Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2023 – 07:48 am GMT

PDB ID	:	2UXL
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 10 in the neutral state, 2nd dataset
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-28
Resolution	:	2.88 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

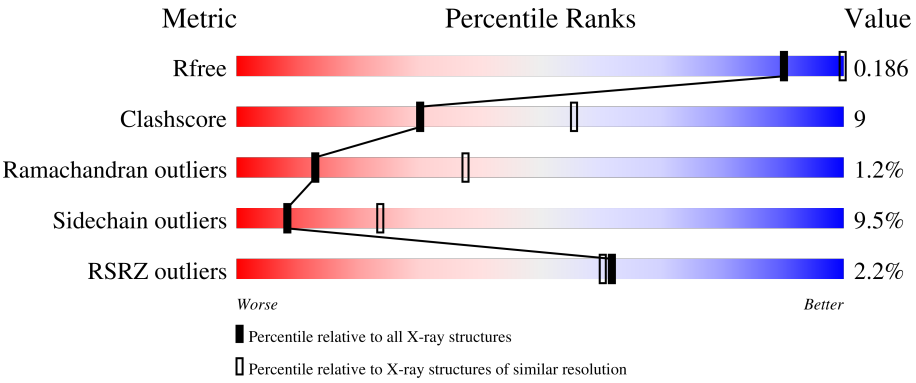
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 70% 19% · 7%
2	L	281	2% 81% 16% ·
3	M	307	3% 75% 20% · ··

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
4	GOL	H	1253	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1285	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
7	UQ2	L	1284[B]	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 7302 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			

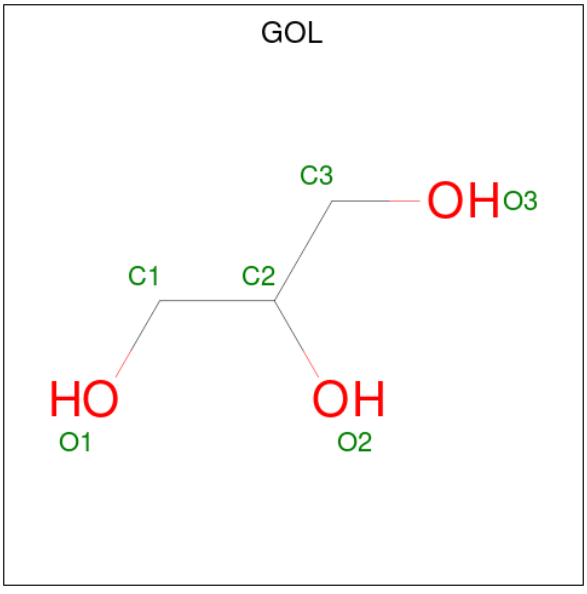
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

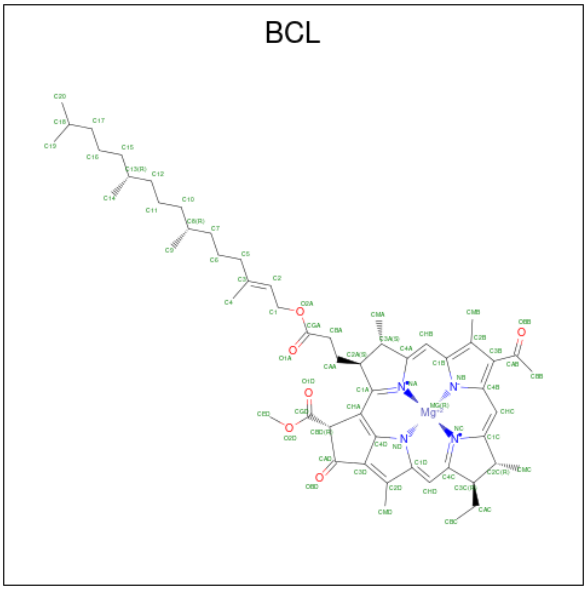
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



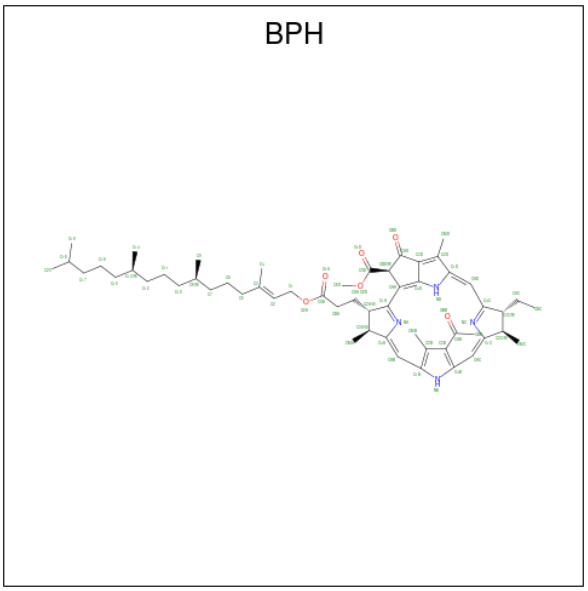
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



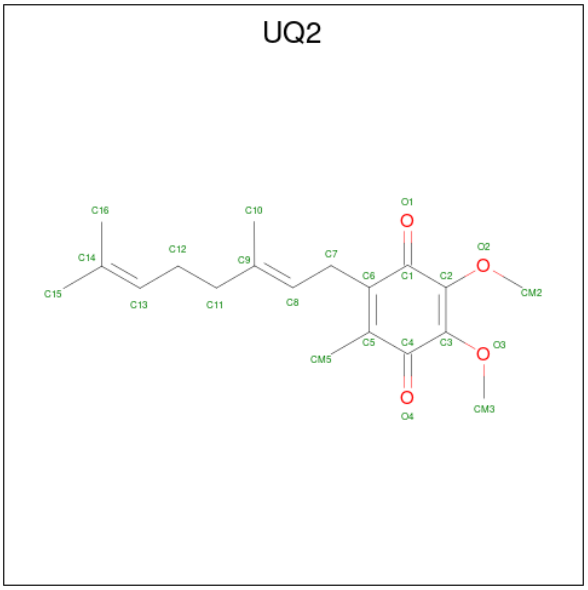
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



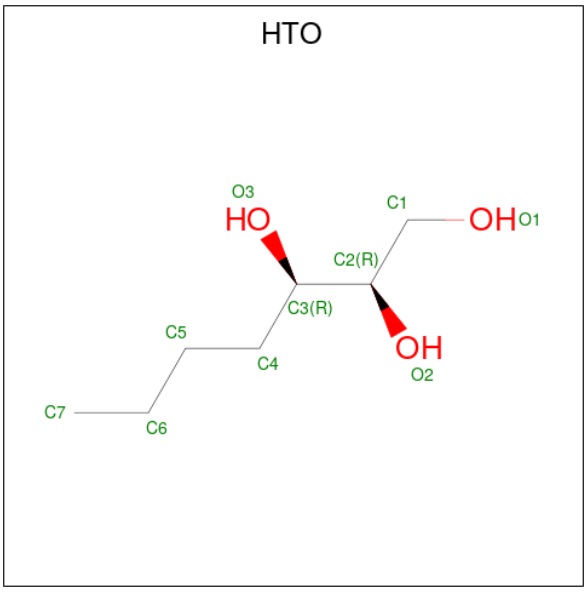
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



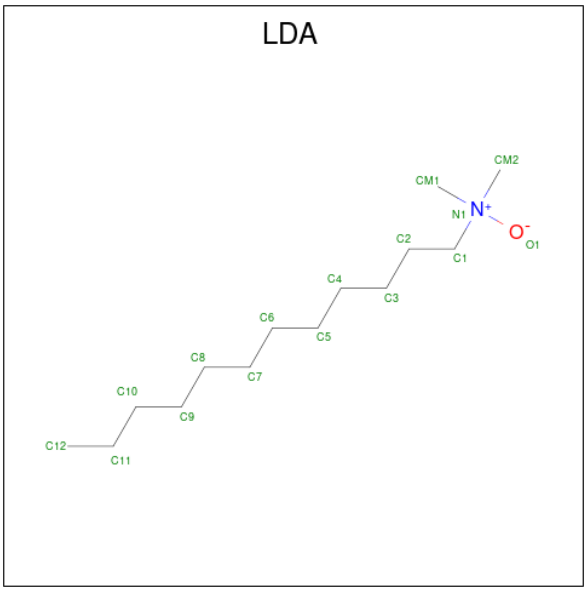
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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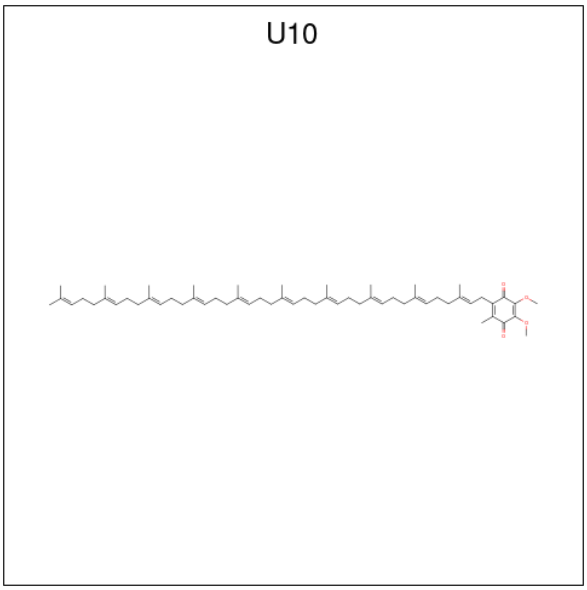
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

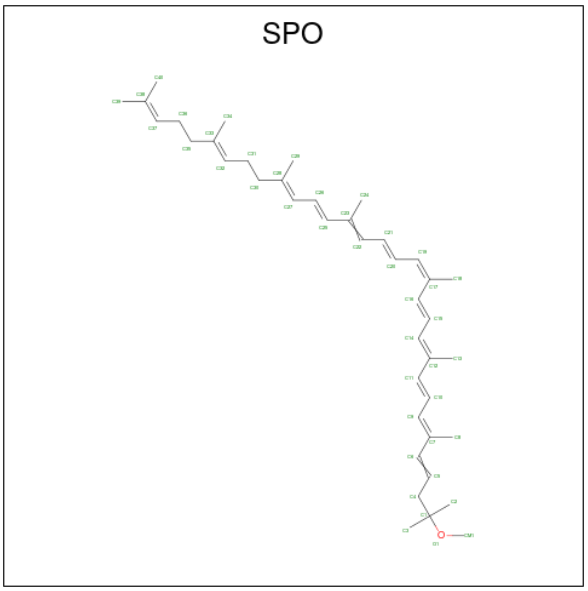
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 13 is water.

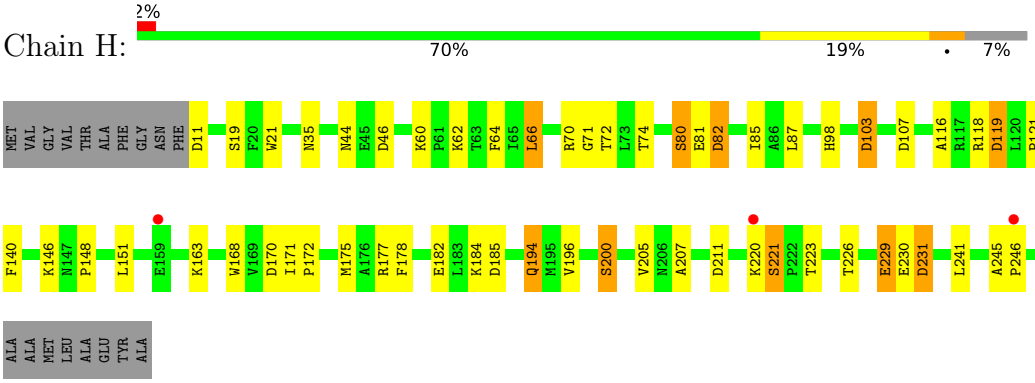
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	76	Total O 76 76	0	0
13	L	68	Total O 68 68	0	0
13	M	58	Total O 58 58	0	0

3 Residue-property plots (i)

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

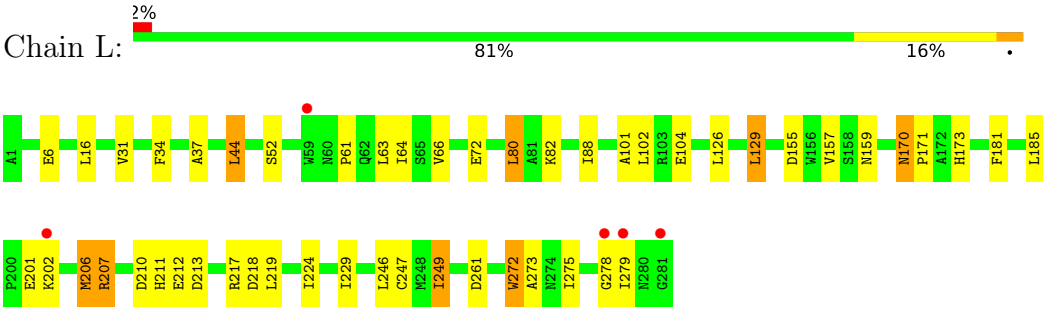
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



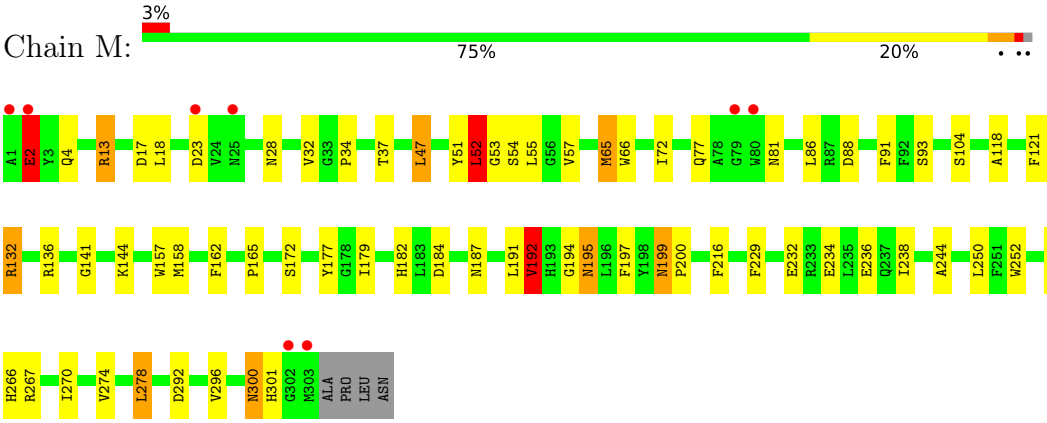
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:



• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.00Å 139.00Å 183.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.88 42.91 – 2.88	Depositor EDS
% Data completeness (in resolution range)	81.2 (119.52-2.88) 77.9 (42.91-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.220 0.179 , 0.186	Depositor DCC
R_{free} test set	1906 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7302	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, GOL, U10, LDA, BCL, HTO, BPH, FE, 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	0.83	2/1906 (0.1%)	0.92	7/2591 (0.3%)
2	L	0.80	0/2320	0.82	4/3175 (0.1%)
3	M	0.78	0/2501	0.81	5/3415 (0.1%)
All	All	0.80	2/6727 (0.0%)	0.85	16/9181 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	122	GLU	CG-CD	5.70	1.60	1.51
1	H	194	GLN	CG-CD	5.07	1.62	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	52	LEU	CA-CB-CG	8.47	134.77	115.30
2	L	261	ASP	CB-CG-OD2	7.19	124.77	118.30
1	H	107	ASP	CB-CG-OD2	5.88	123.59	118.30
3	M	23	ASP	CB-CG-OD2	5.83	123.55	118.30
1	H	103	ASP	CB-CG-OD2	5.79	123.51	118.30
1	H	211	ASP	CB-CG-OD2	5.79	123.51	118.30
2	L	155	ASP	CB-CG-OD2	5.75	123.48	118.30
2	L	218	ASP	CB-CG-OD2	5.74	123.47	118.30
1	H	82	ASP	CB-CG-OD2	5.74	123.47	118.30
1	H	231	ASP	CB-CG-OD2	5.73	123.45	118.30
3	M	184	ASP	CB-CG-OD2	5.71	123.44	118.30
1	H	119	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	185	ASP	CB-CG-OD2	5.23	123.01	118.30
2	L	210	ASP	CB-CG-OD2	5.22	123.00	118.30
3	M	292	ASP	CB-CA-C	-5.16	100.08	110.40
3	M	88	ASP	CB-CG-OD2	5.15	122.94	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	32	0
2	L	2232	0	2187	35	0
3	M	2409	0	2321	41	0
4	H	18	0	24	3	0
4	L	6	0	8	2	0
5	L	132	0	148	3	0
5	M	132	0	148	13	0
6	L	65	0	76	8	0
6	M	65	0	76	11	0
7	L	46	0	52	14	0
8	L	10	0	16	0	0
9	M	48	0	93	3	0
10	M	1	0	0	0	0
11	M	48	0	63	1	0
12	M	42	0	60	1	0
13	H	76	0	0	3	0
13	L	68	0	0	1	0
13	M	58	0	0	2	0
All	All	7302	0	7133	133	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 9.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:1283:BPH:CBB	6:L:1283:BPH:HHC	1.94	0.97
6:M:1309:BPH:CBB	6:M:1309:BPH:HHC	1.94	0.95
5:M:1303:BCL:H91	5:M:1303:BCL:H151	1.53	0.89
7:L:1284[B]:UQ2:C8	7:L:1284[B]:UQ2:H5M1	2.02	0.88
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.55	0.85
6:L:1283:BPH:HHC	6:L:1283:BPH:HBB2	1.60	0.83
2:L:224:ILE:HG22	7:L:1284[B]:UQ2:C8	2.14	0.78
6:M:1309:BPH:HHC	6:M:1309:BPH:HBB3	1.64	0.78
6:M:1309:BPH:HBC3	6:M:1309:BPH:HHD	1.66	0.78
5:M:1303:BCL:HBC1	5:M:1304:BCL:HAA2	1.66	0.77
9:M:1305:LDA:H101	9:M:1306:LDA:H121	1.65	0.77
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.20	0.77
1:H:122:GLU:HG3	3:M:236:GLU:OE1	1.86	0.74
6:L:1283:BPH:CBB	6:L:1283:BPH:CHC	2.67	0.73
6:L:1283:BPH:HHC	6:L:1283:BPH:HBB3	1.70	0.72
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.72	0.71
6:M:1309:BPH:HHC	6:M:1309:BPH:HBB2	1.73	0.69
3:M:194:GLY:O	3:M:195:ASN:HB3	1.93	0.69
2:L:229:ILE:HG12	7:L:1284[B]:UQ2:H5M2	1.75	0.69
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.29	0.68
2:L:170:ASN:HD22	2:L:170:ASN:C	1.98	0.67
9:M:1305:LDA:C10	9:M:1306:LDA:H121	2.26	0.66
6:M:1309:BPH:CBB	6:M:1309:BPH:CHC	2.74	0.65
2:L:212:GLU:HB3	7:L:1284[B]:UQ2:H2M3	1.79	0.65
1:H:80:SER:O	13:H:2025:HOH:O	2.15	0.64
1:H:177:ARG:NH2	3:M:232:GLU:OE2	2.31	0.63
3:M:187:ASN:HD22	5:M:1304:BCL:HBC1	1.65	0.62
2:L:88:ILE:HD11	4:L:1287:GOL:H31	1.83	0.60
2:L:157:VAL:HG21	5:L:1282:BCL:HHD	1.83	0.59
1:H:118[B]:ARG:HH11	1:H:119:ASP:H	1.49	0.59
2:L:278:GLY:HA2	3:M:77:GLN:O	2.03	0.59
6:L:1283:BPH:CHC	6:L:1283:BPH:HBB3	2.32	0.58
1:H:62:LYS:HD2	4:H:1251:GOL:H31	1.84	0.57
1:H:66:LEU:HG	1:H:71:GLY:O	2.03	0.57
5:L:1282:BCL:HBB3	5:L:1285:BCL:H41	1.86	0.57
3:M:77:GLN:HE22	3:M:93:SER:H	1.53	0.57
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.40	0.57
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.87	0.56
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.89	0.55
3:M:199:ASN:HD22	3:M:199:ASN:C	2.09	0.54
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.89	0.54
3:M:53:GLY:O	3:M:57:VAL:HG23	2.07	0.54
1:H:246:PRO:O	1:H:249:LYS:HB2	2.06	0.54
1:H:207:ALA:HA	1:H:241:LEU:HD23	1.90	0.54
5:M:1304:BCL:C2	6:M:1309:BPH:HBB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:101:ALA:O	2:L:104:GLU:HB2	2.10	0.52
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.92	0.52
2:L:212:GLU:CB	7:L:1284[B]:UQ2:H2M3	2.39	0.52
6:M:1309:BPH:HBB3	6:M:1309:BPH:CHC	2.35	0.52
1:H:140:PHE:HA	3:M:13:ARG:O	2.10	0.51
1:H:146:LYS:HE2	1:H:200:SER:O	2.10	0.51
3:M:234:GLU:O	3:M:238:ILE:HG13	2.11	0.51
3:M:296:VAL:O	3:M:300:ASN:ND2	2.44	0.50
2:L:229:ILE:HD13	7:L:1284[B]:UQ2:H111	1.93	0.50
1:H:62:LYS:O	1:H:74:THR:HA	2.12	0.49
5:L:1285:BCL:HMB1	5:L:1285:BCL:HBB3	1.93	0.49
1:H:171:ILE:N	1:H:172:PRO:HD2	2.28	0.49
2:L:189:LEU:HD12	7:L:1284[B]:UQ2:H163	1.94	0.49
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.47	0.49
3:M:270:ILE:O	3:M:274:VAL:HG13	2.13	0.49
3:M:300:ASN:ND2	3:M:300:ASN:N	2.61	0.48
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
1:H:81:GLU:O	1:H:82:ASP:HB2	2.14	0.48
1:H:70:ARG:NH2	1:H:121:PRO:O	2.46	0.48
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.96	0.48
1:H:35:ASN:OD1	3:M:260:ALA:HB1	2.13	0.48
2:L:213:ASP:HB3	2:L:217:ARG:NH1	2.29	0.48
3:M:300:ASN:N	3:M:300:ASN:HD22	2.12	0.47
2:L:80:LEU:HD13	4:L:1287:GOL:H11	1.97	0.47
3:M:192:VAL:O	3:M:192:VAL:HG13	2.15	0.47
6:M:1309:BPH:H2	6:M:1309:BPH:H6C2	1.72	0.47
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.30	0.46
2:L:212:GLU:OE2	7:L:1284[B]:UQ2:O3	2.33	0.46
1:H:21:TRP:CE2	4:H:1253:GOL:H11	2.51	0.46
6:L:1283:BPH:HBC2	6:L:1283:BPH:HHD	1.96	0.46
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.46	0.46
3:M:66:TRP:HD1	3:M:118:ALA:O	1.99	0.46
6:M:1309:BPH:HBC3	6:M:1309:BPH:CHD	2.43	0.46
2:L:34:PHE:HA	2:L:37:ALA:HB3	1.98	0.46
7:L:1284[A]:UQ2:H5M1	7:L:1284[A]:UQ2:H71	1.74	0.46
4:H:1252:GOL:H31	2:L:199:ASN:HA	1.99	0.45
6:L:1283:BPH:HBC2	6:L:1283:BPH:CHD	2.47	0.45
7:L:1284[B]:UQ2:H2M2	7:L:1284[B]:UQ2:O1	2.16	0.45
1:H:44:ASN:HB2	1:H:46:ASP:OD1	2.16	0.45
2:L:170:ASN:HD22	2:L:171:PRO:N	2.14	0.45
3:M:162:PHE:C	3:M:165:PRO:HD2	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1304:BCL:H2	6:M:1309:BPH:HBB3	1.98	0.44
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.99	0.44
2:L:61:PRO:HA	2:L:64:ILE:HD12	1.99	0.44
3:M:2:GLU:H	3:M:4:GLN:HE21	1.65	0.44
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.18	0.44
6:L:1283:BPH:HED3	3:M:252:TRP:CZ3	2.53	0.44
3:M:252:TRP:CD1	11:M:1310:U10:C6	3.00	0.44
1:H:148:PRO:HA	1:H:151:LEU:CD1	2.44	0.43
1:H:194:GLN:NE2	13:H:2062:HOH:O	2.15	0.43
3:M:177:TYR:HD2	12:M:1311:SPO:H19	1.83	0.43
1:H:226:THR:OG1	1:H:229:GLU:HB2	2.18	0.43
1:H:118[B]:ARG:NH1	1:H:119:ASP:H	2.16	0.43
5:M:1303:BCL:HMB1	5:M:1303:BCL:OBB	2.18	0.43
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.53	0.43
3:M:278:LEU:HD23	3:M:278:LEU:HA	1.89	0.43
2:L:229:ILE:HD13	7:L:1284[B]:UQ2:H8	2.01	0.43
2:L:219:LEU:O	3:M:132:ARG:NH1	2.52	0.42
2:L:44:LEU:HD23	2:L:44:LEU:HA	1.95	0.42
2:L:207:ARG:HG3	2:L:211:HIS:CD2	2.54	0.42
7:L:1284[B]:UQ2:H122	7:L:1284[B]:UQ2:H101	1.77	0.42
5:M:1303:BCL:H13	5:M:1303:BCL:H102	1.74	0.42
1:H:249:LYS:N	13:H:2076:HOH:O	2.52	0.42
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.97	0.42
2:L:129:LEU:HD12	2:L:129:LEU:HA	1.82	0.42
2:L:201:GLU:OE2	3:M:141:GLY:HA2	2.19	0.42
3:M:66:TRP:CZ2	3:M:122:MET:CE	3.03	0.42
5:M:1303:BCL:H141	5:M:1303:BCL:H162	1.75	0.42
2:L:159:ASN:HD22	2:L:159:ASN:HA	1.70	0.42
3:M:199:ASN:HA	3:M:200:PRO:HD2	1.95	0.42
9:M:1307:LDA:HM13	13:M:2013:HOH:O	2.19	0.42
7:L:1284[B]:UQ2:H5M1	7:L:1284[B]:UQ2:H8	1.96	0.41
2:L:170:ASN:C	2:L:170:ASN:ND2	2.70	0.41
2:L:249:ILE:HD13	2:L:249:ILE:HA	1.87	0.41
1:H:175:MET:HE3	13:M:2005:HOH:O	2.20	0.41
2:L:170:ASN:HB3	2:L:173:HIS:CB	2.50	0.41
2:L:170:ASN:HA	2:L:171:PRO:HD2	1.91	0.41
1:H:220[B]:LYS:NZ	1:H:221:SER:HB3	2.35	0.41
2:L:279:ILE:HG21	3:M:91:PHE:HB3	2.03	0.41
13:L:2058:HOH:O	3:M:136:ARG:HD3	2.21	0.41
3:M:234:GLU:OE2	3:M:266:HIS:HE1	2.02	0.41
2:L:224:ILE:HG22	7:L:1284[B]:UQ2:H8	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:55:LEU:HD22	3:M:128:SER:HB2	2.03	0.40
2:L:181:PHE:CD2	6:M:1309:BPH:HBB1	2.55	0.40
3:M:34:PRO:O	3:M:47:LEU:HB2	2.20	0.40
2:L:6:GLU:HA	3:M:250:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	242/260 (93%)	226 (93%)	14 (6%)	2 (1%)	19 48
2	L	279/281 (99%)	265 (95%)	11 (4%)	3 (1%)	14 40
3	M	301/307 (98%)	277 (92%)	19 (6%)	5 (2%)	9 28
All	All	822/848 (97%)	768 (93%)	44 (5%)	10 (1%)	13 38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	2	GLU
3	M	52	LEU
1	H	116	ALA
2	L	273	ALA
1	H	245	ALA
2	L	206	MET
2	L	31	VAL
3	M	195	ASN
3	M	179	ILE
3	M	192	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	198/208 (95%)	182 (92%)	16 (8%)	11 31
2	L	220/220 (100%)	200 (91%)	20 (9%)	9 26
3	M	236/240 (98%)	210 (89%)	26 (11%)	6 17
All	All	654/668 (98%)	592 (90%)	62 (10%)	8 24

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	19	SER
1	H	60	LYS
1	H	66	LEU
1	H	72	THR
1	H	80	SER
1	H	103	ASP
1	H	163	LYS
1	H	182	GLU
1	H	184	LYS
1	H	200	SER
1	H	221	SER
1	H	223	THR
1	H	229	GLU
1	H	230	GLU
1	H	231	ASP
2	L	16	LEU
2	L	44	LEU
2	L	52	SER
2	L	63	LEU
2	L	66	VAL
2	L	72	GLU
2	L	80	LEU
2	L	82	LYS
2	L	102	LEU
2	L	126	LEU

