Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2026 – 03:37 am BST

PDB ID	:	2J8C / pdb_00002j8c
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 8 in the neutral state
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2006-10-24
Resolution	:	1.87 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:

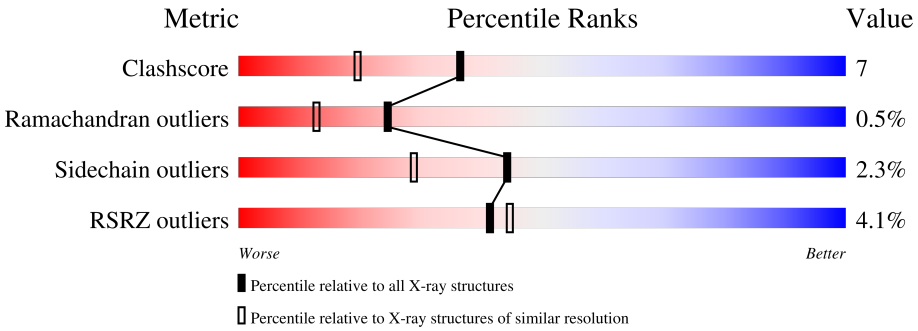
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.87 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))
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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% 82% 10% • 7%
2	L	281	4% 93% 7% •
3	M	307	5% 88% 9% ••

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
10	HTO	L	1291	-	-	-	X
14	PC1	M	1312	X	-	-	-
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 (i)

There are 16 unique types of molecules in this entry. The entry contains 7774 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	1850	1183	321	337	9	0	5	1

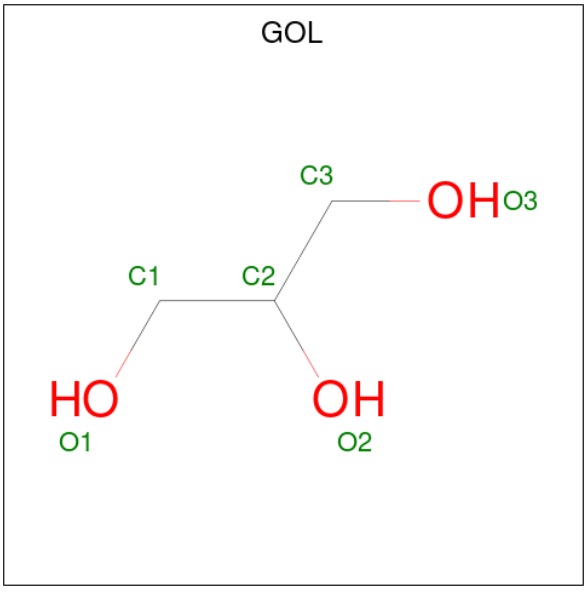
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2239	1513	355	363	8	0	2	0

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

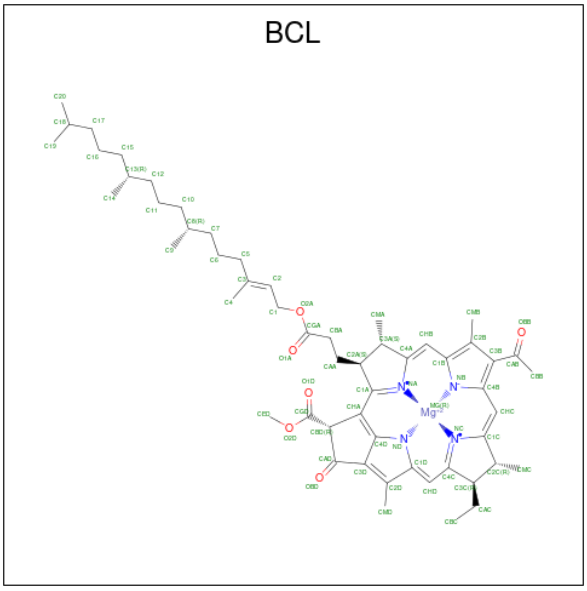
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2411	1607	396	398	10	0	1	1

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



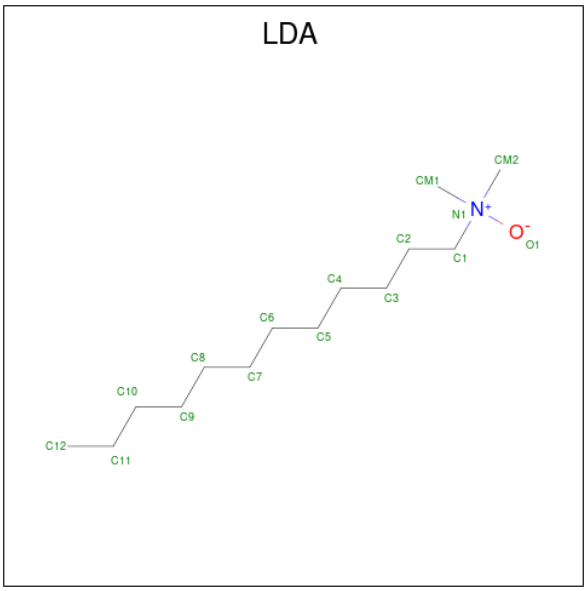
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

