Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 01:28 pm BST

PDB ID	:	2UX5 / pdb_00002ux5
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 9 in the charge-separated state
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-26
Resolution	:	2.21 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 (i) 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 (i)) were used in the production of this report:

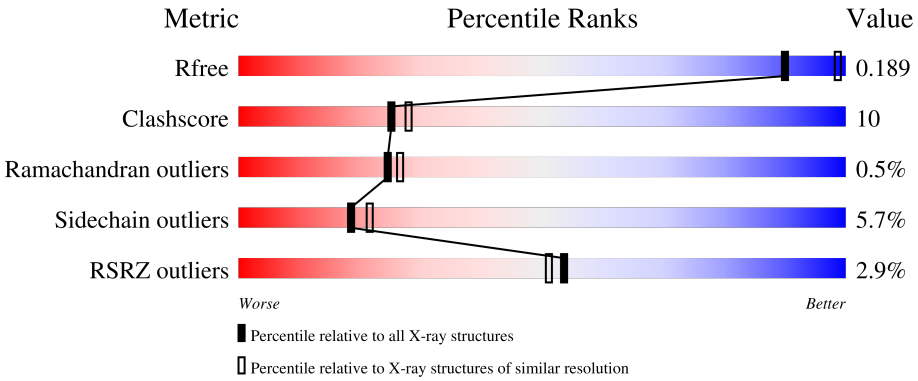
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	3% 77% 14% • 7%
2	L	281	2% 81% 17% •
3	M	307	4% 79% 17% ••

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
5	BCL	L	1282	X	-	-	-
5	BCL	L	1287	X	-	-	-
5	BCL	M	1304	X	-	-	-
5	BCL	M	1305	X	-	-	-
6	LDA	M	1309	-	-	-	X

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 7706 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	1846	1181	319	337	9	0	3	1

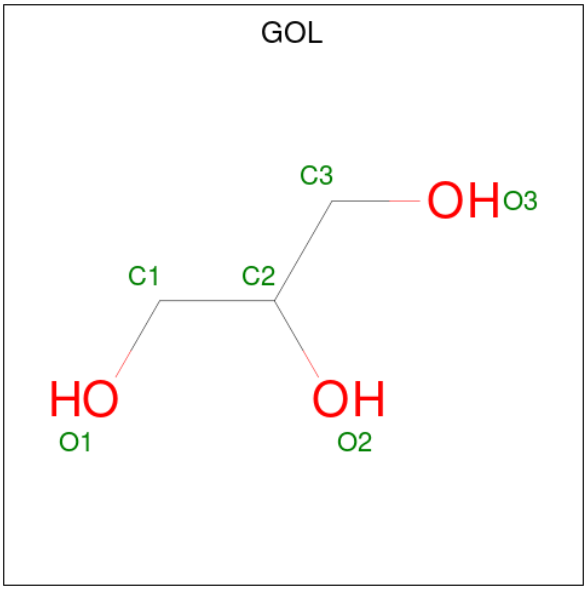
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

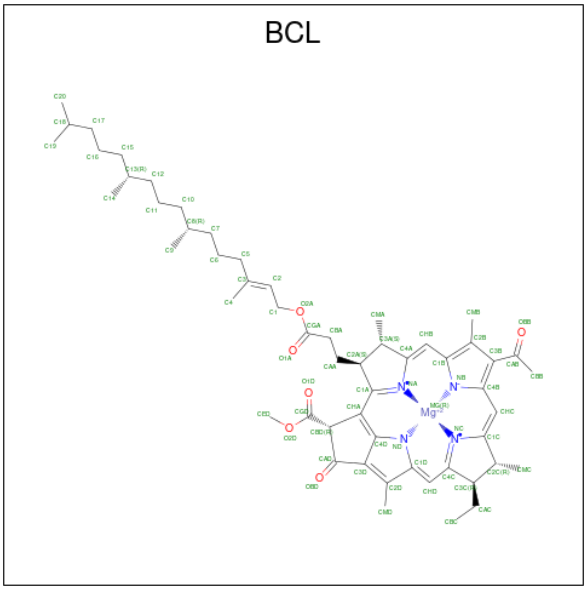
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

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



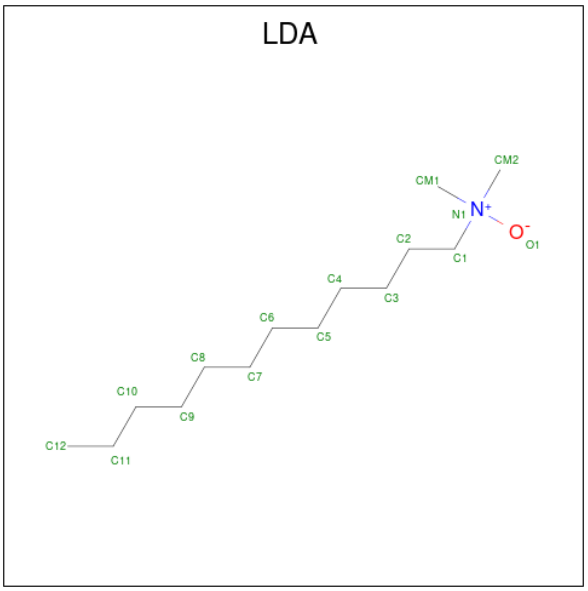
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

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



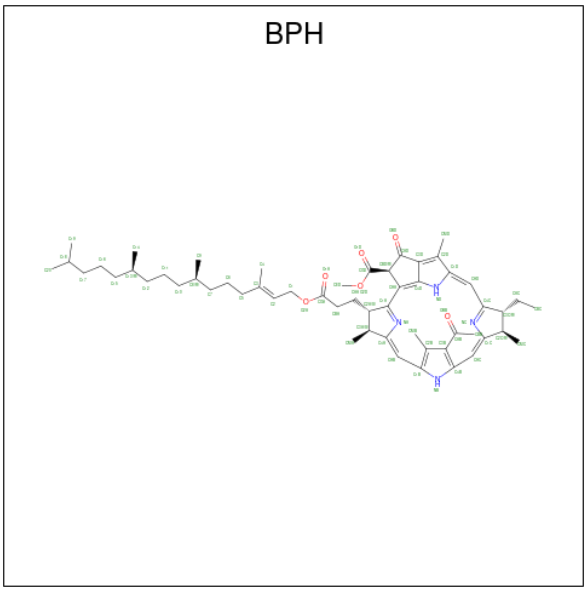
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



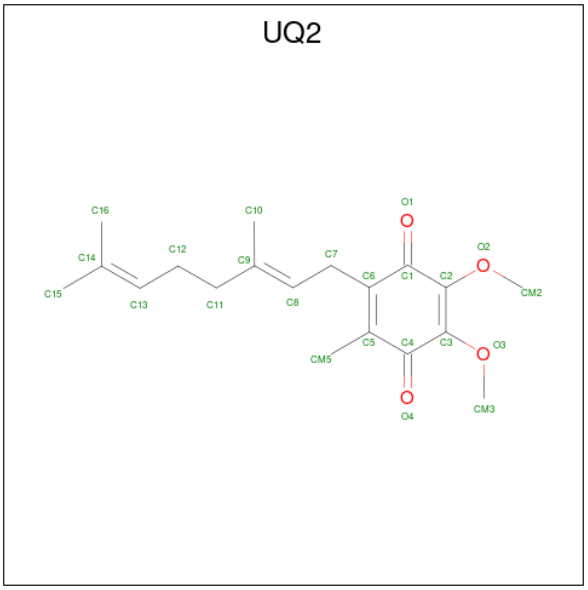
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M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

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



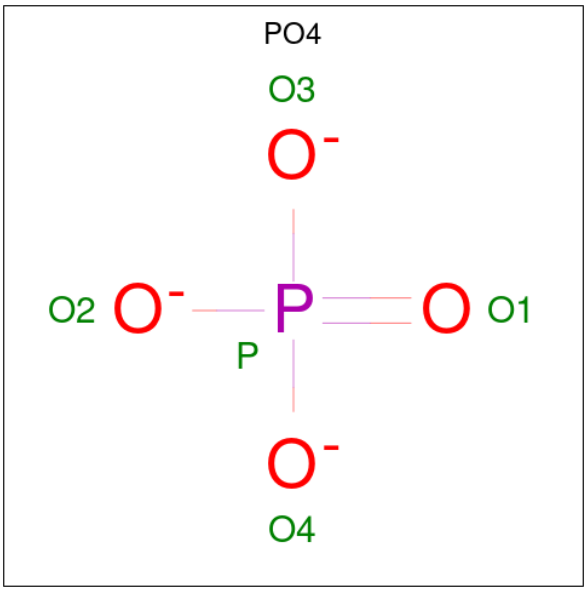
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
			Total	C	N	O		
7	M	1	65	55	4	6	0	0

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



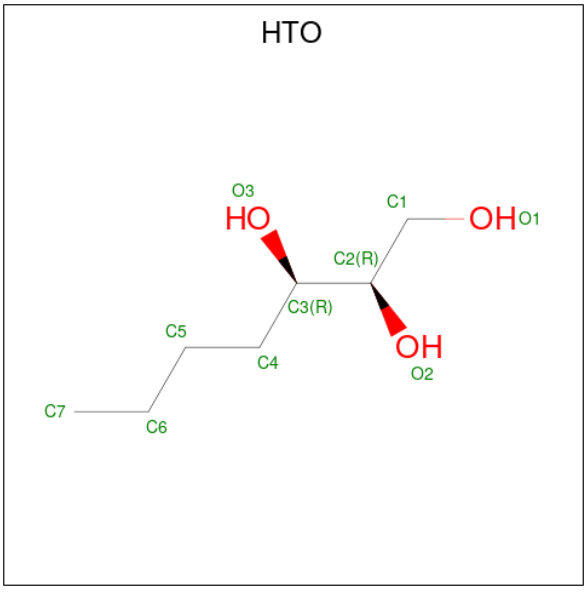
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	46	38	8	0	1

- 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: $C_7H_{16}O_3$).

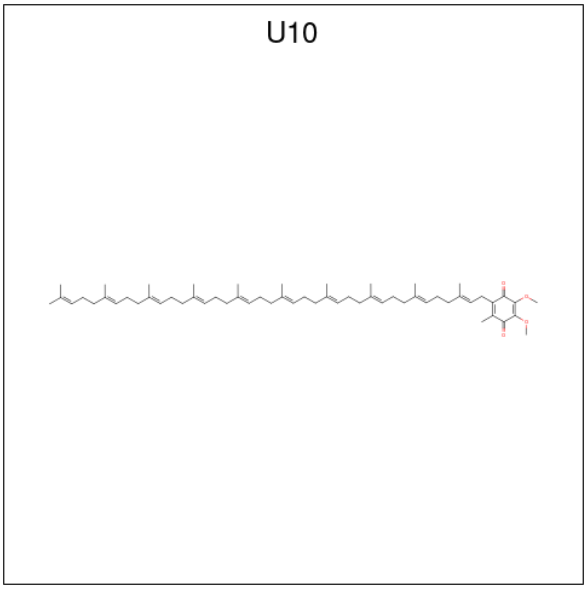


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0

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

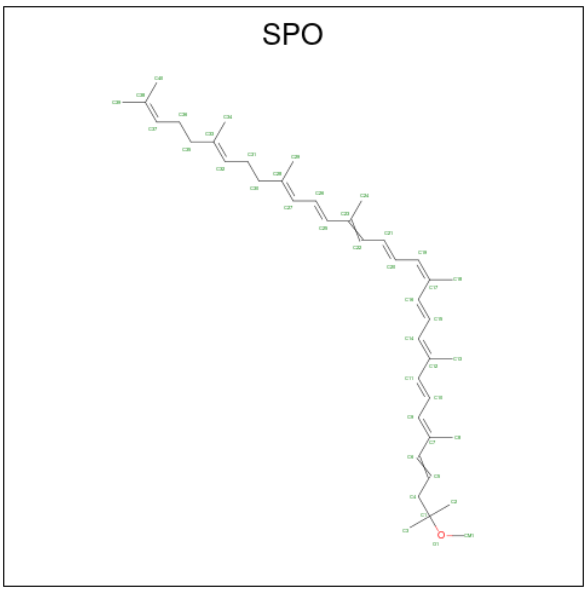
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

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



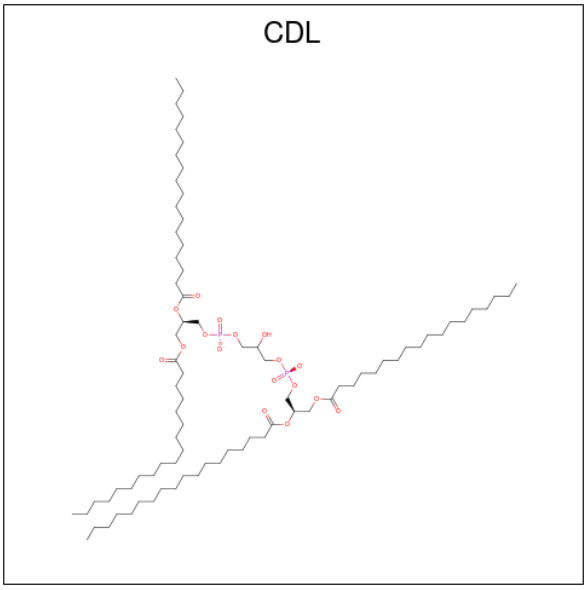
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 48 44 4	0	0

- 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	0	0
			42	41	1		

- 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	0	0
			81	62	17	2		

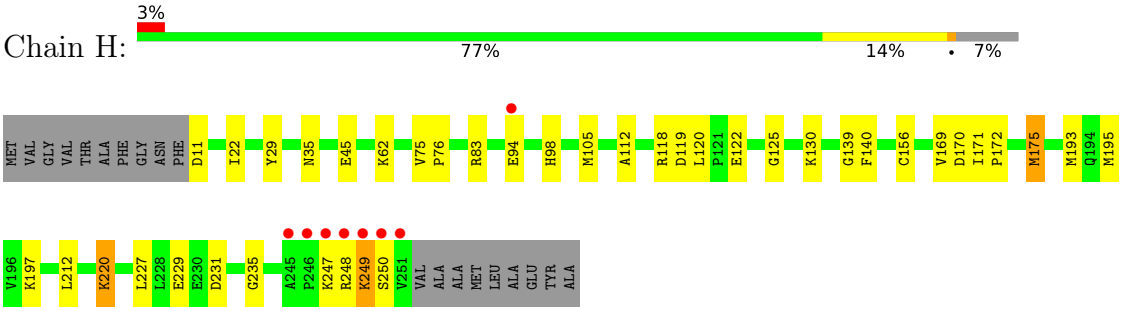
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	167	Total	O	0	0
			167	167		
15	L	115	Total	O	0	0
			115	115		
15	M	124	Total	O	0	0
			124	124		

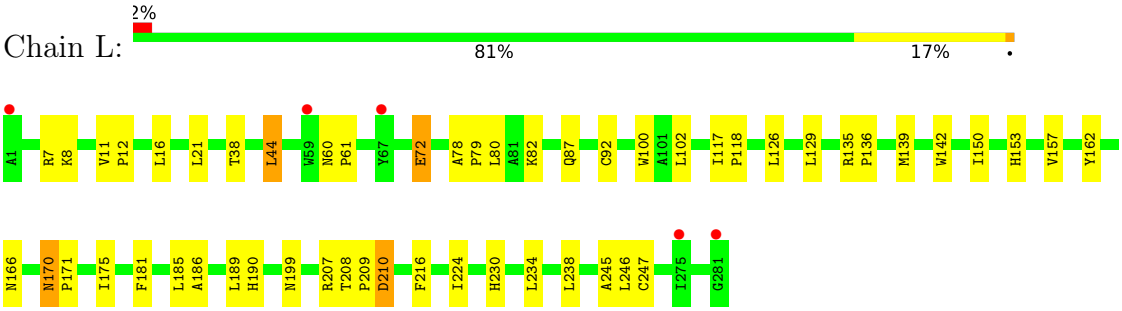
3 Residue-property plots (i)

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.