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Mol	Chain	Res	Type
2	L	129	LEU
2	L	170	ASN
2	L	185	LEU
2	L	202	LYS
2	L	206	MET
2	L	207	ARG
2	L	246	LEU
2	L	247	CYS
2	L	249	ILE
2	L	272	TRP
3	M	2	GLU
3	M	13	ARG
3	M	17	ASP
3	M	18	LEU
3	M	32	VAL
3	M	37	THR
3	M	47	LEU
3	M	52	LEU
3	M	54	SER
3	M	65	MET
3	M	72	ILE
3	M	86	LEU
3	M	104	SER
3	M	132	ARG
3	M	144	LYS
3	M	172	SER
3	M	182	HIS
3	M	191	LEU
3	M	192	VAL
3	M	199	ASN
3	M	216	PHE
3	M	258	PHE
3	M	267	ARG
3	M	278	LEU
3	M	300	ASN
3	M	301	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	62	GLN

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Mol	Chain	Res	Type
2	L	159	ASN
2	L	170	ASN
2	L	264	GLN
3	M	4	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN
3	M	300	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\#\|Z\| > 2$
11	U10	M	1310	-	48,48,63	2.76	13 (27%)	58,61,79	1.70	11 (18%)
5	BCL	M	1304	3	64,74,74	2.02	10 (15%)	78,115,115	2.36	21 (26%)
8	HTO	L	1286	-	9,9,9	0.93	1 (11%)	10,10,10	1.36	2 (20%)
6	BPH	L	1283	-	51,70,70	2.99	7 (13%)	52,101,101	2.11	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	UQ2	L	1284[B]	-	23,23,23	2.67	8 (34%)	28,31,31	1.46	4 (14%)
5	BCL	M	1303	3	64,74,74	2.18	12 (18%)	78,115,115	2.46	26 (33%)
9	LDA	M	1305	-	12,15,15	2.08	1 (8%)	14,17,17	0.73	1 (7%)
4	GOL	H	1252	-	5,5,5	0.27	0	5,5,5	0.57	0
6	BPH	M	1309	-	51,70,70	2.80	8 (15%)	52,101,101	2.45	16 (30%)
4	GOL	L	1287	-	5,5,5	0.40	0	5,5,5	0.45	0
5	BCL	L	1285	2	64,74,74	1.98	13 (20%)	78,115,115	2.78	26 (33%)
7	UQ2	L	1284[A]	-	23,23,23	2.86	8 (34%)	28,31,31	1.49	5 (17%)
9	LDA	M	1306	-	12,15,15	1.91	1 (8%)	14,17,17	0.69	0
4	GOL	H	1253	-	5,5,5	0.39	0	5,5,5	0.40	0
12	SPO	M	1311	-	40,41,41	4.26	12 (30%)	47,50,50	1.96	10 (21%)
5	BCL	L	1282	2	64,74,74	2.09	10 (15%)	78,115,115	2.53	24 (30%)
9	LDA	M	1307	-	12,15,15	2.08	1 (8%)	14,17,17	0.60	0
4	GOL	H	1251	-	5,5,5	0.59	0	5,5,5	0.70	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
11	U10	M	1310	-	-	19/45/69/87	0/1/1/1
5	BCL	M	1304	3	2/2/21/25	12/37/137/137	-
8	HTO	L	1286	-	-	4/10/10/10	-
6	BPH	L	1283	-	-	13/37/105/105	0/5/6/6
7	UQ2	L	1284[B]	-	-	10/15/39/39	0/1/1/1
5	BCL	M	1303	3	2/2/21/25	14/37/137/137	-
9	LDA	M	1305	-	-	5/13/13/13	-
4	GOL	H	1252	-	-	2/4/4/4	-
6	BPH	M	1309	-	-	15/37/105/105	0/5/6/6
4	GOL	L	1287	-	-	2/4/4/4	-
5	BCL	L	1285	2	2/2/21/25	8/37/137/137	-
7	UQ2	L	1284[A]	-	-	7/15/39/39	0/1/1/1
9	LDA	M	1306	-	-	6/13/13/13	-
4	GOL	H	1253	-	-	0/4/4/4	-
12	SPO	M	1311	-	-	17/47/47/47	-
5	BCL	L	1282	2	2/2/21/25	14/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LDA	M	1307	-	-	5/13/13/13	-
4	GOL	H	1251	-	-	2/4/4/4	-

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1283	BPH	OBD-CAD	14.23	1.42	1.22
12	M	1311	SPO	C27-C28	13.79	1.48	1.34
6	M	1309	BPH	OBD-CAD	11.77	1.38	1.22
5	L	1282	BCL	OBD-CAD	11.56	1.42	1.22
5	M	1303	BCL	OBD-CAD	10.67	1.40	1.22
5	M	1304	BCL	OBD-CAD	10.57	1.40	1.22
5	L	1285	BCL	OBD-CAD	9.54	1.38	1.22
12	M	1311	SPO	C14-C12	9.31	1.48	1.35
12	M	1311	SPO	C22-C23	9.20	1.48	1.35
12	M	1311	SPO	C9-C7	8.96	1.47	1.35
12	M	1311	SPO	C19-C17	8.21	1.46	1.35
6	L	1283	BPH	O1D-CGD	8.20	1.41	1.21
6	M	1309	BPH	O1D-CGD	8.14	1.41	1.21
9	M	1307	LDA	O1-N1	-7.06	1.25	1.42
7	L	1284[A]	UQ2	C8-C9	7.03	1.49	1.33
9	M	1305	LDA	O1-N1	-6.88	1.26	1.42
11	M	1310	U10	C33-C34	6.86	1.49	1.33
7	L	1284[B]	UQ2	C8-C9	6.69	1.49	1.33
11	M	1310	U10	C28-C29	6.69	1.49	1.33
12	M	1311	SPO	C32-C33	6.62	1.48	1.33
6	M	1309	BPH	C3D-C2D	6.58	1.51	1.39
6	M	1309	BPH	O1A-CGA	6.52	1.41	1.22
9	M	1306	LDA	O1-N1	-6.52	1.26	1.42
11	M	1310	U10	C13-C14	6.45	1.48	1.33
6	L	1283	BPH	O1A-CGA	6.44	1.41	1.22
11	M	1310	U10	C38-C39	6.41	1.50	1.32
6	L	1283	BPH	C2-C3	6.31	1.48	1.33
5	L	1282	BCL	O1A-CGA	6.31	1.41	1.22
11	M	1310	U10	C18-C19	6.15	1.47	1.33
6	M	1309	BPH	OBB-CAB	6.15	1.41	1.22
5	M	1303	BCL	O1A-CGA	6.02	1.40	1.22
6	L	1283	BPH	OBB-CAB	6.01	1.41	1.22
7	L	1284[A]	UQ2	C13-C14	5.96	1.49	1.32
11	M	1310	U10	C23-C24	5.93	1.47	1.33
11	M	1310	U10	C8-C9	5.88	1.47	1.33
6	M	1309	BPH	C2-C3	5.85	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1285	BCL	O1A-CGA	5.82	1.39	1.22
12	M	1311	SPO	C6-C5	5.82	1.47	1.32
6	L	1283	BPH	C3D-C2D	5.81	1.49	1.39
12	M	1311	SPO	C37-C38	5.79	1.49	1.32
7	L	1284[B]	UQ2	C13-C14	5.77	1.48	1.32
5	M	1304	BCL	O1A-CGA	5.76	1.39	1.22
7	L	1284[A]	UQ2	O3-C3	-5.30	1.23	1.36
12	M	1311	SPO	C26-C25	5.03	1.47	1.34
12	M	1311	SPO	C10-C11	5.02	1.47	1.34
5	M	1303	BCL	C4D-ND	-5.00	1.30	1.37
11	M	1310	U10	O3-C3	-4.73	1.25	1.36
7	L	1284[B]	UQ2	O2-C2	-4.72	1.25	1.36
7	L	1284[A]	UQ2	O2-C2	-4.66	1.25	1.36
5	M	1303	BCL	C4B-NB	4.62	1.39	1.35
12	M	1311	SPO	C15-C16	4.57	1.46	1.34
5	L	1282	BCL	C1B-NB	4.55	1.39	1.35
5	M	1304	BCL	C3D-C4D	-4.55	1.33	1.44
7	L	1284[B]	UQ2	O3-C3	-4.54	1.25	1.36
5	M	1304	BCL	C4D-ND	-4.36	1.31	1.37
12	M	1311	SPO	C21-C20	4.26	1.47	1.36
5	M	1303	BCL	C3D-C4D	-4.22	1.34	1.44
11	M	1310	U10	O4-C4	-4.20	1.26	1.36
5	L	1285	BCL	C3D-C4D	-3.94	1.35	1.44
5	M	1303	BCL	C1B-NB	3.93	1.38	1.35
5	M	1303	BCL	C2-C3	3.83	1.42	1.33
6	M	1309	BPH	O2D-CGD	-3.80	1.23	1.33
7	L	1284[A]	UQ2	C6-C5	3.79	1.42	1.35
5	L	1285	BCL	C2-C3	3.78	1.42	1.33
5	L	1282	BCL	C3D-C4D	-3.77	1.35	1.44
5	L	1285	BCL	C1B-NB	3.63	1.38	1.35
7	L	1284[B]	UQ2	C6-C5	3.35	1.41	1.35
5	M	1303	BCL	O2D-CGD	-3.30	1.25	1.33
5	L	1282	BCL	C2-C3	3.27	1.40	1.33
5	L	1285	BCL	C4D-ND	-3.24	1.33	1.37
5	L	1285	BCL	CHD-C4C	3.22	1.48	1.39
5	L	1285	BCL	C1D-ND	3.10	1.41	1.37
5	L	1282	BCL	C4D-ND	-3.09	1.33	1.37
5	M	1304	BCL	C4B-NB	3.02	1.37	1.35
6	L	1283	BPH	O2D-CGD	-2.95	1.26	1.33
5	L	1285	BCL	C1D-C2D	-2.79	1.39	1.45
5	M	1304	BCL	CHD-C4C	2.76	1.47	1.39
5	L	1285	BCL	C4B-NB	2.76	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1303	BCL	C1D-C2D	-2.75	1.39	1.45
11	M	1310	U10	C6-C1	2.70	1.40	1.35
5	M	1304	BCL	C2-C3	2.69	1.39	1.33
7	L	1284[A]	UQ2	C3-C4	-2.65	1.41	1.48
5	L	1282	BCL	CHD-C4C	2.64	1.46	1.39
5	M	1304	BCL	C1B-NB	2.60	1.37	1.35
5	L	1282	BCL	C4B-NB	2.59	1.37	1.35
7	L	1284[B]	UQ2	C3-C4	-2.57	1.41	1.48
6	M	1309	BPH	O2A-CGA	-2.56	1.25	1.33
5	L	1282	BCL	O2D-CGD	-2.52	1.27	1.33
5	L	1285	BCL	O2A-CGA	-2.51	1.26	1.33
5	M	1304	BCL	O2D-CGD	-2.46	1.27	1.33
11	M	1310	U10	C4-C5	-2.46	1.41	1.48
7	L	1284[A]	UQ2	C2-C1	-2.44	1.41	1.48
5	M	1304	BCL	O2A-CGA	-2.44	1.26	1.33
8	L	1286	HTO	C4-C3	2.29	1.56	1.52
7	L	1284[B]	UQ2	C2-C1	-2.28	1.42	1.48
5	L	1285	BCL	O1D-CGD	2.25	1.26	1.21
5	M	1303	BCL	C3C-C4C	-2.25	1.48	1.51
7	L	1284[A]	UQ2	C7-C6	2.25	1.55	1.51
5	L	1285	BCL	O2D-CGD	-2.24	1.27	1.33
11	M	1310	U10	C6-C5	-2.23	1.40	1.46
5	L	1282	BCL	O2A-CGA	-2.18	1.26	1.33
11	M	1310	U10	C3-C2	-2.18	1.42	1.48
7	L	1284[B]	UQ2	C5-C4	-2.15	1.39	1.47
5	M	1303	BCL	CHD-C4C	2.10	1.45	1.39
5	M	1303	BCL	MG-ND	-2.03	2.01	2.05

