



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:06 pm BST

PDB ID : 2UXK  
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 10 in the charge-separated state  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-28  
Resolution : 2.31 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

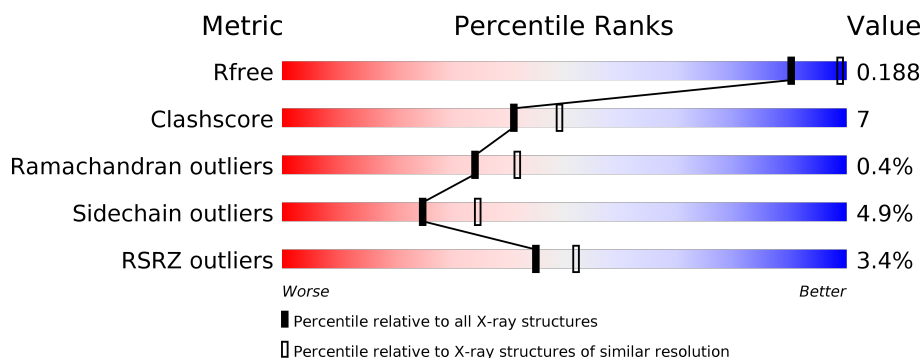
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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>7%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>• 7%</div> </div> </div>
2	L	281	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
3	M	307	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>••</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
5	BCL	L	1282	X	-	-	-
5	BCL	L	1289	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	L	1283	-	-	-	X
6	LDA	L	1286	-	-	-	X
6	LDA	M	1309	-	-	-	X

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7701 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.

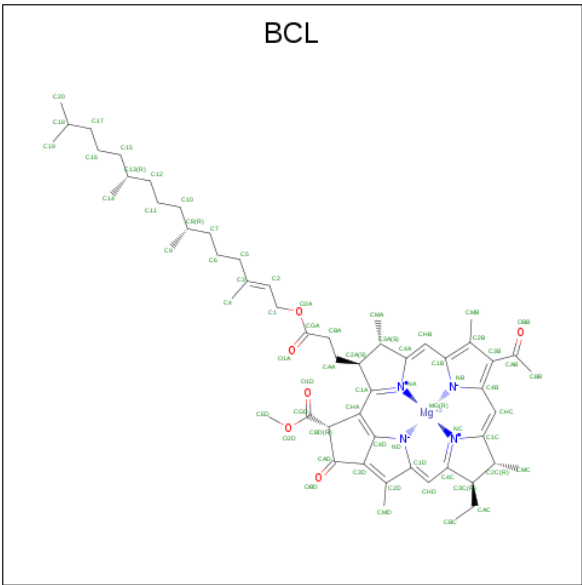
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- 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		

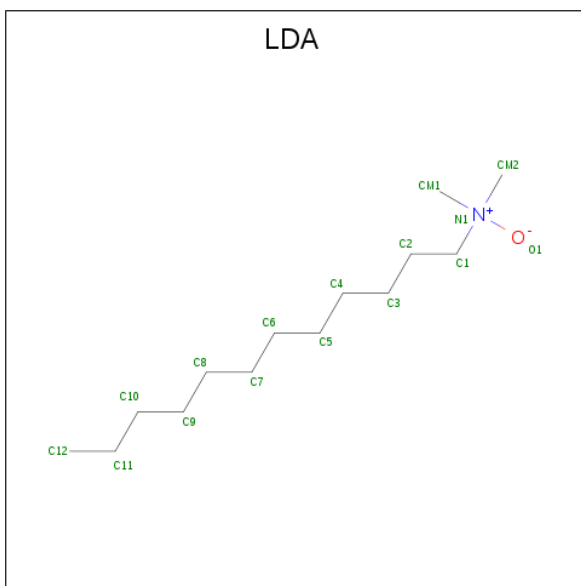
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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		

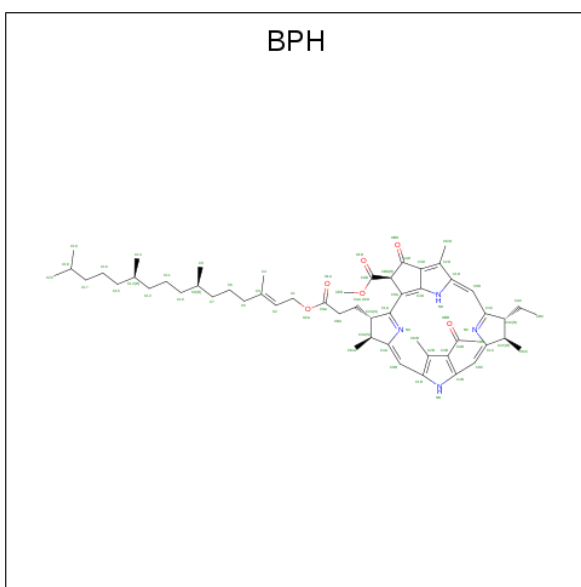
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

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



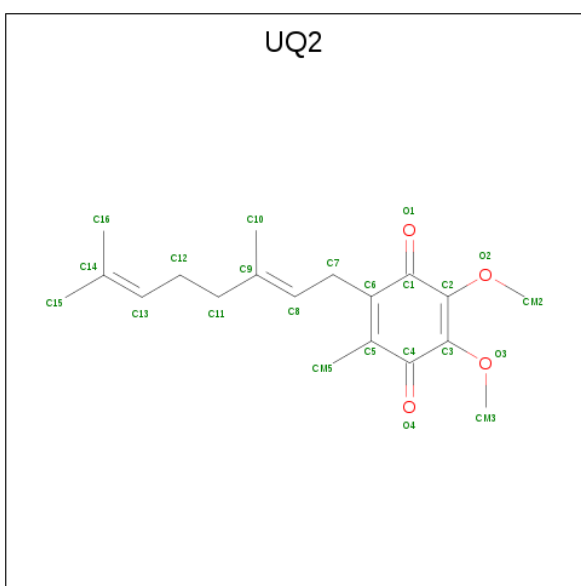
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- 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:  $C_{19}H_{26}O_4$ ).



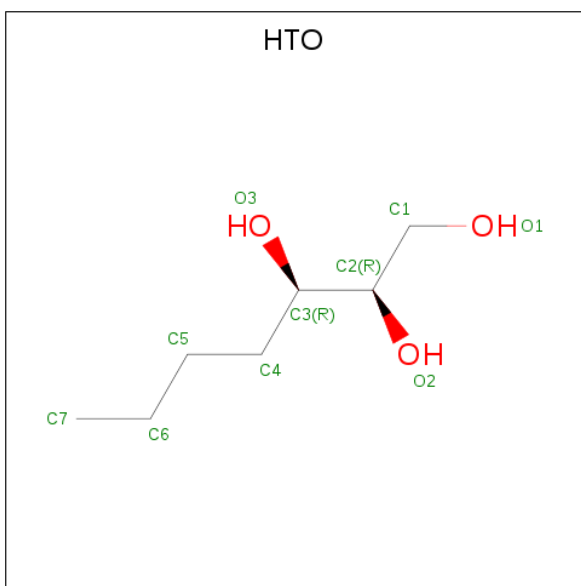
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- 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:  $C_7H_{16}O_3$ ).



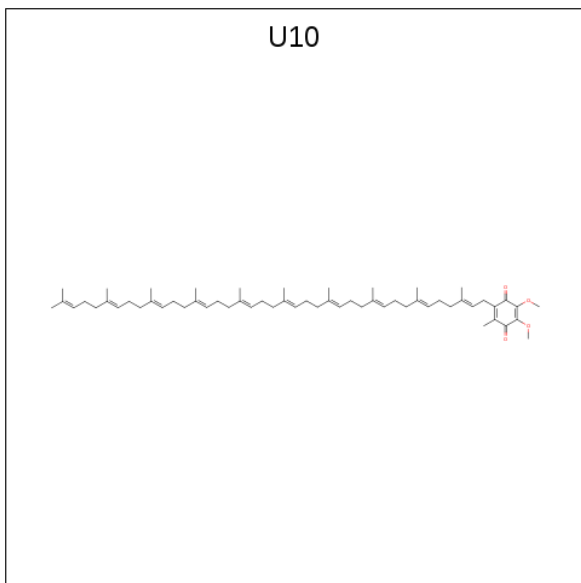
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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



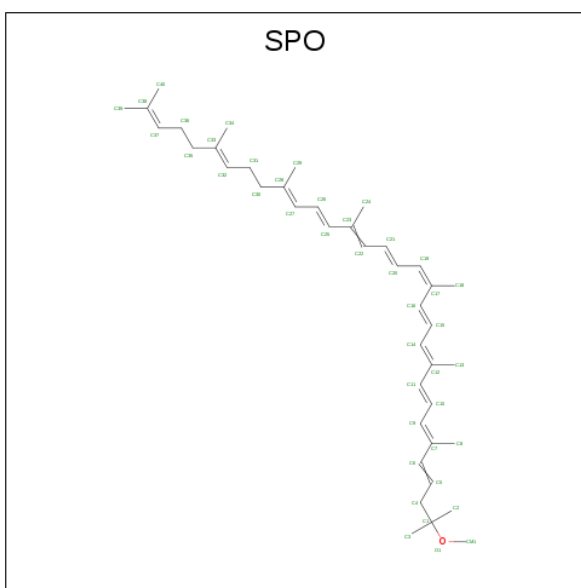
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



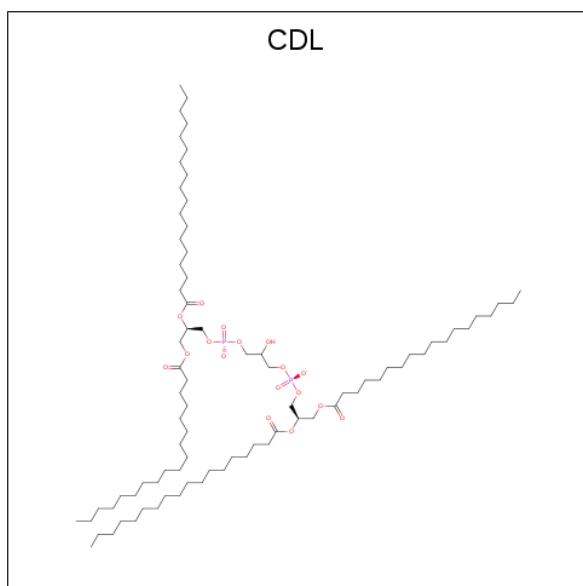
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- 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		

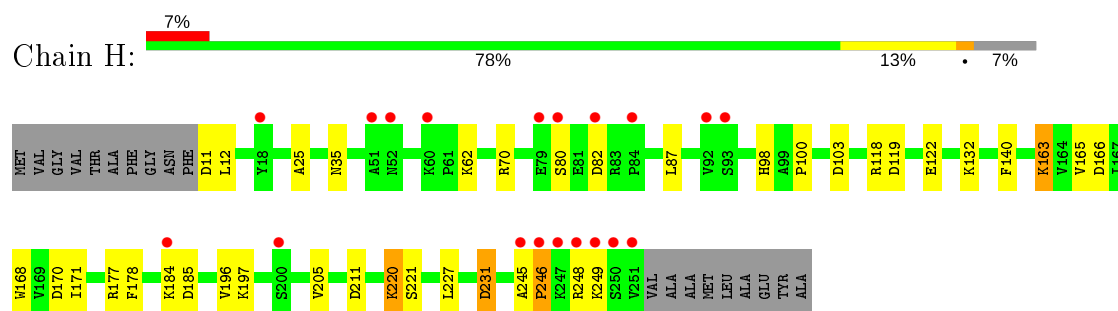
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	127	Total	O	0	0
			127	127		
15	L	127	Total	O	0	0
			127	127		
15	M	147	Total	O	0	0
			147	147		

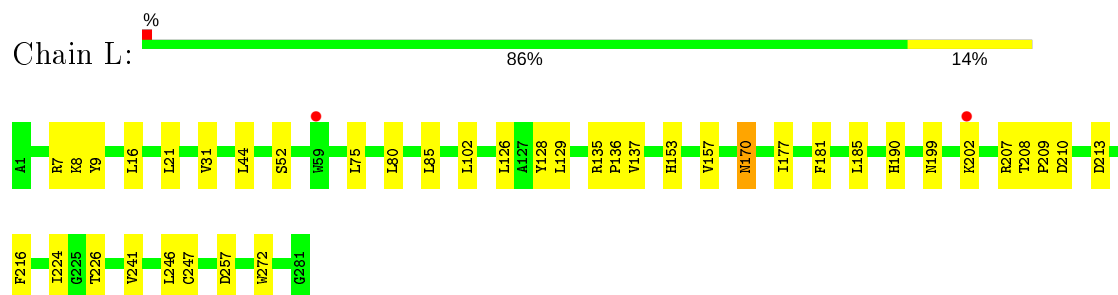
### 3 Residue-property plots [i](#)

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.

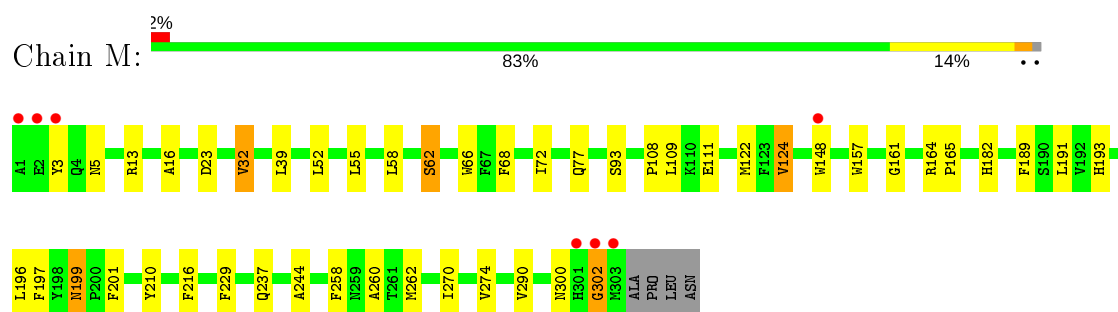
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN



#### • 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 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.02Å 140.02Å 235.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.31 19.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (119.52-2.31) 88.7 (19.95-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.190 , 0.219 0.191 , 0.188	Depositor DCC
$R_{free}$ test set	5612 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7701	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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	0.51	0/1906	0.74	8/2591 (0.3%)
2	L	0.57	0/2320	0.64	1/3175 (0.0%)
3	M	0.57	0/2501	0.64	2/3415 (0.1%)
All	All	0.55	0/6727	0.67	11/9181 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	11	ASP	CB-CG-OD2	6.89	124.50	118.30
1	H	82	ASP	CB-CG-OD2	6.51	124.16	118.30
3	M	23	ASP	CB-CG-OD2	6.06	123.76	118.30
1	H	166	ASP	CB-CG-OD2	6.06	123.75	118.30
3	M	302	GLY	O-C-N	-5.88	113.30	122.70
1	H	211	ASP	CB-CG-OD2	5.77	123.49	118.30
1	H	231	ASP	CB-CG-OD2	5.72	123.44	118.30
1	H	185	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	103	ASP	CB-CG-OD2	5.25	123.03	118.30
2	L	213	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	119	ASP	CB-CG-OD2	5.10	122.89	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	18	0
2	L	2232	0	2187	23	0
3	M	2409	0	2321	32	0
4	H	24	0	32	3	0
4	L	12	0	16	1	0
4	M	6	0	8	2	0
5	L	132	0	148	6	0
5	M	132	0	148	15	0
6	L	64	0	124	3	0
6	M	80	0	155	7	0
7	L	65	0	76	7	0
7	M	65	0	76	11	0
8	L	46	0	52	4	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	1	0
13	M	42	0	60	2	0
14	M	81	0	86	3	0
15	H	127	0	0	2	0
15	L	127	0	0	3	0
15	M	147	0	0	0	0
All	All	7701	0	7429	105	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 7.