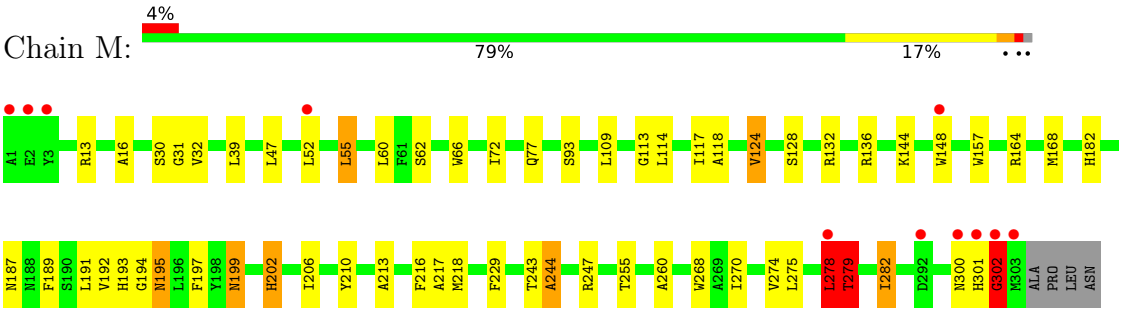
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER PROTEIN M CHAIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.46Å 139.46Å 184.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.21 50.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.21) 96.4 (50.00-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.236 0.196 , 0.189	Depositor DCC
R_{free} test set	3118 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7706	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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: LDA, CDL, SPO, PO4, BCL, HTO, BPH, GOL, FE, U10, UQ2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	H	1.08	3/1906 (0.2%)	1.07	2/2591 (0.1%)
2	L	1.12	6/2320 (0.3%)	1.05	1/3175 (0.0%)
3	M	1.09	8/2501 (0.3%)	1.05	3/3415 (0.1%)
All	All	1.10	17/6727 (0.3%)	1.06	6/9181 (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
3	M	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	278	LEU	CG-CD2	8.65	1.81	1.52
3	M	213	ALA	CA-CB	7.54	1.65	1.53
3	M	218	MET	SD-CE	6.51	1.95	1.79
1	H	250	SER	C-N	-6.41	1.24	1.33
3	M	302	GLY	C-N	-6.31	1.24	1.33
3	M	255	THR	CA-CB	5.91	1.62	1.53
3	M	244	ALA	CA-CB	5.90	1.62	1.53
3	M	282	ILE	CA-CB	5.81	1.61	1.54
2	L	175	ILE	CA-C	5.77	1.59	1.52
2	L	234	LEU	CA-C	5.48	1.59	1.52
2	L	139	MET	SD-CE	5.44	1.93	1.79
1	H	120	LEU	CA-C	5.35	1.57	1.52
1	H	195	MET	SD-CE	-5.33	1.66	1.79
2	L	238	LEU	CA-C	5.18	1.59	1.52
2	L	186	ALA	CA-C	5.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	217	ALA	CA-C	5.13	1.59	1.52
2	L	245	ALA	CA-C	5.11	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	278	LEU	CA-CB-CG	-8.95	84.97	116.30
1	H	83	ARG	N-CA-C	-6.42	102.45	108.22
3	M	202	HIS	N-CA-C	-6.03	104.27	111.69
1	H	139	GLY	N-CA-C	-5.87	96.27	113.30
2	L	230	HIS	N-CA-C	-5.21	105.28	111.69
3	M	279	THR	N-CA-CB	5.15	119.20	110.49

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	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	1846	0	1861	25	0
2	L	2232	0	2187	30	0
3	M	2409	0	2321	51	0
4	H	24	0	32	4	0
4	L	12	0	16	1	0
4	M	6	0	8	1	0
5	L	132	0	148	4	0
5	M	132	0	148	21	0
6	L	32	0	62	2	0
6	M	112	0	217	8	0
7	L	65	0	76	6	0
7	M	65	0	76	14	0
8	L	46	0	52	6	0
9	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	4	0
13	M	42	0	60	2	0
14	M	81	0	86	4	0
15	H	167	0	0	3	0
15	L	115	0	0	2	0
15	M	124	0	0	2	0
All	All	7706	0	7429	143	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 10.

All (143) 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)
3:M:278:LEU:CD2	3:M:278:LEU:CG	1.81	1.56
3:M:278:LEU:CD2	3:M:279:THR:H	1.18	1.55
3:M:278:LEU:CD2	3:M:279:THR:N	1.74	1.38
3:M:278:LEU:HD22	3:M:278:LEU:C	1.56	1.30
3:M:278:LEU:CD2	3:M:278:LEU:HA	1.61	1.28
3:M:278:LEU:CD2	3:M:278:LEU:CA	2.11	1.27
3:M:278:LEU:HD22	3:M:279:THR:N	0.79	1.10
3:M:278:LEU:HA	3:M:278:LEU:HD23	1.20	1.08
3:M:278:LEU:CD2	3:M:278:LEU:C	2.20	0.99
7:L:1285:BPH:HHC	7:L:1285:BPH:HBB3	1.42	0.99
3:M:275:LEU:O	3:M:278:LEU:O	1.83	0.97
1:H:220[A]:LYS:HD2	1:H:229:GLU:OE2	1.71	0.90
3:M:197:PHE:CZ	5:M:1305:BCL:HBB2	2.10	0.86
3:M:197:PHE:HZ	5:M:1305:BCL:HBB2	1.39	0.85
3:M:278:LEU:HD22	3:M:279:THR:CA	2.08	0.83
4:H:1252:GOL:H31	15:H:2003:HOH:O	1.78	0.83
6:M:1306:LDA:H101	6:M:1308:LDA:H121	1.62	0.80
5:M:1305:BCL:HBB3	5:M:1305:BCL:HHC	1.67	0.77
1:H:248:ARG:HA	1:H:249:LYS:HB3	1.67	0.77
3:M:189:PHE:O	3:M:193:HIS:HD2	1.70	0.75
5:M:1305:BCL:HHC	5:M:1305:BCL:CBB	2.18	0.74
7:M:1314:BPH:HBB3	7:M:1314:BPH:HHC	1.68	0.74
6:M:1306:LDA:H101	6:M:1308:LDA:C12	2.19	0.73
7:L:1285:BPH:HHC	7:L:1285:BPH:CBB	2.19	0.72
2:L:181:PHE:CD2	7:M:1314:BPH:HBB1	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:170:ASN:HD22	2:L:170:ASN:C	1.99	0.71
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.71	0.71
2:L:199:ASN:HA	4:L:1290:GOL:H31	1.76	0.68
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.24	0.68
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB2	1.77	0.67
7:M:1314:BPH:HHD	7:M:1314:BPH:HBC3	1.76	0.66
5:M:1304:BCL:HBB3	5:M:1305:BCL:H41	1.76	0.66
6:M:1308:LDA:H112	12:M:1315:U10:H202	1.79	0.65
1:H:35:ASN:OD1	3:M:260:ALA:HB1	1.97	0.65
7:M:1314:BPH:HHC	7:M:1314:BPH:CBB	2.28	0.63
2:L:72:GLU:HG2	15:L:2042:HOH:O	1.97	0.63
3:M:157:TRP:HB2	5:M:1305:BCL:H71	1.81	0.63
1:H:175:MET:HE1	15:M:2097:HOH:O	1.98	0.63
2:L:224:ILE:HG22	8:L:1286[B]:UQ2:H8	1.81	0.63
3:M:77:GLN:HE22	3:M:93:SER:H	1.44	0.62
4:H:1252:GOL:C3	15:H:2003:HOH:O	2.45	0.61
1:H:119:ASP:OD1	1:H:220[A]:LYS:NZ	2.34	0.60
3:M:197:PHE:HZ	5:M:1305:BCL:CBB	2.13	0.60
2:L:181:PHE:HB3	7:M:1314:BPH:HBB2	1.84	0.60
1:H:118[A]:ARG:HD3	15:M:2102:HOH:O	2.01	0.59
7:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.84	0.59
2:L:72:GLU:CG	15:L:2042:HOH:O	2.50	0.58
1:H:169:VAL:HG23	1:H:171:ILE:HD13	1.85	0.58
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.86	0.58
5:L:1282:BCL:HBB3	5:L:1287:BCL:H52	1.85	0.58
3:M:194:GLY:O	3:M:195:ASN:HB3	2.04	0.57
2:L:208:THR:HB	2:L:209:PRO:HD2	1.86	0.57
1:H:11:ASP:OD1	3:M:302:GLY:HA2	2.06	0.56
3:M:62:SER:OG	3:M:124:VAL:HG22	2.05	0.56
1:H:248:ARG:HA	1:H:249:LYS:CB	2.36	0.56
6:L:1284:LDA:H121	8:L:1286[B]:UQ2:C16	2.36	0.55
1:H:62:LYS:HE3	4:H:1252:GOL:H11	1.88	0.55
6:M:1308:LDA:HM22	6:M:1309:LDA:H11	1.89	0.55
2:L:87:GLN:HE21	2:L:142:TRP:CD1	2.26	0.54
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.90	0.54
5:M:1305:BCL:HAA2	5:M:1305:BCL:HBD	1.90	0.54
1:H:171:ILE:HB	1:H:172:PRO:HD3	1.88	0.53
3:M:199:ASN:HD22	3:M:199:ASN:C	2.15	0.52
6:L:1284:LDA:H121	8:L:1286[B]:UQ2:H162	1.90	0.52
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.43	0.52
7:M:1314:BPH:HBB3	7:M:1314:BPH:CHC	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:199:ASN:O	14:M:1317:CDL:HB22	2.09	0.51
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.45	0.51
5:M:1304:BCL:H51	7:M:1314:BPH:HMB2	1.93	0.51
3:M:189:PHE:O	3:M:193:HIS:CD2	2.58	0.51
7:M:1314:BPH:HHD	7:M:1314:BPH:CBC	2.39	0.50
2:L:190:HIS:HA	8:L:1286[B]:UQ2:H5M1	1.94	0.50
5:L:1282:BCL:HBB2	5:L:1282:BCL:HHC	1.94	0.50
3:M:278:LEU:CA	3:M:278:LEU:HD23	1.99	0.49
1:H:122:GLU:HB2	1:H:227:LEU:HD21	1.94	0.49
1:H:140:PHE:HA	3:M:13:ARG:O	2.13	0.49
8:L:1286[A]:UQ2:H152	6:M:1310:LDA:H91	1.95	0.49
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
7:L:1285:BPH:HBB3	7:L:1285:BPH:CHC	2.29	0.48
7:M:1314:BPH:HBC3	7:M:1314:BPH:CHD	2.44	0.48
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.95	0.48
7:L:1285:BPH:CBB	7:L:1285:BPH:CHC	2.89	0.48
5:M:1304:BCL:H102	5:M:1304:BCL:H13	1.64	0.48
1:H:45:GLU:HG3	1:H:94:GLU:OE1	2.14	0.47
5:M:1304:BCL:HBB2	13:M:1316:SPO:H243	1.96	0.47
2:L:181:PHE:HB3	7:M:1314:BPH:CBB	2.44	0.47
3:M:197:PHE:CE1	5:M:1305:BCL:HBB2	2.50	0.47
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.14	0.47
15:H:2003:HOH:O	14:M:1317:CDL:HA32	2.14	0.47
6:M:1309:LDA:H91	12:M:1315:U10:H23	1.97	0.47
3:M:144:LYS:N	14:M:1317:CDL:OB3	2.39	0.47
1:H:75:VAL:HA	1:H:76:PRO:C	2.40	0.46
3:M:278:LEU:CG	3:M:279:THR:N	2.75	0.46
2:L:11:VAL:HB	2:L:12:PRO:HD2	1.96	0.46
2:L:210:ASP:OD1	2:L:210:ASP:N	2.48	0.46
3:M:278:LEU:CD2	3:M:278:LEU:HG	2.22	0.46
3:M:47:LEU:HD12	6:M:1310:LDA:H62	1.97	0.45
5:M:1305:BCL:CBB	5:M:1305:BCL:CHC	2.88	0.45
3:M:109:LEU:O	3:M:114:LEU:HB2	2.16	0.45
2:L:72:GLU:H	2:L:72:GLU:HG3	1.50	0.45
7:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.52	0.45
2:L:44:LEU:HD13	2:L:92:CYS:SG	2.57	0.45
1:H:156:CYS:SG	1:H:248:ARG:HB2	2.57	0.44
12:M:1315:U10:H1M3	12:M:1315:U10:H8	1.98	0.44
3:M:66:TRP:HD1	3:M:118:ALA:O	2.01	0.44
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.82	0.44
6:M:1306:LDA:H32	4:M:1318:GOL:H32	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:ILE:HG23	14:M:1317:CDL:H231	1.99	0.43
1:H:125:GLY:HA2	2:L:208:THR:HG21	2.00	0.43
1:H:105:MET:HE2	1:H:212:LEU:HD13	1.99	0.43
1:H:112:ALA:HA	1:H:235:GLY:O	2.18	0.43
2:L:189:LEU:HB3	8:L:1286[A]:UQ2:H3M3	2.00	0.43
5:M:1304:BCL:H112	5:M:1304:BCL:HMB1	2.00	0.43
2:L:157:VAL:HG11	5:M:1305:BCL:HBB1	2.00	0.43
3:M:113:GLY:O	3:M:117:ILE:HG13	2.18	0.43
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.36	0.43
7:M:1314:BPH:H102	7:M:1314:BPH:H13	1.88	0.43
3:M:268:TRP:CD1	12:M:1315:U10:H111	2.54	0.42
2:L:166:ASN:OD1	2:L:166:ASN:C	2.63	0.42
3:M:132:ARG:O	3:M:136:ARG:HG2	2.20	0.42
2:L:170:ASN:HD22	2:L:171:PRO:N	2.18	0.42
5:M:1305:BCL:H61	7:M:1314:BPH:C4B	2.49	0.42
2:L:117:ILE:N	2:L:118:PRO:HD2	2.35	0.42
1:H:29:TYR:HB2	4:H:1253:GOL:H12	2.01	0.41
2:L:153:HIS:CD2	5:L:1282:BCL:NC	2.88	0.41
3:M:270:ILE:O	3:M:274:VAL:HG13	2.20	0.41
1:H:171:ILE:HB	1:H:172:PRO:CD	2.51	0.41
1:H:171:ILE:N	1:H:172:PRO:HD2	2.36	0.41
3:M:30:SER:OG	3:M:31:GLY:O	2.35	0.41
5:M:1304:BCL:CBB	13:M:1316:SPO:H243	2.51	0.41
7:M:1314:BPH:CBB	7:M:1314:BPH:CHC	2.97	0.41
5:L:1287:BCL:CBB	5:L:1287:BCL:HMB3	2.50	0.41
3:M:164:ARG:O	3:M:168:MET:HG2	2.21	0.41
3:M:278:LEU:CD2	3:M:278:LEU:CD1	2.86	0.41
3:M:278:LEU:HD21	3:M:282:ILE:HG13	2.03	0.41
5:M:1304:BCL:H112	5:M:1304:BCL:HHB	2.02	0.41
5:M:1304:BCL:H71	5:M:1305:BCL:H202	2.03	0.41
3:M:243:THR:O	3:M:247:ARG:HG3	2.20	0.40
2:L:60:ASN:HA	2:L:61:PRO:HD3	1.94	0.40
3:M:77:GLN:NE2	3:M:93:SER:H	2.15	0.40
3:M:278:LEU:HD22	3:M:279:THR:H	0.59	0.40
2:L:185:LEU:HD13	7:M:1314:BPH:ND	2.37	0.40
2:L:78:ALA:O	2:L:79:PRO:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	242/260 (93%)	235 (97%)	6 (2%)	1 (0%)	30 33
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100 100
3	M	301/307 (98%)	289 (96%)	9 (3%)	3 (1%)	12 11
All	All	822/848 (97%)	796 (97%)	22 (3%)	4 (0%)	24 26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	195	ASN
3	M	279	THR
3	M	302	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	198/208 (95%)	191 (96%)	7 (4%)	32 41
2	L	220/220 (100%)	203 (92%)	17 (8%)	12 12
3	M	236/240 (98%)	222 (94%)	14 (6%)	18 20
All	All	654/668 (98%)	616 (94%)	38 (6%)	18 21

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	175	MET
1	H	193	MET
1	H	197	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	231	ASP
1	H	247	LYS
2	L	8	LYS
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	72	GLU
2	L	80	LEU
2	L	82	LYS
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	150	ILE
2	L	170	ASN
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	60	LEU
3	M	72	ILE
3	M	124	VAL
3	M	148	TRP
3	M	182	HIS
3	M	191	LEU
3	M	192	VAL
3	M	199	ASN
3	M	216	PHE
3	M	278	LEU
3	M	301	HIS

