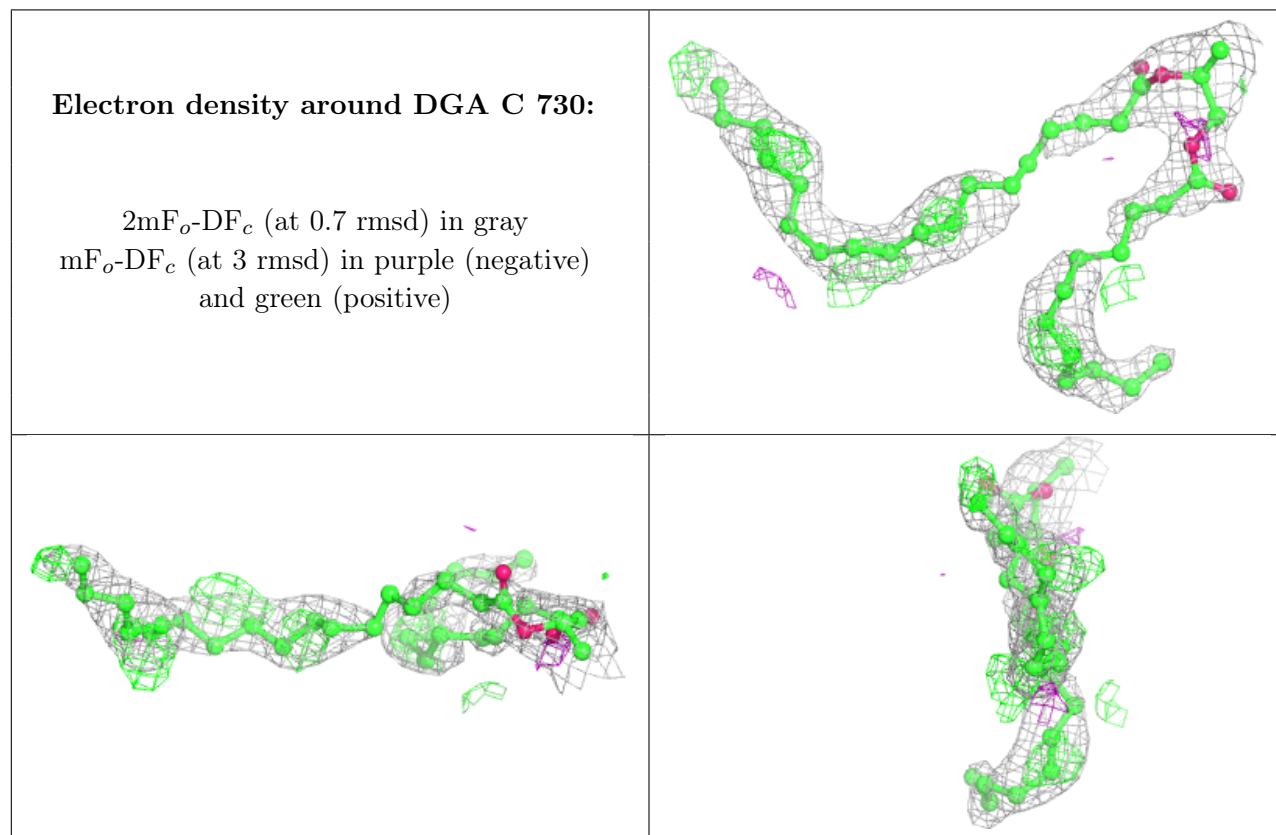
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	GOL	H	284	6/6	0.82	0.21	58,63,65,68	6
10	GOL	L	284	6/6	0.82	0.21	52,65,67,67	6
8	SO4	M	331	5/5	0.82	0.21	60,60,61,62	5
10	GOL	C	366	6/6	0.82	0.22	56,62,63,71	6
9	HTO	C	356	10/10	0.82	0.27	59,72,76,77	10
10	GOL	L	285	6/6	0.82	0.21	51,67,70,71	6
6	LDA	L	708	16/16	0.82	0.21	40,56,68,76	0
8	SO4	C	348	5/5	0.82	0.20	70,73,77,80	5
10	GOL	C	364	6/6	0.83	0.24	52,67,67,68	6
6	LDA	L	703	16/16	0.83	0.40	52,57,61,63	16
10	GOL	H	285	6/6	0.83	0.28	68,70,71,71	6
8	SO4	C	343	5/5	0.83	0.40	52,62,65,66	5
8	SO4	C	353	5/5	0.83	0.38	66,69,72,76	5
8	SO4	M	328	5/5	0.83	0.34	61,62,64,69	5
6	LDA	L	723	16/16	0.84	1.01	55,58,64,68	16
10	GOL	H	278	6/6	0.84	0.20	63,67,68,71	6
6	LDA	H	720	16/16	0.84	0.24	55,69,73,73	16
10	GOL	M	337	6/6	0.84	0.13	68,69,69,70	6
8	SO4	C	349	5/5	0.84	0.42	63,64,71,71	5
8	SO4	H	266	5/5	0.84	0.33	65,66,68,71	5
10	GOL	H	291	6/6	0.85	0.26	74,78,80,81	6
9	HTO	L	276	10/10	0.85	0.48	50,67,70,71	10
8	SO4	C	337[B]	5/5	0.86	0.23	59,64,69,70	5
8	SO4	C	337[A]	5/5	0.86	0.23	59,62,67,67	5
10	GOL	M	336	6/6	0.86	0.17	68,69,70,71	6
8	SO4	H	264	5/5	0.86	0.18	61,67,72,73	5
10	GOL	C	373	6/6	0.86	1.85	60,63,64,65	6
6	LDA	M	713	16/16	0.87	0.18	63,69,84,86	16
10	GOL	C	365	6/6	0.87	0.18	60,67,69,72	6
10	GOL	C	360	6/6	0.87	0.22	44,56,62,71	6
10	GOL	L	282	6/6	0.87	0.15	53,59,59,63	6
10	GOL	L	286	6/6	0.87	0.65	58,63,64,68	6
8	SO4	H	263	5/5	0.87	0.49	75,76,78,79	5
8	SO4	C	352	5/5	0.87	0.35	78,78,81,82	5
8	SO4	H	267	5/5	0.88	0.26	56,64,65,65	5
6	LDA	M	714	16/16	0.88	0.20	70,75,81,82	16
10	GOL	C	377	6/6	0.88	0.12	63,65,67,67	6
8	SO4	C	340	5/5	0.88	0.29	57,71,76,82	5
10	GOL	H	282	6/6	0.88	0.37	59,66,68,69	6
8	SO4	C	344	5/5	0.88	0.38	74,76,79,82	5
10	GOL	H	290	6/6	0.88	0.19	49,59,63,67	6
9	HTO	H	272	10/10	0.89	0.17	61,67,75,80	10