All (105) 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)
2:L:7:ARG:NH1	15:L:2003:HOH:O	1.84	0.84
6:M:1307:LDA:H52	6:M:1308:LDA:H42	1.64	0.80
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.67	0.77
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.50	0.77
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB3	1.68	0.76
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.22	0.74
7:L:1287:BPH:CBB	7:L:1287:BPH:HHC	2.18	0.74
2:L:199:ASN:HA	4:L:1292:GOL:H31	1.68	0.73
7:M:1311:BPH:HBB3	7:M:1311:BPH:HHC	1.69	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1311:BPH:CBB	7:M:1311:BPH:HHC	2.20	0.71
7:M:1311:BPH:HHH	7:M:1311:BPH:HBC3	1.74	0.69
3:M:270:ILE:O	3:M:274:VAL:HG13	1.93	0.69
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.75	0.68
3:M:77:GLN:HE22	3:M:93:SER:H	1.38	0.68
3:M:108:PRO:HG2	3:M:111:GLU:HB2	1.75	0.68
7:L:1287:BPH:HBB3	7:L:1287:BPH:HHC	1.77	0.67
3:M:189:PHE:O	3:M:193:HIS:HD2	1.78	0.67
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.77	0.66
3:M:62:SER:OG	3:M:124:VAL:HG22	1.96	0.66
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.78	0.66
3:M:68:PHE:O	3:M:72:ILE:HG12	1.97	0.65
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.33	0.64
5:M:1303:BCL:CBB	5:M:1303:BCL:HHC	2.28	0.63
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.81	0.63
4:H:1251:GOL:H31	15:H:2001:HOH:O	2.02	0.60
2:L:7:ARG:HD3	15:L:2003:HOH:O	2.02	0.59
3:M:300:ASN:C	3:M:302:GLY:H	2.06	0.59
2:L:170:ASN:C	2:L:170:ASN:HD22	2.06	0.59
3:M:148:TRP:HB3	14:M:1314:CDL:H741	1.84	0.58
3:M:199:ASN:HD22	3:M:199:ASN:C	2.06	0.58
1:H:25:ALA:HB1	4:H:1252:GOL:H12	1.87	0.57
1:H:70:ARG:O	1:H:118[A]:ARG:NH1	2.36	0.56
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.35	0.56
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.36	0.55
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.88	0.55
2:L:226:THR:HG22	8:L:1288[B]:UQ2:H3M3	1.88	0.55
3:M:237:GLN:HB2	3:M:262:MET:HG2	1.89	0.55
3:M:148:TRP:CD1	14:M:1314:CDL:HB62	2.42	0.54
1:H:35:ASN:OD1	3:M:260:ALA:HB1	2.08	0.54
1:H:70:ARG:HB3	1:H:118[A]:ARG:NH1	2.23	0.53
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.90	0.53
7:L:1287:BPH:HBB3	7:L:1287:BPH:CHC	2.38	0.52
7:L:1287:BPH:HBB2	7:L:1287:BPH:HHC	1.92	0.52
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.52
1:H:80:SER:HB2	15:H:2038:HOH:O	2.10	0.51
7:L:1287:BPH:CBB	7:L:1287:BPH:CHC	2.86	0.51
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.93	0.51
2:L:177:ILE:HG12	5:L:1289:BCL:HMB3	1.93	0.51
7:M:1311:BPH:CBB	7:M:1311:BPH:CHC	2.89	0.51
7:L:1287:BPH:HBB2	3:M:210:TYR:HB3	1.94	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1289:BCL:HBB3	5:L:1289:BCL:HMB1	1.93	0.50
5:M:1304:BCL:HHC	5:M:1304:BCL:CBB	2.40	0.50
3:M:148:TRP:HD1	14:M:1314:CDL:HB62	1.77	0.49
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.23	0.49
6:M:1305:LDA:H32	4:M:1315:GOL:H32	1.94	0.49
3:M:189:PHE:O	3:M:193:HIS:CD2	2.64	0.49
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.78	0.49
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.94	0.48
2:L:157:VAL:HG11	5:M:1304:BCL:HBB1	1.95	0.48
6:M:1305:LDA:H12	4:M:1315:GOL:H12	1.95	0.48
2:L:190:HIS:HA	8:L:1288[B]:UQ2:O4	2.14	0.47
6:L:1285:LDA:H22	6:L:1285:LDA:HM21	1.54	0.47
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.49	0.47
5:L:1289:BCL:CBB	5:L:1289:BCL:HMB1	2.45	0.47
1:H:12:LEU:HD23	3:M:290:VAL:HG21	1.96	0.47
6:L:1285:LDA:H41	6:L:1285:LDA:HM11	1.97	0.46
5:L:1282:BCL:HBB3	5:L:1289:BCL:H41	1.97	0.45
3:M:196:LEU:HD12	5:M:1304:BCL:CHD	2.47	0.45
6:L:1283:LDA:H22	6:L:1283:LDA:HM22	1.70	0.45
2:L:257:ASP:HB3	15:L:2114:HOH:O	2.16	0.45
2:L:241:VAL:HG21	7:L:1287:BPH:HBC3	1.99	0.45
3:M:58:LEU:O	3:M:62:SER:HB2	2.17	0.45
1:H:132:LYS:HB2	1:H:171:ILE:HD11	1.98	0.45
12:M:1312:U10:H4M2	12:M:1312:U10:H3M3	1.98	0.45
2:L:208:THR:HB	2:L:209:PRO:HD2	1.99	0.44
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.99	0.44
2:L:224:ILE:H	8:L:1288[B]:UQ2:H103	1.82	0.44
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.86	0.43
3:M:161:GLY:HA3	13:M:1313:SPO:H292	2.00	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HE	2.37	0.43
2:L:8:LYS:HE2	2:L:9:TYR:CE2	2.53	0.42
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.54	0.42
1:H:220[B]:LYS:HG2	1:H:221:SER:N	2.33	0.42
3:M:300:ASN:C	3:M:302:GLY:N	2.72	0.42
1:H:196:VAL:HG12	1:H:205:VAL:HG22	2.02	0.42
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	2.02	0.42
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.00	0.42
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.97	0.42
5:M:1304:BCL:H61	7:M:1311:BPH:C4B	2.49	0.42
2:L:52:SER:HB2	2:L:85:LEU:HD13	2.01	0.42
6:M:1307:LDA:H12	6:M:1308:LDA:HM11	2.02	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:ALA:N	1:H:246:PRO:HD2	2.35	0.41
2:L:185:LEU:HD13	7:M:1311:BPH:ND	2.35	0.41
3:M:199:ASN:HD21	3:M:201:PHE:HB2	1.85	0.41
2:L:75:LEU:HD21	2:L:137:VAL:HA	2.03	0.41
1:H:163:LYS:HE3	1:H:165:VAL:HG12	2.03	0.41
1:H:170:ASP:HB2	1:H:177:ARG:HG3	2.02	0.41
6:M:1307:LDA:H21	6:M:1308:LDA:HM21	2.03	0.41
13:M:1313:SPO:H19	13:M:1313:SPO:H22	1.82	0.41
1:H:140:PHE:HA	3:M:13:ARG:O	2.21	0.40
7:M:1311:BPH:HBC3	7:M:1311:BPH:CHD	2.48	0.40
5:M:1303:BCL:HBB3	5:M:1304:BCL:C4	2.45	0.40
3:M:258:PHE:CG	6:M:1307:LDA:H51	2.56	0.40
8:L:1288[A]:UQ2:H101	8:L:1288[A]:UQ2:H121	1.64	0.40
6:M:1307:LDA:HM11	6:M:1307:LDA:H22	1.86	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	H	242/260 (93%)	234 (97%)	6 (2%)	2 (1%)	19	23
2	L	279/281 (99%)	276 (99%)	2 (1%)	1 (0%)	34	41
3	M	301/307 (98%)	291 (97%)	10 (3%)	0	100	100
All	All	822/848 (97%)	801 (97%)	18 (2%)	3 (0%)	34	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	248	ARG
1	H	246	PRO
2	L	31	VAL

### 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%)	191 (96%)	7 (4%)	36	49
2	L	220/220 (100%)	205 (93%)	15 (7%)	16	20
3	M	236/240 (98%)	225 (95%)	11 (5%)	26	36
All	All	654/668 (98%)	621 (95%)	33 (5%)	25	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	163	LYS
1	H	184	LYS
1	H	197	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	249	LYS
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	80	LEU
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
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	32	VAL
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	M	62	SER
3	M	109	LEU
3	M	124	VAL
3	M	182	HIS
3	M	191	LEU
3	M	199	ASN
3	M	216	PHE

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	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	L	1293	-	5,5,5	0.40	0	5,5,5	0.30	0
4	GOL	H	1251	-	5,5,5	0.50	0	5,5,5	0.65	0
4	GOL	H	1254	-	5,5,5	0.40	0	5,5,5	0.21	0
12	U10	M	1312	-	48,48,63	2.72	13 (27%)	58,61,79	1.47	12 (20%)
6	LDA	L	1284	-	12,15,15	2.06	1 (8%)	14,17,17	0.55	0
5	BCL	M	1303	3	58,74,74	2.19	6 (10%)	69,115,115	2.06	18 (26%)
5	BCL	L	1282	2	58,74,74	2.14	8 (13%)	69,115,115	2.09	16 (23%)
4	GOL	H	1253	-	5,5,5	0.40	0	5,5,5	0.19	0
6	LDA	L	1285	-	12,15,15	1.94	1 (8%)	14,17,17	0.41	0
7	BPH	M	1311	-	64,70,70	3.01	18 (28%)	76,101,101	1.58	16 (21%)
6	LDA	M	1308	-	12,15,15	2.08	1 (8%)	14,17,17	0.59	0
6	LDA	L	1283	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
4	GOL	H	1252	-	5,5,5	0.44	0	5,5,5	0.40	0
4	GOL	L	1292	-	5,5,5	0.25	0	5,5,5	0.55	0
7	BPH	L	1287	-	64,70,70	3.02	16 (25%)	76,101,101	1.81	18 (23%)
13	SPO	M	1313	-	40,41,41	4.02	12 (30%)	47,50,50	2.03	16 (34%)
8	UQ2	L	1288[A]	-	23,23,23	2.72	8 (34%)	28,31,31	1.10	2 (7%)
10	HTO	L	1291	-	9,9,9	0.33	0	10,10,10	0.61	0
8	UQ2	L	1288[B]	-	23,23,23	2.65	8 (34%)	28,31,31	1.73	8 (28%)
14	CDL	M	1314	-	80,80,99	2.06	18 (22%)	86,92,111	3.11	12 (13%)
6	LDA	M	1309	-	12,15,15	2.06	1 (8%)	14,17,17	0.46	0
6	LDA	M	1305	-	12,15,15	2.05	1 (8%)	14,17,17	0.37	0
5	BCL	L	1289	2	58,74,74	2.28	8 (13%)	69,115,115	1.96	17 (24%)
5	BCL	M	1304	3	58,74,74	2.33	7 (12%)	69,115,115	2.20	22 (31%)
6	LDA	M	1307	-	12,15,15	1.95	1 (8%)	14,17,17	0.52	0
6	LDA	L	1286	-	12,15,15	1.96	1 (8%)	14,17,17	0.55	0
4	GOL	M	1315	-	5,5,5	0.34	0	5,5,5	0.41	0
9	PO4	L	1290	-	4,4,4	0.90	0	6,6,6	0.44	0
6	LDA	M	1306	-	12,15,15	2.02	1 (8%)	14,17,17	0.45	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
4	GOL	L	1293	-	-	0/4/4/4	-
4	GOL	H	1251	-	-	2/4/4/4	-
4	GOL	H	1254	-	-	1/4/4/4	-
12	U10	M	1312	-	-	12/45/69/87	0/1/1/1
6	LDA	L	1284	-	-	6/13/13/13	-
5	BCL	M	1303	3	2/2/21/25	17/37/137/137	-
5	BCL	L	1282	2	2/2/21/25	7/37/137/137	-
4	GOL	H	1253	-	-	2/4/4/4	-
6	LDA	L	1285	-	-	11/13/13/13	-
7	BPH	M	1311	-	-	18/54/105/105	0/5/6/6
6	LDA	M	1308	-	-	4/13/13/13	-
6	LDA	L	1283	-	-	9/13/13/13	-
4	GOL	H	1252	-	-	4/4/4/4	-
4	GOL	L	1292	-	-	2/4/4/4	-
7	BPH	L	1287	-	-	8/54/105/105	0/5/6/6
13	SPO	M	1313	-	-	4/47/47/47	-
8	UQ2	L	1288[A]	-	-	7/15/39/39	0/1/1/1
10	HTO	L	1291	-	-	9/10/10/10	-
8	UQ2	L	1288[B]	-	-	7/15/39/39	0/1/1/1
14	CDL	M	1314	-	-	54/91/91/110	-
6	LDA	M	1309	-	-	4/13/13/13	-
6	LDA	M	1305	-	-	3/13/13/13	-
5	BCL	L	1289	2	2/2/21/25	12/37/137/137	-
5	BCL	M	1304	3	2/2/21/25	5/37/137/137	-
6	LDA	M	1307	-	-	8/13/13/13	-
6	LDA	L	1286	-	-	8/13/13/13	-
4	GOL	M	1315	-	-	2/4/4/4	-
6	LDA	M	1306	-	-	7/13/13/13	-

