Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 03:06 pm GMT

PDB ID	:	2UWW
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 6.5 in the neutral state
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-23
Resolution	:	2.05 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:

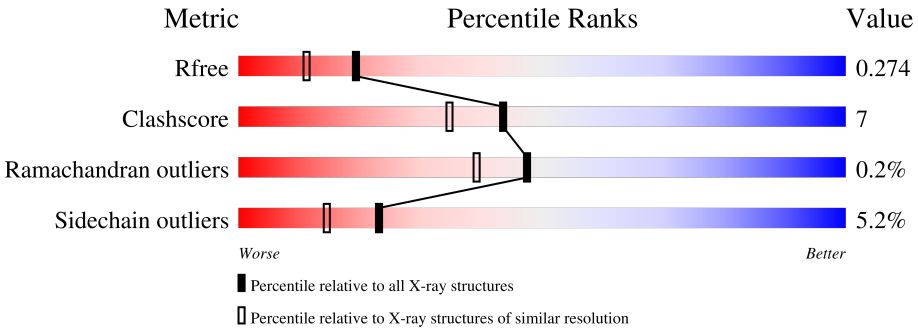
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)

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%

Mol	Chain	Length	Quality of chain
1	H	260	81% 10% • 7%
2	L	281	88% 10% •
3	M	307	86% 12% ••

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	1252	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1282	X	-	-	-
5	BCL	L	1290	X	-	-	-
5	BCL	M	1304	X	-	-	-
5	BCL	M	1305	X	-	-	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 7772 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
			Total	C	N	O	S			
1	H	241	1830	1169	315	337	9	0	0	1

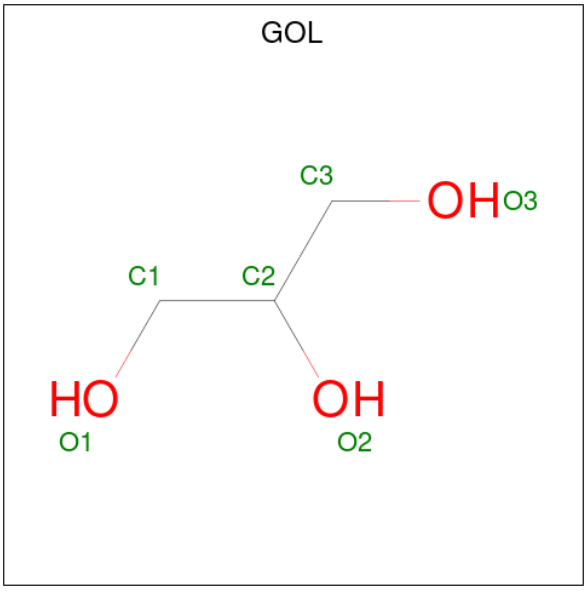
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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

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

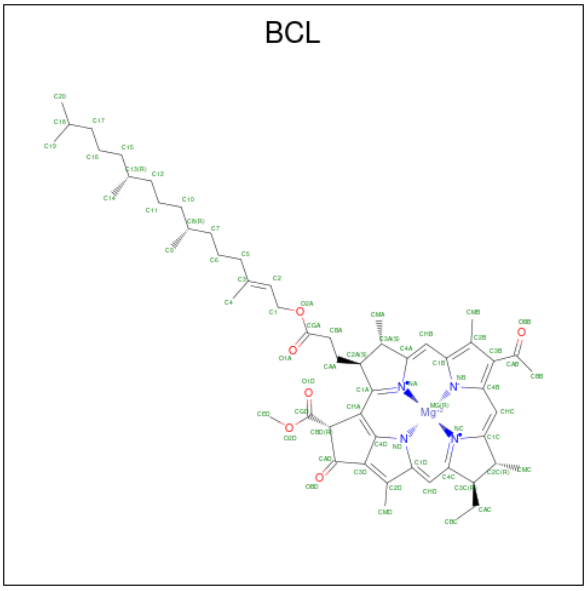
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

- 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	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

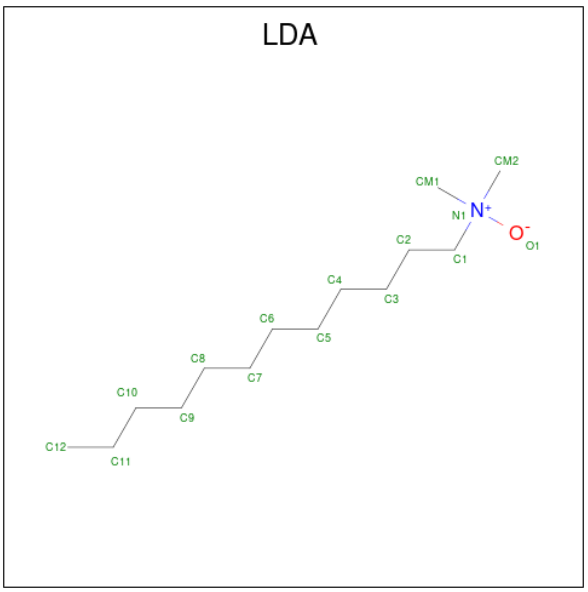
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

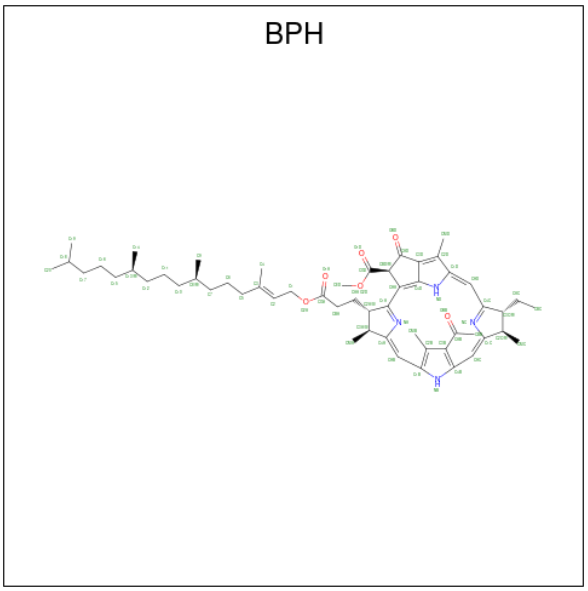
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

$C_{14}H_{31}NO$).



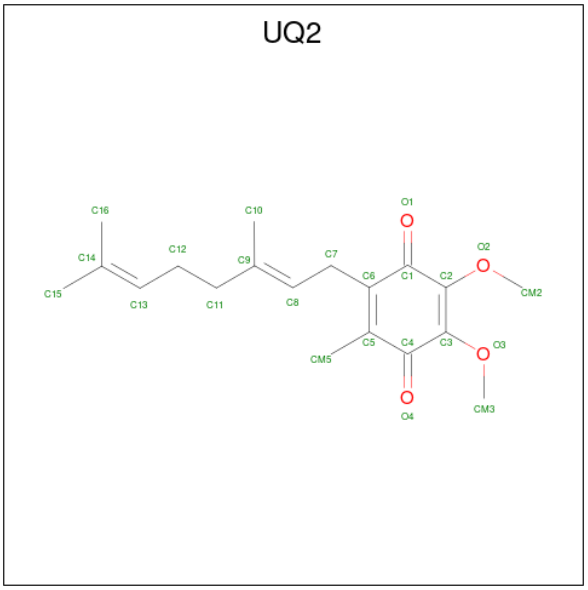
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



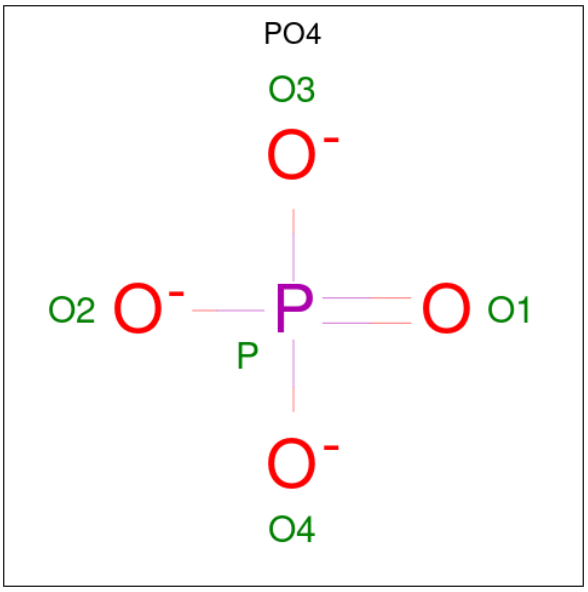
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C N O 65 55 4 6	0	0
7	M	1	Total C N O 65 55 4 6	0	0

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



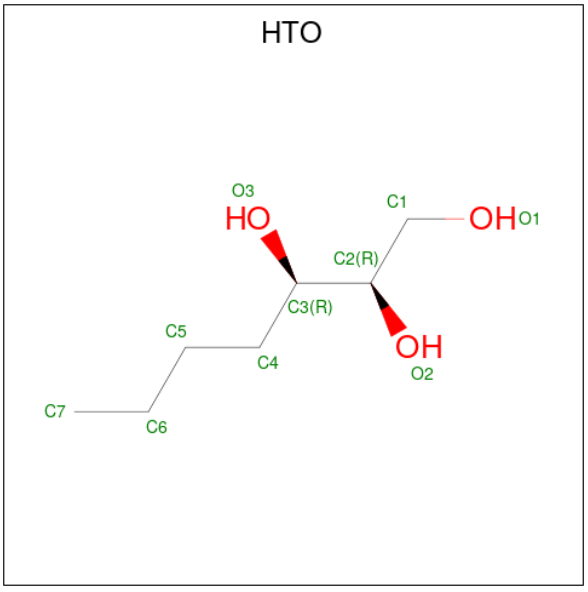
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 46 38 8	0	1

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



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

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

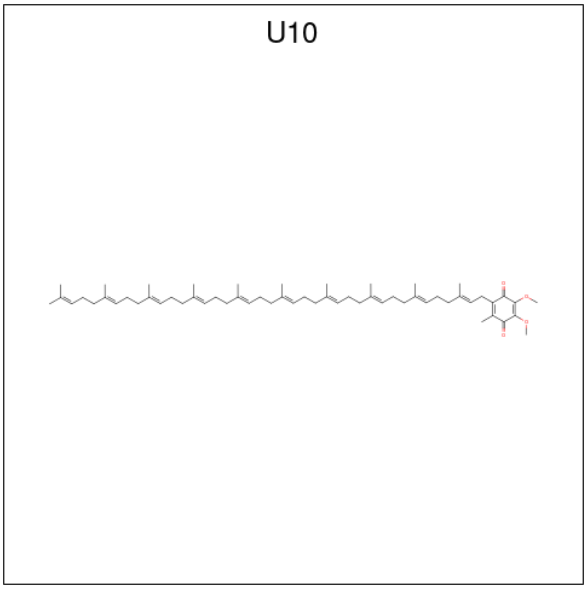


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0

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

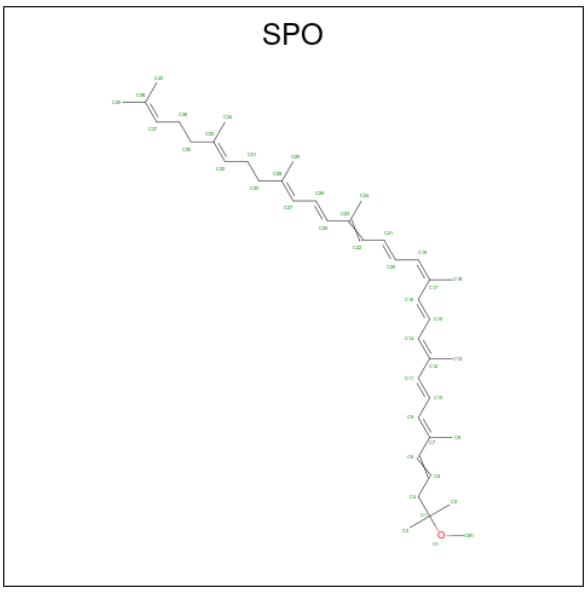
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

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



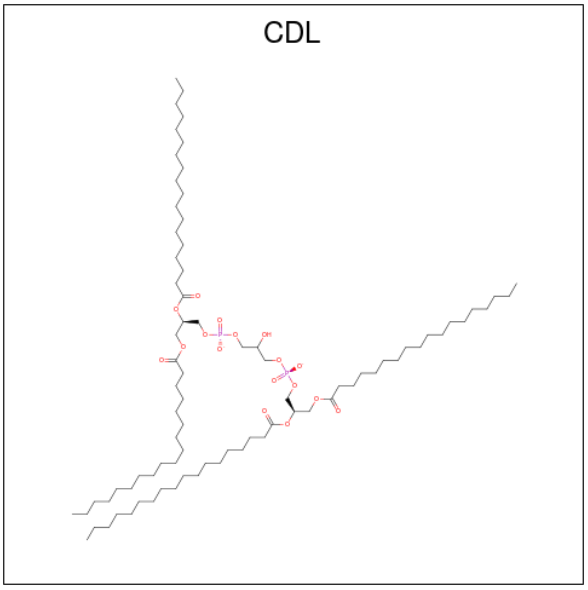
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 48 44 4	0	0

- 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 42 41 1	0	0

- 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 81 62 17 2	0	0

- Molecule 15 is water.