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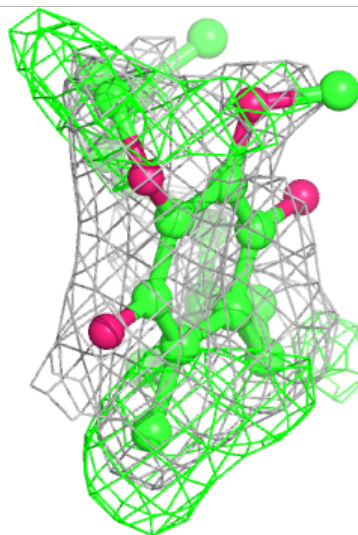
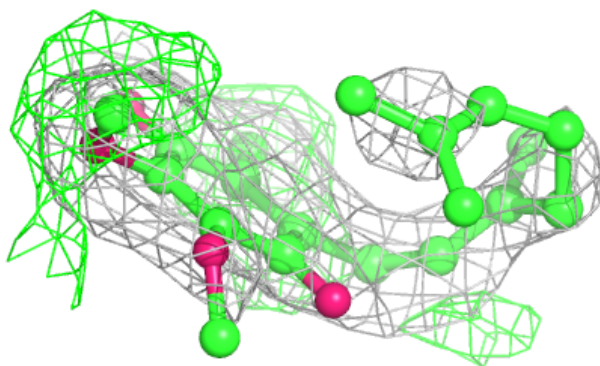
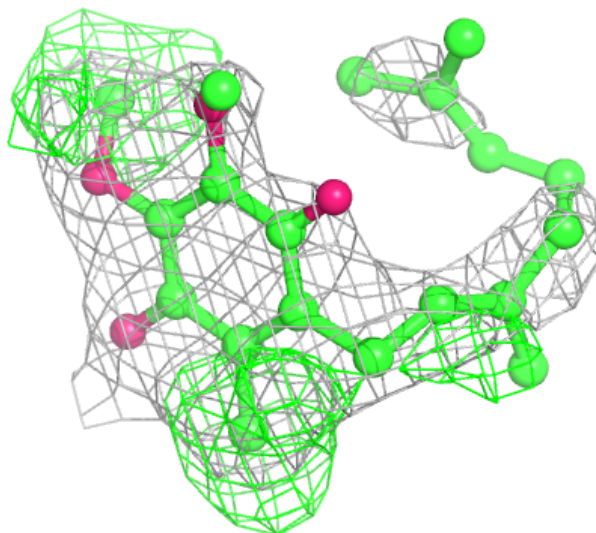
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	GOL	L	283	6/6	0.89	0.13	59,63,68,70	6
10	GOL	C	368	6/6	0.89	0.19	62,63,68,70	6
8	SO4	H	261[A]	5/5	0.90	0.19	52,58,64,65	5
10	GOL	H	286	6/6	0.90	0.33	67,67,69,70	6
10	GOL	C	362	6/6	0.90	0.38	51,57,63,63	6
6	LDA	M	704	16/16	0.90	0.22	49,80,87,87	16
8	SO4	H	261[B]	5/5	0.90	0.19	47,54,61,61	5
16	NS5	M	600	40/40	0.90	0.14	42,54,95,96	0
8	SO4	C	342	5/5	0.90	0.24	63,68,71,75	5
8	SO4	H	268	5/5	0.90	0.54	63,66,70,72	5
15	MQ9	M	501	58/58	0.91	0.17	31,41,92,98	0
6	LDA	H	701	16/16	0.91	0.26	43,57,71,73	0
10	GOL	C	361	6/6	0.91	0.24	60,64,72,75	6
8	SO4	C	346	5/5	0.93	0.25	57,65,71,72	5
10	GOL	M	335	6/6	0.93	0.10	44,54,60,68	6
8	SO4	C	339	5/5	0.93	0.36	69,71,75,80	5
10	GOL	L	281	6/6	0.94	0.41	54,58,66,68	6
8	SO4	C	345	5/5	0.94	0.23	66,68,72,72	5
8	SO4	M	327	5/5	0.94	0.22	53,58,68,75	5
10	GOL	M	334	6/6	0.94	0.18	40,56,66,69	6
8	SO4	C	341	5/5	0.95	0.17	67,74,80,81	5
6	LDA	H	721	16/16	0.95	0.14	50,66,69,69	0
10	GOL	H	275	6/6	0.95	0.27	59,62,64,67	0
11	BCB	M	401	66/66	0.95	0.17	28,34,58,66	0
11	BCB	M	400	66/66	0.95	0.18	34,40,109,121	0
8	SO4	H	260	5/5	0.96	0.09	59,63,68,71	5
11	BCB	L	401	66/66	0.96	0.14	27,35,64,75	0
10	GOL	C	359	6/6	0.96	0.44	44,50,54,55	6
8	SO4	C	338	5/5	0.96	0.19	53,57,60,64	5
12	BPB	L	402	65/65	0.96	0.13	32,39,48,51	0
12	BPB	M	402	65/65	0.96	0.13	33,41,124,132	0
8	SO4	M	326	5/5	0.97	0.18	56,61,62,62	5
8	SO4	H	259	5/5	0.97	0.13	60,62,67,69	5
11	BCB	L	400	66/66	0.97	0.18	28,36,48,52	0
5	HEC	C	403	43/43	0.98	0.15	32,36,41,42	0
5	HEC	C	402	43/43	0.98	0.09	39,44,52,60	0
5	HEC	C	401	43/43	0.98	0.10	41,46,55,58	0
5	HEC	C	404	43/43	0.98	0.09	32,38,51,64	0
8	SO4	M	325	5/5	0.99	0.17	64,67,78,79	0
8	SO4	H	262	5/5	0.99	0.12	41,43,45,47	5
8	SO4	M	324	5/5	0.99	0.11	47,52,61,63	0
14	FE2	M	500	1/1	1.00	0.14	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



