



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:48 pm BST

PDB ID : 2UX4  
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 9 in the charge-separated state, 2nd dataset  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-26  
Resolution : 2.51 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.

---

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 : 2.11  
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) : 2.11

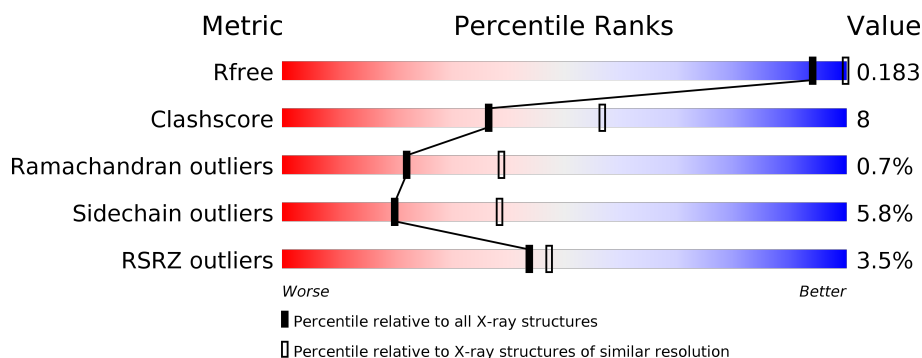
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	H	260	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>
2	L	281	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>12%</div> </div> </div>
3	M	307	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>16%</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
14	CDL	M	1314	-	-	-	X
4	GOL	H	1253	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	L	1283	-	-	-	X
6	LDA	L	1285	-	-	-	X
6	LDA	M	1309	-	-	-	X
6	LDA	M	1709	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7671 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 REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	3	1
			1846	1181	319	337	9			

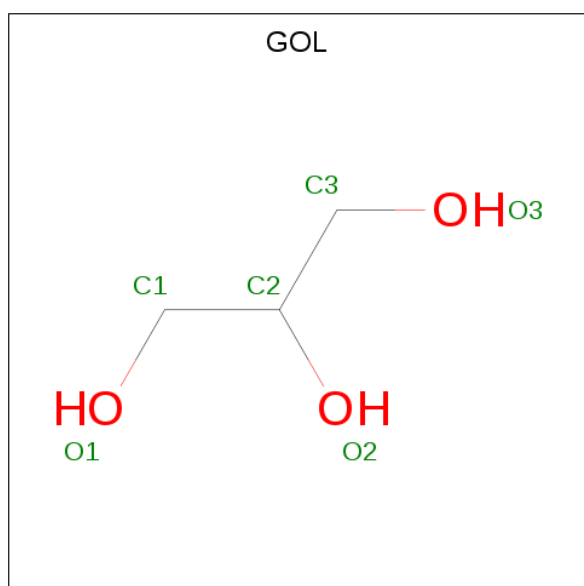
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

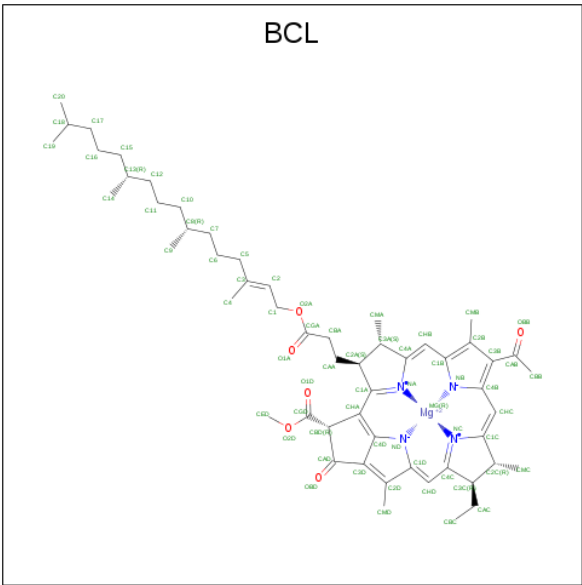
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

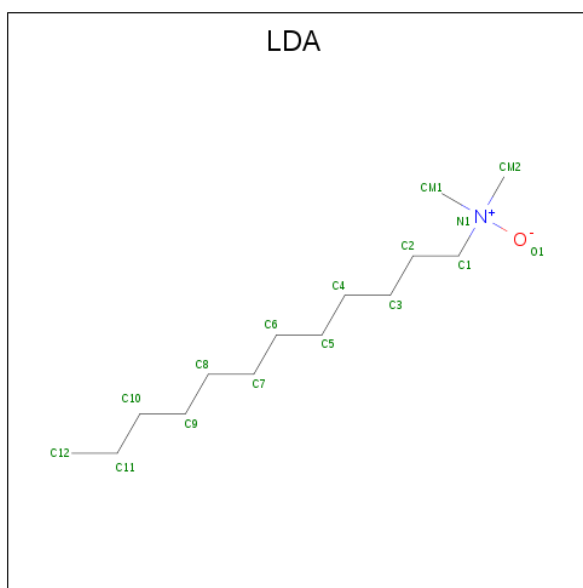
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

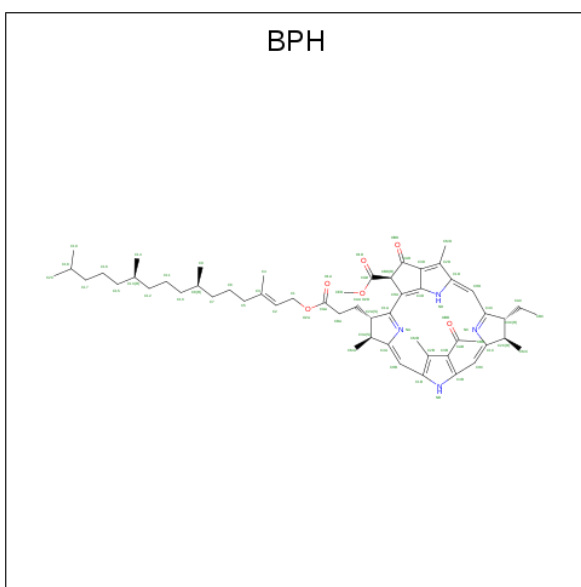
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C<sub>14</sub>H<sub>31</sub>NO).



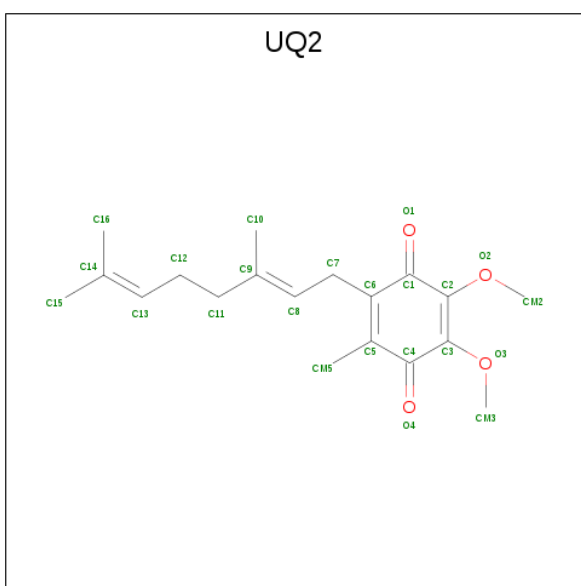
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



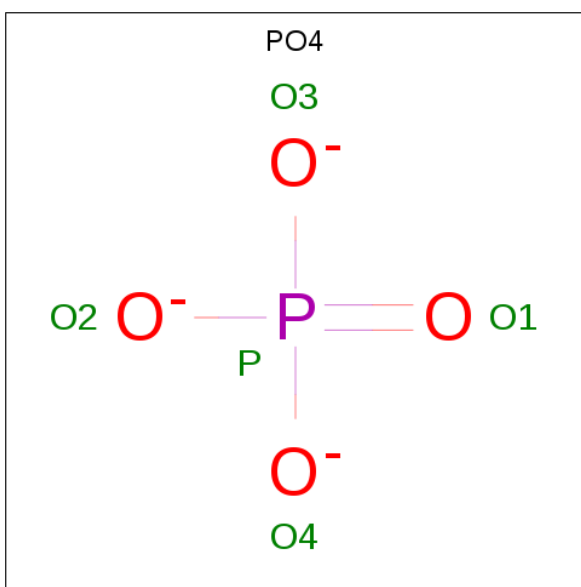
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (three-letter code: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



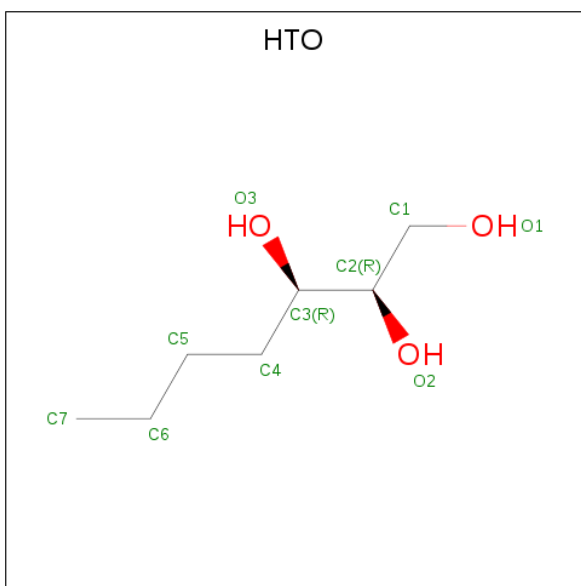
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).

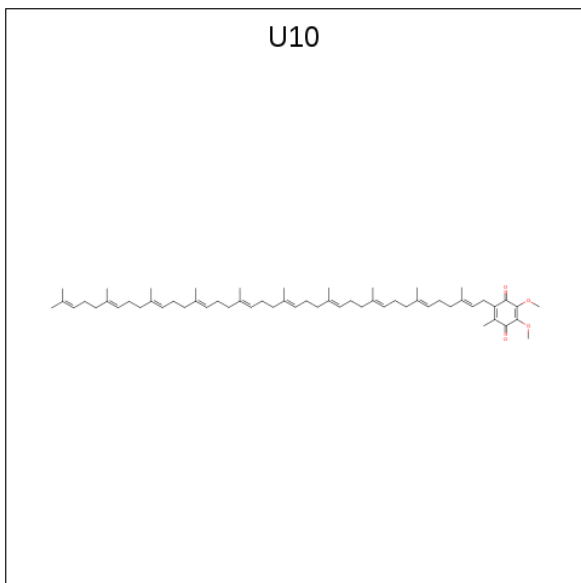


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

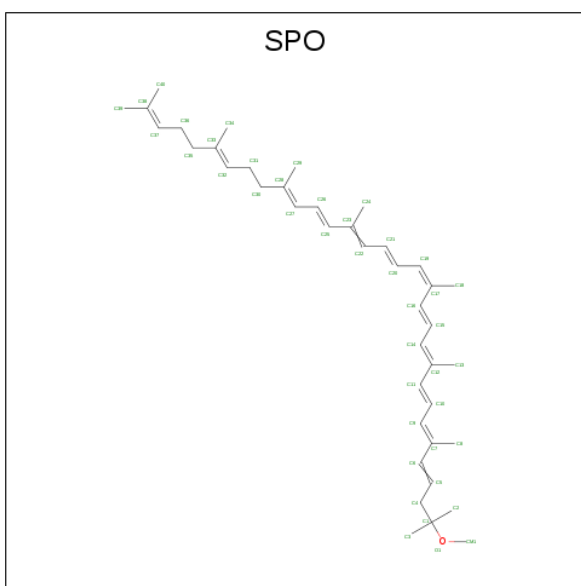
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



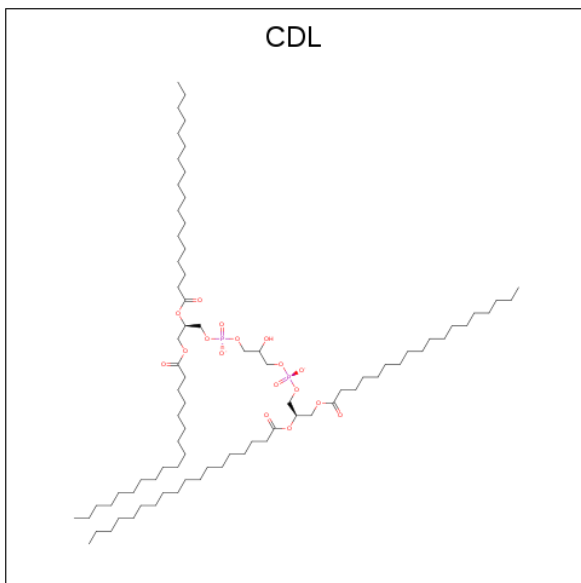
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

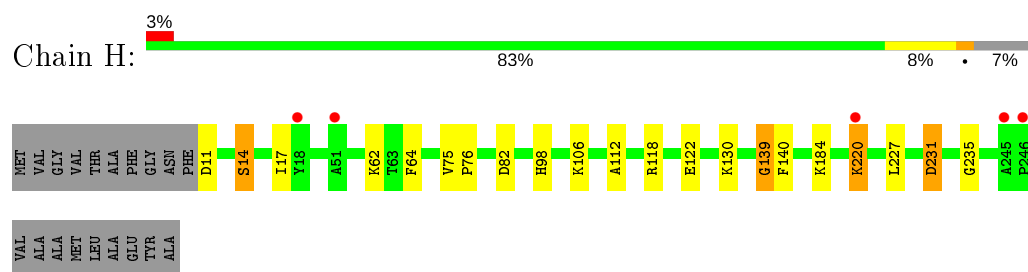
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	149	Total	O	0	0
			149	149		
15	L	111	Total	O	0	0
			111	111		
15	M	111	Total	O	0	0
			111	111		

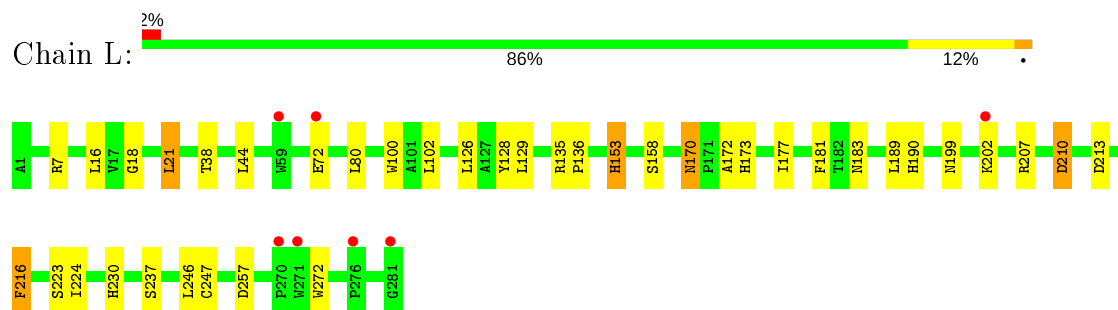
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

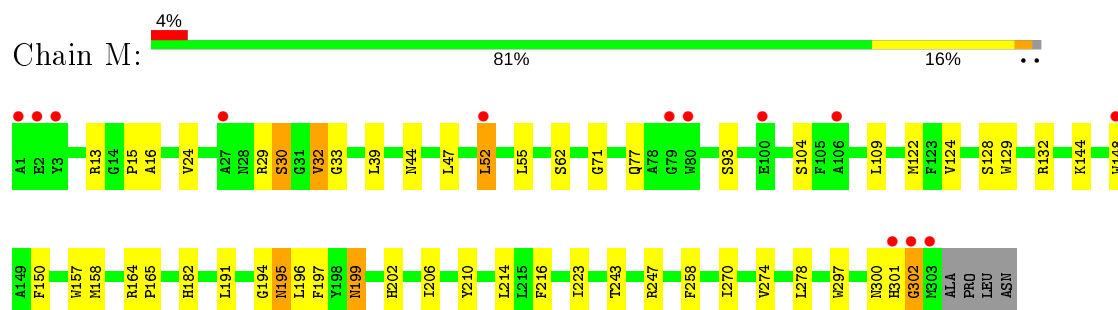
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN