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	OBD-CAD	13.94	1.41	1.22
5	L	1289	BCL	OBD-CAD	13.75	1.41	1.22
13	M	1313	SPO	C27-C28	12.83	1.47	1.34
5	L	1282	BCL	OBD-CAD	12.76	1.40	1.22
7	L	1287	BPH	OBD-CAD	12.69	1.40	1.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1303	BCL	OBD-CAD	12.64	1.40	1.22
7	M	1311	BPH	OBD-CAD	12.44	1.39	1.22
7	L	1287	BPH	OBG-CAB	9.91	1.45	1.23
13	M	1313	SPO	C19-C17	9.10	1.47	1.35
13	M	1313	SPO	C22-C23	8.67	1.47	1.35
13	M	1313	SPO	C9-C7	8.38	1.46	1.35
7	M	1311	BPH	OBG-CAB	8.21	1.41	1.23
13	M	1313	SPO	C14-C12	7.98	1.46	1.35
7	M	1311	BPH	O1D-CGD	7.96	1.41	1.21
7	L	1287	BPH	O1D-CGD	7.39	1.39	1.21
6	M	1308	LDA	O1-N1	-7.12	1.25	1.42
6	L	1284	LDA	O1-N1	-7.06	1.25	1.42
6	M	1309	LDA	O1-N1	-7.02	1.25	1.42
8	L	1288[A]	UQ2	C8-C9	6.96	1.49	1.33
6	L	1283	LDA	O1-N1	-6.93	1.25	1.42
6	M	1305	LDA	O1-N1	-6.91	1.26	1.42
6	M	1306	LDA	O1-N1	-6.90	1.26	1.42
14	M	1314	CDL	C32-C31	-6.78	1.27	1.52
6	L	1286	LDA	O1-N1	-6.72	1.26	1.42
6	M	1307	LDA	O1-N1	-6.70	1.26	1.42
14	M	1314	CDL	C11-CA5	-6.70	1.31	1.50
6	L	1285	LDA	O1-N1	-6.63	1.26	1.42
12	M	1312	U10	C33-C34	6.55	1.48	1.33
12	M	1312	U10	C18-C19	6.52	1.48	1.33
13	M	1313	SPO	C32-C33	6.48	1.48	1.33
7	M	1311	BPH	C2-C3	6.33	1.48	1.33
7	M	1311	BPH	O1A-CGA	6.32	1.41	1.22
12	M	1312	U10	C28-C29	6.25	1.48	1.33
12	M	1312	U10	C13-C14	6.25	1.48	1.33
8	L	1288[B]	UQ2	C8-C9	6.20	1.47	1.33
12	M	1312	U10	C8-C9	6.11	1.47	1.33
7	L	1287	BPH	O1A-CGA	6.07	1.40	1.22
12	M	1312	U10	C23-C24	6.07	1.47	1.33
13	M	1313	SPO	C37-C38	6.06	1.49	1.32
7	L	1287	BPH	C2-C3	6.04	1.47	1.33
5	L	1289	BCL	O1A-CGA	5.96	1.40	1.22
7	L	1287	BPH	CHB-C1B	5.94	1.50	1.38
5	M	1304	BCL	O1A-CGA	5.91	1.40	1.22
5	M	1303	BCL	O1A-CGA	5.89	1.40	1.22
7	M	1311	BPH	CHB-C1B	5.82	1.50	1.38
8	L	1288[B]	UQ2	O2-C2	-5.66	1.23	1.36
5	L	1282	BCL	O1A-CGA	5.62	1.39	1.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1287	BPH	CHC-C1C	5.52	1.47	1.36
8	L	1288[A]	UQ2	C13-C14	5.50	1.48	1.32
12	M	1312	U10	C38-C39	5.45	1.48	1.32
7	M	1311	BPH	C3D-C2D	5.44	1.49	1.39
13	M	1313	SPO	C6-C5	5.34	1.46	1.32
8	L	1288[B]	UQ2	C13-C14	5.29	1.47	1.32
7	L	1287	BPH	C3D-C2D	5.16	1.48	1.39
12	M	1312	U10	O3-C3	-5.08	1.24	1.36
5	M	1303	BCL	C1B-NB	4.94	1.39	1.35
7	M	1311	BPH	CHC-C1C	4.91	1.46	1.36
8	L	1288[A]	UQ2	O3-C3	-4.80	1.25	1.36
14	M	1314	CDL	OA6-CA5	4.74	1.47	1.34
14	M	1314	CDL	OB6-CB5	4.72	1.47	1.34
14	M	1314	CDL	OA8-CA7	4.71	1.47	1.33
8	L	1288[B]	UQ2	O3-C3	-4.70	1.25	1.36
8	L	1288[A]	UQ2	O2-C2	-4.70	1.25	1.36
13	M	1313	SPO	C26-C25	4.69	1.46	1.34
14	M	1314	CDL	OB8-CB7	4.65	1.46	1.33
5	M	1304	BCL	C1B-NB	4.59	1.39	1.35
14	M	1314	CDL	C16-C15	-4.54	1.26	1.51
14	M	1314	CDL	C17-C16	-4.49	1.26	1.51
12	M	1312	U10	O4-C4	-4.40	1.26	1.36
13	M	1313	SPO	C10-C11	4.24	1.45	1.34
7	M	1311	BPH	CHD-C4C	4.23	1.48	1.38
13	M	1313	SPO	C15-C16	4.23	1.45	1.34
7	M	1311	BPH	C3D-CAD	-4.19	1.38	1.47
7	L	1287	BPH	CHC-C4B	4.18	1.50	1.40
5	M	1304	BCL	C4B-NB	4.13	1.38	1.35
7	L	1287	BPH	C3D-CAD	-4.04	1.39	1.47
7	M	1311	BPH	CHC-C4B	3.89	1.49	1.40
5	L	1289	BCL	C4B-NB	3.80	1.38	1.35
14	M	1314	CDL	C13-C12	-3.80	1.30	1.51
13	M	1313	SPO	C21-C20	3.76	1.45	1.36
7	L	1287	BPH	CHD-C4C	3.72	1.47	1.38
5	L	1289	BCL	C1B-NB	3.70	1.38	1.35
7	M	1311	BPH	C1B-C2B	-3.57	1.38	1.45
5	M	1303	BCL	C2-C3	3.54	1.41	1.33
8	L	1288[B]	UQ2	C3-C4	-3.52	1.38	1.48
14	M	1314	CDL	C19-C18	-3.47	1.32	1.51
8	L	1288[A]	UQ2	C6-C5	3.43	1.41	1.35
5	M	1303	BCL	O2D-CGD	-3.41	1.24	1.33
14	M	1314	CDL	C20-C19	-3.33	1.32	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1289	BCL	C2-C3	3.32	1.40	1.33
14	M	1314	CDL	C34-C33	-3.31	1.33	1.51
14	M	1314	CDL	C33-C32	-3.24	1.33	1.51
14	M	1314	CDL	C37-C36	-3.17	1.33	1.51
14	M	1314	CDL	C79-C78	-3.14	1.33	1.51
14	M	1314	CDL	C80-C79	-3.09	1.34	1.51
5	L	1282	BCL	C1B-NB	3.03	1.37	1.35
14	M	1314	CDL	C22-C21	-3.01	1.34	1.51
7	M	1311	BPH	O2D-CGD	-3.00	1.25	1.33
12	M	1312	U10	C6-C1	2.97	1.40	1.35
7	L	1287	BPH	C1B-C2B	-2.90	1.39	1.45
7	M	1311	BPH	CHB-C4A	2.90	1.47	1.40
5	L	1289	BCL	O2D-CGD	-2.86	1.26	1.33
5	M	1304	BCL	O2D-CGD	-2.85	1.26	1.33
5	L	1282	BCL	C2-C3	2.83	1.39	1.33
5	L	1282	BCL	O2D-CGD	-2.73	1.26	1.33
5	M	1304	BCL	C2-C3	2.73	1.39	1.33
8	L	1288[A]	UQ2	C2-C1	-2.68	1.41	1.48
7	L	1287	BPH	CHB-C4A	2.68	1.46	1.40
12	M	1312	U10	C4-C5	-2.67	1.41	1.48
8	L	1288[B]	UQ2	C2-C1	-2.66	1.41	1.48
7	M	1311	BPH	C1D-CHD	2.65	1.51	1.41
8	L	1288[A]	UQ2	C3-C4	-2.61	1.41	1.48
5	L	1282	BCL	C4B-NB	2.61	1.37	1.35
7	L	1287	BPH	O2D-CGD	-2.52	1.27	1.33
5	L	1282	BCL	O2A-CGA	-2.50	1.26	1.33
8	L	1288[B]	UQ2	C6-C1	-2.49	1.39	1.46
12	M	1312	U10	C3-C2	-2.45	1.41	1.48
8	L	1288[B]	UQ2	C6-C5	2.42	1.39	1.35
7	M	1311	BPH	O2A-CGA	-2.40	1.26	1.33
7	M	1311	BPH	C1A-NA	-2.32	1.33	1.37
5	M	1303	BCL	C3D-CAD	-2.30	1.40	1.46
5	L	1282	BCL	O1D-CGD	2.26	1.26	1.21
5	L	1289	BCL	C3D-CAD	-2.26	1.40	1.46
5	M	1304	BCL	O2A-CGA	-2.25	1.26	1.33
7	L	1287	BPH	O2A-CGA	-2.25	1.26	1.33
7	L	1287	BPH	C1D-CHD	2.19	1.49	1.41
8	L	1288[A]	UQ2	C5-C4	-2.19	1.39	1.47
5	L	1289	BCL	O2A-CGA	-2.18	1.26	1.33
12	M	1312	U10	C6-C5	-2.14	1.40	1.46
7	M	1311	BPH	C1C-NC	-2.09	1.33	1.37
14	M	1314	CDL	C12-C11	-2.09	1.44	1.52