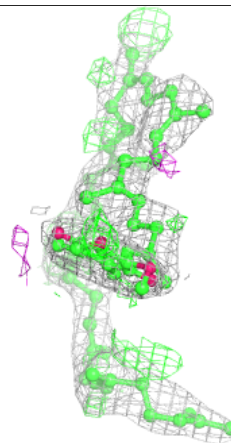
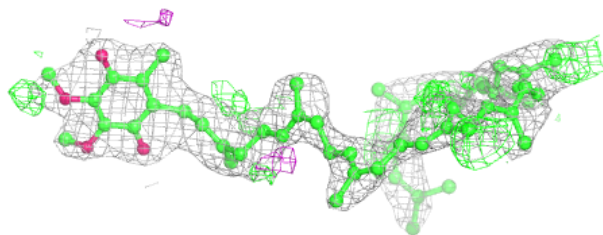
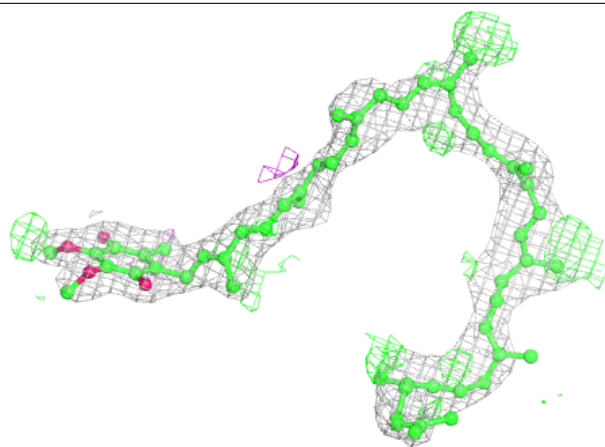
**Electron density around UQ9 L 503:**