#### • Molecule 2: REACTION CENTER PROTEIN L CHAIN



#### • Molecule 3: REACTION CENTER PROTEIN M CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.58Å 139.58Å 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.51 29.45 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.51) 90.9 (29.45-2.51)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190 , 0.211 0.184 , 0.183	Depositor DCC
$R_{free}$ test set	3493 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, FE, SPO, U10, UQ2

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	H	0.53	0/1906	0.74	4/2591 (0.2%)
2	L	0.56	0/2320	0.64	2/3175 (0.1%)
3	M	0.54	0/2501	0.63	0/3415
All	All	0.54	0/6727	0.66	6/9181 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	L	213	ASP	CB-CG-OD2	6.87	124.49	118.30
1	H	82	ASP	CB-CG-OD2	6.09	123.78	118.30
1	H	11	ASP	CB-CG-OD2	5.91	123.62	118.30
1	H	139	GLY	N-CA-C	-5.89	98.37	113.10
1	H	231	ASP	CB-CG-OD2	5.67	123.40	118.30
2	L	257	ASP	CB-CG-OD2	5.36	123.12	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	H	1846	0	1861	16	0
2	L	2232	0	2187	26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	M	2409	0	2321	37	0
4	H	24	0	32	1	0
4	L	12	0	16	1	0
4	M	6	0	8	2	0
5	L	132	0	148	7	0
5	M	132	0	148	24	0
6	L	48	0	93	7	0
6	M	96	0	186	10	0
7	L	65	0	76	7	0
7	M	65	0	76	12	0
8	L	46	0	52	6	0
9	L	5	0	0	0	0
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	0	0
13	M	42	0	60	4	0
14	M	81	0	82	2	0
15	H	149	0	0	3	0
15	L	111	0	0	1	0
15	M	111	0	0	1	0
All	All	7671	0	7425	116	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 (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.25	1.10
1:H:248:ARG:HA	1:H:249:LYS:CB	1.95	0.96
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.87
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.15	0.80
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.66	0.77
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.21	0.75
7:L:1286:BPH:HHC	7:L:1286:BPH:HBB3	1.67	0.75
2:L:224:ILE:HG22	8:L:1287[A]:UQ2:H8	1.72	0.72
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.73	0.71
1:H:248:ARG:CA	1:H:249:LYS:HB2	2.12	0.70
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.73	0.69
3:M:243:THR:O	3:M:247:ARG:HG3	1.94	0.68
7:L:1286:BPH:HHC	7:L:1286:BPH:CBB	2.23	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB2	1.79	0.65
5:M:1303:BCL:CBB	5:M:1303:BCL:HHC	2.28	0.64
5:M:1303:BCL:HMA2	6:M:1309:LDA:H112	1.79	0.64
7:M:1311:BPH:HBB3	7:M:1311:BPH:HHC	1.78	0.63
5:M:1303:BCL:H203	13:M:1313:SPO:H10	1.81	0.62
3:M:300:ASN:C	3:M:302:GLY:H	2.02	0.62
1:H:220[B]:LYS:NZ	15:H:2135:HOH:O	2.34	0.61
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.36	0.60
6:M:1305:LDA:H12	4:M:1315:GOL:H12	1.83	0.60
2:L:189:LEU:CD2	7:M:1311:BPH:HMD2	2.32	0.60
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.19	0.59
6:M:1307:LDA:H52	6:M:1308:LDA:H62	1.84	0.59
3:M:77:GLN:HE22	3:M:93:SER:H	1.49	0.59
2:L:170:ASN:C	2:L:170:ASN:HD22	2.06	0.58
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.34	0.58
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.86	0.57
7:L:1286:BPH:HBB1	3:M:210:TYR:CD2	2.41	0.56
5:L:1282:BCL:HBB3	5:L:1288:BCL:H52	1.87	0.56
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.88	0.55
4:H:1251:GOL:H32	15:H:2003:HOH:O	2.06	0.54
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.86	0.54
2:L:199:ASN:HA	4:L:1291:GOL:H31	1.91	0.53
1:H:140:PHE:HA	3:M:13:ARG:O	2.09	0.53
3:M:270:ILE:O	3:M:274:VAL:HG13	2.09	0.53
3:M:199:ASN:HD22	3:M:199:ASN:C	2.11	0.53
3:M:24:VAL:HG21	3:M:29:ARG:NH1	2.24	0.53
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.91	0.53
3:M:144:LYS:N	14:M:1314:CDL:OB3	2.38	0.53
3:M:62:SER:OG	3:M:124:VAL:HG22	2.09	0.52
1:H:112:ALA:HA	1:H:235:GLY:O	2.10	0.52
1:H:248:ARG:CA	1:H:249:LYS:CB	2.78	0.52
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.90	0.52
6:M:1305:LDA:H32	4:M:1315:GOL:H32	1.91	0.52
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.45	0.52
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.57	0.52
6:L:1284:LDA:H11	3:M:33:GLY:HA2	1.91	0.51
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.92	0.51
7:M:1311:BPH:CBB	7:M:1311:BPH:HHC	2.40	0.51
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.40	0.51
3:M:194:GLY:O	3:M:195:ASN:HB3	2.10	0.51
7:L:1286:BPH:CHC	7:L:1286:BPH:HBB3	2.38	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1288:BCL:HMB1	5:L:1288:BCL:CBB	2.41	0.51
2:L:190:HIS:HA	8:L:1287[A]:UQ2:O4	2.11	0.51
2:L:189:LEU:HD23	7:M:1311:BPH:HMD2	1.92	0.51
2:L:18:GLY:O	2:L:21:LEU:HB2	2.12	0.50
3:M:258:PHE:CG	6:M:1307:LDA:H51	2.46	0.50
2:L:210:ASP:OD1	2:L:210:ASP:N	2.45	0.49
6:L:1285:LDA:H42	6:M:1309:LDA:H81	1.94	0.49
6:M:1305:LDA:H101	6:M:1307:LDA:H121	1.95	0.49
5:L:1288:BCL:C1C	5:M:1304:BCL:HBB3	2.43	0.49
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.95	0.49
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.49	0.48
7:L:1286:BPH:ND	3:M:214:LEU:HD13	2.28	0.48
1:H:75:VAL:HA	1:H:76:PRO:C	2.35	0.47
1:H:14:SER:HA	1:H:17:ILE:HG22	1.97	0.47
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.50	0.47
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.44	0.46
3:M:150:PHE:CD1	7:M:1311:BPH:C3D	2.98	0.46
5:L:1288:BCL:HMB2	5:M:1304:BCL:HHB	1.98	0.46
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.19	0.46
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.81	0.45
6:L:1284:LDA:H62	3:M:47:LEU:HD12	1.99	0.44
7:L:1286:BPH:CHC	7:L:1286:BPH:CBB	2.94	0.44
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.99	0.44
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.85	0.44
3:M:297:TRP:CE2	3:M:302:GLY:HA2	2.53	0.44
3:M:197:PHE:CE1	5:M:1304:BCL:HHC	2.52	0.44
6:M:1307:LDA:H22	6:M:1307:LDA:HM11	1.54	0.44
3:M:300:ASN:C	3:M:302:GLY:N	2.70	0.44
6:M:1307:LDA:H41	6:M:1308:LDA:H42	1.99	0.44
2:L:189:LEU:HD13	2:L:216:PHE:HZ	1.81	0.44
5:M:1303:BCL:H101	5:M:1304:BCL:H171	2.00	0.43
3:M:196:LEU:HD12	5:M:1304:BCL:C1D	2.49	0.43
3:M:71:GLY:HA3	13:M:1313:SPO:H42	2.00	0.43
1:H:139:GLY:H	3:M:15:PRO:HD3	1.84	0.43
1:H:130:LYS:HD2	15:L:2087:HOH:O	2.19	0.42
3:M:129:TRP:O	3:M:132:ARG:HB3	2.19	0.42
3:M:194:GLY:O	3:M:195:ASN:CB	2.67	0.42
2:L:224:ILE:HD12	8:L:1287[B]:UQ2:H102	2.01	0.42
5:L:1282:BCL:HMB1	5:L:1288:BCL:H142	2.02	0.42
6:L:1285:LDA:H21	6:L:1285:LDA:HM21	1.90	0.42
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.55	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.02	0.42
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.84	0.42
6:L:1285:LDA:H121	8:L:1287[A]:UQ2:H161	2.01	0.42
5:M:1303:BCL:H102	5:M:1303:BCL:H13	1.72	0.42
2:L:170:ASN:ND2	2:L:172:ALA:H	2.18	0.42
5:M:1303:BCL:HBB2	13:M:1313:SPO:H243	2.02	0.42
7:M:1311:BPH:H141	7:M:1311:BPH:H161	1.90	0.42
1:H:118[A]:ARG:HD3	15:M:2089:HOH:O	2.20	0.41
2:L:224:ILE:CG2	8:L:1287[A]:UQ2:H8	2.46	0.41
5:M:1303:BCL:CBB	13:M:1313:SPO:H243	2.51	0.41
5:M:1303:BCL:HBB3	5:M:1303:BCL:HHC	2.01	0.41
6:L:1285:LDA:H121	8:L:1287[A]:UQ2:C16	2.50	0.41
6:L:1283:LDA:H22	6:L:1283:LDA:HM11	1.86	0.41
15:H:2003:HOH:O	14:M:1314:CDL:HA32	2.20	0.41
2:L:183:ASN:ND2	2:L:237:SER:HB3	2.36	0.41
7:M:1311:BPH:H2	7:M:1311:BPH:H6C2	1.94	0.41
3:M:122:MET:HE3	5:M:1304:BCL:H142	2.03	0.41
6:M:1309:LDA:HM11	6:M:1309:LDA:H21	1.75	0.41
2:L:189:LEU:HD21	7:M:1311:BPH:HMD2	2.02	0.40
5:M:1303:BCL:CBB	5:M:1303:BCL:CHC	2.99	0.40
2:L:223:SER:O	3:M:44:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	H	242/260 (93%)	233 (96%)	8 (3%)	1 (0%)	34	54
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
3	M	301/307 (98%)	287 (95%)	9 (3%)	5 (2%)	9	16
All	All	822/848 (97%)	790 (96%)	26 (3%)	6 (1%)	22	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	301	HIS
3	M	52	LEU
3	M	195	ASN
3	M	30	SER
3	M	302	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	198/208 (95%)	189 (96%)	9 (4%)	27	51
2	L	220/220 (100%)	202 (92%)	18 (8%)	11	22
3	M	236/240 (98%)	224 (95%)	12 (5%)	24	45
All	All	654/668 (98%)	615 (94%)	39 (6%)	20	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	SER
1	H	106	LYS
1	H	184	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	247	LYS
1	H	249	LYS
1	H	250	SER
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	72	GLU
2	L	80	LEU
2	L	102	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	126	LEU
2	L	129	LEU
2	L	153	HIS
2	L	158	SER
2	L	170	ASN
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
2	L	272	TRP
3	M	30	SER
3	M	32	VAL
3	M	39	LEU
3	M	52	LEU
3	M	104	SER
3	M	109	LEU
3	M	148	TRP
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE
3	M	278	LEU

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

Mol	Chain	Res	Type
1	H	98	HIS
2	L	159	ASN
2	L	170	ASN
2	L	183	ASN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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$
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.25	0
6	LDA	L	1285	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
14	CDL	M	1314	-	80,80,99	2.33	18 (22%)	86,92,111	4.01	15 (17%)
4	GOL	H	1251	-	5,5,5	0.52	0	5,5,5	0.73	0
6	LDA	M	1309	-	12,15,15	2.01	1 (8%)	14,17,17	0.45	0
4	GOL	H	1253	-	5,5,5	0.35	0	5,5,5	0.28	0
6	LDA	L	1284	-	12,15,15	2.04	1 (8%)	14,17,17	0.50	0
13	SPO	M	1313	-	40,41,41	4.16	12 (30%)	47,50,50	1.89	11 (23%)
12	U10	M	1312	-	48,48,63	2.69	12 (25%)	58,61,79	1.65	12 (20%)
9	PO4	L	1289	-	4,4,4	0.84	0	6,6,6	0.48	0
6	LDA	M	1308	-	12,15,15	2.05	1 (8%)	14,17,17	0.46	0
5	BCL	M	1304	3	58,74,74	2.21	8 (13%)	69,115,115	1.95	18 (26%)
4	GOL	L	1292	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	L	1291	-	5,5,5	0.32	0	5,5,5	0.51	0
5	BCL	L	1282	2	58,74,74	2.17	8 (13%)	69,115,115	2.21	20 (28%)
5	BCL	M	1303	3	58,74,74	2.26	9 (15%)	69,115,115	1.98	14 (20%)
4	GOL	M	1315	-	5,5,5	0.33	0	5,5,5	0.31	0
10	HTO	L	1290	-	9,9,9	0.43	0	10,10,10	0.57	0
6	LDA	L	1283	-	12,15,15	2.03	1 (8%)	14,17,17	0.49	0
6	LDA	M	1307	-	12,15,15	2.00	1 (8%)	14,17,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	UQ2	L	1287[A]	-	23,23,23	2.67	8 (34%)	28,31,31	1.61	5 (17%)
6	LDA	M	1306	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
8	UQ2	L	1287[B]	-	23,23,23	2.76	7 (30%)	28,31,31	1.18	1 (3%)
4	GOL	H	1252	-	5,5,5	0.38	0	5,5,5	0.22	0
6	LDA	M	1305	-	12,15,15	2.10	1 (8%)	14,17,17	0.49	0
7	BPH	M	1311	-	64,70,70	3.01	17 (26%)	76,101,101	1.66	15 (19%)
6	LDA	M	1709	-	12,15,15	2.02	1 (8%)	14,17,17	0.51	0
5	BCL	L	1288	2	58,74,74	2.18	8 (13%)	69,115,115	2.00	17 (24%)
7	BPH	L	1286	-	64,70,70	3.02	17 (26%)	76,101,101	1.67	13 (17%)

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
4	GOL	H	1254	-	-	0/4/4/4	-
6	LDA	L	1285	-	-	9/13/13/13	-
14	CDL	M	1314	-	-	46/91/91/110	-
4	GOL	H	1251	-	-	4/4/4/4	-
6	LDA	M	1309	-	-	12/13/13/13	-
4	GOL	H	1253	-	-	1/4/4/4	-
6	LDA	L	1284	-	-	4/13/13/13	-
13	SPO	M	1313	-	-	24/47/47/47	-
12	U10	M	1312	-	-	13/45/69/87	0/1/1/1
6	LDA	M	1308	-	-	5/13/13/13	-
5	BCL	M	1304	3	2/2/21/25	9/37/137/137	-
4	GOL	L	1292	-	-	4/4/4/4	-
4	GOL	L	1291	-	-	2/4/4/4	-
5	BCL	L	1282	2	2/2/21/25	9/37/137/137	-
5	BCL	M	1303	3	2/2/21/25	16/37/137/137	-
4	GOL	M	1315	-	-	3/4/4/4	-
10	HTO	L	1290	-	-	7/10/10/10	-
6	LDA	L	1283	-	-	6/13/13/13	-
6	LDA	M	1307	-	-	8/13/13/13	-
8	UQ2	L	1287[A]	-	-	8/15/39/39	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1306	-	-	7/13/13/13	-
8	UQ2	L	1287[B]	-	-	8/15/39/39	0/1/1/1
4	GOL	H	1252	-	-	4/4/4/4	-
6	LDA	M	1305	-	-	5/13/13/13	-
7	BPH	M	1311	-	-	24/54/105/105	0/5/6/6
6	LDA	M	1709	-	-	8/13/13/13	-
5	BCL	L	1288	2	2/2/21/25	9/37/137/137	-
7	BPH	L	1286	-	-	14/54/105/105	0/5/6/6