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



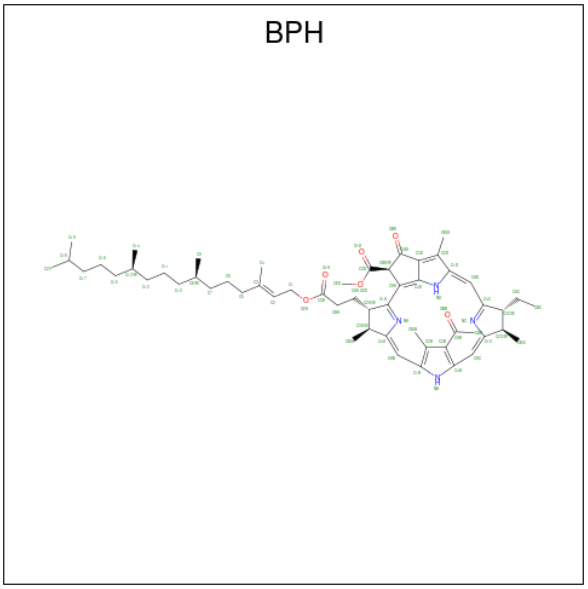
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



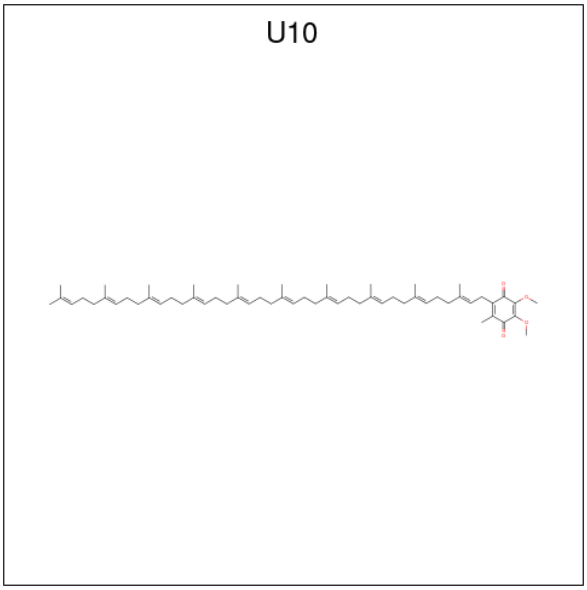
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0

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



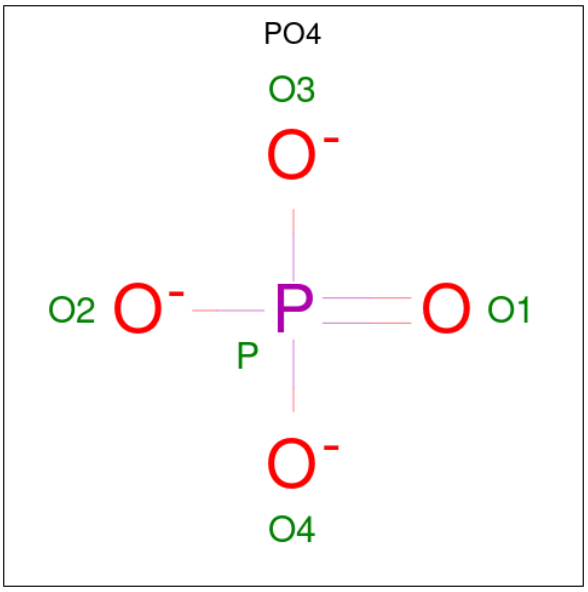
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



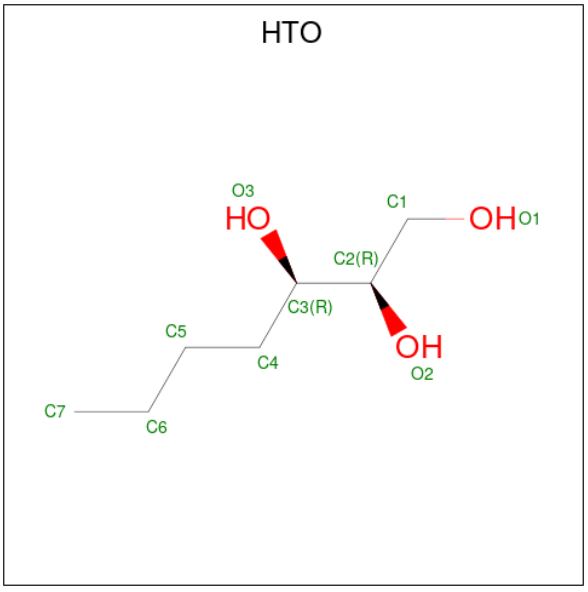
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		
8	M	1	Total	C	O	0	0
			48	44	4		

- 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: $C_7H_{16}O_3$).

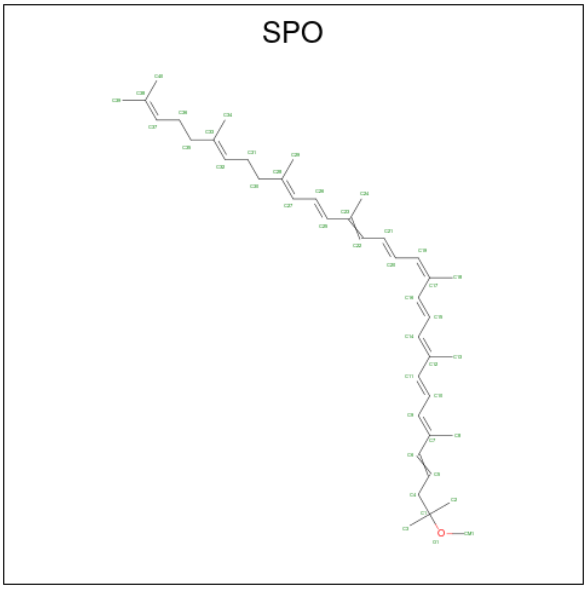


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0
10	L	1	Total C O 10 7 3	0	0