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

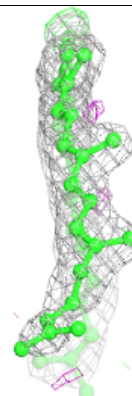
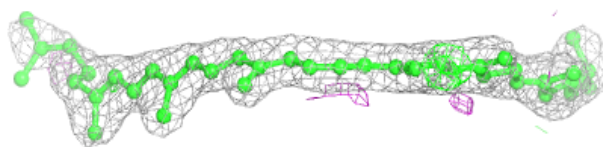
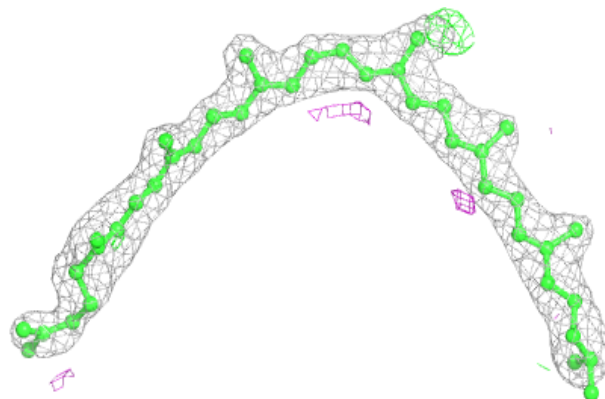


**Electron density around UQ9 L 502:**

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and green (positive)

**Electron density around NS5 M 600:**

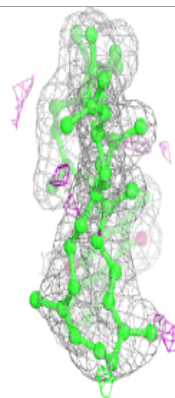
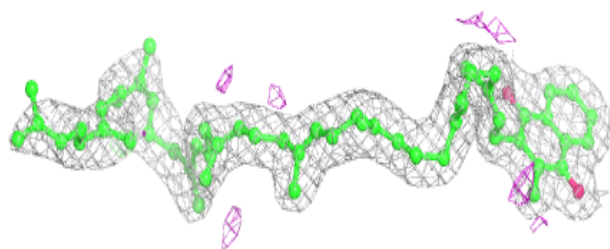
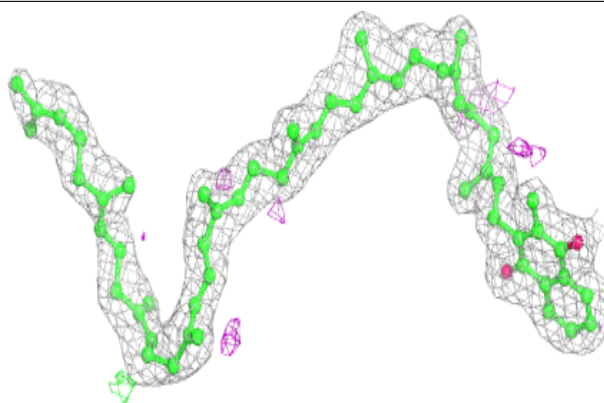
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



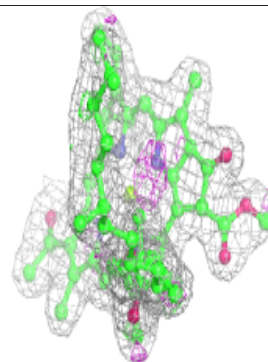
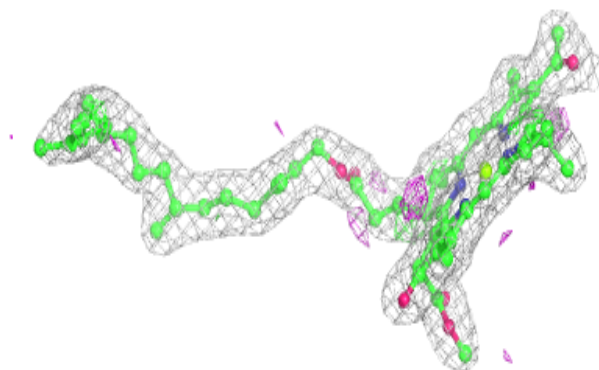
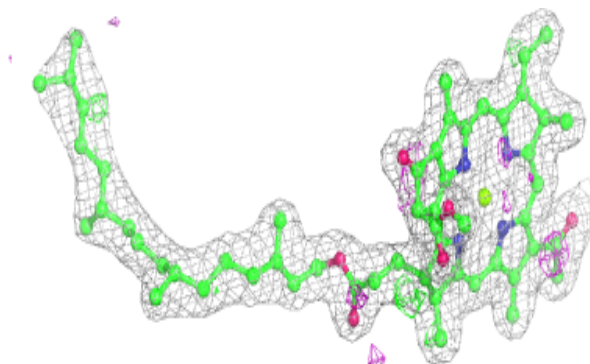