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	OBD-CAD	13.41	1.41	1.22
5	M	1303	BCL	OBD-CAD	13.35	1.41	1.22
7	L	1286	BPH	OBD-CAD	12.97	1.40	1.22
5	L	1282	BCL	OBD-CAD	12.89	1.40	1.22
7	M	1311	BPH	OBD-CAD	12.82	1.40	1.22
5	L	1288	BCL	OBD-CAD	12.79	1.40	1.22
13	M	1313	SPO	C27-C28	12.67	1.47	1.34
13	M	1313	SPO	C9-C7	9.40	1.48	1.35
13	M	1313	SPO	C22-C23	9.29	1.48	1.35
13	M	1313	SPO	C14-C12	9.25	1.48	1.35
13	M	1313	SPO	C19-C17	8.90	1.47	1.35
7	L	1286	BPH	OBB-CAB	8.47	1.41	1.23
7	L	1286	BPH	O1D-CGD	8.05	1.41	1.21
7	M	1311	BPH	OBB-CAB	7.83	1.40	1.23
7	M	1311	BPH	O1D-CGD	7.79	1.40	1.21
14	M	1314	CDL	C11-CA5	-7.36	1.29	1.50
6	L	1285	LDA	O1-N1	-7.12	1.25	1.42
6	M	1305	LDA	O1-N1	-7.07	1.25	1.42
6	M	1306	LDA	O1-N1	-7.00	1.25	1.42
6	M	1308	LDA	O1-N1	-7.00	1.25	1.42
6	L	1284	LDA	O1-N1	-7.00	1.25	1.42
6	L	1283	LDA	O1-N1	-6.94	1.25	1.42
6	M	1709	LDA	O1-N1	-6.92	1.26	1.42
6	M	1307	LDA	O1-N1	-6.89	1.26	1.42
14	M	1314	CDL	C32-C31	-6.86	1.26	1.52
6	M	1309	LDA	O1-N1	-6.86	1.26	1.42
8	L	1287[B]	UQ2	C8-C9	6.80	1.49	1.33
12	M	1312	U10	C33-C34	6.72	1.49	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1312	U10	C13-C14	6.65	1.48	1.33
7	L	1286	BPH	CHB-C1B	6.53	1.51	1.38
7	L	1286	BPH	O1A-CGA	6.41	1.41	1.22
5	M	1303	BCL	O1A-CGA	6.37	1.41	1.22
8	L	1287[A]	UQ2	C8-C9	6.36	1.48	1.33
7	L	1286	BPH	C2-C3	6.34	1.48	1.33
5	M	1304	BCL	O1A-CGA	6.33	1.41	1.22
13	M	1313	SPO	C32-C33	6.31	1.48	1.33
7	M	1311	BPH	CHB-C1B	6.30	1.50	1.38
7	M	1311	BPH	C2-C3	6.26	1.48	1.33
7	M	1311	BPH	O1A-CGA	6.08	1.40	1.22
12	M	1312	U10	C18-C19	6.07	1.47	1.33
12	M	1312	U10	C8-C9	5.98	1.47	1.33
5	L	1288	BCL	O1A-CGA	5.91	1.40	1.22
5	L	1282	BCL	O1A-CGA	5.90	1.40	1.22
14	M	1314	CDL	C12-C11	-5.85	1.30	1.52
12	M	1312	U10	C23-C24	5.84	1.47	1.33
14	M	1314	CDL	C34-C33	-5.81	1.19	1.51
14	M	1314	CDL	C33-C32	-5.76	1.19	1.51
12	M	1312	U10	C28-C29	5.75	1.46	1.33
13	M	1313	SPO	C37-C38	5.72	1.48	1.32
8	L	1287[A]	UQ2	C13-C14	5.69	1.48	1.32
7	M	1311	BPH	CHC-C1C	5.68	1.47	1.36
13	M	1313	SPO	C6-C5	5.52	1.46	1.32
12	M	1312	U10	C38-C39	5.41	1.47	1.32
7	L	1286	BPH	C3D-C2D	5.40	1.49	1.39
8	L	1287[B]	UQ2	C13-C14	5.40	1.47	1.32
7	M	1311	BPH	C3D-C2D	5.25	1.48	1.39
8	L	1287[A]	UQ2	O2-C2	-5.25	1.24	1.36
8	L	1287[B]	UQ2	O2-C2	-5.11	1.24	1.36
8	L	1287[B]	UQ2	O3-C3	-5.06	1.24	1.36
14	M	1314	CDL	OB6-CB5	4.94	1.48	1.34
13	M	1313	SPO	C15-C16	4.76	1.46	1.34
12	M	1312	U10	O4-C4	-4.76	1.25	1.36
8	L	1287[A]	UQ2	O3-C3	-4.73	1.25	1.36
7	L	1286	BPH	CHC-C1C	4.69	1.45	1.36
14	M	1314	CDL	OA6-CA5	4.66	1.47	1.34
13	M	1313	SPO	C10-C11	4.59	1.46	1.34
14	M	1314	CDL	OA8-CA7	4.58	1.46	1.33
13	M	1313	SPO	C26-C25	4.52	1.46	1.34
12	M	1312	U10	O3-C3	-4.52	1.25	1.36
14	M	1314	CDL	C17-C16	-4.49	1.26	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1314	CDL	C16-C15	-4.48	1.26	1.51
7	L	1286	BPH	C3D-CAD	-4.47	1.38	1.47
14	M	1314	CDL	C20-C19	-4.42	1.26	1.51
7	M	1311	BPH	CHC-C4B	4.42	1.50	1.40
14	M	1314	CDL	C19-C18	-4.36	1.27	1.51
14	M	1314	CDL	OB8-CB7	4.33	1.46	1.33
5	M	1303	BCL	C1B-NB	4.05	1.38	1.35
7	M	1311	BPH	C3D-CAD	-4.01	1.39	1.47
13	M	1313	SPO	C21-C20	3.89	1.46	1.36
14	M	1314	CDL	C13-C12	-3.76	1.30	1.51
5	L	1288	BCL	C2-C3	3.68	1.41	1.33
7	M	1311	BPH	CHD-C4C	3.58	1.47	1.38
7	L	1286	BPH	CHC-C4B	3.58	1.48	1.40
8	L	1287[B]	UQ2	C6-C5	3.57	1.41	1.35
5	L	1282	BCL	C4B-NB	3.55	1.38	1.35
12	M	1312	U10	C6-C1	3.52	1.41	1.35
7	L	1286	BPH	CHD-C4C	3.46	1.46	1.38
8	L	1287[A]	UQ2	C3-C4	-3.27	1.39	1.48
5	L	1288	BCL	C4B-NB	3.23	1.38	1.35
5	L	1282	BCL	C2-C3	3.21	1.40	1.33
7	M	1311	BPH	C1B-C2B	-3.19	1.38	1.45
12	M	1312	U10	C4-C5	-3.18	1.39	1.48
8	L	1287[B]	UQ2	C3-C4	-3.11	1.39	1.48
7	L	1286	BPH	O2D-CGD	-3.10	1.25	1.33
14	M	1314	CDL	C37-C36	-3.09	1.34	1.51
14	M	1314	CDL	C79-C78	-3.09	1.34	1.51
14	M	1314	CDL	C80-C79	-3.05	1.34	1.51
5	M	1303	BCL	C4B-NB	3.05	1.37	1.35
5	L	1288	BCL	C1B-NB	3.03	1.37	1.35
5	M	1303	BCL	C2-C3	3.02	1.40	1.33
7	L	1286	BPH	CHB-C4A	3.00	1.47	1.40
14	M	1314	CDL	C22-C21	-3.00	1.34	1.51
7	M	1311	BPH	O2D-CGD	-2.96	1.26	1.33
7	M	1311	BPH	CHB-C4A	2.94	1.47	1.40
5	L	1282	BCL	C1B-NB	2.83	1.37	1.35
8	L	1287[B]	UQ2	C2-C1	-2.82	1.40	1.48
5	M	1304	BCL	C2-C3	2.81	1.39	1.33
5	L	1282	BCL	C3D-CAD	-2.75	1.39	1.46
5	M	1304	BCL	C4B-NB	2.71	1.37	1.35
8	L	1287[A]	UQ2	C6-C5	2.71	1.40	1.35
7	M	1311	BPH	O2A-CGA	-2.70	1.25	1.33
5	M	1304	BCL	C3D-CAD	-2.67	1.39	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1311	BPH	C1D-CHD	2.63	1.51	1.41
5	L	1288	BCL	C3D-CAD	-2.62	1.39	1.46
5	L	1288	BCL	O2D-CGD	-2.56	1.27	1.33
5	L	1282	BCL	O2D-CGD	-2.55	1.27	1.33
8	L	1287[A]	UQ2	C6-C1	-2.54	1.39	1.46
5	L	1282	BCL	O2A-CGA	-2.52	1.25	1.33
7	L	1286	BPH	C1B-C2B	-2.52	1.40	1.45
5	M	1303	BCL	O2D-CGD	-2.49	1.27	1.33
8	L	1287[A]	UQ2	C2-C1	-2.40	1.42	1.48
7	L	1286	BPH	O2A-CGA	-2.39	1.26	1.33
5	M	1304	BCL	O2A-CGA	-2.37	1.26	1.33
5	M	1303	BCL	C3D-CAD	-2.32	1.40	1.46
5	M	1304	BCL	O2D-CGD	-2.32	1.27	1.33
5	L	1288	BCL	O2A-CGA	-2.28	1.26	1.33
5	M	1303	BCL	O1D-CGD	2.26	1.26	1.21
7	L	1286	BPH	C1A-NA	-2.21	1.33	1.37
12	M	1312	U10	C3-C2	-2.20	1.42	1.48
7	L	1286	BPH	C1D-CHD	2.19	1.49	1.41
5	M	1304	BCL	C3C-C4C	-2.03	1.49	1.51
7	M	1311	BPH	C4C-NC	-2.02	1.33	1.37
5	M	1303	BCL	O2A-CGA	-2.01	1.27	1.33