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1285	BCL	C1D-ND-C4D	10.52	113.81	106.33
5	L	1285	BCL	C2D-C1D-ND	-10.22	102.57	110.10
6	M	1309	BPH	O2D-CGD-CBD	9.03	122.44	111.00
6	M	1309	BPH	OBD-CAD-CBD	-8.41	113.48	125.82
5	M	1304	BCL	C2D-C1D-ND	-8.21	104.06	110.10
5	M	1303	BCL	C1D-ND-C4D	7.50	111.66	106.33
5	M	1304	BCL	C1D-ND-C4D	7.00	111.31	106.33
5	L	1285	BCL	CMB-C2B-C1B	-6.95	117.78	128.46
5	L	1282	BCL	CMB-C2B-C1B	-6.82	117.98	128.46
5	L	1282	BCL	O2D-CGD-CBD	6.69	123.15	111.27
5	M	1303	BCL	C2D-C1D-ND	-6.68	105.18	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BCL	CMB-C2B-C1B	-6.63	118.27	128.46
5	L	1285	BCL	CHD-C1D-ND	-6.51	118.47	124.45
5	L	1282	BCL	C4A-NA-C1A	6.42	109.59	106.71
5	M	1303	BCL	C1C-NC-C4C	-6.36	103.85	106.71
5	L	1282	BCL	C4B-CHC-C1C	-6.34	117.57	130.12
5	M	1303	BCL	O2D-CGD-CBD	6.13	122.17	111.27
6	L	1283	BPH	O2D-CGD-CBD	6.07	118.68	111.00
5	L	1282	BCL	C2D-C1D-ND	-6.01	105.68	110.10
5	M	1303	BCL	CMB-C2B-C1B	-5.88	119.43	128.46
5	L	1285	BCL	CHB-C4A-NA	-5.69	116.64	124.51
5	M	1304	BCL	CMD-C2D-C1D	5.36	134.15	124.71
12	M	1311	SPO	C21-C22-C23	-5.27	119.79	127.31
6	L	1283	BPH	C1C-C2C-C3C	-5.14	97.95	102.84
5	M	1303	BCL	CHD-C1D-ND	-5.11	119.75	124.45
6	M	1309	BPH	O2D-CGD-O1D	-5.10	113.87	123.84
5	M	1303	BCL	C1-O2A-CGA	4.95	129.43	116.44
5	L	1282	BCL	CHD-C4C-NC	-4.91	119.62	125.08
5	M	1304	BCL	CMB-C2B-C3B	4.86	133.78	124.68
12	M	1311	SPO	C20-C19-C17	-4.80	120.46	127.31
5	M	1304	BCL	C4B-CHC-C1C	-4.75	120.72	130.12
5	M	1303	BCL	C4A-NA-C1A	4.68	108.81	106.71
5	L	1285	BCL	CMB-C2B-C3B	4.66	133.40	124.68
12	M	1311	SPO	C10-C9-C7	-4.61	120.74	127.31
5	L	1282	BCL	CHD-C1D-ND	-4.59	120.23	124.45
5	M	1303	BCL	C4B-CHC-C1C	-4.59	121.03	130.12
5	L	1282	BCL	CMD-C2D-C1D	4.57	132.76	124.71
5	L	1285	BCL	CED-O2D-CGD	4.53	126.17	115.94
12	M	1311	SPO	C15-C14-C12	-4.51	120.87	127.31
5	L	1282	BCL	C1D-ND-C4D	4.50	109.53	106.33
6	M	1309	BPH	CMA-C3A-C4A	-4.48	104.56	114.38
6	L	1283	BPH	CMD-C2D-C3D	-4.43	116.38	124.68
11	M	1310	U10	C32-C33-C34	-4.37	117.15	127.66
5	L	1282	BCL	CMB-C2B-C3B	4.36	132.84	124.68
11	M	1310	U10	C10-C9-C11	4.19	122.32	115.27
5	L	1285	BCL	C4B-CHC-C1C	-4.18	121.84	130.12
5	L	1282	BCL	C1C-NC-C4C	4.03	108.52	106.71
5	L	1285	BCL	CMD-C2D-C1D	4.03	131.81	124.71
5	L	1282	BCL	C1D-CHD-C4C	-4.00	116.98	126.62
5	M	1304	BCL	O2D-CGD-CBD	3.95	118.29	111.27
6	L	1283	BPH	C4-C3-C5	3.90	121.84	115.27
11	M	1310	U10	C25-C24-C26	3.90	121.83	115.27
6	L	1283	BPH	C1-C2-C3	-3.87	119.35	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1283	BPH	CED-O2D-CGD	3.82	124.58	115.94
5	L	1285	BCL	O2A-CGA-CBA	3.79	123.80	111.91
6	M	1309	BPH	C1-C2-C3	-3.74	119.58	126.04
5	M	1304	BCL	CMD-C2D-C3D	-3.73	119.02	127.61
7	L	1284[A]	UQ2	C6-C5-C4	3.67	122.08	119.18
6	M	1309	BPH	CMD-C2D-C3D	-3.59	117.97	124.68
11	M	1310	U10	C30-C29-C31	3.56	121.25	115.27
5	M	1304	BCL	C1D-CHD-C4C	-3.53	118.10	126.62
5	M	1303	BCL	CMD-C2D-C1D	3.53	130.93	124.71
11	M	1310	U10	C17-C18-C19	-3.52	119.18	127.66
6	L	1283	BPH	CMC-C2C-C1C	-3.50	106.70	114.38
5	L	1285	BCL	CHA-C1A-NA	-3.50	118.38	126.40
5	L	1282	BCL	C1B-CHB-C4A	-3.48	123.23	130.12
6	M	1309	BPH	CAC-C3C-C2C	-3.41	105.74	114.26
6	M	1309	BPH	C1A-C2A-C3A	-3.40	99.60	102.84
5	M	1304	BCL	O2A-CGA-CBA	3.40	122.58	111.91
6	L	1283	BPH	O1D-CGD-CBD	-3.34	119.18	124.74
6	L	1283	BPH	OBD-CAD-CBD	-3.34	120.92	125.82
5	L	1282	BCL	CHC-C1C-NC	-3.33	119.90	124.51
5	L	1285	BCL	CMD-C2D-C3D	-3.25	120.13	127.61
5	L	1285	BCL	C1B-CHB-C4A	-3.25	123.68	130.12
5	M	1303	BCL	CMB-C2B-C3B	3.24	130.74	124.68
11	M	1310	U10	C22-C23-C24	-3.24	119.87	127.66
5	M	1304	BCL	C4-C3-C5	3.22	120.69	115.27
5	M	1304	BCL	CHD-C4C-NC	-3.19	121.53	125.08
5	M	1303	BCL	C2A-C3A-C4A	3.19	107.02	101.87
5	M	1303	BCL	O1D-CGD-CBD	-3.19	117.96	124.48
5	L	1282	BCL	O2D-CGD-O1D	-3.16	117.66	123.84
5	M	1303	BCL	CHA-C1A-NA	-3.15	119.19	126.40
5	L	1285	BCL	O2D-CGD-CBD	3.14	116.86	111.27
5	L	1282	BCL	CMD-C2D-C3D	-3.13	120.41	127.61
5	L	1285	BCL	C1D-CHD-C4C	-3.08	119.19	126.62
5	M	1304	BCL	C1B-CHB-C4A	-3.04	124.09	130.12
12	M	1311	SPO	C29-C28-C30	3.01	120.33	115.27
6	M	1309	BPH	C1C-C2C-C3C	-2.99	99.99	102.84
7	L	1284[B]	UQ2	C10-C9-C11	2.98	120.28	115.27
5	M	1303	BCL	C1D-CHD-C4C	-2.97	119.45	126.62
8	L	1286	HTO	O3-C3-C4	2.97	115.62	109.15
5	L	1285	BCL	C1-O2A-CGA	2.96	124.21	116.44
5	M	1303	BCL	O2A-CGA-CBA	2.95	121.18	111.91
8	L	1286	HTO	C5-C4-C3	2.95	119.02	114.18
5	M	1303	BCL	CHB-C4A-NA	-2.94	120.44	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1282	BCL	C1-O2A-CGA	2.88	123.99	116.44
5	L	1285	BCL	CHA-C4D-ND	2.86	138.48	132.50
5	M	1303	BCL	C1B-CHB-C4A	-2.84	124.50	130.12
5	M	1304	BCL	CHA-C1A-NA	-2.82	119.94	126.40
5	M	1304	BCL	CHB-C4A-NA	-2.80	120.63	124.51
5	M	1304	BCL	C1-O2A-CGA	2.80	123.80	116.44
11	M	1310	U10	C1M-C1-C6	-2.77	119.89	124.40
6	L	1283	BPH	O2A-CGA-CBA	2.77	120.59	111.91
5	L	1282	BCL	C11-C10-C8	-2.75	107.02	115.92
5	M	1304	BCL	C3C-C4C-CHD	-2.72	117.59	123.39
7	L	1284[B]	UQ2	CM2-O2-C2	2.71	126.07	116.47
7	L	1284[A]	UQ2	C7-C6-C1	2.70	121.73	118.48
12	M	1311	SPO	C18-C17-C19	-2.70	119.14	122.92
5	L	1285	BCL	C3D-C4D-ND	-2.70	105.87	110.24
7	L	1284[B]	UQ2	C6-C5-C4	2.68	121.30	119.18
6	L	1283	BPH	C4B-NB-C1B	-2.68	101.59	107.09
12	M	1311	SPO	C8-C7-C9	-2.66	119.19	122.92
5	L	1285	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
5	L	1282	BCL	CHA-C1A-NA	-2.64	120.34	126.40
5	L	1282	BCL	C2A-C3A-C4A	2.64	106.13	101.87
5	M	1303	BCL	O2A-C1-C2	2.61	115.50	108.64
6	M	1309	BPH	C1-O2A-CGA	2.60	123.28	116.44
5	L	1282	BCL	C4-C3-C5	2.59	119.62	115.27
5	L	1282	BCL	O1D-CGD-CBD	-2.59	119.19	124.48
5	M	1303	BCL	CAA-C2A-C3A	-2.57	105.73	112.78
6	M	1309	BPH	C4-C3-C5	2.52	119.50	115.27
5	M	1303	BCL	OBB-CAB-C3B	-2.49	115.58	119.99
5	M	1303	BCL	CHC-C1C-NC	-2.48	121.08	124.51
5	L	1282	BCL	CMA-C3A-C4A	-2.46	105.16	111.77
5	L	1285	BCL	O2D-CGD-O1D	-2.45	119.05	123.84
5	L	1285	BCL	CHC-C1C-NC	-2.45	121.13	124.51
6	L	1283	BPH	C1A-C2A-C3A	-2.44	100.52	102.84
7	L	1284[B]	UQ2	CM3-O3-C3	2.44	125.11	116.47
7	L	1284[A]	UQ2	C5-C6-C1	-2.40	117.32	119.58
5	M	1304	BCL	O2A-CGA-O1A	-2.39	117.56	123.59
5	L	1285	BCL	O2A-CGA-O1A	-2.38	117.60	123.59
6	M	1309	BPH	O2A-CGA-CBA	2.36	119.31	111.91
5	M	1304	BCL	CHD-C1D-ND	-2.36	122.29	124.45
5	M	1303	BCL	C3C-C4C-CHD	-2.36	118.36	123.39
12	M	1311	SPO	C40-C38-C39	2.35	119.79	114.60
11	M	1310	U10	C27-C28-C29	-2.35	122.01	127.66
11	M	1310	U10	C7-C8-C9	-2.30	122.96	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1285	BCL	C3C-C4C-CHD	-2.29	118.50	123.39
7	L	1284[A]	UQ2	C10-C9-C11	2.27	119.09	115.27
6	M	1309	BPH	O2A-CGA-O1A	-2.22	118.00	123.59
5	M	1304	BCL	CBA-CAA-C2A	-2.21	107.33	113.86
5	M	1303	BCL	CMD-C2D-C3D	-2.21	122.53	127.61
6	M	1309	BPH	CBC-CAC-C3C	-2.19	109.36	113.77
11	M	1310	U10	C25-C24-C23	-2.19	118.07	123.68
12	M	1311	SPO	C34-C33-C35	2.18	118.94	115.27
5	L	1285	BCL	C16-C15-C13	-2.18	108.89	115.92
6	M	1309	BPH	C3D-CAD-CBD	2.15	110.43	107.61
12	M	1311	SPO	C8-C7-C6	2.13	121.43	118.08
6	M	1309	BPH	C4B-NB-C1B	-2.11	102.76	107.09
11	M	1310	U10	C35-C34-C36	2.08	118.78	115.27
5	M	1303	BCL	CHD-C4C-NC	2.08	127.38	125.08
5	L	1285	BCL	OBB-CAB-C3B	-2.06	116.33	119.99
7	L	1284[A]	UQ2	CM2-O2-C2	2.05	123.72	116.47
5	L	1285	BCL	C4-C3-C5	2.04	118.70	115.27
5	L	1282	BCL	O2A-CGA-CBA	2.03	118.28	111.91
5	M	1303	BCL	O2D-CGD-O1D	-2.03	119.87	123.84
6	L	1283	BPH	CMB-C2B-C3B	2.02	128.46	124.68
9	M	1305	LDA	CM1-N1-C1	2.01	114.47	110.23
5	M	1304	BCL	CHA-C4D-ND	2.00	136.69	132.50

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C13
5	L	1282	BCL	C8
5	L	1285	BCL	C13
5	L	1285	BCL	C8
5	M	1303	BCL	C13
5	M	1303	BCL	C8
5	M	1304	BCL	C13
5	M	1304	BCL	C8