**Electron density around MQ9 M 501:**

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

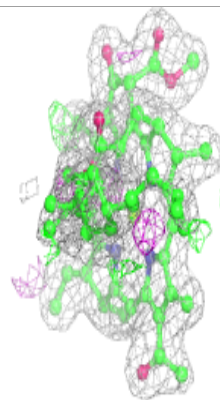
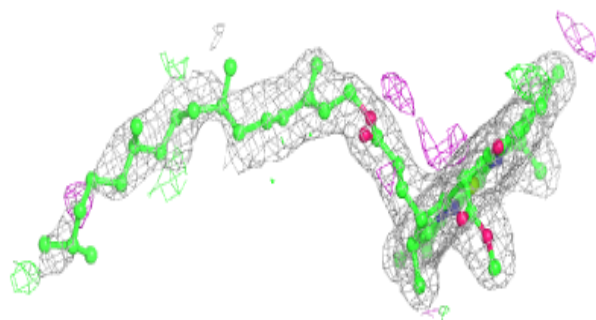
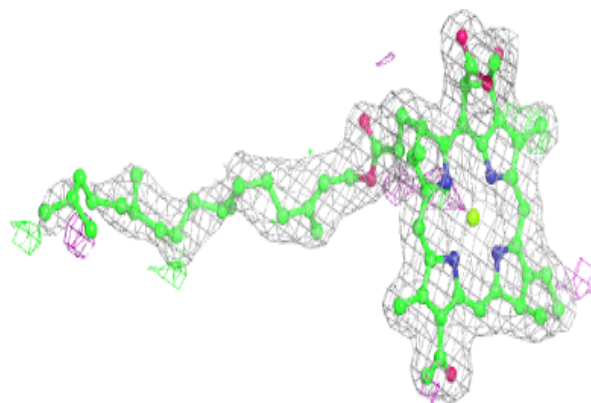
**Electron density around BCB M 401:**

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

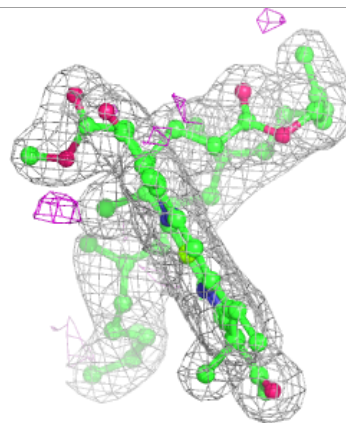
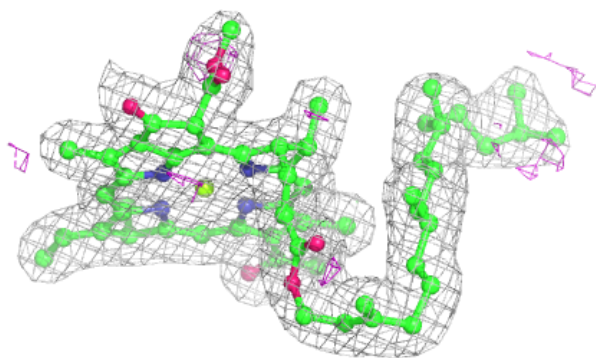
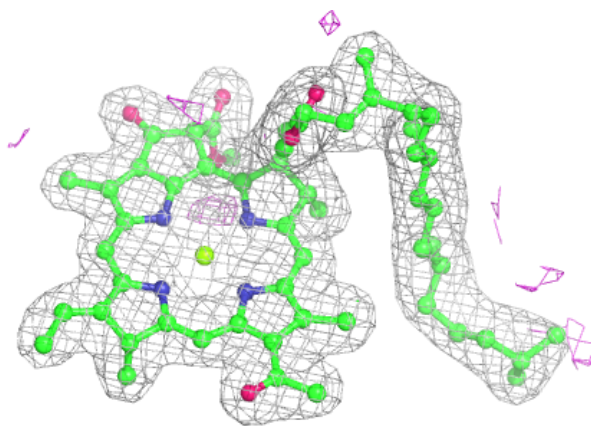


