Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:49 AM UTC

PDB ID	:	2UWU / pdb_00002uwu
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 6.5 in the neutral state, 2nd dataset
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-23
Resolution	:	2.04 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:

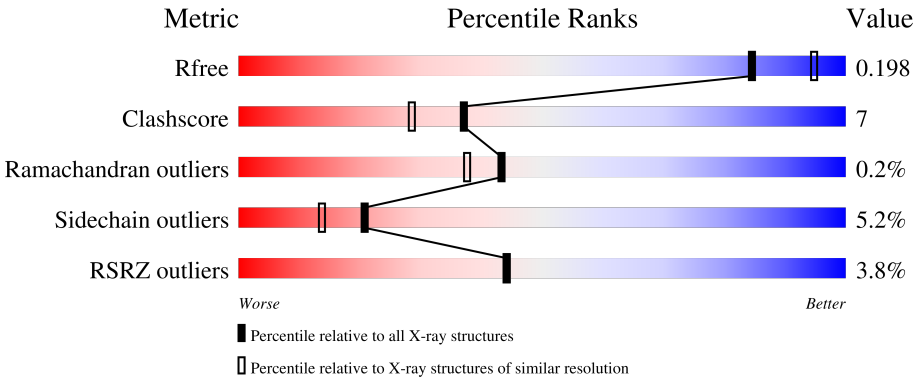
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.04 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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% 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% 82% 9% · 7%
2	L	281	4% 88% 11% ·
3	M	307	5% 83% 14% ••

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	1251	-	-	X	-
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7785 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

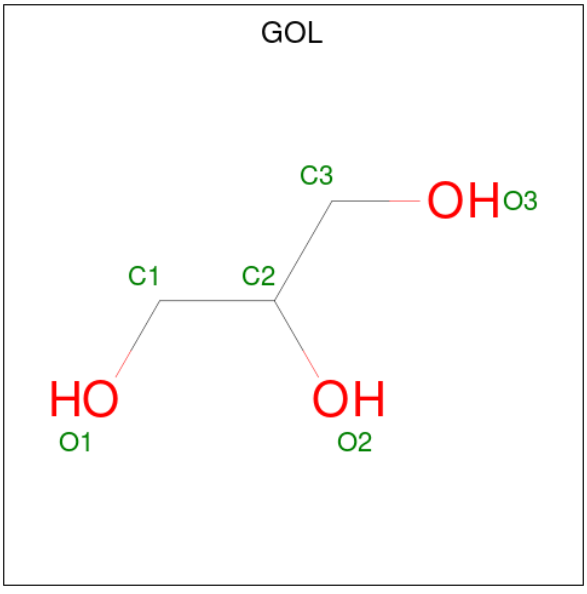
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

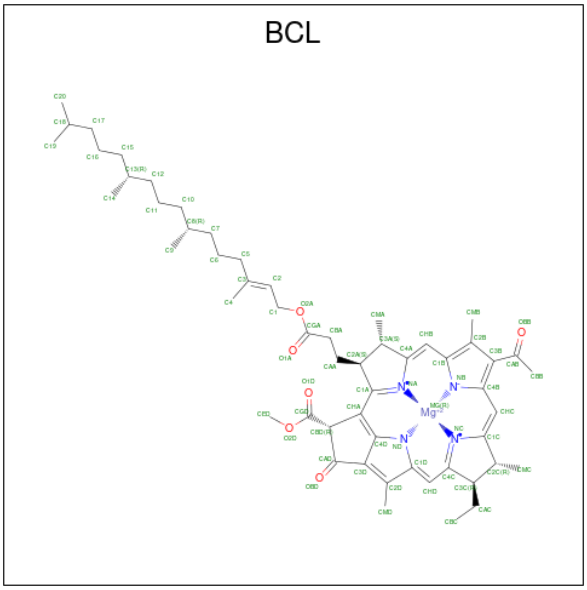
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



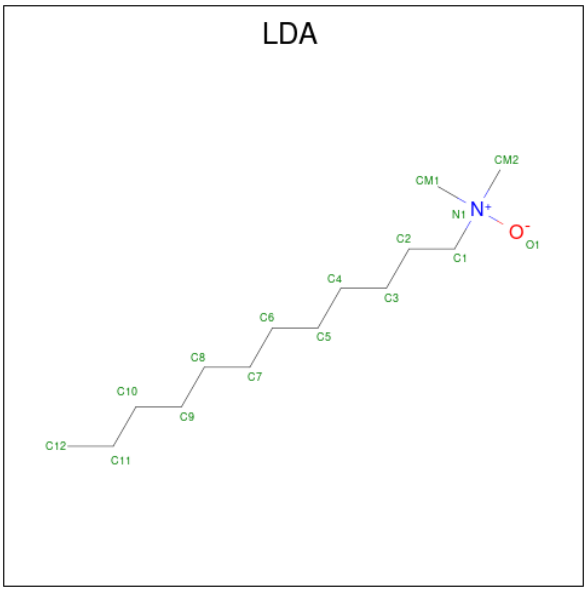
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

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



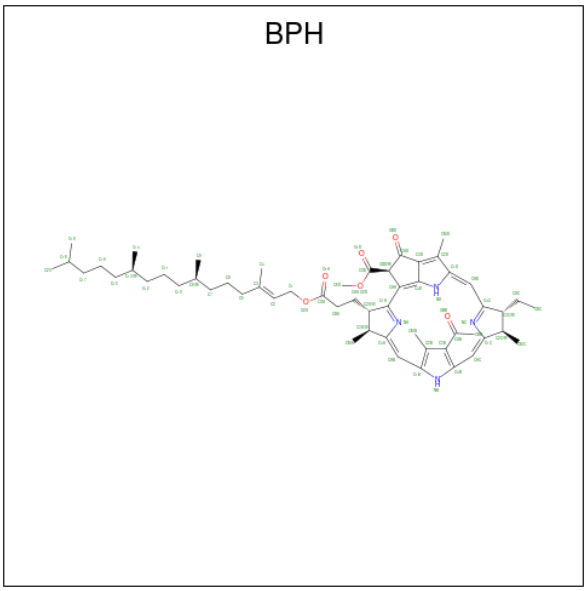
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



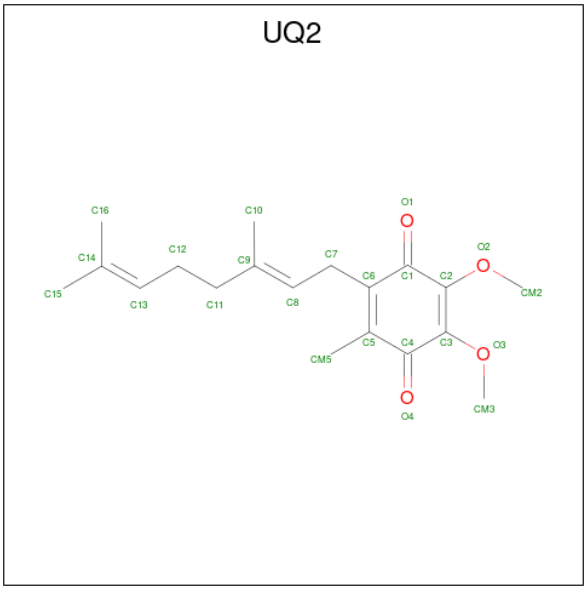
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M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

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



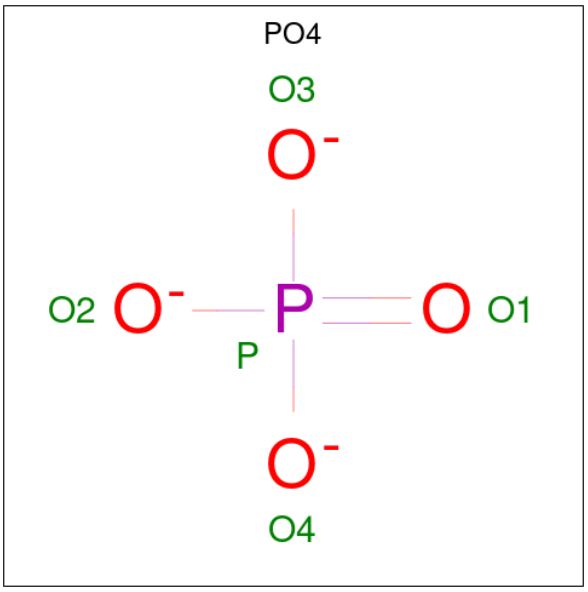
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C N O 65 55 4 6	0	0
7	M	1	Total C N O 65 55 4 6	0	0

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



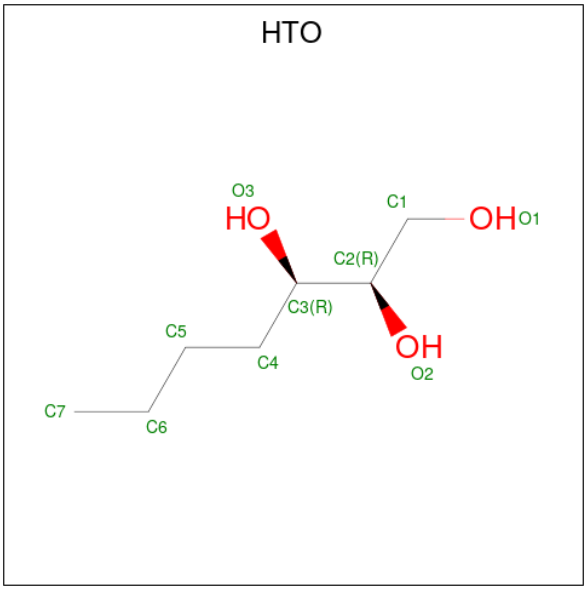
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total C O 46 38 8	0	1

- Molecule 9 is PHOSPHATE ION (CCD ID: 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 (CCD ID: HTO) (formula: $C_7H_{16}O_3$).

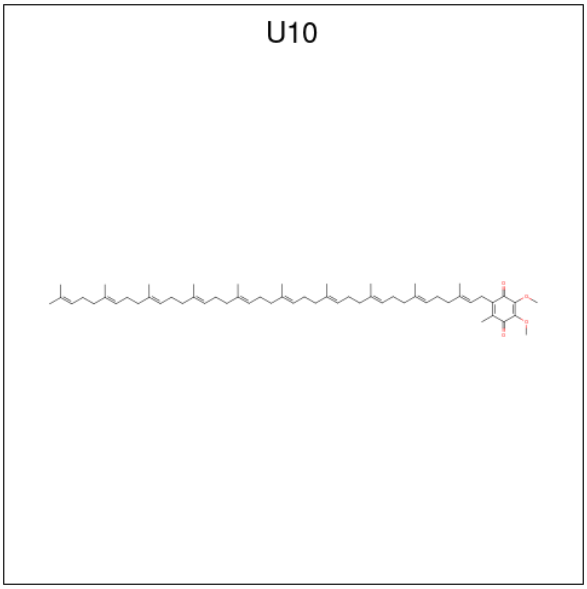


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0
10	L	1	Total C O 10 7 3	0	0

- Molecule 11 is FE (III) ION (CCD ID: FE) (formula: Fe).

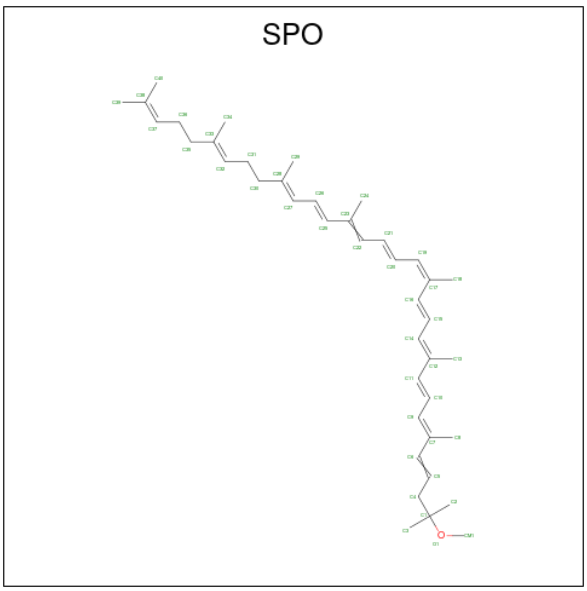
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

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



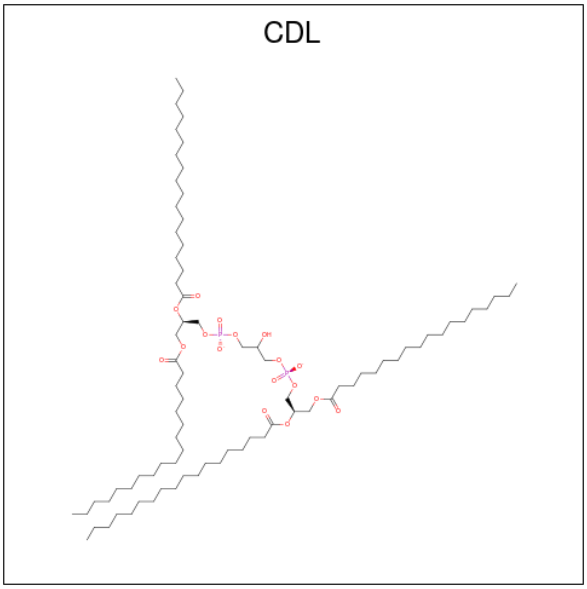
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 48 44 4	0	0

- Molecule 13 is SPHEROIDENE (CCD ID: 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 (CCD ID: 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.