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1314	CDL	C33-C32-C31	18.27	178.87	113.19
14	M	1314	CDL	C13-C12-C11	12.79	159.15	113.19
14	M	1314	CDL	C17-C16-C15	12.53	178.05	114.42
14	M	1314	CDL	C35-C34-C33	12.51	177.91	114.42
14	M	1314	CDL	C34-C33-C32	12.33	177.02	114.42
14	M	1314	CDL	C20-C19-C18	12.19	176.33	114.42
14	M	1314	CDL	C12-C11-CA5	11.59	155.76	113.62
5	L	1282	BCL	CMB-C2B-C1B	-7.73	116.58	128.46
5	M	1303	BCL	CMB-C2B-C1B	-7.54	116.88	128.46
5	M	1304	BCL	CMB-C2B-C1B	-7.45	117.01	128.46
5	L	1288	BCL	CMB-C2B-C1B	-7.34	117.18	128.46
5	L	1282	BCL	C1C-NC-C4C	-6.24	103.90	106.71
5	L	1288	BCL	C4A-NA-C1A	5.82	109.32	106.71
7	L	1286	BPH	C4D-C3D-CAD	5.75	111.51	107.87
5	L	1282	BCL	O2D-CGD-CBD	5.72	121.43	111.27
5	L	1282	BCL	C4A-NA-C1A	5.64	109.24	106.71
7	M	1311	BPH	O2D-CGD-CBD	5.60	121.22	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1286	BPH	O2D-CGD-CBD	5.59	121.21	111.27
5	M	1303	BCL	C4A-NA-C1A	5.47	109.17	106.71
14	M	1314	CDL	OA6-CA5-C11	5.28	122.88	111.50
7	M	1311	BPH	CHC-C4B-NB	-4.92	114.64	124.93
5	L	1288	BCL	CMB-C2B-C3B	4.88	133.80	124.68
12	M	1312	U10	C30-C29-C31	4.87	123.47	115.27
5	M	1303	BCL	O2D-CGD-CBD	4.86	119.91	111.27
5	M	1304	BCL	CMB-C2B-C3B	4.81	133.68	124.68
5	M	1303	BCL	CMB-C2B-C3B	4.78	133.62	124.68
5	M	1304	BCL	C1D-CHD-C4C	-4.75	118.88	125.88
13	M	1313	SPO	C10-C9-C7	-4.52	120.86	127.31
7	L	1286	BPH	OBD-CAD-C3D	-4.49	120.52	127.98
5	L	1282	BCL	CMB-C2B-C3B	4.49	133.07	124.68
7	M	1311	BPH	OBD-CAD-CBD	-4.42	119.58	125.89
13	M	1313	SPO	C20-C19-C17	-4.38	121.05	127.31
5	M	1304	BCL	O2D-CGD-CBD	4.36	119.02	111.27
13	M	1313	SPO	C3-C1-C4	-4.08	104.59	110.86
5	L	1282	BCL	C1D-CHD-C4C	-4.04	119.92	125.88
5	L	1282	BCL	C4B-CHC-C1C	-4.01	122.18	130.12
5	L	1288	BCL	O2D-CGD-CBD	3.95	118.28	111.27
5	L	1288	BCL	C1C-NC-C4C	-3.92	104.94	106.71
5	M	1303	BCL	C1-O2A-CGA	3.87	126.60	116.44
5	M	1303	BCL	C1D-CHD-C4C	-3.86	120.19	125.88
12	M	1312	U10	C10-C9-C11	3.81	121.67	115.27
12	M	1312	U10	C27-C28-C29	-3.70	118.76	127.66
7	M	1311	BPH	OBD-CAD-C3D	-3.68	121.87	127.98
14	M	1314	CDL	OB6-CB5-C51	3.65	119.37	111.50
5	M	1303	BCL	C1B-CHB-C4A	-3.65	122.89	130.12
8	L	1287[A]	UQ2	CM5-C5-C6	-3.55	118.61	124.40
13	M	1313	SPO	C29-C28-C30	3.51	121.17	115.27
5	M	1304	BCL	CED-O2D-CGD	3.51	123.87	115.94
5	M	1304	BCL	C4B-CHC-C1C	-3.45	123.29	130.12
8	L	1287[A]	UQ2	C10-C9-C11	3.40	120.99	115.27
5	L	1288	BCL	CMD-C2D-C3D	-3.34	118.44	124.68
7	L	1286	BPH	C1C-NC-C4C	-3.32	107.62	110.54
5	L	1288	BCL	O2A-CGA-CBA	3.29	122.22	111.91
13	M	1313	SPO	C15-C14-C12	-3.28	122.64	127.31
5	L	1288	BCL	CED-O2D-CGD	3.25	123.28	115.94
7	L	1286	BPH	CED-O2D-CGD	3.21	123.21	115.94
5	L	1282	BCL	C4-C3-C5	3.19	120.64	115.27
7	M	1311	BPH	O1D-CGD-CBD	-3.14	118.07	124.48
5	M	1304	BCL	C3C-C4C-CHD	-3.05	116.87	123.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1312	U10	C35-C34-C36	3.03	120.37	115.27
7	M	1311	BPH	C4D-C3D-CAD	3.03	109.78	107.87
5	M	1304	BCL	O2A-CGA-CBA	3.01	121.36	111.91
12	M	1312	U10	C17-C18-C19	-2.97	120.51	127.66
5	M	1304	BCL	C1B-CHB-C4A	-2.94	124.29	130.12
5	L	1282	BCL	CHA-C1A-NA	-2.93	119.70	126.40
12	M	1312	U10	C22-C23-C24	-2.92	120.63	127.66
5	L	1288	BCL	C4B-CHC-C1C	-2.91	124.36	130.12
7	M	1311	BPH	C2B-C1B-NB	2.90	114.17	109.79
14	M	1314	CDL	OB8-CB7-C71	2.83	120.79	111.91
8	L	1287[A]	UQ2	O1-C1-C6	-2.82	116.60	121.55
7	M	1311	BPH	CMD-C2D-C3D	-2.82	119.40	124.68
7	L	1286	BPH	O2A-CGA-CBA	2.82	120.75	111.91
14	M	1314	CDL	OA8-CA7-C31	2.78	120.64	111.91
5	M	1303	BCL	CHB-C4A-NA	-2.78	120.67	124.51
13	M	1313	SPO	C21-C22-C23	-2.77	123.35	127.31
5	M	1304	BCL	CMD-C2D-C3D	-2.76	119.51	124.68
7	L	1286	BPH	C4A-NA-C1A	2.76	110.37	108.14
7	M	1311	BPH	CBC-CAC-C3C	-2.72	107.41	113.47
12	M	1312	U10	C25-C24-C26	2.71	119.83	115.27
7	L	1286	BPH	C2B-C1B-NB	2.68	113.83	109.79
7	M	1311	BPH	C3B-C2B-C1B	-2.66	102.00	105.87
5	L	1288	BCL	C1-O2A-CGA	2.66	123.41	116.44
5	M	1304	BCL	C4-C3-C5	2.64	119.72	115.27
5	M	1304	BCL	O2D-CGD-O1D	-2.64	118.67	123.84
5	L	1288	BCL	C1B-CHB-C4A	-2.64	124.89	130.12
5	L	1282	BCL	O2A-CGA-CBA	2.63	120.16	111.91
5	L	1282	BCL	CHB-C4A-NA	-2.60	120.91	124.51
5	L	1282	BCL	C3C-C4C-CHD	-2.58	117.87	123.39
5	M	1303	BCL	C4B-CHC-C1C	-2.57	125.02	130.12
5	M	1303	BCL	O2A-CGA-CBA	2.56	119.94	111.91
14	M	1314	CDL	C32-C31-CA7	2.55	122.89	113.62
8	L	1287[A]	UQ2	CM3-O3-C3	2.55	125.50	116.47
5	M	1303	BCL	O2D-CGD-O1D	-2.54	118.87	123.84
5	M	1303	BCL	CMA-C3A-C4A	-2.53	104.98	111.77
12	M	1312	U10	C20-C19-C21	2.52	119.52	115.27
13	M	1313	SPO	C40-C38-C39	2.52	120.17	114.60
5	M	1304	BCL	C16-C15-C13	-2.52	107.78	115.92
13	M	1313	SPO	C34-C33-C35	2.51	119.50	115.27
5	L	1282	BCL	O1D-CGD-CBD	-2.51	119.35	124.48
12	M	1312	U10	C30-C29-C28	-2.48	117.31	123.68
5	L	1288	BCL	C2A-C3A-C4A	2.47	105.85	101.87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1311	BPH	C1C-NC-C4C	-2.44	108.40	110.54
5	M	1304	BCL	C4A-NA-C1A	2.43	107.80	106.71
7	L	1286	BPH	O2D-CGD-O1D	-2.42	119.11	123.84
5	M	1303	BCL	CHA-C1A-NA	-2.40	120.89	126.40
5	L	1282	BCL	O2D-CGD-O1D	-2.37	119.20	123.84
12	M	1312	U10	C15-C14-C16	2.37	119.25	115.27
7	L	1286	BPH	O1D-CGD-CBD	-2.36	119.65	124.48
13	M	1313	SPO	C31-C32-C33	-2.34	122.03	127.66
5	M	1304	BCL	CAC-C3C-C4C	-2.33	107.40	112.58
7	M	1311	BPH	O2A-CGA-CBA	2.32	119.18	111.91
8	L	1287[A]	UQ2	C7-C8-C9	-2.31	122.94	126.79
7	M	1311	BPH	CED-O2D-CGD	2.31	121.15	115.94
5	L	1282	BCL	C1B-CHB-C4A	-2.30	125.55	130.12
5	L	1288	BCL	C2A-C1A-CHA	-2.29	119.85	123.86
5	L	1288	BCL	C1D-CHD-C4C	-2.29	122.51	125.88
5	L	1282	BCL	C2A-C3A-C4A	2.26	105.51	101.87
13	M	1313	SPO	C13-C12-C11	2.25	121.62	118.08
5	M	1304	BCL	CHD-C4C-NC	-2.24	122.59	125.08
5	M	1304	BCL	C1-C2-C3	-2.24	122.18	126.04
5	L	1282	BCL	O2A-CGA-O1A	-2.23	117.95	123.59
7	M	1311	BPH	C1-O2A-CGA	2.23	122.30	116.44
14	M	1314	CDL	OA6-CA5-OA7	-2.23	118.31	123.70
12	M	1312	U10	C4M-O4-C4	2.22	124.33	116.47
14	M	1314	CDL	OA8-CA7-OA9	-2.17	118.11	123.59
5	L	1282	BCL	C1-O2A-CGA	2.16	122.11	116.44
7	L	1286	BPH	O2A-CGA-O1A	-2.14	118.19	123.59
5	M	1303	BCL	CED-O2D-CGD	2.12	120.74	115.94
5	L	1288	BCL	CHB-C4A-NA	-2.12	121.58	124.51
14	M	1314	CDL	OB8-CB7-OB9	-2.11	118.26	123.59
12	M	1312	U10	C41-C39-C40	2.10	119.24	114.60
7	L	1286	BPH	OBD-CAD-CBD	-2.08	122.92	125.89
7	M	1311	BPH	CHC-C1C-NC	-2.08	122.74	125.20
7	L	1286	BPH	CMD-C2D-C3D	-2.07	120.81	124.68
5	M	1304	BCL	C7-C6-C5	-2.05	107.79	113.36
5	L	1282	BCL	C1-C2-C3	-2.05	122.50	126.04
13	M	1313	SPO	C18-C17-C19	-2.03	120.08	122.92
5	L	1288	BCL	C4-C3-C5	2.02	118.67	115.27
5	L	1282	BCL	CED-O2D-CGD	2.02	120.51	115.94
5	L	1288	BCL	CHA-C1A-NA	-2.02	121.78	126.40
8	L	1287[B]	UQ2	C16-C14-C15	2.01	119.04	114.60

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1303	BCL	C8
5	M	1303	BCL	C13
5	L	1288	BCL	C8
5	L	1288	BCL	C13

All (269) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	M	1314	CDL	CA3-OA5-PA1-OA3
14	M	1314	CDL	CB3-OB5-PB2-OB2
14	M	1314	CDL	CB3-OB5-PB2-OB3
4	H	1251	GOL	O1-C1-C2-O2
4	H	1251	GOL	O1-C1-C2-C3
6	M	1309	LDA	C2-C1-N1-O1
6	M	1309	LDA	C2-C1-N1-CM1
6	M	1309	LDA	N1-C1-C2-C3
13	M	1313	SPO	C4-C1-O1-CM1
13	M	1313	SPO	C1-C4-C5-C6
13	M	1313	SPO	C4-C5-C6-C7
13	M	1313	SPO	C6-C7-C9-C10
13	M	1313	SPO	C8-C7-C9-C10
13	M	1313	SPO	C9-C10-C11-C12
13	M	1313	SPO	C15-C16-C17-C18
13	M	1313	SPO	C15-C16-C17-C19
13	M	1313	SPO	C19-C20-C21-C22
13	M	1313	SPO	C36-C37-C38-C39
13	M	1313	SPO	C36-C37-C38-C40
4	L	1292	GOL	O1-C1-C2-C3
4	L	1291	GOL	C1-C2-C3-O3
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
10	L	1290	HTO	O3-C3-C4-C5
12	M	1312	U10	C27-C28-C29-C30
12	M	1312	U10	C27-C28-C29-C31
12	M	1312	U10	C34-C36-C37-C38
8	L	1287[A]	UQ2	C7-C8-C9-C10
8	L	1287[A]	UQ2	C7-C8-C9-C11
8	L	1287[A]	UQ2	C12-C13-C14-C16
8	L	1287[B]	UQ2	C12-C11-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
8	L	1287[B]	UQ2	C12-C11-C9-C10
4	H	1252	GOL	O1-C1-C2-C3
6	M	1305	LDA	C2-C1-N1-O1
6	M	1305	LDA	C2-C1-N1-CM1
6	M	1305	LDA	C2-C1-N1-CM2
7	M	1311	BPH	C4C-C3C-CAC-CBC
7	M	1311	BPH	C2C-C1C-CHC-C4B
7	M	1311	BPH	NC-C1C-CHC-C4B
7	M	1311	BPH	NB-C4B-CHC-C1C
7	M	1311	BPH	C4B-C3B-CAB-CBB
7	M	1311	BPH	C4B-C3B-CAB-OB
7	M	1311	BPH	O2A-C1-C2-C3
7	M	1311	BPH	C1-C2-C3-C4
7	L	1286	BPH	C2C-C1C-CHC-C4B
7	L	1286	BPH	NC-C1C-CHC-C4B
7	L	1286	BPH	C4B-C3B-CAB-CBB
7	L	1286	BPH	C4B-C3B-CAB-OB
7	L	1286	BPH	O2A-C1-C2-C3
5	L	1282	BCL	C3-C5-C6-C7
14	M	1314	CDL	C20-C21-C22-C23
14	M	1314	CDL	C33-C34-C35-C36
14	M	1314	CDL	C78-C79-C80-C81
10	L	1290	HTO	O1-C1-C2-O2
8	L	1287[A]	UQ2	C12-C13-C14-C15
14	M	1314	CDL	OA9-CA7-OA8-CA6
14	M	1314	CDL	OB9-CB7-OB8-CB6
14	M	1314	CDL	C31-CA7-OA8-CA6
7	L	1286	BPH	CBD-CGD-O2D-CED
14	M	1314	CDL	C71-CB7-OB8-CB6
5	M	1303	BCL	C10-C11-C12-C13
13	M	1313	SPO	C33-C35-C36-C37
12	M	1312	U10	C29-C31-C32-C33
8	L	1287[B]	UQ2	C7-C8-C9-C10
8	L	1287[B]	UQ2	C7-C8-C9-C11
14	M	1314	CDL	C17-C18-C19-C20
14	M	1314	CDL	CB5-C51-C52-C53
5	L	1282	BCL	C11-C10-C8-C9
5	L	1288	BCL	C11-C12-C13-C14
14	M	1314	CDL	CB7-C71-C72-C73
5	L	1282	BCL	C13-C15-C16-C17
7	L	1286	BPH	NB-C4B-CHC-C1C
5	M	1303	BCL	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	L	1282	BCL	C5-C6-C7-C8
5	L	1288	BCL	C15-C16-C17-C18
8	L	1287[A]	UQ2	C9-C11-C12-C13
14	M	1314	CDL	CA7-C31-C32-C33
5	L	1288	BCL	C10-C11-C12-C13
14	M	1314	CDL	C11-CA5-OA6-CA4
13	M	1313	SPO	C13-C12-C14-C15
13	M	1313	SPO	C18-C17-C19-C20
13	M	1313	SPO	C21-C22-C23-C24
6	L	1285	LDA	C7-C8-C9-C10
14	M	1314	CDL	C12-C13-C14-C15
14	M	1314	CDL	CA5-C11-C12-C13
6	M	1308	LDA	C11-C10-C9-C8
6	M	1307	LDA	C7-C8-C9-C10
6	L	1283	LDA	C3-C4-C5-C6
13	M	1313	SPO	C16-C17-C19-C20
14	M	1314	CDL	C72-C73-C74-C75
6	L	1284	LDA	C7-C8-C9-C10
6	L	1285	LDA	C4-C5-C6-C7
14	M	1314	CDL	C15-C16-C17-C18
6	L	1284	LDA	C6-C7-C8-C9
6	M	1305	LDA	C2-C3-C4-C5
14	M	1314	CDL	C14-C15-C16-C17
4	H	1251	GOL	C1-C2-C3-O3
4	H	1253	GOL	O1-C1-C2-C3
4	L	1292	GOL	C1-C2-C3-O3
4	H	1252	GOL	C1-C2-C3-O3
14	M	1314	CDL	OA7-CA5-OA6-CA4
6	M	1306	LDA	C3-C4-C5-C6
7	L	1286	BPH	C8-C10-C11-C12
14	M	1314	CDL	C71-C72-C73-C74
6	M	1307	LDA	C4-C5-C6-C7
7	M	1311	BPH	C8-C10-C11-C12
6	L	1283	LDA	C6-C7-C8-C9
8	L	1287[B]	UQ2	C12-C13-C14-C15
6	L	1285	LDA	C3-C4-C5-C6
6	L	1283	LDA	C5-C6-C7-C8
6	L	1285	LDA	C2-C3-C4-C5
10	L	1290	HTO	O1-C1-C2-C3
4	L	1292	GOL	O1-C1-C2-O2
4	L	1292	GOL	O2-C2-C3-O3
4	L	1291	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	L	1283	LDA	C11-C10-C9-C8
6	M	1306	LDA	C2-C3-C4-C5
6	M	1709	LDA	C1-C2-C3-C4
14	M	1314	CDL	C19-C20-C21-C22
5	M	1304	BCL	C15-C16-C17-C18
5	M	1303	BCL	C8-C10-C11-C12
7	M	1311	BPH	C15-C16-C17-C18
5	L	1288	BCL	C8-C10-C11-C12
6	M	1307	LDA	C1-C2-C3-C4
5	L	1288	BCL	C13-C15-C16-C17
7	M	1311	BPH	C16-C17-C18-C19
6	L	1285	LDA	C5-C6-C7-C8
5	L	1288	BCL	C2A-CAA-CBA-CGA
6	M	1309	LDA	C7-C8-C9-C10
6	M	1306	LDA	C6-C7-C8-C9
6	M	1309	LDA	C6-C7-C8-C9
6	M	1309	LDA	C2-C3-C4-C5
6	M	1309	LDA	C11-C10-C9-C8
5	M	1303	BCL	CBD-CGD-O2D-CED
14	M	1314	CDL	C74-C75-C76-C77
7	L	1286	BPH	C2-C3-C5-C6
6	L	1284	LDA	C1-C2-C3-C4
5	L	1282	BCL	C14-C13-C15-C16
14	M	1314	CDL	C16-C17-C18-C19
7	M	1311	BPH	C5-C6-C7-C8
6	M	1308	LDA	C5-C6-C7-C8
6	L	1283	LDA	C2-C3-C4-C5
7	M	1311	BPH	C2C-C3C-CAC-CBC
7	L	1286	BPH	O1D-CGD-O2D-CED
14	M	1314	CDL	CA3-CA4-CA6-OA8
6	M	1306	LDA	C1-C2-C3-C4
6	L	1285	LDA	C9-C10-C11-C12
6	L	1283	LDA	C9-C10-C11-C12
14	M	1314	CDL	C40-C41-C42-C43
8	L	1287[B]	UQ2	C12-C13-C14-C16
4	H	1252	GOL	O2-C2-C3-O3
5	M	1303	BCL	C4-C3-C5-C6
7	M	1311	BPH	C4-C3-C5-C6
7	L	1286	BPH	C4-C3-C5-C6
6	M	1309	LDA	C1-C2-C3-C4
6	M	1305	LDA	C11-C10-C9-C8
6	M	1307	LDA	C3-C4-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	M	1314	CDL	C18-C19-C20-C21
13	M	1313	SPO	C3-C1-O1-CM1
13	M	1313	SPO	C11-C12-C14-C15
13	M	1313	SPO	C21-C22-C23-C25
6	M	1307	LDA	C5-C6-C7-C8
7	M	1311	BPH	C16-C17-C18-C20
13	M	1313	SPO	C3-C1-C4-C5
6	M	1306	LDA	C9-C10-C11-C12
6	L	1285	LDA	C11-C10-C9-C8
5	M	1304	BCL	C12-C13-C15-C16
7	M	1311	BPH	C6-C7-C8-C10
7	M	1311	BPH	C11-C12-C13-C15
5	L	1288	BCL	C11-C12-C13-C15
6	L	1285	LDA	C1-C2-C3-C4
5	M	1304	BCL	C14-C13-C15-C16
7	M	1311	BPH	C6-C7-C8-C9
7	M	1311	BPH	C11-C12-C13-C14
10	L	1290	HTO	C2-C3-C4-C5
6	L	1285	LDA	N1-C1-C2-C3
6	M	1306	LDA	N1-C1-C2-C3
6	M	1709	LDA	N1-C1-C2-C3
7	M	1311	BPH	C13-C15-C16-C17
14	M	1314	CDL	OA5-CA3-CA4-CA6
5	M	1303	BCL	C2-C3-C5-C6
7	M	1311	BPH	C2-C3-C5-C6
14	M	1314	CDL	C80-C81-C82-C83
6	M	1308	LDA	C7-C8-C9-C10
6	M	1307	LDA	C11-C10-C9-C8
10	L	1290	HTO	C1-C2-C3-O3
6	M	1309	LDA	C5-C6-C7-C8
12	M	1312	U10	C35-C34-C36-C37
5	M	1303	BCL	O1D-CGD-O2D-CED
4	H	1251	GOL	O2-C2-C3-O3
14	M	1314	CDL	OA5-CA3-CA4-OA6
14	M	1314	CDL	C37-C38-C39-C40
14	M	1314	CDL	OA6-CA4-CA6-OA8
8	L	1287[B]	UQ2	C9-C11-C12-C13
6	L	1284	LDA	C2-C3-C4-C5
5	M	1303	BCL	C14-C13-C15-C16
5	M	1303	BCL	C4C-C3C-CAC-CBC
7	L	1286	BPH	C4C-C3C-CAC-CBC
14	M	1314	CDL	C21-C22-C23-C24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	M	1307	LDA	C2-C3-C4-C5
5	L	1282	BCL	C12-C13-C15-C16
13	M	1313	SPO	C12-C14-C15-C16
7	M	1311	BPH	C2B-C3B-CAB-OB8
7	L	1286	BPH	CAD-CBD-CGD-O2D
5	M	1304	BCL	C3-C5-C6-C7
14	M	1314	CDL	OB6-CB4-CB6-OB8
4	M	1315	GOL	O1-C1-C2-O2
6	M	1308	LDA	C4-C5-C6-C7
6	M	1309	LDA	C9-C10-C11-C12
6	M	1709	LDA	C7-C8-C9-C10
5	M	1303	BCL	C11-C10-C8-C7
14	M	1314	CDL	C31-C32-C33-C34
6	M	1709	LDA	C6-C7-C8-C9
6	M	1306	LDA	C7-C8-C9-C10
5	M	1304	BCL	C11-C10-C8-C9
5	M	1303	BCL	C6-C7-C8-C9
4	H	1252	GOL	O1-C1-C2-O2
7	M	1311	BPH	C2B-C3B-CAB-CBB
5	M	1304	BCL	C8-C10-C11-C12
8	L	1287[A]	UQ2	C4-C3-O3-CM3
5	M	1303	BCL	C2-C1-O2A-CGA
6	M	1709	LDA	C3-C4-C5-C6
13	M	1313	SPO	C2-C1-O1-CM1
14	M	1314	CDL	CA3-OA5-PA1-OA2
6	M	1709	LDA	C11-C10-C9-C8
5	M	1303	BCL	C11-C10-C8-C9
6	M	1307	LDA	N1-C1-C2-C3
12	M	1312	U10	C33-C34-C36-C37
14	M	1314	CDL	C81-C82-C83-C84
13	M	1313	SPO	C17-C19-C20-C21
14	M	1314	CDL	C36-C37-C38-C39
5	L	1288	BCL	C2-C1-O2A-CGA
10	L	1290	HTO	C4-C5-C6-C7
5	M	1304	BCL	C11-C12-C13-C14
14	M	1314	CDL	C79-C80-C81-C82
14	M	1314	CDL	CB3-CB4-CB6-OB8
6	M	1709	LDA	C5-C6-C7-C8
12	M	1312	U10	C5-C4-O4-C4M
8	L	1287[B]	UQ2	C1-C2-O2-CM2
12	M	1312	U10	C14-C16-C17-C18
6	M	1309	LDA	C3-C4-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	M	1315	GOL	C1-C2-C3-O3
12	M	1312	U10	C25-C24-C26-C27
8	L	1287[A]	UQ2	C12-C11-C9-C10
5	M	1304	BCL	C16-C17-C18-C19
6	M	1308	LDA	C2-C3-C4-C5
5	M	1303	BCL	C6-C7-C8-C10
5	L	1282	BCL	C1-C2-C3-C4
7	L	1286	BPH	C1-C2-C3-C4
5	M	1304	BCL	CAA-CBA-CGA-O2A
12	M	1312	U10	C30-C29-C31-C32
7	M	1311	BPH	CAD-CBD-CGD-O2D
5	L	1288	BCL	CAD-CBD-CGD-O2D
12	M	1312	U10	C23-C24-C26-C27
12	M	1312	U10	C31-C32-C33-C34
6	M	1309	LDA	C2-C1-N1-CM2
5	L	1282	BCL	CHA-CBD-CGD-O1D
5	L	1282	BCL	CHA-CBD-CGD-O2D
14	M	1314	CDL	C52-C51-CB5-OB6
8	L	1287[A]	UQ2	C12-C11-C9-C8
6	M	1709	LDA	C2-C3-C4-C5
13	M	1313	SPO	C2-C1-C4-C5
12	M	1312	U10	C3-C4-O4-C4M
10	L	1290	HTO	C3-C4-C5-C6
14	M	1314	CDL	CA3-OA5-PA1-OA4
14	M	1314	CDL	C52-C51-CB5-OB7
4	M	1315	GOL	O2-C2-C3-O3
14	M	1314	CDL	C76-C77-C78-C79
14	M	1314	CDL	C72-C71-CB7-OB8