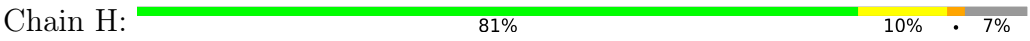
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	198	Total O 198 198	0	0
15	L	132	Total O 132 132	0	0
15	M	158	Total O 158 158	0	0

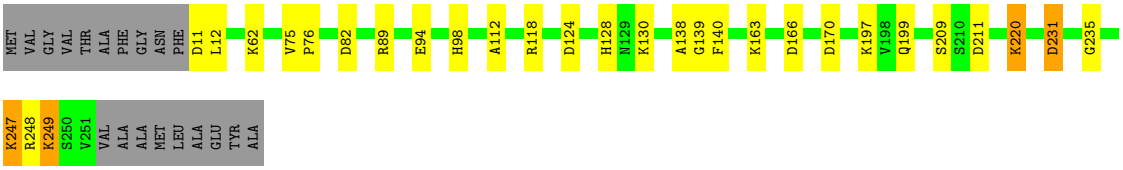
3 Residue-property plots (i)

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. 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. 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

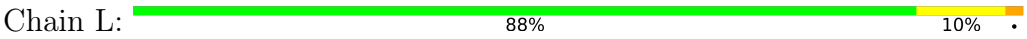
Chain H:

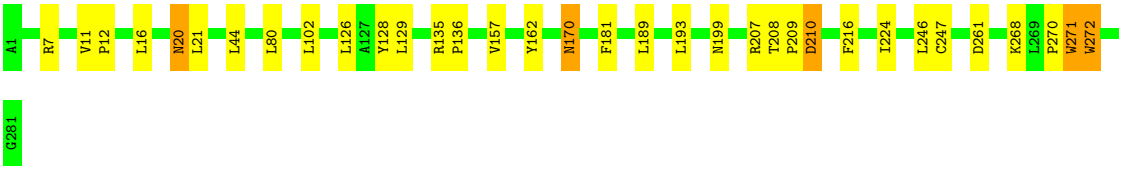




- Molecule 2: REACTION CENTER PROTEIN L CHAIN

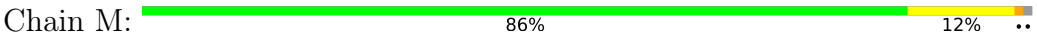
Chain L:

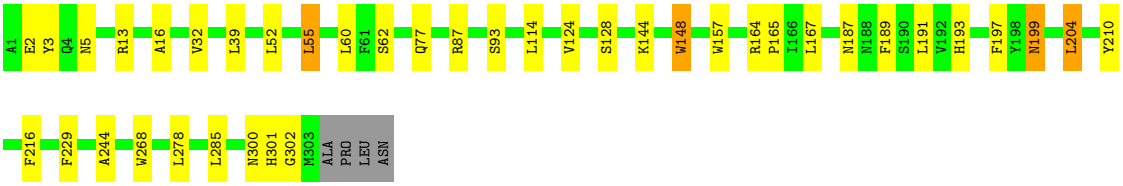




- Molecule 3: REACTION CENTER PROTEIN M CHAIN

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	138.69Å 138.69Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.05 29.81 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.2 (119.52-2.05) 89.3 (29.81-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.233 0.271 , 0.274	Depositor DCC
R_{free} test set	2639 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	33.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7772	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: BPH, CDL, BCL, SPO, UQ2, PO4, GOL, HTO, FE, U10, LDA

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	0.68	0/1878	0.77	5/2555 (0.2%)
2	L	0.69	0/2320	0.69	0/3175
3	M	0.68	0/2501	0.70	1/3415 (0.0%)
All	All	0.69	0/6699	0.72	6/9145 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	204	LEU	CB-CG-CD1	5.70	120.68	111.00
1	H	82	ASP	CB-CG-OD2	5.69	123.42	118.30
1	H	211	ASP	CB-CG-OD2	5.47	123.23	118.30
1	H	231	ASP	CB-CG-OD2	5.34	123.10	118.30
1	H	139	GLY	N-CA-C	-5.27	99.92	113.10
1	H	166	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	138	ALA	Peptide

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	1830	0	1836	18	0
2	L	2232	0	2187	23	0
3	M	2409	0	2321	26	0
4	H	24	0	32	5	0
4	L	12	0	16	1	0
4	M	6	0	8	0	0
5	L	132	0	148	6	0
5	M	132	0	148	20	0
6	L	80	0	155	1	0
6	M	64	0	124	3	0
7	L	65	0	76	6	0
7	M	65	0	76	9	0
8	L	46	0	52	7	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	84	3	0
15	H	198	0	0	5	1
15	L	132	0	0	1	1
15	M	158	0	0	0	0
All	All	7772	0	7402	98	1

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 (98) 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)
7:L:1288:BPH:HBB3	7:L:1288:BPH:HHC	1.37	1.02
1:H:220:LYS:HD3	15:H:2181:HOH:O	1.75	0.86
5:L:1282:BCL:HBB2	5:L:1282:BCL:HHC	1.59	0.85
1:H:62:LYS:HE3	4:H:1252:GOL:H11	1.60	0.84
3:M:197:PHE:HZ	5:M:1305:BCL:HBB2	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:197:PHE:CZ	5:M:1305:BCL:HBB2	2.16	0.80
1:H:248:ARG:HA	1:H:249:LYS:CB	2.11	0.79
7:L:1288:BPH:HHC	7:L:1288:BPH:CBB	2.14	0.77
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.67	0.75
7:M:1311:BPH:HHC	7:M:1311:BPH:HBB3	1.69	0.74
4:H:1252:GOL:C3	15:H:2003:HOH:O	2.38	0.71
6:M:1306:LDA:H81	6:M:1308:LDA:H121	1.73	0.70
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.28	0.68
3:M:189:PHE:O	3:M:193:HIS:HD2	1.77	0.67
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.77	0.66
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.27	0.63
7:M:1311:BPH:HHC	7:M:1311:BPH:CBB	2.28	0.63
5:M:1305:BCL:CBB	5:M:1305:BCL:HHC	2.28	0.63
2:L:261:ASP:OD1	15:L:2120:HOH:O	2.16	0.62
4:H:1252:GOL:H31	15:H:2003:HOH:O	1.96	0.62
3:M:144:LYS:N	14:M:1314:CDL:OB3	2.27	0.61
7:L:1288:BPH:HBB3	7:L:1288:BPH:CHC	2.22	0.61
4:H:1252:GOL:H32	15:H:2003:HOH:O	1.99	0.60
2:L:199:ASN:O	14:M:1314:CDL:HB22	2.02	0.59
5:M:1304:BCL:HBB3	5:M:1305:BCL:H41	1.83	0.59
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.34	0.58
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.85	0.57
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.22	0.56
2:L:170:ASN:HD22	2:L:170:ASN:C	2.09	0.56
3:M:157:TRP:HB2	5:M:1305:BCL:H71	1.88	0.56
7:L:1288:BPH:CBB	7:L:1288:BPH:CHC	2.81	0.55
1:H:128:HIS:HE1	15:H:2125:HOH:O	1.88	0.55
7:L:1288:BPH:HBB2	3:M:210:TYR:HB3	1.90	0.55
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.56	0.54
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.35	0.54
1:H:248:ARG:HA	1:H:249:LYS:HB3	1.91	0.53
3:M:189:PHE:O	3:M:193:HIS:CD2	2.61	0.53
3:M:77:GLN:HE22	3:M:93:SER:H	1.54	0.53
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.39	0.53
5:M:1305:BCL:HBB2	5:M:1305:BCL:HHC	1.91	0.53
1:H:197:LYS:HE3	1:H:199:GLN:NE2	2.24	0.52
1:H:209:SER:OG	1:H:247:LYS:HD3	2.10	0.52
5:M:1304:BCL:HBB2	13:M:1313:SPO:H243	1.92	0.52
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.74	0.52
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.51
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:189:LEU:CD1	8:L:1289[A]:UQ2:H121	2.40	0.51
1:H:75:VAL:HA	1:H:76:PRO:C	2.31	0.51
5:L:1290:BCL:CBB	5:L:1290:BCL:HMB1	2.41	0.50
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB2	1.94	0.50
6:M:1308:LDA:H52	6:M:1309:LDA:H42	1.93	0.50
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.94	0.50
5:M:1304:BCL:CBB	13:M:1313:SPO:H243	2.42	0.50
2:L:157:VAL:HG11	5:M:1305:BCL:HBB1	1.94	0.49
5:M:1305:BCL:HAA2	5:M:1305:BCL:HBD	1.95	0.49
3:M:167:LEU:HD12	3:M:285:LEU:HD11	1.94	0.48
3:M:199:ASN:HD22	3:M:199:ASN:C	2.16	0.48
1:H:62:LYS:CE	4:H:1252:GOL:H11	2.39	0.48
2:L:271:TRP:CD1	2:L:271:TRP:N	2.79	0.48
3:M:197:PHE:HZ	5:M:1305:BCL:CBB	2.19	0.48
8:L:1289[A]:UQ2:H71	8:L:1289[A]:UQ2:H5M1	1.67	0.47
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.47	0.47
3:M:300:ASN:C	3:M:302:GLY:H	2.17	0.47
1:H:248:ARG:CA	1:H:249:LYS:HB2	2.43	0.47
5:M:1305:BCL:HHC	5:M:1305:BCL:HBB3	1.97	0.46
2:L:199:ASN:HA	4:L:1293:GOL:H31	1.98	0.46
6:L:1287:LDA:H121	8:L:1289[A]:UQ2:H161	1.97	0.46
5:L:1282:BCL:H192	7:L:1288:BPH:H7C2	1.98	0.46
2:L:208:THR:HB	2:L:209:PRO:HD2	1.98	0.46
2:L:193:LEU:HD23	8:L:1289[A]:UQ2:C4	2.46	0.45
1:H:112:ALA:HA	1:H:235:GLY:O	2.17	0.45
5:L:1290:BCL:HMB1	5:L:1290:BCL:HBB3	1.99	0.45
3:M:60:LEU:HD11	7:M:1311:BPH:H161	1.98	0.44
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.44
2:L:11:VAL:HB	2:L:12:PRO:HD2	1.99	0.44
5:M:1305:BCL:CBB	5:M:1305:BCL:CHC	2.94	0.44
1:H:89:ARG:NH2	1:H:94:GLU:HG2	2.33	0.43
2:L:224:ILE:HG22	8:L:1289[A]:UQ2:H8	2.00	0.43
1:H:140:PHE:HA	3:M:13:ARG:O	2.19	0.43
3:M:62:SER:OG	3:M:124:VAL:HG22	2.18	0.43
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.19	0.43
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.54	0.43
5:M:1304:BCL:H102	5:M:1304:BCL:H13	1.39	0.42
2:L:20:ASN:N	2:L:20:ASN:HD22	2.17	0.42
5:M:1304:BCL:HMB2	7:M:1311:BPH:HMB3	2.01	0.42
5:M:1304:BCL:H71	5:M:1305:BCL:H202	2.02	0.42
5:M:1304:BCL:H101	5:M:1305:BCL:H171	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1311:BPH:H7C2	7:M:1311:BPH:H112	1.81	0.41
8:L:1289[A]:UQ2:H101	8:L:1289[A]:UQ2:H122	1.88	0.41
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.20	0.41
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.56	0.41
3:M:278:LEU:HD21	14:M:1314:CDL:H782	2.01	0.41
3:M:268:TRP:CD1	12:M:1312:U10:H111	2.56	0.41
6:M:1308:LDA:C5	6:M:1309:LDA:H42	2.52	0.40
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.57	0.40
3:M:197:PHE:CE1	5:M:1305:BCL:HBB2	2.56	0.40
2:L:270:PRO:HG2	2:L:271:TRP:CD1	2.57	0.40
8:L:1289[B]:UQ2:H121	8:L:1289[B]:UQ2:H101	1.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:2050:HOH:O	15:L:2077:HOH:O[6_655]	2.18	0.02

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	239/260 (92%)	235 (98%)	3 (1%)	1 (0%)	34 24
2	L	279/281 (99%)	274 (98%)	5 (2%)	0	100 100
3	M	301/307 (98%)	290 (96%)	10 (3%)	1 (0%)	41 31
All	All	819/848 (97%)	799 (98%)	18 (2%)	2 (0%)	47 39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS

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Mol	Chain	Res	Type
3	M	301	HIS

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	195/208 (94%)	188 (96%)	7 (4%)	35 28
2	L	220/220 (100%)	203 (92%)	17 (8%)	13 5
3	M	236/240 (98%)	226 (96%)	10 (4%)	30 22
All	All	651/668 (98%)	617 (95%)	34 (5%)	23 14

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	12	LEU
1	H	118	ARG
1	H	163	LYS
1	H	220	LYS
1	H	231	ASP
1	H	247	LYS
2	L	16	LEU
2	L	20	ASN
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	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS

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Mol	Chain	Res	Type
2	L	268	LYS
2	L	271	TRP
2	L	272	TRP
3	M	2	GLU
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	114	LEU
3	M	148	TRP
3	M	191	LEU
3	M	199	ASN
3	M	204	LEU
3	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	141	HIS
2	L	20	ASN
2	L	159	ASN
2	L	170	ASN
2	L	183	ASN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

5.3.3 RNA (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 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	$\#\|Z\| > 2$
7	BPH	M	1311	-	51,70,70	2.71	9 (17%)	52,101,101	1.91	13 (25%)
6	LDA	L	1283	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
4	GOL	H	1255	-	5,5,5	0.35	0	5,5,5	0.35	0
13	SPO	M	1313	-	40,41,41	3.90	12 (30%)	47,50,50	2.07	17 (36%)
8	UQ2	L	1289[A]	-	23,23,23	2.58	8 (34%)	28,31,31	1.82	8 (28%)
5	BCL	L	1290	2	64,74,74	1.99	10 (15%)	78,115,115	2.11	22 (28%)
6	LDA	M	1307	-	12,15,15	2.04	1 (8%)	14,17,17	0.60	0
6	LDA	M	1308	-	12,15,15	1.93	1 (8%)	14,17,17	0.64	0
8	UQ2	L	1289[B]	-	23,23,23	2.66	8 (34%)	28,31,31	1.25	4 (14%)
6	LDA	L	1285	-	12,15,15	2.05	1 (8%)	14,17,17	0.55	0
6	LDA	M	1306	-	12,15,15	1.91	1 (8%)	14,17,17	0.68	0
4	GOL	H	1252	-	5,5,5	0.56	0	5,5,5	1.11	0
6	LDA	M	1309	-	12,15,15	2.05	1 (8%)	14,17,17	0.57	0
6	LDA	L	1284	-	12,15,15	2.02	1 (8%)	14,17,17	0.54	0
14	CDL	M	1314	-	80,80,99	2.01	15 (18%)	86,92,111	2.85	13 (15%)
10	HTO	L	1292	-	9,9,9	0.38	0	10,10,10	0.63	0
4	GOL	H	1253	-	5,5,5	0.38	0	5,5,5	0.29	0
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.27	0
5	BCL	M	1304	3	64,74,74	1.95	10 (15%)	78,115,115	2.00	13 (16%)
4	GOL	L	1294	-	5,5,5	0.37	0	5,5,5	0.26	0
6	LDA	L	1286	-	12,15,15	2.05	1 (8%)	14,17,17	0.67	0
12	U10	M	1312	-	48,48,63	2.64	11 (22%)	58,61,79	1.57	12 (20%)
5	BCL	M	1305	3	64,74,74	2.06	13 (20%)	78,115,115	2.00	21 (26%)
6	LDA	L	1287	-	12,15,15	2.08	1 (8%)	14,17,17	0.59	0
5	BCL	L	1282	2	64,74,74	2.02	13 (20%)	78,115,115	1.92	19 (24%)
4	GOL	L	1293	-	5,5,5	0.40	0	5,5,5	0.74	0
9	PO4	L	1291	-	4,4,4	0.97	0	6,6,6	0.67	0
4	GOL	M	1315	-	5,5,5	0.36	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BPH	L	1288	-	51,70,70	2.58	8 (15%)	52,101,101	1.92	11 (21%)

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
7	BPH	M	1311	-	-	18/37/105/105	0/5/6/6
6	LDA	L	1283	-	-	6/13/13/13	-
4	GOL	H	1255	-	-	2/4/4/4	-
13	SPO	M	1313	-	-	13/47/47/47	-
8	UQ2	L	1289[A]	-	-	8/15/39/39	0/1/1/1
5	BCL	L	1290	2	2/2/21/25	14/37/137/137	-
6	LDA	M	1307	-	-	6/13/13/13	-
6	LDA	M	1308	-	-	7/13/13/13	-
8	UQ2	L	1289[B]	-	-	6/15/39/39	0/1/1/1
6	LDA	L	1285	-	-	6/13/13/13	-
6	LDA	M	1306	-	-	4/13/13/13	-
4	GOL	H	1252	-	-	0/4/4/4	-
6	LDA	M	1309	-	-	8/13/13/13	-
6	LDA	L	1284	-	-	7/13/13/13	-
14	CDL	M	1314	-	-	55/91/91/110	-
10	HTO	L	1292	-	-	7/10/10/10	-
4	GOL	H	1253	-	-	2/4/4/4	-
4	GOL	H	1254	-	-	0/4/4/4	-
4	GOL	L	1294	-	-	4/4/4/4	-
5	BCL	M	1304	3	2/2/21/25	14/37/137/137	-
6	LDA	L	1286	-	-	5/13/13/13	-
12	U10	M	1312	-	-	7/45/69/87	0/1/1/1
5	BCL	M	1305	3	2/2/21/25	6/37/137/137	-
6	LDA	L	1287	-	-	9/13/13/13	-
5	BCL	L	1282	2	2/2/21/25	12/37/137/137	-
4	GOL	L	1293	-	-	2/4/4/4	-
4	GOL	M	1315	-	-	2/4/4/4	-
7	BPH	L	1288	-	-	5/37/105/105	0/5/6/6