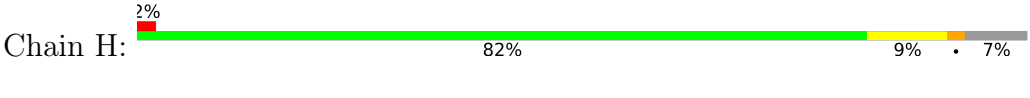
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	213	Total O 213 213	0	0
15	L	136	Total O 136 136	0	0
15	M	148	Total O 148 148	0	0

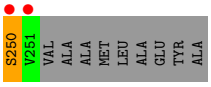
3 Residue-property plots (i)

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

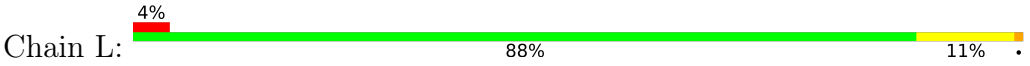
Chain H:

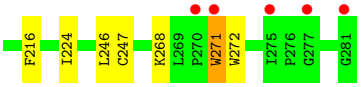




• Molecule 2: REACTION CENTER PROTEIN L CHAIN

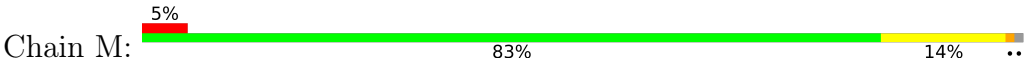
Chain L:

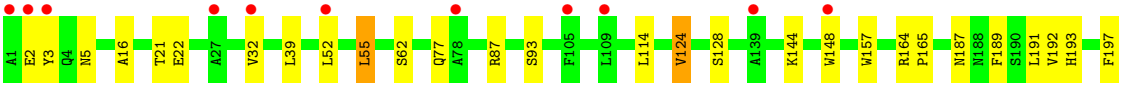




• Molecule 3: REACTION CENTER PROTEIN M CHAIN

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	139.45Å 139.45Å 184.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.04 119.52 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.2 (119.52-2.04) 88.1 (119.52-2.04)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.208 , 0.232 0.199 , 0.198	Depositor DCC
R_{free} test set	2580 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7785	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: UQ2, PO4, GOL, LDA, U10, SPO, CDL, BCL, BPH, HTO, FE

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	0.88	1/1878 (0.1%)	0.94	3/2555 (0.1%)
2	L	0.88	0/2320	0.94	0/3175
3	M	0.90	4/2501 (0.2%)	0.93	0/3415
All	All	0.89	5/6699 (0.1%)	0.94	3/9145 (0.0%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	302	GLY	C-N	-6.71	1.24	1.33
1	H	250	SER	C-N	-6.44	1.24	1.33
3	M	262	MET	SD-CE	-6.40	1.63	1.79
3	M	218	MET	SD-CE	6.21	1.95	1.79
3	M	213	ALA	CA-CB	5.20	1.61	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	248	ARG	CA-C-N	5.67	131.91	121.70
1	H	248	ARG	C-N-CA	5.67	131.91	121.70
1	H	139	GLY	N-CA-C	-5.01	98.78	113.30

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	19	0
2	L	2232	0	2187	24	0
3	M	2409	0	2321	32	0
4	H	24	0	32	5	0
4	L	12	0	16	1	0
5	L	132	0	148	4	0
5	M	132	0	148	18	0
6	L	48	0	93	2	0
6	M	96	0	186	5	0
7	L	65	0	76	7	0
7	M	65	0	76	12	0
8	L	46	0	52	4	0
9	L	5	0	0	0	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	48	0	63	0	0
13	M	42	0	60	3	0
14	M	81	0	86	5	0
15	H	213	0	0	5	0
15	L	136	0	0	0	0
15	M	148	0	0	1	0
All	All	7785	0	7412	105	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1286:BPH:HHC	7:L:1286:BPH:HBB3	1.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.40	0.85
2:L:271:TRP:H	2:L:271:TRP:CD1	1.92	0.83
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.13	0.82
5:L:1282:BCL:HBB2	5:L:1282:BCL:HHC	1.62	0.82
1:H:248:ARG:HA	1:H:249:LYS:CB	2.17	0.73
2:L:181:PHE:CD2	7:M:1312:BPH:HBB1	2.23	0.73
1:H:248:ARG:HA	1:H:249:LYS:HB3	1.73	0.71
7:L:1286:BPH:HHC	7:L:1286:BPH:CBB	2.20	0.71
3:M:62:SER:OG	3:M:124:VAL:HG22	1.91	0.71
2:L:181:PHE:HB3	7:M:1312:BPH:HBB2	1.72	0.71
4:H:1251:GOL:C3	15:H:2009:HOH:O	2.41	0.68
7:M:1312:BPH:HBC3	7:M:1312:BPH:HHD	1.76	0.68
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.25	0.67
3:M:144:LYS:N	14:M:1315:CDL:OB3	2.25	0.64
3:M:189:PHE:O	3:M:193:HIS:HD2	1.80	0.64
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.77	0.64
4:H:1251:GOL:H31	15:H:2009:HOH:O	1.96	0.63
7:M:1312:BPH:HHC	7:M:1312:BPH:HBB3	1.81	0.63
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB3	1.81	0.63
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.81	0.62
2:L:170:ASN:HD22	2:L:170:ASN:C	2.09	0.61
3:M:300:ASN:C	3:M:302:GLY:H	2.10	0.60
6:L:1284:LDA:H111	6:L:1284:LDA:H62	1.84	0.59
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.02	0.59
5:M:1303:BCL:HHC	5:M:1303:BCL:CBB	2.33	0.58
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.85	0.58
2:L:181:PHE:HB3	7:M:1312:BPH:CBB	2.34	0.58
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.33	0.58
5:M:1303:BCL:H61	7:M:1312:BPH:HMB2	1.87	0.57
2:L:199:ASN:HA	4:L:1292:GOL:H31	1.87	0.57
5:M:1303:BCL:HBB2	13:M:1314:SPO:H243	1.86	0.57
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.87	0.56
2:L:157:VAL:HG11	5:M:1304:BCL:HBB1	1.87	0.56
7:M:1312:BPH:HHC	7:M:1312:BPH:CBB	2.36	0.55
6:M:1307:LDA:H81	6:M:1308:LDA:H62	1.89	0.55
7:L:1286:BPH:HBB3	7:L:1286:BPH:CHC	2.27	0.55
2:L:224:ILE:HG22	8:L:1287[B]:UQ2:H8	1.88	0.55
3:M:77:GLN:HE22	3:M:93:SER:H	1.53	0.54
5:M:1303:BCL:CBB	13:M:1314:SPO:H243	2.37	0.54
4:H:1251:GOL:H32	15:H:2009:HOH:O	2.04	0.54
1:H:75:VAL:HA	1:H:76:PRO:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1282:BCL:H192	7:L:1286:BPH:H7C2	1.89	0.53
7:M:1312:BPH:HBB3	7:M:1312:BPH:CHC	2.39	0.52
2:L:193:LEU:HD23	8:L:1287[B]:UQ2:C4	2.40	0.52
3:M:189:PHE:O	3:M:193:HIS:CD2	2.63	0.52
1:H:62:LYS:CE	4:H:1251:GOL:H11	2.40	0.51
15:H:2009:HOH:O	14:M:1315:CDL:HA32	2.10	0.51
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.29	0.51
3:M:199:ASN:HD22	3:M:199:ASN:C	2.18	0.51
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.93	0.51
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.76	0.50
2:L:199:ASN:O	14:M:1315:CDL:HB22	2.12	0.49
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.17	0.49
2:L:208:THR:HB	2:L:209:PRO:HD2	1.95	0.49
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.47	0.49
7:L:1286:BPH:CBB	7:L:1286:BPH:CHC	2.88	0.49
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.95	0.49
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.93	0.49
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.46	0.48
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.94	0.48
3:M:300:ASN:C	3:M:302:GLY:N	2.72	0.47
5:M:1303:BCL:H13	5:M:1303:BCL:H102	1.65	0.47
3:M:270:ILE:O	3:M:274:VAL:HG13	2.15	0.47
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.50	0.47
1:H:112:ALA:HA	1:H:235:GLY:O	2.15	0.46
1:H:209:SER:OG	1:H:247:LYS:HD2	2.16	0.46
5:M:1303:BCL:HHC	5:M:1303:BCL:HBB2	1.97	0.46
3:M:258:PHE:HB3	6:M:1307:LDA:H31	1.97	0.46
6:M:1310:LDA:H62	7:M:1312:BPH:H162	1.97	0.46
7:L:1286:BPH:HBB1	3:M:210:TYR:CD2	2.51	0.46
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.51	0.45
6:M:1305:LDA:H92	6:M:1307:LDA:H121	1.99	0.45
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.99	0.45
2:L:189:LEU:HB3	8:L:1287[A]:UQ2:H3M3	1.99	0.44
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.44
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.66	0.44
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.83	0.44
3:M:16:ALA:HB1	3:M:32:VAL:HG11	2.01	0.43
8:L:1287[A]:UQ2:H101	8:L:1287[A]:UQ2:H121	1.74	0.43
3:M:278:LEU:HD21	14:M:1315:CDL:H782	2.00	0.43
7:M:1312:BPH:HBC3	7:M:1312:BPH:CHD	2.47	0.42
2:L:72:GLU:H	2:L:72:GLU:HG3	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:LYS:HE3	15:H:2123:HOH:O	2.19	0.42
7:M:1312:BPH:HHD	7:M:1312:BPH:CBC	2.48	0.42
2:L:178:SER:HB3	6:L:1285:LDA:H62	2.02	0.42
3:M:148:TRP:NE1	14:M:1315:CDL:OB6	2.52	0.42
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.20	0.42
1:H:175:MET:HE1	15:M:2116:HOH:O	2.20	0.42
3:M:187:ASN:HD22	5:M:1304:BCL:CBC	2.32	0.42
5:M:1303:BCL:H101	5:M:1304:BCL:H171	2.02	0.42
6:M:1307:LDA:H32	6:M:1308:LDA:H42	2.02	0.42
7:M:1312:BPH:CBB	7:M:1312:BPH:CHC	2.98	0.42
1:H:18:TYR:CZ	1:H:22:ILE:HD11	2.55	0.41
2:L:210:ASP:OD1	2:L:210:ASP:N	2.52	0.41
1:H:12:LEU:HD23	3:M:290:VAL:HG21	2.01	0.41
3:M:21:THR:O	3:M:22:GLU:C	2.63	0.41
2:L:271:TRP:CD1	2:L:271:TRP:N	2.72	0.41
3:M:243:THR:O	3:M:247:ARG:HG3	2.21	0.40
1:H:248:ARG:HA	1:H:249:LYS:HB2	2.00	0.40
3:M:157:TRP:CE2	13:M:1314:SPO:H293	2.56	0.40
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.95	0.40
1:H:60:LYS:HA	1:H:61:PRO:HD3	1.94	0.40
1:H:156:CYS:SG	1:H:248:ARG:HB2	2.61	0.40
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	239/260 (92%)	236 (99%)	2 (1%)	1 (0%)	30 22
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100 100
3	M	301/307 (98%)	289 (96%)	11 (4%)	1 (0%)	36 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	819/848 (97%)	797 (97%)	20 (2%)	2 (0%)	43 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
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%)	189 (97%)	6 (3%)	35 30
2	L	220/220 (100%)	203 (92%)	17 (8%)	12 6
3	M	236/240 (98%)	225 (95%)	11 (5%)	23 17
All	All	651/668 (98%)	617 (95%)	34 (5%)	21 14

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

Mol	Chain	Res	Type
1	H	118	ARG
1	H	163	LYS
1	H	220	LYS
1	H	231	ASP
1	H	247	LYS
1	H	250	SER
2	L	16	LEU
2	L	20	ASN
2	L	21	LEU
2	L	44	LEU
2	L	72	GLU
2	L	80	LEU
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	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
2	L	268	LYS
2	L	271	TRP
3	M	2	GLU
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	114	LEU
3	M	124	VAL
3	M	191	LEU
3	M	192	VAL
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	44	ASN
1	H	68	HIS
1	H	98	HIS
1	H	199	GLN
2	L	20	ASN
2	L	159	ASN
2	L	170	ASN
2	L	183	ASN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	H	1253	-	5,5,5	0.41	0	5,5,5	0.21	0
12	U10	M	1313	-	48,48,63	2.68	12 (25%)	60,61,79	1.58	12 (20%)
4	GOL	L	1292	-	5,5,5	0.38	0	5,5,5	0.79	0
4	GOL	H	1251	-	5,5,5	0.64	0	5,5,5	1.09	0
6	LDA	M	1309	-	13,15,15	2.16	2 (15%)	14,17,17	0.61	0
4	GOL	L	1293	-	5,5,5	0.37	0	5,5,5	0.37	0
10	HTO	L	1291	-	9,9,9	0.34	0	10,10,10	0.97	1 (10%)
6	LDA	M	1305	-	13,15,15	2.03	2 (15%)	14,17,17	0.60	1 (7%)
14	CDL	M	1315	-	80,80,99	2.15	16 (20%)	86,92,111	2.85	17 (19%)
7	BPH	L	1286	-	59,70,70	2.59	11 (18%)	59,101,101	2.81	20 (33%)
6	LDA	L	1284	-	13,15,15	2.12	2 (15%)	14,17,17	0.60	0
5	BCL	M	1304	3	69,74,74	1.92	12 (17%)	79,115,115	1.77	17 (21%)
6	LDA	M	1306	-	13,15,15	2.13	2 (15%)	14,17,17	0.51	0
7	BPH	M	1312	-	59,70,70	2.75	12 (20%)	59,101,101	2.41	17 (28%)
4	GOL	H	1252	-	5,5,5	0.41	0	5,5,5	0.42	0
6	LDA	L	1283	-	13,15,15	2.10	2 (15%)	14,17,17	0.47	0
6	LDA	L	1285	-	13,15,15	2.27	2 (15%)	14,17,17	0.59	0
5	BCL	L	1282	2	69,74,74	1.81	9 (13%)	79,115,115	1.87	19 (24%)
13	SPO	M	1314	-	41,41,41	2.62	12 (29%)	47,50,50	2.34	22 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	UQ2	L	1287[A]	-	23,23,23	2.71	8 (34%)	30,31,31	1.30	5 (16%)
8	UQ2	L	1287[B]	-	23,23,23	2.62	8 (34%)	30,31,31	1.78	8 (26%)
4	GOL	H	1254	-	5,5,5	0.36	0	5,5,5	0.36	0
6	LDA	M	1308	-	13,15,15	2.21	2 (15%)	14,17,17	0.58	0
9	PO4	L	1289	-	4,4,4	0.94	0	6,6,6	0.72	0
10	HTO	L	1290	-	9,9,9	0.41	0	10,10,10	0.63	0
6	LDA	M	1307	-	13,15,15	2.16	2 (15%)	14,17,17	0.72	0
5	BCL	L	1288	2	69,74,74	1.82	8 (11%)	79,115,115	1.93	22 (27%)
6	LDA	M	1310	-	13,15,15	2.18	2 (15%)	14,17,17	0.60	0
5	BCL	M	1303	3	69,74,74	1.82	8 (11%)	79,115,115	1.80	16 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	1253	-	-	0/4/4/4	-
12	U10	M	1313	-	-	12/45/69/87	0/1/1/1
4	GOL	L	1292	-	-	2/4/4/4	-
4	GOL	H	1251	-	-	2/4/4/4	-
6	LDA	M	1309	-	-	6/13/13/13	-
4	GOL	L	1293	-	-	4/4/4/4	-
10	HTO	L	1291	-	-	2/10/10/10	-
6	LDA	M	1305	-	-	7/13/13/13	-
14	CDL	M	1315	-	-	52/91/91/110	-
7	BPH	L	1286	-	-	4/37/105/105	0/5/6/6
6	LDA	L	1284	-	-	5/13/13/13	-
5	BCL	M	1304	3	2/2/21/25	6/41/137/137	-
6	LDA	M	1306	-	-	5/13/13/13	-
7	BPH	M	1312	-	-	13/37/105/105	0/5/6/6
4	GOL	H	1252	-	-	4/4/4/4	-
6	LDA	L	1283	-	-	8/13/13/13	-
6	LDA	L	1285	-	-	9/13/13/13	-
5	BCL	L	1282	2	2/2/21/25	13/41/137/137	-
13	SPO	M	1314	-	-	13/47/47/47	-
8	UQ2	L	1287[A]	-	-	5/15/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	UQ2	L	1287[B]	-	-	8/15/39/39	0/1/1/1
4	GOL	H	1254	-	-	0/4/4/4	-
6	LDA	M	1308	-	-	6/13/13/13	-
10	HTO	L	1290	-	-	7/10/10/10	-
6	LDA	M	1307	-	-	6/13/13/13	-
5	BCL	L	1288	2	2/2/21/25	11/41/137/137	-
6	LDA	M	1310	-	-	5/13/13/13	-
5	BCL	M	1303	3	2/2/21/25	11/41/137/137	-