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

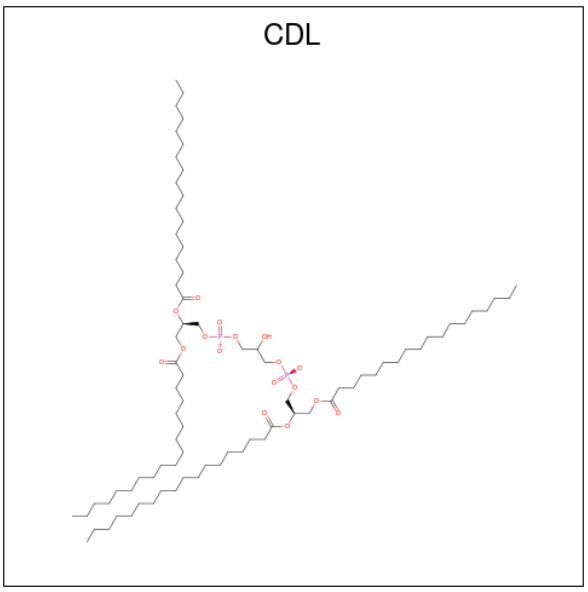
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



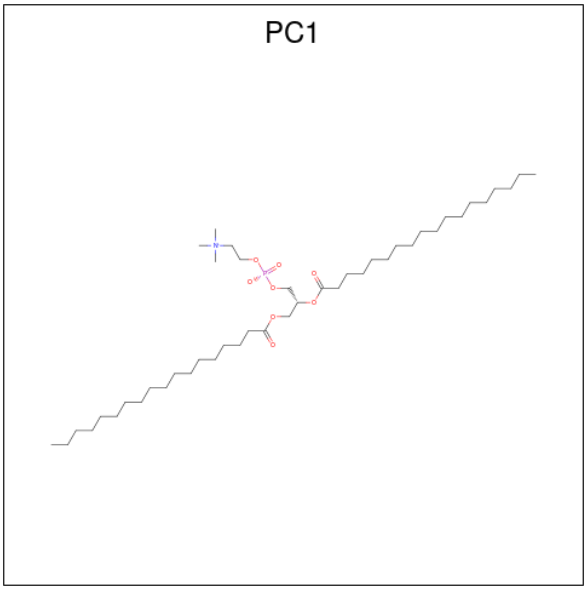
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 42 41 1	0	0

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



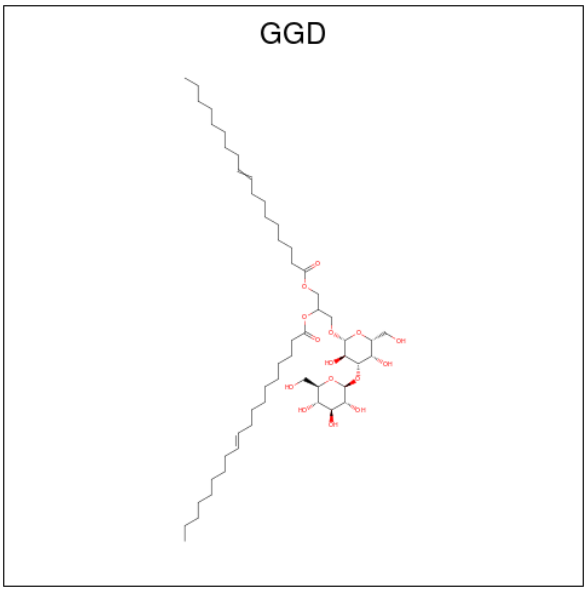
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 14 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 15 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY] -1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (CCD ID: GGD) (formula: $C_{52}H_{94}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	M	1	Total	C	O	0	0
			57	42	15		

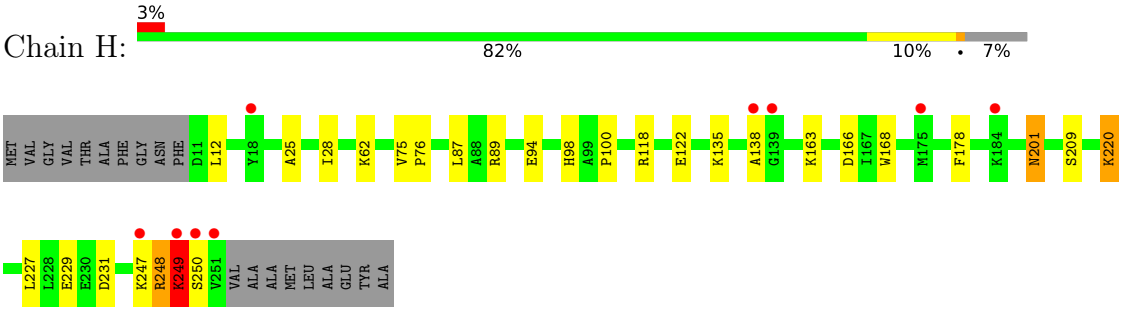
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	172	Total	O	0	0
			172	172		
16	L	116	Total	O	0	0
			116	116		
16	M	127	Total	O	0	0
			127	127		

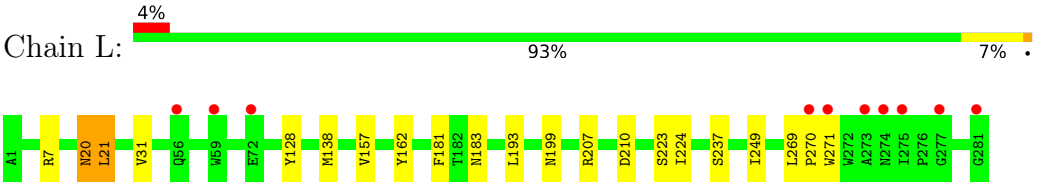
3 Residue-property plots (i)

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.