All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1314	CDL	C33-C32-C31	15.92	170.41	113.19
14	M	1314	CDL	C17-C16-C15	12.48	177.80	114.42
14	M	1314	CDL	C12-C11-CA5	9.64	148.68	113.62
5	M	1304	BCL	C1C-NC-C4C	9.02	110.76	106.71
14	M	1314	CDL	C13-C12-C11	7.93	141.69	113.19
14	M	1314	CDL	C35-C34-C33	7.65	153.26	114.42
5	L	1289	BCL	CMB-C2B-C1B	-7.55	116.87	128.46
5	L	1282	BCL	CMB-C2B-C1B	-7.16	117.45	128.46
14	M	1314	CDL	C34-C33-C32	6.89	149.42	114.42
5	M	1303	BCL	CMB-C2B-C1B	-6.76	118.07	128.46
14	M	1314	CDL	C20-C19-C18	6.58	147.81	114.42
7	L	1287	BPH	C4D-C3D-CAD	6.08	111.72	107.87
5	M	1303	BCL	C4A-NA-C1A	6.01	109.41	106.71
5	M	1304	BCL	CMB-C2B-C1B	-5.89	119.41	128.46
5	M	1304	BCL	C1D-CHD-C4C	-5.78	117.34	125.88
5	L	1282	BCL	O2D-CGD-CBD	5.43	120.92	111.27
7	M	1311	BPH	O2D-CGD-CBD	5.26	120.62	111.27
13	M	1313	SPO	C10-C9-C7	-5.24	119.84	127.31
7	L	1287	BPH	O2D-CGD-CBD	5.22	120.54	111.27
5	L	1289	BCL	CMB-C2B-C3B	5.19	134.40	124.68
5	M	1303	BCL	O2D-CGD-CBD	5.04	120.23	111.27
5	L	1282	BCL	C4A-NA-C1A	4.90	108.91	106.71
5	M	1303	BCL	CMB-C2B-C3B	4.85	133.76	124.68
5	L	1289	BCL	C4A-NA-C1A	4.61	108.78	106.71
5	L	1282	BCL	C4B-CHC-C1C	-4.54	121.14	130.12
7	M	1311	BPH	CHC-C4B-NB	-4.47	115.57	124.93
5	L	1282	BCL	CMB-C2B-C3B	4.47	133.03	124.68
7	L	1287	BPH	CED-O2D-CGD	4.43	125.96	115.94
5	M	1304	BCL	O2D-CGD-CBD	4.41	119.10	111.27
5	M	1303	BCL	C1D-CHD-C4C	-4.40	119.39	125.88
5	L	1282	BCL	C1D-CHD-C4C	-4.31	119.51	125.88
13	M	1313	SPO	C21-C22-C23	-4.28	121.20	127.31
5	M	1303	BCL	C1-O2A-CGA	4.24	127.56	116.44
14	M	1314	CDL	OA6-CA5-C11	4.21	120.58	111.50
14	M	1314	CDL	OB6-CB5-C51	4.15	120.44	111.50
8	L	1288[B]	UQ2	CM5-C5-C6	-4.03	117.83	124.40
5	L	1289	BCL	CHB-C4A-NA	-4.00	118.97	124.51
5	L	1282	BCL	OBD-CAD-CBD	-4.00	120.18	125.89
12	M	1312	U10	C30-C29-C31	3.95	121.92	115.27
5	M	1304	BCL	CMB-C2B-C3B	3.94	132.04	124.68
7	M	1311	BPH	C4D-C3D-CAD	3.90	110.34	107.87
7	L	1287	BPH	OBD-CAD-CBD	-3.87	120.36	125.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1313	SPO	C20-C19-C17	-3.79	121.90	127.31
13	M	1313	SPO	C15-C14-C12	-3.68	122.06	127.31
7	L	1287	BPH	OBD-CAD-C3D	-3.56	122.07	127.98
7	L	1287	BPH	O1D-CGD-CBD	-3.53	117.25	124.48
13	M	1313	SPO	C29-C28-C30	3.49	121.15	115.27
5	M	1304	BCL	CED-O2D-CGD	3.49	123.84	115.94
13	M	1313	SPO	C8-C7-C6	3.46	123.52	118.08
5	M	1304	BCL	O2A-CGA-CBA	3.43	122.67	111.91
7	M	1311	BPH	OBD-CAD-CBD	-3.40	121.04	125.89
7	L	1287	BPH	C2B-C1B-NB	3.39	114.91	109.79
5	L	1289	BCL	O2D-CGD-CBD	3.39	117.29	111.27
7	M	1311	BPH	OBD-CAD-C3D	-3.35	122.41	127.98
5	L	1289	BCL	C4B-CHC-C1C	-3.33	123.52	130.12
5	M	1304	BCL	C1B-CHB-C4A	-3.28	123.61	130.12
5	M	1303	BCL	O2D-CGD-O1D	-3.22	117.54	123.84
5	L	1289	BCL	O2A-CGA-CBA	3.16	121.82	111.91
5	M	1303	BCL	C1B-CHB-C4A	-3.12	123.93	130.12
5	M	1303	BCL	O2A-CGA-CBA	3.10	121.65	111.91
7	L	1287	BPH	C1C-NC-C4C	-3.10	107.82	110.54
5	L	1289	BCL	C1-O2A-CGA	3.07	124.49	116.44
5	M	1304	BCL	C4B-CHC-C1C	-3.03	124.11	130.12
8	L	1288[B]	UQ2	C7-C8-C9	-3.02	121.76	126.79
7	L	1287	BPH	CBB-CAB-C3B	-3.02	113.98	120.43
8	L	1288[B]	UQ2	CM3-O3-C3	3.01	127.12	116.47
5	M	1303	BCL	C1C-NC-C4C	2.98	108.05	106.71
5	L	1289	BCL	CED-O2D-CGD	2.97	122.66	115.94
5	M	1304	BCL	C4-C3-C5	2.95	120.24	115.27
13	M	1313	SPO	C13-C12-C11	2.89	122.64	118.08
5	M	1304	BCL	C16-C15-C13	-2.87	106.63	115.92
5	L	1282	BCL	O2A-CGA-CBA	2.87	120.91	111.91
7	M	1311	BPH	C2B-C1B-NB	2.85	114.10	109.79
7	M	1311	BPH	CED-O2D-CGD	2.85	122.39	115.94
14	M	1314	CDL	OB8-CB7-C71	2.85	120.84	111.91
5	M	1304	BCL	O2D-CGD-O1D	-2.83	118.31	123.84
13	M	1313	SPO	C21-C20-C19	-2.79	117.76	123.47
12	M	1312	U10	C25-C24-C26	2.78	119.95	115.27
7	M	1311	BPH	C1-O2A-CGA	2.77	123.72	116.44
5	L	1282	BCL	O2D-CGD-O1D	-2.75	118.46	123.84
5	L	1289	BCL	CMA-C3A-C4A	-2.74	104.41	111.77
13	M	1313	SPO	C8-C7-C9	-2.74	119.09	122.92
7	M	1311	BPH	CMD-C2D-C3D	-2.73	119.57	124.68
13	M	1313	SPO	C34-C33-C35	2.73	119.86	115.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1289	BCL	C1D-CHD-C4C	-2.72	121.86	125.88
13	M	1313	SPO	C15-C16-C17	-2.71	118.80	126.42
14	M	1314	CDL	C32-C31-CA7	2.70	123.45	113.62
12	M	1312	U10	C22-C23-C24	-2.70	121.16	127.66
5	L	1282	BCL	C1B-CHB-C4A	-2.69	124.78	130.12
12	M	1312	U10	C17-C18-C19	-2.69	121.18	127.66
5	L	1282	BCL	C2A-C3A-C4A	2.67	106.19	101.87
5	L	1289	BCL	CMD-C2D-C3D	-2.62	119.77	124.68
12	M	1312	U10	C15-C14-C16	2.62	119.68	115.27
7	M	1311	BPH	CAC-C3C-C2C	-2.62	107.72	114.26
5	M	1303	BCL	OBD-CAD-CBD	-2.62	122.15	125.89
7	M	1311	BPH	O2D-CGD-O1D	-2.61	118.74	123.84
12	M	1312	U10	C35-C34-C36	2.60	119.65	115.27
12	M	1312	U10	C10-C9-C11	2.60	119.65	115.27
7	L	1287	BPH	CHC-C4B-NB	-2.57	119.55	124.93
14	M	1314	CDL	OA8-CA7-C31	2.57	119.97	111.91
5	M	1303	BCL	CMA-C3A-C4A	-2.55	104.92	111.77
5	L	1282	BCL	C4-C3-C5	2.54	119.55	115.27
5	L	1289	BCL	CHA-C1A-NA	-2.54	120.58	126.40
7	L	1287	BPH	C7-C6-C5	-2.53	106.48	113.36
13	M	1313	SPO	C20-C21-C22	-2.51	118.33	123.47
5	M	1303	BCL	CHA-C1A-NA	-2.47	120.73	126.40
5	M	1304	BCL	CHD-C4C-NC	-2.47	122.33	125.08
5	L	1289	BCL	O2D-CGD-O1D	-2.46	119.02	123.84
8	L	1288[B]	UQ2	C16-C14-C15	2.43	119.97	114.60
8	L	1288[A]	UQ2	C10-C9-C11	2.43	119.35	115.27
12	M	1312	U10	C27-C28-C29	-2.43	121.82	127.66
12	M	1312	U10	C4M-O4-C4	2.40	124.99	116.47
5	L	1289	BCL	O2A-CGA-O1A	-2.38	117.58	123.59
7	L	1287	BPH	CMB-C2B-C1B	2.38	128.73	125.06
8	L	1288[B]	UQ2	C10-C9-C11	2.36	119.23	115.27
7	L	1287	BPH	O2A-CGA-CBA	2.35	119.28	111.91
5	L	1282	BCL	C1-O2A-CGA	2.33	122.55	116.44
5	L	1289	BCL	C1B-CHB-C4A	-2.32	125.52	130.12
12	M	1312	U10	C30-C29-C28	-2.31	117.74	123.68
5	L	1282	BCL	C1-C2-C3	-2.30	122.06	126.04
12	M	1312	U10	C41-C39-C40	2.30	119.69	114.60
8	L	1288[B]	UQ2	O4-C4-C3	-2.30	116.05	120.93
8	L	1288[A]	UQ2	CM2-O2-C2	2.29	124.59	116.47
12	M	1312	U10	C12-C13-C14	-2.29	122.14	127.66
8	L	1288[B]	UQ2	O1-C1-C6	-2.26	117.59	121.55
13	M	1313	SPO	C14-C15-C16	-2.25	116.19	123.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	C11-C12-C13	-2.25	108.66	115.92
5	M	1304	BCL	C1-O2A-CGA	2.24	122.33	116.44
5	M	1303	BCL	O2A-C1-C2	2.23	114.50	108.64
13	M	1313	SPO	C24-C23-C25	2.22	121.57	118.08
7	M	1311	BPH	C3B-C2B-C1B	-2.21	102.65	105.87
5	M	1304	BCL	CMD-C2D-C3D	-2.21	120.55	124.68
5	M	1304	BCL	C4A-NA-C1A	2.20	107.69	106.71
5	L	1289	BCL	C2A-C3A-C4A	2.19	105.41	101.87
13	M	1313	SPO	C11-C12-C14	-2.16	115.62	118.94
7	L	1287	BPH	C3B-C2B-C1B	-2.16	102.72	105.87
5	M	1303	BCL	CHB-C4A-NA	-2.15	121.53	124.51
5	L	1282	BCL	CHD-C4C-NC	-2.14	122.70	125.08
5	M	1304	BCL	OBD-CAD-CBD	-2.13	122.85	125.89
5	M	1303	BCL	C4B-CHC-C1C	-2.12	125.91	130.12
5	M	1304	BCL	C7-C6-C5	-2.11	107.62	113.36
7	L	1287	BPH	OB B-CAB-C3B	2.11	124.31	120.41
7	L	1287	BPH	C1-C2-C3	-2.11	122.40	126.04
13	M	1313	SPO	C9-C10-C11	-2.10	116.65	123.22
7	L	1287	BPH	C1-O2A-CGA	2.10	121.95	116.44
7	M	1311	BPH	C4-C3-C5	2.10	118.80	115.27
5	M	1304	BCL	C3C-C4C-CHD	-2.10	118.91	123.39
5	M	1304	BCL	CHC-C1C-NC	-2.07	121.65	124.51
8	L	1288[B]	UQ2	C12-C13-C14	-2.07	120.67	127.75
7	M	1311	BPH	CHD-C4C-NC	-2.07	122.75	125.20
7	L	1287	BPH	O2A-CGA-O1A	-2.06	118.39	123.59
5	L	1282	BCL	O2A-CGA-O1A	-2.05	118.42	123.59
5	M	1303	BCL	C2A-C3A-C4A	2.05	105.18	101.87
7	M	1311	BPH	C1-C2-C3	-2.04	122.51	126.04
7	M	1311	BPH	O2A-CGA-CBA	2.04	118.30	111.91
5	M	1304	BCL	CAC-C3C-C4C	-2.03	108.07	112.58
5	M	1304	BCL	CHA-C1A-NA	-2.00	121.81	126.40

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1303	BCL	C8
5	M	1303	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	L	1289	BCL	C8
5	L	1289	BCL	C13
5	M	1304	BCL	C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C13

All (233) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1251	GOL	C1-C2-C3-O3
12	M	1312	U10	C27-C28-C29-C30
12	M	1312	U10	C27-C28-C29-C31
12	M	1312	U10	C29-C31-C32-C33
12	M	1312	U10	C32-C33-C34-C35
12	M	1312	U10	C32-C33-C34-C36
12	M	1312	U10	C34-C36-C37-C38
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
5	L	1282	BCL	C6-C7-C8-C9
6	L	1285	LDA	C2-C1-N1-O1
6	L	1285	LDA	C2-C1-N1-CM2
6	L	1285	LDA	N1-C1-C2-C3
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
4	L	1292	GOL	C1-C2-C3-O3
7	L	1287	BPH	C2C-C1C-CHC-C4B
7	L	1287	BPH	NC-C1C-CHC-C4B
13	M	1313	SPO	C8-C7-C9-C10
8	L	1288[A]	UQ2	C12-C11-C9-C8
8	L	1288[A]	UQ2	C12-C11-C9-C10
8	L	1288[A]	UQ2	C9-C11-C12-C13
10	L	1291	HTO	C1-C2-C3-O3
10	L	1291	HTO	C1-C2-C3-C4
10	L	1291	HTO	O2-C2-C3-O3
10	L	1291	HTO	O2-C2-C3-C4
10	L	1291	HTO	O3-C3-C4-C5
14	M	1314	CDL	CA2-OA2-PA1-OA3
14	M	1314	CDL	CA3-OA5-PA1-OA3
14	M	1314	CDL	C51-CB5-OB6-CB4
6	L	1286	LDA	N1-C1-C2-C3
6	M	1306	LDA	C2-C1-N1-CM1
8	L	1288[B]	UQ2	C12-C13-C14-C15
8	L	1288[B]	UQ2	C12-C13-C14-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
14	M	1314	CDL	OB9-CB7-OB8-CB6
14	M	1314	CDL	OB7-CB5-OB6-CB4
12	M	1312	U10	C35-C34-C36-C37
14	M	1314	CDL	C20-C21-C22-C23
14	M	1314	CDL	C78-C79-C80-C81
5	M	1303	BCL	C3-C5-C6-C7
14	M	1314	CDL	C31-CA7-OA8-CA6
14	M	1314	CDL	C71-CB7-OB8-CB6
10	L	1291	HTO	O1-C1-C2-O2
8	L	1288[A]	UQ2	C12-C13-C14-C16
8	L	1288[B]	UQ2	C7-C8-C9-C10
8	L	1288[B]	UQ2	C7-C8-C9-C11
14	M	1314	CDL	OA9-CA7-OA8-CA6
7	L	1287	BPH	NB-C4B-CHC-C1C
8	L	1288[B]	UQ2	C9-C11-C12-C13
8	L	1288[A]	UQ2	C12-C13-C14-C15
5	M	1303	BCL	C15-C16-C17-C18
5	L	1289	BCL	C11-C12-C13-C14
5	M	1303	BCL	C10-C11-C12-C13
5	L	1289	BCL	C13-C15-C16-C17
4	H	1251	GOL	O2-C2-C3-O3
14	M	1314	CDL	CB5-C51-C52-C53
14	M	1314	CDL	CB7-C71-C72-C73
5	M	1303	BCL	C2-C1-O2A-CGA
5	L	1289	BCL	C11-C10-C8-C7
13	M	1313	SPO	C9-C10-C11-C12
7	M	1311	BPH	C5-C6-C7-C8
5	M	1303	BCL	C8-C10-C11-C12
7	M	1311	BPH	C10-C11-C12-C13
12	M	1312	U10	C33-C34-C36-C37
5	L	1289	BCL	C15-C16-C17-C18
10	L	1291	HTO	O1-C1-C2-C3
6	L	1283	LDA	C6-C7-C8-C9
6	M	1307	LDA	C3-C4-C5-C6
6	M	1307	LDA	C4-C5-C6-C7
6	M	1306	LDA	C4-C5-C6-C7
5	L	1282	BCL	C16-C17-C18-C20
6	L	1285	LDA	C7-C8-C9-C10
14	M	1314	CDL	C15-C16-C17-C18
6	M	1308	LDA	C6-C7-C8-C9
14	M	1314	CDL	C72-C73-C74-C75
14	M	1314	CDL	CA5-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
13	M	1313	SPO	C6-C7-C9-C10
6	L	1284	LDA	C7-C8-C9-C10
6	L	1284	LDA	C6-C7-C8-C9
6	M	1305	LDA	C2-C3-C4-C5
6	L	1283	LDA	C11-C10-C9-C8
14	M	1314	CDL	C74-C75-C76-C77
14	M	1314	CDL	C80-C81-C82-C83
6	M	1308	LDA	C4-C5-C6-C7
6	L	1286	LDA	C5-C6-C7-C8
14	M	1314	CDL	C31-C32-C33-C34
6	L	1286	LDA	C4-C5-C6-C7
6	L	1284	LDA	C2-C3-C4-C5
6	L	1283	LDA	C2-C3-C4-C5
6	L	1286	LDA	C11-C10-C9-C8
14	M	1314	CDL	C16-C17-C18-C19
6	L	1285	LDA	C5-C6-C7-C8
5	L	1289	BCL	C10-C11-C12-C13
6	M	1309	LDA	C3-C4-C5-C6
6	L	1283	LDA	C3-C4-C5-C6
6	L	1285	LDA	C3-C4-C5-C6
14	M	1314	CDL	C32-C33-C34-C35
7	L	1287	BPH	C4-C3-C5-C6
7	L	1287	BPH	C2-C3-C5-C6
4	L	1292	GOL	O2-C2-C3-O3
14	M	1314	CDL	C18-C19-C20-C21
5	L	1282	BCL	C16-C17-C18-C19
6	M	1309	LDA	C1-C2-C3-C4
7	M	1311	BPH	C15-C16-C17-C18
5	L	1282	BCL	C3-C5-C6-C7
6	L	1286	LDA	C1-C2-C3-C4
14	M	1314	CDL	OA7-CA5-OA6-CA4
6	L	1283	LDA	C5-C6-C7-C8
6	L	1286	LDA	C2-C3-C4-C5
6	M	1308	LDA	C7-C8-C9-C10
5	M	1303	BCL	C2-C3-C5-C6
7	M	1311	BPH	C11-C12-C13-C15
6	M	1307	LDA	C7-C8-C9-C10
6	M	1308	LDA	C1-C2-C3-C4
5	L	1282	BCL	C5-C6-C7-C8
12	M	1312	U10	C37-C38-C39-C41
14	M	1314	CDL	C37-C38-C39-C40
7	M	1311	BPH	C16-C17-C18-C19