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1313	SPO	C27-C28	12.68	1.47	1.34
7	M	1311	BPH	OBD-CAD	12.28	1.39	1.22
7	L	1288	BPH	OBD-CAD	10.54	1.37	1.22
5	M	1305	BCL	OBD-CAD	10.14	1.40	1.22
5	L	1282	BCL	OBD-CAD	9.72	1.39	1.22
5	L	1290	BCL	OBD-CAD	9.56	1.39	1.22
5	M	1304	BCL	OBD-CAD	9.51	1.38	1.22
13	M	1313	SPO	C9-C7	9.14	1.47	1.35
13	M	1313	SPO	C19-C17	8.46	1.47	1.35
13	M	1313	SPO	C14-C12	7.77	1.46	1.35
13	M	1313	SPO	C22-C23	7.65	1.45	1.35
7	L	1288	BPH	OBB-CAB	7.21	1.45	1.22
6	L	1287	LDA	O1-N1	-7.16	1.25	1.42
6	L	1285	LDA	O1-N1	-7.04	1.25	1.42
6	L	1286	LDA	O1-N1	-7.03	1.25	1.42
6	M	1309	LDA	O1-N1	-7.03	1.25	1.42
7	M	1311	BPH	O1D-CGD	7.02	1.38	1.21
6	M	1307	LDA	O1-N1	-6.99	1.25	1.42
6	L	1284	LDA	O1-N1	-6.94	1.25	1.42
6	L	1283	LDA	O1-N1	-6.92	1.26	1.42
12	M	1312	U10	C33-C34	6.84	1.49	1.33
14	M	1314	CDL	C11-CA5	-6.73	1.31	1.50
7	L	1288	BPH	O1D-CGD	6.71	1.38	1.21
6	M	1308	LDA	O1-N1	-6.63	1.26	1.42
8	L	1289[B]	UQ2	C8-C9	6.60	1.48	1.33
6	M	1306	LDA	O1-N1	-6.56	1.26	1.42
14	M	1314	CDL	C32-C31	-6.42	1.28	1.52
7	L	1288	BPH	C2-C3	6.32	1.48	1.33
7	M	1311	BPH	C2-C3	6.28	1.48	1.33
5	L	1290	BCL	O1A-CGA	6.27	1.41	1.22
12	M	1312	U10	C8-C9	6.25	1.48	1.33
12	M	1312	U10	C13-C14	6.24	1.48	1.33
7	M	1311	BPH	OBB-CAB	6.20	1.42	1.22
13	M	1313	SPO	C32-C33	6.17	1.47	1.33
12	M	1312	U10	C28-C29	6.11	1.47	1.33
7	L	1288	BPH	O1A-CGA	6.07	1.40	1.22
8	L	1289[A]	UQ2	C8-C9	6.07	1.47	1.33
7	M	1311	BPH	O1A-CGA	5.97	1.40	1.22
5	M	1305	BCL	O1A-CGA	5.88	1.40	1.22
12	M	1312	U10	C18-C19	5.82	1.46	1.33
12	M	1312	U10	C23-C24	5.72	1.46	1.33
13	M	1313	SPO	C37-C38	5.66	1.48	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	O1A-CGA	5.64	1.39	1.22
8	L	1289[A]	UQ2	C13-C14	5.52	1.48	1.32
5	L	1282	BCL	O1A-CGA	5.46	1.38	1.22
5	L	1290	BCL	C1B-NB	5.45	1.40	1.35
12	M	1312	U10	C38-C39	5.32	1.47	1.32
8	L	1289[A]	UQ2	O2-C2	-5.30	1.23	1.36
8	L	1289[B]	UQ2	C13-C14	5.21	1.47	1.32
13	M	1313	SPO	C6-C5	5.20	1.45	1.32
8	L	1289[B]	UQ2	O2-C2	-4.97	1.24	1.36
5	L	1282	BCL	C1B-NB	4.87	1.39	1.35
14	M	1314	CDL	OA6-CA5	4.84	1.48	1.34
14	M	1314	CDL	OA8-CA7	4.74	1.47	1.33
7	M	1311	BPH	C3D-C2D	4.73	1.47	1.39
8	L	1289[B]	UQ2	O3-C3	-4.70	1.25	1.36
7	L	1288	BPH	C3D-C2D	4.68	1.47	1.39
14	M	1314	CDL	OB6-CB5	4.58	1.47	1.34
8	L	1289[A]	UQ2	O3-C3	-4.53	1.25	1.36
13	M	1313	SPO	C10-C11	4.50	1.46	1.34
14	M	1314	CDL	C17-C16	-4.49	1.26	1.51
14	M	1314	CDL	C19-C18	-4.48	1.26	1.51
14	M	1314	CDL	C16-C15	-4.48	1.26	1.51
5	L	1282	BCL	C4D-ND	-4.46	1.31	1.37
14	M	1314	CDL	OB8-CB7	4.41	1.46	1.33
14	M	1314	CDL	C20-C19	-4.40	1.26	1.51
5	M	1305	BCL	C1B-NB	4.34	1.39	1.35
5	M	1305	BCL	C4B-NB	4.19	1.39	1.35
13	M	1313	SPO	C26-C25	4.16	1.45	1.34
13	M	1313	SPO	C15-C16	4.11	1.45	1.34
12	M	1312	U10	O4-C4	-4.07	1.26	1.36
5	M	1305	BCL	C4D-ND	-3.98	1.32	1.37
5	M	1304	BCL	C3D-C4D	-3.97	1.35	1.44
12	M	1312	U10	O3-C3	-3.92	1.27	1.36
5	M	1304	BCL	C1B-NB	3.83	1.38	1.35
12	M	1312	U10	C6-C1	3.80	1.42	1.35
5	L	1290	BCL	C4B-NB	3.57	1.38	1.35
5	L	1282	BCL	C4B-NB	3.53	1.38	1.35
13	M	1313	SPO	C21-C20	3.53	1.45	1.36
5	M	1305	BCL	C3D-C4D	-3.52	1.36	1.44
5	L	1282	BCL	C3D-C4D	-3.50	1.36	1.44
5	M	1304	BCL	C4D-ND	-3.38	1.33	1.37
5	M	1304	BCL	C4B-NB	3.34	1.38	1.35
5	M	1304	BCL	C2-C3	3.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1290	BCL	C2-C3	3.28	1.40	1.33
8	L	1289[B]	UQ2	C6-C5	3.26	1.41	1.35
5	L	1290	BCL	C4D-ND	-3.26	1.33	1.37
7	L	1288	BPH	O2D-CGD	-3.26	1.25	1.33
14	M	1314	CDL	C37-C36	-3.15	1.33	1.51
8	L	1289[A]	UQ2	C3-C4	-3.11	1.39	1.48
14	M	1314	CDL	C79-C78	-3.10	1.34	1.51
7	M	1311	BPH	O2D-CGD	-3.09	1.25	1.33
5	L	1290	BCL	O2D-CGD	-3.09	1.25	1.33
14	M	1314	CDL	C80-C79	-3.06	1.34	1.51
5	L	1290	BCL	C3D-C4D	-3.05	1.37	1.44
8	L	1289[B]	UQ2	C3-C4	-3.05	1.40	1.48
14	M	1314	CDL	C22-C21	-3.00	1.34	1.51
14	M	1314	CDL	C13-C12	-2.99	1.34	1.51
8	L	1289[B]	UQ2	C2-C1	-2.86	1.40	1.48
7	M	1311	BPH	O2A-CGA	-2.83	1.25	1.33
5	L	1282	BCL	O2A-CGA	-2.82	1.25	1.33
8	L	1289[A]	UQ2	C6-C5	2.80	1.40	1.35
5	M	1305	BCL	C2-C3	2.79	1.39	1.33
12	M	1312	U10	C4-C5	-2.76	1.40	1.48
7	M	1311	BPH	CBD-CGD	-2.65	1.48	1.52
5	M	1304	BCL	O2D-CGD	-2.63	1.26	1.33
5	L	1282	BCL	O2D-CGD	-2.58	1.26	1.33
5	L	1290	BCL	CHD-C4C	2.54	1.46	1.39
8	L	1289[A]	UQ2	C6-C1	-2.53	1.39	1.46
5	L	1282	BCL	C1D-C2D	-2.53	1.40	1.45
5	L	1282	BCL	C2-C3	2.51	1.39	1.33
7	L	1288	BPH	O2A-CGA	-2.47	1.26	1.33
5	M	1305	BCL	O2D-CGD	-2.45	1.27	1.33
5	M	1304	BCL	CHD-C4C	2.42	1.46	1.39
5	M	1304	BCL	O2A-CGA	-2.33	1.26	1.33
8	L	1289[A]	UQ2	C2-C1	-2.28	1.42	1.48
5	M	1305	BCL	O2A-CGA	-2.26	1.26	1.33
5	M	1305	BCL	C3B-C2B	-2.26	1.35	1.39
5	M	1305	BCL	CHD-C4C	2.22	1.45	1.39
5	L	1282	BCL	MG-ND	-2.20	2.01	2.05
5	L	1290	BCL	O2A-CGA	-2.13	1.27	1.33
5	M	1305	BCL	C1D-C2D	-2.11	1.41	1.45
5	L	1282	BCL	O1D-CGD	2.10	1.26	1.21
5	M	1305	BCL	OBB-CAB	2.09	1.29	1.22
8	L	1289[B]	UQ2	C6-C1	-2.09	1.40	1.46
5	L	1282	BCL	CHD-C4C	2.06	1.45	1.39