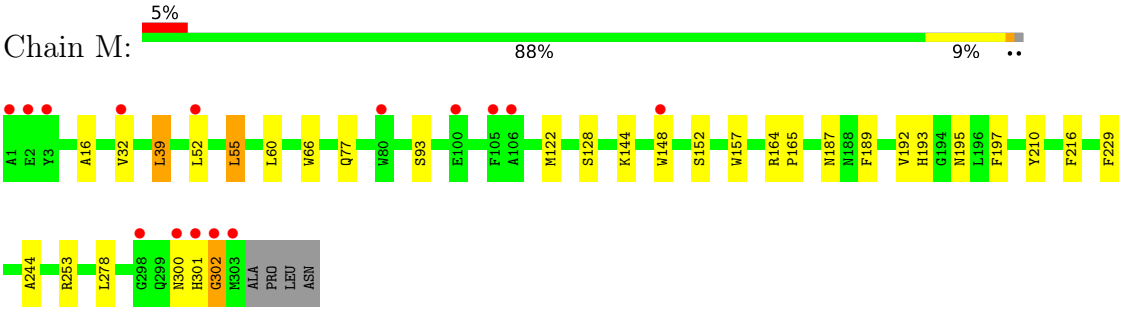
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• 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	138.69Å 138.69Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 1.87 119.52 – 1.87	Depositor EDS
% Data completeness (in resolution range)	87.0 (119.52-1.87) 87.0 (119.52-1.87)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.178 , 0.196 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7774	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: CDL, BCL, BPH, GOL, SPO, GGD, HTO, PO4, FE, LDA, U10, PC1

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	0.74	1/1930 (0.1%)	0.86	2/2621 (0.1%)
2	L	0.75	0/2339	0.81	0/3203
3	M	0.74	1/2508 (0.0%)	0.83	0/3424
All	All	0.74	2/6777 (0.0%)	0.83	2/9248 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	302	GLY	C-N	-7.07	1.23	1.33
1	H	250	SER	C-N	-6.33	1.24	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	248	ARG	CA-C-N	5.56	131.71	121.70
1	H	248	ARG	C-N-CA	5.56	131.71	121.70

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	1850	0	1873	30	0
2	L	2239	0	2185	22	0
3	M	2411	0	2319	23	0
4	H	24	0	32	8	0
4	L	18	0	24	2	0
5	L	132	0	147	4	0
5	M	132	0	148	16	0
6	L	48	0	93	0	0
6	M	32	0	62	2	0
7	L	65	0	76	4	0
7	M	65	0	76	12	0
8	L	46	0	46	5	0
8	M	48	0	63	1	0
9	L	5	0	0	0	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	42	0	60	4	0
13	M	81	0	90	8	0
14	M	43	0	60	0	0
15	M	57	0	67	2	0
16	H	172	0	0	4	1
16	L	116	0	0	1	0
16	M	127	0	0	1	0
All	All	7774	0	7453	106	1