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
14	M	1314	CDL	C11-CA5-OA6-CA4
7	M	1311	BPH	C13-C15-C16-C17
6	M	1307	LDA	C2-C3-C4-C5
5	M	1303	BCL	C4-C3-C5-C6
5	L	1289	BCL	C11-C10-C8-C9
14	M	1314	CDL	C71-C72-C73-C74
5	M	1303	BCL	C16-C17-C18-C20
14	M	1314	CDL	CA3-OA5-PA1-OA2
6	M	1309	LDA	C5-C6-C7-C8
6	L	1283	LDA	C1-C2-C3-C4
10	L	1291	HTO	C4-C5-C6-C7
14	M	1314	CDL	C12-C13-C14-C15
14	M	1314	CDL	C33-C34-C35-C36
6	L	1283	LDA	C9-C10-C11-C12
7	M	1311	BPH	C16-C17-C18-C20
6	L	1285	LDA	C1-C2-C3-C4
6	M	1307	LDA	C9-C10-C11-C12
6	L	1286	LDA	C9-C10-C11-C12
6	L	1284	LDA	C1-C2-C3-C4
5	M	1303	BCL	C11-C12-C13-C15
7	M	1311	BPH	C11-C12-C13-C14
7	M	1311	BPH	C14-C13-C15-C16
5	M	1304	BCL	C14-C13-C15-C16
14	M	1314	CDL	C14-C15-C16-C17
14	M	1314	CDL	C17-C18-C19-C20
6	L	1284	LDA	N1-C1-C2-C3
6	L	1283	LDA	N1-C1-C2-C3
6	M	1307	LDA	N1-C1-C2-C3
6	L	1285	LDA	C4-C5-C6-C7
14	M	1314	CDL	C40-C41-C42-C43
14	M	1314	CDL	CA3-CA4-CA6-OA8
14	M	1314	CDL	CB3-CB4-CB6-OB8
7	L	1287	BPH	O2A-C1-C2-C3
12	M	1312	U10	C37-C38-C39-C40
6	L	1285	LDA	C11-C10-C9-C8
4	M	1315	GOL	O1-C1-C2-O2
6	L	1285	LDA	C6-C7-C8-C9
5	L	1289	BCL	C2-C1-O2A-CGA
5	L	1289	BCL	C8-C10-C11-C12
14	M	1314	CDL	C75-C76-C77-C78
14	M	1314	CDL	C81-C82-C83-C84
5	M	1303	BCL	C4C-C3C-CAC-CBC

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	C16-C17-C18-C19
7	M	1311	BPH	C12-C13-C15-C16
5	M	1304	BCL	C12-C13-C15-C16
7	M	1311	BPH	CAD-CBD-CGD-O2D
7	L	1287	BPH	CAD-CBD-CGD-O2D
5	L	1289	BCL	CAD-CBD-CGD-O2D
14	M	1314	CDL	OB5-CB3-CB4-OB6
6	L	1285	LDA	C2-C1-N1-CM1
6	L	1283	LDA	C2-C1-N1-CM2
5	M	1304	BCL	CHA-CBD-CGD-O1D
6	M	1306	LDA	C2-C1-N1-CM2
14	M	1314	CDL	OA6-CA4-CA6-OA8
14	M	1314	CDL	OB6-CB4-CB6-OB8
4	H	1253	GOL	O2-C2-C3-O3
4	H	1252	GOL	O1-C1-C2-O2
4	H	1252	GOL	O2-C2-C3-O3
4	M	1315	GOL	O1-C1-C2-C3
14	M	1314	CDL	CA3-OA5-PA1-OA4
5	M	1304	BCL	C16-C17-C18-C19
14	M	1314	CDL	OA5-CA3-CA4-CA6
5	M	1303	BCL	C12-C13-C15-C16
14	M	1314	CDL	OA5-CA3-CA4-OA6
6	M	1309	LDA	C2-C3-C4-C5
6	M	1306	LDA	C7-C8-C9-C10
6	M	1307	LDA	C5-C6-C7-C8
8	L	1288[B]	UQ2	C4-C3-O3-CM3
6	M	1305	LDA	C4-C5-C6-C7
14	M	1314	CDL	C21-C22-C23-C24
5	M	1303	BCL	C11-C12-C13-C14
10	L	1291	HTO	C3-C4-C5-C6
13	M	1313	SPO	C33-C35-C36-C37
14	M	1314	CDL	C73-C74-C75-C76
12	M	1312	U10	C5-C4-O4-C4M
7	L	1287	BPH	C8-C10-C11-C12
6	M	1307	LDA	C6-C7-C8-C9
6	M	1305	LDA	C9-C10-C11-C12
5	L	1289	BCL	C11-C12-C13-C15
6	M	1306	LDA	C1-C2-C3-C4
14	M	1314	CDL	C53-C54-C55-C56
5	L	1289	BCL	C5-C6-C7-C8
14	M	1314	CDL	OB5-CB3-CB4-CB6
14	M	1314	CDL	C76-C77-C78-C79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	M	1306	LDA	C6-C7-C8-C9
5	M	1304	BCL	CAA-CBA-CGA-O2A
4	H	1254	GOL	O1-C1-C2-C3
4	H	1253	GOL	C1-C2-C3-O3
4	H	1252	GOL	C1-C2-C3-O3
5	L	1282	BCL	C4C-C3C-CAC-CBC
8	L	1288[A]	UQ2	C1-C2-O2-CM2
5	L	1289	BCL	C16-C17-C18-C20
5	M	1303	BCL	C14-C13-C15-C16
7	M	1311	BPH	O2A-C1-C2-C3
5	M	1303	BCL	O1A-CGA-O2A-C1
6	L	1284	LDA	C4-C5-C6-C7
14	M	1314	CDL	C72-C71-CB7-OB8
5	L	1282	BCL	CHA-CBD-CGD-O2D
14	M	1314	CDL	C52-C51-CB5-OB6
14	M	1314	CDL	C55-C56-C57-C58
8	L	1288[A]	UQ2	C3-C2-O2-CM2
4	H	1252	GOL	O1-C1-C2-C3
14	M	1314	CDL	CA2-OA2-PA1-OA5
6	M	1306	LDA	C9-C10-C11-C12
14	M	1314	CDL	CA2-OA2-PA1-OA4
14	M	1314	CDL	C72-C71-CB7-OB9
14	M	1314	CDL	C79-C80-C81-C82
6	L	1286	LDA	C3-C4-C5-C6
8	L	1288[B]	UQ2	C12-C11-C9-C10
7	M	1311	BPH	C8-C10-C11-C12
14	M	1314	CDL	C52-C51-CB5-OB7
12	M	1312	U10	C3-C4-O4-C4M

There are no ring outliers.

20 monomers are involved in 62 short contacts:

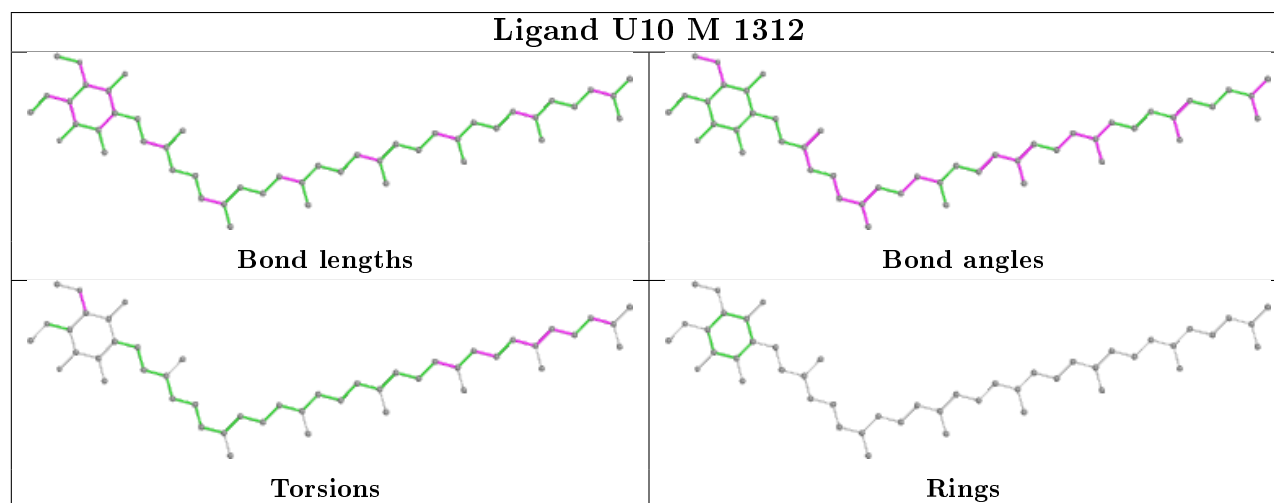
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	2	0
12	M	1312	U10	1	0
5	M	1303	BCL	4	0
5	L	1282	BCL	3	0
6	L	1285	LDA	2	0
7	M	1311	BPH	11	0
6	M	1308	LDA	3	0
6	L	1283	LDA	1	0
4	H	1252	GOL	1	0

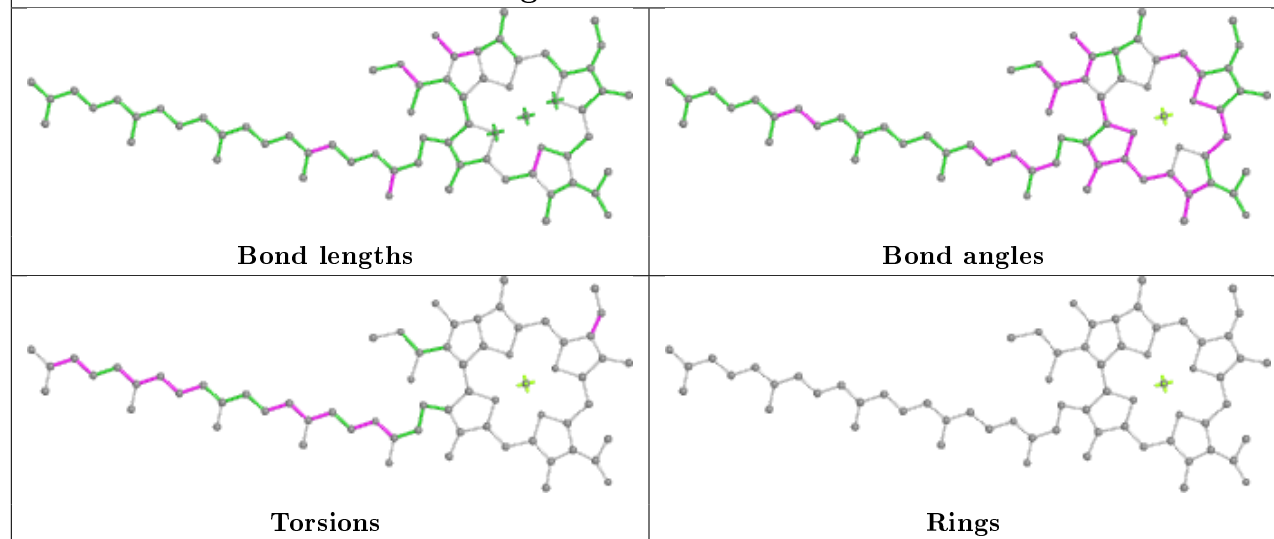
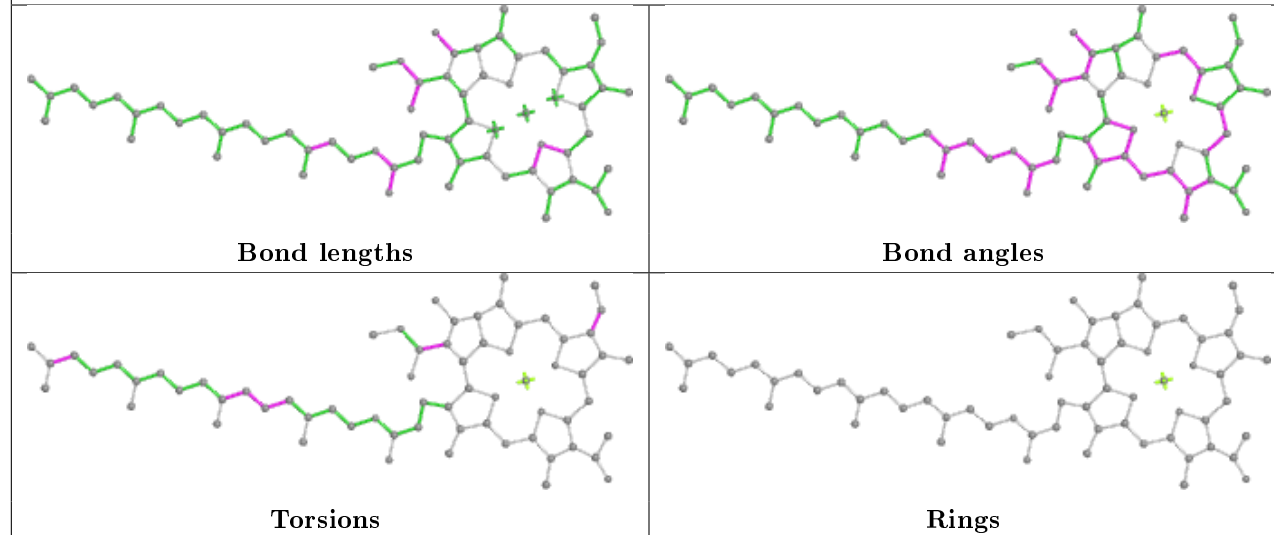
*Continued on next page...*