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

Mol	Chain	Res	Type
1	H	44	ASN

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Mol	Chain	Res	Type
1	H	98	HIS
1	H	129	ASN
2	L	159	ASN
2	L	170	ASN
2	L	258	GLN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
5	BCL	M	1305	3	69,74,74	2.02	11 (15%)	83,115,115	2.05	20 (24%)
14	CDL	M	1317	-	80,80,99	2.13	17 (21%)	86,92,111	3.42	17 (19%)
4	GOL	H	1254	-	5,5,5	0.36	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	LDA	L	1284	-	12,15,15	2.07	1 (8%)	14,17,17	0.68	0
4	GOL	M	1318	-	5,5,5	0.35	0	5,5,5	0.36	0
6	LDA	M	1312	-	12,15,15	2.00	1 (8%)	14,17,17	0.54	0
5	BCL	L	1287	2	69,74,74	1.99	8 (11%)	83,115,115	1.94	22 (26%)
6	LDA	M	1308	-	12,15,15	1.93	1 (8%)	14,17,17	0.52	0
6	LDA	M	1306	-	12,15,15	2.13	1 (8%)	14,17,17	0.67	1 (7%)
10	HTO	L	1289	-	9,9,9	0.47	0	10,10,10	0.61	0
5	BCL	M	1304	3	69,74,74	1.99	11 (15%)	83,115,115	1.80	17 (20%)
6	LDA	L	1283	-	12,15,15	2.00	1 (8%)	14,17,17	0.46	0
4	GOL	H	1255	-	5,5,5	0.38	0	5,5,5	0.36	0
8	UQ2	L	1286[A]	-	23,23,23	2.71	8 (34%)	28,31,31	1.29	3 (10%)
13	SPO	M	1316	-	40,41,41	3.95	12 (30%)	47,50,50	2.20	17 (36%)
7	BPH	M	1314	-	59,70,70	2.60	11 (18%)	61,101,101	2.60	20 (32%)
8	UQ2	L	1286[B]	-	23,23,23	2.62	8 (34%)	28,31,31	1.80	7 (25%)
6	LDA	M	1311	-	12,15,15	2.03	1 (8%)	14,17,17	0.55	0
6	LDA	M	1309	-	12,15,15	2.02	1 (8%)	14,17,17	0.41	0
12	U10	M	1315	-	48,48,63	2.66	12 (25%)	58,61,79	1.82	13 (22%)
9	PO4	L	1288	-	4,4,4	0.73	0	6,6,6	0.49	0
6	LDA	M	1310	-	12,15,15	2.03	1 (8%)	14,17,17	0.57	0
5	BCL	L	1282	2	69,74,74	1.92	9 (13%)	83,115,115	1.93	20 (24%)
7	BPH	L	1285	-	59,70,70	2.71	12 (20%)	61,101,101	2.77	20 (32%)
6	LDA	M	1307	-	12,15,15	2.04	1 (8%)	14,17,17	0.49	0
4	GOL	H	1253	-	5,5,5	0.52	0	5,5,5	0.56	0
4	GOL	L	1290	-	5,5,5	0.44	0	5,5,5	0.85	0
4	GOL	L	1291	-	5,5,5	0.34	0	5,5,5	0.27	0
4	GOL	H	1252	-	5,5,5	0.61	0	5,5,5	1.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	M	1305	3	2/2/21/25	6/41/137/137	-
14	CDL	M	1317	-	-	46/91/91/110	-
4	GOL	H	1254	-	-	2/4/4/4	-
6	LDA	L	1284	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	M	1318	-	-	1/4/4/4	-
6	LDA	M	1312	-	-	8/13/13/13	-
5	BCL	L	1287	2	2/2/21/25	9/41/137/137	-
6	LDA	M	1308	-	-	6/13/13/13	-
6	LDA	M	1306	-	-	4/13/13/13	-
10	HTO	L	1289	-	-	5/10/10/10	-
5	BCL	M	1304	3	2/2/21/25	14/41/137/137	-
6	LDA	L	1283	-	-	5/13/13/13	-
4	GOL	H	1255	-	-	1/4/4/4	-
8	UQ2	L	1286[A]	-	-	6/15/39/39	0/1/1/1
13	SPO	M	1316	-	-	13/47/47/47	-
7	BPH	M	1314	-	-	17/37/105/105	0/5/6/6
8	UQ2	L	1286[B]	-	-	5/15/39/39	0/1/1/1
6	LDA	M	1311	-	-	6/13/13/13	-
6	LDA	M	1309	-	-	5/13/13/13	-
12	U10	M	1315	-	-	13/45/69/87	0/1/1/1
6	LDA	M	1310	-	-	5/13/13/13	-
5	BCL	L	1282	2	2/2/21/25	8/41/137/137	-
7	BPH	L	1285	-	-	6/37/105/105	0/5/6/6
6	LDA	M	1307	-	-	6/13/13/13	-
4	GOL	H	1253	-	-	2/4/4/4	-
4	GOL	L	1290	-	-	2/4/4/4	-
4	GOL	L	1291	-	-	4/4/4/4	-
4	GOL	H	1252	-	-	0/4/4/4	-

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1285	BPH	OBD-CAD	12.74	1.40	1.22
13	M	1316	SPO	C27-C28	12.43	1.47	1.34
7	M	1314	BPH	OBD-CAD	12.13	1.39	1.22
5	M	1305	BCL	OBD-CAD	11.35	1.42	1.22
5	L	1287	BCL	OBD-CAD	10.70	1.40	1.22
5	L	1282	BCL	OBD-CAD	10.43	1.40	1.22
5	M	1304	BCL	OBD-CAD	10.41	1.40	1.22
13	M	1316	SPO	C9-C7	8.99	1.47	1.35
13	M	1316	SPO	C19-C17	8.99	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1316	SPO	C14-C12	8.13	1.46	1.35
13	M	1316	SPO	C22-C23	7.75	1.46	1.35
7	L	1285	BPH	OBB-CAB	7.12	1.44	1.22
6	M	1306	LDA	O1-N1	-7.10	1.25	1.42
6	L	1284	LDA	O1-N1	-7.10	1.25	1.42
6	M	1307	LDA	O1-N1	-6.97	1.25	1.42
12	M	1315	U10	C33-C34	6.95	1.49	1.33
6	M	1310	LDA	O1-N1	-6.95	1.25	1.42
6	M	1311	LDA	O1-N1	-6.94	1.25	1.42
6	M	1309	LDA	O1-N1	-6.85	1.26	1.42
7	L	1285	BPH	O1D-CGD	6.85	1.38	1.21
8	L	1286[A]	UQ2	C8-C9	6.78	1.49	1.33
6	M	1312	LDA	O1-N1	-6.78	1.26	1.42
6	L	1283	LDA	O1-N1	-6.76	1.26	1.42
14	M	1317	CDL	C32-C31	-6.69	1.27	1.52
12	M	1315	U10	C13-C14	6.68	1.49	1.33
7	M	1314	BPH	O1D-CGD	6.67	1.37	1.21
6	M	1308	LDA	O1-N1	-6.61	1.26	1.42
13	M	1316	SPO	C32-C33	6.55	1.48	1.33
7	L	1285	BPH	O1A-CGA	6.44	1.41	1.22
7	M	1314	BPH	C2-C3	6.41	1.48	1.33
8	L	1286[B]	UQ2	C8-C9	6.04	1.47	1.33
7	L	1285	BPH	C2-C3	6.01	1.47	1.33
7	M	1314	BPH	O1A-CGA	5.98	1.40	1.22
12	M	1315	U10	C28-C29	5.96	1.47	1.33
5	M	1304	BCL	O1A-CGA	5.94	1.40	1.22
13	M	1316	SPO	C37-C38	5.91	1.49	1.32
5	L	1287	BCL	O1A-CGA	5.89	1.40	1.22
12	M	1315	U10	C8-C9	5.85	1.47	1.33
14	M	1317	CDL	C11-CA5	-5.85	1.33	1.50
5	L	1282	BCL	O1A-CGA	5.80	1.39	1.22
7	M	1314	BPH	OBB-CAB	5.70	1.40	1.22
12	M	1315	U10	C23-C24	5.67	1.46	1.33
8	L	1286[B]	UQ2	C13-C14	5.64	1.48	1.32
12	M	1315	U10	C18-C19	5.63	1.46	1.33
12	M	1315	U10	C38-C39	5.47	1.48	1.32
7	M	1314	BPH	C3D-C2D	5.33	1.49	1.39
14	M	1317	CDL	C33-C32	-5.26	1.22	1.51
5	M	1305	BCL	O1A-CGA	5.24	1.38	1.22
8	L	1286[B]	UQ2	O2-C2	-5.24	1.24	1.36
8	L	1286[A]	UQ2	C13-C14	5.20	1.47	1.32
8	L	1286[A]	UQ2	O2-C2	-5.17	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1317	CDL	OB6-CB5	5.15	1.48	1.34
14	M	1317	CDL	OA6-CA5	4.93	1.48	1.34
13	M	1316	SPO	C6-C5	4.92	1.44	1.32
14	M	1317	CDL	OA8-CA7	4.89	1.47	1.33
13	M	1316	SPO	C10-C11	4.67	1.46	1.34
8	L	1286[A]	UQ2	O3-C3	-4.66	1.25	1.36
7	L	1285	BPH	C3D-C2D	4.63	1.47	1.39
14	M	1317	CDL	OB8-CB7	4.62	1.46	1.33
8	L	1286[B]	UQ2	O3-C3	-4.56	1.25	1.36
13	M	1316	SPO	C15-C16	4.56	1.46	1.34
14	M	1317	CDL	C34-C33	-4.52	1.26	1.51
7	M	1314	BPH	C3D-CAD	-4.27	1.38	1.47
14	M	1317	CDL	C17-C16	-4.26	1.27	1.51
14	M	1317	CDL	C16-C15	-4.12	1.28	1.51
14	M	1317	CDL	C13-C12	-4.11	1.28	1.51
5	M	1304	BCL	C4D-ND	-4.09	1.32	1.37
13	M	1316	SPO	C26-C25	4.06	1.45	1.34
5	L	1282	BCL	C4D-ND	-4.04	1.32	1.37
5	L	1287	BCL	O2D-CGD	-4.03	1.23	1.33
5	L	1287	BCL	C4D-ND	-4.02	1.32	1.37
14	M	1317	CDL	C20-C19	-3.96	1.29	1.51
5	M	1304	BCL	MG-ND	-3.96	1.97	2.05
5	L	1287	BCL	C2-C3	3.94	1.42	1.33
12	M	1315	U10	O3-C3	-3.90	1.27	1.36
5	M	1305	BCL	C3D-C4D	-3.83	1.35	1.44
14	M	1317	CDL	C19-C18	-3.78	1.30	1.51
5	M	1305	BCL	C4D-ND	-3.66	1.32	1.37
12	M	1315	U10	C6-C1	3.57	1.41	1.35
7	L	1285	BPH	C3D-CAD	-3.54	1.40	1.47
12	M	1315	U10	O4-C4	-3.49	1.28	1.36
13	M	1316	SPO	C21-C20	3.48	1.45	1.36
5	L	1282	BCL	C2-C3	3.42	1.41	1.33
5	M	1304	BCL	O2D-CGD	-3.41	1.24	1.33
8	L	1286[B]	UQ2	C3-C4	-3.38	1.39	1.48
5	M	1304	BCL	C3D-C4D	-3.37	1.36	1.44
7	L	1285	BPH	O2A-CGA	-3.35	1.23	1.33
8	L	1286[A]	UQ2	C6-C5	3.34	1.41	1.35
7	M	1314	BPH	C4D-ND	-3.18	1.34	1.38
7	M	1314	BPH	O2D-CGD	-3.14	1.25	1.33
12	M	1315	U10	C4-C5	-3.12	1.39	1.48
8	L	1286[A]	UQ2	C3-C4	-3.08	1.40	1.48
5	M	1304	BCL	C2-C3	3.06	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1317	CDL	C79-C78	-3.04	1.34	1.51
7	L	1285	BPH	O2D-CGD	-3.03	1.25	1.33
14	M	1317	CDL	C37-C36	-3.01	1.34	1.51
14	M	1317	CDL	C80-C79	-2.99	1.34	1.51
14	M	1317	CDL	C22-C21	-2.94	1.35	1.51
7	L	1285	BPH	C3D-C4D	-2.87	1.37	1.41
5	M	1305	BCL	C2-C3	2.76	1.39	1.33
5	L	1282	BCL	O2A-CGA	-2.76	1.25	1.33
5	L	1282	BCL	C3D-C4D	-2.71	1.38	1.44
8	L	1286[B]	UQ2	C6-C5	2.71	1.40	1.35
5	M	1305	BCL	O2D-CGD	-2.70	1.26	1.33
8	L	1286[B]	UQ2	C6-C1	-2.68	1.39	1.46
5	M	1304	BCL	C1D-C2D	-2.64	1.40	1.45
7	M	1314	BPH	O2A-CGA	-2.61	1.25	1.33
12	M	1315	U10	O3-C3M	-2.59	1.39	1.45
5	L	1282	BCL	C1D-C2D	-2.50	1.40	1.45
7	L	1285	BPH	C2C-C3C	-2.49	1.52	1.54
5	M	1304	BCL	O2A-CGA	-2.45	1.26	1.33
5	L	1282	BCL	MG-ND	-2.43	2.01	2.05
5	L	1287	BCL	C3D-C4D	-2.40	1.38	1.44
5	M	1305	BCL	OBB-CAB	2.39	1.28	1.23
7	M	1314	BPH	C3D-C4D	-2.30	1.38	1.41
8	L	1286[B]	UQ2	C2-C1	-2.28	1.42	1.48
5	M	1305	BCL	O2D-CED	-2.26	1.40	1.45
8	L	1286[A]	UQ2	C2-C1	-2.22	1.42	1.48
5	M	1305	BCL	MG-NA	2.20	2.11	2.06
5	L	1282	BCL	O2D-CGD	-2.19	1.27	1.33
5	L	1287	BCL	CHD-C4C	2.17	1.45	1.39
5	M	1304	BCL	CHD-C4C	2.15	1.45	1.39
5	M	1305	BCL	O2A-CGA	-2.15	1.27	1.33
5	M	1305	BCL	C3C-C4C	2.06	1.54	1.51
5	L	1287	BCL	C1B-NB	2.06	1.40	1.37
8	L	1286[A]	UQ2	O2-CM2	-2.03	1.40	1.45
7	L	1285	BPH	CHA-CBD	2.02	1.53	1.51
5	M	1304	BCL	C3C-C4C	-2.01	1.49	1.51