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1314	CDL	C20-C19-C18	11.98	175.25	114.42
14	M	1314	CDL	C17-C16-C15	11.86	174.65	114.42
14	M	1314	CDL	C13-C12-C11	9.67	147.97	113.19
14	M	1314	CDL	C34-C33-C32	9.18	161.05	114.42
7	L	1288	BPH	O2D-CGD-CBD	8.73	122.05	111.00
5	M	1304	BCL	CMB-C2B-C1B	-7.88	116.34	128.46
7	M	1311	BPH	O2D-CGD-CBD	7.44	120.43	111.00
14	M	1314	CDL	C33-C32-C31	7.35	139.63	113.19
5	M	1304	BCL	C1D-ND-C4D	6.56	111.00	106.33
5	L	1290	BCL	CMB-C2B-C1B	-6.32	118.75	128.46
5	M	1304	BCL	C2D-C1D-ND	-6.00	105.68	110.10
5	L	1282	BCL	O2D-CGD-CBD	5.80	121.57	111.27
5	L	1290	BCL	C1C-NC-C4C	-5.78	104.11	106.71
14	M	1314	CDL	C12-C11-CA5	5.68	134.27	113.62
5	M	1305	BCL	CMB-C2B-C1B	-5.51	120.00	128.46
5	L	1282	BCL	CMB-C2B-C1B	-5.44	120.10	128.46
14	M	1314	CDL	OA6-CA5-C11	5.14	122.57	111.50
5	L	1282	BCL	C1D-ND-C4D	5.09	109.95	106.33
5	L	1290	BCL	CMD-C2D-C1D	5.05	133.62	124.71
5	L	1290	BCL	C4A-NA-C1A	4.99	108.95	106.71
5	M	1305	BCL	C2D-C1D-ND	-4.82	106.55	110.10
13	M	1313	SPO	C10-C9-C7	-4.71	120.59	127.31
5	M	1304	BCL	CMB-C2B-C3B	4.70	133.48	124.68
5	L	1282	BCL	C2D-C1D-ND	-4.68	106.65	110.10
5	M	1305	BCL	C1C-NC-C4C	4.68	108.81	106.71
12	M	1312	U10	C30-C29-C31	4.50	122.84	115.27
5	L	1290	BCL	C1D-ND-C4D	4.40	109.46	106.33
13	M	1313	SPO	C20-C19-C17	-4.37	121.07	127.31
5	M	1305	BCL	CMD-C2D-C1D	4.33	132.34	124.71
5	L	1282	BCL	CMD-C2D-C1D	4.32	132.32	124.71
5	M	1305	BCL	O2D-CGD-CBD	4.29	118.89	111.27
7	L	1288	BPH	O1D-CGD-CBD	-4.23	117.70	124.74
7	M	1311	BPH	OBD-CAD-CBD	-4.23	119.62	125.82
5	M	1305	BCL	C1D-ND-C4D	4.22	109.34	106.33
5	L	1290	BCL	CMB-C2B-C3B	4.19	132.53	124.68
5	M	1304	BCL	O2D-CGD-CBD	4.18	118.70	111.27
5	L	1290	BCL	C2D-C1D-ND	-4.15	107.04	110.10
13	M	1313	SPO	C21-C22-C23	-4.11	121.44	127.31
14	M	1314	CDL	OB6-CB5-C51	4.08	120.30	111.50
7	M	1311	BPH	O1D-CGD-CBD	-4.07	117.96	124.74
8	L	1289[A]	UQ2	C10-C9-C11	3.92	121.87	115.27
14	M	1314	CDL	C35-C34-C33	3.92	134.30	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	1289[A]	UQ2	CM5-C5-C6	-3.89	118.06	124.40
5	L	1290	BCL	O2D-CGD-CBD	3.80	118.02	111.27
13	M	1313	SPO	C29-C28-C30	3.71	121.52	115.27
5	M	1304	BCL	C1-O2A-CGA	3.65	126.03	116.44
13	M	1313	SPO	C15-C14-C12	-3.63	122.13	127.31
12	M	1312	U10	C25-C24-C26	3.59	121.30	115.27
5	M	1305	BCL	C4A-NA-C1A	3.59	108.32	106.71
5	M	1305	BCL	OBB-CAB-C3B	3.58	126.34	119.99
5	M	1305	BCL	O2A-CGA-CBA	3.48	122.83	111.91
7	M	1311	BPH	CED-O2D-CGD	3.42	123.67	115.94
7	L	1288	BPH	OBD-CAD-CBD	-3.41	120.82	125.82
5	M	1305	BCL	C16-C15-C13	-3.38	104.98	115.92
8	L	1289[A]	UQ2	O1-C1-C6	-3.34	115.69	121.55
5	L	1290	BCL	CMA-C3A-C4A	-3.34	102.80	111.77
8	L	1289[A]	UQ2	CM3-O3-C3	3.28	128.11	116.47
5	M	1304	BCL	O2A-CGA-CBA	3.28	122.20	111.91
12	M	1312	U10	C10-C9-C11	3.25	120.74	115.27
5	L	1282	BCL	C4-C3-C5	3.25	120.73	115.27
7	M	1311	BPH	CAC-C3C-C4C	3.25	120.99	113.73
5	M	1305	BCL	CMB-C2B-C3B	3.22	130.70	124.68
5	M	1304	BCL	CMD-C2D-C1D	3.17	130.30	124.71
5	L	1282	BCL	CMB-C2B-C3B	3.14	130.56	124.68
12	M	1312	U10	C15-C14-C16	3.13	120.53	115.27
5	L	1290	BCL	C4B-CHC-C1C	-3.11	123.97	130.12
5	L	1290	BCL	CMD-C2D-C3D	-3.06	120.57	127.61
5	M	1305	BCL	CED-O2D-CGD	3.04	122.81	115.94
5	L	1282	BCL	O2A-CGA-CBA	3.04	121.44	111.91
5	M	1304	BCL	C4B-CHC-C1C	-3.03	124.11	130.12
14	M	1314	CDL	OA8-CA7-C31	3.00	121.33	111.91
7	M	1311	BPH	CMB-C2B-C3B	3.00	130.28	124.68
7	L	1288	BPH	CED-O2D-CGD	2.99	122.70	115.94
5	L	1290	BCL	O2A-CGA-CBA	2.96	121.20	111.91
5	M	1304	BCL	O1D-CGD-CBD	-2.93	118.48	124.48
5	L	1290	BCL	CHD-C4C-NC	-2.90	121.86	125.08
5	M	1305	BCL	C1D-CHD-C4C	-2.82	119.82	126.62
12	M	1312	U10	C22-C23-C24	-2.81	120.90	127.66
14	M	1314	CDL	OB8-CB7-C71	2.80	120.70	111.91
13	M	1313	SPO	C20-C21-C22	-2.80	117.75	123.47
5	M	1304	BCL	CED-O2D-CGD	2.76	122.18	115.94
5	L	1282	BCL	C4A-NA-C1A	2.75	107.94	106.71
5	M	1305	BCL	C7-C6-C5	-2.75	105.90	113.36
5	L	1290	BCL	CED-O2D-CGD	2.74	122.14	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	1313	SPO	C40-C38-C39	2.71	120.58	114.60
7	L	1288	BPH	C4B-NB-C1B	-2.70	101.55	107.09
5	L	1290	BCL	C1-O2A-CGA	2.69	123.49	116.44
8	L	1289[A]	UQ2	C7-C8-C9	-2.68	122.33	126.79
13	M	1313	SPO	C14-C15-C16	-2.68	114.86	123.22
12	M	1312	U10	C12-C13-C14	-2.67	121.22	127.66
5	L	1282	BCL	C4B-CHC-C1C	-2.67	124.83	130.12
7	L	1288	BPH	O2A-CGA-CBA	2.67	120.27	111.91
13	M	1313	SPO	C34-C33-C35	2.65	119.73	115.27
7	M	1311	BPH	CMA-C3A-C4A	-2.61	108.65	114.38
7	M	1311	BPH	CBA-CAA-C2A	-2.59	106.25	113.81
5	L	1282	BCL	CMD-C2D-C3D	-2.59	121.66	127.61
14	M	1314	CDL	OA6-CA5-OA7	-2.59	117.45	123.70
5	L	1290	BCL	C3C-C4C-CHD	-2.58	117.87	123.39
5	L	1282	BCL	C1-O2A-CGA	2.58	123.20	116.44
5	L	1282	BCL	O1D-CGD-CBD	-2.55	119.26	124.48
7	L	1288	BPH	C4C-C3C-C2C	-2.55	100.41	102.84
5	M	1305	BCL	CMD-C2D-C3D	-2.55	121.75	127.61
5	L	1282	BCL	C1B-CHB-C4A	-2.55	125.07	130.12
5	M	1305	BCL	O2D-CGD-O1D	-2.54	118.88	123.84
12	M	1312	U10	C30-C29-C28	-2.53	117.20	123.68
5	L	1282	BCL	CAA-C2A-C3A	-2.52	105.88	112.78
7	L	1288	BPH	O2A-CGA-O1A	-2.50	117.29	123.59
13	M	1313	SPO	C13-C12-C11	2.48	121.99	118.08
5	L	1290	BCL	C2A-C3A-C4A	2.48	105.87	101.87
5	L	1290	BCL	O2A-CGA-O1A	-2.47	117.35	123.59
5	L	1282	BCL	C1D-CHD-C4C	-2.44	120.74	126.62
13	M	1313	SPO	C25-C23-C22	-2.42	115.23	118.94
5	M	1305	BCL	CBB-CAB-C3B	-2.40	113.20	120.34
5	L	1282	BCL	O2D-CGD-O1D	-2.39	119.16	123.84
13	M	1313	SPO	C8-C7-C6	2.35	121.78	118.08
12	M	1312	U10	C35-C34-C36	2.34	119.21	115.27
5	M	1305	BCL	C3C-C4C-CHD	-2.34	118.40	123.39
13	M	1313	SPO	C16-C17-C19	-2.33	115.37	118.94
13	M	1313	SPO	C24-C23-C25	2.32	121.74	118.08
8	L	1289[B]	UQ2	C16-C14-C15	2.32	119.73	114.60
5	M	1304	BCL	O2A-CGA-O1A	-2.31	117.75	123.59
8	L	1289[A]	UQ2	C16-C14-C15	2.30	119.69	114.60
5	M	1304	BCL	CHA-C1A-NA	-2.29	121.15	126.40
12	M	1312	U10	O5-C5-C4	-2.29	116.06	120.93
13	M	1313	SPO	C27-C26-C25	-2.29	116.07	123.22
8	L	1289[B]	UQ2	C10-C9-C11	2.28	119.11	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1311	BPH	C1-O2A-CGA	2.28	122.42	116.44
7	M	1311	BPH	C1-C2-C3	-2.26	122.13	126.04
5	L	1290	BCL	C14-C13-C12	2.24	119.42	111.29
5	M	1305	BCL	CHD-C1D-ND	-2.22	122.41	124.45
12	M	1312	U10	C27-C28-C29	-2.22	122.31	127.66
7	M	1311	BPH	CBC-CAC-C3C	2.20	118.19	113.77
12	M	1312	U10	C41-C39-C40	2.19	119.45	114.60
13	M	1313	SPO	C31-C32-C33	-2.19	122.38	127.66
7	L	1288	BPH	C1-C2-C3	-2.18	122.28	126.04
5	L	1282	BCL	O2A-CGA-O1A	-2.17	118.11	123.59
12	M	1312	U10	C20-C19-C21	2.17	118.92	115.27
5	L	1290	BCL	CHD-C1D-C2D	2.15	130.00	125.48
5	L	1290	BCL	O2D-CGD-O1D	-2.15	119.63	123.84
7	L	1288	BPH	C4A-C3A-C2A	-2.15	100.79	102.84
5	L	1290	BCL	C1D-CHD-C4C	-2.15	121.45	126.62
14	M	1314	CDL	CA4-OA6-CA5	-2.12	112.57	117.79
5	L	1282	BCL	C1-C2-C3	-2.09	122.43	126.04
8	L	1289[B]	UQ2	C12-C13-C14	-2.07	120.66	127.75
13	M	1313	SPO	C10-C11-C12	-2.06	120.62	126.42
8	L	1289[A]	UQ2	CM2-O2-C2	2.05	123.74	116.47
7	M	1311	BPH	CAC-C3C-C2C	-2.05	109.14	114.26
7	M	1311	BPH	O2A-CGA-CBA	2.04	118.32	111.91
7	L	1288	BPH	C1C-C2C-C3C	-2.02	100.91	102.84
8	L	1289[B]	UQ2	CM2-O2-C2	2.01	123.60	116.47
5	M	1305	BCL	O2A-CGA-O1A	-2.01	118.52	123.59
8	L	1289[A]	UQ2	O4-C4-C3	-2.01	116.67	120.93
5	M	1305	BCL	C4B-C3B-CAB	2.00	130.99	127.13

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	L	1290	BCL	C8
5	L	1290	BCL	C13
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	M	1305	BCL	C8
5	M	1305	BCL	C13

All (235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1253	GOL	O1-C1-C2-C3
4	L	1293	GOL	C1-C2-C3-O3
4	L	1294	GOL	C1-C2-C3-O3
4	L	1294	GOL	O2-C2-C3-O3
5	L	1290	BCL	C14-C13-C15-C16
5	M	1304	BCL	C1-C2-C3-C4
5	M	1304	BCL	C1-C2-C3-C5
6	L	1287	LDA	N1-C1-C2-C3
7	M	1311	BPH	C4C-C3C-CAC-CBC
7	M	1311	BPH	C2C-C3C-CAC-CBC
7	M	1311	BPH	C1-C2-C3-C4
8	L	1289[A]	UQ2	C7-C8-C9-C10
8	L	1289[A]	UQ2	C7-C8-C9-C11
8	L	1289[A]	UQ2	C12-C13-C14-C16
8	L	1289[B]	UQ2	C12-C11-C9-C8
8	L	1289[B]	UQ2	C12-C11-C9-C10
10	L	1292	HTO	C1-C2-C3-O3
10	L	1292	HTO	C1-C2-C3-C4
10	L	1292	HTO	O2-C2-C3-O3
10	L	1292	HTO	O2-C2-C3-C4
12	M	1312	U10	C27-C28-C29-C30
12	M	1312	U10	C27-C28-C29-C31
12	M	1312	U10	C29-C31-C32-C33
13	M	1313	SPO	C3-C1-O1-CM1
13	M	1313	SPO	C4-C1-O1-CM1
13	M	1313	SPO	C4-C5-C6-C7
13	M	1313	SPO	C8-C7-C9-C10
13	M	1313	SPO	C36-C37-C38-C39
13	M	1313	SPO	C36-C37-C38-C40
14	M	1314	CDL	CA3-OA5-PA1-OA3
14	M	1314	CDL	CB3-OB5-PB2-OB4
14	M	1314	CDL	OB7-CB5-OB6-CB4
5	M	1304	BCL	C10-C11-C12-C13
8	L	1289[B]	UQ2	C12-C13-C14-C15
14	M	1314	CDL	OA9-CA7-OA8-CA6
14	M	1314	CDL	C31-CA7-OA8-CA6
14	M	1314	CDL	C51-CB5-OB6-CB4
8	L	1289[B]	UQ2	C12-C13-C14-C16
8	L	1289[A]	UQ2	C12-C11-C9-C10
12	M	1312	U10	C30-C29-C31-C32
8	L	1289[A]	UQ2	C12-C11-C9-C8
14	M	1314	CDL	C20-C21-C22-C23
14	M	1314	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
8	L	1289[A]	UQ2	C12-C13-C14-C15
14	M	1314	CDL	C15-C16-C17-C18
14	M	1314	CDL	OB9-CB7-OB8-CB6
13	M	1313	SPO	C19-C20-C21-C22
5	M	1304	BCL	C3-C5-C6-C7
14	M	1314	CDL	C71-CB7-OB8-CB6
8	L	1289[A]	UQ2	C9-C11-C12-C13
7	M	1311	BPH	C5-C6-C7-C8
14	M	1314	CDL	O1-C1-CB2-OB2
12	M	1312	U10	C28-C29-C31-C32
5	L	1282	BCL	C6-C7-C8-C9
5	L	1290	BCL	C6-C7-C8-C9
5	M	1305	BCL	C11-C10-C8-C9
5	M	1304	BCL	C8-C10-C11-C12
5	L	1290	BCL	C10-C11-C12-C13
5	L	1290	BCL	C11-C10-C8-C7
5	M	1305	BCL	C6-C7-C8-C10
7	M	1311	BPH	C11-C10-C8-C7
13	M	1313	SPO	C33-C35-C36-C37
5	L	1290	BCL	C15-C16-C17-C18
12	M	1312	U10	C31-C32-C33-C34
14	M	1314	CDL	CA3-OA5-PA1-OA2
14	M	1314	CDL	CB3-OB5-PB2-OB2
6	M	1308	LDA	C4-C5-C6-C7
6	L	1284	LDA	C6-C7-C8-C9
6	M	1307	LDA	C6-C7-C8-C9
6	L	1285	LDA	C7-C8-C9-C10
13	M	1313	SPO	C6-C7-C9-C10
10	L	1292	HTO	O1-C1-C2-O2
7	M	1311	BPH	C16-C17-C18-C20
14	M	1314	CDL	C71-C72-C73-C74
5	L	1290	BCL	C11-C10-C8-C9
6	L	1284	LDA	C7-C8-C9-C10
6	M	1308	LDA	C2-C3-C4-C5
6	M	1309	LDA	C5-C6-C7-C8
14	M	1314	CDL	C53-C54-C55-C56
7	M	1311	BPH	C13-C15-C16-C17
4	H	1255	GOL	O1-C1-C2-C3
4	L	1294	GOL	O1-C1-C2-C3
4	M	1315	GOL	O1-C1-C2-C3
6	M	1308	LDA	C3-C4-C5-C6
6	L	1287	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
6	M	1309	LDA	C7-C8-C9-C10
6	M	1309	LDA	C2-C3-C4-C5
6	L	1284	LDA	C2-C3-C4-C5
14	M	1314	CDL	C17-C18-C19-C20
14	M	1314	CDL	C80-C81-C82-C83
14	M	1314	CDL	C19-C20-C21-C22
6	L	1287	LDA	C7-C8-C9-C10
6	L	1287	LDA	C3-C4-C5-C6
5	M	1304	BCL	C4-C3-C5-C6
7	M	1311	BPH	C2-C3-C5-C6
14	M	1314	CDL	C11-CA5-OA6-CA4
14	M	1314	CDL	C52-C53-C54-C55
4	H	1253	GOL	O1-C1-C2-O2
4	L	1294	GOL	O1-C1-C2-O2
4	M	1315	GOL	O1-C1-C2-O2
6	L	1283	LDA	C3-C4-C5-C6
6	M	1306	LDA	C7-C8-C9-C10
14	M	1314	CDL	C11-C12-C13-C14
6	L	1286	LDA	C3-C4-C5-C6
14	M	1314	CDL	C16-C17-C18-C19
14	M	1314	CDL	CA2-C1-CB2-OB2
6	M	1306	LDA	C3-C4-C5-C6
6	M	1308	LDA	C7-C8-C9-C10
14	M	1314	CDL	OA7-CA5-OA6-CA4
5	M	1304	BCL	C2-C1-O2A-CGA
6	L	1287	LDA	C2-C3-C4-C5
14	M	1314	CDL	C74-C75-C76-C77
6	L	1283	LDA	C5-C6-C7-C8
14	M	1314	CDL	C32-C33-C34-C35
6	L	1285	LDA	C11-C10-C9-C8
7	M	1311	BPH	C10-C11-C12-C13
6	L	1286	LDA	C4-C5-C6-C7
6	L	1287	LDA	C11-C10-C9-C8
7	M	1311	BPH	C4-C3-C5-C6
5	L	1282	BCL	C12-C13-C15-C16
7	L	1288	BPH	C2-C3-C5-C6
5	L	1282	BCL	C16-C17-C18-C19
6	L	1287	LDA	C5-C6-C7-C8
6	M	1308	LDA	C5-C6-C7-C8
14	M	1314	CDL	CA5-C11-C12-C13
7	M	1311	BPH	C16-C17-C18-C19
7	L	1288	BPH	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
7	M	1311	BPH	C11-C12-C13-C14
6	L	1286	LDA	C6-C7-C8-C9
5	L	1282	BCL	C16-C17-C18-C20
14	M	1314	CDL	OA5-CA3-CA4-CA6
6	L	1285	LDA	C1-C2-C3-C4
13	M	1313	SPO	C1-C4-C5-C6
6	M	1307	LDA	C3-C4-C5-C6
14	M	1314	CDL	C12-C13-C14-C15
14	M	1314	CDL	C54-C55-C56-C57
6	L	1284	LDA	C1-C2-C3-C4
14	M	1314	CDL	CA3-CA4-CA6-OA8
5	L	1282	BCL	C13-C15-C16-C17
6	L	1287	LDA	C9-C10-C11-C12
6	M	1307	LDA	C1-C2-C3-C4
14	M	1314	CDL	C81-C82-C83-C84
6	L	1285	LDA	C9-C10-C11-C12
13	M	1313	SPO	C21-C22-C23-C24
5	L	1290	BCL	C8-C10-C11-C12
6	L	1283	LDA	C9-C10-C11-C12
14	M	1314	CDL	C14-C15-C16-C17
14	M	1314	CDL	C40-C41-C42-C43
14	M	1314	CDL	CB7-C71-C72-C73
13	M	1313	SPO	C2-C1-O1-CM1
5	M	1304	BCL	C2-C3-C5-C6
5	M	1304	BCL	C11-C12-C13-C15
5	M	1305	BCL	C12-C13-C15-C16
7	M	1311	BPH	C11-C12-C13-C15
5	L	1282	BCL	C14-C13-C15-C16
5	M	1304	BCL	C11-C12-C13-C14
6	L	1285	LDA	N1-C1-C2-C3
6	M	1307	LDA	N1-C1-C2-C3
6	M	1308	LDA	N1-C1-C2-C3
6	M	1309	LDA	N1-C1-C2-C3
6	M	1307	LDA	C2-C3-C4-C5
7	L	1288	BPH	C8-C10-C11-C12
8	L	1289[B]	UQ2	C9-C11-C12-C13
6	M	1309	LDA	C11-C10-C9-C8
10	L	1292	HTO	C4-C5-C6-C7
7	M	1311	BPH	C8-C10-C11-C12
7	M	1311	BPH	O2A-C1-C2-C3
14	M	1314	CDL	OA5-CA3-CA4-OA6
14	M	1314	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
5	M	1304	BCL	C11-C10-C8-C9
5	M	1305	BCL	C14-C13-C15-C16
14	M	1314	CDL	C72-C73-C74-C75
5	M	1304	BCL	C4C-C3C-CAC-CBC
14	M	1314	CDL	C39-C40-C41-C42
5	L	1290	BCL	C16-C17-C18-C19
5	L	1282	BCL	C6-C7-C8-C10
5	L	1290	BCL	C12-C13-C15-C16
5	M	1304	BCL	C11-C10-C8-C7
5	L	1290	BCL	C13-C15-C16-C17
6	L	1287	LDA	C1-C2-C3-C4
5	M	1304	BCL	CAD-CBD-CGD-O2D
7	M	1311	BPH	CAD-CBD-CGD-O2D
10	L	1292	HTO	O3-C3-C4-C5
6	M	1306	LDA	C2-C3-C4-C5
8	L	1289[B]	UQ2	C1-C2-O2-CM2
6	M	1309	LDA	C2-C1-N1-CM1
6	M	1309	LDA	C2-C1-N1-CM2
13	M	1313	SPO	C21-C22-C23-C25
14	M	1314	CDL	OA6-CA4-CA6-OA8
4	L	1293	GOL	O2-C2-C3-O3
6	L	1286	LDA	C9-C10-C11-C12
6	L	1283	LDA	C11-C10-C9-C8
14	M	1314	CDL	C55-C56-C57-C58
14	M	1314	CDL	CA3-OA5-PA1-OA4
14	M	1314	CDL	CB3-OB5-PB2-OB3
14	M	1314	CDL	OB5-CB3-CB4-CB6
5	L	1282	BCL	C3-C5-C6-C7
14	M	1314	CDL	CA7-C31-C32-C33
14	M	1314	CDL	CB2-C1-CA2-OA2
6	L	1283	LDA	C6-C7-C8-C9
6	L	1284	LDA	C11-C10-C9-C8
5	L	1282	BCL	C8-C10-C11-C12
6	L	1286	LDA	C2-C3-C4-C5
6	M	1308	LDA	C6-C7-C8-C9
6	M	1307	LDA	C7-C8-C9-C10
7	M	1311	BPH	C1-C2-C3-C5
5	L	1290	BCL	C11-C12-C13-C14
14	M	1314	CDL	C1-CB2-OB2-PB2
6	L	1284	LDA	C4-C5-C6-C7
4	H	1255	GOL	O1-C1-C2-O2
6	L	1285	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	M	1314	CDL	C31-C32-C33-C34
14	M	1314	CDL	C75-C76-C77-C78
7	M	1311	BPH	C11-C10-C8-C9
7	L	1288	BPH	O2A-C1-C2-C3
5	M	1305	BCL	C11-C10-C8-C7
8	L	1289[A]	UQ2	C3-C2-O2-CM2
5	L	1282	BCL	C5-C6-C7-C8
12	M	1312	U10	C5-C4-O4-C4M
6	L	1284	LDA	C9-C10-C11-C12
5	L	1290	BCL	C2-C1-O2A-CGA
6	L	1283	LDA	C2-C3-C4-C5
6	M	1306	LDA	C11-C10-C9-C8
14	M	1314	CDL	C13-C14-C15-C16
5	L	1282	BCL	C11-C12-C13-C14
14	M	1314	CDL	O1-C1-CA2-OA2
5	L	1290	BCL	CAD-CBD-CGD-O2D
7	L	1288	BPH	CAD-CBD-CGD-O2D
14	M	1314	CDL	C21-C22-C23-C24
14	M	1314	CDL	C72-C71-CB7-OB8
5	L	1282	BCL	CHA-CBD-CGD-O1D
14	M	1314	CDL	C72-C71-CB7-OB9
5	M	1305	BCL	CAA-CBA-CGA-O2A
5	L	1290	BCL	C5-C6-C7-C8
6	M	1309	LDA	C2-C1-N1-O1