*Continued from previous page...*

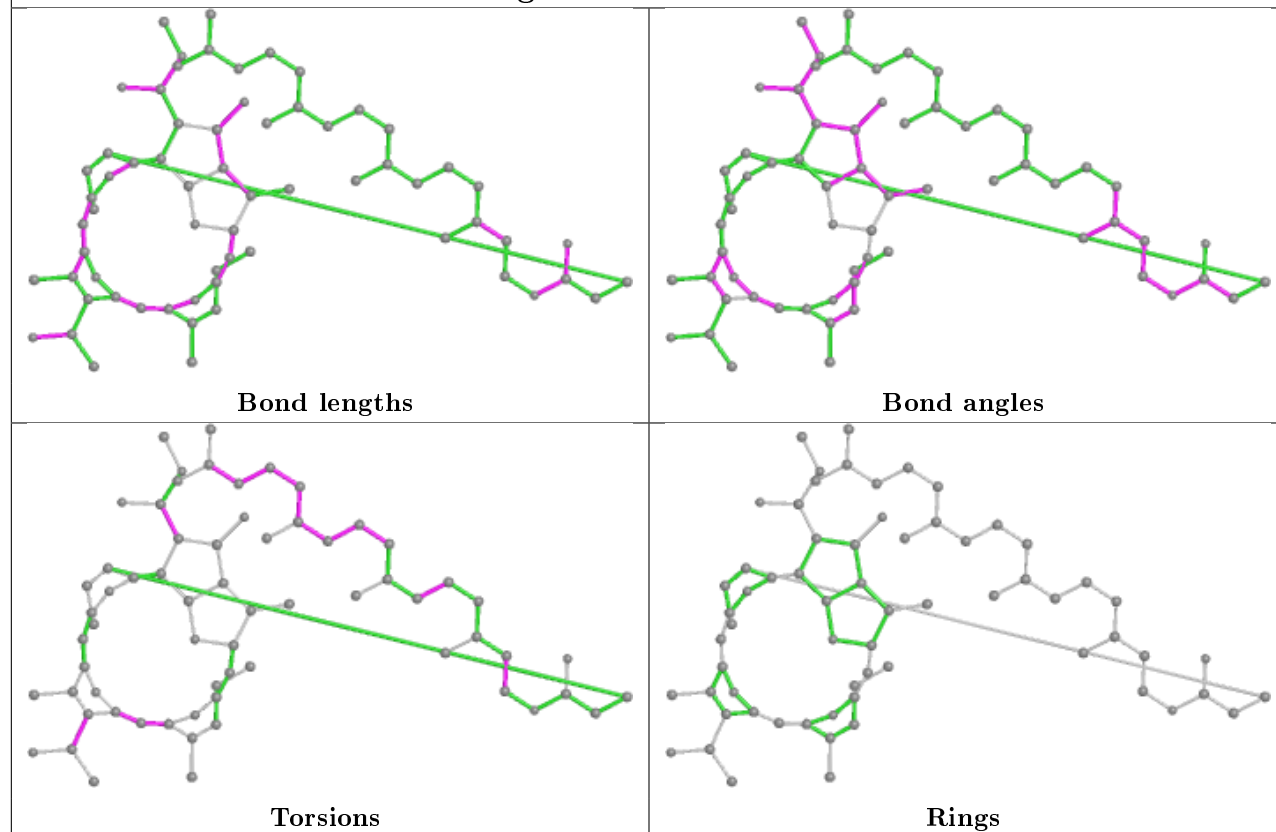
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1292	GOL	1	0
7	L	1287	BPH	7	0
13	M	1313	SPO	2	0
8	L	1288[A]	UQ2	1	0
8	L	1288[B]	UQ2	3	0
14	M	1314	CDL	3	0
6	M	1305	LDA	2	0
5	L	1289	BCL	4	0
5	M	1304	BCL	13	0
6	M	1307	LDA	5	0
4	M	1315	GOL	2	0

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

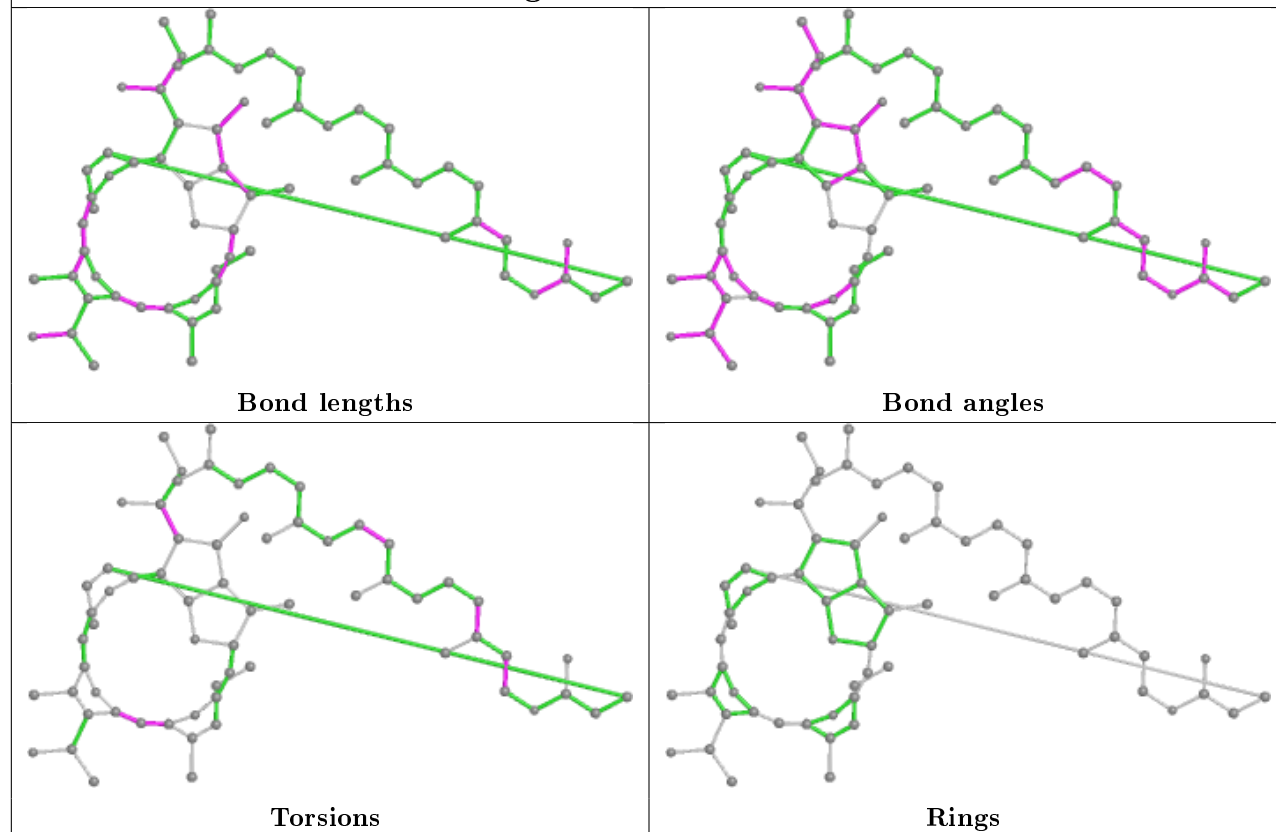


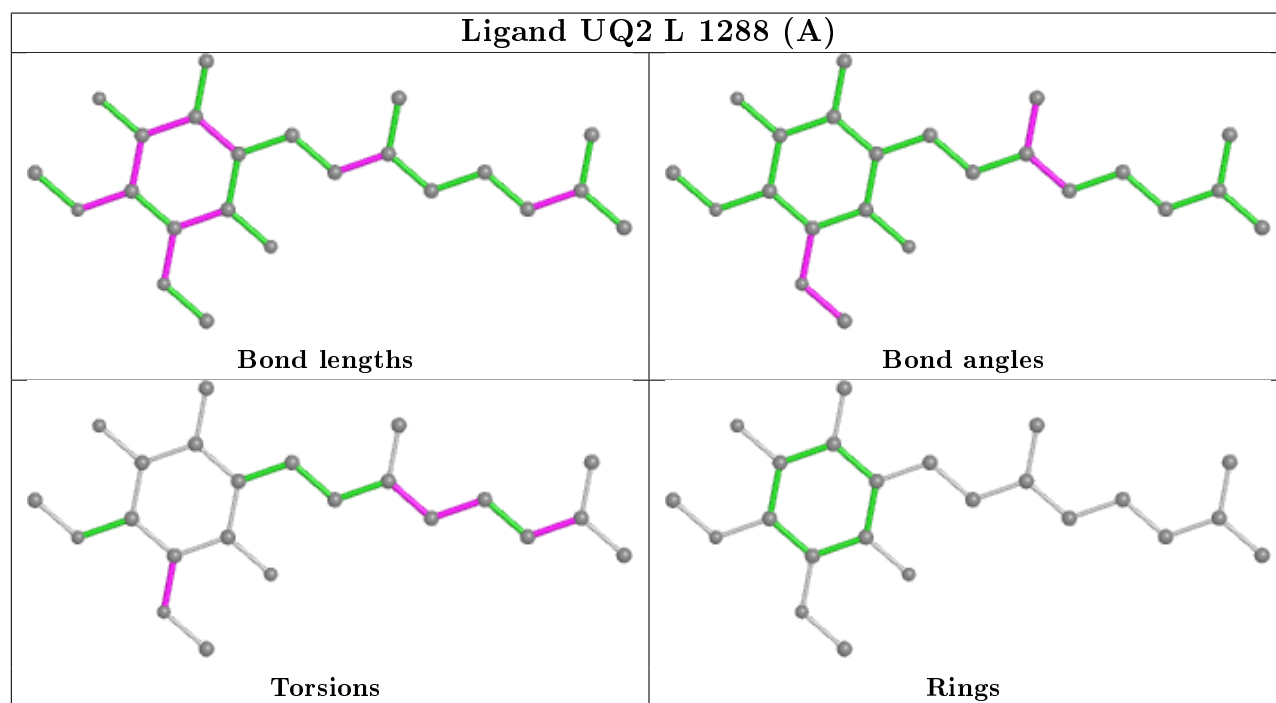
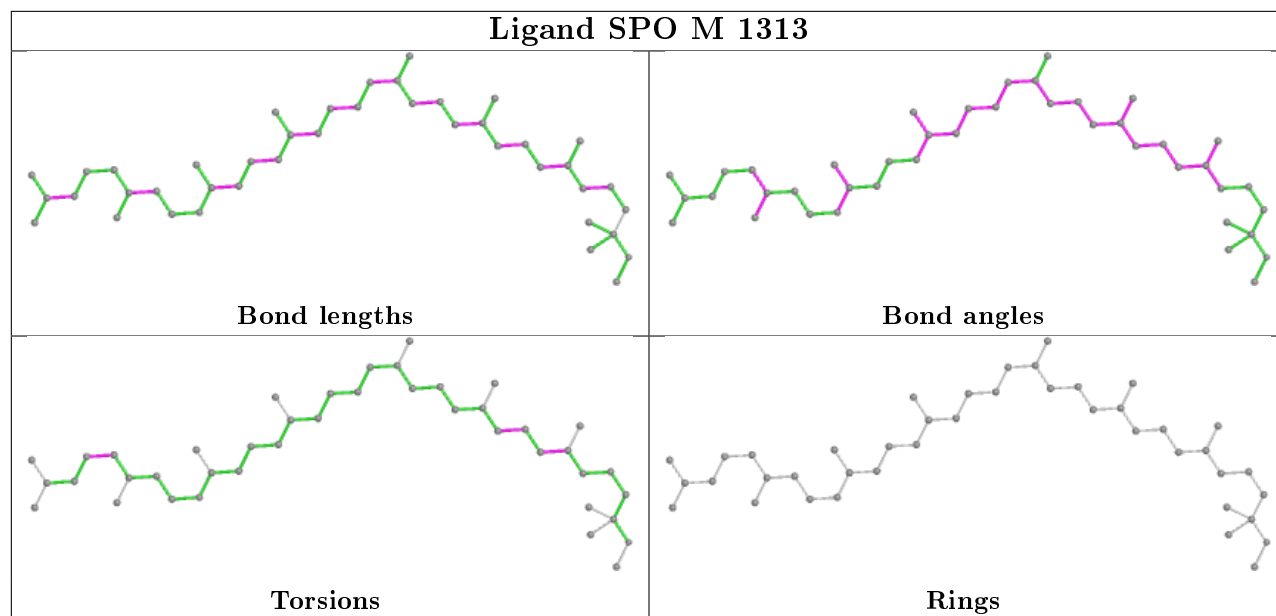
**Ligand BCL M 1303****Ligand BCL L 1282**