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1317	CDL	C33-C32-C31	18.11	178.30	113.19
14	M	1317	CDL	C17-C16-C15	11.38	172.22	114.42
14	M	1317	CDL	C12-C11-CA5	10.77	152.78	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	M	1317	CDL	C20-C19-C18	10.10	165.72	114.42
7	M	1314	BPH	O2D-CGD-CBD	9.96	123.62	111.00
7	L	1285	BPH	O2D-CGD-CBD	9.50	123.04	111.00
14	M	1317	CDL	C35-C34-C33	8.41	157.13	114.42
7	L	1285	BPH	C2B-C1B-NB	7.98	115.03	109.53
14	M	1317	CDL	C34-C33-C32	7.77	153.85	114.42
7	M	1314	BPH	C2B-C1B-NB	7.74	114.87	109.53
14	M	1317	CDL	C13-C12-C11	7.44	139.94	113.19
5	M	1305	BCL	C1C-NC-C4C	-7.43	103.37	106.71
7	M	1314	BPH	OBD-CAD-C3D	-6.71	116.85	127.98
5	L	1287	BCL	CMB-C2B-C1B	-6.42	115.59	125.37
5	L	1287	BCL	C2B-C1B-NB	-6.13	106.12	110.23
5	L	1282	BCL	O2D-CGD-CBD	6.12	122.15	111.27
5	M	1304	BCL	CMB-C2B-C1B	-5.65	116.76	125.37
13	M	1316	SPO	C15-C14-C12	-5.60	119.32	127.31
5	M	1305	BCL	CMB-C2B-C1B	-5.58	116.86	125.37
14	M	1317	CDL	OA6-CA5-C11	5.56	123.48	111.50
13	M	1316	SPO	C20-C19-C17	-5.55	119.39	127.31
7	L	1285	BPH	C2D-C1D-ND	5.44	113.28	109.53
7	L	1285	BPH	C4D-ND-C1D	-5.23	103.51	108.83
7	L	1285	BPH	OBD-CAD-CBD	-5.16	118.25	125.82
12	M	1315	U10	C30-C29-C31	5.04	123.75	115.27
7	L	1285	BPH	C3D-C4D-ND	5.01	114.55	107.72
5	L	1282	BCL	C1D-ND-C4D	4.89	109.81	106.33
7	L	1285	BPH	O1D-CGD-CBD	-4.86	116.64	124.74
5	M	1304	BCL	C1D-ND-C4D	4.80	109.74	106.33
5	M	1305	BCL	C2D-C1D-ND	-4.77	106.59	110.10
5	L	1287	BCL	CMD-C2D-C1D	4.73	133.04	124.71
7	M	1314	BPH	C2D-C1D-ND	4.72	112.78	109.53
5	M	1305	BCL	CMD-C2D-C1D	4.68	132.96	124.71
7	M	1314	BPH	C3D-C4D-ND	4.65	114.05	107.72
5	L	1282	BCL	CMB-C2B-C1B	-4.63	118.32	125.37
7	L	1285	BPH	C1B-NB-C4B	-4.61	101.69	108.83
7	L	1285	BPH	OBD-CAD-C3D	-4.57	120.39	127.98
5	L	1282	BCL	C1C-NC-C4C	-4.55	104.66	106.71
5	L	1282	BCL	C2B-C1B-NB	-4.49	107.22	110.23
7	M	1314	BPH	OBD-CAD-CBD	-4.46	119.28	125.82
5	M	1304	BCL	O2D-CGD-CBD	4.39	119.07	111.27
13	M	1316	SPO	C10-C9-C7	-4.37	121.08	127.31
13	M	1316	SPO	C21-C22-C23	-4.36	121.09	127.31
5	L	1282	BCL	C2D-C1D-ND	-4.34	106.90	110.10
7	M	1314	BPH	O2D-CGD-O1D	-4.33	115.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BCL	C2D-C1D-ND	-4.28	106.95	110.10
5	M	1305	BCL	O2D-CGD-CBD	4.25	118.83	111.27
12	M	1315	U10	C15-C14-C16	4.24	122.40	115.27
8	L	1286[B]	UQ2	CM5-C5-C6	-4.24	117.49	124.40
5	M	1305	BCL	C1D-ND-C4D	4.21	109.33	106.33
7	L	1285	BPH	CED-O2D-CGD	4.21	125.45	115.94
12	M	1315	U10	C25-C24-C26	4.12	122.19	115.27
5	M	1305	BCL	CED-O2D-CGD	4.05	125.10	115.94
12	M	1315	U10	C10-C9-C11	3.99	121.98	115.27
5	L	1287	BCL	C1D-ND-C4D	3.85	109.07	106.33
5	M	1304	BCL	C1-O2A-CGA	3.73	126.23	116.44
5	L	1287	BCL	O2A-CGA-CBA	3.71	123.55	111.91
5	M	1305	BCL	O2A-CGA-CBA	3.71	123.54	111.91
5	M	1305	BCL	C2B-C1B-NB	-3.68	107.77	110.23
7	M	1314	BPH	C4D-ND-C1D	-3.67	105.10	108.83
5	L	1287	BCL	C1-O2A-CGA	3.63	125.97	116.44
14	M	1317	CDL	OB6-CB5-C51	3.62	119.31	111.50
13	M	1316	SPO	C29-C28-C30	3.55	121.24	115.27
5	L	1287	BCL	C2D-C1D-ND	-3.53	107.50	110.10
5	M	1304	BCL	C2B-C1B-NB	-3.45	107.92	110.23
5	L	1287	BCL	O2D-CGD-O1D	-3.35	117.30	123.84
5	M	1304	BCL	CMA-C3A-C4A	-3.33	102.82	111.77
7	L	1285	BPH	C4A-C3A-C2A	-3.32	99.68	102.84
5	L	1282	BCL	C4-C3-C5	3.29	120.81	115.27
12	M	1315	U10	C17-C18-C19	-3.22	119.90	127.66
8	L	1286[B]	UQ2	C10-C9-C11	3.22	120.68	115.27
7	L	1285	BPH	C4D-CHA-CBD	-3.21	107.06	108.52
7	L	1285	BPH	O2A-CGA-O1A	-3.21	115.48	123.59
5	M	1304	BCL	O2A-CGA-CBA	3.18	121.87	111.91
7	M	1314	BPH	C4D-CHA-CBD	-3.14	107.10	108.52
7	M	1314	BPH	CAC-C3C-C2C	-3.13	106.44	114.26
5	M	1304	BCL	CMB-C2B-C3B	3.11	134.34	125.93
5	L	1282	BCL	CMD-C2D-C1D	3.10	130.18	124.71
5	L	1287	BCL	CMB-C2B-C3B	3.08	134.25	125.93
5	L	1282	BCL	O2A-CGA-CBA	3.08	121.56	111.91
8	L	1286[B]	UQ2	CM3-O3-C3	3.06	127.32	116.47
5	L	1282	BCL	CHC-C4B-NB	-3.05	121.03	124.26
13	M	1316	SPO	C24-C23-C25	3.02	122.83	118.08
7	M	1314	BPH	CMA-C3A-C4A	-3.00	107.81	114.38
14	M	1317	CDL	OB8-CB7-C71	2.98	121.27	111.91
7	L	1285	BPH	C3B-C4B-NB	2.97	112.48	108.04
7	M	1314	BPH	O2A-CGA-CBA	2.96	121.21	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	1286[B]	UQ2	O1-C1-C6	-2.92	116.42	121.55
7	M	1314	BPH	C1B-NB-C4B	-2.92	104.31	108.83
14	M	1317	CDL	OA8-CA7-C31	2.90	121.01	111.91
5	L	1282	BCL	O2D-CGD-O1D	-2.90	118.17	123.84
5	M	1304	BCL	CAA-C2A-C3A	-2.89	104.86	112.78
12	M	1315	U10	C27-C28-C29	-2.89	120.70	127.66
5	L	1287	BCL	C2A-C3A-C4A	2.88	106.52	101.87
7	M	1314	BPH	CMD-C2D-C3D	-2.85	119.35	124.68
12	M	1315	U10	C30-C29-C28	-2.82	116.45	123.68
5	L	1287	BCL	CMD-C2D-C3D	-2.81	121.15	127.61
5	M	1305	BCL	CMB-C2B-C3B	2.80	133.50	125.93
5	L	1287	BCL	C14-C13-C12	2.80	121.42	111.29
5	M	1305	BCL	OBB-CAB-C3B	2.79	125.57	120.41
5	M	1305	BCL	O2D-CGD-O1D	-2.79	118.39	123.84
5	M	1304	BCL	C4A-NA-C1A	2.78	107.96	106.71
12	M	1315	U10	C11-C9-C8	-2.76	115.53	121.12
12	M	1315	U10	C22-C23-C24	-2.74	121.06	127.66
5	M	1305	BCL	CMD-C2D-C3D	-2.72	121.36	127.61
5	M	1304	BCL	O2D-CGD-O1D	-2.71	118.54	123.84
5	M	1304	BCL	CED-O2D-CGD	2.69	122.03	115.94
13	M	1316	SPO	C15-C16-C17	-2.69	118.87	126.42
5	M	1305	BCL	C3C-C4C-CHD	-2.68	117.67	123.39
7	L	1285	BPH	C4C-C3C-C2C	-2.67	100.30	102.84
13	M	1316	SPO	C8-C7-C6	2.67	122.28	118.08
5	M	1304	BCL	CMD-C2D-C1D	2.65	129.39	124.71
7	M	1314	BPH	CBA-CAA-C2A	-2.64	106.08	113.81
5	L	1287	BCL	O2D-CGD-CBD	2.64	115.96	111.27
5	L	1287	BCL	C11-C12-C13	2.64	124.44	115.92
5	L	1282	BCL	O2A-CGA-O1A	-2.63	116.94	123.59
7	L	1285	BPH	C1-C2-C3	-2.63	121.50	126.04
8	L	1286[A]	UQ2	O2-C2-C3	-2.61	113.80	123.64
12	M	1315	U10	C41-C39-C40	2.58	120.30	114.60
14	M	1317	CDL	OA6-CA5-OA7	-2.57	117.49	123.70
5	M	1304	BCL	CAB-C3B-C2B	-2.56	124.50	128.34
13	M	1316	SPO	C20-C21-C22	-2.56	118.23	123.47
13	M	1316	SPO	C25-C23-C22	-2.55	115.03	118.94
7	L	1285	BPH	CMA-C3A-C4A	-2.54	108.81	114.38
7	L	1285	BPH	C11-C10-C8	-2.52	107.77	115.92
5	M	1305	BCL	C4A-NA-C1A	2.51	107.83	106.71
5	M	1305	BCL	C1-C2-C3	-2.50	121.71	126.04
5	L	1282	BCL	C2A-C3A-C4A	2.48	105.87	101.87
13	M	1316	SPO	C27-C26-C25	-2.47	115.52	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1314	BPH	C4A-C3A-C2A	-2.47	100.49	102.84
5	L	1282	BCL	CAB-C3B-C2B	-2.46	124.65	128.34
13	M	1316	SPO	C13-C12-C11	2.45	121.93	118.08
5	M	1305	BCL	CBB-CAB-C3B	-2.44	115.22	120.43
12	M	1315	U10	C7-C8-C9	2.44	130.85	126.79
5	L	1282	BCL	CAC-C3C-C2C	-2.42	108.22	114.26
7	L	1285	BPH	O2A-CGA-CBA	2.41	119.46	111.91
5	L	1282	BCL	O1D-CGD-CBD	-2.40	119.57	124.48
8	L	1286[A]	UQ2	C10-C9-C11	2.39	119.30	115.27
13	M	1316	SPO	C34-C33-C35	2.38	119.28	115.27
5	L	1287	BCL	CHD-C4C-NC	2.38	127.72	125.08
5	M	1305	BCL	C7-C6-C5	-2.37	106.91	113.36
5	L	1287	BCL	C3C-C4C-CHD	-2.37	118.33	123.39
13	M	1316	SPO	C14-C15-C16	-2.36	115.86	123.22
5	L	1282	BCL	CMB-C2B-C3B	2.35	132.26	125.93
12	M	1315	U10	C16-C14-C13	-2.34	116.38	121.12
7	M	1314	BPH	C4C-C3C-C2C	-2.34	100.61	102.84
5	L	1287	BCL	CAA-C2A-C1A	-2.31	104.41	111.97
5	L	1282	BCL	CHC-C4B-C3B	-2.29	124.20	132.35
5	M	1304	BCL	C3C-C4C-CHD	-2.29	118.51	123.39
13	M	1316	SPO	C3-C1-C4	-2.28	107.35	110.86
5	M	1304	BCL	O2A-C1-C2	2.28	114.62	108.64
7	M	1314	BPH	CED-O2D-CGD	2.25	121.03	115.94
14	M	1317	CDL	C32-C31-CA7	2.25	121.81	113.62
7	M	1314	BPH	O1D-CGD-CBD	-2.25	121.00	124.74
5	L	1287	BCL	CHB-C1B-NB	2.24	126.63	124.26
5	M	1305	BCL	CAC-C3C-C2C	-2.23	108.68	114.26
14	M	1317	CDL	C80-C79-C78	2.23	125.73	114.42
5	L	1287	BCL	CHB-C4A-NA	-2.20	121.47	124.51
5	L	1287	BCL	O2A-CGA-O1A	-2.20	118.03	123.59
5	L	1282	BCL	C5-C3-C2	-2.20	116.66	121.12
13	M	1316	SPO	C40-C38-C39	2.15	119.34	114.60
8	L	1286[B]	UQ2	O4-C4-C3	-2.12	116.43	120.93
14	M	1317	CDL	C81-C80-C79	2.12	125.19	114.42
14	M	1317	CDL	C22-C21-C20	2.12	125.18	114.42
14	M	1317	CDL	OB8-CB7-OB9	-2.09	118.32	123.59
13	M	1316	SPO	C31-C32-C33	-2.09	122.63	127.66
8	L	1286[A]	UQ2	C16-C14-C15	2.09	119.21	114.60
12	M	1315	U10	C12-C13-C14	-2.08	122.64	127.66
5	M	1305	BCL	C16-C15-C13	-2.07	109.23	115.92
8	L	1286[B]	UQ2	C16-C14-C15	2.05	119.12	114.60
6	M	1306	LDA	O1-N1-C1	2.04	114.29	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	1286[B]	UQ2	C6-C5-C4	2.04	120.80	119.18
7	M	1314	BPH	CMB-C2B-C3B	2.03	128.47	124.68
5	L	1287	BCL	C11-C10-C8	2.02	122.46	115.92
5	L	1287	BCL	C12-C11-C10	-2.01	104.00	113.24
7	L	1285	BPH	CMC-C2C-C1C	-2.01	109.98	114.38
5	L	1282	BCL	CHA-C1A-NA	-2.01	121.80	126.40

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C13
5	L	1282	BCL	C8
5	L	1287	BCL	C13
5	L	1287	BCL	C8
5	M	1304	BCL	C13
5	M	1304	BCL	C8
5	M	1305	BCL	C13
5	M	1305	BCL	C8