All (155) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	C1-C2-C3-O3
4	L	1287	GOL	O1-C1-C2-C3
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
5	M	1304	BCL	C1A-C2A-CAA-CBA
5	M	1304	BCL	C3A-C2A-CAA-CBA
6	M	1309	BPH	C1-C2-C3-C4
7	L	1284[A]	UQ2	C7-C8-C9-C10
7	L	1284[A]	UQ2	C7-C8-C9-C11
7	L	1284[A]	UQ2	C12-C11-C9-C8
7	L	1284[A]	UQ2	C12-C13-C14-C15
7	L	1284[A]	UQ2	C12-C13-C14-C16
7	L	1284[B]	UQ2	C1-C6-C7-C8
7	L	1284[B]	UQ2	C12-C11-C9-C10
7	L	1284[B]	UQ2	C12-C13-C14-C16
8	L	1286	HTO	O1-C1-C2-O2
8	L	1286	HTO	O1-C1-C2-C3
8	L	1286	HTO	O3-C3-C4-C5
9	M	1305	LDA	C2-C1-N1-O1
9	M	1305	LDA	C2-C1-N1-CM1
9	M	1306	LDA	N1-C1-C2-C3
11	M	1310	U10	C14-C16-C17-C18
11	M	1310	U10	C22-C23-C24-C25
11	M	1310	U10	C22-C23-C24-C26
11	M	1310	U10	C28-C29-C31-C32
11	M	1310	U10	C30-C29-C31-C32
11	M	1310	U10	C32-C33-C34-C35
11	M	1310	U10	C32-C33-C34-C36
11	M	1310	U10	C37-C38-C39-C41
12	M	1311	SPO	C6-C7-C9-C10
12	M	1311	SPO	C8-C7-C9-C10
12	M	1311	SPO	C9-C10-C11-C12
12	M	1311	SPO	C14-C15-C16-C17
12	M	1311	SPO	C15-C16-C17-C18
12	M	1311	SPO	C15-C16-C17-C19
12	M	1311	SPO	C16-C17-C19-C20
12	M	1311	SPO	C18-C17-C19-C20
12	M	1311	SPO	C19-C20-C21-C22
12	M	1311	SPO	C21-C22-C23-C24
7	L	1284[B]	UQ2	C12-C13-C14-C15
7	L	1284[A]	UQ2	C12-C11-C9-C10
11	M	1310	U10	C35-C34-C36-C37
7	L	1284[B]	UQ2	C12-C11-C9-C8
7	L	1284[B]	UQ2	C7-C8-C9-C10
7	L	1284[B]	UQ2	C7-C8-C9-C11
5	L	1282	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
5	L	1285	BCL	CBD-CGD-O2D-CED
5	M	1303	BCL	C10-C11-C12-C13
11	M	1310	U10	C37-C38-C39-C40
12	M	1311	SPO	C36-C37-C38-C40
11	M	1310	U10	C34-C36-C37-C38
5	M	1303	BCL	C8-C10-C11-C12
5	L	1282	BCL	C6-C7-C8-C9
5	L	1282	BCL	C14-C13-C15-C16
5	M	1303	BCL	C14-C13-C15-C16
12	M	1311	SPO	C24-C23-C25-C26
12	M	1311	SPO	C22-C23-C25-C26
5	L	1285	BCL	C13-C15-C16-C17
6	L	1283	BPH	C8-C10-C11-C12
12	M	1311	SPO	C36-C37-C38-C39
11	M	1310	U10	C27-C28-C29-C30
5	M	1303	BCL	C2-C1-O2A-CGA
5	M	1304	BCL	C6-C7-C8-C10
6	M	1309	BPH	C12-C13-C15-C16
5	L	1282	BCL	C15-C16-C17-C18
7	L	1284[B]	UQ2	C9-C11-C12-C13
11	M	1310	U10	C29-C31-C32-C33
5	L	1285	BCL	C15-C16-C17-C18
6	L	1283	BPH	C5-C6-C7-C8
5	L	1282	BCL	C8-C10-C11-C12
5	M	1303	BCL	C13-C15-C16-C17
12	M	1311	SPO	C13-C12-C14-C15
9	M	1306	LDA	C2-C3-C4-C5
9	M	1307	LDA	C4-C5-C6-C7
5	L	1285	BCL	O1D-CGD-O2D-CED
12	M	1311	SPO	C11-C12-C14-C15
12	M	1311	SPO	C21-C22-C23-C25
5	L	1285	BCL	C11-C12-C13-C14
6	M	1309	BPH	C11-C12-C13-C14
5	L	1282	BCL	O1D-CGD-O2D-CED
9	M	1306	LDA	C4-C5-C6-C7
8	L	1286	HTO	C2-C3-C4-C5
4	H	1251	GOL	C1-C2-C3-O3
9	M	1306	LDA	C5-C6-C7-C8
11	M	1310	U10	C19-C21-C22-C23
5	M	1304	BCL	C13-C15-C16-C17
6	M	1309	BPH	C5-C6-C7-C8
6	M	1309	BPH	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	C3-C5-C6-C7
6	M	1309	BPH	C1-C2-C3-C5
4	L	1287	GOL	O1-C1-C2-O2
9	M	1307	LDA	C1-C2-C3-C4
5	L	1285	BCL	C11-C12-C13-C15
6	L	1283	BPH	C11-C10-C8-C7
6	M	1309	BPH	C11-C12-C13-C15
6	M	1309	BPH	C3-C5-C6-C7
6	M	1309	BPH	C16-C17-C18-C19
5	M	1304	BCL	C15-C16-C17-C18
9	M	1305	LDA	C4-C5-C6-C7
9	M	1307	LDA	C2-C3-C4-C5
11	M	1310	U10	C33-C34-C36-C37
6	L	1283	BPH	C11-C10-C8-C9
6	L	1283	BPH	C11-C12-C13-C14
6	M	1309	BPH	C14-C13-C15-C16
5	M	1304	BCL	C16-C17-C18-C20
7	L	1284[B]	UQ2	C5-C6-C7-C8
9	M	1306	LDA	C3-C4-C5-C6
5	M	1303	BCL	C4-C3-C5-C6
9	M	1305	LDA	C2-C3-C4-C5
5	L	1282	BCL	C6-C7-C8-C10
5	L	1285	BCL	C11-C10-C8-C7
5	M	1303	BCL	C2-C3-C5-C6
5	M	1303	BCL	C12-C13-C15-C16
6	L	1283	BPH	C11-C12-C13-C15
7	L	1284[B]	UQ2	C3-C2-O2-CM2
11	M	1310	U10	C24-C26-C27-C28
9	M	1307	LDA	C5-C6-C7-C8
4	H	1252	GOL	O2-C2-C3-O3
6	M	1309	BPH	C16-C17-C18-C20
11	M	1310	U10	C5-C4-O4-C4M
6	M	1309	BPH	C6-C7-C8-C9
5	L	1282	BCL	C13-C15-C16-C17
6	M	1309	BPH	C6-C7-C8-C10
11	M	1310	U10	C27-C28-C29-C31
6	L	1283	BPH	C3-C5-C6-C7
5	M	1303	BCL	CAD-CBD-CGD-O2D
5	M	1304	BCL	CAD-CBD-CGD-O2D
6	M	1309	BPH	CAD-CBD-CGD-O2D
9	M	1305	LDA	C2-C1-N1-CM2
5	M	1304	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
6	L	1283	BPH	C16-C17-C18-C20
6	M	1309	BPH	C8-C10-C11-C12
5	L	1282	BCL	C11-C10-C8-C7
5	L	1282	BCL	C12-C13-C15-C16
5	M	1303	BCL	C11-C10-C8-C7
5	L	1282	BCL	C11-C10-C8-C9
5	M	1303	BCL	C11-C10-C8-C9
9	M	1307	LDA	C9-C10-C11-C12
7	L	1284[A]	UQ2	C1-C2-O2-CM2
9	M	1306	LDA	C11-C10-C9-C8
5	M	1304	BCL	C12-C13-C15-C16
5	M	1304	BCL	C16-C17-C18-C19
5	M	1304	BCL	C14-C13-C15-C16
5	L	1282	BCL	C1-C2-C3-C4
5	L	1285	BCL	C1-C2-C3-C4
11	M	1310	U10	C20-C19-C21-C22
6	L	1283	BPH	C14-C13-C15-C16
5	M	1304	BCL	O2A-C1-C2-C3
6	L	1283	BPH	O2A-C1-C2-C3
5	L	1282	BCL	CHA-CBD-CGD-O1D
5	L	1282	BCL	CHA-CBD-CGD-O2D
4	H	1251	GOL	O2-C2-C3-O3
6	L	1283	BPH	C6-C7-C8-C9
6	L	1283	BPH	C4-C3-C5-C6
6	L	1283	BPH	C6-C7-C8-C10

There are no ring outliers.

17 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	1310	U10	1	0
5	M	1304	BCL	9	0
6	L	1283	BPH	8	0
7	L	1284[B]	UQ2	13	0
5	M	1303	BCL	6	0
9	M	1305	LDA	2	0
4	H	1252	GOL	1	0
6	M	1309	BPH	11	0
4	L	1287	GOL	2	0
5	L	1285	BCL	2	0
7	L	1284[A]	UQ2	1	0
9	M	1306	LDA	2	0

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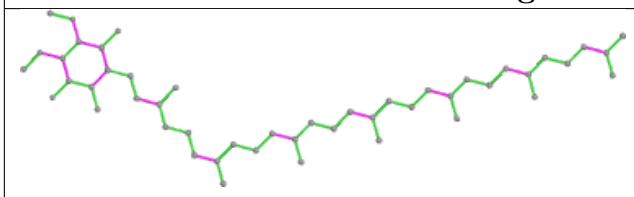
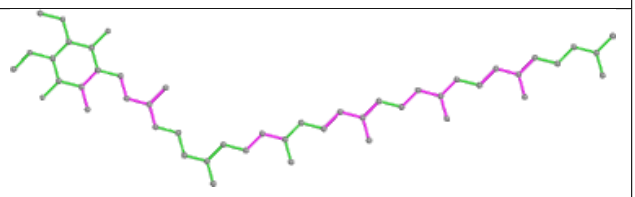
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1253	GOL	1	0
12	M	1311	SPO	1	0
5	L	1282	BCL	2	0
9	M	1307	LDA	1	0
4	H	1251	GOL	1	0

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 then 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.

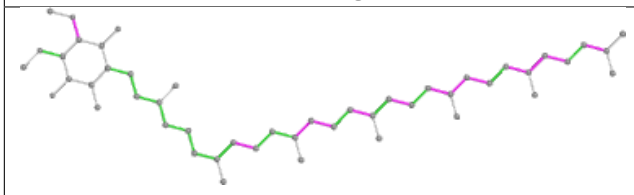
Ligand U10 M 1310



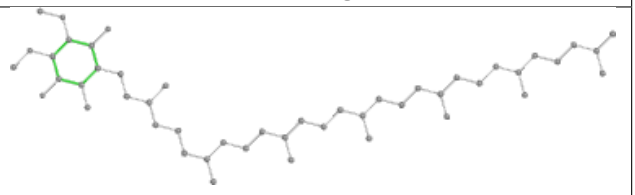
Bond lengths



Bond angles

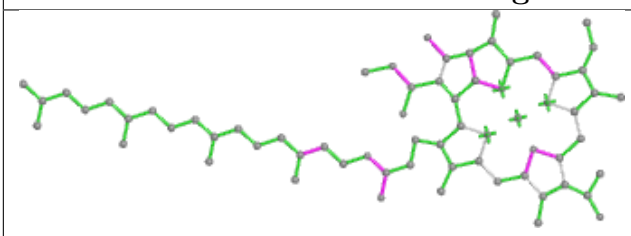


Torsions

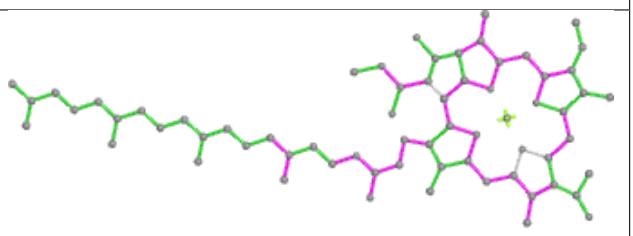


Rings

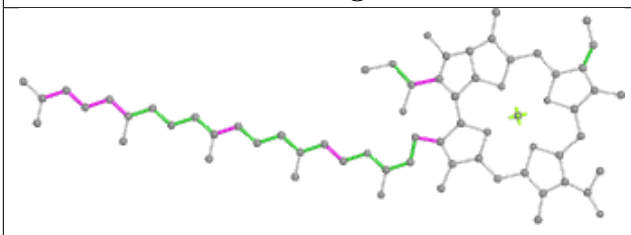
Ligand BCL M 1304



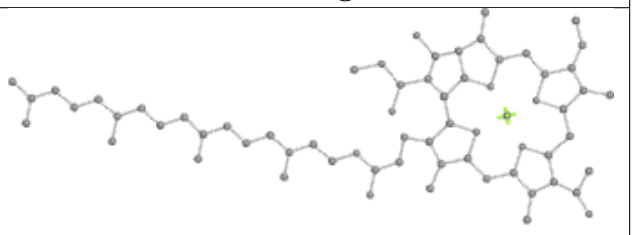
Bond lengths



Bond angles

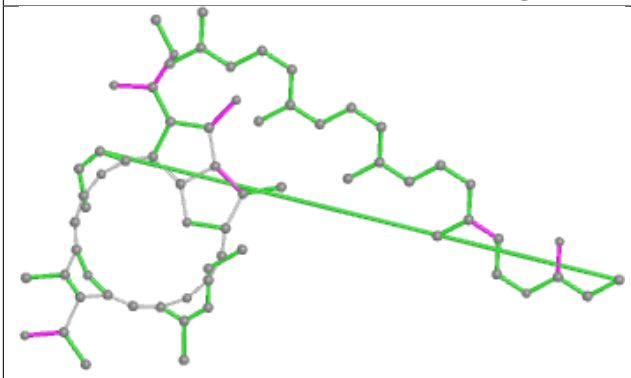


Torsions

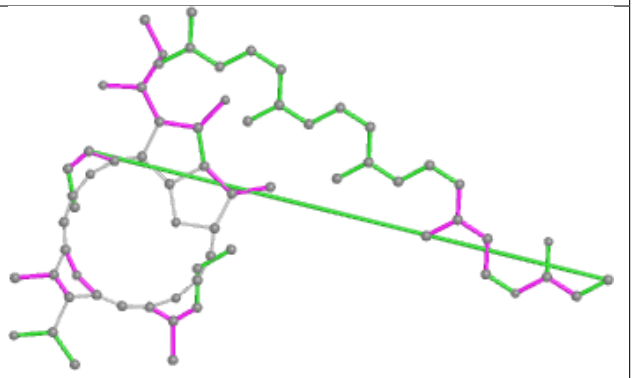


Rings

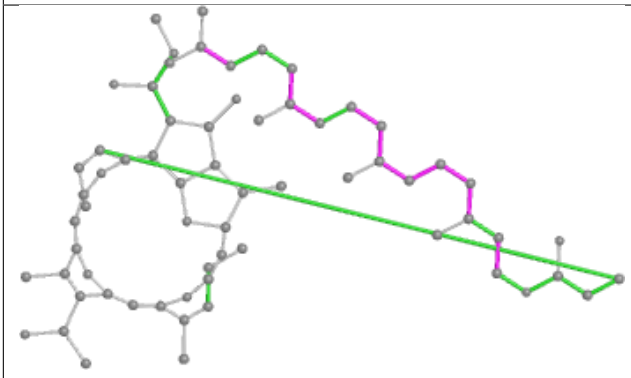
Ligand BPH L 1283



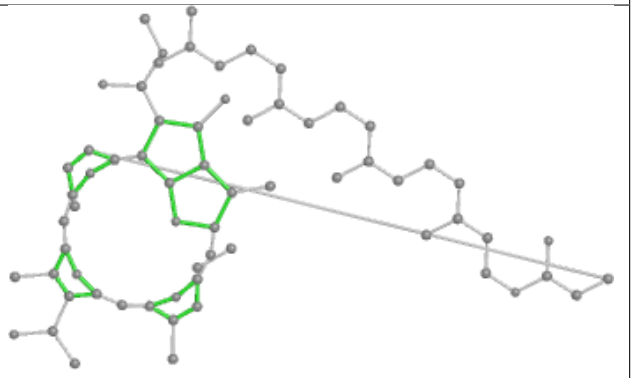
Bond lengths



Bond angles

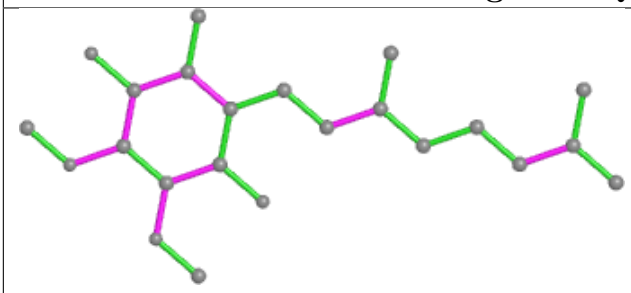


Torsions

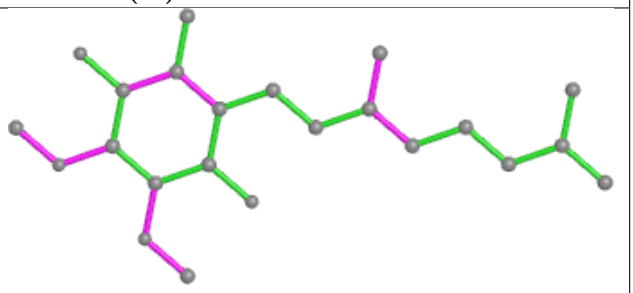


Rings

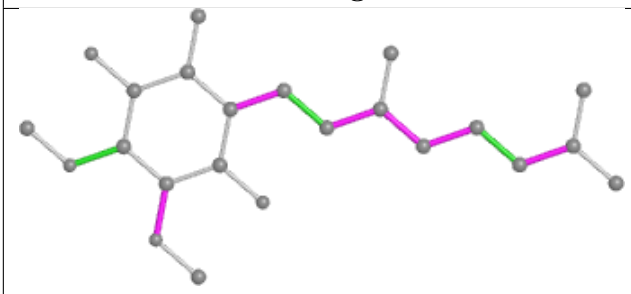
Ligand UQ2 L 1284 (B)