## Ligand BPH M 1311

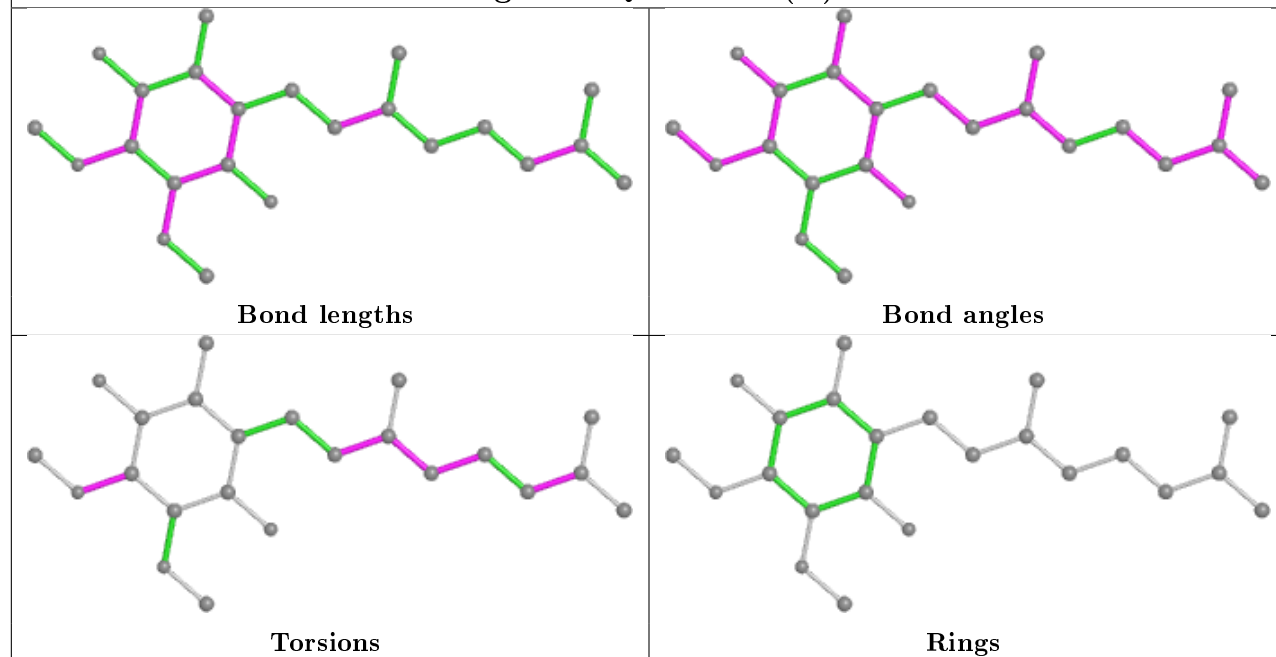


## Ligand BPH L 1287

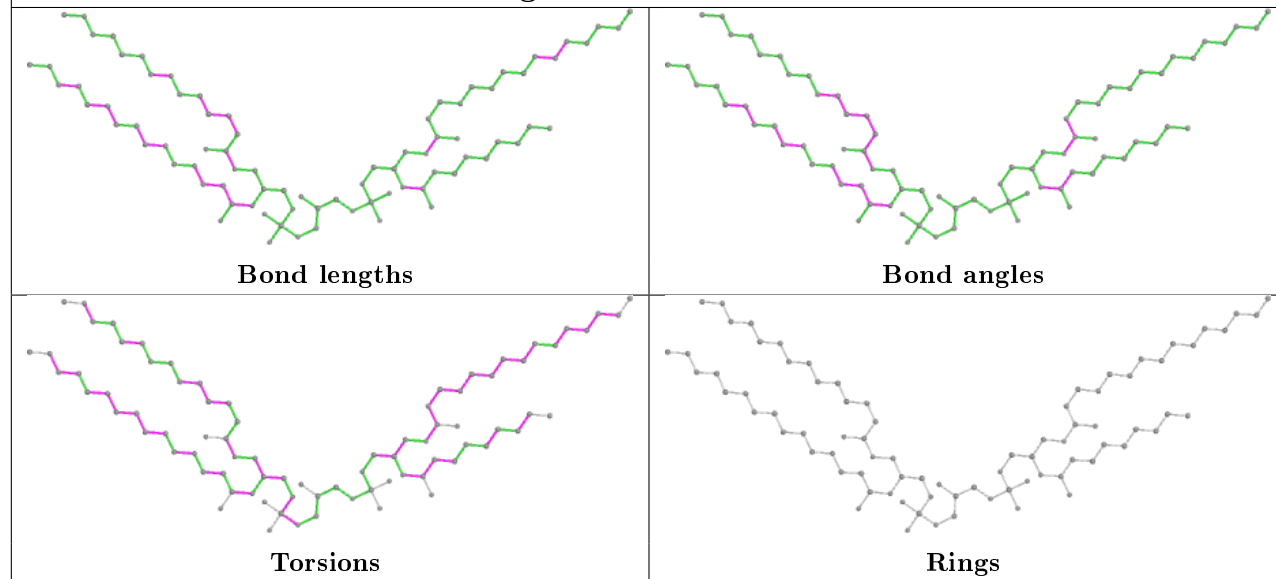


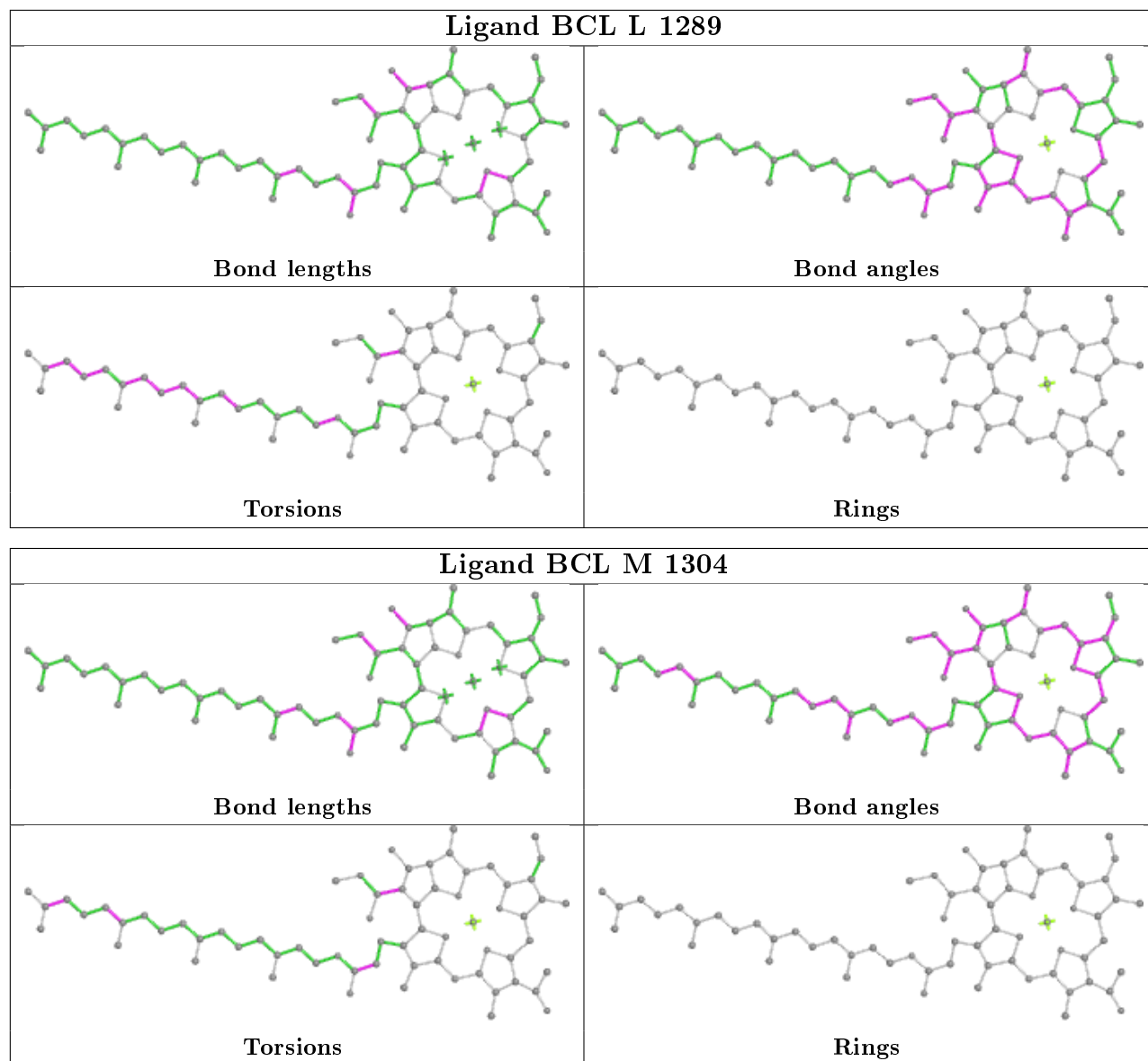


## Ligand UQ2 L 1288 (B)



## Ligand CDL M 1314





## 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%)	-0.02	19 (7%)	12 17	39, 49, 63, 103	0
2	L	281/281 (100%)	-0.62	2 (0%)	87 91	31, 41, 53, 59	0
3	M	303/307 (98%)	-0.63	7 (2%)	60 67	32, 41, 54, 79	0
All	All	825/848 (97%)	-0.45	28 (3%)	45 52	31, 44, 58, 103	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	15.1
1	H	250	SER	13.4
1	H	247	LYS	7.9
3	M	1	ALA	6.7
1	H	246	PRO	5.8
1	H	249	LYS	5.6
1	H	248	ARG	5.4
3	M	302	GLY	5.3
3	M	301	HIS	5.2
1	H	92	VAL	4.0
1	H	245	ALA	3.8
3	M	2	GLU	3.7
3	M	3	TYR	3.5
2	L	59	TRP	3.4
1	H	18	TYR	3.4
3	M	148	TRP	3.0
1	H	51	ALA	2.6
1	H	84	PRO	2.6
1	H	79	GLU	2.4
1	H	82	ASP	2.3
2	L	202	LYS	2.2
1	H	93	SER	2.2
1	H	184	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	52	ASN	2.2
1	H	200	SER	2.1
1	H	80	SER	2.1
3	M	303	MET	2.1
1	H	60	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å <sup>2</sup> )	Q<0.9
6	LDA	M	1309	16/16	-0.14	0.50	119,123,128,128	0
6	LDA	L	1286	16/16	0.04	0.41	97,103,111,111	0
6	LDA	L	1283	16/16	0.06	0.48	80,97,107,108	0
6	LDA	M	1308	16/16	0.22	0.36	116,117,121,121	0
14	CDL	M	1314	81/100	0.32	0.43	110,119,127,127	0
6	LDA	L	1285	16/16	0.35	0.31	76,86,98,98	0
4	GOL	H	1254	6/6	0.48	0.38	115,115,115,116	0
6	LDA	L	1284	16/16	0.53	0.31	106,107,110,111	0
4	GOL	H	1251	6/6	0.54	0.40	69,72,73,74	0
4	GOL	H	1252	6/6	0.56	0.37	91,93,93,93	0
4	GOL	H	1253	6/6	0.56	0.35	108,108,109,109	0
6	LDA	M	1305	16/16	0.61	0.27	61,74,78,79	0
6	LDA	M	1306	16/16	0.69	0.25	81,83,86,87	0
4	GOL	M	1315	6/6	0.75	0.20	105,106,106,106	0
4	GOL	L	1293	6/6	0.76	0.18	90,92,92,93	0
10	HTO	L	1291	10/10	0.77	0.27	72,76,77,78	0
6	LDA	M	1307	16/16	0.78	0.21	71,75,79,79	0
9	PO4	L	1290	5/5	0.79	0.34	170,170,171,171	0

*Continued on next page...*

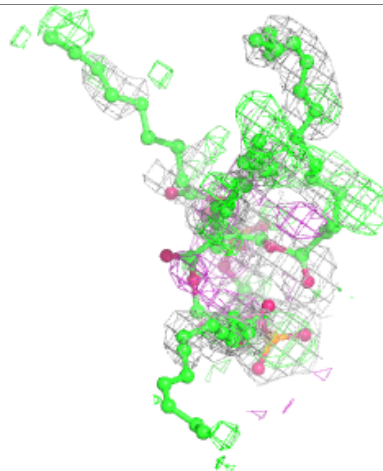
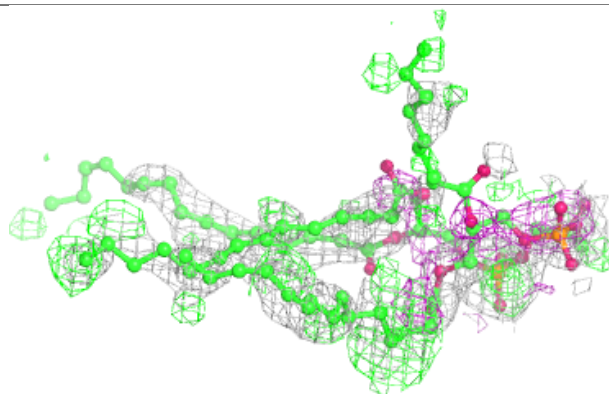
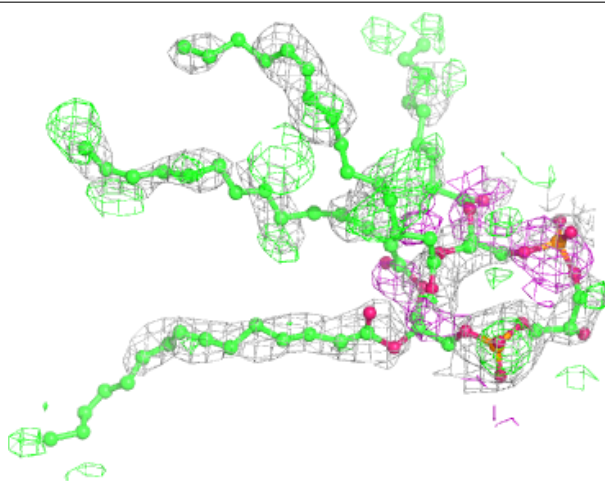
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	L	1292	6/6	0.86	0.18	62,65,66,68	0
13	SPO	M	1313	42/42	0.87	0.17	38,44,62,66	0
8	UQ2	L	1288[B]	23/23	0.90	0.20	36,40,47,47	23
8	UQ2	L	1288[A]	23/23	0.90	0.20	28,38,56,57	23
12	U10	M	1312	48/63	0.90	0.13	36,49,77,78	0
7	BPH	M	1311	65/65	0.93	0.11	30,37,87,89	0
5	BCL	M	1303	66/66	0.95	0.09	28,31,70,71	0
5	BCL	M	1304	66/66	0.96	0.11	27,33,48,55	0
7	BPH	L	1287	65/65	0.97	0.10	27,35,42,45	0
5	BCL	L	1282	66/66	0.97	0.07	28,32,57,60	0
5	BCL	L	1289	66/66	0.97	0.12	28,34,50,56	0
11	FE	M	1310	1/1	0.99	0.02	34,34,34,34	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.

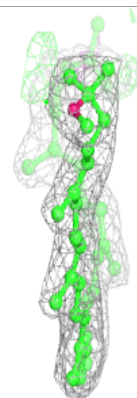
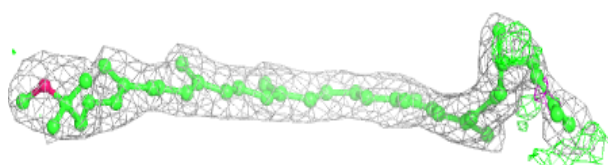
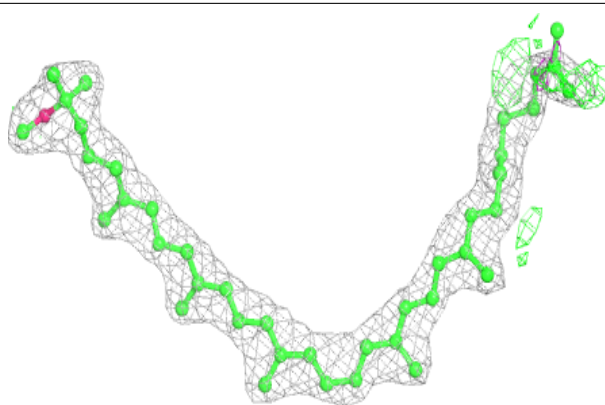
**Electron density around CDL M 1314:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

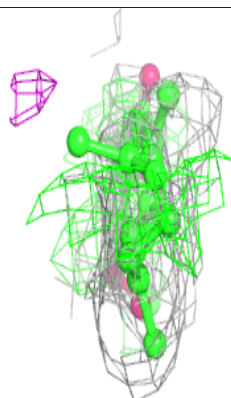
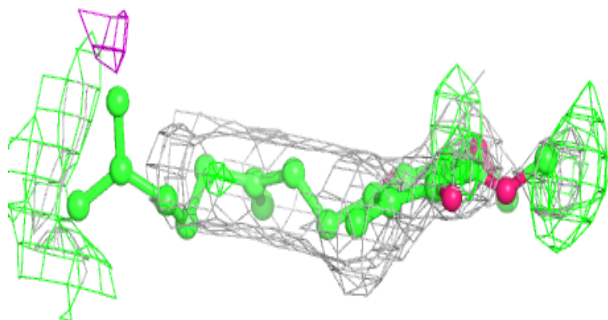
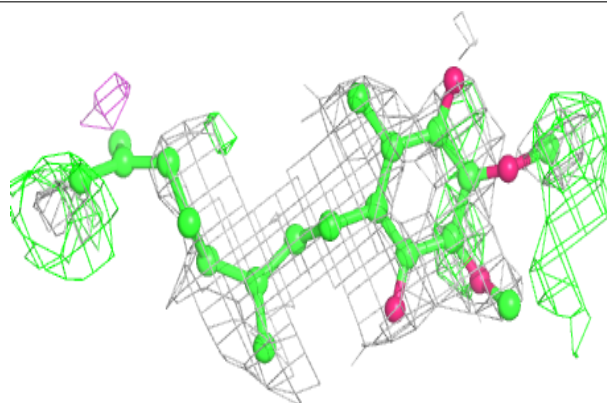