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

All (106) 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)
1:H:248:ARG:HA	1:H:249[A]:LYS:HB2	1.33	1.06
7:M:1308:BPH:HHC	7:M:1308:BPH:HBB3	1.39	1.01
4:H:1251:GOL:H32	16:H:2002:HOH:O	1.67	0.93
7:L:1286:BPH:HHC	7:L:1286:BPH:HBB3	1.58	0.85
5:L:1282:BCL:HBB2	5:L:1282:BCL:HHC	1.59	0.85
1:H:201:ASN:H	1:H:201:ASN:HD22	1.29	0.79
7:L:1286:BPH:HHC	7:L:1286:BPH:CBB	2.13	0.78
1:H:248:ARG:CA	1:H:249[A]:LYS:HB2	2.14	0.77
4:H:1251:GOL:C3	16:H:2002:HOH:O	2.29	0.77
2:L:199:ASN:O	13:M:1311:CDL:HB22	1.85	0.76
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.68	0.75
1:H:62:LYS:HE3	4:H:1251:GOL:H11	1.70	0.74
2:L:20:ASN:C	2:L:20:ASN:HD22	1.96	0.74
2:L:224:ILE:H	8:L:1287[A]:U10:H8	1.55	0.72
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.54	0.72
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.24	0.72
7:M:1308:BPH:HHC	7:M:1308:BPH:CBB	2.19	0.68
5:M:1303:BCL:HBB2	12:M:1310:SPO:H243	1.75	0.68
1:H:248:ARG:HA	1:H:249[B]:LYS:HB3	1.76	0.68
1:H:248:ARG:HA	1:H:249[B]:LYS:HB2	1.70	0.68
3:M:77:GLN:HE22	3:M:93:SER:H	1.42	0.68
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.24	0.67
8:L:1287[A]:U10:H4M1	16:L:2090:HOH:O	1.93	0.66
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.77	0.66
2:L:181:PHE:HB3	7:M:1308:BPH:HBB2	1.78	0.66
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.77	0.65
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.26	0.65
5:M:1303:BCL:H71	5:M:1304:BCL:H202	1.78	0.65
3:M:300:ASN:C	3:M:302:GLY:H	2.03	0.65
5:M:1303:BCL:CBB	12:M:1310:SPO:H243	2.27	0.65
1:H:62:LYS:HZ1	4:H:1251:GOL:H11	1.63	0.63
3:M:148:TRP:HE1	13:M:1311:CDL:HB31	1.65	0.61
1:H:62:LYS:CE	4:H:1251:GOL:H11	2.30	0.60
7:M:1308:BPH:H5C2	7:M:1308:BPH:H142	1.82	0.60
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.21	0.58
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB3	1.85	0.57
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.51	0.57
1:H:201:ASN:H	1:H:201:ASN:ND2	1.99	0.56
1:H:209:SER:OG	1:H:247:LYS:HD3	2.05	0.56
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.88	0.56
2:L:181:PHE:CD2	7:M:1308:BPH:HBB1	2.40	0.56
7:M:1308:BPH:HBC3	7:M:1308:BPH:HHD	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220[A]:LYS:HG2	1:H:229:GLU:OE2	2.06	0.55
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.71	0.54
3:M:189:PHE:O	3:M:193:HIS:HD2	1.90	0.54
1:H:201:ASN:HD22	1:H:201:ASN:N	2.00	0.54
2:L:199:ASN:HA	4:L:1292:GOL:H31	1.91	0.52
5:M:1303:BCL:HHC	5:M:1303:BCL:CBB	2.39	0.52
3:M:253:ARG:NH1	15:M:1313:GGD:HC31	2.25	0.52
2:L:181:PHE:HB3	7:M:1308:BPH:CBB	2.39	0.52
7:M:1308:BPH:HBB3	7:M:1308:BPH:CHC	2.26	0.51
1:H:28:ILE:HG22	16:H:2169:HOH:O	2.11	0.51
3:M:144:LYS:H	13:M:1311:CDL:PB2	2.33	0.51
7:L:1286:BPH:HBB3	7:L:1286:BPH:CHC	2.35	0.50
1:H:62:LYS:NZ	4:H:1251:GOL:H11	2.25	0.50
3:M:278:LEU:HD21	13:M:1311:CDL:H782	1.94	0.50
3:M:300:ASN:C	3:M:302:GLY:N	2.70	0.50
1:H:89:ARG:NH2	1:H:94:GLU:HG2	2.27	0.49
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	1.94	0.49
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.47
3:M:39:LEU:HD12	6:M:1306:LDA:H112	1.96	0.47
1:H:62:LYS:HE3	4:H:1251:GOL:C1	2.43	0.47
1:H:118[B]:ARG:HD2	16:M:2106:HOH:O	2.15	0.46
3:M:148:TRP:CD2	13:M:1311:CDL:H522	2.51	0.46
5:L:1282:BCL:H92	15:M:1313:GGD:H401	1.97	0.46
1:H:135:LYS:HE3	1:H:166:ASP:OD2	2.15	0.46
1:H:25:ALA:HB1	4:H:1252:GOL:H11	1.99	0.45
13:M:1311:CDL:H512	13:M:1311:CDL:H321	1.99	0.45
2:L:138:MET:SD	2:L:249:ILE:HD11	2.56	0.45
8:L:1287[A]:U10:H71	8:L:1287[A]:U10:H1M3	1.72	0.45
2:L:223:SER:OG	8:L:1287[A]:U10:O5	2.29	0.44
8:M:1309:U10:H4M2	8:M:1309:U10:O3	2.17	0.44
7:M:1308:BPH:H121	7:M:1308:BPH:H8	1.74	0.44
4:L:1294:GOL:H32	6:M:1305:LDA:HM22	2.00	0.44
3:M:229:PHE:HB2	3:M:244:ALA:HB2	2.00	0.44
13:M:1311:CDL:OA8	13:M:1311:CDL:HB4	2.18	0.44
1:H:248:ARG:CA	1:H:249[B]:LYS:HB2	2.46	0.43
3:M:144:LYS:N	13:M:1311:CDL:OB3	2.44	0.43
5:M:1304:BCL:HBB2	5:M:1304:BCL:HHC	1.98	0.43
2:L:20:ASN:HD22	2:L:21:LEU:N	2.16	0.43
3:M:152:SER:OG	3:M:278:LEU:HG	2.19	0.43
3:M:55:LEU:HD22	3:M:128:SER:HB2	2.01	0.43
2:L:157:VAL:HG11	5:M:1304:BCL:HBB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.00	0.43
1:H:220[A]:LYS:CG	1:H:229:GLU:OE2	2.67	0.43
2:L:183:ASN:ND2	2:L:237[B]:SER:OG	2.52	0.43
5:M:1304:BCL:H172	7:M:1308:BPH:H9C2	2.00	0.43
7:M:1308:BPH:CBB	7:M:1308:BPH:CHC	2.92	0.42
5:M:1303:BCL:H203	12:M:1310:SPO:H10	2.01	0.42
2:L:269:LEU:HD13	2:L:271[A]:TRP:CZ2	2.55	0.42
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.53	0.42
2:L:270:PRO:HG2	2:L:271[B]:TRP:CD1	2.54	0.42
1:H:168:TRP:HB2	1:H:178:PHE:HB2	2.01	0.41
3:M:60:LEU:HD11	7:M:1308:BPH:H161	2.02	0.41
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.03	0.41
2:L:20:ASN:C	2:L:20:ASN:ND2	2.68	0.41
3:M:157:TRP:CE2	12:M:1310:SPO:H293	2.56	0.41
2:L:193:LEU:HD23	8:L:1287[A]:U10:C2	2.52	0.40
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.56	0.40
1:H:118[B]:ARG:NH2	16:H:2086:HOH:O	2.24	0.40
3:M:164:ARG:HB3	3:M:165:PRO:HD3	2.02	0.40
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.94	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:H:2039:HOH:O	16:H:2039:HOH:O[4_555]	1.66	0.54

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	245/260 (94%)	241 (98%)	2 (1%)	2 (1%)	16 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	L	281/281 (100%)	275 (98%)	5 (2%)	1 (0%)	30 18
3	M	302/307 (98%)	293 (97%)	7 (2%)	2 (1%)	18 7
All	All	828/848 (98%)	809 (98%)	14 (2%)	5 (1%)	24 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	301	HIS
3	M	195	ASN
2	L	31	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	200/208 (96%)	190 (95%)	10 (5%)	22 7
2	L	221/220 (100%)	217 (98%)	4 (2%)	51 38
3	M	237/240 (99%)	232 (98%)	5 (2%)	47 32
All	All	658/668 (98%)	639 (97%)	19 (3%)	44 20