There are no ring outliers.

17 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1311	BPH	9	0
13	M	1313	SPO	2	0
8	L	1289[A]	UQ2	6	0
5	L	1290	BCL	2	0
6	M	1308	LDA	3	0
8	L	1289[B]	UQ2	1	0
6	M	1306	LDA	1	0
4	H	1252	GOL	5	0
6	M	1309	LDA	2	0
14	M	1314	CDL	3	0
5	M	1304	BCL	9	0
12	M	1312	U10	1	0
5	M	1305	BCL	14	0

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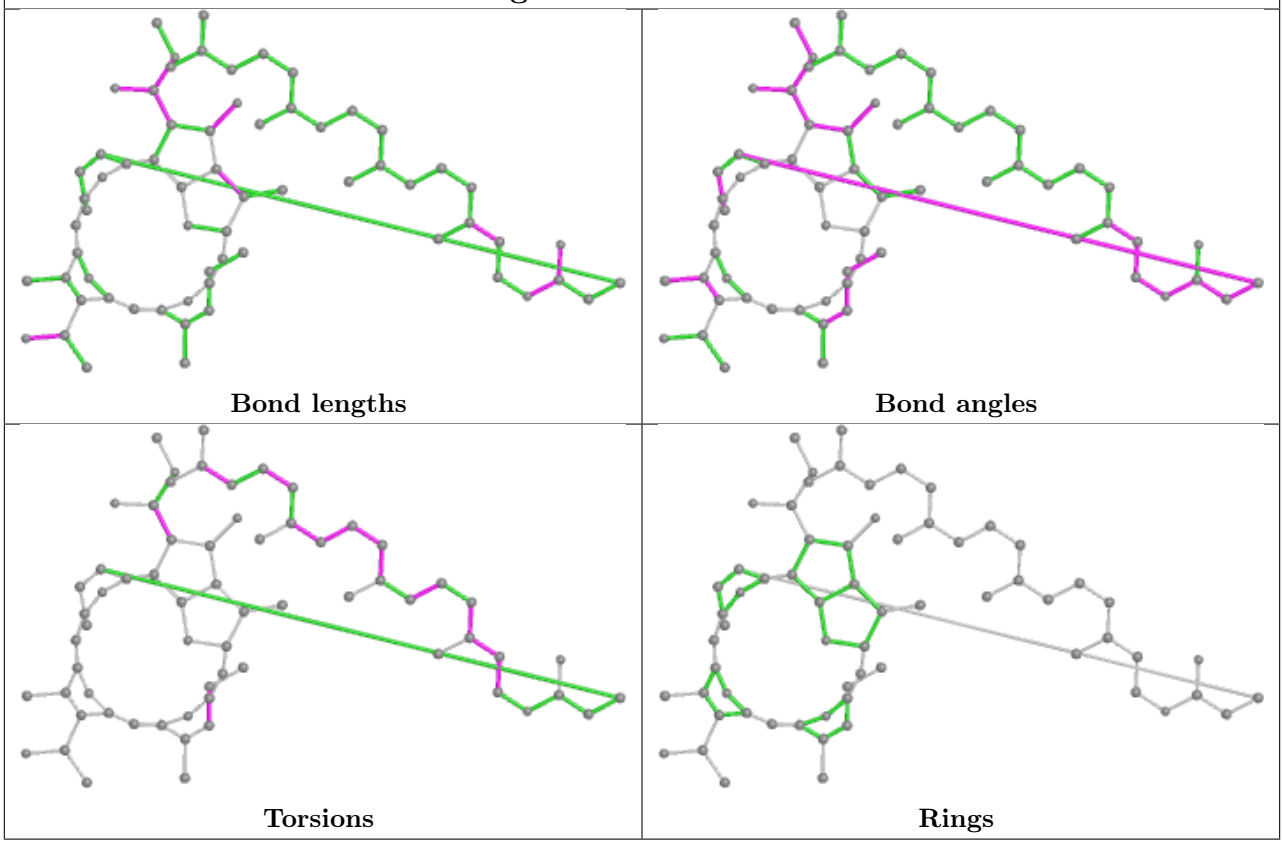
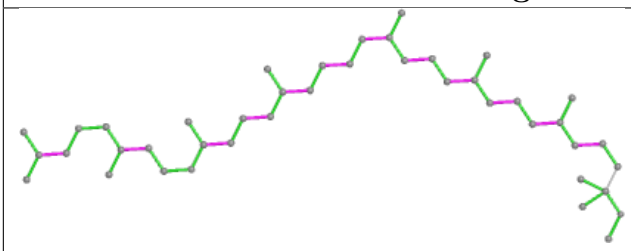
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1287	LDA	1	0
5	L	1282	BCL	4	0
4	L	1293	GOL	1	0
7	L	1288	BPH	6	0

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.

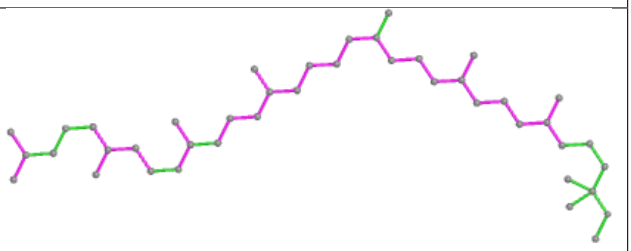
Ligand BPH M 1311



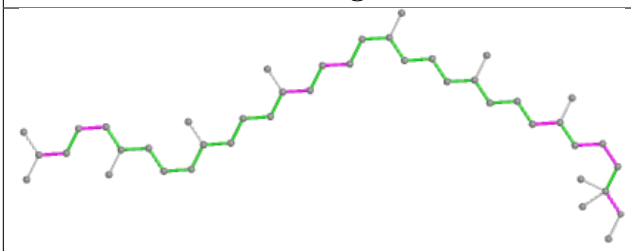
Ligand SPO M 1313



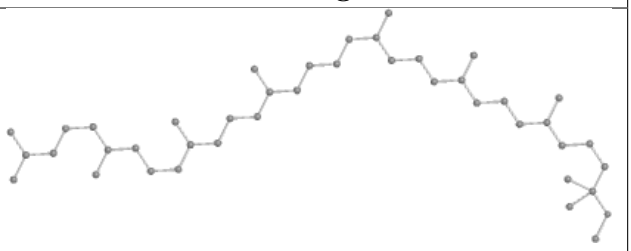
Bond lengths



Bond angles

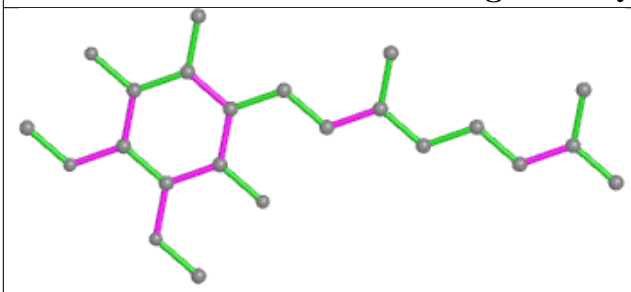


Torsions

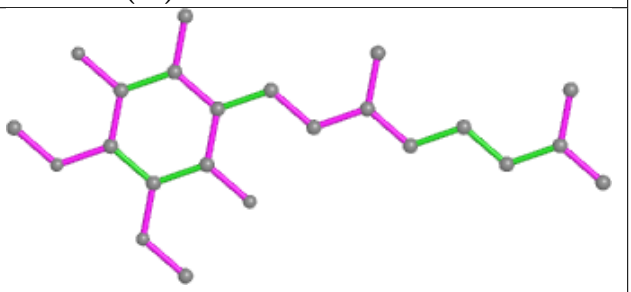


Rings

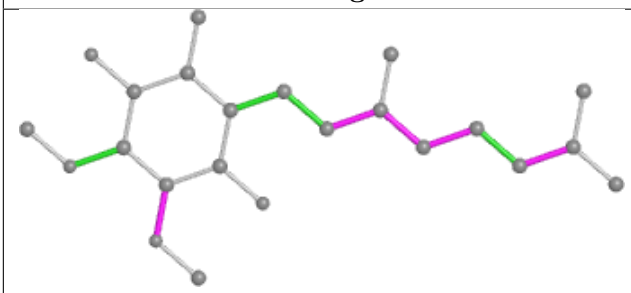
Ligand UQ2 L 1289 (A)