All (214) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1253	GOL	O1-C1-C2-C3
4	L	1290	GOL	C1-C2-C3-O3
4	L	1291	GOL	C1-C2-C3-O3
4	L	1291	GOL	O2-C2-C3-O3
5	M	1304	BCL	C1-C2-C3-C4
5	M	1304	BCL	C1-C2-C3-C5
5	M	1304	BCL	C14-C13-C15-C16
6	M	1307	LDA	C2-C1-N1-CM1
6	M	1307	LDA	C2-C1-N1-CM2
7	M	1314	BPH	O2A-C1-C2-C3
8	L	1286[A]	UQ2	C12-C13-C14-C15
8	L	1286[B]	UQ2	C7-C8-C9-C10
8	L	1286[B]	UQ2	C7-C8-C9-C11
8	L	1286[B]	UQ2	C12-C13-C14-C16
10	L	1289	HTO	O3-C3-C4-C5
12	M	1315	U10	C27-C28-C29-C30
12	M	1315	U10	C27-C28-C29-C31
12	M	1315	U10	C29-C31-C32-C33
13	M	1316	SPO	C4-C1-O1-CM1
13	M	1316	SPO	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	M	1316	SPO	C6-C7-C9-C10
13	M	1316	SPO	C8-C7-C9-C10
14	M	1317	CDL	CA2-OA2-PA1-OA3
14	M	1317	CDL	CA3-OA5-PA1-OA3
14	M	1317	CDL	CB3-OB5-PB2-OB2
14	M	1317	CDL	CB3-OB5-PB2-OB3
8	L	1286[A]	UQ2	C12-C13-C14-C16
13	M	1316	SPO	C36-C37-C38-C39
13	M	1316	SPO	C36-C37-C38-C40
12	M	1315	U10	C37-C38-C39-C41
14	M	1317	CDL	C20-C21-C22-C23
14	M	1317	CDL	C78-C79-C80-C81
8	L	1286[B]	UQ2	C12-C13-C14-C15
8	L	1286[A]	UQ2	C7-C8-C9-C10
14	M	1317	CDL	OB9-CB7-OB8-CB6
5	L	1282	BCL	C3-C5-C6-C7
14	M	1317	CDL	C71-CB7-OB8-CB6
6	M	1312	LDA	C6-C7-C8-C9
5	M	1304	BCL	C10-C11-C12-C13
8	L	1286[A]	UQ2	C12-C11-C9-C10
8	L	1286[A]	UQ2	C12-C11-C9-C8
12	M	1315	U10	C24-C26-C27-C28
14	M	1317	CDL	C33-C34-C35-C36
12	M	1315	U10	C37-C38-C39-C40
8	L	1286[A]	UQ2	C7-C8-C9-C11
14	M	1317	CDL	C31-CA7-OA8-CA6
5	L	1287	BCL	C15-C16-C17-C18
14	M	1317	CDL	C15-C16-C17-C18
14	M	1317	CDL	O1-C1-CB2-OB2
5	M	1305	BCL	C11-C10-C8-C9
5	M	1305	BCL	C15-C16-C17-C18
14	M	1317	CDL	CB7-C71-C72-C73
5	L	1287	BCL	C11-C10-C8-C7
5	L	1287	BCL	C11-C12-C13-C15
5	M	1304	BCL	C8-C10-C11-C12
13	M	1316	SPO	C9-C10-C11-C12
5	L	1282	BCL	C5-C6-C7-C8
7	M	1314	BPH	C13-C15-C16-C17
14	M	1317	CDL	OA9-CA7-OA8-CA6
5	L	1287	BCL	C13-C15-C16-C17
5	M	1304	BCL	C5-C6-C7-C8
10	L	1289	HTO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	M	1310	LDA	C4-C5-C6-C7
14	M	1317	CDL	C54-C55-C56-C57
14	M	1317	CDL	C71-C72-C73-C74
7	M	1314	BPH	C16-C17-C18-C20
6	M	1308	LDA	C6-C7-C8-C9
14	M	1317	CDL	C32-C33-C34-C35
6	L	1284	LDA	C11-C10-C9-C8
6	M	1309	LDA	C6-C7-C8-C9
14	M	1317	CDL	C12-C13-C14-C15
6	L	1284	LDA	C4-C5-C6-C7
4	H	1254	GOL	O1-C1-C2-C3
4	L	1291	GOL	O1-C1-C2-C3
5	M	1305	BCL	C13-C15-C16-C17
6	L	1283	LDA	C3-C4-C5-C6
6	M	1307	LDA	C6-C7-C8-C9
6	M	1310	LDA	C6-C7-C8-C9
14	M	1317	CDL	C16-C17-C18-C19
5	L	1282	BCL	C16-C17-C18-C19
5	L	1282	BCL	C16-C17-C18-C20
7	M	1314	BPH	C5-C6-C7-C8
6	M	1310	LDA	C7-C8-C9-C10
6	L	1284	LDA	C7-C8-C9-C10
14	M	1317	CDL	C18-C19-C20-C21
6	M	1312	LDA	C3-C4-C5-C6
7	M	1314	BPH	C16-C17-C18-C19
4	H	1253	GOL	O1-C1-C2-O2
4	L	1290	GOL	O2-C2-C3-O3
6	M	1306	LDA	C2-C3-C4-C5
6	L	1284	LDA	C3-C4-C5-C6
6	M	1309	LDA	C1-C2-C3-C4
6	M	1312	LDA	C5-C6-C7-C8
5	L	1282	BCL	C12-C13-C15-C16
7	M	1314	BPH	C11-C12-C13-C15
14	M	1317	CDL	OA7-CA5-OA6-CA4
6	M	1311	LDA	C1-C2-C3-C4
6	M	1312	LDA	C2-C3-C4-C5
14	M	1317	CDL	C53-C54-C55-C56
14	M	1317	CDL	C11-CA5-OA6-CA4
6	L	1283	LDA	C5-C6-C7-C8
14	M	1317	CDL	C19-C20-C21-C22
7	M	1314	BPH	C11-C12-C13-C14
7	M	1314	BPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
6	L	1284	LDA	C5-C6-C7-C8
6	L	1284	LDA	C1-C2-C3-C4
6	L	1283	LDA	C1-C2-C3-C4
13	M	1316	SPO	C1-C4-C5-C6
14	M	1317	CDL	CA2-C1-CB2-OB2
6	M	1308	LDA	C2-C3-C4-C5
6	M	1311	LDA	C9-C10-C11-C12
4	L	1291	GOL	O1-C1-C2-O2
13	M	1316	SPO	C18-C17-C19-C20
7	L	1285	BPH	C4-C3-C5-C6
6	L	1283	LDA	C9-C10-C11-C12
13	M	1316	SPO	C2-C1-O1-CM1
13	M	1316	SPO	C3-C1-O1-CM1
13	M	1316	SPO	C16-C17-C19-C20
6	M	1309	LDA	C9-C10-C11-C12
6	M	1312	LDA	C7-C8-C9-C10
14	M	1317	CDL	C40-C41-C42-C43
5	M	1305	BCL	C11-C10-C8-C7
7	L	1285	BPH	C2-C3-C5-C6
5	L	1282	BCL	C14-C13-C15-C16
6	L	1283	LDA	C2-C3-C4-C5
6	L	1284	LDA	C2-C3-C4-C5
10	L	1289	HTO	C2-C3-C4-C5
6	L	1284	LDA	N1-C1-C2-C3
6	M	1311	LDA	N1-C1-C2-C3
6	M	1312	LDA	N1-C1-C2-C3
14	M	1317	CDL	C74-C75-C76-C77
7	M	1314	BPH	C8-C10-C11-C12
14	M	1317	CDL	OA5-CA3-CA4-CA6
12	M	1315	U10	C14-C16-C17-C18
12	M	1315	U10	C30-C29-C31-C32
6	L	1284	LDA	C9-C10-C11-C12
6	M	1307	LDA	C7-C8-C9-C10
7	L	1285	BPH	O2A-C1-C2-C3
14	M	1317	CDL	CA3-OA5-PA1-OA2
6	M	1311	LDA	C3-C4-C5-C6
6	M	1311	LDA	C11-C10-C9-C8
4	M	1318	GOL	O1-C1-C2-O2
7	L	1285	BPH	C8-C10-C11-C12
5	L	1287	BCL	C2-C1-O2A-CGA
5	L	1282	BCL	C6-C7-C8-C9
5	L	1287	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
6	M	1311	LDA	C6-C7-C8-C9
5	M	1304	BCL	C4C-C3C-CAC-CBC
5	M	1304	BCL	C12-C13-C15-C16
7	M	1314	BPH	C6-C7-C8-C10
14	M	1317	CDL	C72-C73-C74-C75
6	M	1307	LDA	C4-C5-C6-C7
5	L	1287	BCL	CAD-CBD-CGD-O2D
13	M	1316	SPO	C26-C27-C28-C29
14	M	1317	CDL	OA5-CA3-CA4-OA6
6	M	1308	LDA	C1-C2-C3-C4
14	M	1317	CDL	OB6-CB4-CB6-OB8
5	M	1304	BCL	C11-C12-C13-C14
7	M	1314	BPH	C2C-C3C-CAC-CBC
6	M	1308	LDA	C7-C8-C9-C10
12	M	1315	U10	C20-C19-C21-C22
12	M	1315	U10	C28-C29-C31-C32
14	M	1317	CDL	CA2-OA2-PA1-OA4
14	M	1317	CDL	CA3-OA5-PA1-OA4
6	M	1307	LDA	C2-C1-N1-O1
10	L	1289	HTO	C4-C5-C6-C7
5	M	1304	BCL	C6-C7-C8-C10
5	L	1287	BCL	C11-C10-C8-C9
7	L	1285	BPH	C11-C10-C8-C9
7	M	1314	BPH	C6-C7-C8-C9
4	H	1254	GOL	O1-C1-C2-O2
8	L	1286[B]	UQ2	C4-C3-O3-CM3
14	M	1317	CDL	C31-C32-C33-C34
6	M	1306	LDA	C4-C5-C6-C7
14	M	1317	CDL	C81-C82-C83-C84
14	M	1317	CDL	CA2-OA2-PA1-OA5
5	M	1304	BCL	C6-C7-C8-C9
6	M	1310	LDA	C1-C2-C3-C4
6	M	1308	LDA	C3-C4-C5-C6
10	L	1289	HTO	O1-C1-C2-C3
14	M	1317	CDL	C1-CB2-OB2-PB2
14	M	1317	CDL	C80-C81-C82-C83
6	M	1306	LDA	N1-C1-C2-C3
6	M	1312	LDA	C4-C5-C6-C7
12	M	1315	U10	C5-C4-O4-C4M
5	M	1305	BCL	CAA-CBA-CGA-O2A
12	M	1315	U10	C18-C19-C21-C22
14	M	1317	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
4	H	1255	GOL	O2-C2-C3-O3
7	M	1314	BPH	C2-C3-C5-C6
5	L	1287	BCL	C2A-CAA-CBA-CGA
6	M	1306	LDA	C9-C10-C11-C12
6	M	1312	LDA	C1-C2-C3-C4
6	M	1308	LDA	C11-C10-C9-C8
5	L	1282	BCL	C1-C2-C3-C4
7	M	1314	BPH	C1-C2-C3-C4
6	M	1309	LDA	C4-C5-C6-C7
5	M	1304	BCL	C4-C3-C5-C6
5	M	1305	BCL	C10-C11-C12-C13
14	M	1317	CDL	C72-C71-CB7-OB8
5	M	1304	BCL	CAD-CBD-CGD-O2D
7	L	1285	BPH	CAD-CBD-CGD-O2D
7	M	1314	BPH	CAD-CBD-CGD-O2D
14	M	1317	CDL	CB3-CB4-OB6-CB5
6	M	1310	LDA	C2-C1-N1-CM2
7	M	1314	BPH	CHA-CBD-CGD-O1D
12	M	1315	U10	C31-C32-C33-C34
14	M	1317	CDL	C32-C31-CA7-OA8
6	M	1309	LDA	C11-C10-C9-C8
14	M	1317	CDL	C72-C71-CB7-OB9
7	M	1314	BPH	C4-C3-C5-C6
14	M	1317	CDL	CB2-C1-CA2-OA2
5	M	1304	BCL	C11-C12-C13-C15
14	M	1317	CDL	C32-C31-CA7-OA9

There are no ring outliers.

20 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1305	BCL	13	0
14	M	1317	CDL	4	0
6	L	1284	LDA	2	0
4	M	1318	GOL	1	0
5	L	1287	BCL	2	0
6	M	1308	LDA	4	0
6	M	1306	LDA	3	0
5	M	1304	BCL	10	0
8	L	1286[A]	UQ2	2	0
13	M	1316	SPO	2	0
7	M	1314	BPH	14	0

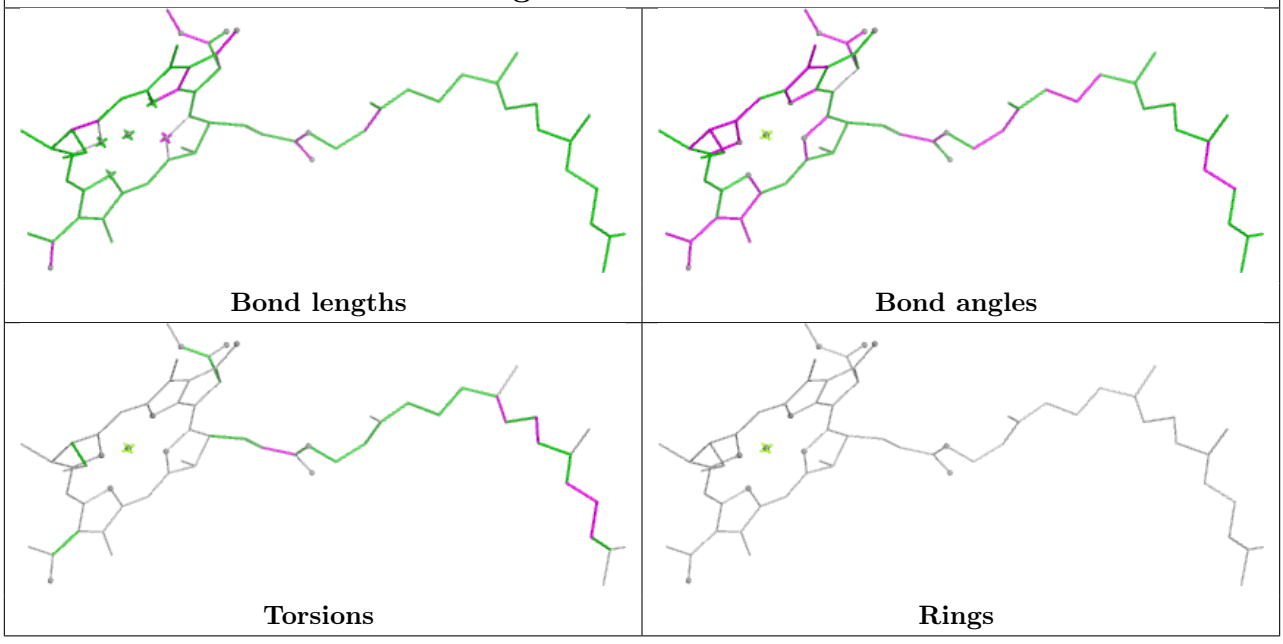
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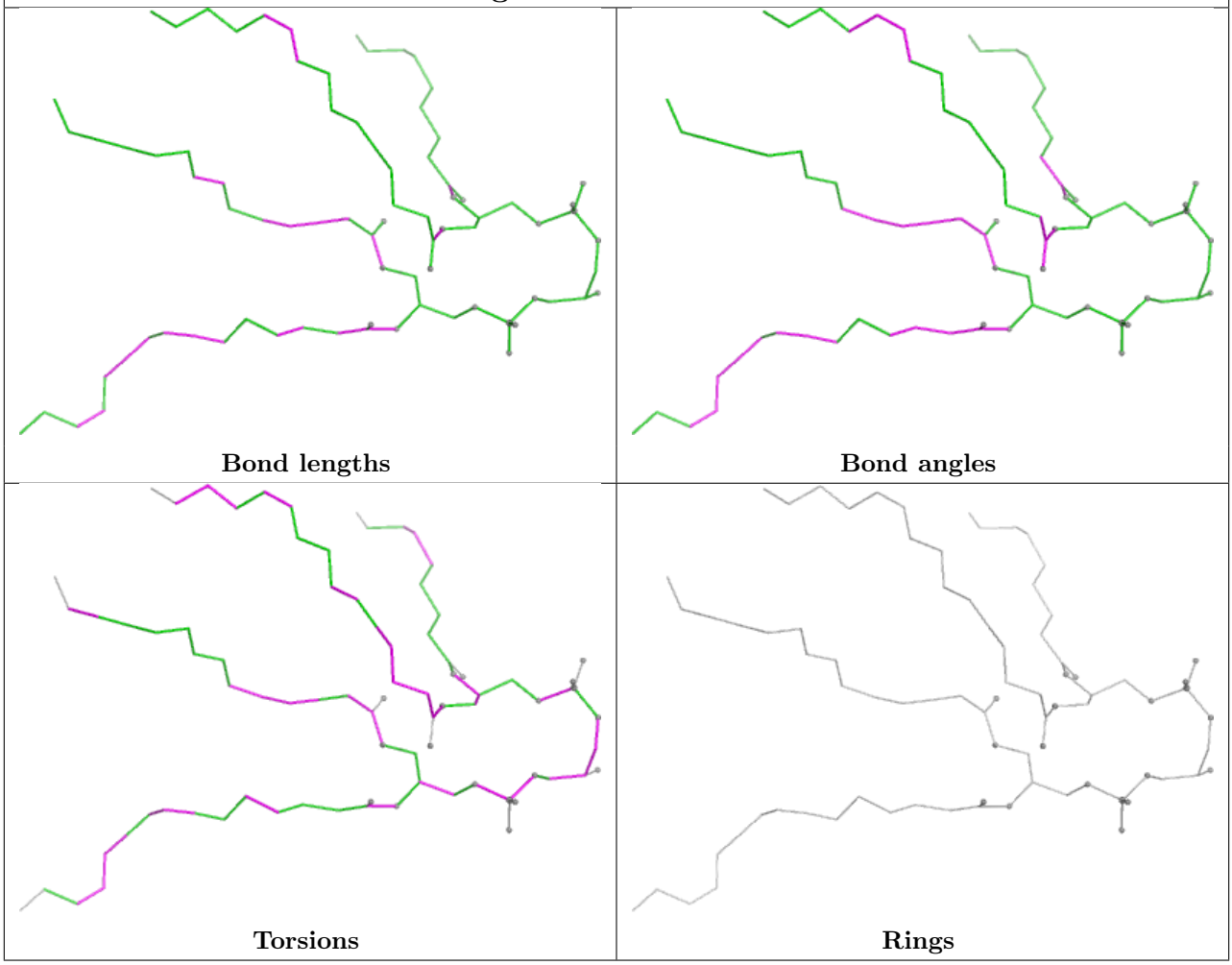
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1286[B]	UQ2	4	0
6	M	1309	LDA	2	0
12	M	1315	U10	4	0
6	M	1310	LDA	2	0
5	L	1282	BCL	3	0
7	L	1285	BPH	6	0
4	H	1253	GOL	1	0
4	L	1290	GOL	1	0
4	H	1252	GOL	3	0

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.