There are no ring outliers.

20 monomers are involved in 72 short contacts:

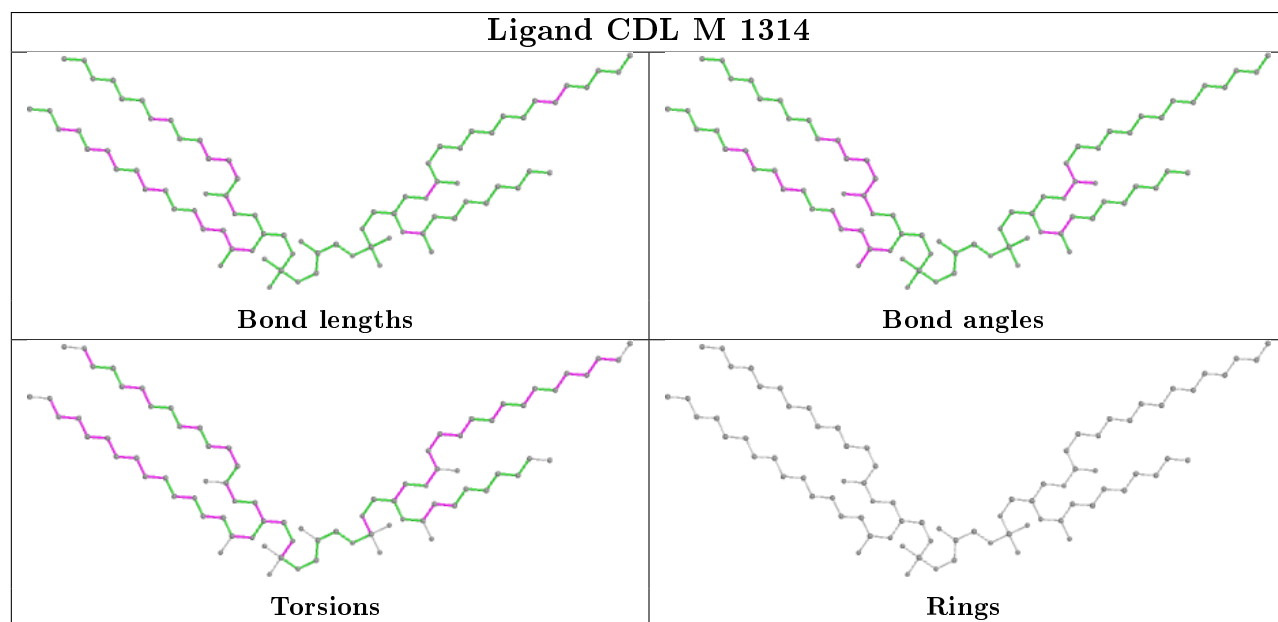
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1285	LDA	4	0
14	M	1314	CDL	2	0
4	H	1251	GOL	1	0
6	M	1309	LDA	3	0
6	L	1284	LDA	2	0
13	M	1313	SPO	4	0
6	M	1308	LDA	2	0
5	M	1304	BCL	15	0
4	L	1291	GOL	1	0

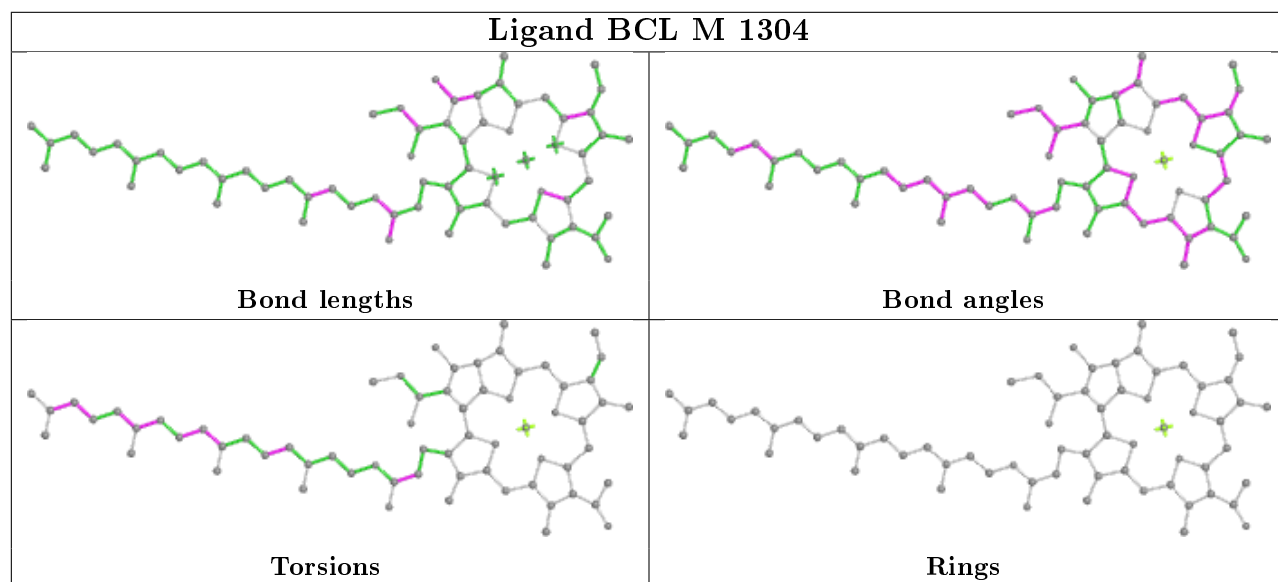
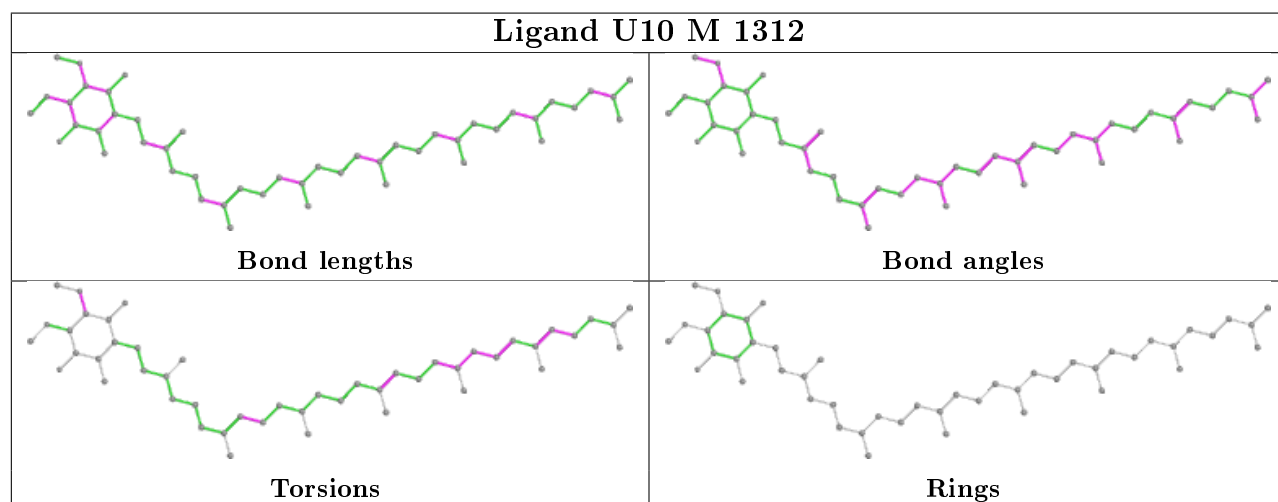
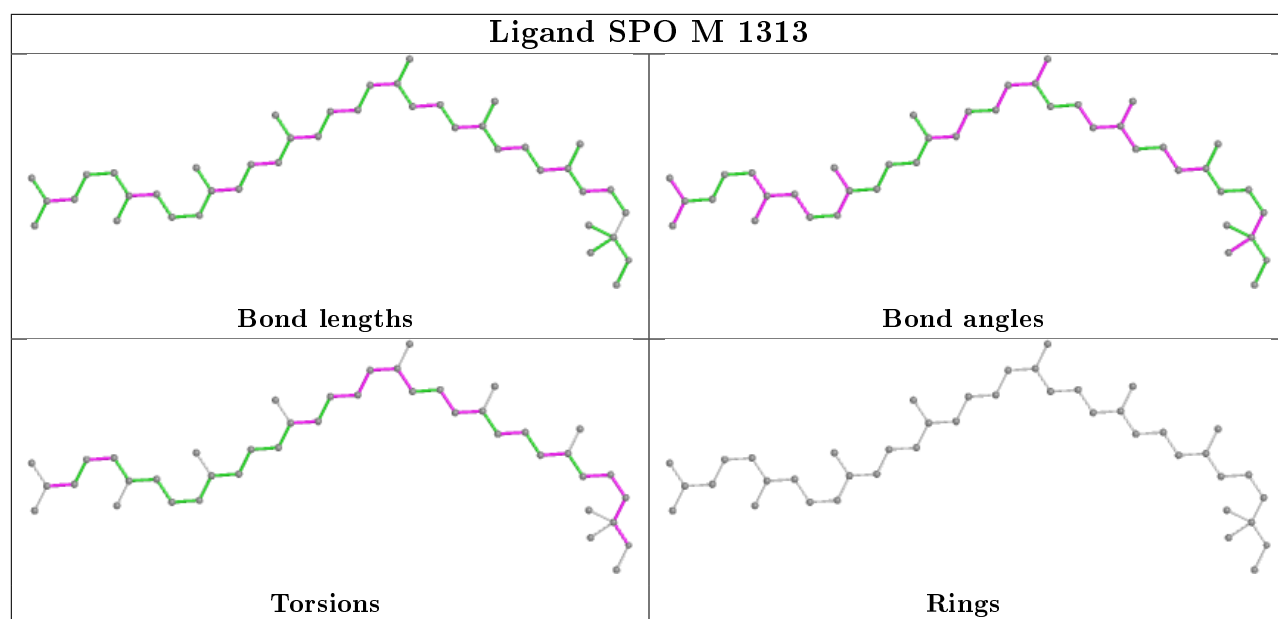
*Continued on next page...*