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1312	BPH	OBD-CAD	13.17	1.39	1.22
7	L	1286	BPH	OBD-CAD	11.15	1.37	1.22
5	M	1304	BCL	OBD-CAD	10.63	1.40	1.22
5	M	1303	BCL	OBD-CAD	10.19	1.40	1.22
5	L	1282	BCL	OBD-CAD	10.19	1.40	1.22
5	L	1288	BCL	OBD-CAD	9.60	1.39	1.22
14	M	1315	CDL	C11-CA5	-7.70	1.28	1.50
7	L	1286	BPH	OBB-CAB	7.51	1.44	1.22
12	M	1313	U10	C33-C34	7.35	1.50	1.33
7	M	1312	BPH	O1D-CGD	7.19	1.39	1.21
8	L	1287[A]	UQ2	C8-C9	6.92	1.49	1.33
7	L	1286	BPH	O1D-CGD	6.86	1.38	1.21
6	M	1309	LDA	O1-N1	-6.68	1.25	1.42
6	M	1306	LDA	O1-N1	-6.61	1.25	1.42
6	L	1285	LDA	O1-N1	-6.61	1.26	1.42
7	L	1286	BPH	C2-C3	6.61	1.48	1.33
6	M	1308	LDA	O1-N1	-6.61	1.26	1.42
6	M	1310	LDA	O1-N1	-6.60	1.26	1.42
6	L	1283	LDA	O1-N1	-6.60	1.26	1.42
6	L	1284	LDA	O1-N1	-6.58	1.26	1.42
13	M	1314	SPO	C32-C33	6.55	1.48	1.33
5	L	1288	BCL	O1A-CGA	6.55	1.42	1.22
7	M	1312	BPH	C2-C3	6.53	1.48	1.33
8	L	1287[B]	UQ2	C8-C9	6.48	1.48	1.33
12	M	1313	U10	C13-C14	6.42	1.47	1.33
7	M	1312	BPH	OBB-CAB	6.38	1.41	1.22
7	L	1286	BPH	O1A-CGA	6.31	1.41	1.22
12	M	1313	U10	C8-C9	6.22	1.47	1.33
6	M	1305	LDA	O1-N1	-6.20	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1313	U10	C28-C29	6.16	1.47	1.33
6	M	1307	LDA	O1-N1	-6.09	1.27	1.42
12	M	1313	U10	C23-C24	6.00	1.46	1.33
7	M	1312	BPH	O1A-CGA	5.84	1.39	1.22
12	M	1313	U10	C18-C19	5.77	1.46	1.33
5	M	1303	BCL	O1A-CGA	5.68	1.39	1.22
13	M	1314	SPO	C37-C38	5.61	1.49	1.32
8	L	1287[B]	UQ2	O2-C2	-5.61	1.23	1.36
5	M	1304	BCL	O1A-CGA	5.58	1.39	1.22
8	L	1287[B]	UQ2	C13-C14	5.36	1.48	1.32
12	M	1313	U10	C38-C39	5.25	1.48	1.32
13	M	1314	SPO	C9-C7	5.23	1.47	1.35
5	L	1282	BCL	O1A-CGA	5.22	1.38	1.22
7	M	1312	BPH	C3D-C2D	5.16	1.48	1.39
8	L	1287[A]	UQ2	C13-C14	5.15	1.47	1.32
14	M	1315	CDL	C19-C18	-5.10	1.26	1.51
14	M	1315	CDL	C17-C16	-5.07	1.26	1.51
14	M	1315	CDL	C16-C15	-5.07	1.26	1.51
14	M	1315	CDL	C20-C19	-5.06	1.26	1.51
8	L	1287[A]	UQ2	O2-C2	-5.05	1.24	1.36
14	M	1315	CDL	OA8-CA7	4.96	1.47	1.33
13	M	1314	SPO	C6-C5	4.86	1.45	1.32
14	M	1315	CDL	C32-C31	-4.81	1.34	1.52
6	M	1307	LDA	C1-N1	-4.79	1.46	1.51
13	M	1314	SPO	C19-C17	4.78	1.46	1.35
6	L	1285	LDA	C1-N1	-4.73	1.46	1.51
14	M	1315	CDL	OB6-CB5	4.73	1.47	1.34
14	M	1315	CDL	OA6-CA5	4.71	1.47	1.34
13	M	1314	SPO	C14-C12	4.64	1.46	1.35
13	M	1314	SPO	C22-C23	4.63	1.46	1.35
8	L	1287[A]	UQ2	O3-C3	-4.62	1.25	1.36
7	L	1286	BPH	C3D-C2D	4.55	1.47	1.39
14	M	1315	CDL	OB8-CB7	4.52	1.46	1.33
7	M	1312	BPH	C3D-CAD	-4.41	1.39	1.47
13	M	1314	SPO	C10-C11	4.38	1.46	1.34
8	L	1287[B]	UQ2	O3-C3	-4.34	1.26	1.36
6	M	1308	LDA	C1-N1	-4.28	1.47	1.51
13	M	1314	SPO	C26-C25	4.15	1.45	1.34
13	M	1314	SPO	C15-C16	4.11	1.45	1.34
6	M	1310	LDA	C1-N1	-4.10	1.47	1.51
7	L	1286	BPH	C3D-CAD	-3.99	1.40	1.47
12	M	1313	U10	O3-C3	-3.95	1.27	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1309	LDA	C1-N1	-3.89	1.47	1.51
13	M	1314	SPO	C27-C28	3.87	1.47	1.35
5	M	1303	BCL	C3D-C4D	-3.85	1.35	1.44
14	M	1315	CDL	C34-C33	-3.79	1.32	1.51
6	M	1306	LDA	C1-N1	-3.76	1.47	1.51
12	M	1313	U10	C6-C1	3.74	1.41	1.35
6	L	1284	LDA	C1-N1	-3.65	1.47	1.51
12	M	1313	U10	O4-C4	-3.57	1.28	1.36
8	L	1287[A]	UQ2	C6-C5	3.55	1.41	1.35
5	L	1282	BCL	C3D-C4D	-3.52	1.36	1.44
5	M	1304	BCL	C3D-C4D	-3.49	1.36	1.44
14	M	1315	CDL	C79-C78	-3.47	1.34	1.51
6	L	1283	LDA	C1-N1	-3.47	1.47	1.51
14	M	1315	CDL	C37-C36	-3.46	1.34	1.51
6	M	1305	LDA	C1-N1	-3.45	1.47	1.51
14	M	1315	CDL	C80-C79	-3.43	1.34	1.51
5	L	1288	BCL	C2-C3	3.43	1.41	1.33
13	M	1314	SPO	C21-C20	3.41	1.45	1.36
14	M	1315	CDL	C22-C21	-3.40	1.34	1.51
5	L	1288	BCL	O2D-CGD	-3.37	1.24	1.33
5	L	1288	BCL	C3D-C4D	-3.33	1.36	1.44
5	M	1303	BCL	C2-C3	3.24	1.40	1.33
8	L	1287[A]	UQ2	C3-C4	-3.18	1.39	1.48
8	L	1287[B]	UQ2	C3-C4	-3.12	1.39	1.48
5	M	1304	BCL	C2-C3	3.10	1.40	1.33
7	L	1286	BPH	O2D-CGD	-3.02	1.25	1.33
5	L	1282	BCL	C2-C3	2.98	1.39	1.33
7	M	1312	BPH	O2A-CGA	-2.95	1.24	1.33
12	M	1313	U10	C4-C5	-2.93	1.40	1.48
5	L	1282	BCL	C1D-C2D	-2.92	1.39	1.45
14	M	1315	CDL	C33-C32	-2.85	1.37	1.51
5	L	1288	BCL	CHD-C4C	2.81	1.47	1.39
8	L	1287[B]	UQ2	C6-C5	2.69	1.40	1.35
7	L	1286	BPH	C3D-C4D	-2.68	1.37	1.41
8	L	1287[A]	UQ2	C2-C1	-2.68	1.41	1.48
5	M	1304	BCL	O2D-CGD	-2.67	1.26	1.33
5	M	1303	BCL	CHD-C4C	2.67	1.46	1.39
7	M	1312	BPH	O2D-CGD	-2.65	1.26	1.33
7	M	1312	BPH	C4D-ND	-2.64	1.34	1.38
7	M	1312	BPH	C3D-C4D	-2.63	1.37	1.41
8	L	1287[B]	UQ2	C6-C1	-2.58	1.39	1.46
5	M	1303	BCL	O2D-CGD	-2.57	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	OBB-CAB	2.52	1.28	1.23
5	M	1304	BCL	CBB-CAB	-2.50	1.45	1.50
5	L	1282	BCL	O2A-CGA	-2.47	1.26	1.33
5	M	1304	BCL	CHD-C4C	2.43	1.46	1.39
5	M	1304	BCL	C1D-C2D	-2.42	1.40	1.45
7	L	1286	BPH	O2A-CGA	-2.37	1.26	1.33
5	M	1304	BCL	C1D-ND	2.33	1.40	1.37
8	L	1287[B]	UQ2	C2-C1	-2.29	1.42	1.48
5	L	1282	BCL	O2D-CGD	-2.27	1.27	1.33
5	M	1303	BCL	O2A-CGA	-2.25	1.26	1.33
5	L	1282	BCL	C1B-NB	2.23	1.40	1.37
7	L	1286	BPH	C4D-ND	-2.17	1.35	1.38
7	M	1312	BPH	O2D-CED	-2.14	1.40	1.45
5	L	1288	BCL	C1B-NB	2.14	1.40	1.37
5	M	1304	BCL	O2A-CGA	-2.10	1.27	1.33
5	M	1303	BCL	C1D-C2D	-2.09	1.41	1.45
8	L	1287[A]	UQ2	O2-CM2	-2.08	1.40	1.45
12	M	1313	U10	O3-C3M	-2.07	1.40	1.45
5	L	1282	BCL	MG-ND	-2.05	2.01	2.05
5	M	1304	BCL	MG-NA	2.04	2.11	2.06
5	L	1288	BCL	O2A-CGA	-2.01	1.27	1.33