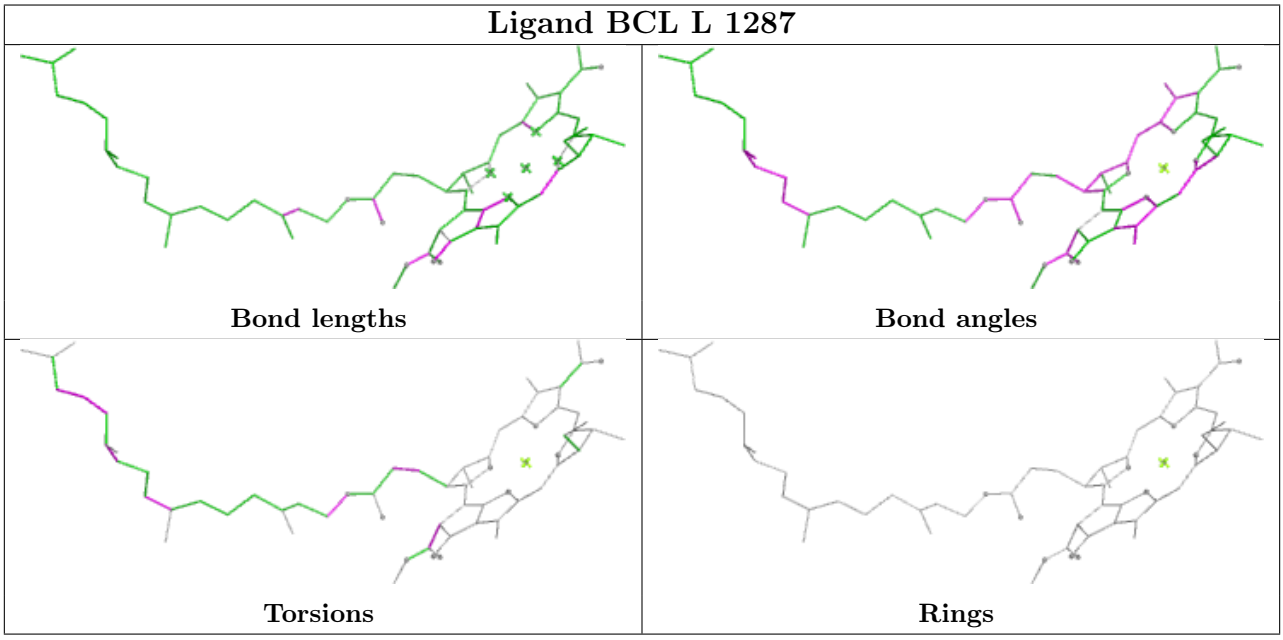
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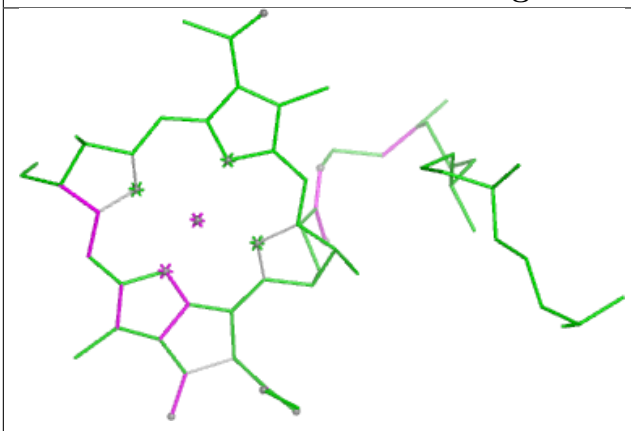
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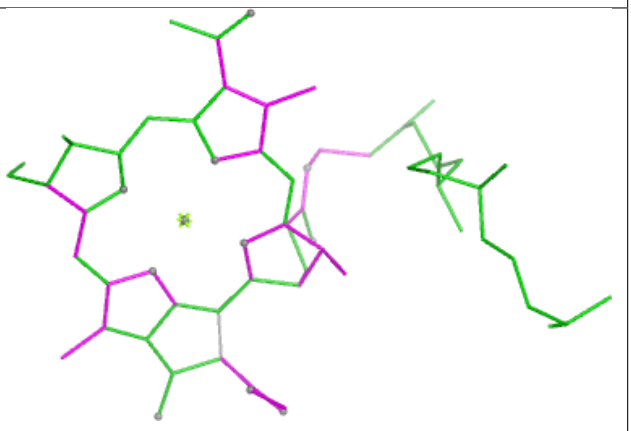
Ligand BCL L 1287



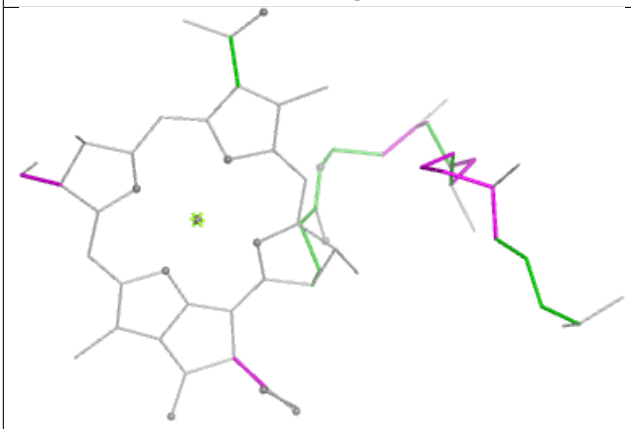
Ligand BCL M 1304



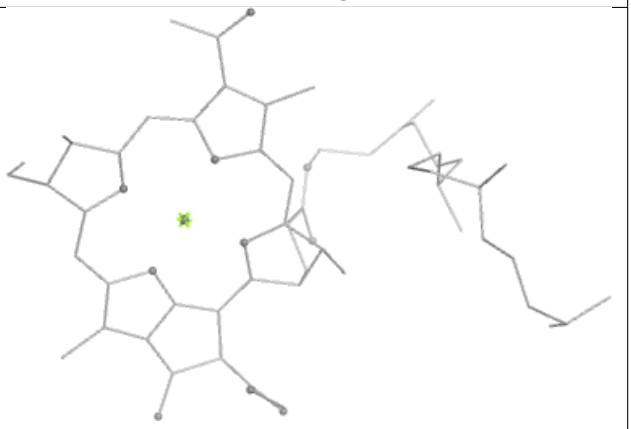
Bond lengths



Bond angles

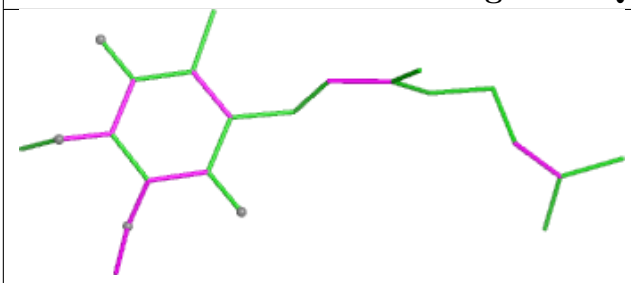


Torsions

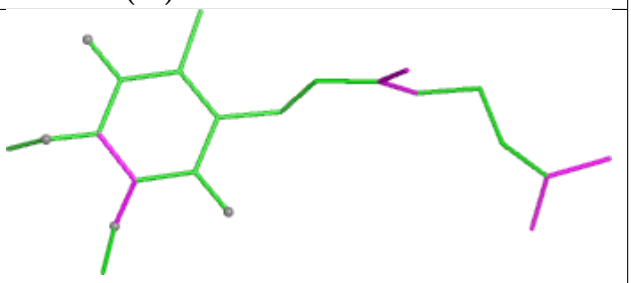


Rings

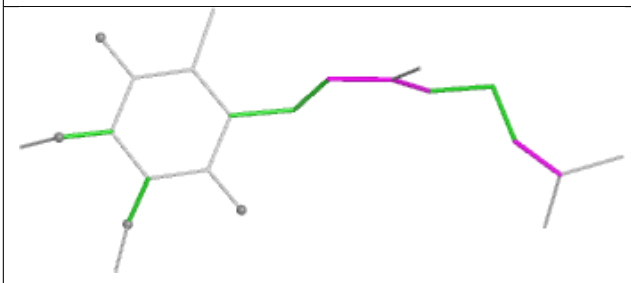
Ligand UQ2 L 1286 (A)



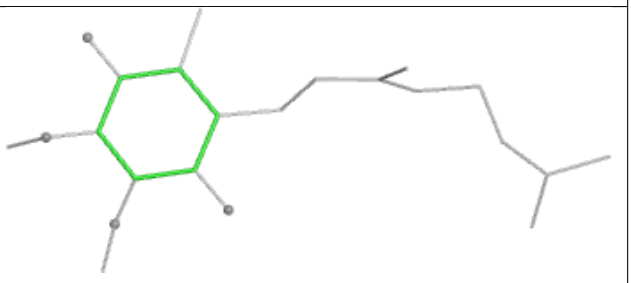
Bond lengths



Bond angles

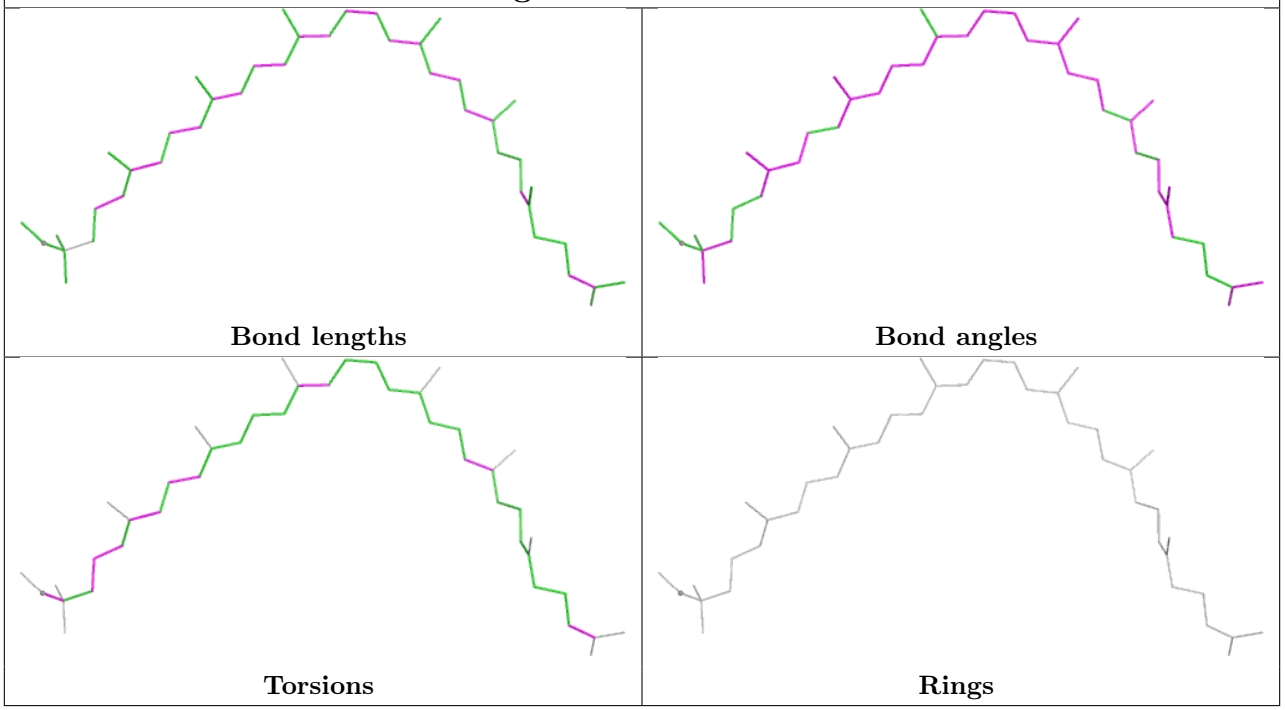


Torsions

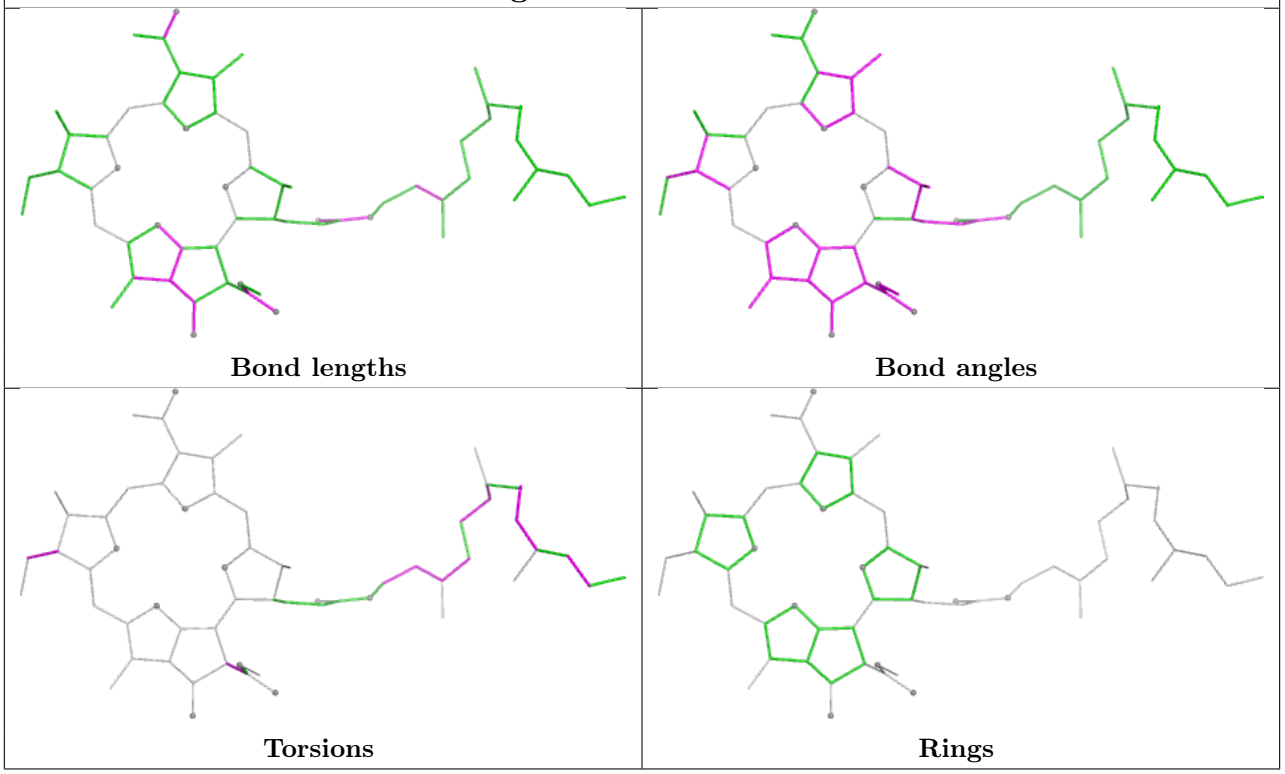


Rings

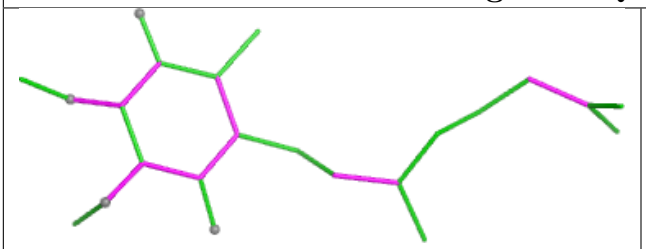
Ligand SPO M 1316



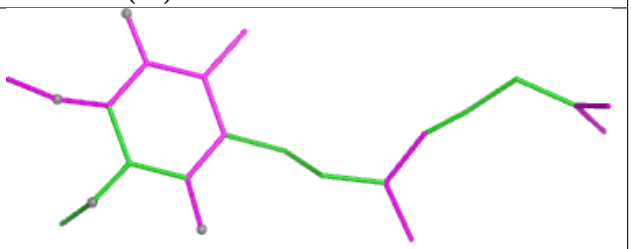
Ligand BPH M 1314



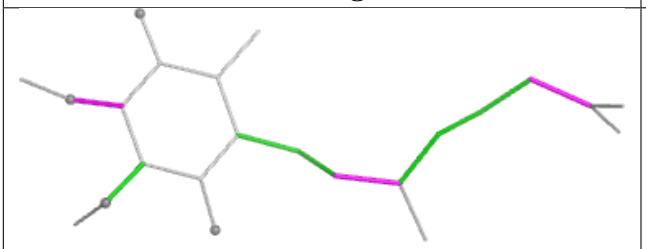
Ligand UQ2 L 1286 (B)



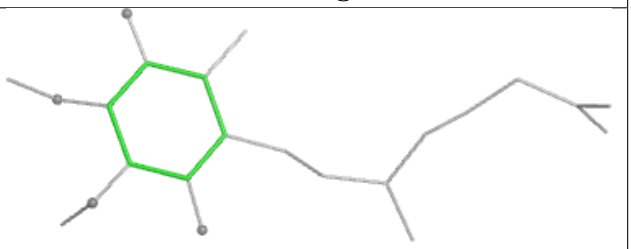
Bond lengths



Bond angles

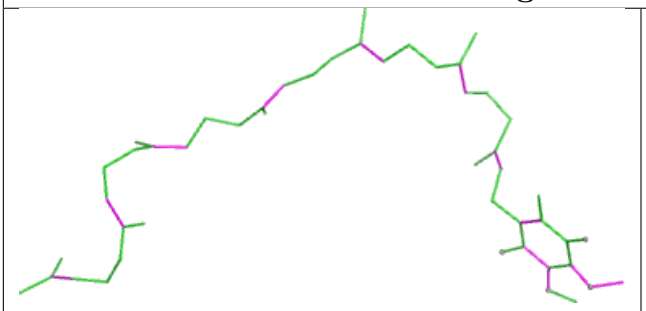


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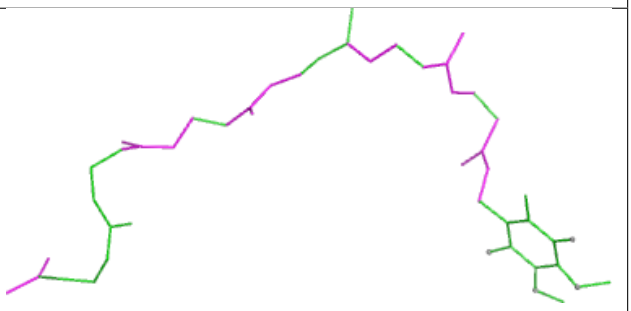