**Electron density around BCB M 400:**

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

**Electron density around BCB L 401:**

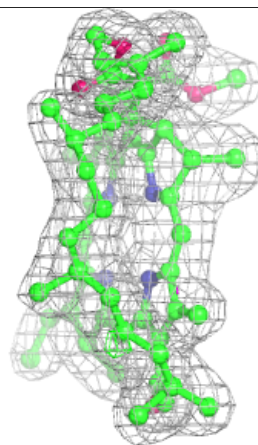
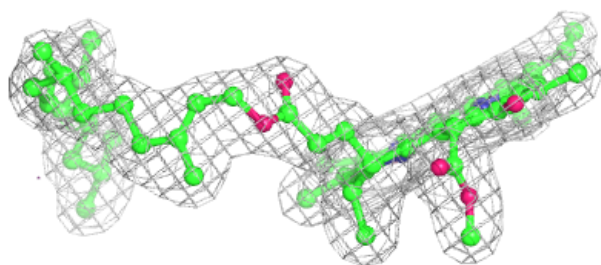
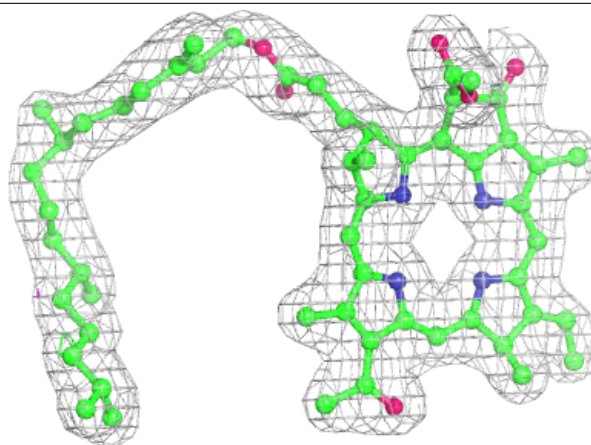
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



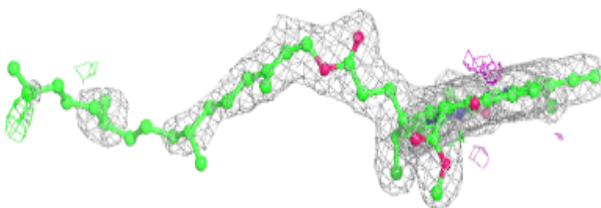
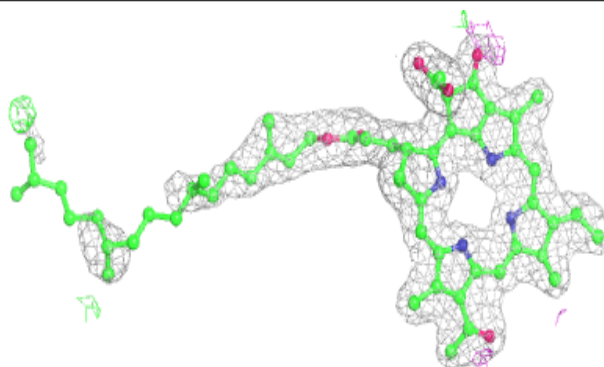


**Electron density around BPB L 402:**

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

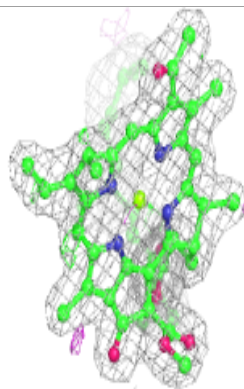
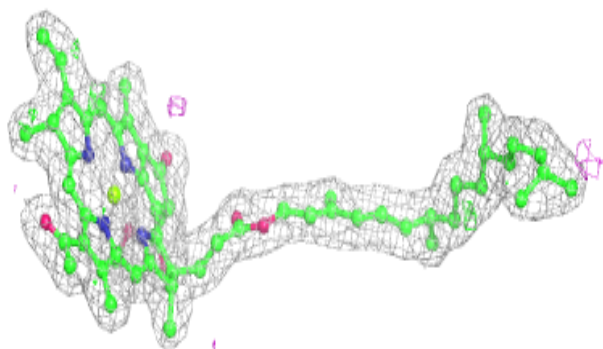
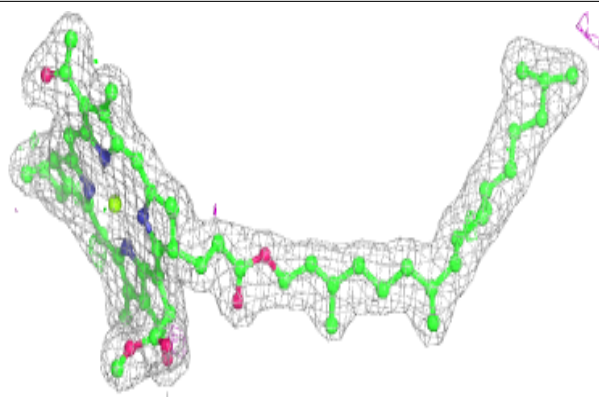
**Electron density around BPB M 402:**