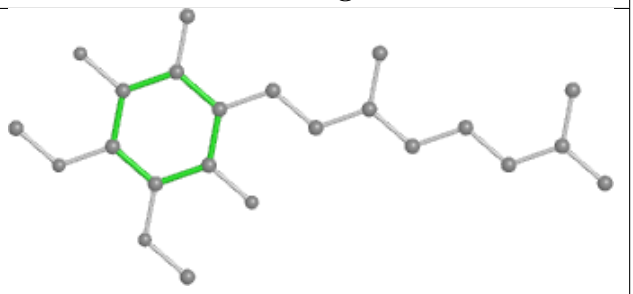
Bond lengths



Bond angles

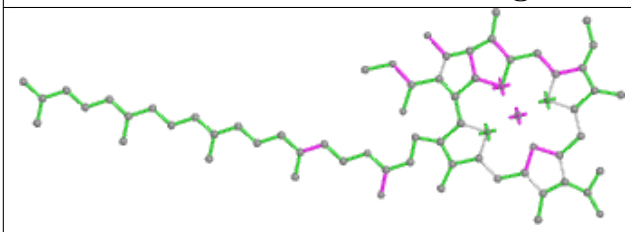


Torsions

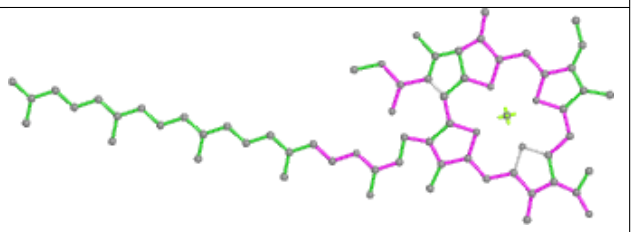


Rings

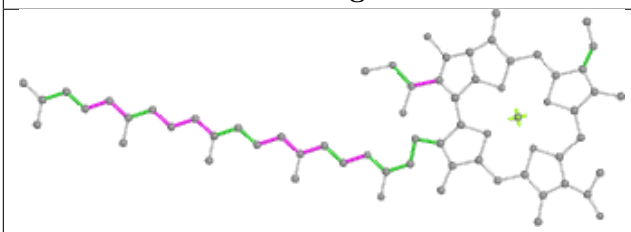
Ligand BCL M 1303



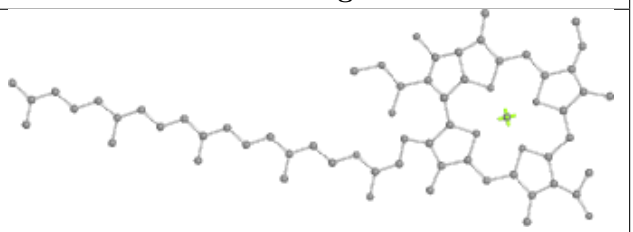
Bond lengths



Bond angles

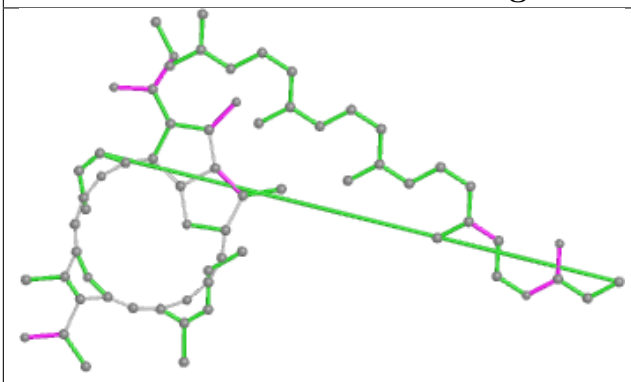


Torsions

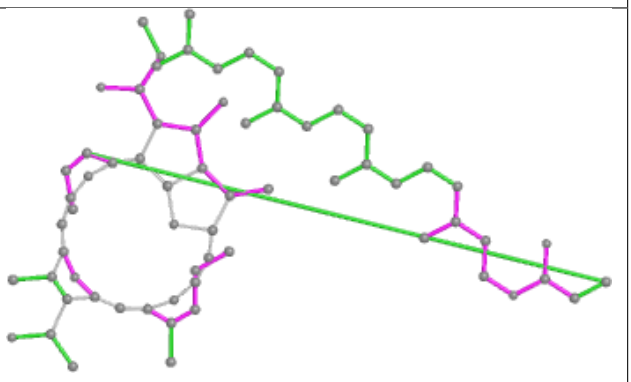


Rings

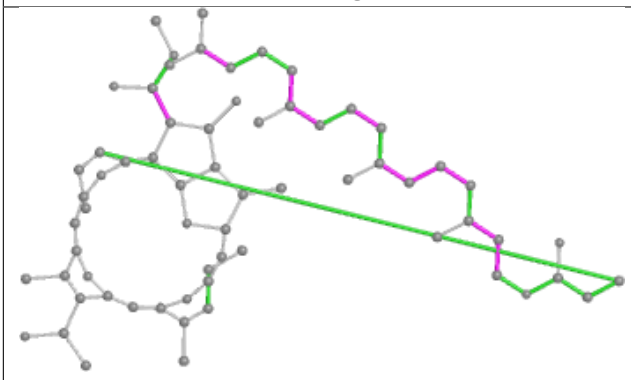
Ligand BPH M 1309



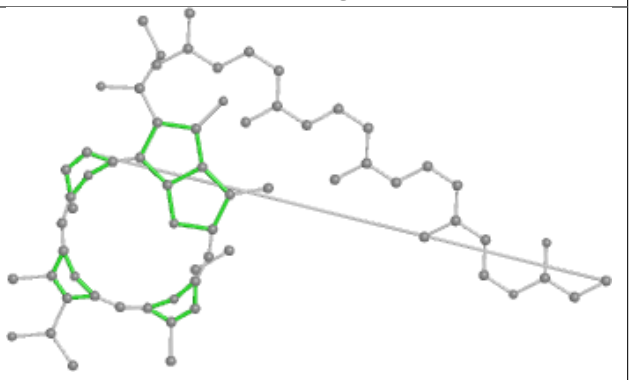
Bond lengths



Bond angles

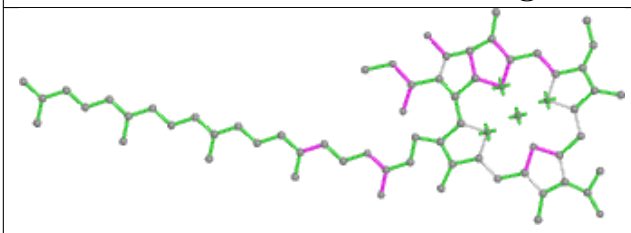


Torsions

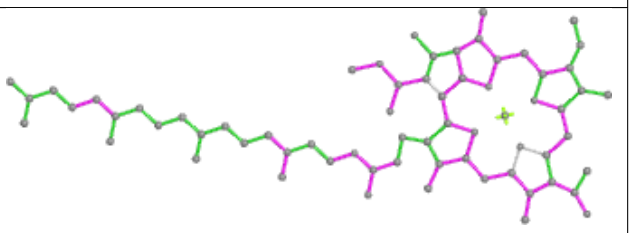


Rings

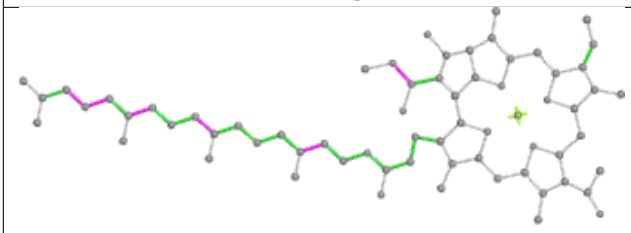
Ligand BCL L 1285



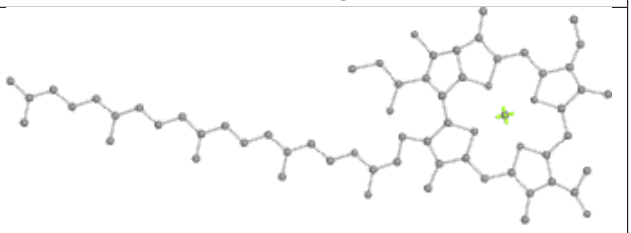
Bond lengths



Bond angles

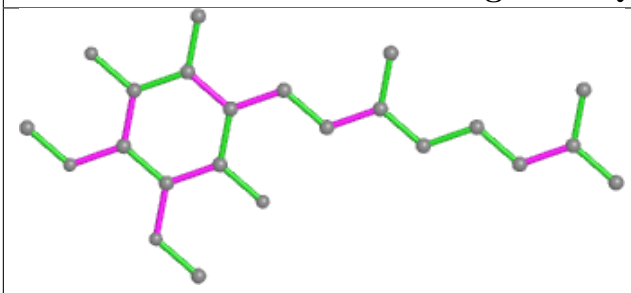


Torsions

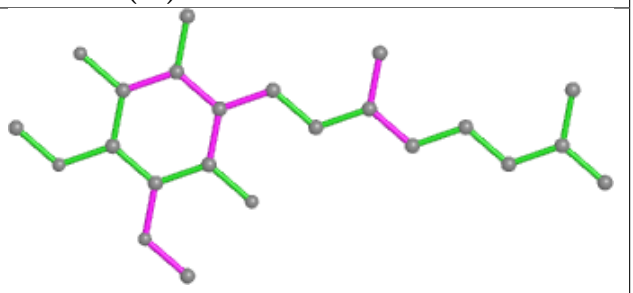


Rings

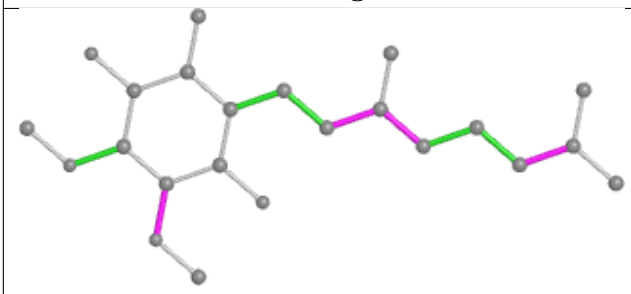
Ligand UQ2 L 1284 (A)