Rings

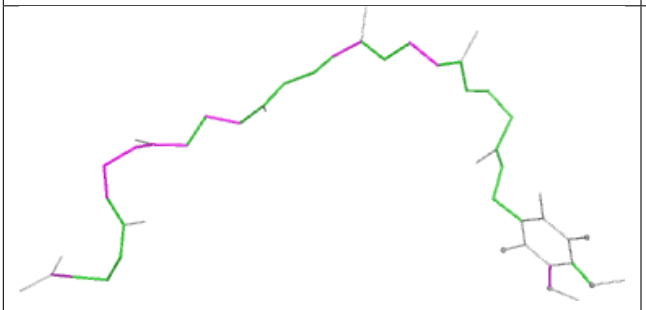
Ligand U10 M 1315



Bond lengths



Bond angles

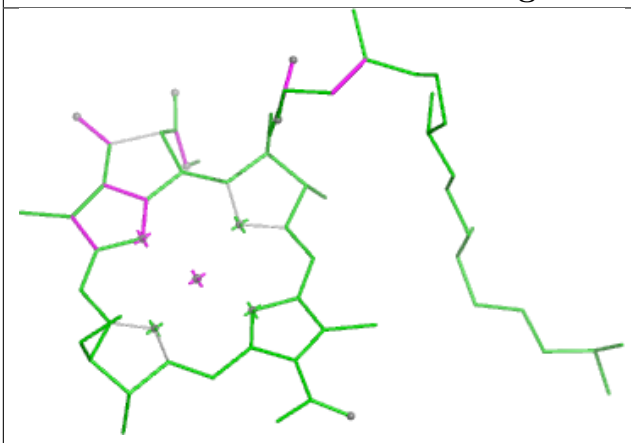


Torsions

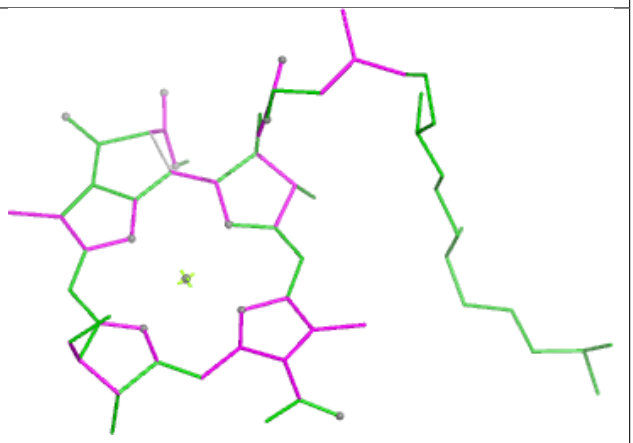


Rings

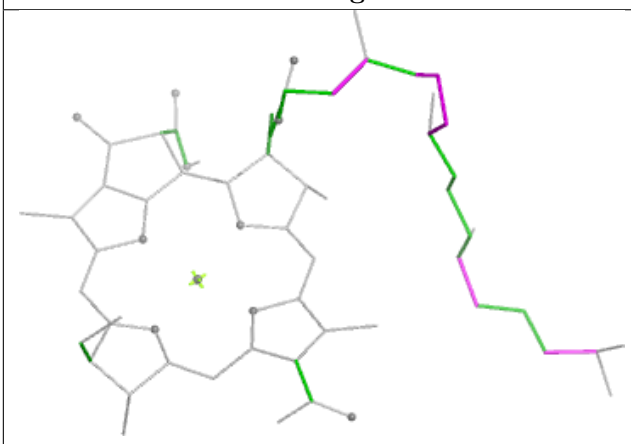
Ligand BCL L 1282



Bond lengths



Bond angles

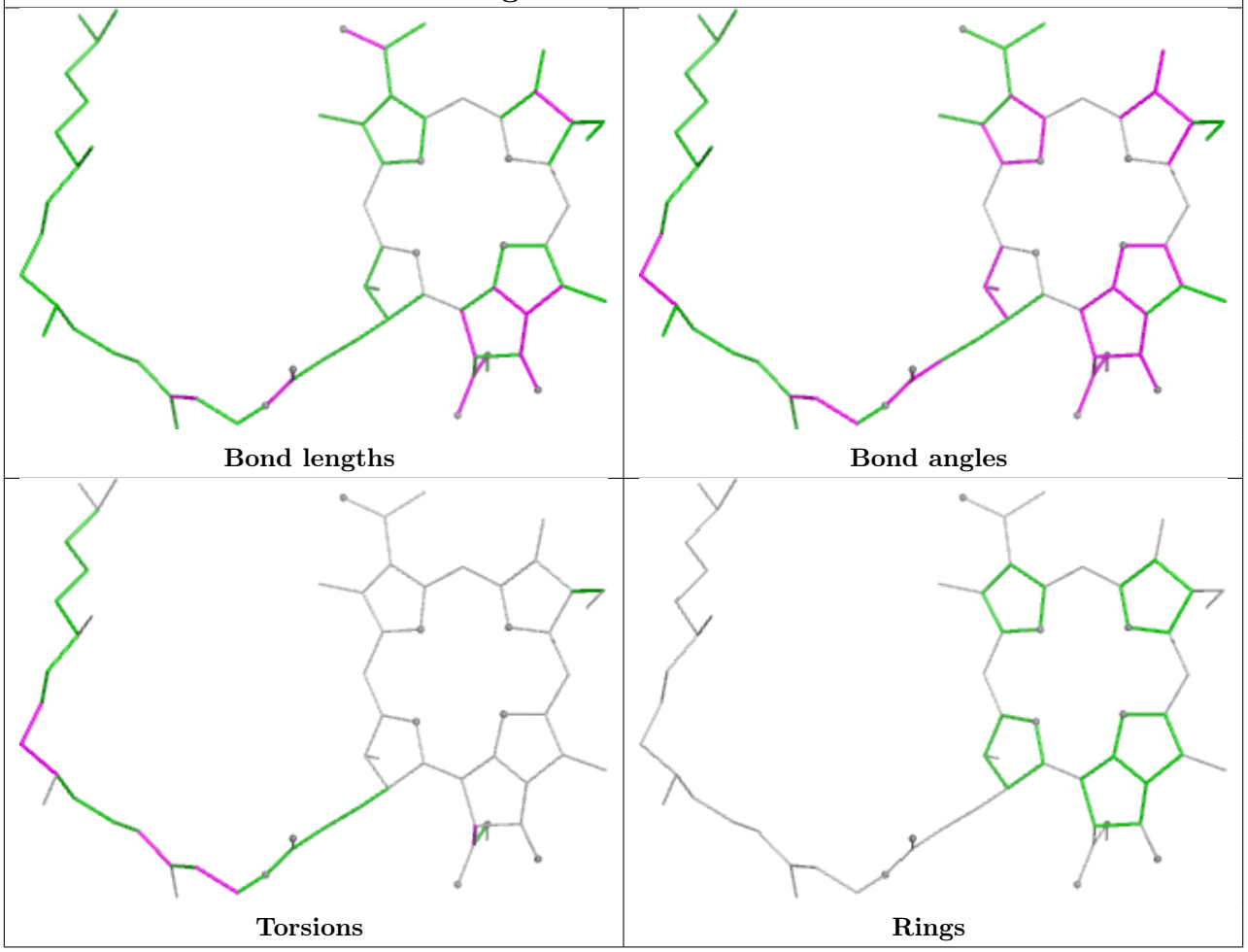


Torsions



Rings

Ligand BPH L 1285



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%)	-0.09	8 (3%)	49	46	23, 39, 51, 96	3 (1%)
2	L	281/281 (100%)	0.00	5 (1%)	67	65	27, 37, 61, 67	0
3	M	303/307 (98%)	0.05	11 (3%)	46	43	24, 41, 63, 75	0
All	All	825/848 (97%)	-0.00	24 (2%)	53	51	23, 39, 61, 96	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	303	MET	6.9
3	M	1	ALA	5.3
3	M	148	TRP	5.2
1	H	249	LYS	4.8
1	H	250	SER	4.8
3	M	278	LEU	4.3
1	H	251	VAL	4.0
3	M	3	TYR	3.8
3	M	52	LEU	3.6
1	H	245	ALA	3.2
2	L	59	TRP	2.9
3	M	2	GLU	2.8
3	M	292	ASP	2.7
3	M	302	GLY	2.6
1	H	248	ARG	2.5
3	M	301	HIS	2.5
2	L	275	ILE	2.4
2	L	281	GLY	2.2
1	H	247	LYS	2.2
2	L	1	ALA	2.2
2	L	67	TYR	2.2
1	H	94	GLU	2.2
3	M	300	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	246	PRO	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
6	LDA	M	1309	16/16	0.52	0.42	98,102,109,110	0
6	LDA	M	1312	16/16	0.54	0.39	78,90,101,101	0
14	CDL	M	1317	81/100	0.63	0.36	78,104,124,124	0
6	LDA	M	1310	16/16	0.66	0.36	110,113,119,120	0
6	LDA	L	1283	16/16	0.68	0.31	61,91,105,105	0
6	LDA	M	1311	16/16	0.71	0.28	95,104,112,113	0
6	LDA	L	1284	16/16	0.71	0.27	109,110,114,114	0
6	LDA	M	1306	16/16	0.71	0.28	54,70,75,76	0
4	GOL	H	1253	6/6	0.77	0.21	74,77,77,80	0
6	LDA	M	1308	16/16	0.78	0.22	61,67,75,75	0
8	UQ2	L	1286[B]	23/23	0.81	0.20	32,41,50,51	23
8	UQ2	L	1286[A]	23/23	0.81	0.20	36,41,50,52	23
4	GOL	H	1254	6/6	0.82	0.18	103,104,105,105	0
4	GOL	H	1255	6/6	0.82	0.19	101,101,102,102	0
4	GOL	L	1290	6/6	0.82	0.18	49,57,57,61	0
6	LDA	M	1307	16/16	0.82	0.22	66,69,80,80	0
10	HTO	L	1289	10/10	0.84	0.27	85,87,88,89	0
9	PO4	L	1288	5/5	0.84	0.11	89,89,90,90	0
4	GOL	L	1291	6/6	0.86	0.20	94,95,96,96	0
4	GOL	M	1318	6/6	0.87	0.12	83,84,84,85	0
4	GOL	H	1252	6/6	0.88	0.20	46,60,63,65	0
12	U10	M	1315	48/63	0.91	0.14	26,45,73,75	0

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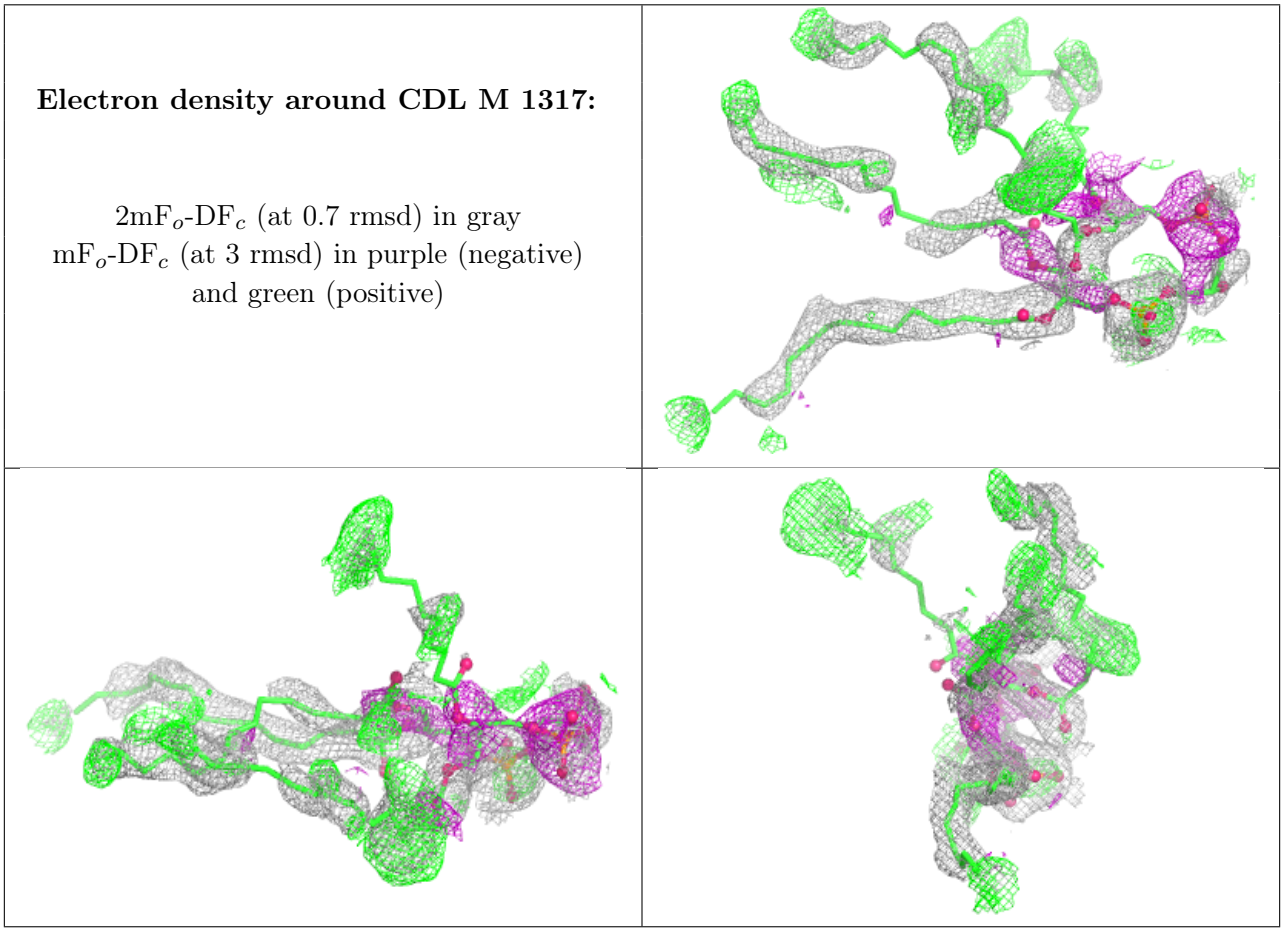
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	SPO	M	1316	42/42	0.92	0.13	36,49,68,72	0
5	BCL	L	1282	66/66	0.95	0.08	24,32,59,63	0
7	BPH	M	1314	65/65	0.95	0.10	26,41,98,101	0
5	BCL	M	1304	66/66	0.95	0.09	21,32,75,76	0
7	BPH	L	1285	65/65	0.96	0.07	23,31,44,48	0
5	BCL	M	1305	66/66	0.96	0.08	22,29,59,67	0
5	BCL	L	1287	66/66	0.96	0.07	19,30,50,57	0
11	FE	M	1313	1/1	0.99	0.04	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 1317:

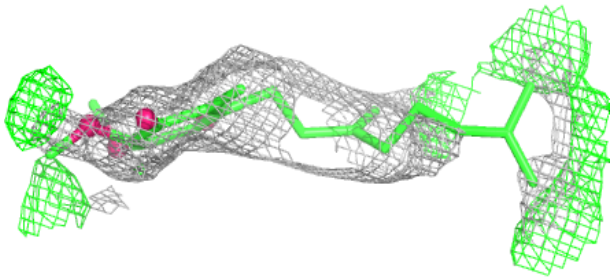
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

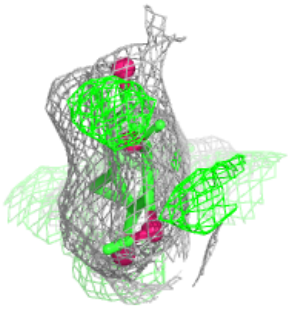


Electron density around UQ2 L 1286 (B):

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

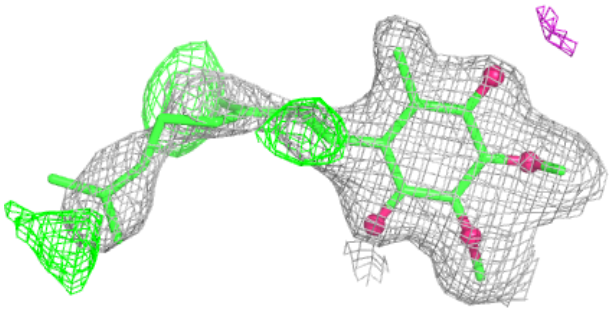


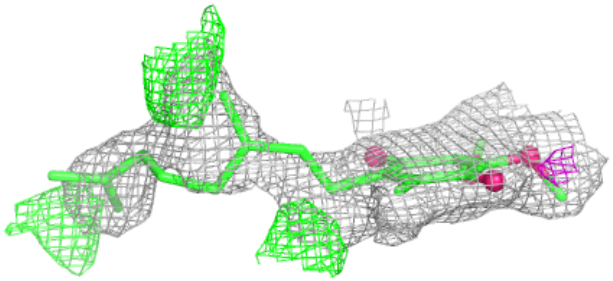


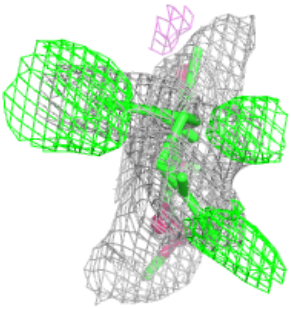


Electron density around UQ2 L 1286 (A):