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



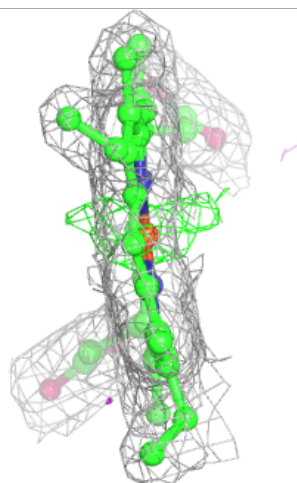
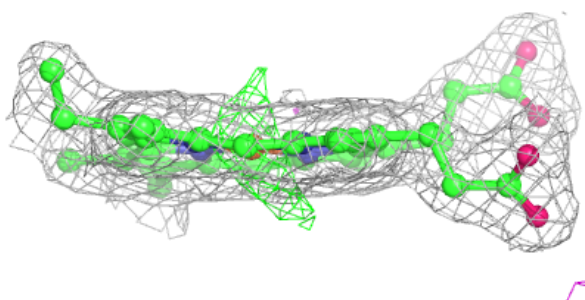
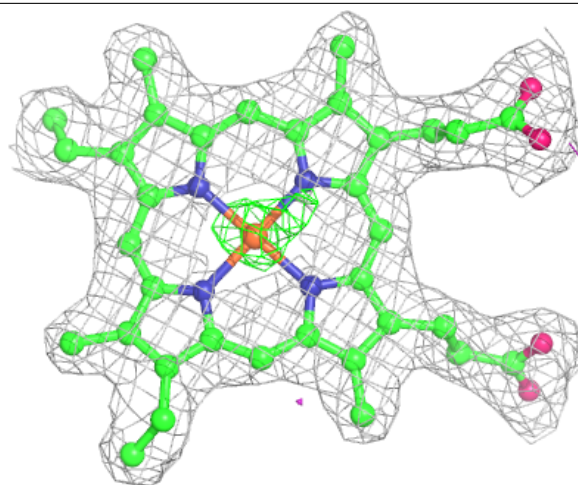
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and green (positive)



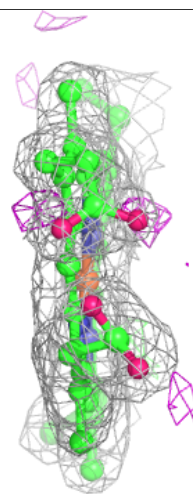
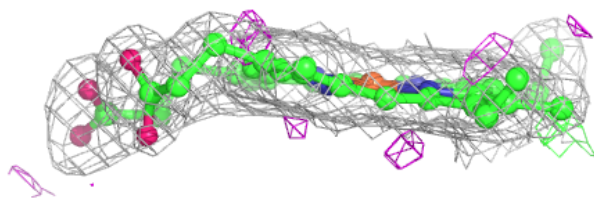
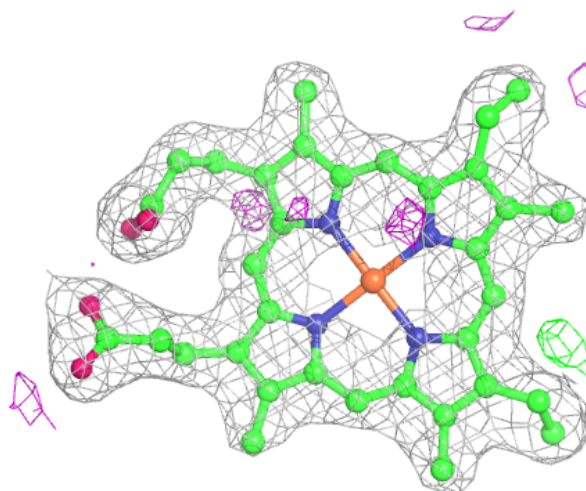
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and green (positive)