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	163[A]	LYS
1	H	163[B]	LYS
1	H	201	ASN
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	220[C]	LYS
1	H	231	ASP
1	H	249[A]	LYS

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Mol	Chain	Res	Type
1	H	249[B]	LYS
2	L	20	ASN
2	L	21	LEU
2	L	207	ARG
2	L	210	ASP
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	192	VAL
3	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	141	HIS
1	H	201	ASN
2	L	20	ASN
2	L	159	ASN
2	L	183	ASN
2	L	264	GLN
3	M	4	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	300	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 1 is monoatomic - leaving 28 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	$\#\|Z\| > 2$
6	LDA	L	1284	-	12,15,15	2.03	1 (8%)	14,17,17	0.45	0
9	PO4	L	1289	-	4,4,4	1.04	0	6,6,6	0.75	0
12	SPO	M	1310	-	40,41,41	3.83	12 (30%)	47,50,50	2.27	20 (42%)
6	LDA	M	1305	-	12,15,15	2.03	1 (8%)	14,17,17	0.48	0
10	HTO	L	1290	-	9,9,9	0.29	0	10,10,10	0.79	1 (10%)
4	GOL	L	1293	-	5,5,5	0.41	0	5,5,5	0.27	0
4	GOL	L	1294	-	5,5,5	0.36	0	5,5,5	0.18	0
5	BCL	M	1304	3	69,74,74	1.85	13 (18%)	83,115,115	1.86	21 (25%)
7	BPH	M	1308	-	59,70,70	2.57	12 (20%)	61,101,101	2.77	20 (32%)
15	GGD	M	1313	-	58,58,68	2.14	12 (20%)	72,72,82	1.79	18 (25%)
5	BCL	M	1303	3	69,74,74	1.78	11 (15%)	83,115,115	1.69	15 (18%)
8	U10	L	1287[A]	-	23,23,63	2.49	8 (34%)	28,31,79	1.89	7 (25%)
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.25	0
13	CDL	M	1311	-	79,79,99	1.89	16 (20%)	84,90,111	2.71	14 (16%)
8	U10	L	1287[B]	-	23,23,63	2.70	8 (34%)	28,31,79	1.27	3 (10%)
4	GOL	H	1252	-	5,5,5	0.43	0	5,5,5	0.39	0
4	GOL	H	1251	-	5,5,5	0.48	0	5,5,5	0.81	0
4	GOL	L	1292	-	5,5,5	0.46	0	5,5,5	0.86	0
10	HTO	L	1291	-	9,9,9	0.33	0	10,10,10	0.87	1 (10%)
6	LDA	L	1283	-	12,15,15	2.02	1 (8%)	14,17,17	0.45	0
8	U10	M	1309	-	48,48,63	2.54	11 (22%)	58,61,79	1.59	11 (18%)
6	LDA	M	1306	-	12,15,15	2.01	1 (8%)	14,17,17	0.54	0
5	BCL	L	1282	2	69,74,74	1.79	11 (15%)	83,115,115	1.89	22 (26%)
14	PC1	M	1312	-	42,42,53	1.74	8 (19%)	48,50,61	1.32	6 (12%)
5	BCL	L	1288	2	69,74,74	1.75	11 (15%)	83,115,115	1.86	21 (25%)
7	BPH	L	1286	-	59,70,70	2.46	12 (20%)	61,101,101	2.56	18 (29%)
4	GOL	H	1253	-	5,5,5	0.36	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	LDA	L	1285	-	12,15,15	2.07	1 (8%)	14,17,17	0.58	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
6	LDA	L	1284	-	-	7/13/13/13	-
12	SPO	M	1310	-	-	6/47/47/47	-
6	LDA	M	1305	-	-	5/13/13/13	-
10	HTO	L	1290	-	-	10/10/10/10	-
4	GOL	L	1293	-	-	2/4/4/4	-
4	GOL	L	1294	-	-	1/4/4/4	-
5	BCL	M	1304	3	2/2/21/25	10/41/137/137	-
7	BPH	M	1308	-	-	17/37/105/105	0/5/6/6
15	GGD	M	1313	-	-	19/47/87/97	0/2/2/2
5	BCL	M	1303	3	2/2/21/25	18/41/137/137	-
8	U10	L	1287[A]	-	-	7/15/39/87	0/1/1/1
4	GOL	H	1254	-	-	0/4/4/4	-
13	CDL	M	1311	-	-	50/88/88/110	-
8	U10	L	1287[B]	-	-	8/15/39/87	0/1/1/1
4	GOL	H	1252	-	-	2/4/4/4	-
4	GOL	H	1251	-	-	2/4/4/4	-
4	GOL	L	1292	-	-	2/4/4/4	-
10	HTO	L	1291	-	-	9/10/10/10	-
6	LDA	L	1283	-	-	7/13/13/13	-
8	U10	M	1309	-	-	6/45/69/87	0/1/1/1
6	LDA	M	1306	-	-	7/13/13/13	-
5	BCL	L	1282	2	2/2/21/25	9/41/137/137	-
14	PC1	M	1312	-	1/1/5/5	25/46/46/57	-
5	BCL	L	1288	2	2/2/21/25	10/41/137/137	-
7	BPH	L	1286	-	-	6/37/105/105	0/5/6/6
4	GOL	H	1253	-	-	2/4/4/4	-
6	LDA	L	1285	-	-	10/13/13/13	-