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mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

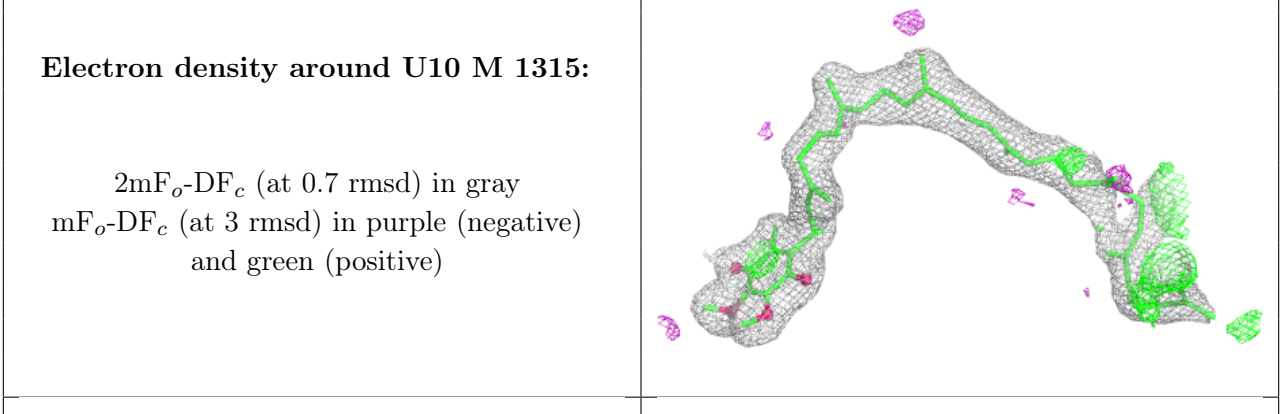






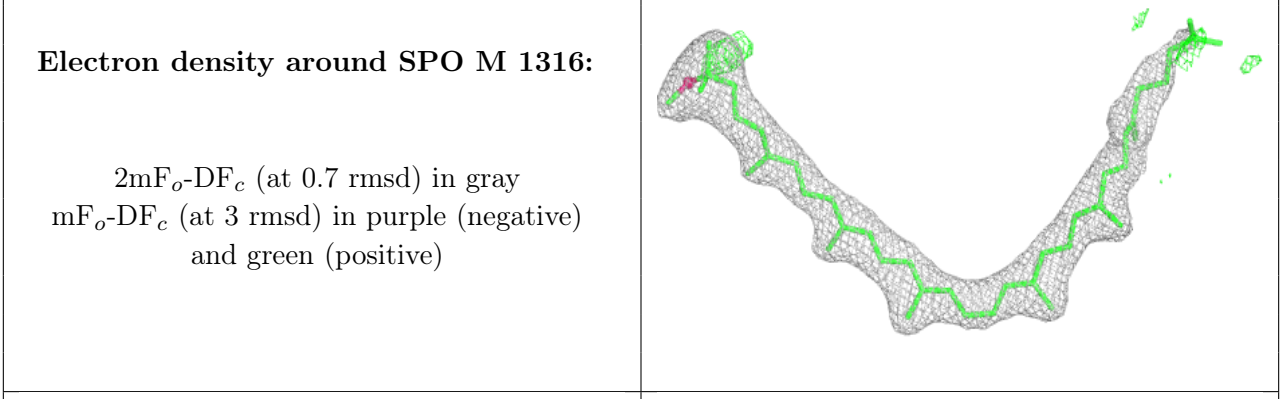
Electron density around U10 M 1315:

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



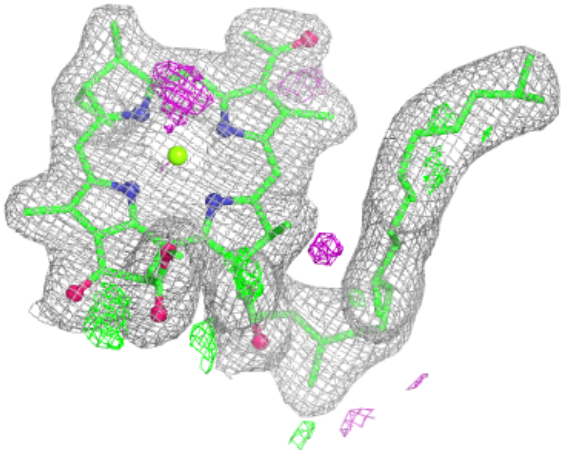
Electron density around SPO M 1316:

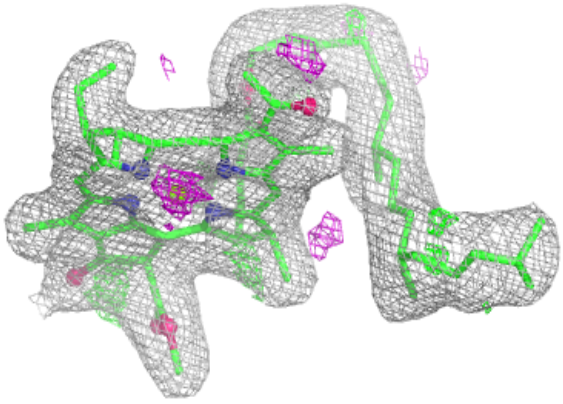
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

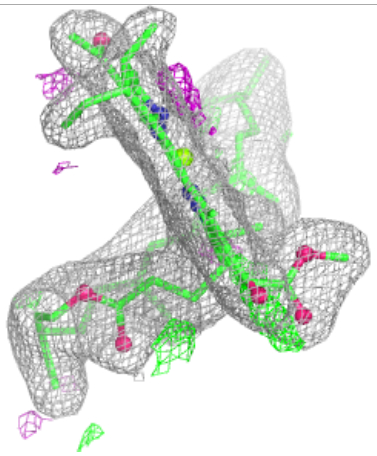


Electron density around BCL L 1282:

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

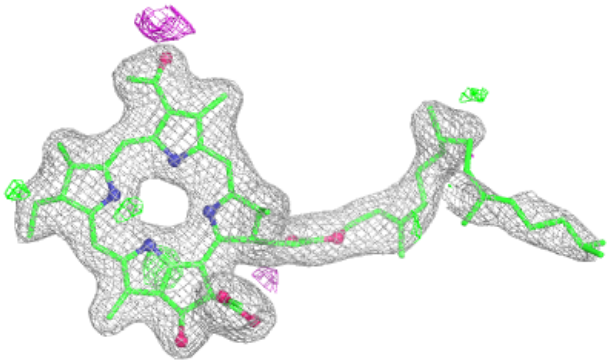


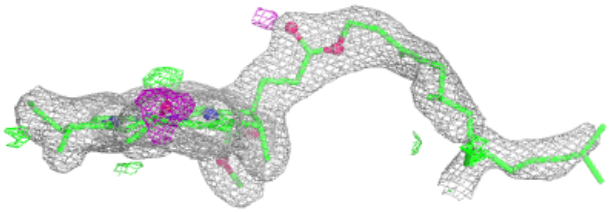


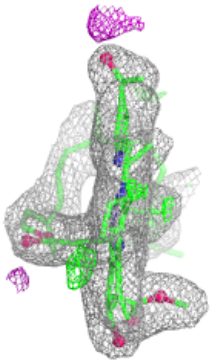


Electron density around BPH M 1314:

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

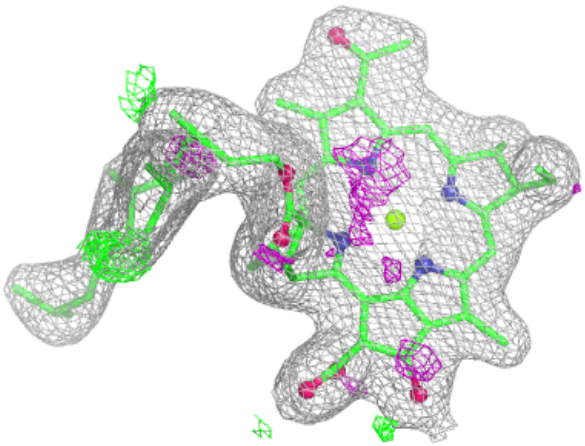


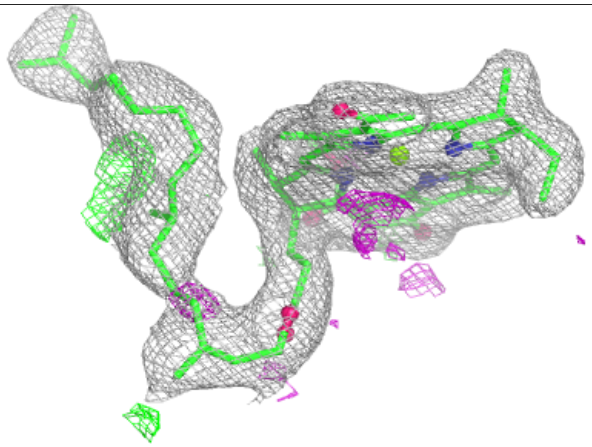


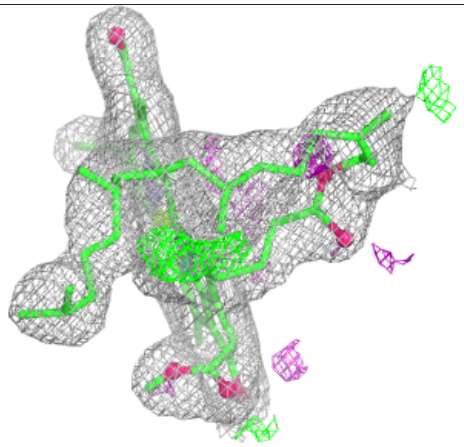


Electron density around BCL M 1304:

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

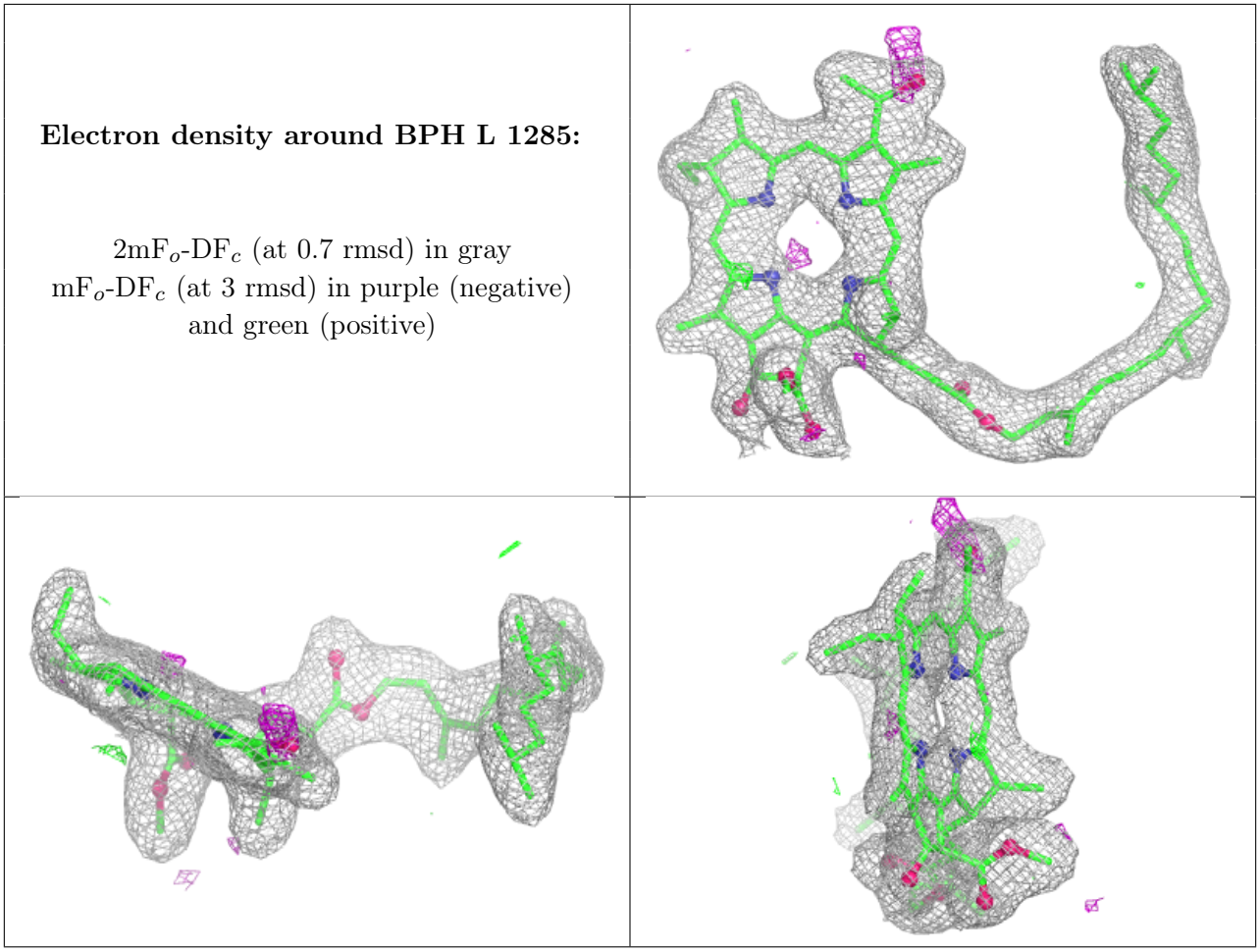






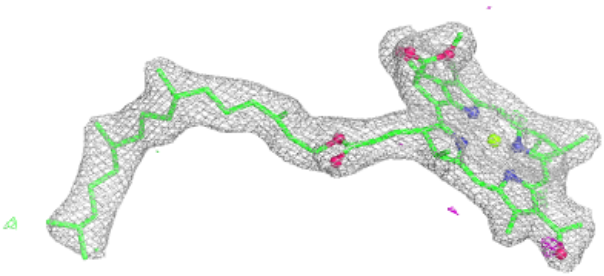
Electron density around BPH L 1285:

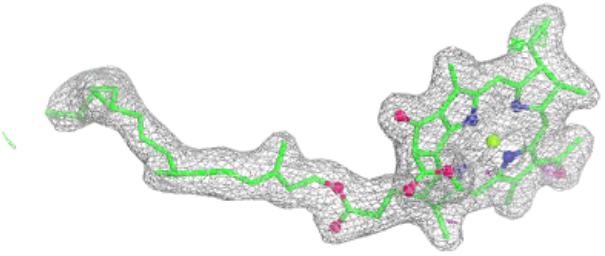
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

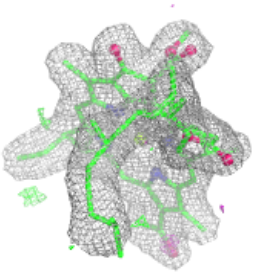


Electron density around BCL M 1305:

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

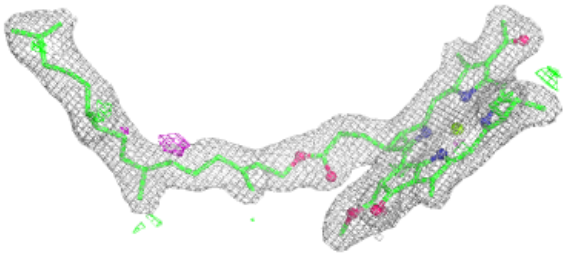


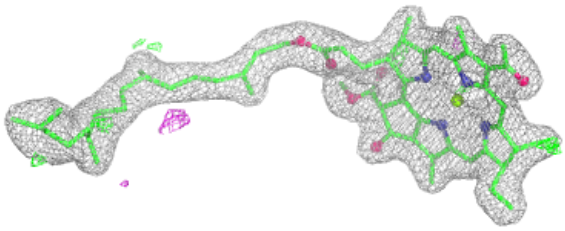


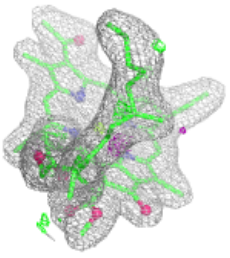


Electron density around BCL L 1287:

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







6.5 Other polymers (i)

There are no such residues in this entry.