**Electron density around SPO M 1313:**

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

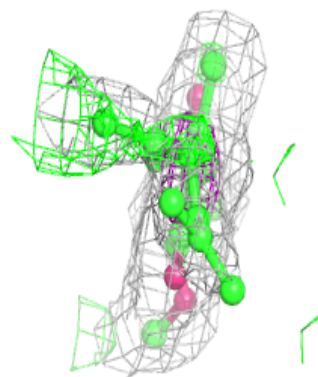
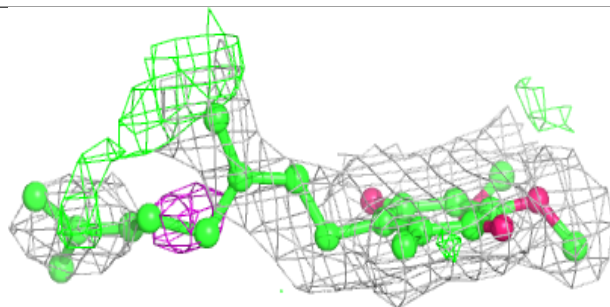
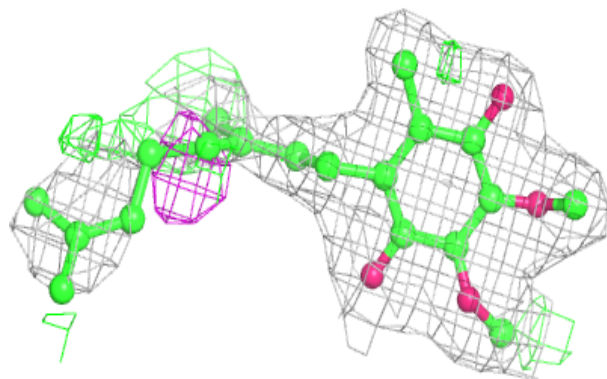
**Electron density around UQ2 L 1288 (B):**

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

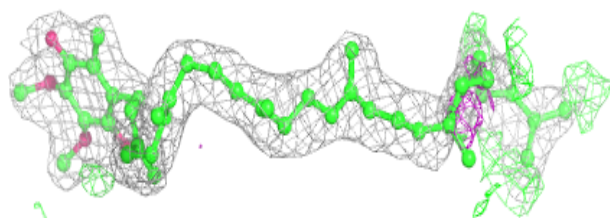
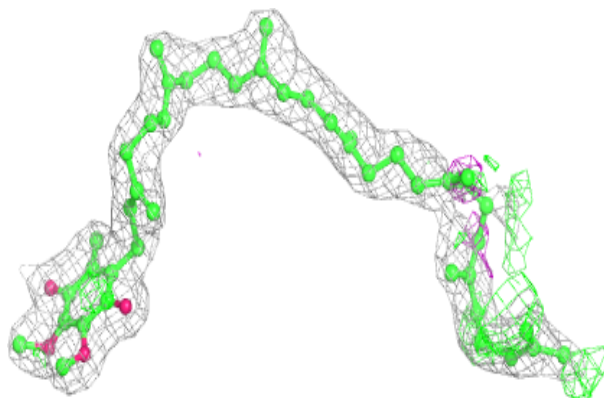


**Electron density around UQ2 L 1288 (A):**

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

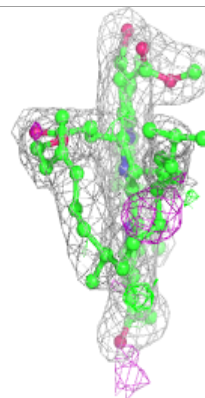
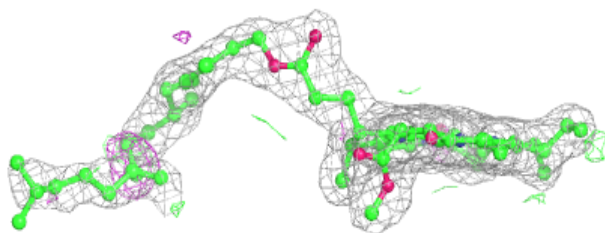
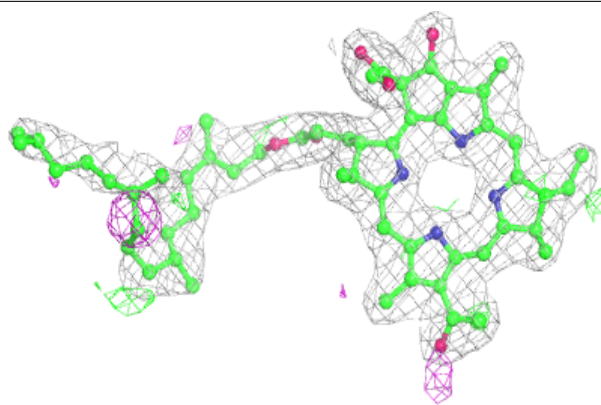
**Electron density around U10 M 1312:**

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



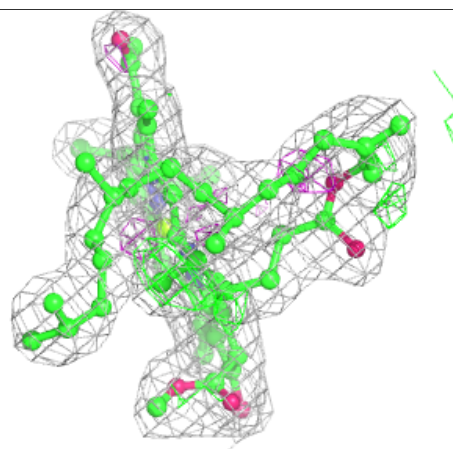
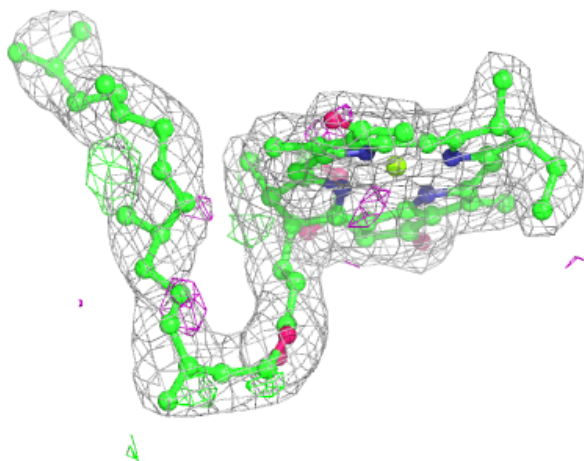
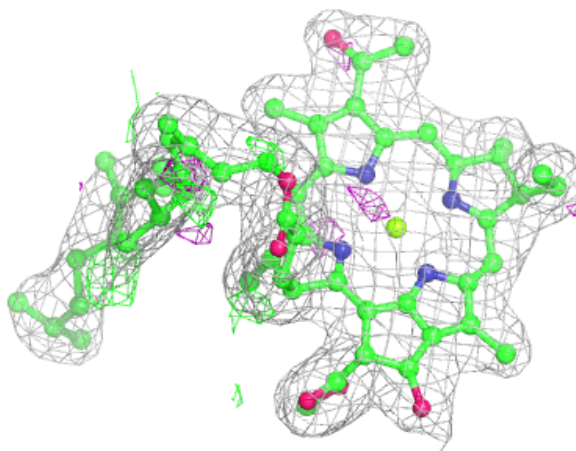
**Electron density around BPH M 1311:**

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



**Electron density around BCL M 1303:**

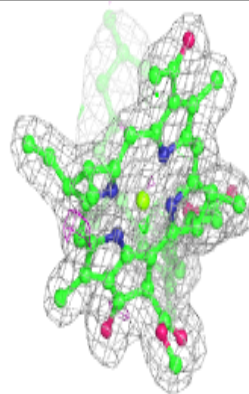
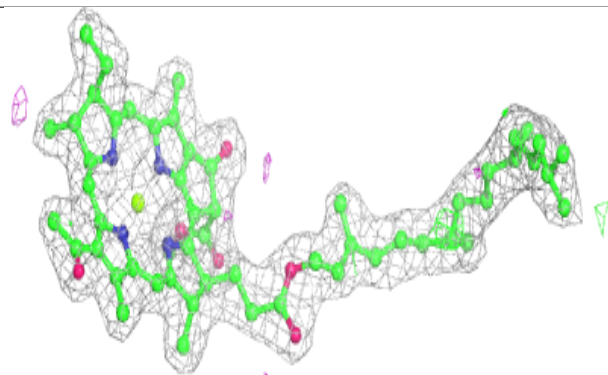
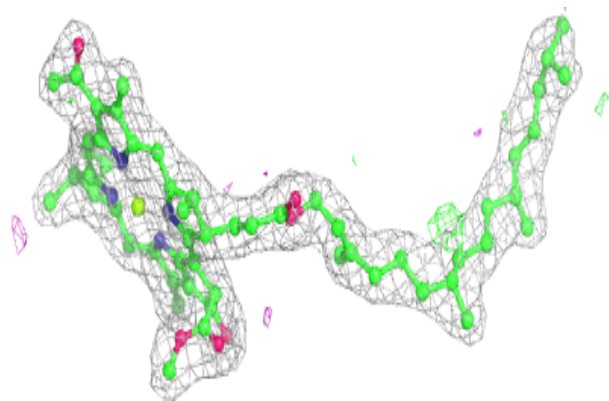
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BCL M 1304:**

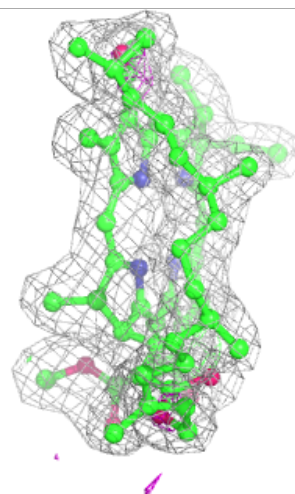
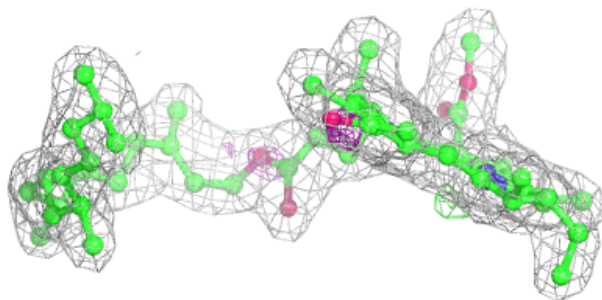
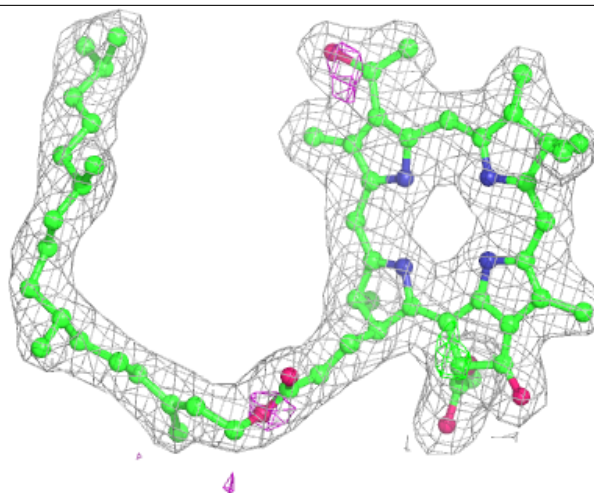
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





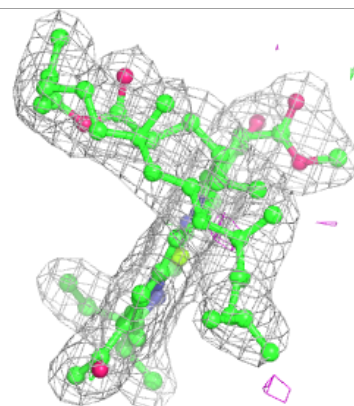
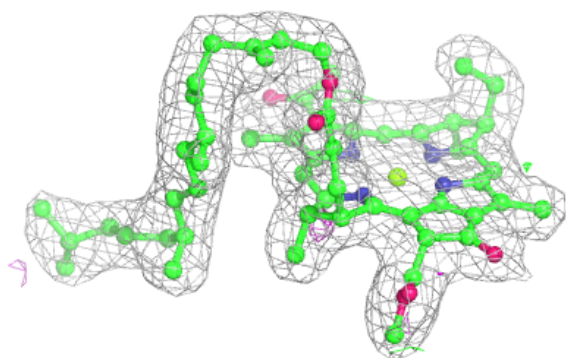
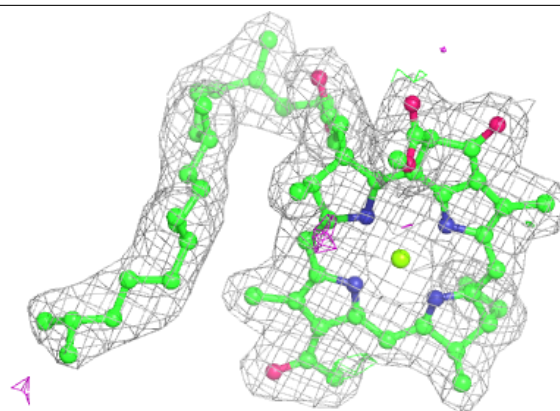
**Electron density around BPH L 1287:**

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

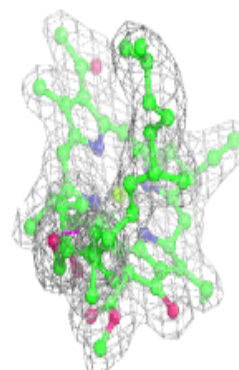
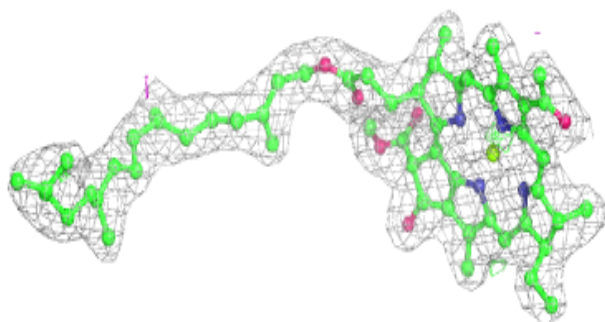
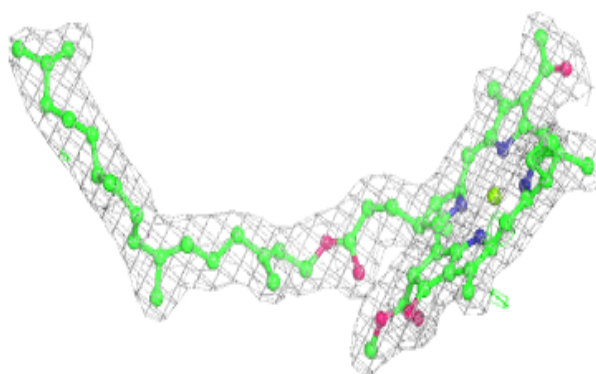


**Electron density around BCL L 1282:**

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

**Electron density around BCL L 1289:**

$2mF_o-DF_c$  (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.