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1310	SPO	C27-C28	12.95	1.47	1.34
7	M	1308	BPH	OBD-CAD	11.84	1.38	1.22
7	L	1286	BPH	OBD-CAD	10.36	1.36	1.22
5	L	1282	BCL	OBD-CAD	9.22	1.38	1.22
5	M	1304	BCL	OBD-CAD	9.10	1.38	1.22
5	M	1303	BCL	OBD-CAD	8.84	1.37	1.22
5	L	1288	BCL	OBD-CAD	8.57	1.37	1.22
12	M	1310	SPO	C9-C7	8.22	1.46	1.35
12	M	1310	SPO	C19-C17	8.20	1.46	1.35
12	M	1310	SPO	C22-C23	7.95	1.46	1.35
12	M	1310	SPO	C14-C12	7.55	1.45	1.35
6	L	1285	LDA	O1-N1	-7.11	1.25	1.42
13	M	1311	CDL	C11-CA5	-6.98	1.30	1.50
6	L	1284	LDA	O1-N1	-6.96	1.25	1.42
6	L	1283	LDA	O1-N1	-6.92	1.26	1.42
6	M	1306	LDA	O1-N1	-6.91	1.26	1.42
6	M	1305	LDA	O1-N1	-6.83	1.26	1.42
7	L	1286	BPH	O1D-CGD	6.83	1.38	1.21
7	M	1308	BPH	O1D-CGD	6.54	1.37	1.21
8	M	1309	U10	C33-C34	6.53	1.48	1.33
7	L	1286	BPH	OBB-CAB	6.48	1.42	1.22
8	M	1309	U10	C28-C29	6.47	1.48	1.33
8	L	1287[B]	U10	C8-C9	6.36	1.48	1.33
7	M	1308	BPH	OBB-CAB	6.36	1.42	1.22
12	M	1310	SPO	C32-C33	6.24	1.47	1.33
8	M	1309	U10	C13-C14	6.11	1.47	1.33
8	L	1287[A]	U10	C8-C9	6.08	1.47	1.33
7	M	1308	BPH	C2-C3	6.04	1.47	1.33
5	M	1303	BCL	O1A-CGA	5.94	1.40	1.22
12	M	1310	SPO	C37-C38	5.91	1.49	1.32
7	L	1286	BPH	O1A-CGA	5.79	1.39	1.22
5	M	1304	BCL	O1A-CGA	5.78	1.39	1.22
7	L	1286	BPH	C2-C3	5.70	1.46	1.33
15	M	1313	GGD	C14-CC5	-5.68	1.34	1.50
7	M	1308	BPH	O1A-CGA	5.66	1.39	1.22
5	L	1288	BCL	O1A-CGA	5.56	1.39	1.22
8	M	1309	U10	C18-C19	5.47	1.46	1.33
15	M	1313	GGD	C31-CC7	-5.46	1.34	1.50
14	M	1312	PC1	C22-C21	-5.40	1.34	1.50
8	M	1309	U10	C23-C24	5.33	1.45	1.33
8	M	1309	U10	C8-C9	5.31	1.45	1.33
8	L	1287[A]	U10	C13-C14	5.31	1.47	1.32
8	L	1287[B]	U10	O3-C3	-5.25	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1287[B]	U10	C13-C14	5.24	1.47	1.32
8	L	1287[B]	U10	O4-C4	-5.23	1.24	1.36
15	M	1313	GGD	CC3-CC4	-5.11	1.35	1.50
15	M	1313	GGD	C15-C14	-5.06	1.33	1.52
12	M	1310	SPO	C6-C5	5.05	1.45	1.32
5	L	1282	BCL	O1A-CGA	5.03	1.37	1.22
8	L	1287[A]	U10	O4-C4	-5.02	1.24	1.36
8	M	1309	U10	C38-C39	5.02	1.46	1.32
7	M	1308	BPH	C3D-C2D	4.94	1.48	1.39
15	M	1313	GGD	CC6-CC4	-4.93	1.35	1.50
13	M	1311	CDL	OB6-CB5	4.81	1.47	1.34
7	L	1286	BPH	C3D-C2D	4.73	1.47	1.39
13	M	1311	CDL	OA8-CA7	4.69	1.47	1.33
15	M	1313	GGD	C36-C37	-4.63	1.33	1.52
14	M	1312	PC1	O31-C31	4.63	1.46	1.33
15	M	1313	GGD	C20-C21	-4.52	1.34	1.52
13	M	1311	CDL	C12-C11	-4.51	1.35	1.52
13	M	1311	CDL	OA6-CA5	4.44	1.46	1.34
14	M	1312	PC1	O21-C21	4.39	1.46	1.34
13	M	1311	CDL	OB8-CB7	4.38	1.46	1.33
15	M	1313	GGD	OC6-CC5	4.36	1.46	1.34
13	M	1311	CDL	C20-C19	-4.33	1.27	1.51
8	M	1309	U10	C6-C1	4.27	1.43	1.35
7	M	1308	BPH	C3D-CAD	-4.24	1.38	1.47
8	L	1287[A]	U10	O3-C3	-4.19	1.26	1.36
12	M	1310	SPO	C26-C25	4.16	1.45	1.34
15	M	1313	GGD	OC8-CC7	4.09	1.45	1.33
7	L	1286	BPH	C3D-CAD	-3.99	1.39	1.47
13	M	1311	CDL	C13-C12	-3.97	1.29	1.51
12	M	1310	SPO	C10-C11	3.84	1.44	1.34
5	M	1304	BCL	C3D-C4D	-3.82	1.35	1.44
12	M	1310	SPO	C15-C16	3.81	1.44	1.34
5	L	1288	BCL	C4D-ND	-3.81	1.32	1.37