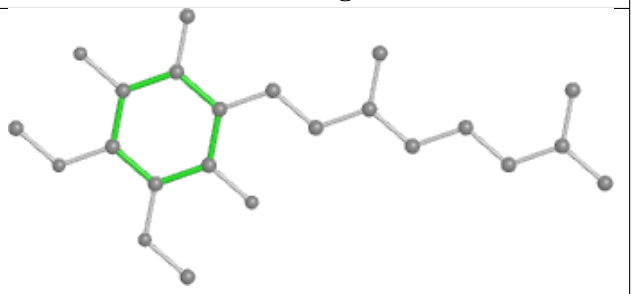
Bond lengths



Bond angles

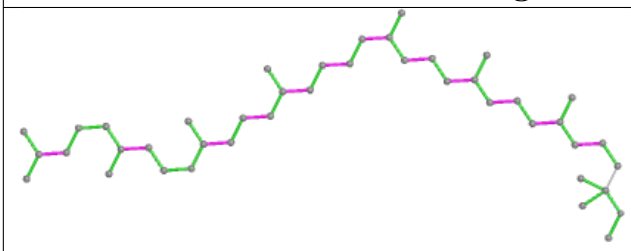


Torsions

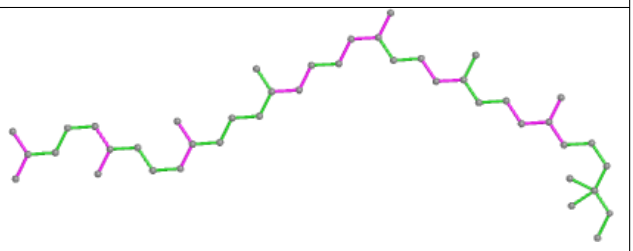


Rings

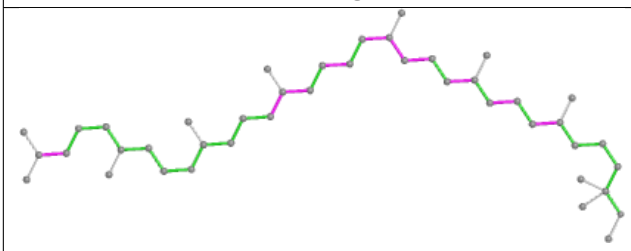
Ligand SPO M 1311



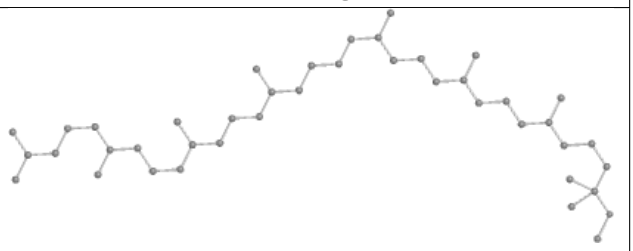
Bond lengths



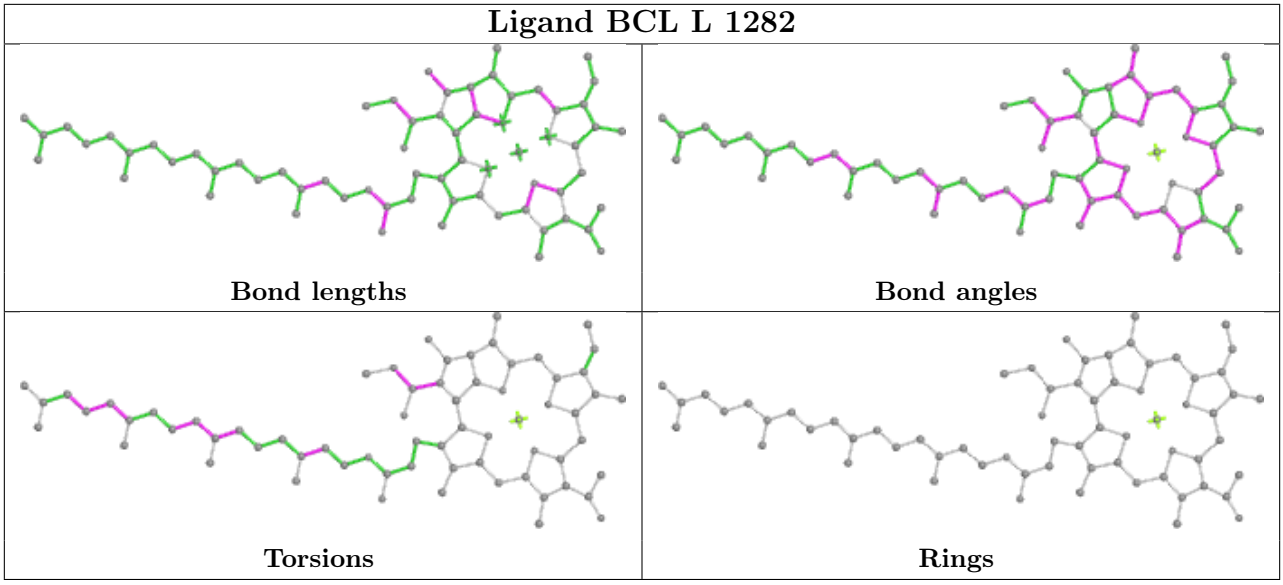
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	H	241/260 (92%)	-0.42	5 (2%)	63	62	36, 51, 66, 102	0
2	L	281/281 (100%)	-0.65	5 (1%)	68	67	32, 44, 69, 84	0
3	M	303/307 (98%)	-0.45	8 (2%)	56	53	34, 51, 76, 104	0
All	All	825/848 (97%)	-0.51	18 (2%)	62	60	32, 49, 72, 104	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	4.1
2	L	281	GLY	3.6
1	H	249	LYS	3.4
1	H	220[A]	LYS	3.3
1	H	250	SER	3.3
3	M	79	GLY	3.0
2	L	279	ILE	2.9
3	M	302	GLY	2.9
2	L	202	LYS	2.8
2	L	59	TRP	2.8
3	M	303	MET	2.7
3	M	23	ASP	2.7
3	M	25	ASN	2.5
1	H	159	GLU	2.2
3	M	2	GLU	2.2
3	M	80	TRP	2.2
1	H	246	PRO	2.2
2	L	278	GLY	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

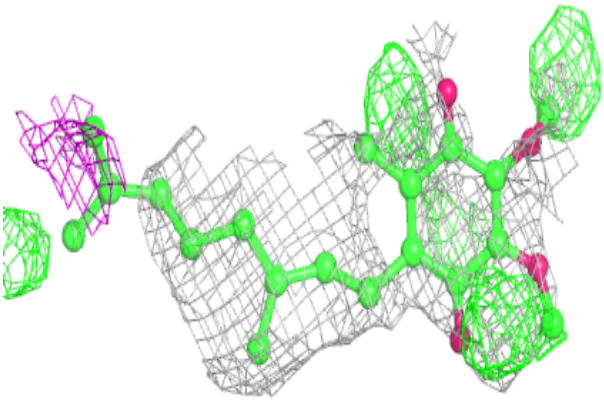
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

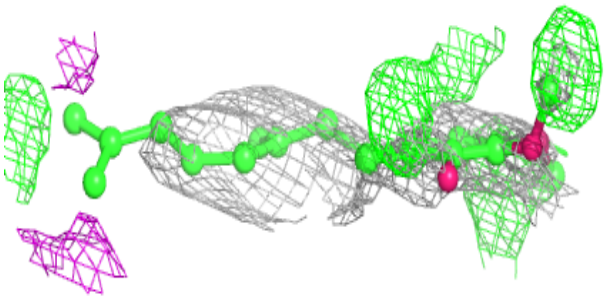
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	H	1253	6/6	0.67	0.45	113,114,115,116	0
4	GOL	H	1251	6/6	0.82	0.39	69,77,81,82	0
9	LDA	M	1307	16/16	0.83	0.32	98,102,114,115	0
7	UQ2	L	1284[B]	23/23	0.84	0.32	31,35,43,45	23
7	UQ2	L	1284[A]	23/23	0.84	0.32	51,59,74,74	23
4	GOL	L	1287	6/6	0.86	0.48	85,86,86,87	0
9	LDA	M	1305	16/16	0.87	0.26	74,83,86,87	0
4	GOL	H	1252	6/6	0.88	0.41	81,84,85,87	0
8	HTO	L	1286	10/10	0.88	0.48	71,83,83,84	0
9	LDA	M	1306	16/16	0.91	0.26	49,62,72,72	0
11	U10	M	1310	48/63	0.92	0.22	42,52,81,82	0
6	BPH	M	1309	65/65	0.94	0.21	39,48,109,110	0
12	SPO	M	1311	42/42	0.96	0.26	47,59,82,85	0
6	BPH	L	1283	65/65	0.97	0.15	25,35,53,55	0
5	BCL	M	1303	66/66	0.98	0.15	29,41,93,96	0
5	BCL	M	1304	66/66	0.98	0.16	32,40,59,68	0
5	BCL	L	1282	66/66	0.98	0.13	31,40,64,75	0
5	BCL	L	1285	66/66	0.98	0.14	30,37,55,60	0
10	FE	M	1308	1/1	0.99	0.07	41,41,41,41	0

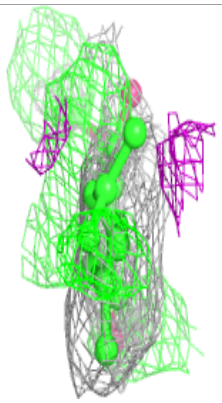
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ2 L 1284 (B):

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

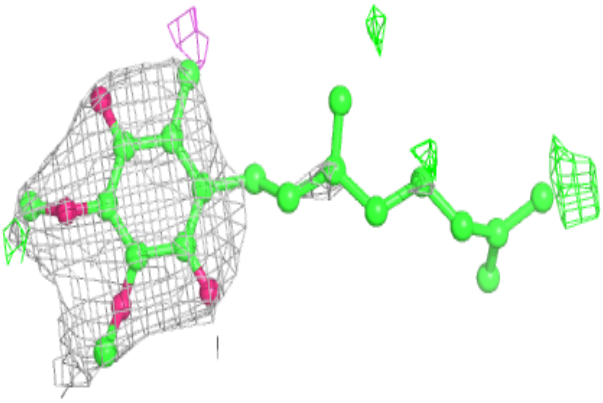


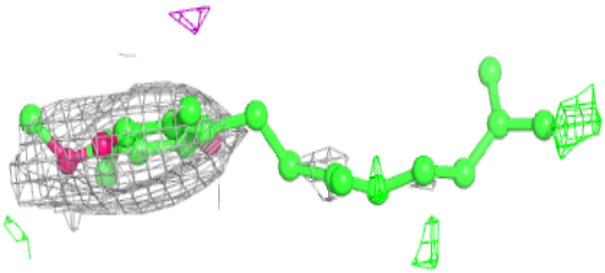


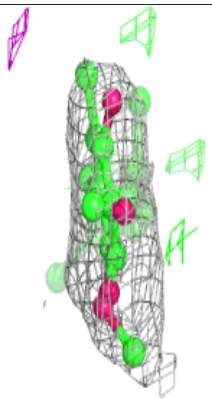


Electron density around UQ2 L 1284 (A):

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

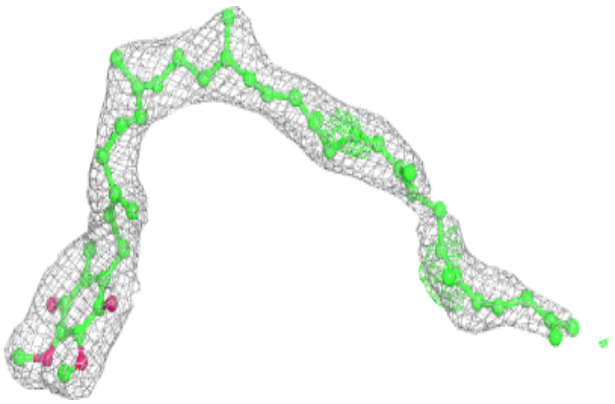


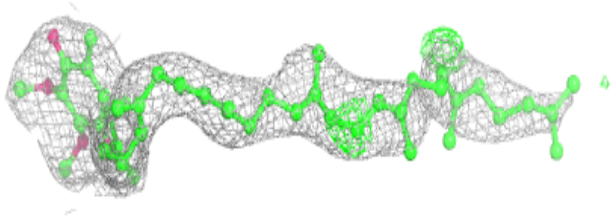




Electron density around U10 M 1310:

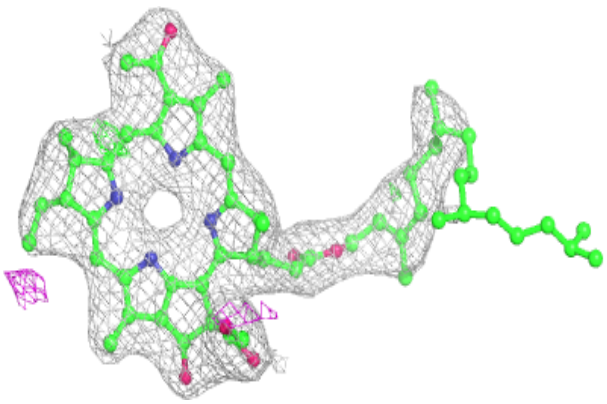
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

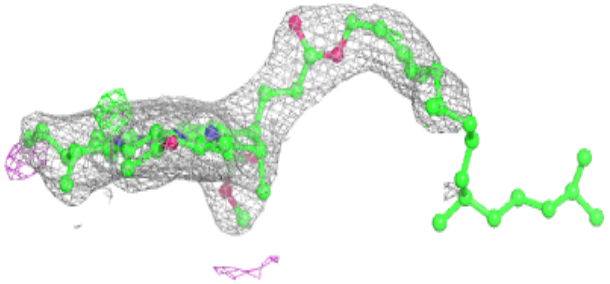


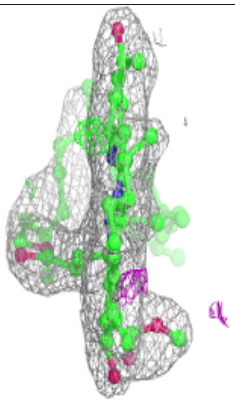


Electron density around BPH M 1309:

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

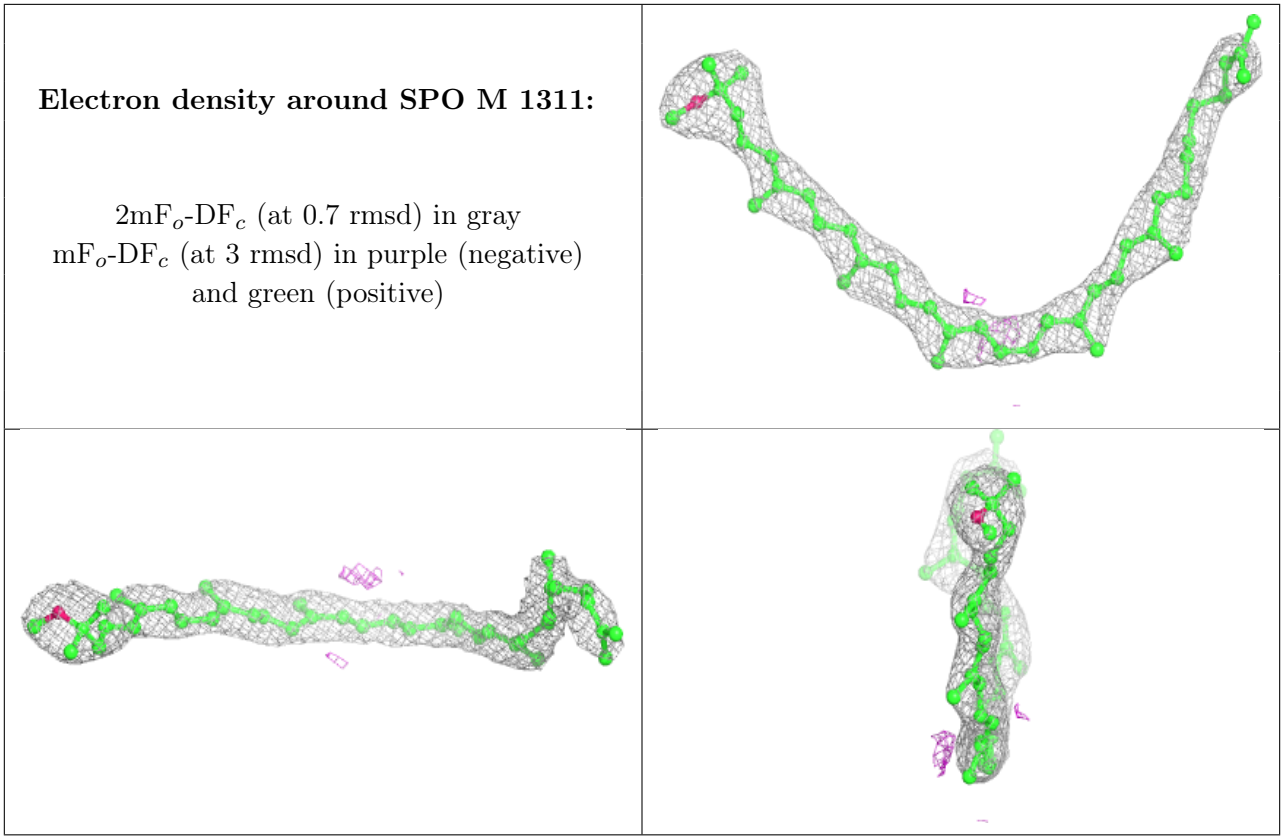






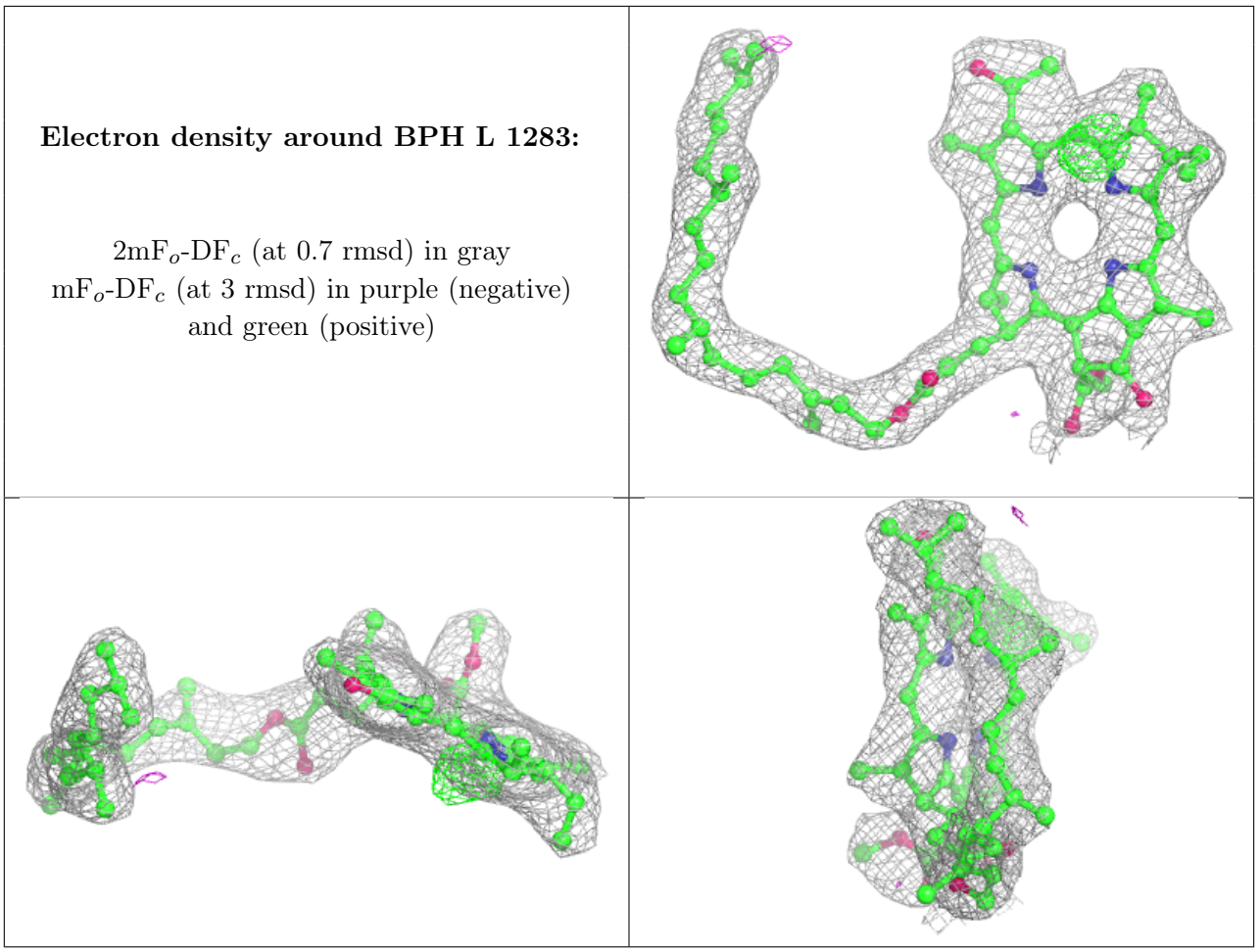
Electron density around SPO M 1311:

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



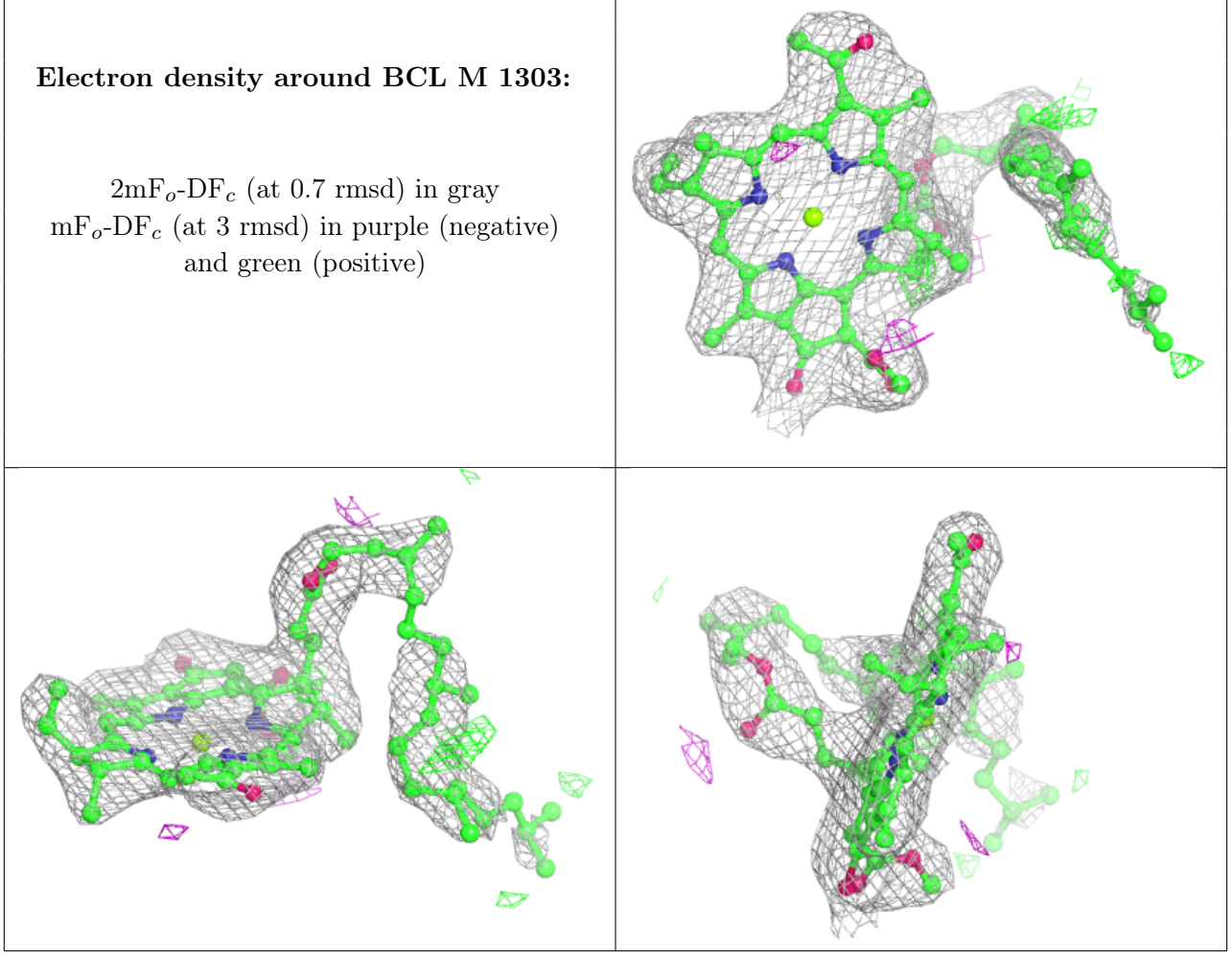
Electron density around BPH L 1283:

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



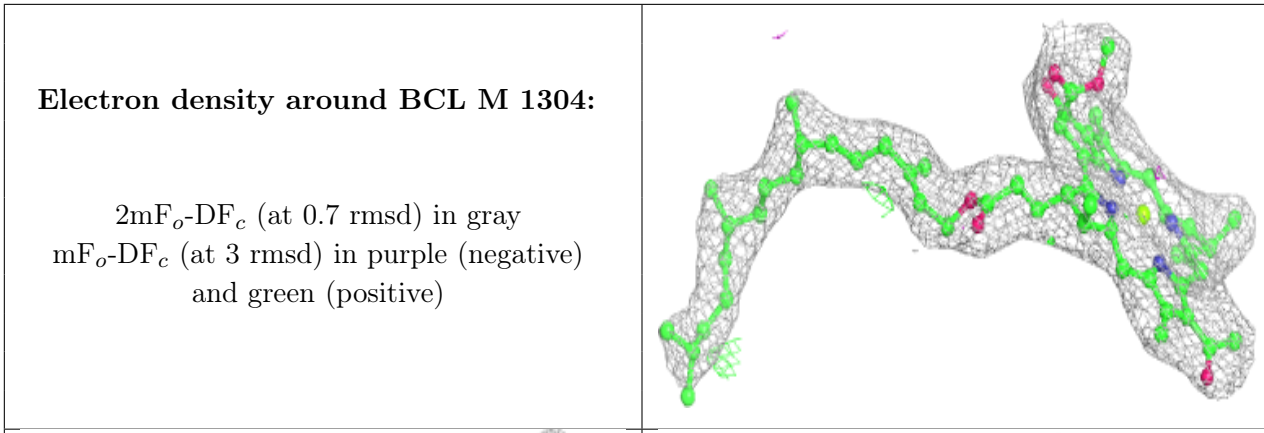
Electron density around BCL M 1303:

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



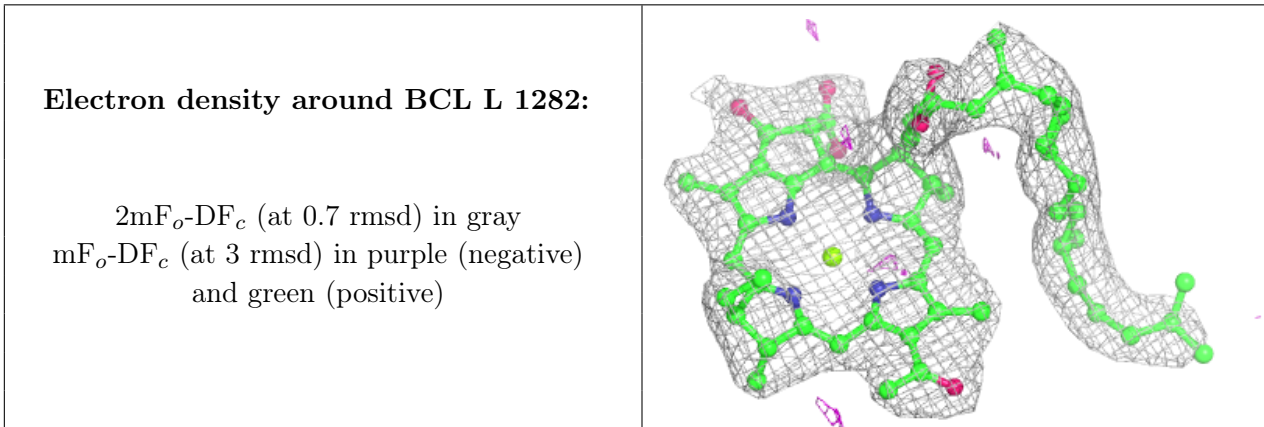
Electron density around BCL M 1304:

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



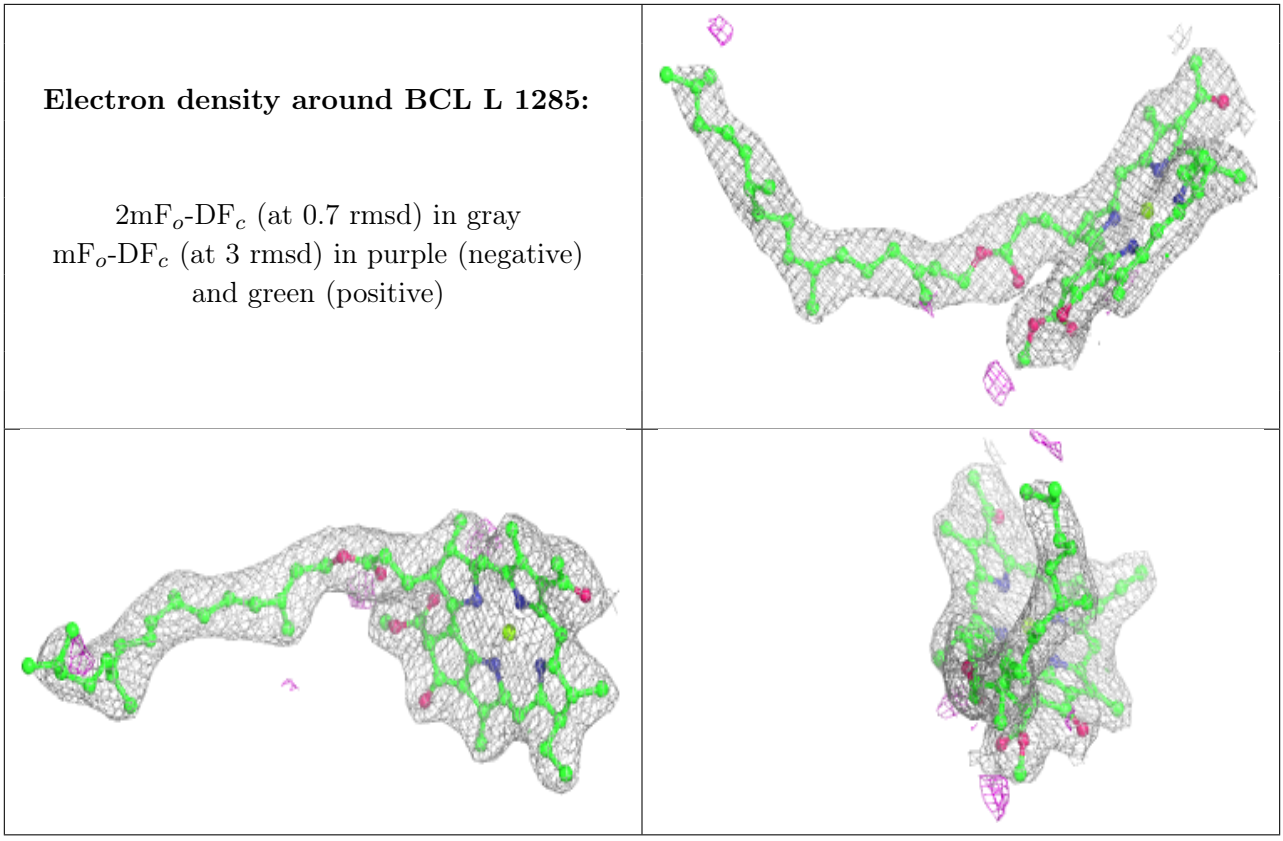
Electron density around BCL L 1282:

$2mF_o$-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 1285:

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



6.5 Other polymers (i)

There are no such residues in this entry.