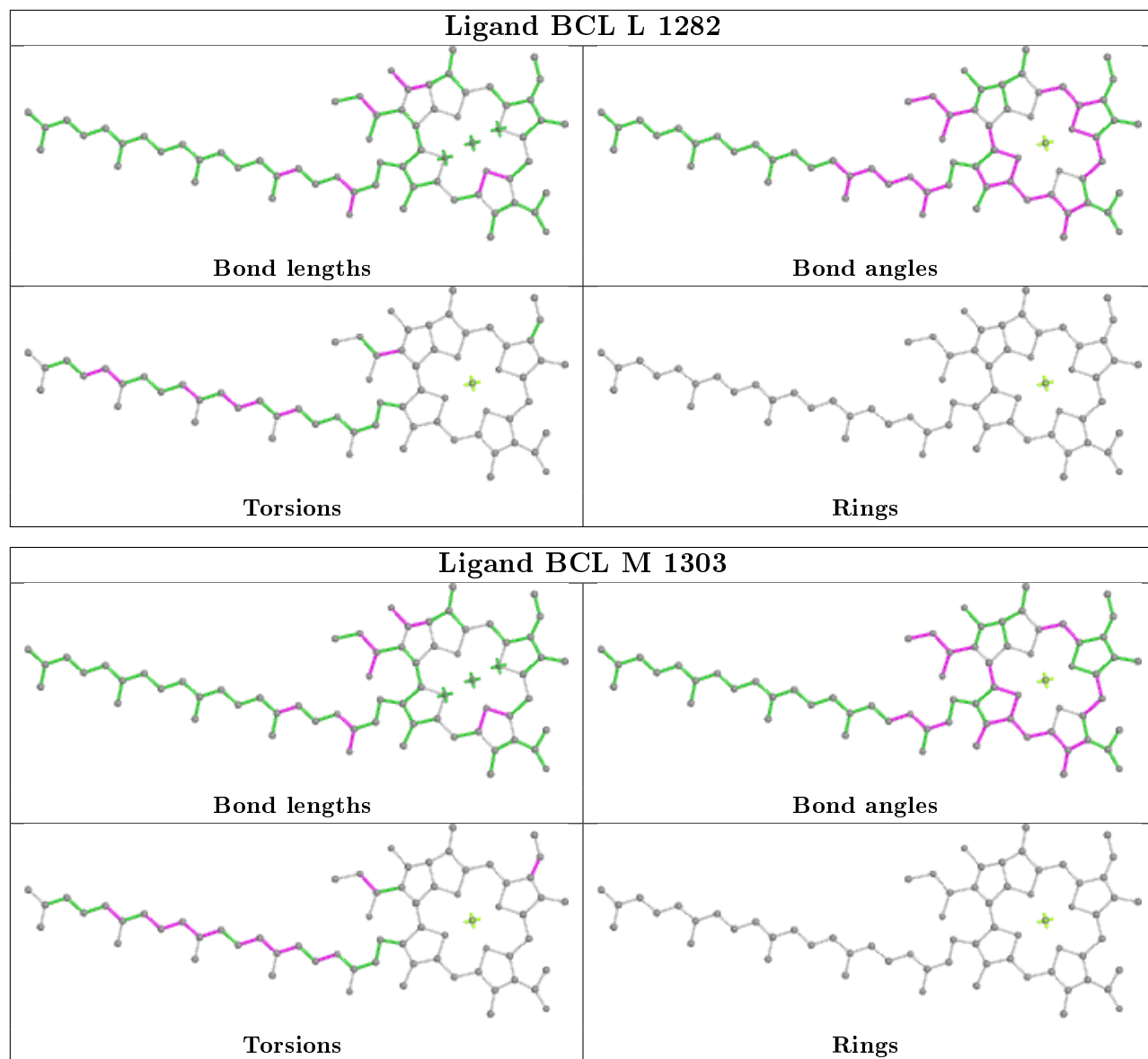
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1282	BCL	4	0
5	M	1303	BCL	11	0
4	M	1315	GOL	2	0
6	L	1283	LDA	1	0
6	M	1307	LDA	5	0
8	L	1287[A]	UQ2	5	0
8	L	1287[B]	UQ2	1	0
6	M	1305	LDA	3	0
7	M	1311	BPH	12	0
5	L	1288	BCL	5	0
7	L	1286	BPH	7	0

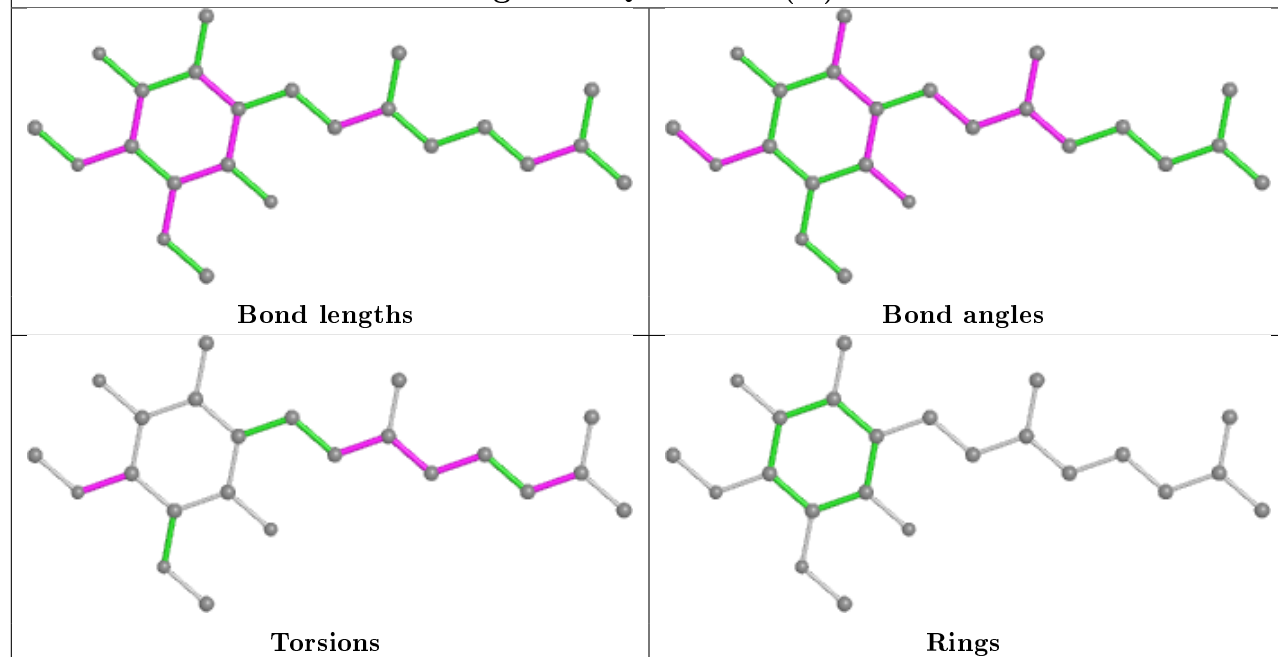
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



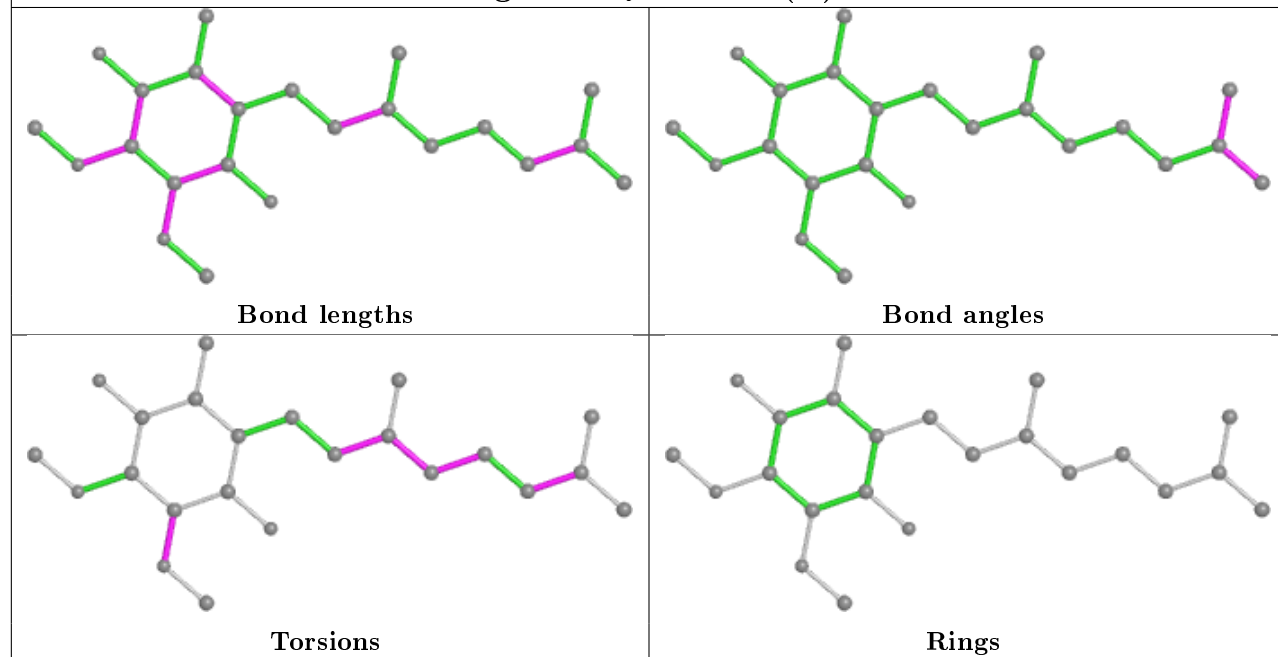




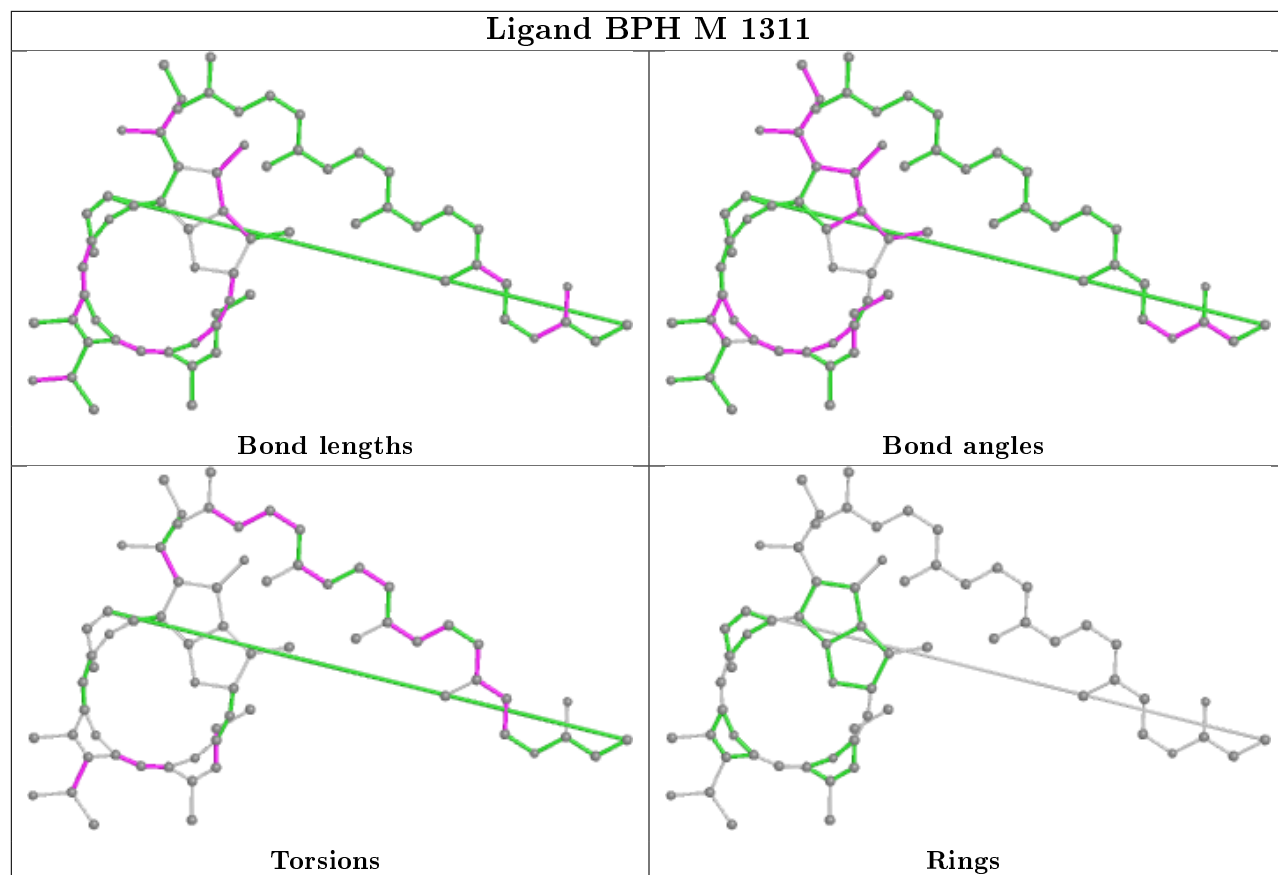
## Ligand UQ2 L 1287 (A)



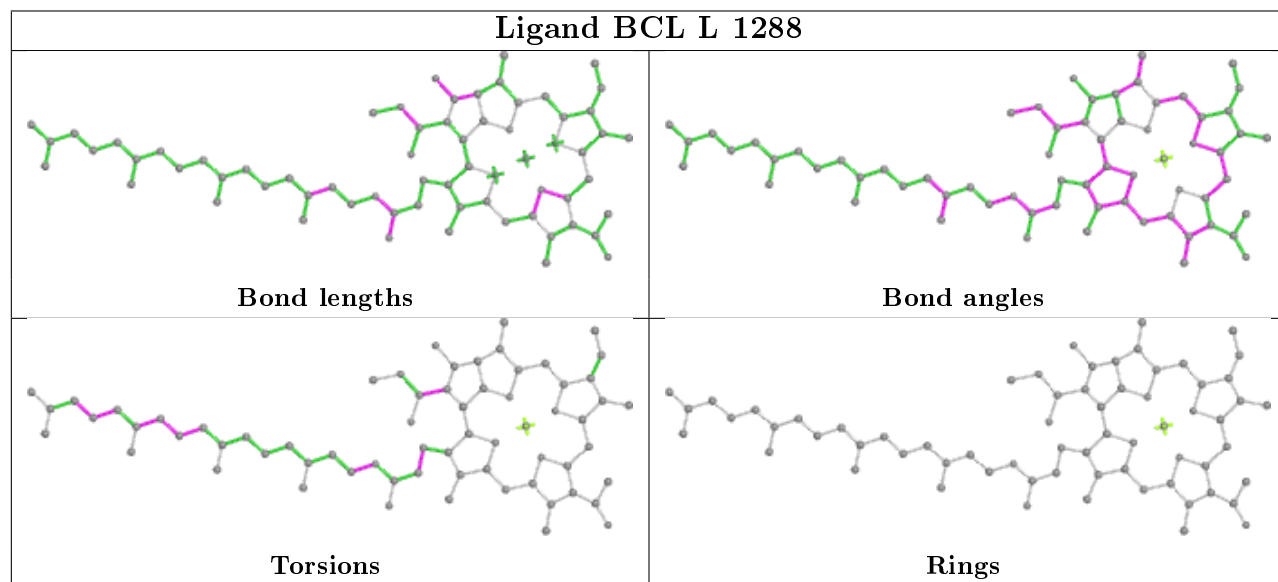
## Ligand UQ2 L 1287 (B)