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1315	CDL	C20-C19-C18	12.93	179.75	114.37
14	M	1315	CDL	C17-C16-C15	11.30	171.48	114.37
14	M	1315	CDL	C35-C34-C33	10.02	165.03	114.37
7	M	1312	BPH	O2D-CGD-CBD	9.66	121.56	110.95
7	L	1286	BPH	O2D-CGD-CBD	9.22	121.08	110.95
7	L	1286	BPH	C2B-C1B-NB	9.13	116.03	109.43
14	M	1315	CDL	C33-C32-C31	7.63	141.18	113.13
14	M	1315	CDL	C12-C11-CA5	6.99	139.31	113.69
7	L	1286	BPH	C2D-C1D-ND	6.94	114.44	109.43
7	M	1312	BPH	C2B-C1B-NB	6.59	114.19	109.43
5	L	1282	BCL	O2D-CGD-CBD	6.49	122.58	111.23
13	M	1314	SPO	C4-C5-C6	-6.40	115.92	124.91
5	L	1282	BCL	C1D-ND-C4D	5.82	110.39	106.31
5	M	1303	BCL	C1D-ND-C4D	5.79	110.38	106.31
5	M	1303	BCL	CMB-C2B-C1B	-5.75	116.67	125.42
7	L	1286	BPH	C1B-NB-C4B	-5.73	100.46	108.82
7	M	1312	BPH	C2D-C1D-ND	5.45	113.37	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1315	CDL	C13-C12-C11	5.35	132.79	113.13
14	M	1315	CDL	C34-C33-C32	5.31	141.20	114.37
5	L	1288	BCL	C1C-NC-C4C	-5.05	104.37	106.68
7	M	1312	BPH	C3D-C4D-ND	4.99	114.11	107.71
12	M	1313	U10	C30-C29-C31	4.99	123.88	115.23
5	M	1304	BCL	CMD-C2D-C1D	4.98	133.50	124.73
7	L	1286	BPH	O1D-CGD-CBD	-4.92	117.26	124.72
13	M	1314	SPO	C15-C14-C12	-4.92	120.38	127.28
5	L	1288	BCL	O2D-CGD-CBD	4.91	119.82	111.23
7	L	1286	BPH	C3D-C4D-ND	4.82	113.88	107.71
7	L	1286	BPH	C4D-ND-C1D	-4.81	103.11	108.87
5	L	1288	BCL	CMD-C2D-C1D	4.76	133.11	124.73
5	L	1288	BCL	C1D-ND-C4D	4.74	109.64	106.31
7	L	1286	BPH	OBD-CAD-CBD	-4.73	118.88	125.82
14	M	1315	CDL	OA6-CA5-C11	4.70	121.66	111.48
5	M	1303	BCL	O2D-CGD-CBD	4.63	119.33	111.23
7	L	1286	BPH	CED-O2D-CGD	4.56	126.26	115.92
5	M	1304	BCL	O2D-CGD-CBD	4.53	119.14	111.23
5	M	1304	BCL	CMB-C2B-C1B	-4.46	118.62	125.42
14	M	1315	CDL	OB6-CB5-C51	4.39	120.97	111.48
5	M	1303	BCL	C1-O2A-CGA	4.37	127.22	116.65
13	M	1314	SPO	C20-C19-C17	-4.25	121.32	127.28
13	M	1314	SPO	C10-C9-C7	-4.19	121.40	127.28
5	M	1303	BCL	C2D-C1D-ND	-4.12	106.04	110.13
7	M	1312	BPH	C4D-ND-C1D	-4.05	104.02	108.87
5	M	1304	BCL	O2A-CGA-CBA	4.04	124.16	111.83
13	M	1314	SPO	C26-C27-C28	-4.04	122.01	127.69
5	L	1282	BCL	CMD-C2D-C1D	4.03	131.82	124.73
8	L	1287[B]	UQ2	CM5-C5-C6	-3.91	118.02	124.45
5	L	1288	BCL	CMB-C2B-C1B	-3.87	119.53	125.42
7	M	1312	BPH	OBD-CAD-CBD	-3.79	120.26	125.82
7	M	1312	BPH	O1D-CGD-CBD	-3.69	119.12	124.72
5	L	1288	BCL	O2D-CGD-O1D	-3.68	116.69	123.85
13	M	1314	SPO	C29-C28-C30	3.64	121.55	115.23
5	L	1282	BCL	C2D-C1D-ND	-3.59	106.57	110.13
7	L	1286	BPH	C3B-C4B-NB	3.56	113.23	108.05
5	M	1304	BCL	CED-O2D-CGD	3.54	123.94	115.92
5	M	1304	BCL	C16-C15-C13	-3.44	104.54	115.97
8	L	1287[B]	UQ2	C10-C9-C11	3.39	121.12	115.23
13	M	1314	SPO	C21-C22-C23	-3.38	122.54	127.28
13	M	1314	SPO	C13-C12-C11	3.36	123.22	118.09
5	L	1282	BCL	O2A-CGA-CBA	3.35	122.06	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	1313	U10	C10-C9-C11	3.35	121.05	115.23
5	M	1303	BCL	O2A-CGA-CBA	3.32	121.96	111.83
5	L	1288	BCL	C2D-C1D-ND	-3.31	106.85	110.13
14	M	1315	CDL	OA8-CA7-C31	3.29	121.85	111.83
5	L	1288	BCL	C4A-NA-C1A	3.28	108.18	106.68
7	M	1312	BPH	CED-O2D-CGD	3.26	123.31	115.92
8	L	1287[B]	UQ2	CM3-O3-C3	3.23	127.84	116.47
5	L	1282	BCL	C4-C3-C5	3.22	120.81	115.23
5	L	1282	BCL	O1D-CGD-CBD	-3.22	118.17	124.52
7	M	1312	BPH	OBD-CAD-C3D	-3.21	122.88	127.89
5	M	1304	BCL	C4A-NA-C1A	3.20	108.14	106.68
5	M	1303	BCL	CMA-C3A-C4A	-3.19	103.20	111.77
5	L	1288	BCL	C1-O2A-CGA	3.15	124.29	116.65
8	L	1287[B]	UQ2	O1-C1-C6	-3.15	115.70	121.79
7	L	1286	BPH	OBB-CAB-C3B	3.14	125.24	119.99
5	M	1304	BCL	C1D-ND-C4D	3.13	108.51	106.31
7	L	1286	BPH	OBD-CAD-C3D	-3.10	123.05	127.89
5	M	1303	BCL	O1D-CGD-CBD	-3.09	118.42	124.52
13	M	1314	SPO	C20-C21-C22	-3.08	117.22	123.52
12	M	1313	U10	C15-C14-C16	3.03	120.49	115.23
5	L	1282	BCL	C1-O2A-CGA	3.03	123.98	116.65
7	M	1312	BPH	C1B-NB-C4B	-3.02	104.42	108.82
5	L	1282	BCL	C1-C2-C3	-2.99	121.29	126.20
5	L	1282	BCL	C2B-C1B-NB	-2.98	107.24	110.33
12	M	1313	U10	C22-C23-C24	-2.96	120.85	127.62
5	L	1288	BCL	O2A-CGA-CBA	2.94	120.80	111.83
14	M	1315	CDL	OB8-CB7-C71	2.92	120.74	111.83
5	M	1304	BCL	OBB-CAB-C3B	2.92	125.59	120.43
5	L	1288	BCL	C3C-C4C-CHD	-2.92	117.24	123.39
5	M	1303	BCL	CMD-C2D-C1D	2.92	129.87	124.73
12	M	1313	U10	C20-C19-C21	2.89	120.25	115.23
7	M	1312	BPH	C4D-CHA-CBD	-2.88	107.08	108.45
5	L	1288	BCL	CMD-C2D-C3D	-2.88	121.09	127.69
5	M	1303	BCL	C2B-C1B-NB	-2.86	107.36	110.33
5	L	1282	BCL	C4A-NA-C1A	2.85	107.98	106.68
5	M	1304	BCL	CBB-CAB-C3B	-2.85	114.40	120.40
13	M	1314	SPO	C8-C7-C6	2.79	122.35	118.09
5	L	1288	BCL	C2B-C1B-NB	-2.77	107.45	110.33
5	L	1282	BCL	CMB-C2B-C1B	-2.76	121.21	125.42
12	M	1313	U10	C25-C24-C26	2.76	120.02	115.23
5	L	1288	BCL	C2A-C3A-C4A	2.74	106.29	101.87
5	M	1304	BCL	CMD-C2D-C3D	-2.72	121.45	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1288	BCL	C1D-CHD-C4C	-2.69	120.12	126.62
8	L	1287[A]	UQ2	C10-C9-C11	2.69	119.89	115.23
7	M	1312	BPH	C1-C2-C3	-2.68	121.80	126.20
12	M	1313	U10	C27-C28-C29	-2.67	121.51	127.62
5	L	1288	BCL	C14-C13-C12	2.65	120.73	111.27
7	M	1312	BPH	CMA-C3A-C4A	-2.64	108.91	114.61
5	L	1288	BCL	CMA-C3A-C4A	-2.61	104.77	111.77
13	M	1314	SPO	C14-C15-C16	-2.57	115.76	123.20
5	M	1303	BCL	CED-O2D-CGD	2.55	121.70	115.92
5	L	1288	BCL	C1-C2-C3	2.54	130.36	126.20
7	L	1286	BPH	CMA-C3A-C4A	-2.52	109.18	114.61
12	M	1313	U10	C30-C29-C28	-2.52	117.16	123.63
5	M	1304	BCL	C2D-C1D-ND	-2.52	107.64	110.13
8	L	1287[B]	UQ2	C7-C8-C9	-2.51	122.51	126.83
8	L	1287[B]	UQ2	C7-C6-C5	-2.50	120.61	124.89
5	L	1282	BCL	C2A-C3A-C4A	2.49	105.90	101.87
5	M	1304	BCL	O2D-CGD-O1D	-2.48	119.01	123.85
5	M	1303	BCL	CMB-C2B-C3B	2.47	133.45	125.67
7	L	1286	BPH	O2A-CGA-CBA	2.44	119.29	111.83
5	L	1288	BCL	O2A-CGA-O1A	-2.44	117.53	123.63
12	M	1313	U10	O5-C5-C4	-2.43	115.88	121.03
5	L	1282	BCL	CMD-C2D-C3D	-2.43	122.13	127.69
13	M	1314	SPO	C34-C33-C35	2.41	119.41	115.23
5	L	1288	BCL	CED-O2D-CGD	2.41	121.38	115.92
12	M	1313	U10	C12-C13-C14	-2.41	122.11	127.62
13	M	1314	SPO	C16-C17-C19	-2.38	115.27	119.01
7	M	1312	BPH	O2A-CGA-CBA	2.37	119.05	111.83
13	M	1314	SPO	C27-C26-C25	-2.37	116.34	123.20
5	L	1282	BCL	O2D-CGD-O1D	-2.36	119.25	123.85
7	L	1286	BPH	C1C-C2C-C3C	-2.35	100.60	102.84
7	M	1312	BPH	O2D-CGD-O1D	-2.33	119.31	123.85
13	M	1314	SPO	C18-C17-C16	2.31	121.62	118.09
13	M	1314	SPO	C24-C23-C25	2.31	121.62	118.09
5	M	1304	BCL	C3C-C4C-CHD	-2.29	118.56	123.39
7	L	1286	BPH	C1-O2A-CGA	2.29	122.20	116.65
12	M	1313	U10	C35-C34-C36	2.29	119.21	115.23
14	M	1315	CDL	OA6-CA5-OA7	-2.28	118.36	123.70
5	L	1288	BCL	CMA-C3A-C2A	-2.27	105.19	113.98
7	L	1286	BPH	O2A-CGA-O1A	-2.26	117.97	123.63
7	M	1312	BPH	CMB-C2B-C3B	2.25	129.18	124.68
5	M	1303	BCL	O2A-CGA-O1A	-2.23	118.04	123.63
13	M	1314	SPO	C40-C38-C39	2.22	119.70	114.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BCL	O2A-CGA-O1A	-2.22	118.08	123.63
5	L	1282	BCL	CAA-C2A-C1A	-2.21	104.72	111.97
13	M	1314	SPO	C25-C23-C22	-2.21	115.53	119.01
12	M	1313	U10	C7-C6-C1	-2.21	121.10	124.89
7	L	1286	BPH	C4C-C3C-C2C	-2.20	100.74	102.84
7	L	1286	BPH	CBB-CAB-C3B	-2.20	113.77	120.34
8	L	1287[A]	UQ2	C16-C14-C15	2.19	119.64	114.59
5	L	1282	BCL	CAA-C2A-C3A	-2.19	107.08	113.00
13	M	1314	SPO	C21-C20-C19	-2.19	119.04	123.52
5	L	1288	BCL	CHD-C1D-C2D	2.18	130.02	125.49
8	L	1287[B]	UQ2	C16-C14-C15	2.17	119.58	114.59
8	L	1287[A]	UQ2	O2-C2-C3	-2.17	115.43	123.64
7	M	1312	BPH	C1-O2A-CGA	2.16	121.87	116.65
13	M	1314	SPO	C9-C10-C11	-2.15	116.97	123.20
5	M	1303	BCL	CHA-C1A-NA	-2.14	121.55	126.39
8	L	1287[A]	UQ2	C7-C6-C5	-2.11	121.27	124.89
14	M	1315	CDL	CA4-OA6-CA5	-2.11	112.75	117.80
8	L	1287[B]	UQ2	CM2-O2-C2	2.11	123.89	116.47
14	M	1315	CDL	OB8-CB7-OB9	-2.11	118.36	123.63
14	M	1315	CDL	OA8-CA7-OA9	-2.11	118.36	123.63
5	M	1303	BCL	C3C-C4C-CHD	-2.09	118.99	123.39
10	L	1291	HTO	C5-C4-C3	-2.09	110.69	114.11
5	L	1282	BCL	CHA-C1A-NA	-2.07	121.71	126.39
5	M	1303	BCL	C2A-C3A-C4A	2.05	105.18	101.87
8	L	1287[A]	UQ2	C12-C13-C14	-2.05	120.81	127.64
13	M	1314	SPO	C31-C32-C33	-2.05	122.94	127.62
14	M	1315	CDL	C22-C21-C20	2.03	124.62	114.37
5	L	1282	BCL	C1D-CHD-C4C	-2.02	121.74	126.62
7	L	1286	BPH	C4A-C3A-C2A	-2.02	100.91	102.84
13	M	1314	SPO	C15-C16-C17	-2.02	120.82	126.36
14	M	1315	CDL	C80-C79-C78	2.01	124.55	114.37
5	M	1304	BCL	CAB-C3B-C2B	-2.01	123.56	127.74
5	M	1304	BCL	C2B-C1B-NB	-2.00	108.25	110.33
6	M	1305	LDA	O1-N1-C1	2.00	114.18	109.27

All (8) chirality outliers are listed below:

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

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

All (226) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	O1-C1-C2-C3
4	L	1292	GOL	C1-C2-C3-O3
4	L	1293	GOL	O1-C1-C2-C3
4	L	1293	GOL	C1-C2-C3-O3
5	L	1288	BCL	C11-C10-C8-C7
5	L	1288	BCL	C11-C12-C13-C14
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
5	M	1304	BCL	C11-C10-C8-C9
6	M	1305	LDA	C2-C1-N1-O1
6	M	1305	LDA	C2-C1-N1-CM1
6	M	1305	LDA	C2-C1-N1-CM2
6	M	1306	LDA	C2-C1-N1-CM1
6	M	1306	LDA	C2-C1-N1-CM2
6	M	1309	LDA	C2-C1-N1-O1
6	M	1309	LDA	C2-C1-N1-CM2
8	L	1287[B]	UQ2	C7-C8-C9-C10
8	L	1287[B]	UQ2	C7-C8-C9-C11
10	L	1290	HTO	C1-C2-C3-O3
10	L	1290	HTO	C1-C2-C3-C4
10	L	1290	HTO	O2-C2-C3-O3
10	L	1290	HTO	O2-C2-C3-C4
10	L	1290	HTO	O3-C3-C4-C5
12	M	1313	U10	C27-C28-C29-C30
12	M	1313	U10	C27-C28-C29-C31
12	M	1313	U10	C33-C34-C36-C37
12	M	1313	U10	C35-C34-C36-C37
13	M	1314	SPO	C3-C1-O1-CM1
13	M	1314	SPO	C4-C1-O1-CM1
13	M	1314	SPO	C4-C5-C6-C7
13	M	1314	SPO	C19-C20-C21-C22
13	M	1314	SPO	C36-C37-C38-C39
14	M	1315	CDL	CA3-OA5-PA1-OA2
14	M	1315	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
14	M	1315	CDL	CB3-OB5-PB2-OB2
14	M	1315	CDL	CB3-OB5-PB2-OB4
14	M	1315	CDL	C51-CB5-OB6-CB4
14	M	1315	CDL	OA9-CA7-OA8-CA6
8	L	1287[B]	UQ2	C12-C13-C14-C15
8	L	1287[B]	UQ2	C12-C13-C14-C16
13	M	1314	SPO	C36-C37-C38-C40
14	M	1315	CDL	OB7-CB5-OB6-CB4
14	M	1315	CDL	C31-CA7-OA8-CA6
8	L	1287[A]	UQ2	C12-C11-C9-C10
14	M	1315	CDL	C78-C79-C80-C81
14	M	1315	CDL	OB9-CB7-OB8-CB6
14	M	1315	CDL	C20-C21-C22-C23
12	M	1313	U10	C37-C38-C39-C41
14	M	1315	CDL	O1-C1-CB2-OB2
14	M	1315	CDL	C71-CB7-OB8-CB6
8	L	1287[A]	UQ2	C12-C11-C9-C8
8	L	1287[B]	UQ2	C9-C11-C12-C13
12	M	1313	U10	C29-C31-C32-C33
13	M	1314	SPO	C33-C35-C36-C37
5	M	1303	BCL	C10-C11-C12-C13
14	M	1315	CDL	C18-C19-C20-C21
5	L	1282	BCL	C6-C7-C8-C9
5	L	1288	BCL	C6-C7-C8-C9
5	L	1288	BCL	C14-C13-C15-C16
12	M	1313	U10	C37-C38-C39-C40
4	H	1251	GOL	O1-C1-C2-O2
4	H	1252	GOL	O1-C1-C2-O2
5	L	1288	BCL	C10-C11-C12-C13
14	M	1315	CDL	CB5-C51-C52-C53
7	M	1312	BPH	C5-C6-C7-C8
7	M	1312	BPH	C13-C15-C16-C17
8	L	1287[B]	UQ2	C12-C11-C9-C8
14	M	1315	CDL	CA2-C1-CB2-OB2
8	L	1287[B]	UQ2	C12-C11-C9-C10
13	M	1314	SPO	C21-C22-C23-C24
4	H	1251	GOL	O1-C1-C2-C3
4	H	1252	GOL	C1-C2-C3-O3
8	L	1287[A]	UQ2	C12-C13-C14-C15
13	M	1314	SPO	C21-C22-C23-C25
7	M	1312	BPH	C16-C17-C18-C20
6	M	1305	LDA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
14	M	1315	CDL	C15-C16-C17-C18
7	M	1312	BPH	C16-C17-C18-C19
5	M	1304	BCL	C12-C13-C15-C16
6	L	1285	LDA	C2-C3-C4-C5
14	M	1315	CDL	C52-C53-C54-C55
14	M	1315	CDL	C51-C52-C53-C54
6	M	1309	LDA	C6-C7-C8-C9
6	M	1309	LDA	C7-C8-C9-C10
5	L	1282	BCL	C13-C15-C16-C17
6	L	1285	LDA	C3-C4-C5-C6
14	M	1315	CDL	C16-C17-C18-C19
14	M	1315	CDL	C11-CA5-OA6-CA4
6	M	1306	LDA	C6-C7-C8-C9
6	L	1285	LDA	C5-C6-C7-C8
6	M	1307	LDA	C1-C2-C3-C4
6	M	1305	LDA	C11-C10-C9-C8
6	L	1283	LDA	C3-C4-C5-C6
13	M	1314	SPO	C24-C23-C25-C26
13	M	1314	SPO	C1-C4-C5-C6
6	M	1308	LDA	C2-C3-C4-C5
6	M	1308	LDA	C5-C6-C7-C8
6	M	1308	LDA	C7-C8-C9-C10
14	M	1315	CDL	C71-C72-C73-C74
5	M	1303	BCL	C8-C10-C11-C12
6	L	1285	LDA	C1-C2-C3-C4
14	M	1315	CDL	C11-C12-C13-C14
6	M	1308	LDA	C11-C10-C9-C8
5	L	1282	BCL	C3-C5-C6-C7
14	M	1315	CDL	C14-C15-C16-C17
5	M	1303	BCL	C2-C1-O2A-CGA
12	M	1313	U10	C30-C29-C31-C32
4	L	1293	GOL	O2-C2-C3-O3
6	L	1283	LDA	C5-C6-C7-C8
6	L	1284	LDA	C4-C5-C6-C7
14	M	1315	CDL	C80-C81-C82-C83
14	M	1315	CDL	OA5-CA3-CA4-CA6
14	M	1315	CDL	OA7-CA5-OA6-CA4
6	M	1307	LDA	C7-C8-C9-C10
5	L	1282	BCL	C16-C17-C18-C19
7	L	1286	BPH	C4-C3-C5-C6
7	L	1286	BPH	C2-C3-C5-C6
6	M	1307	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
14	M	1315	CDL	CA3-CA4-CA6-OA8
5	L	1288	BCL	C8-C10-C11-C12
6	M	1310	LDA	C1-C2-C3-C4
14	M	1315	CDL	C19-C20-C21-C22
6	M	1308	LDA	C1-C2-C3-C4
7	L	1286	BPH	O2A-C1-C2-C3
7	M	1312	BPH	O2A-C1-C2-C3
6	L	1285	LDA	C4-C5-C6-C7
7	L	1286	BPH	C8-C10-C11-C12
6	L	1283	LDA	C6-C7-C8-C9
5	L	1282	BCL	C16-C17-C18-C20
12	M	1313	U10	C31-C32-C33-C34
6	L	1285	LDA	C6-C7-C8-C9
14	M	1315	CDL	C55-C56-C57-C58
8	L	1287[A]	UQ2	C12-C13-C14-C16
6	L	1283	LDA	C9-C10-C11-C12
6	L	1284	LDA	C11-C10-C9-C8
6	L	1285	LDA	C11-C10-C9-C8
6	L	1285	LDA	C9-C10-C11-C12
13	M	1314	SPO	C2-C1-O1-CM1
14	M	1315	CDL	C81-C82-C83-C84
6	L	1284	LDA	C7-C8-C9-C10
6	M	1306	LDA	C7-C8-C9-C10
4	L	1292	GOL	O2-C2-C3-O3
5	M	1304	BCL	C14-C13-C15-C16
7	M	1312	BPH	C11-C10-C8-C9
5	L	1288	BCL	C12-C13-C15-C16
5	M	1304	BCL	C11-C10-C8-C7
7	M	1312	BPH	C11-C10-C8-C7
6	M	1307	LDA	C4-C5-C6-C7
6	L	1284	LDA	C6-C7-C8-C9
5	M	1303	BCL	C4-C3-C5-C6
14	M	1315	CDL	OA5-CA3-CA4-OA6
14	M	1315	CDL	OB5-CB3-CB4-OB6
10	L	1290	HTO	O1-C1-C2-O2
14	M	1315	CDL	C53-C54-C55-C56
5	M	1303	BCL	C2-C3-C5-C6
7	M	1312	BPH	C1-C2-C3-C5
5	M	1303	BCL	C14-C13-C15-C16
6	M	1305	LDA	C7-C8-C9-C10
12	M	1313	U10	C34-C36-C37-C38
14	M	1315	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	O2-C2-C3-O3
4	L	1293	GOL	O1-C1-C2-O2
13	M	1314	SPO	C22-C23-C25-C26
14	M	1315	CDL	C32-C33-C34-C35
12	M	1313	U10	C28-C29-C31-C32
14	M	1315	CDL	C74-C75-C76-C77
6	M	1309	LDA	C2-C3-C4-C5
5	L	1282	BCL	C5-C6-C7-C8
6	M	1309	LDA	C2-C1-N1-CM1
14	M	1315	CDL	C38-C39-C40-C41
14	M	1315	CDL	C21-C22-C23-C24
6	L	1283	LDA	C11-C10-C9-C8
5	M	1304	BCL	C5-C6-C7-C8
14	M	1315	CDL	OB5-CB3-CB4-CB6
5	L	1282	BCL	C6-C7-C8-C10
5	M	1303	BCL	C11-C10-C8-C7
6	L	1283	LDA	C2-C3-C4-C5
6	M	1306	LDA	C2-C1-N1-O1
6	L	1284	LDA	C5-C6-C7-C8
14	M	1315	CDL	OA6-CA4-CA6-OA8
8	L	1287[A]	UQ2	C1-C2-O2-CM2
14	M	1315	CDL	C37-C38-C39-C40
5	L	1282	BCL	CHA-CBD-CGD-O1D
5	L	1282	BCL	CHA-CBD-CGD-O2D
14	M	1315	CDL	CA3-OA5-PA1-OA4
14	M	1315	CDL	CB3-OB5-PB2-OB3
6	M	1310	LDA	C7-C8-C9-C10
10	L	1290	HTO	C4-C5-C6-C7
5	L	1288	BCL	C13-C15-C16-C17
14	M	1315	CDL	C33-C34-C35-C36
14	M	1315	CDL	CB7-C71-C72-C73
6	L	1285	LDA	N1-C1-C2-C3
5	M	1303	BCL	C11-C10-C8-C9
7	M	1312	BPH	C11-C12-C13-C14
5	L	1288	BCL	C2-C1-O2A-CGA
6	M	1308	LDA	C4-C5-C6-C7
5	L	1282	BCL	C14-C13-C15-C16
5	L	1282	BCL	C2B-C3B-CAB-OBB
7	M	1312	BPH	C1-C2-C3-C4
8	L	1287[B]	UQ2	C3-C2-O2-CM2
6	M	1307	LDA	C9-C10-C11-C12
7	M	1312	BPH	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	M	1305	LDA	C1-C2-C3-C4
7	M	1312	BPH	C11-C12-C13-C15
14	M	1315	CDL	C12-C13-C14-C15
5	L	1282	BCL	C8-C10-C11-C12
14	M	1315	CDL	C1-CB2-OB2-PB2
10	L	1291	HTO	C3-C4-C5-C6
12	M	1313	U10	C5-C4-O4-C4M
14	M	1315	CDL	CB2-C1-CA2-OA2
5	M	1304	BCL	CAA-CBA-CGA-O2A
5	L	1288	BCL	C16-C17-C18-C19
5	M	1303	BCL	C11-C12-C13-C14
5	L	1288	BCL	C16-C17-C18-C20
6	M	1310	LDA	N1-C1-C2-C3
7	M	1312	BPH	C2-C3-C5-C6
6	M	1310	LDA	C5-C6-C7-C8
6	M	1307	LDA	C5-C6-C7-C8
6	L	1283	LDA	C2-C1-N1-CM2
10	L	1291	HTO	C4-C5-C6-C7
14	M	1315	CDL	CA5-C11-C12-C13
5	L	1282	BCL	C2B-C3B-CAB-CBB
14	M	1315	CDL	C75-C76-C77-C78
6	L	1283	LDA	C2-C1-N1-O1
6	M	1310	LDA	C6-C7-C8-C9
14	M	1315	CDL	C72-C71-CB7-OB8

There are no ring outliers.

17 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1292	GOL	1	0
4	H	1251	GOL	5	0
6	M	1305	LDA	1	0
14	M	1315	CDL	5	0
7	L	1286	BPH	7	0
6	L	1284	LDA	1	0
5	M	1304	BCL	12	0
7	M	1312	BPH	12	0
6	L	1285	LDA	1	0
5	L	1282	BCL	4	0
13	M	1314	SPO	3	0
8	L	1287[A]	UQ2	2	0
8	L	1287[B]	UQ2	2	0

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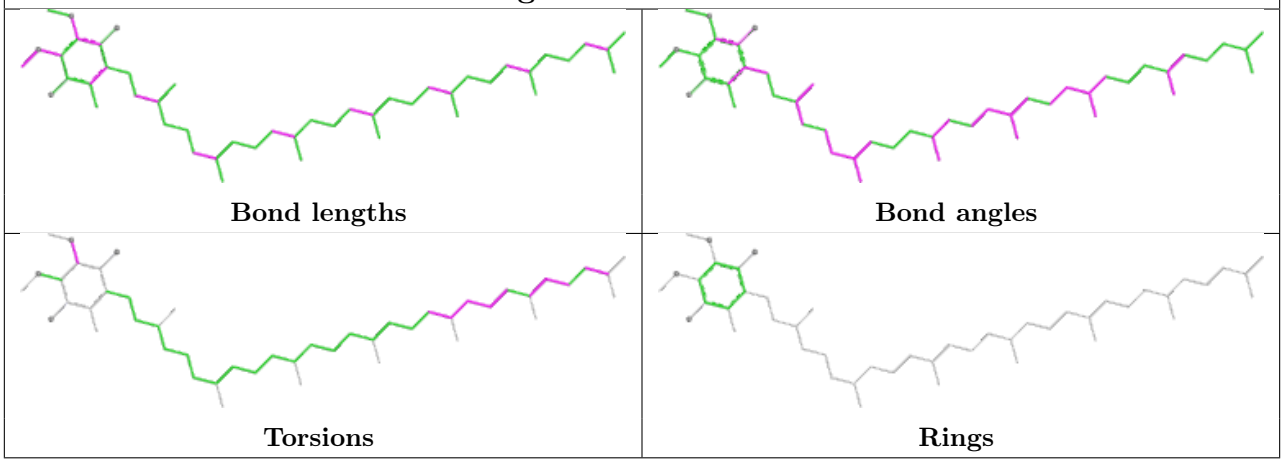
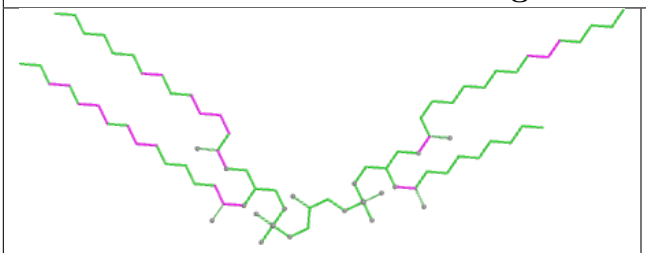
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1308	LDA	2	0
6	M	1307	LDA	4	0
6	M	1310	LDA	1	0
5	M	1303	BCL	8	0

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.