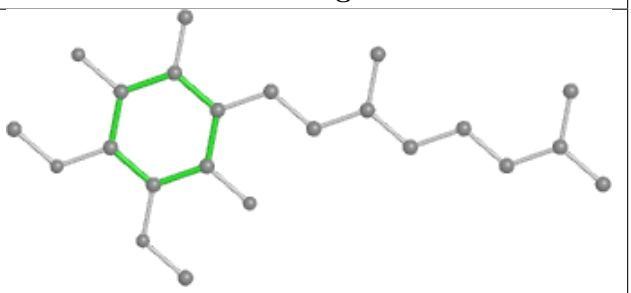
Bond lengths



Bond angles

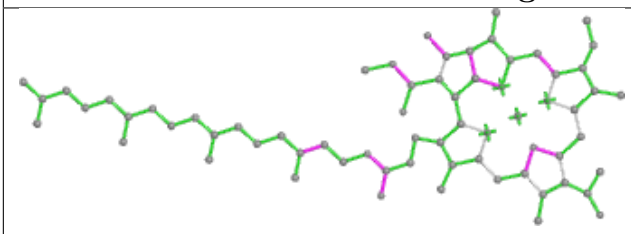


Torsions

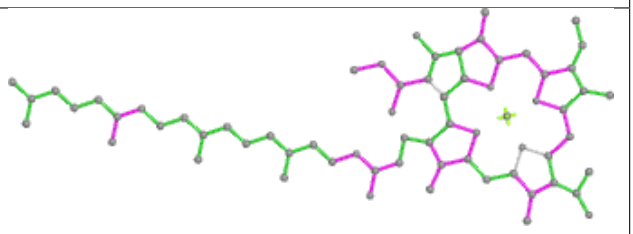


Rings

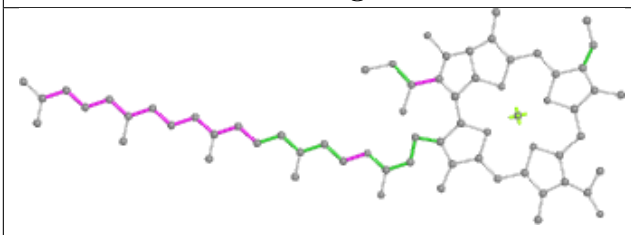
Ligand BCL L 1290



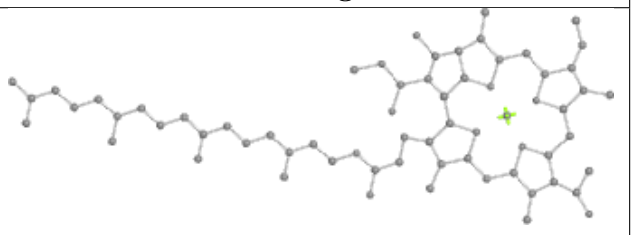
Bond lengths



Bond angles

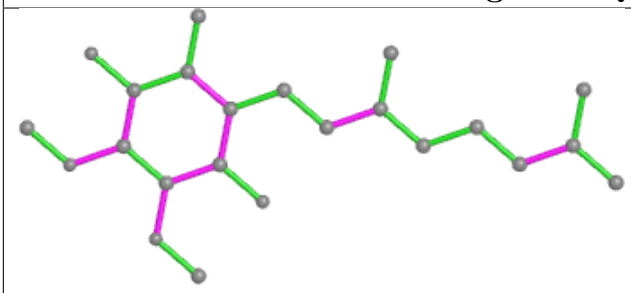


Torsions

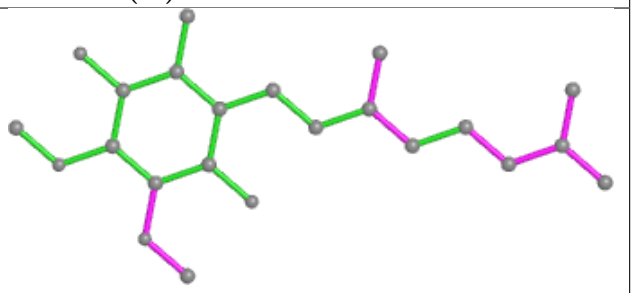


Rings

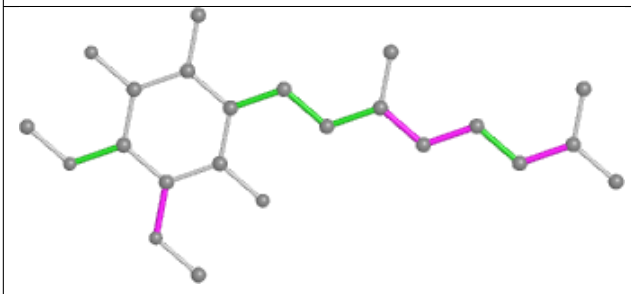
Ligand UQ2 L 1289 (B)