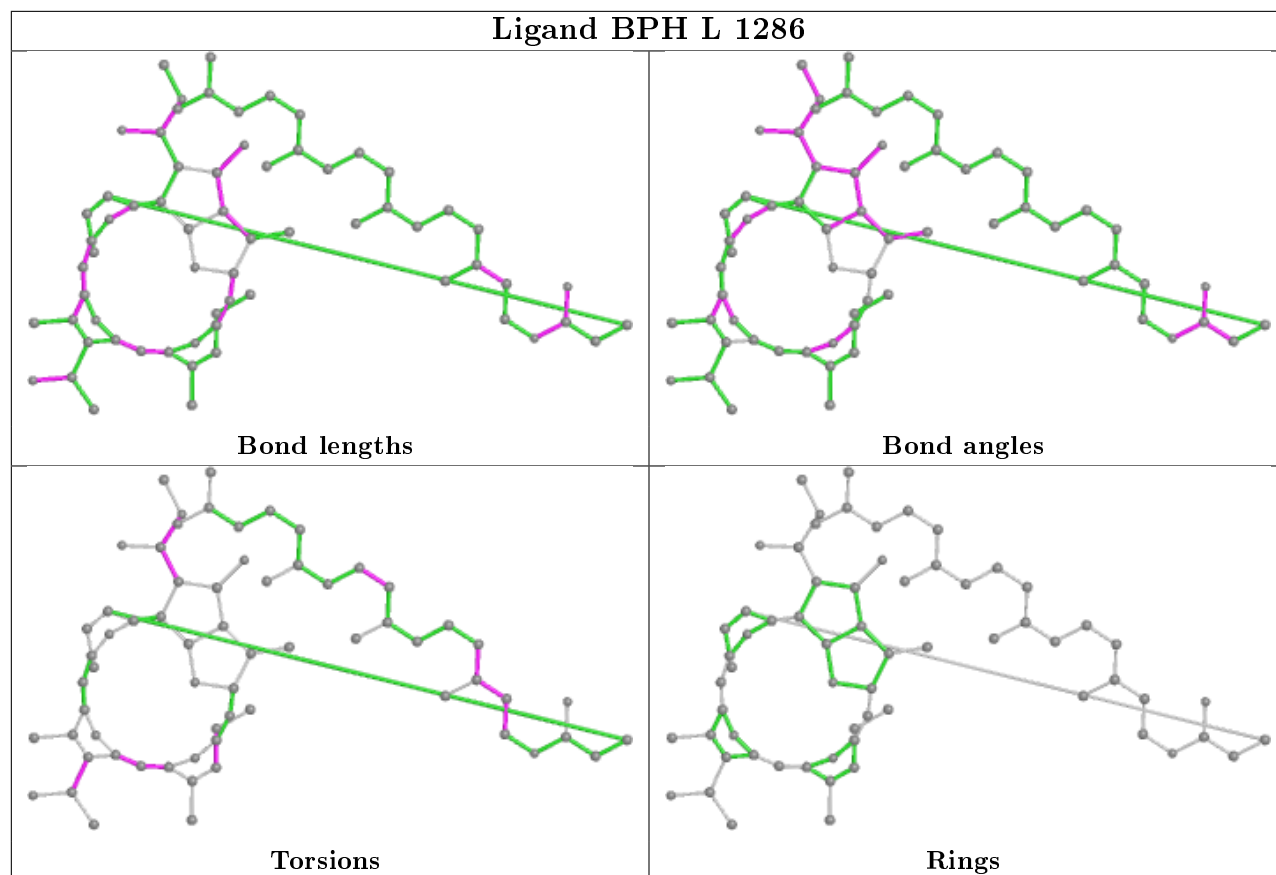


## Ligand BPH M 1311



## Ligand BCL L 1288





## 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	H	241/260 (92%)	-0.39	9 (3%) 41 45	33, 43, 53, 85	0
2	L	281/281 (100%)	-0.53	7 (2%) 57 61	30, 39, 61, 68	0
3	M	303/307 (98%)	-0.38	13 (4%) 35 38	29, 44, 69, 76	0
All	All	825/848 (97%)	-0.43	29 (3%) 44 47	29, 42, 63, 85	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	6.3
3	M	1	ALA	5.4
1	H	249	LYS	4.6
1	H	251	VAL	4.4
3	M	148	TRP	4.4
3	M	301	HIS	3.9
3	M	302	GLY	3.8
2	L	59	TRP	3.8
3	M	2	GLU	3.5
3	M	303	MET	3.4
3	M	52	LEU	3.2
1	H	247	LYS	2.9
2	L	281	GLY	2.8
3	M	106	ALA	2.7
2	L	271	TRP	2.7
3	M	80	TRP	2.7
2	L	270	PRO	2.5
2	L	72	GLU	2.5
1	H	245	ALA	2.5
1	H	51	ALA	2.4
3	M	27	ALA	2.4
3	M	100	GLU	2.4
3	M	3	TYR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	246	PRO	2.2
1	H	220[A]	LYS	2.2
2	L	202	LYS	2.2
1	H	18	TYR	2.1
2	L	276	PRO	2.1
3	M	79	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
6	LDA	M	1309	16/16	0.12	0.55	94,102,110,110	0
6	LDA	L	1283	16/16	0.27	0.48	86,103,111,111	0
6	LDA	M	1709	16/16	0.40	0.49	92,100,107,107	0
14	CDL	M	1314	81/100	0.50	0.50	96,107,120,121	0
6	LDA	M	1308	16/16	0.53	0.39	90,97,105,105	0
6	LDA	L	1284	16/16	0.59	0.32	98,102,109,109	0
6	LDA	L	1285	16/16	0.67	0.41	106,109,111,111	0
4	GOL	H	1253	6/6	0.74	0.41	102,103,104,104	0
10	HTO	L	1290	10/10	0.74	0.36	74,77,77,78	0
4	GOL	L	1292	6/6	0.79	0.25	85,87,87,87	0
4	GOL	H	1254	6/6	0.79	0.21	102,102,103,103	0
6	LDA	M	1307	16/16	0.80	0.24	64,68,77,77	0
6	LDA	M	1306	16/16	0.80	0.33	72,74,84,84	0
6	LDA	M	1305	16/16	0.80	0.28	50,63,70,71	0
4	GOL	M	1315	6/6	0.80	0.22	85,86,86,87	0
4	GOL	H	1251	6/6	0.83	0.23	65,68,70,71	0
8	UQ2	L	1287[A]	23/23	0.84	0.31	39,42,51,52	23

*Continued on next page...*

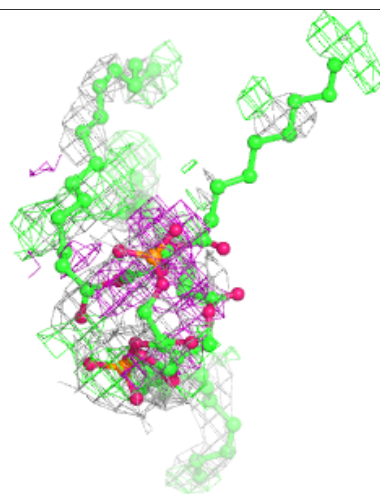
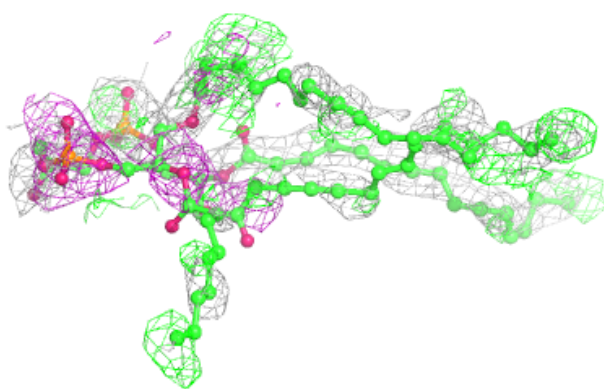
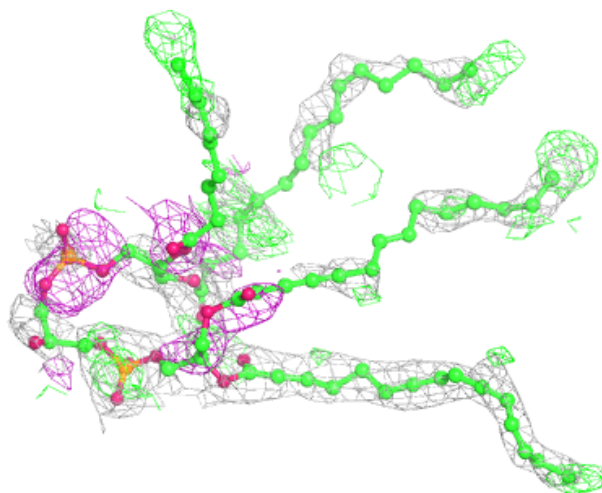
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	UQ2	L	1287[B]	23/23	0.84	0.31	40,43,47,48	23
13	SPO	M	1313	42/42	0.86	0.21	38,51,68,71	0
4	GOL	H	1252	6/6	0.88	0.31	88,89,89,89	0
4	GOL	L	1291	6/6	0.89	0.19	47,52,53,54	0
7	BPH	M	1311	65/65	0.91	0.17	35,42,94,95	0
12	U10	M	1312	48/63	0.93	0.15	30,39,68,69	0
9	PO4	L	1289	5/5	0.95	0.26	103,103,103,103	0
5	BCL	M	1303	66/66	0.96	0.14	26,31,80,81	0
5	BCL	L	1282	66/66	0.97	0.12	30,34,51,54	0
5	BCL	M	1304	66/66	0.97	0.16	25,31,53,59	0
5	BCL	L	1288	66/66	0.97	0.13	25,30,48,52	0
7	BPH	L	1286	65/65	0.98	0.13	25,30,39,40	0
11	FE	M	1310	1/1	0.99	0.02	32,32,32,32	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.

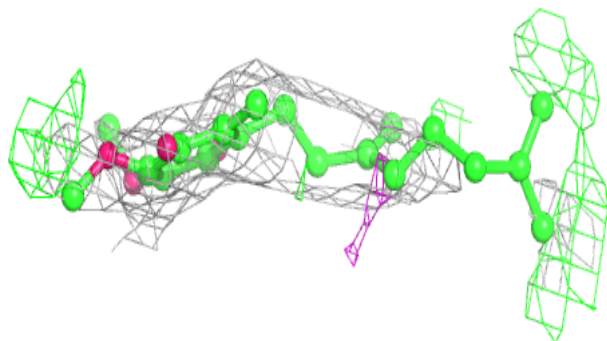
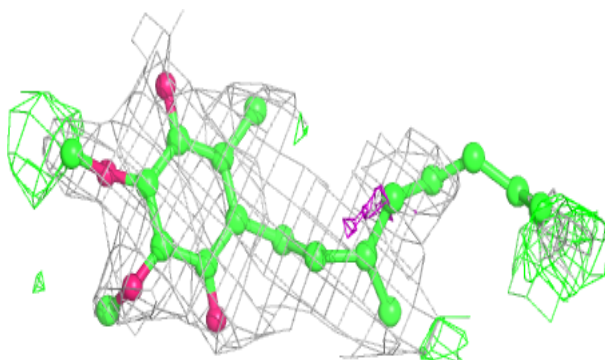
**Electron density around CDL M 1314:**

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

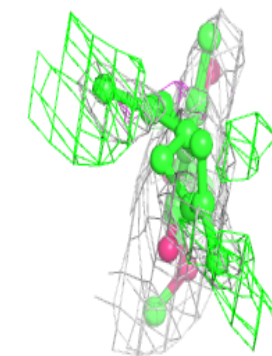
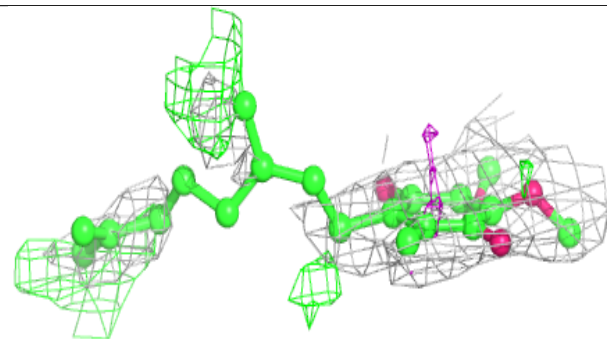
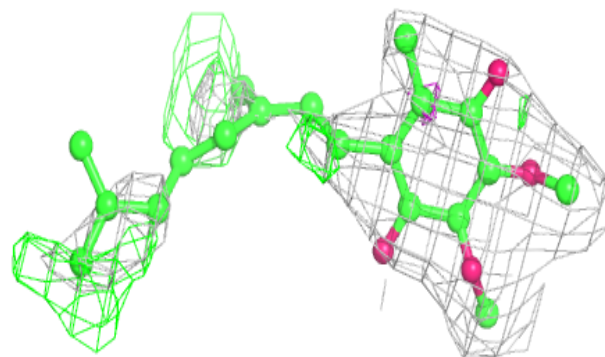


**Electron density around UQ2 L 1287 (A):**

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

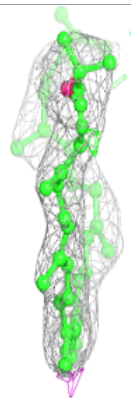
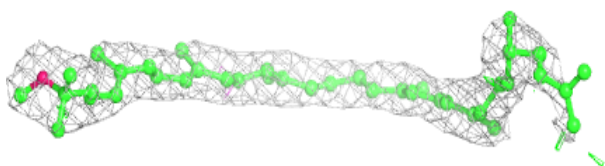
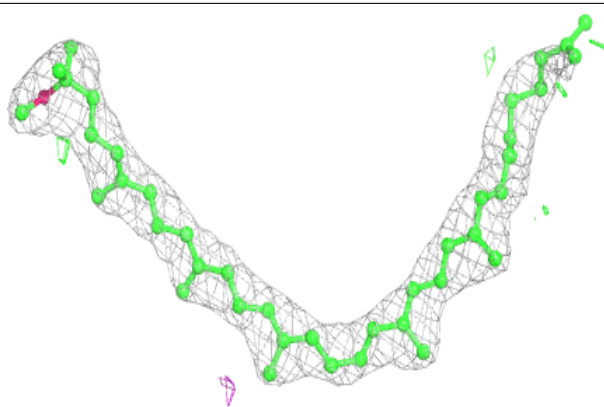
**Electron density around UQ2 L 1287 (B):**