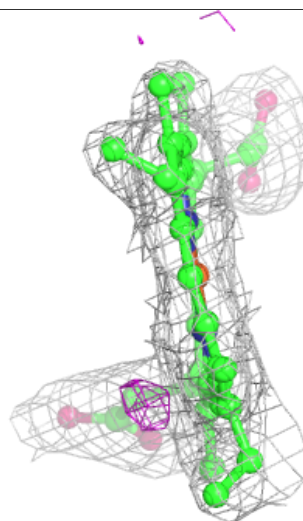
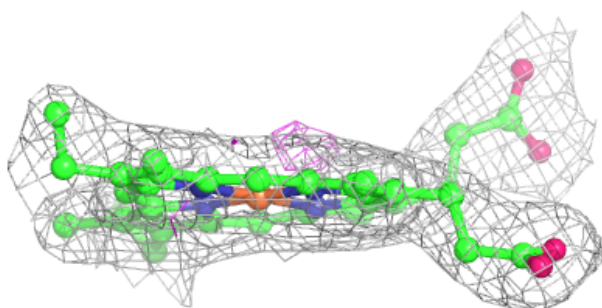
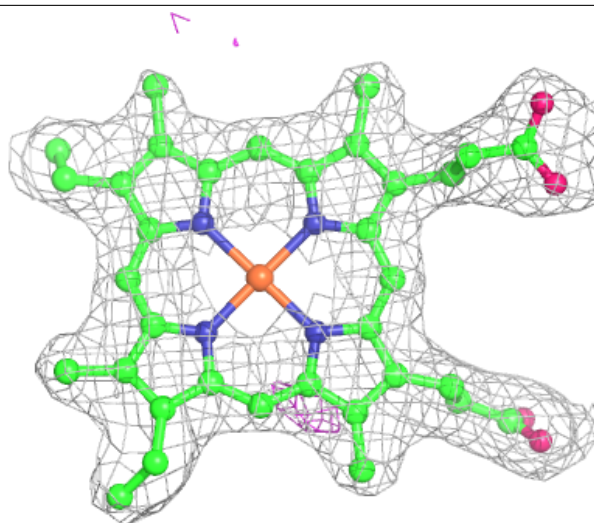
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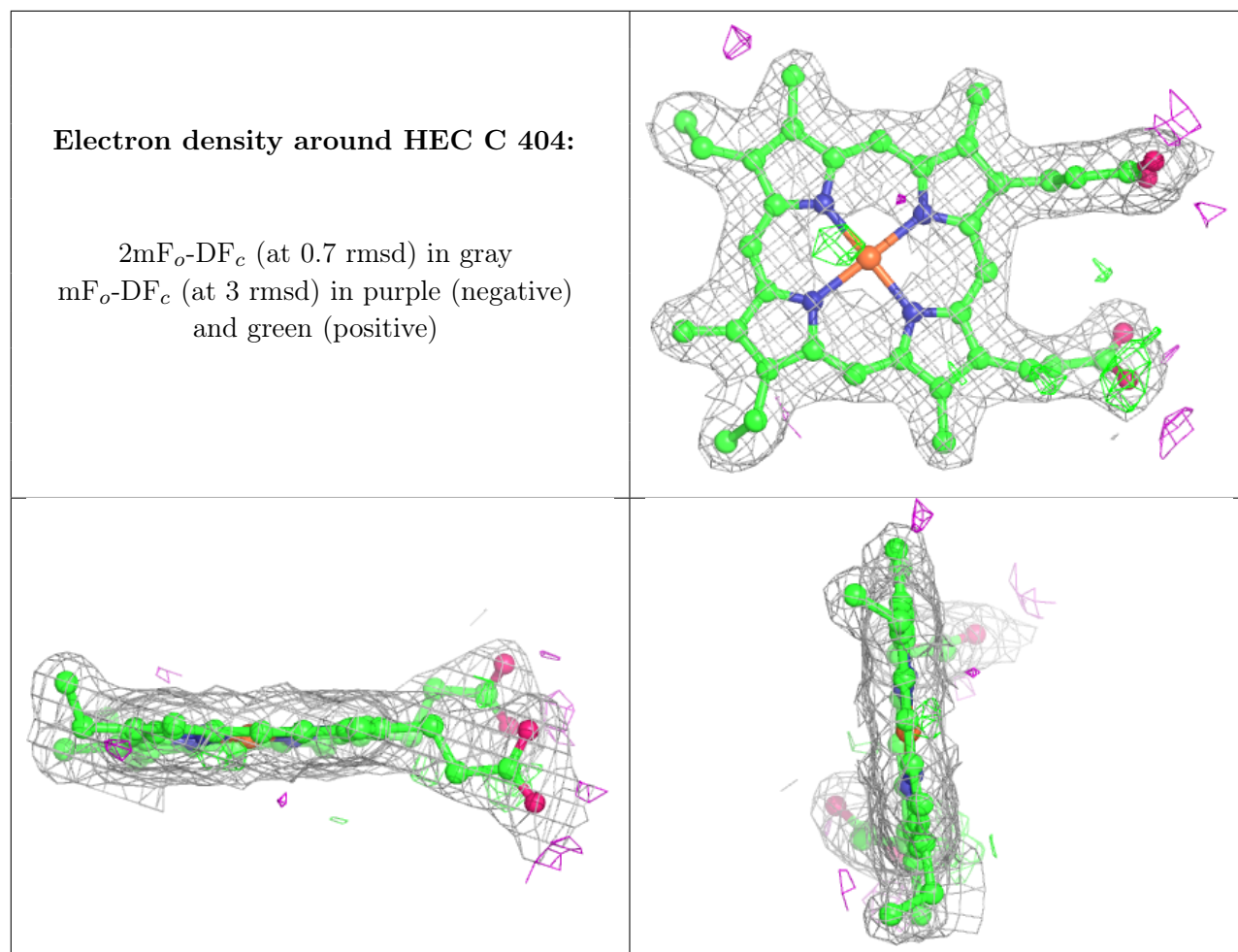
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.