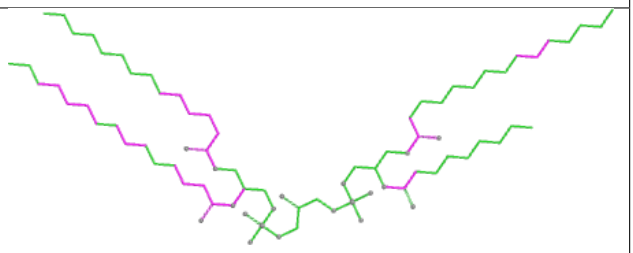
Ligand U10 M 1313



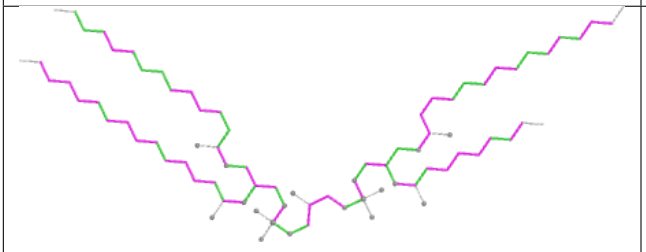
Ligand CDL M 1315



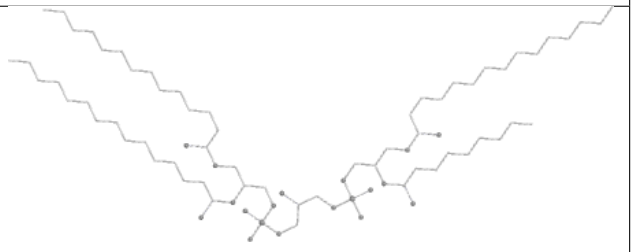
Bond lengths



Bond angles

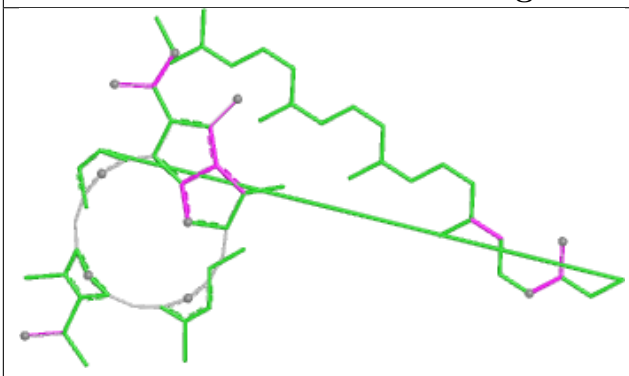


Torsions

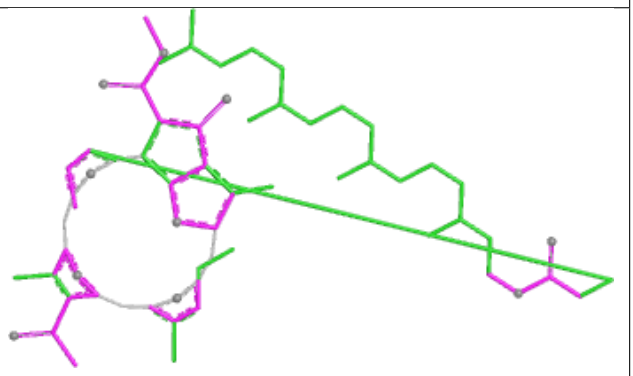


Rings

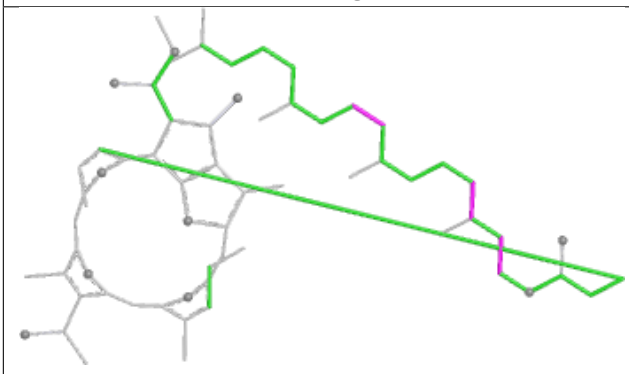
Ligand BPH L 1286



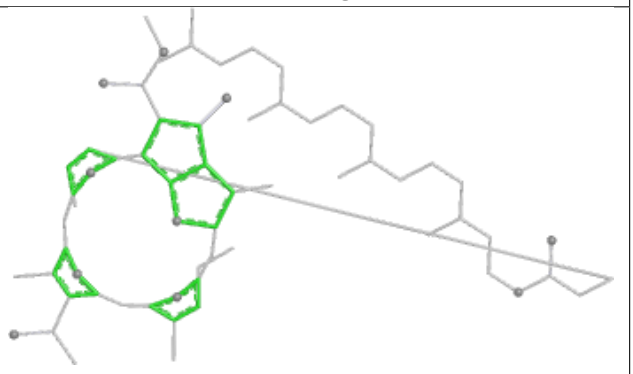
Bond lengths



Bond angles

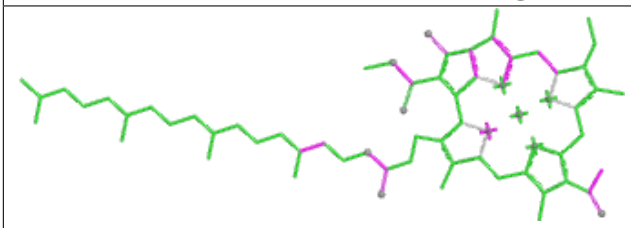


Torsions

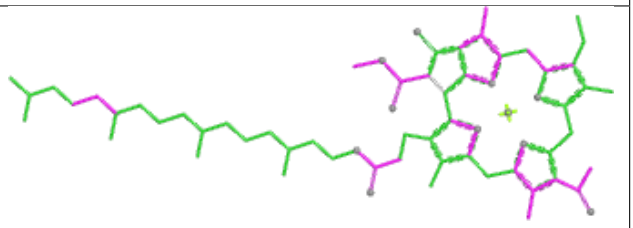


Rings

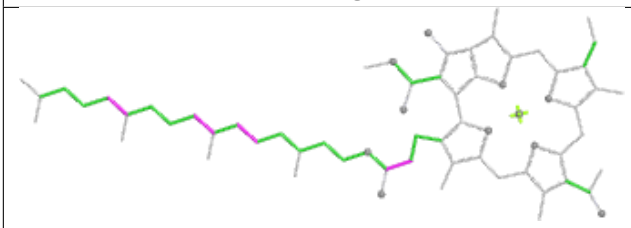
Ligand BCL M 1304



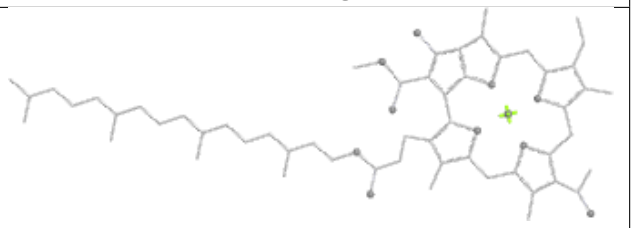
Bond lengths



Bond angles

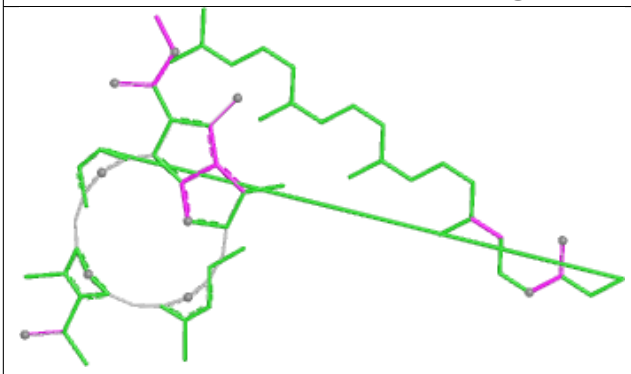


Torsions

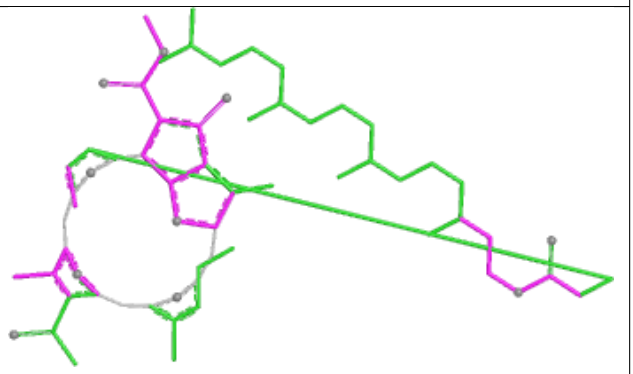


Rings

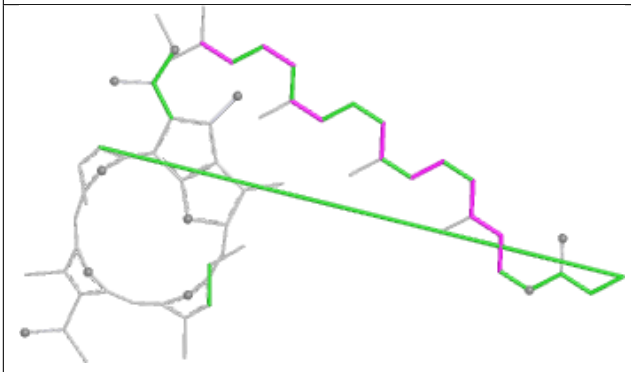
Ligand BPH M 1312



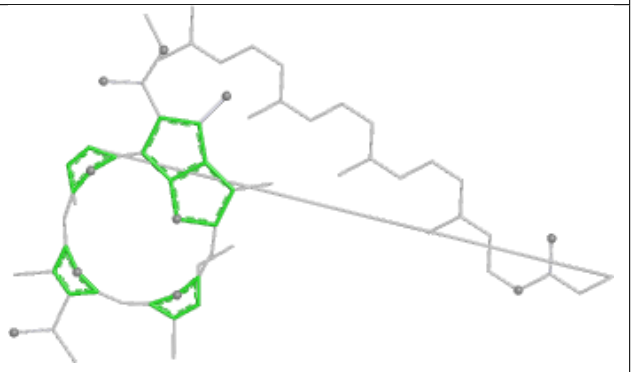
Bond lengths



Bond angles

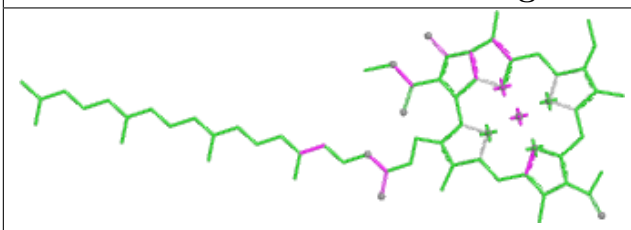


Torsions

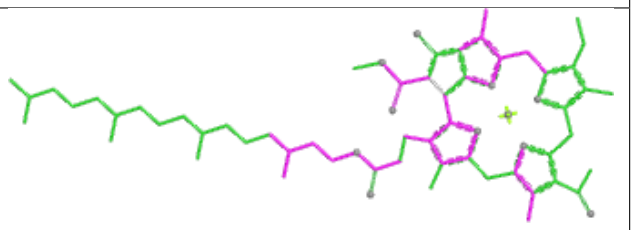


Rings

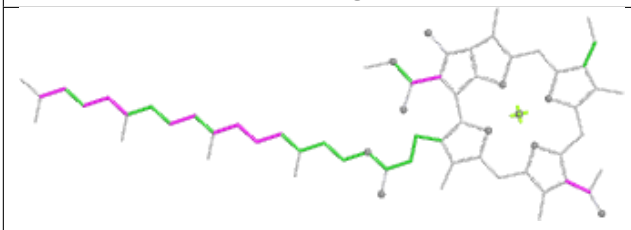
Ligand BCL L 1282



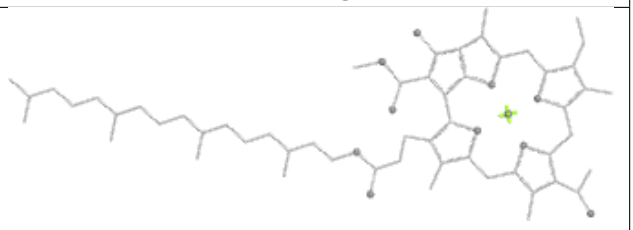
Bond lengths



Bond angles

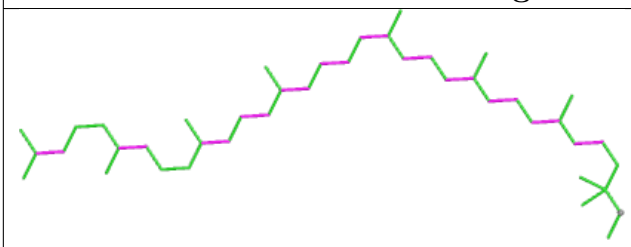


Torsions

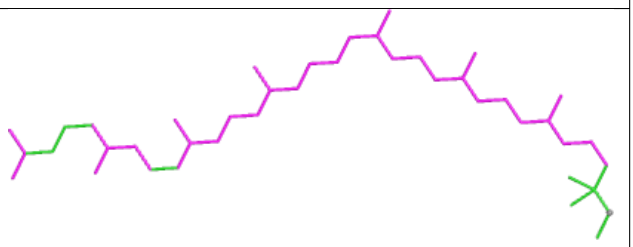


Rings

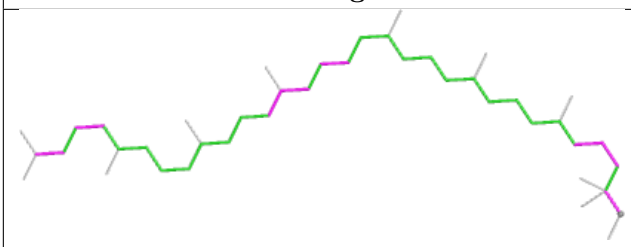
Ligand SPO M 1314



Bond lengths



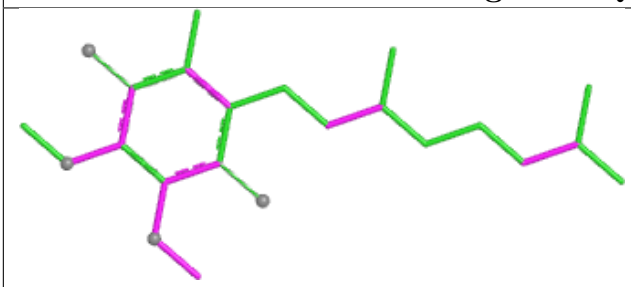
Bond angles



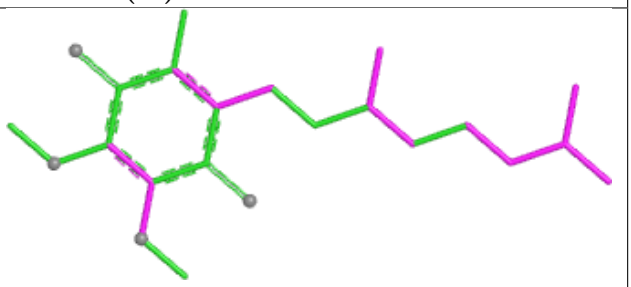
Torsions

Rings

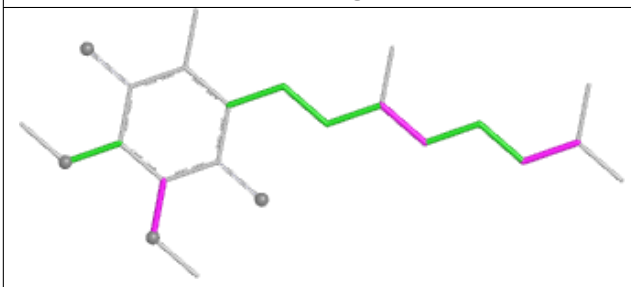
Ligand UQ2 L 1287 (A)



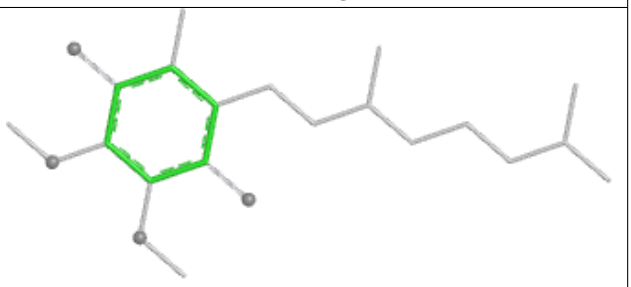
Bond lengths



Bond angles

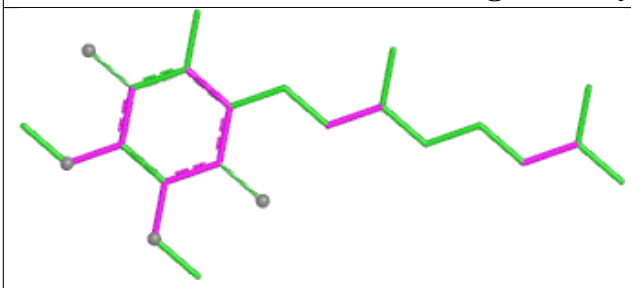


Torsions

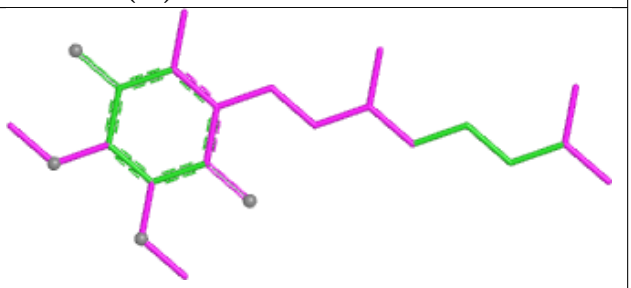


Rings

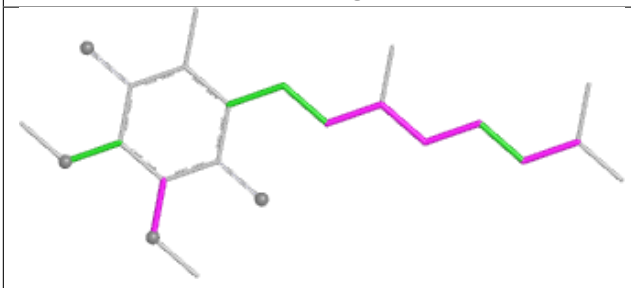
Ligand UQ2 L 1287 (B)