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

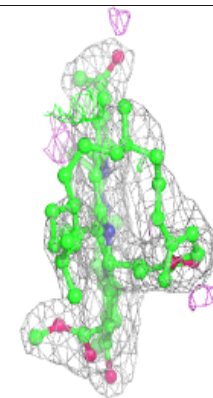
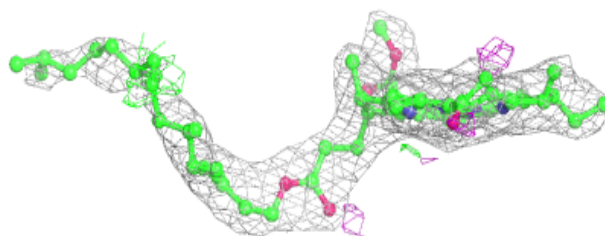
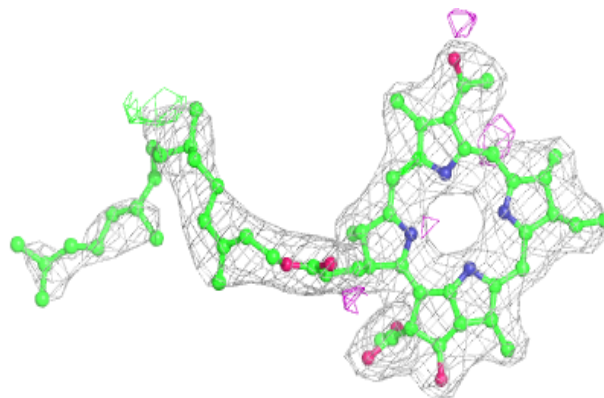


**Electron density around SPO M 1313:**

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

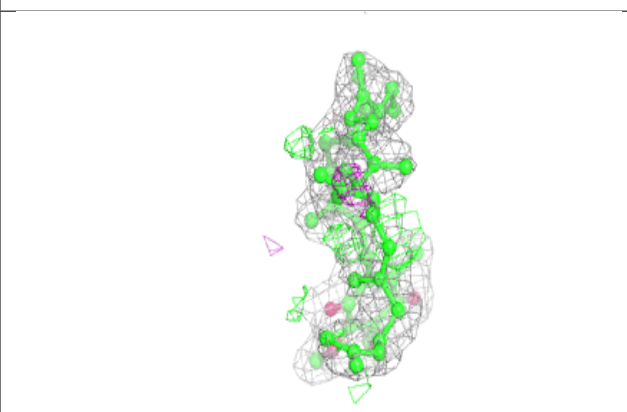
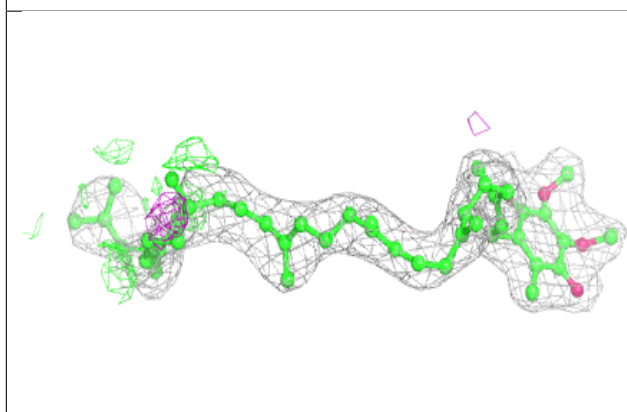
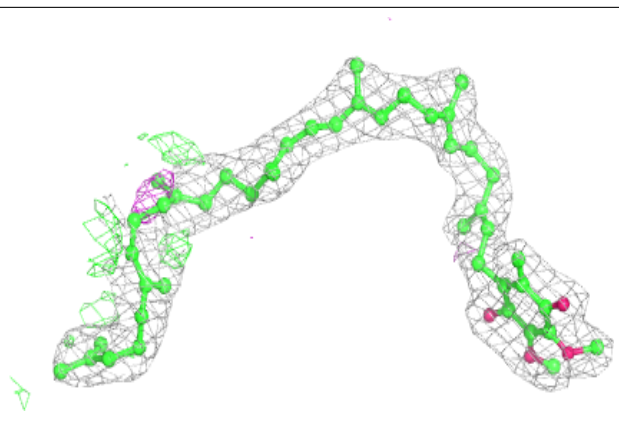
**Electron density around BPH M 1311:**

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



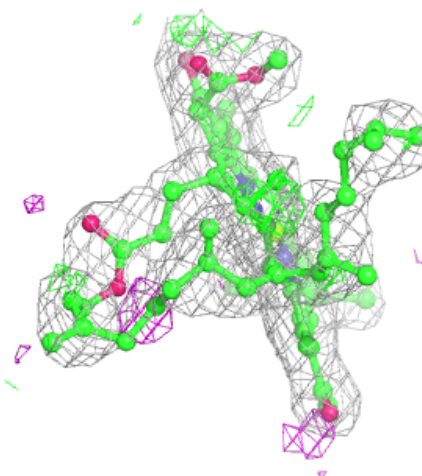
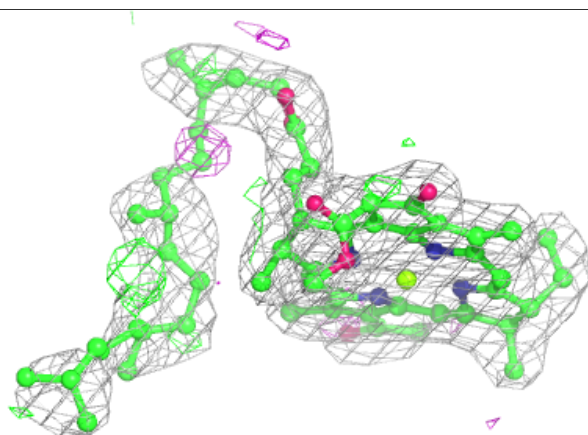
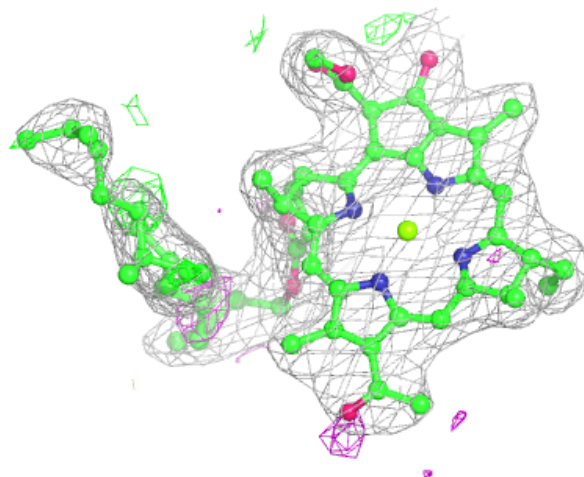
**Electron density around U10 M 1312:**

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



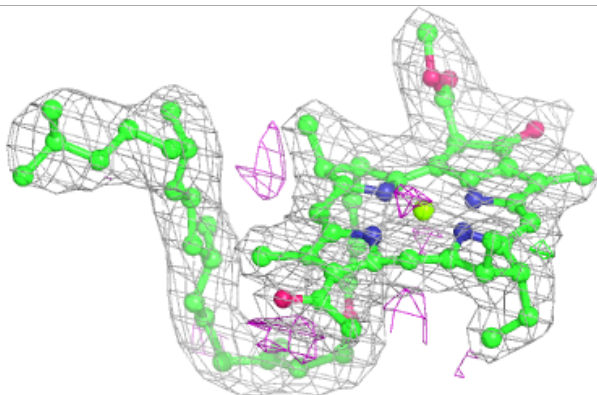
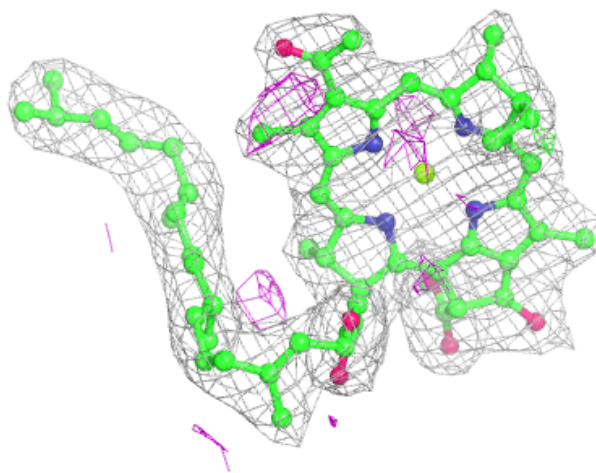
**Electron density around BCL M 1303:**

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



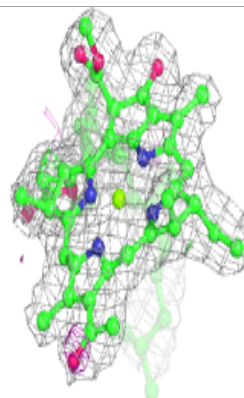
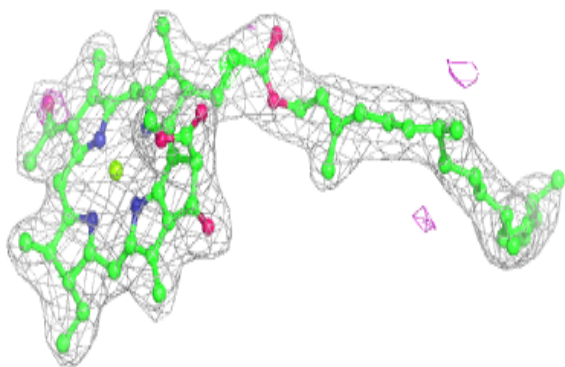
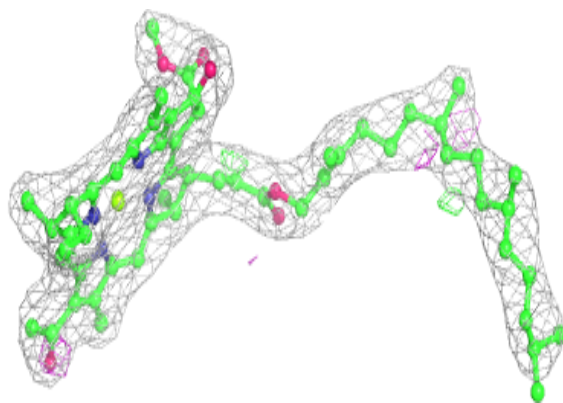
**Electron density around BCL L 1282:**

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

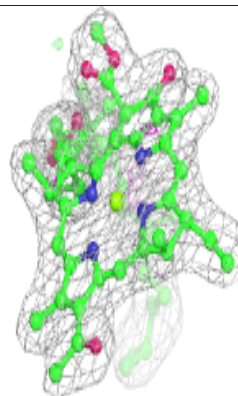
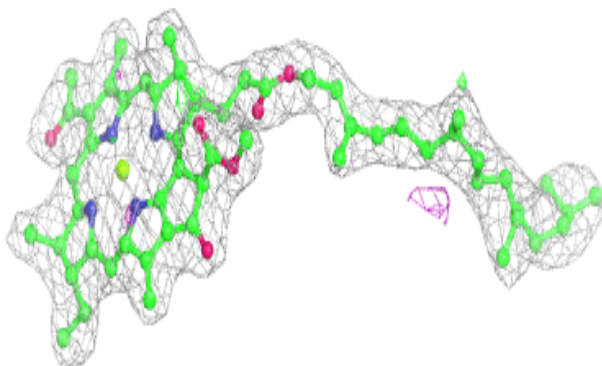
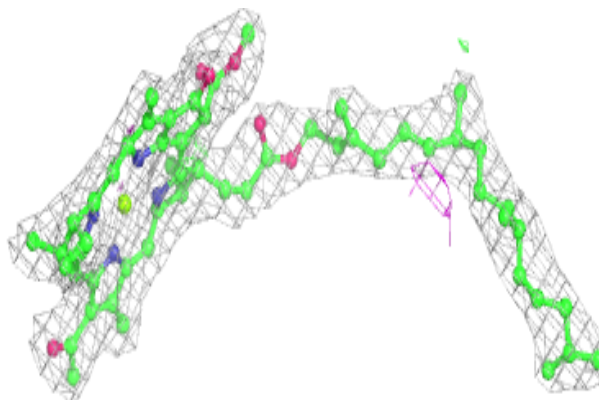


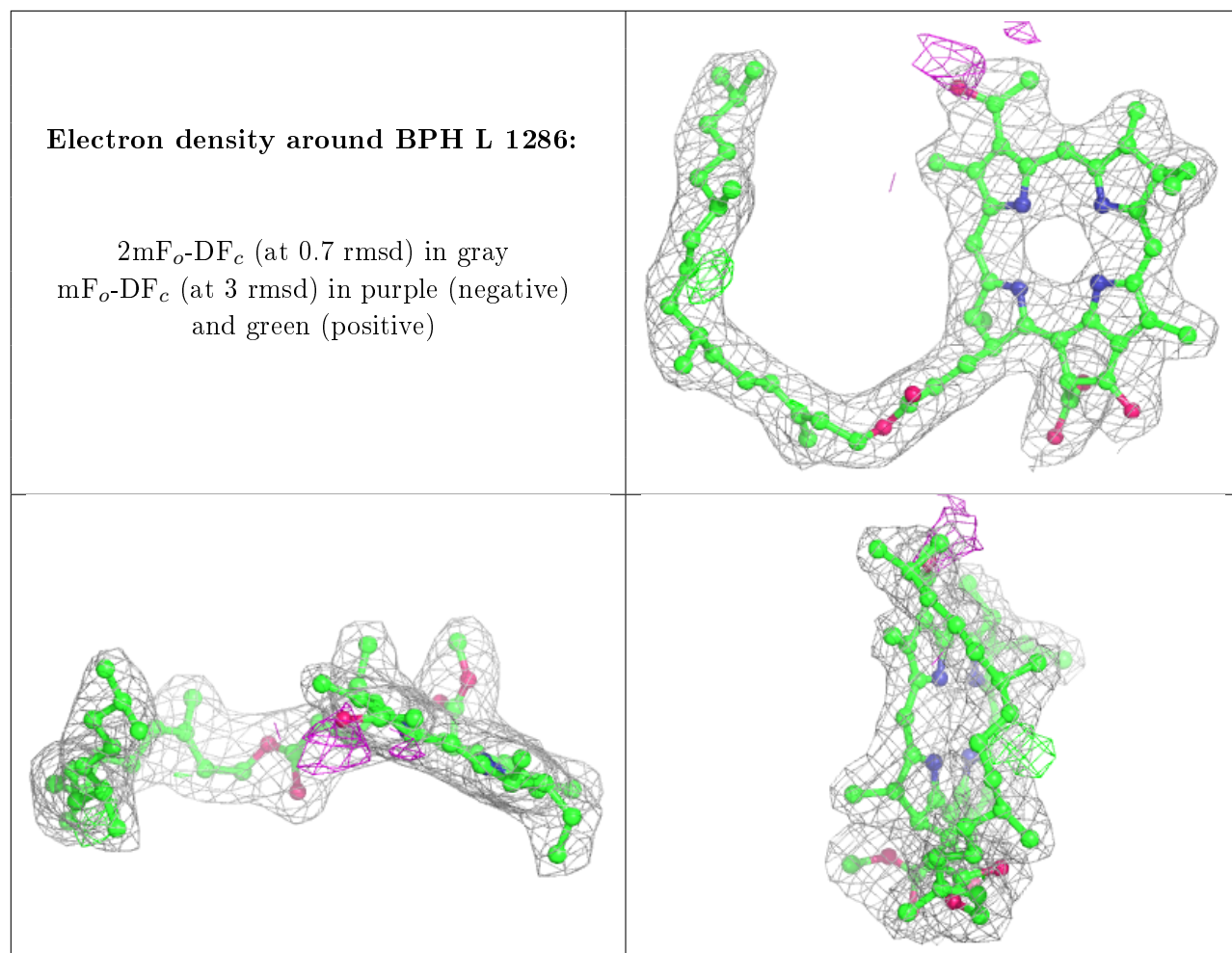
**Electron density around BCL M 1304:**

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

**Electron density around BCL L 1288:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.