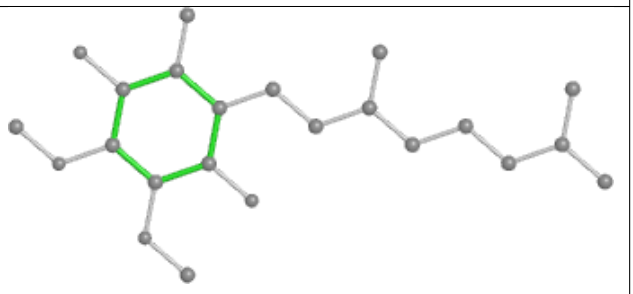
Bond lengths



Bond angles

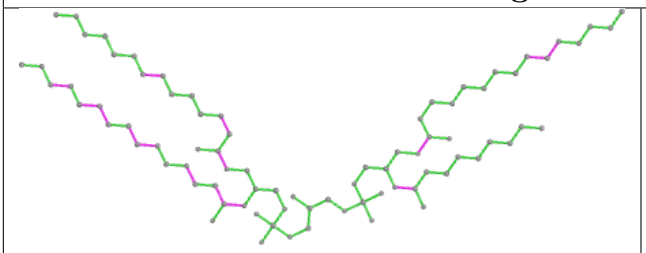


Torsions

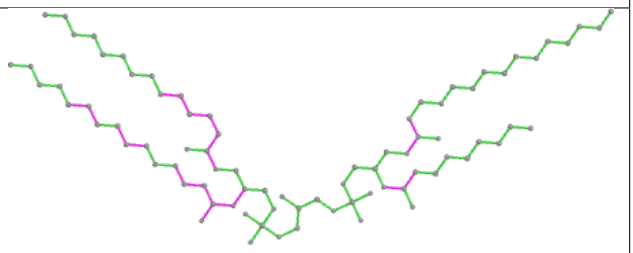


Rings

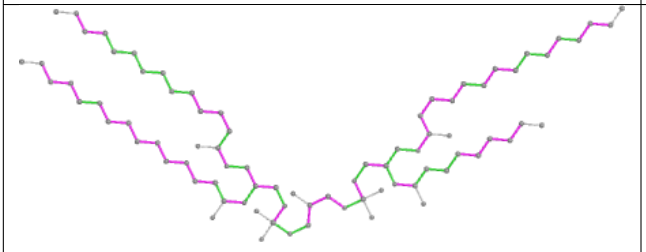
Ligand CDL M 1314



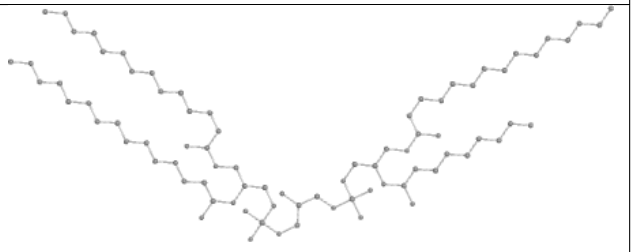
Bond lengths



Bond angles

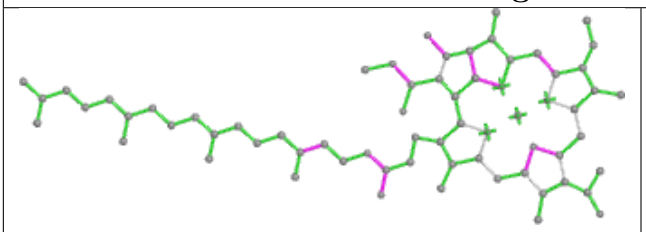


Torsions

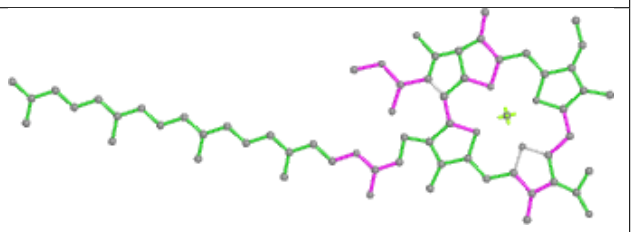


Rings

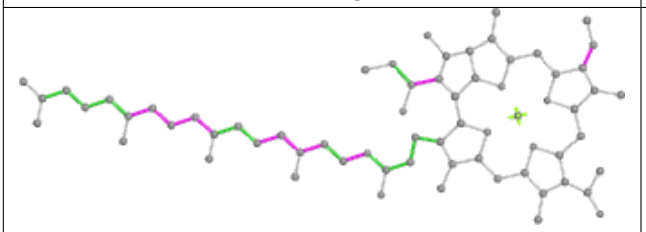
Ligand BCL M 1304



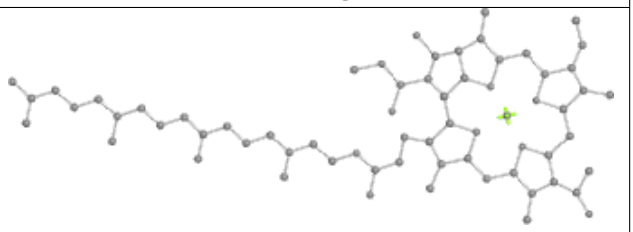
Bond lengths



Bond angles

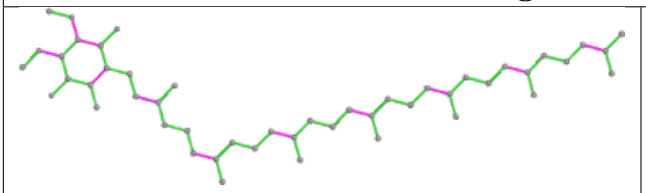


Torsions

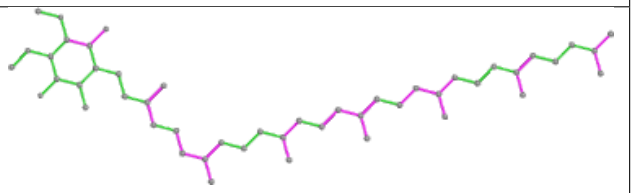


Rings

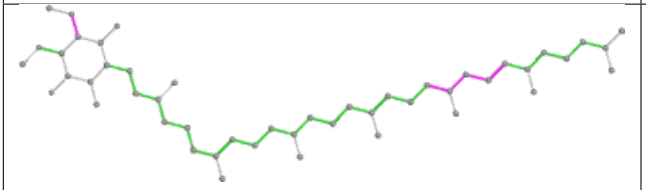
Ligand U10 M 1312



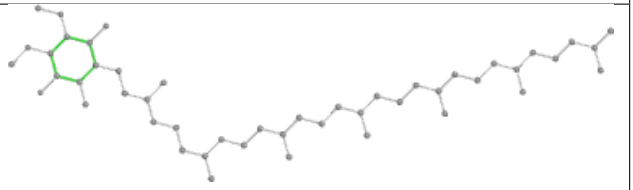
Bond lengths



Bond angles

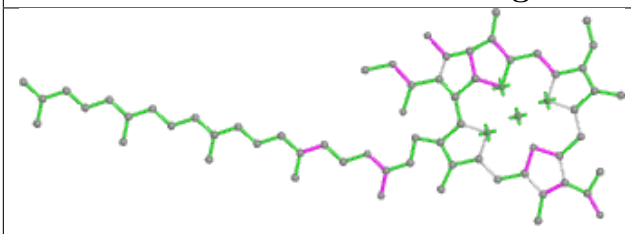


Torsions

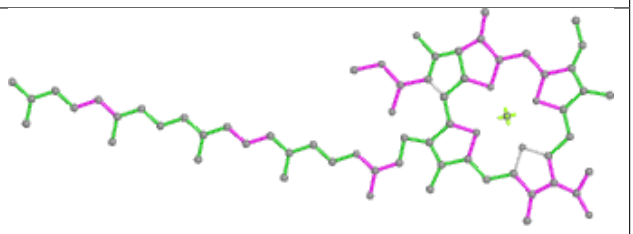


Rings

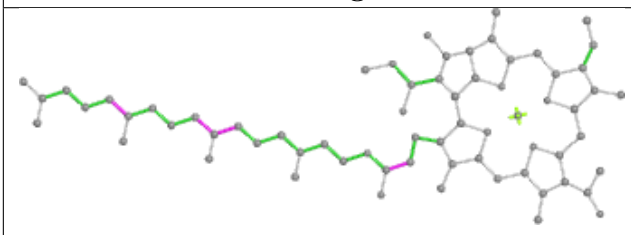
Ligand BCL M 1305



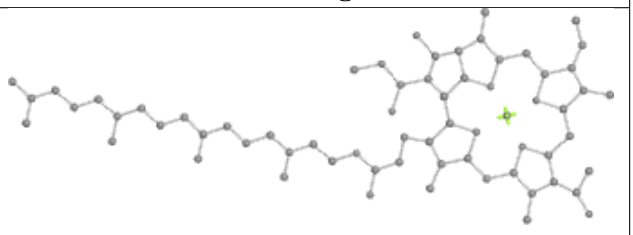
Bond lengths



Bond angles

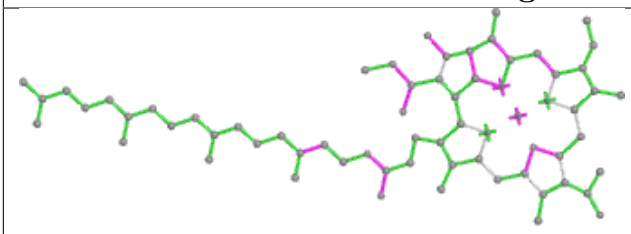


Torsions

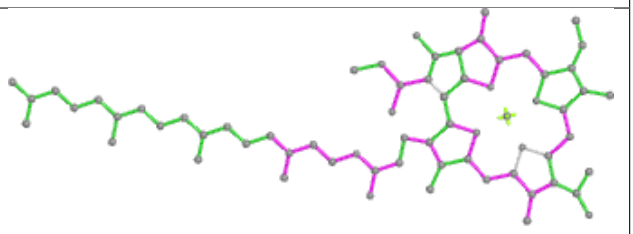


Rings

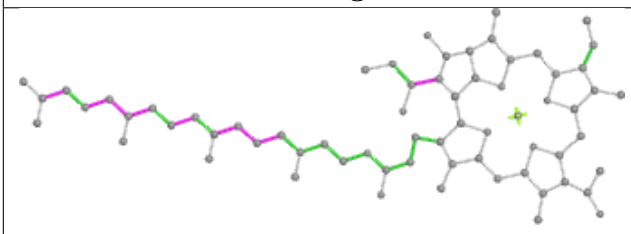
Ligand BCL L 1282



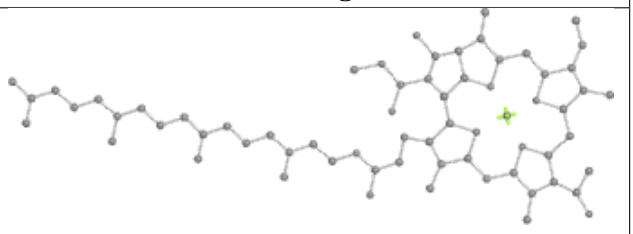
Bond lengths



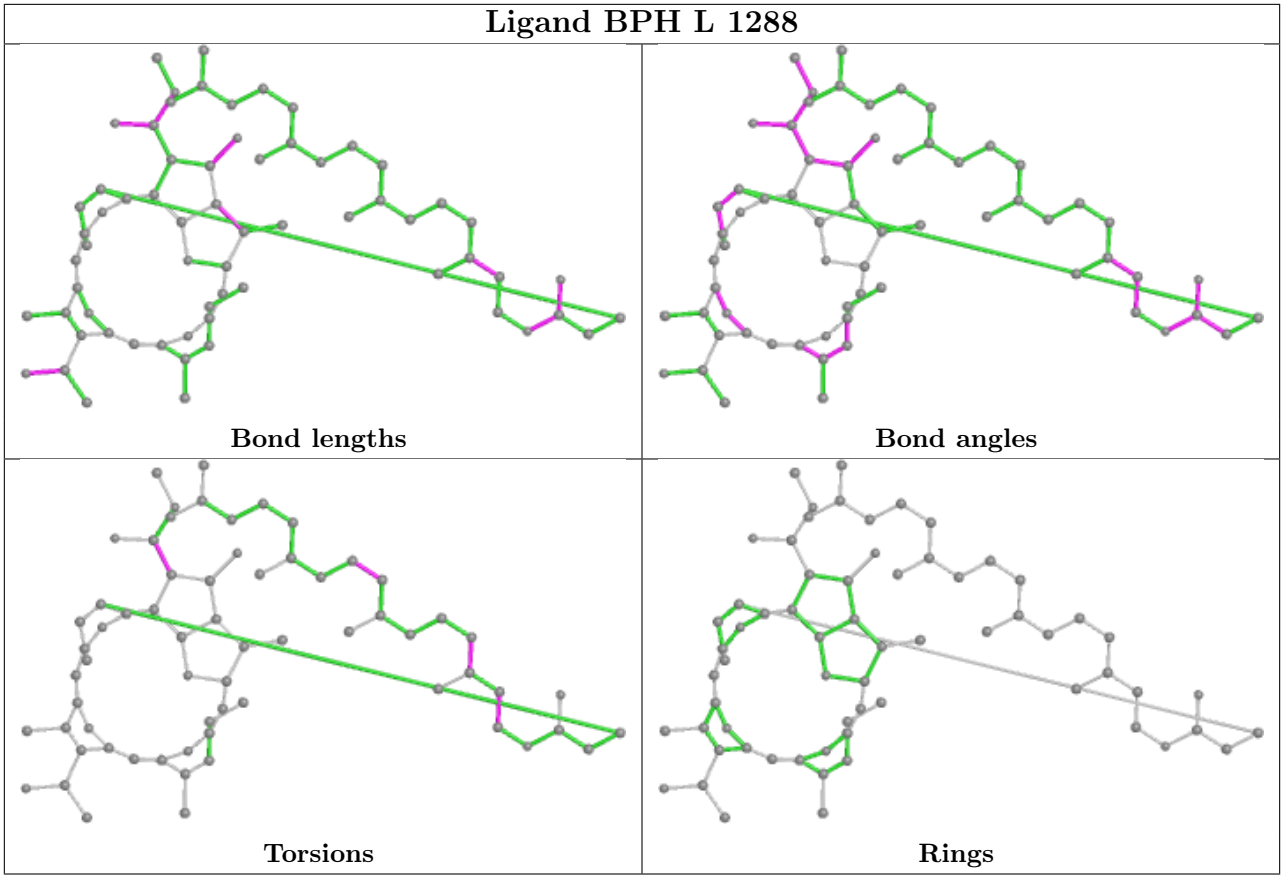
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

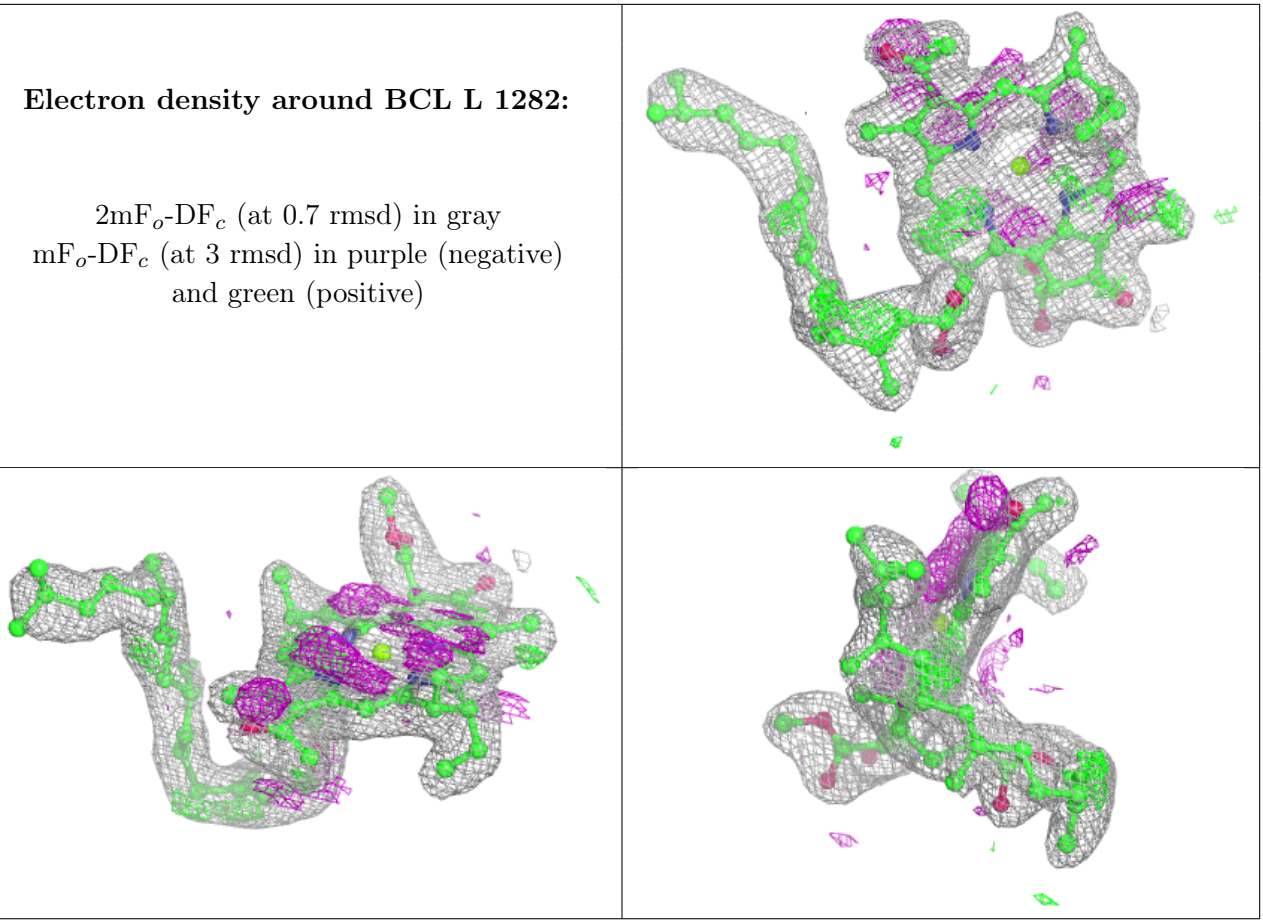
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

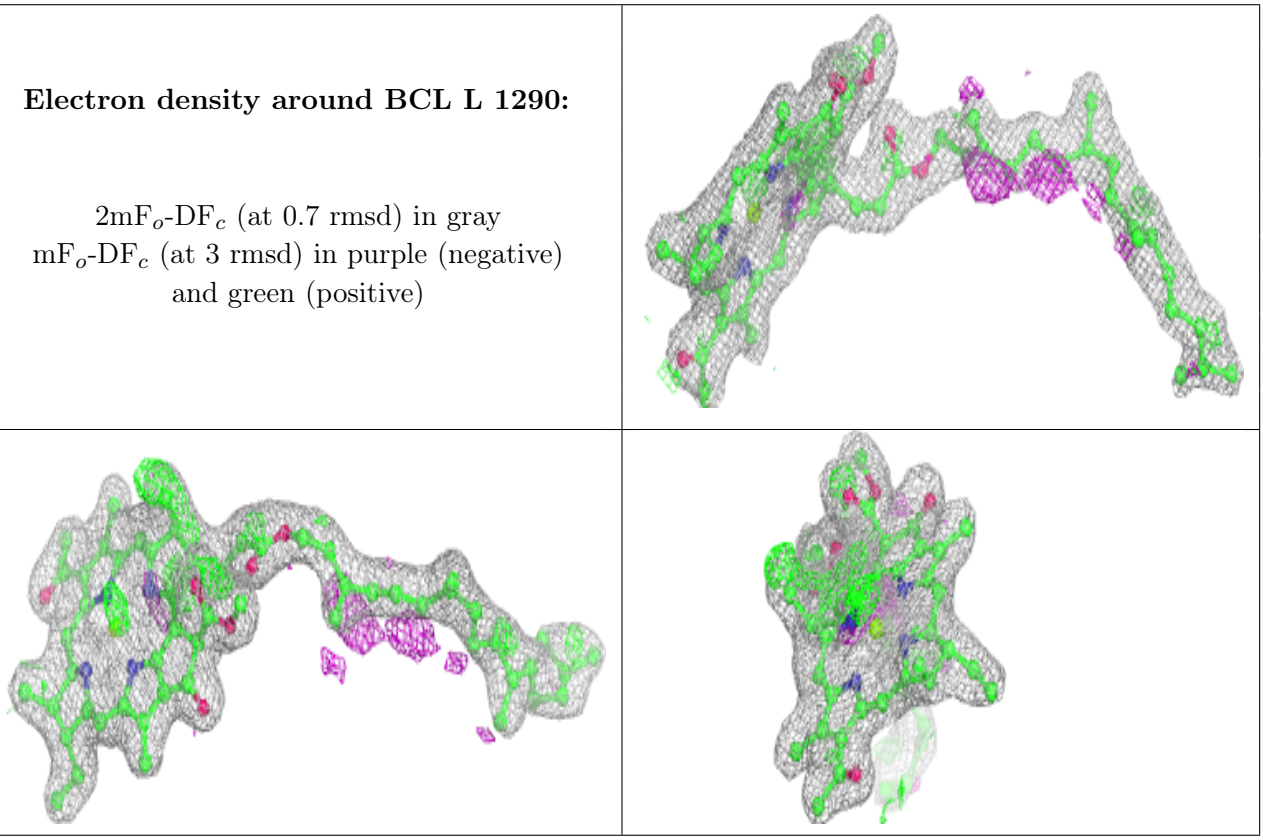
Electron density around BCL L 1282:

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



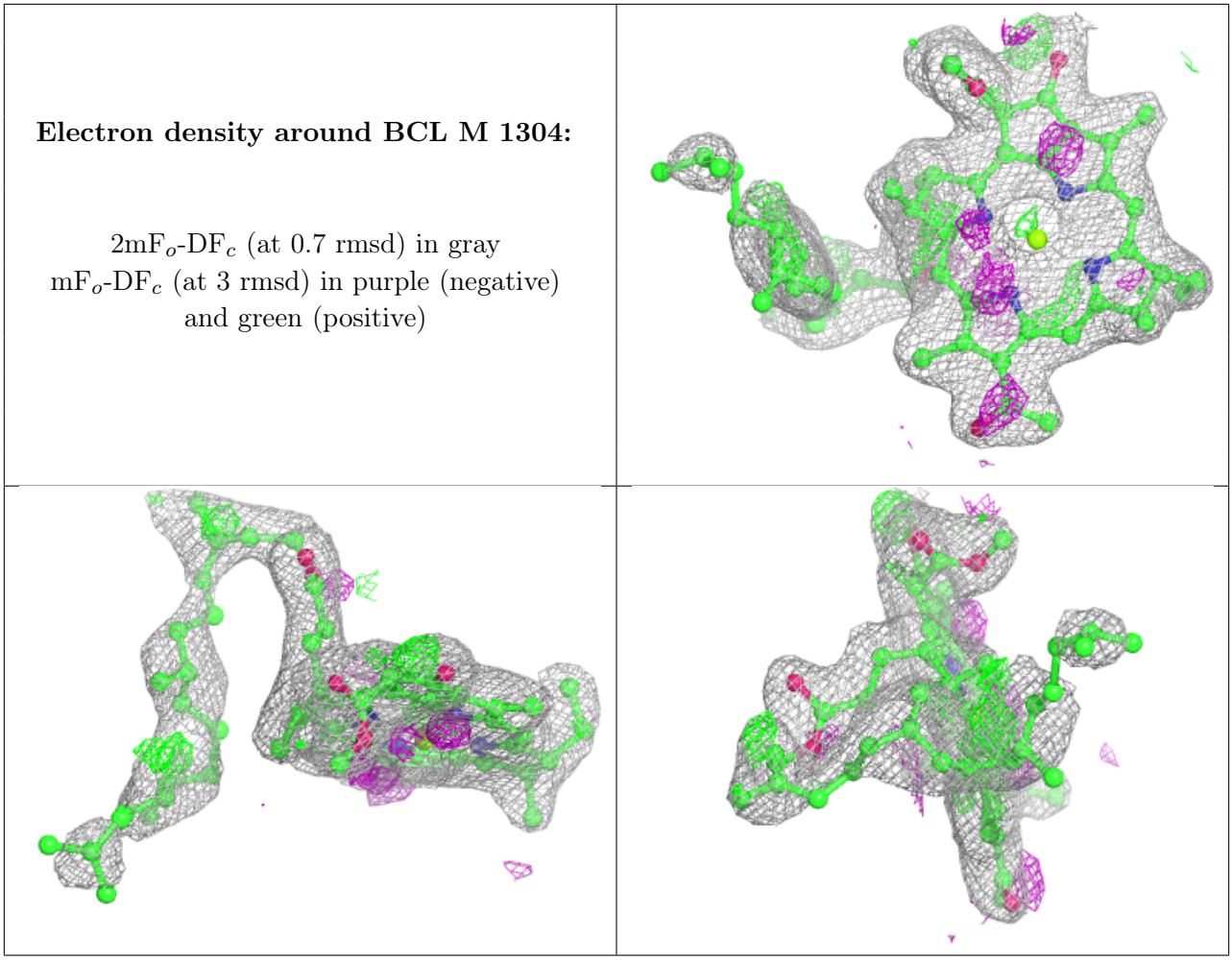
Electron density around BCL L 1290:

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



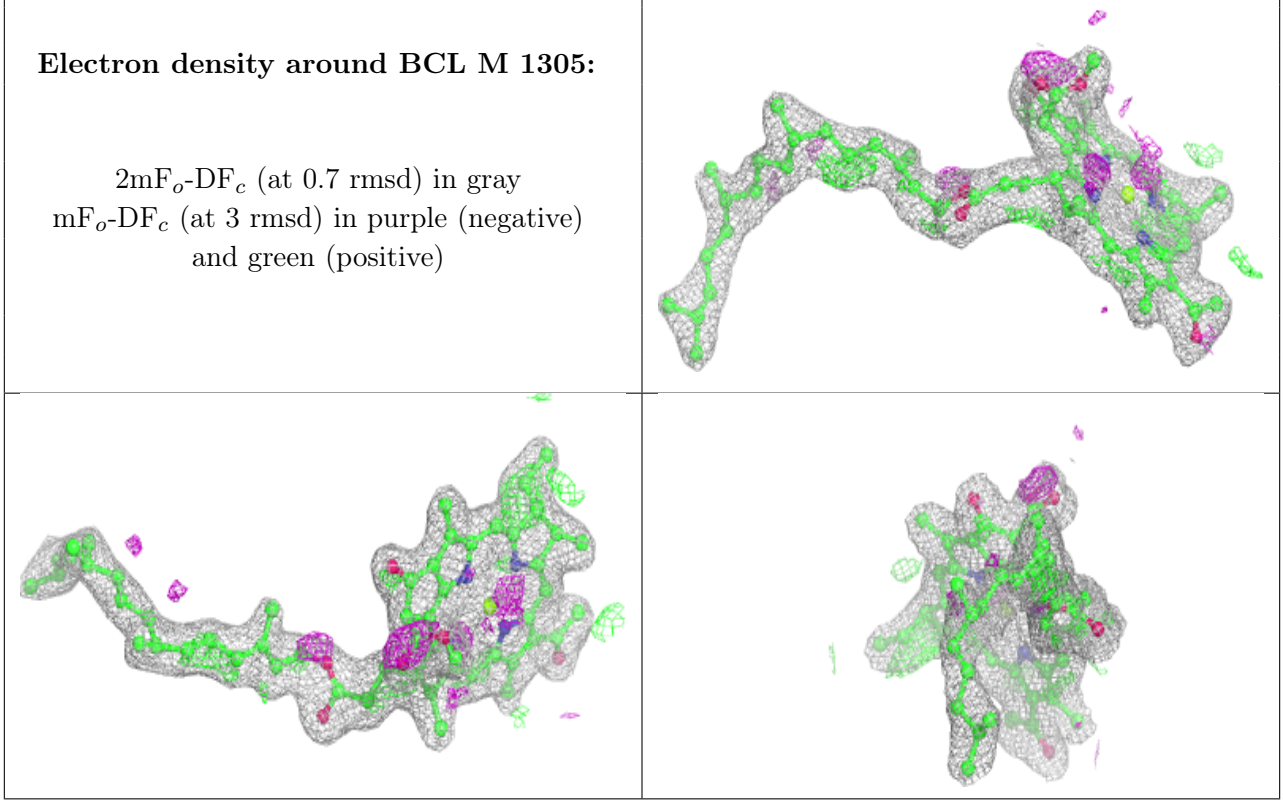
Electron density around BCL M 1304:

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



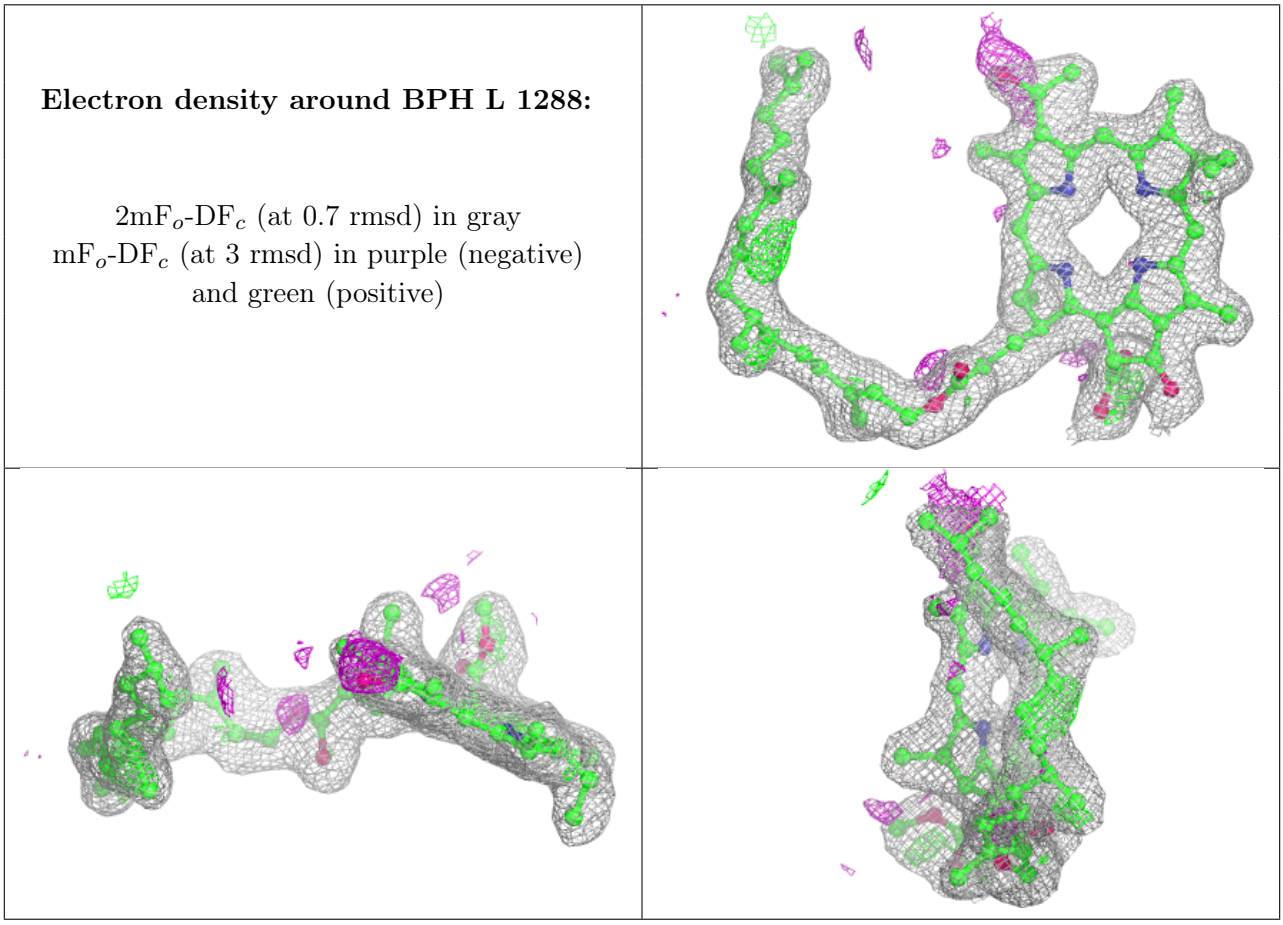
Electron density around BCL M 1305:

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



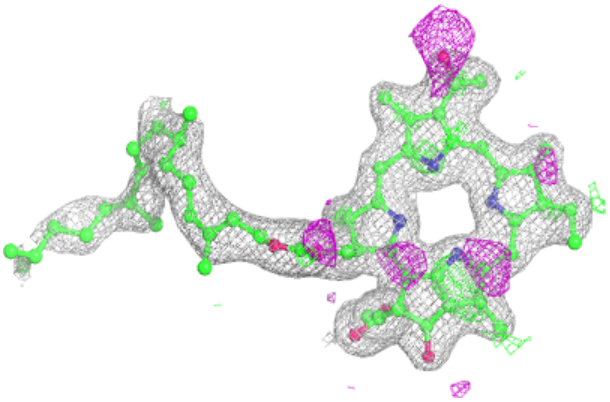
Electron density around BPH L 1288:

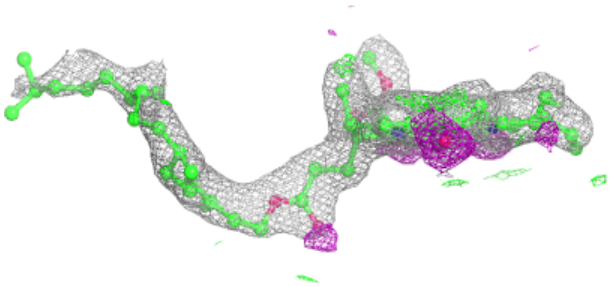
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BPH M 1311:

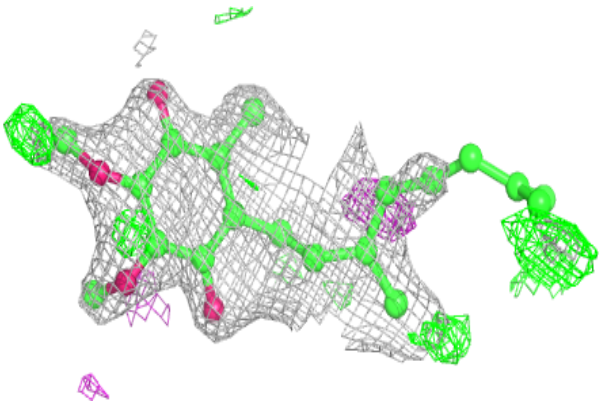
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

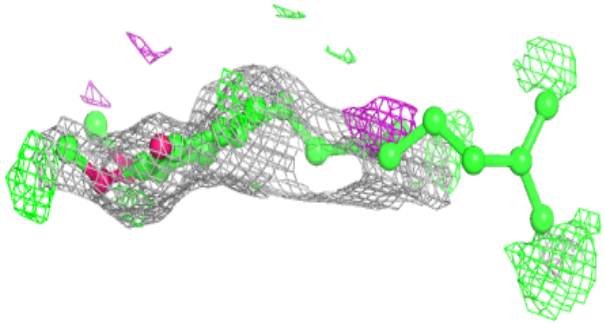


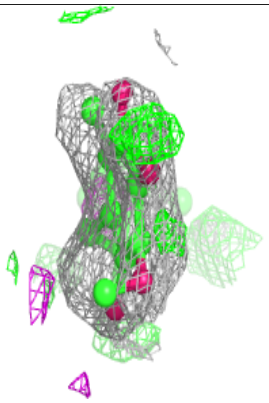


Electron density around UQ2 L 1289 (A):

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

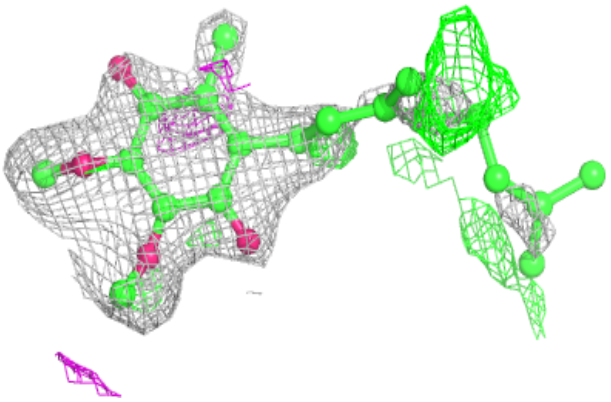


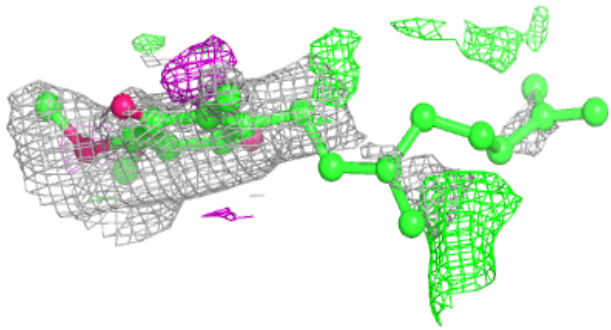


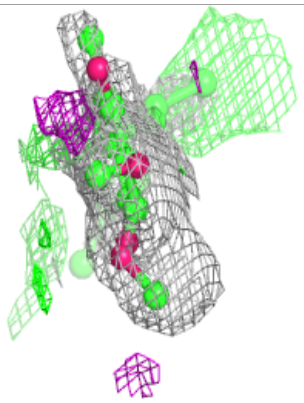


Electron density around UQ2 L 1289 (B):

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

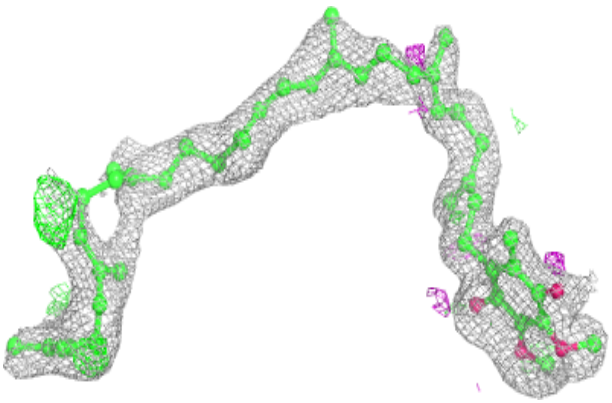


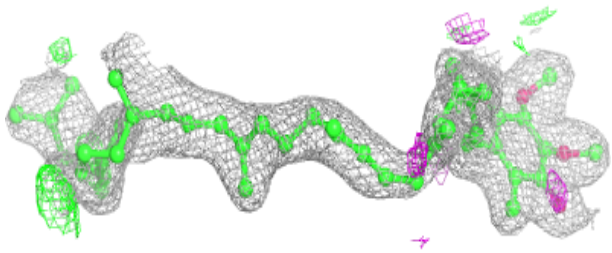


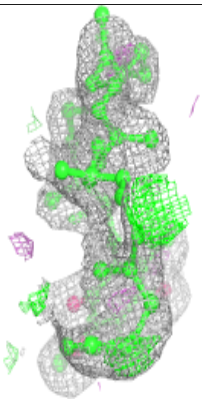


Electron density around U10 M 1312:

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

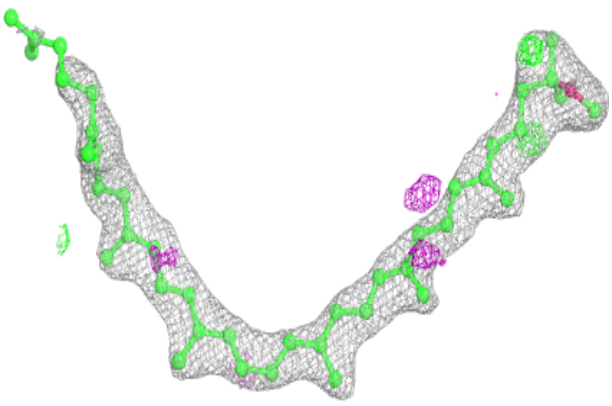


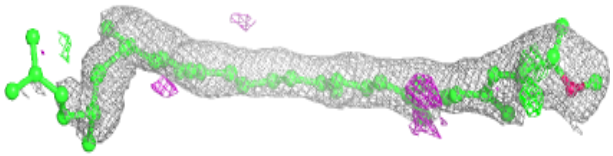


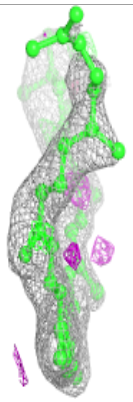


Electron density around SPO M 1313:

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

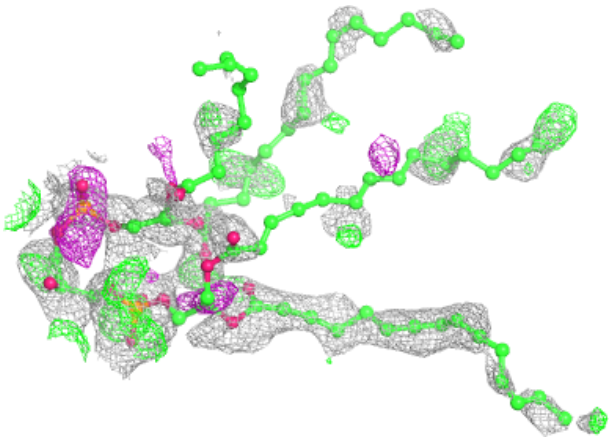


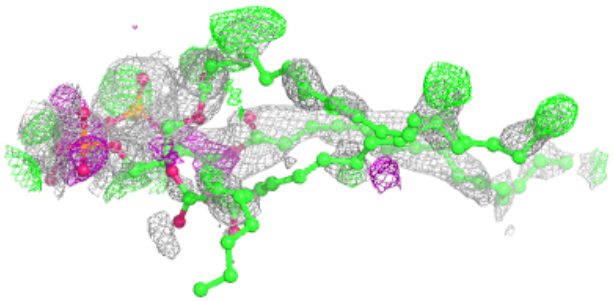


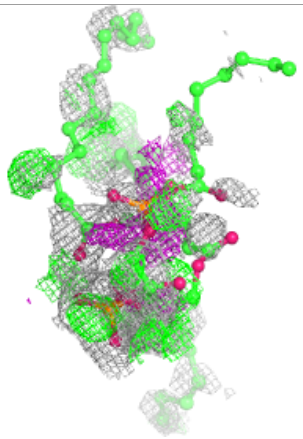


Electron density around CDL M 1314:

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







6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.