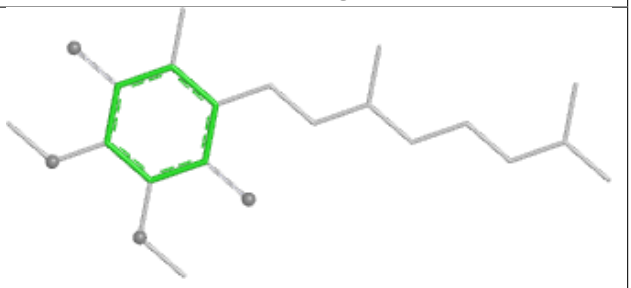
Bond lengths



Bond angles

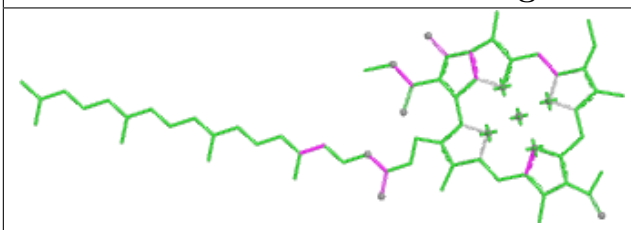


Torsions

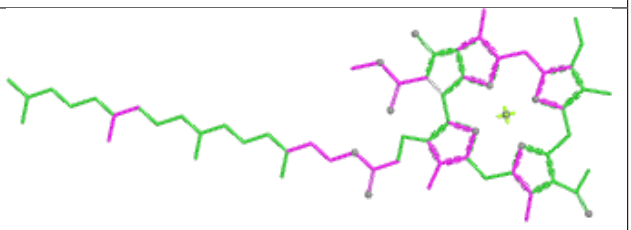


Rings

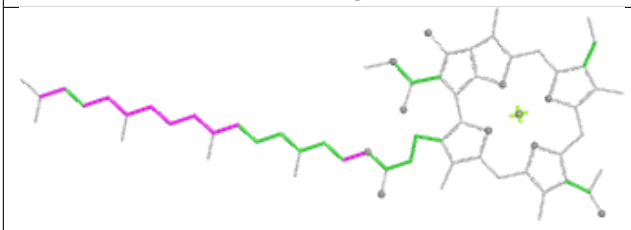
Ligand BCL L 1288



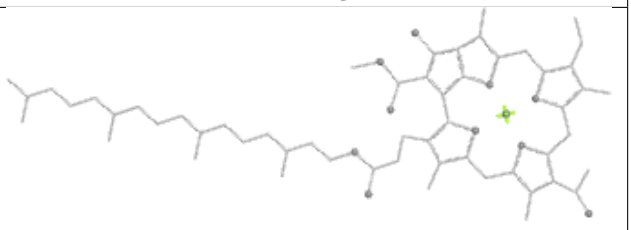
Bond lengths



Bond angles

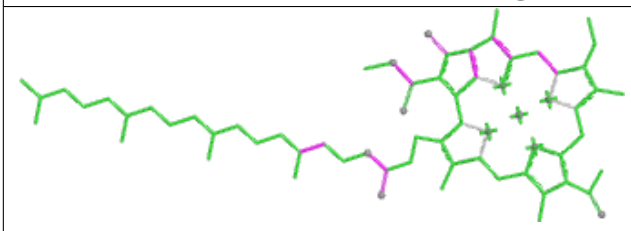


Torsions

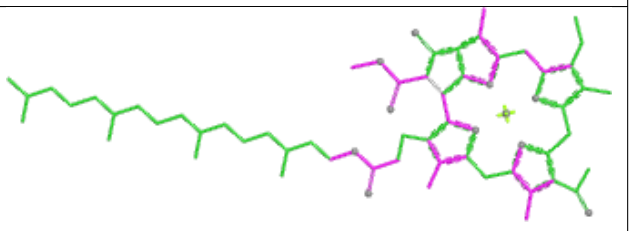


Rings

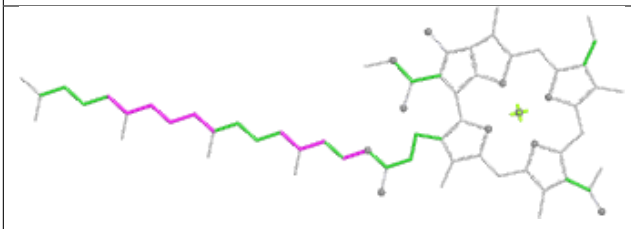
Ligand BCL M 1303



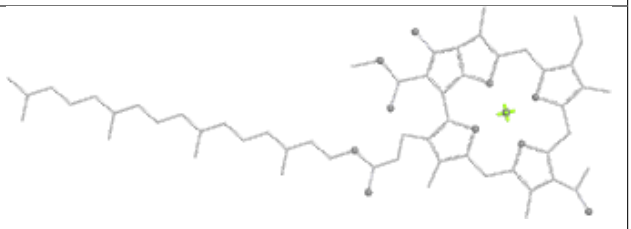
Bond lengths



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%)	0.05	5 (2%)	63	65	29, 37, 49, 79	0
2	L	281/281 (100%)	0.33	12 (4%)	40	40	27, 36, 58, 66	0
3	M	303/307 (98%)	0.32	14 (4%)	37	37	26, 40, 60, 72	0
All	All	825/848 (97%)	0.25	31 (3%)	44	44	26, 37, 58, 79	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	3	TYR	5.0
2	L	59	TRP	4.2
3	M	1	ALA	3.9
3	M	301	HIS	3.6
3	M	2	GLU	3.5
2	L	271	TRP	3.4
3	M	148	TRP	3.4
3	M	302	GLY	3.3
3	M	109	LEU	3.3
2	L	277	GLY	2.9
2	L	67	TYR	2.8
1	H	249	LYS	2.7
1	H	250	SER	2.7
2	L	56	GLN	2.6
3	M	27	ALA	2.5
2	L	51	TRP	2.4
2	L	1	ALA	2.4
3	M	300	ASN	2.4
1	H	18	TYR	2.3
2	L	281	GLY	2.3
1	H	251	VAL	2.3
3	M	139	ALA	2.3
3	M	105	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	53	ALA	2.2
2	L	270	PRO	2.2
3	M	52	LEU	2.1
2	L	54	VAL	2.1
3	M	32	VAL	2.1
2	L	275	ILE	2.0
3	M	78	ALA	2.0
1	H	220	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides 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
10	HTO	L	1291	10/10	0.49	0.38	111,114,114,115	0
6	LDA	L	1284	16/16	0.62	0.38	71,83,95,95	0
6	LDA	M	1308	16/16	0.71	0.37	97,100,104,105	0
14	CDL	M	1315	81/100	0.71	0.30	64,97,111,113	0
6	LDA	M	1309	16/16	0.74	0.31	96,98,104,104	0
6	LDA	L	1285	16/16	0.76	0.29	101,105,111,111	0
6	LDA	M	1310	16/16	0.77	0.31	90,96,104,104	0
6	LDA	M	1305	16/16	0.79	0.25	41,67,76,76	0
6	LDA	M	1307	16/16	0.80	0.21	58,60,64,65	0
6	LDA	L	1283	16/16	0.80	0.26	80,99,109,110	0
6	LDA	M	1306	16/16	0.83	0.28	66,71,83,83	0
4	GOL	H	1254	6/6	0.84	0.14	104,104,105,105	0
8	UQ2	L	1287[A]	23/23	0.84	0.20	27,36,51,51	23
8	UQ2	L	1287[B]	23/23	0.84	0.20	28,36,52,53	23
4	GOL	H	1251	6/6	0.84	0.16	47,59,62,62	0

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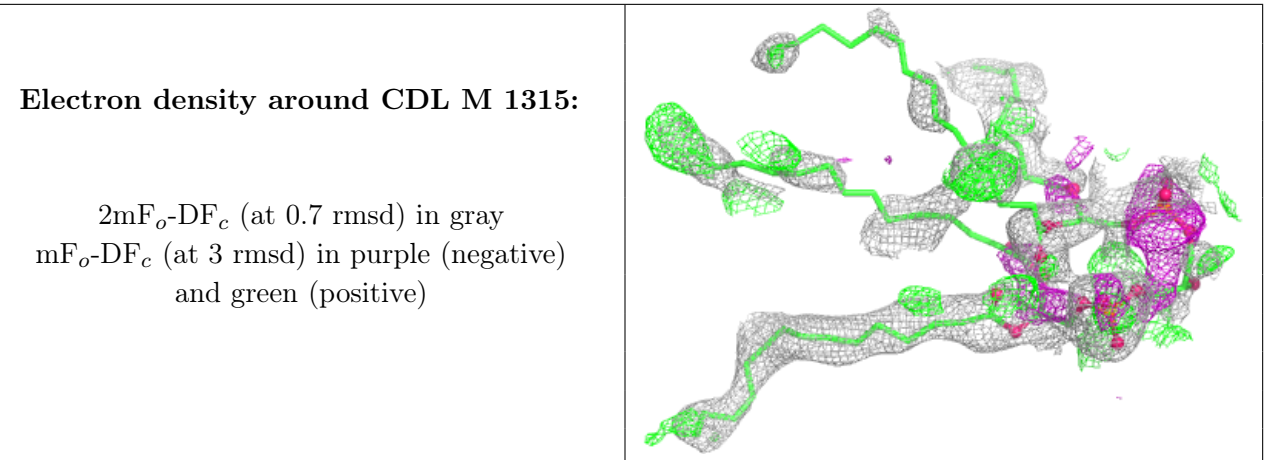
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	H	1252	6/6	0.84	0.13	74,75,75,77	0
4	GOL	L	1293	6/6	0.85	0.18	98,99,99,99	0
4	GOL	L	1292	6/6	0.85	0.19	49,56,57,60	0
10	HTO	L	1290	10/10	0.86	0.23	85,88,88,88	0
4	GOL	H	1253	6/6	0.88	0.18	113,114,114,114	0
13	SPO	M	1314	42/42	0.91	0.13	38,49,68,71	0
12	U10	M	1313	48/63	0.91	0.14	26,42,67,69	0
9	PO4	L	1289	5/5	0.95	0.06	62,63,64,64	0
5	BCL	L	1282	66/66	0.95	0.09	25,30,57,59	0
7	BPH	M	1312	65/65	0.95	0.10	29,37,93,95	0
5	BCL	M	1303	66/66	0.96	0.10	26,33,79,81	0
5	BCL	M	1304	66/66	0.96	0.08	26,30,54,62	0
7	BPH	L	1286	65/65	0.96	0.08	22,29,41,42	0
5	BCL	L	1288	66/66	0.96	0.08	25,31,48,55	0
11	FE	M	1311	1/1	0.99	0.05	26,26,26,26	0

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

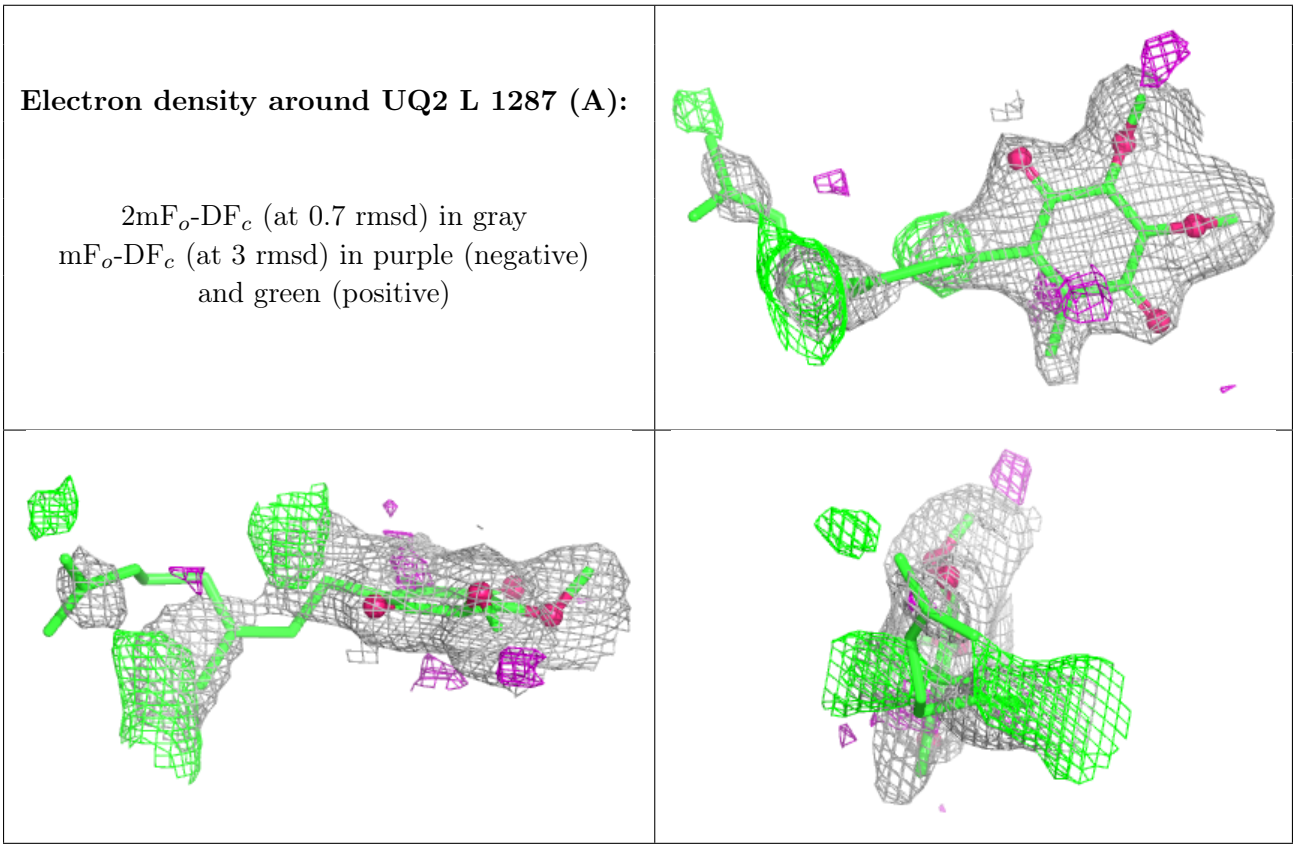
Electron density around CDL M 1315:

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



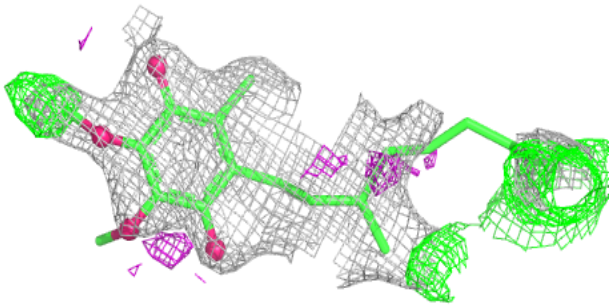
Electron density around UQ2 L 1287 (A):

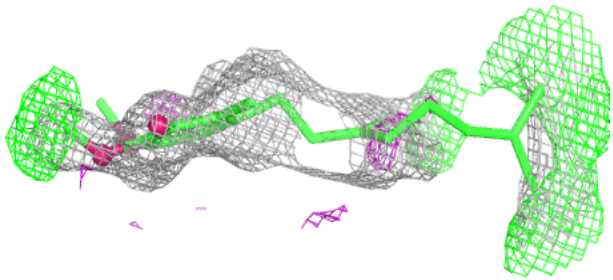
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

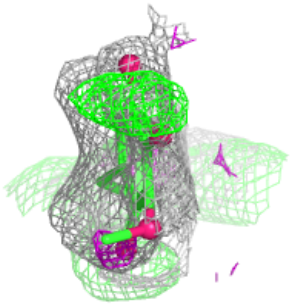


Electron density around UQ2 L 1287 (B):

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

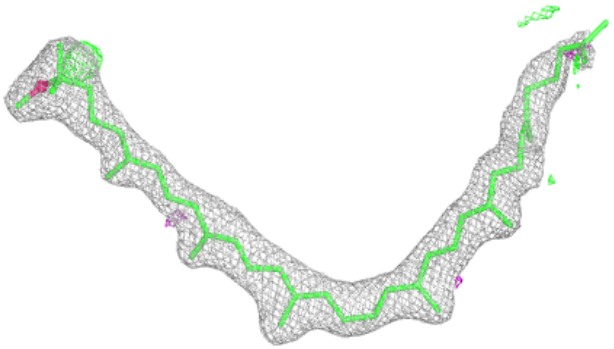


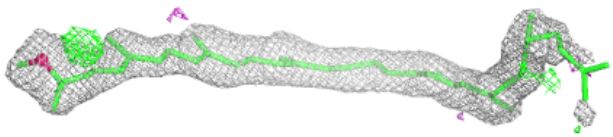


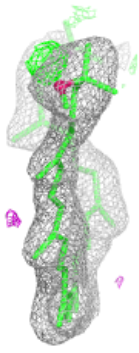


Electron density around SPO M 1314:

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

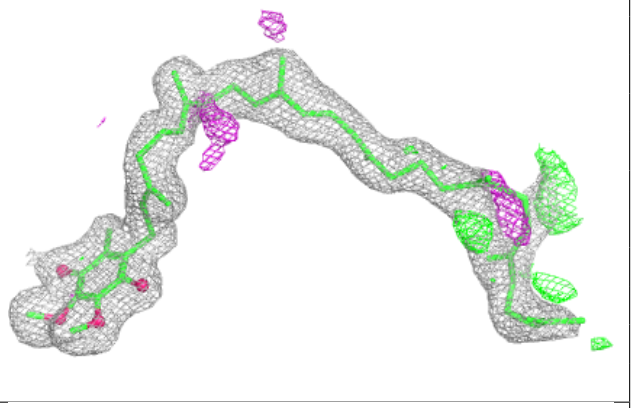


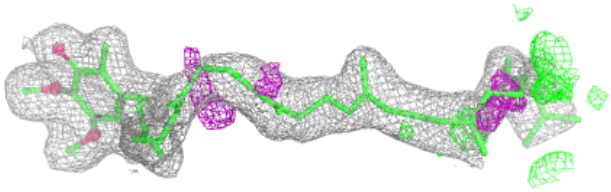


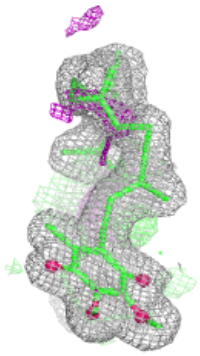


Electron density around U10 M 1313:

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

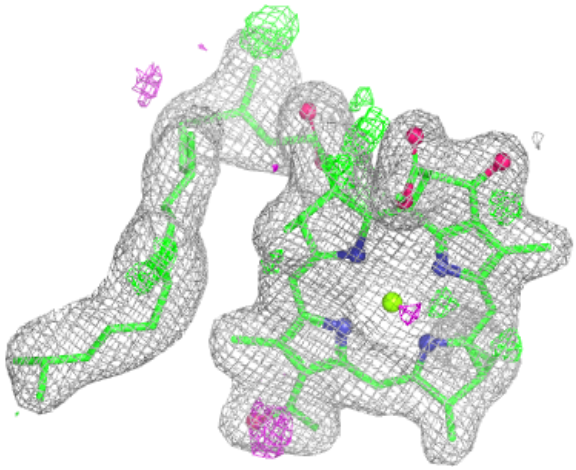


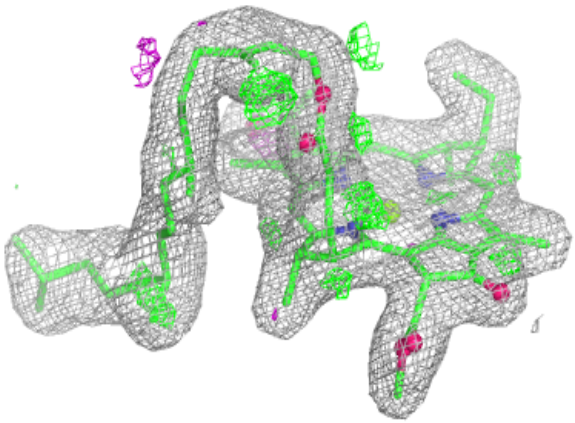


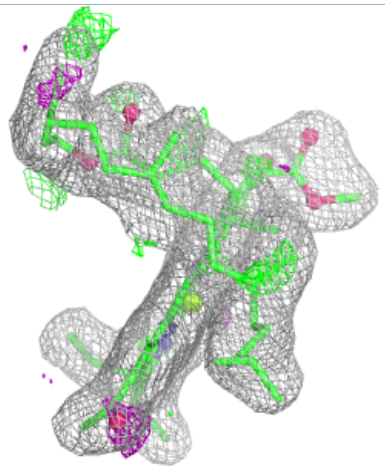


Electron density around BCL L 1282:

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

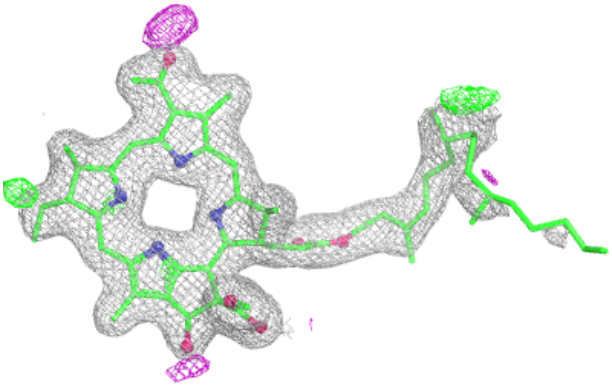


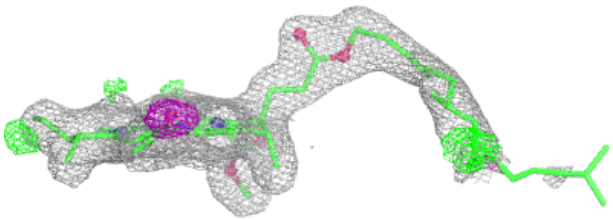


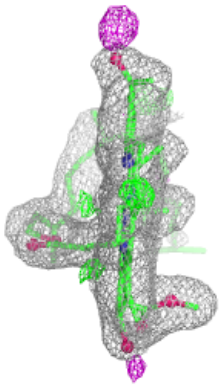


Electron density around BPH M 1312:

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

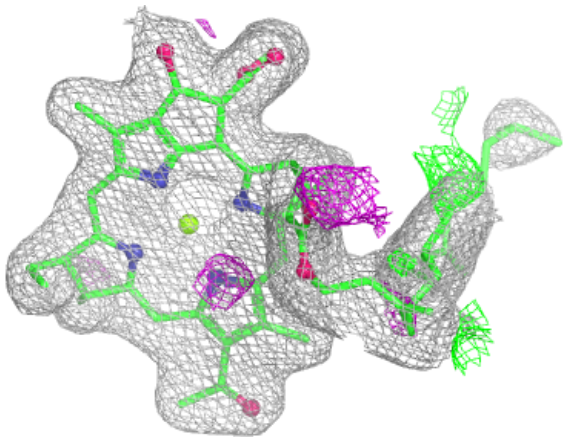


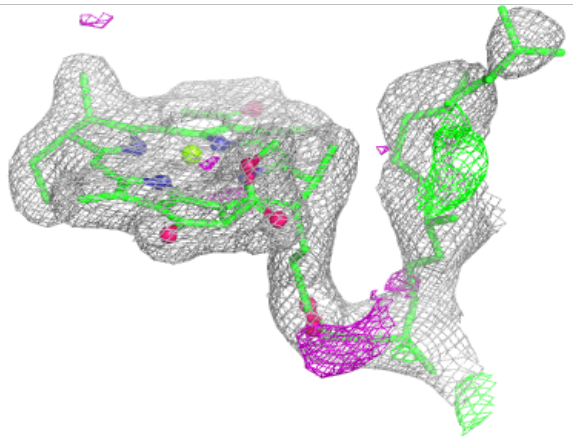


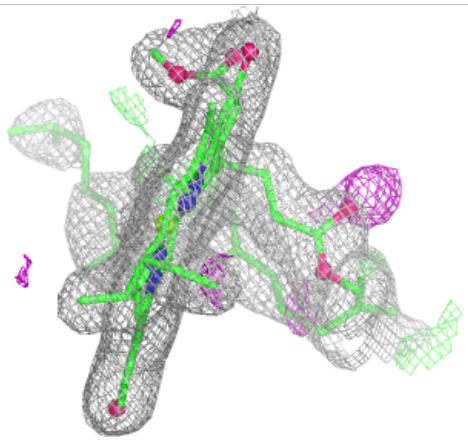


Electron density around BCL M 1303:

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

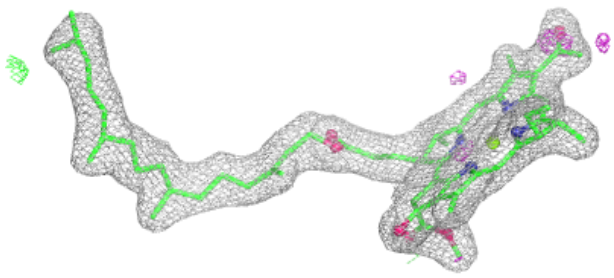


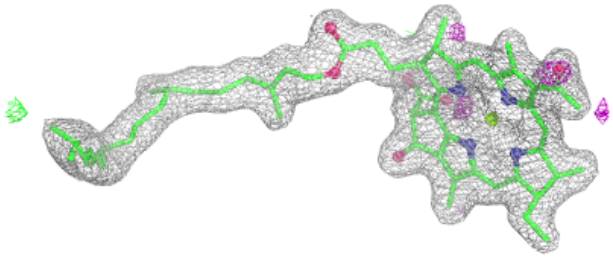


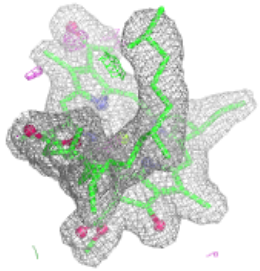


Electron density around BCL M 1304:

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

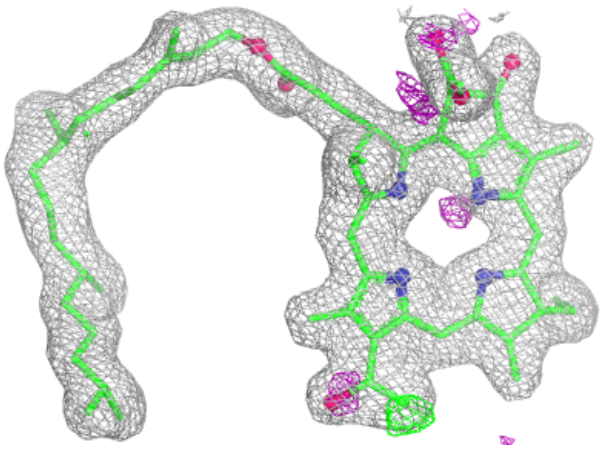


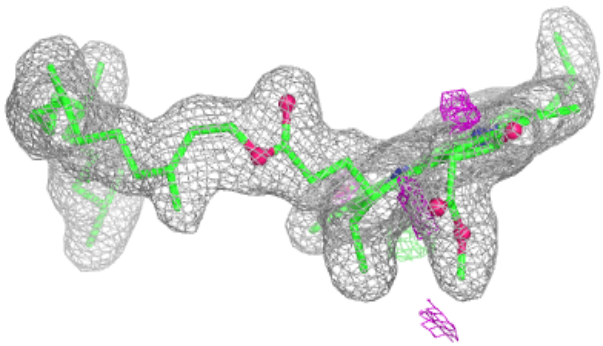


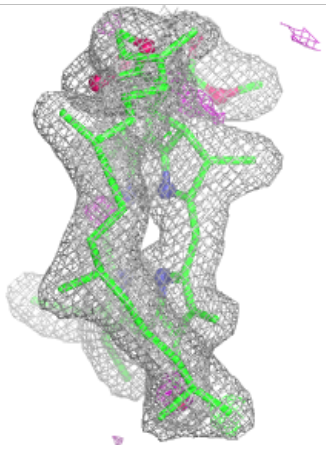


Electron density around BPH L 1286:

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

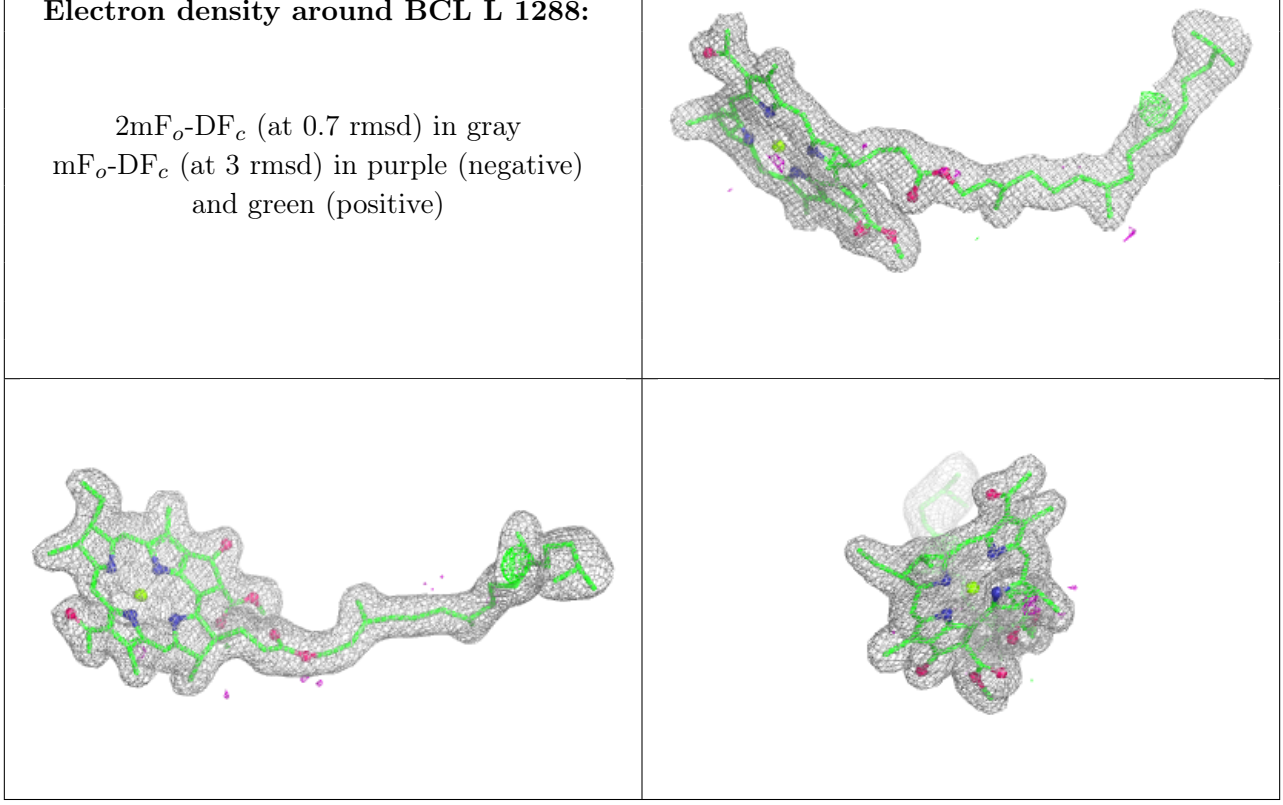






Electron density around BCL L 1288:

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



6.5 Other polymers

There are no such residues in this entry.