5	L	1282	BCL	C3D-C4D	-3.68	1.35	1.44
13	M	1311	CDL	C17-C16	-3.64	1.31	1.51
8	M	1309	U10	O3-C3	-3.59	1.28	1.36
8	M	1309	U10	O4-C4	-3.58	1.28	1.36
5	M	1303	BCL	C3D-C4D	-3.55	1.36	1.44
5	M	1304	BCL	OBB-CAB	3.47	1.30	1.23
15	M	1313	GGD	C39-C38	3.45	1.51	1.31
5	L	1282	BCL	CBB-CAB	-3.33	1.43	1.50
12	M	1310	SPO	C21-C20	3.29	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1287[B]	U10	C6-C1	3.28	1.41	1.35
15	M	1313	GGD	C20-C19	-3.17	1.33	1.51
5	M	1303	BCL	C4D-ND	-3.17	1.33	1.37
5	L	1288	BCL	C3D-C4D	-3.17	1.37	1.44
5	M	1304	BCL	CBB-CAB	-3.17	1.43	1.50
13	M	1311	CDL	C32-C31	-3.16	1.40	1.52
7	L	1286	BPH	C3D-C4D	-3.16	1.36	1.41
5	L	1288	BCL	O2D-CGD	-3.14	1.25	1.33
15	M	1313	GGD	C22-C23	3.13	1.53	1.29
14	M	1312	PC1	C39-C38	-3.10	1.34	1.51
8	L	1287[B]	U10	C3-C2	-3.08	1.40	1.48
5	M	1303	BCL	O2D-CGD	-3.06	1.25	1.33
8	L	1287[B]	U10	C4-C5	-3.02	1.40	1.48
13	M	1311	CDL	C79-C78	-3.02	1.34	1.51
14	M	1312	PC1	C36-C35	3.01	1.68	1.51
5	M	1303	BCL	C2-C3	3.01	1.40	1.33
13	M	1311	CDL	C34-C33	-3.01	1.25	1.49
13	M	1311	CDL	C80-C79	-3.00	1.34	1.51
5	M	1303	BCL	CHD-C4C	3.00	1.47	1.39
13	M	1311	CDL	C22-C21	-2.97	1.34	1.51
5	L	1282	BCL	O2D-CGD	-2.94	1.26	1.33
5	M	1304	BCL	C2-C3	2.92	1.40	1.33
7	M	1308	BPH	O2D-CGD	-2.91	1.26	1.33
5	L	1288	BCL	C2-C3	2.87	1.39	1.33
7	L	1286	BPH	O2D-CGD	-2.84	1.26	1.33
8	M	1309	U10	C4-C5	-2.82	1.40	1.48
13	M	1311	CDL	C19-C18	-2.79	1.35	1.51
5	L	1282	BCL	C1D-C2D	-2.77	1.39	1.45
5	L	1282	BCL	OBB-CAB	2.75	1.29	1.23
8	L	1287[A]	U10	C4-C5	-2.74	1.41	1.48
8	L	1287[A]	U10	C3-C2	-2.71	1.41	1.48
14	M	1312	PC1	C37-C36	2.70	1.66	1.51
5	L	1282	BCL	C4D-ND	-2.69	1.34	1.37
5	L	1282	BCL	C2-C3	2.66	1.39	1.33
7	M	1308	BPH	O2A-CGA	-2.66	1.25	1.33
7	M	1308	BPH	C3D-C4D	-2.66	1.37	1.41
5	M	1304	BCL	C1D-C2D	-2.62	1.40	1.45
13	M	1311	CDL	C16-C15	-2.58	1.37	1.51
14	M	1312	PC1	C12-N	-2.57	1.42	1.51
7	M	1308	BPH	CBD-CGD	-2.53	1.49	1.52
14	M	1312	PC1	C3A-C39	-2.49	1.34	1.51
5	M	1303	BCL	CBB-CAB	-2.48	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1288	BCL	C1D-ND	2.47	1.40	1.37
8	L	1287[A]	U10	C6-C1	2.43	1.39	1.35
5	M	1304	BCL	CHD-C4C	2.42	1.46	1.39
5	M	1304	BCL	C1D-ND	2.41	1.40	1.37
5	L	1288	BCL	C1D-C2D	-2.38	1.40	1.45
5	M	1304	BCL	O2A-CGA	-2.34	1.26	1.33
5	L	1288	BCL	CHD-C4C	2.30	1.45	1.39
7	L	1286	BPH	O2A-CGA	-2.30	1.26	1.33
5	M	1304	BCL	C4D-ND	-2.29	1.34	1.37
5	L	1288	BCL	O2A-CGA	-2.26	1.26	1.33
5	L	1282	BCL	O2A-CGA	-2.25	1.26	1.33
7	M	1308	BPH	C4D-ND	-2.24	1.35	1.38
7	L	1286	BPH	CBD-CGD	-2.22	1.49	1.52
5	L	1288	BCL	C1B-NB	2.21	1.40	1.37
8	L	1287[A]	U10	C6-C5	-2.21	1.40	1.46
5	L	1282	BCL	CHD-C4C	2.20	1.45	1.39
7	L	1286	BPH	C4D-ND	-2.10	1.35	1.38
8	L	1287[B]	U10	C6-C5	-2.09	1.40	1.46
5	M	1303	BCL	O2A-CGA	-2.06	1.27	1.33
5	M	1303	BCL	OBB-CAB	2.05	1.27	1.23
5	M	1304	BCL	MG-NA	2.03	2.11	2.06
5	M	1303	BCL	C1D-C2D	-2.02	1.41	1.45
5	M	1304	BCL	CHC-C4B	2.00	1.43	1.39

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	1311	CDL	C13-C12-C11	12.96	159.78	113.19
13	M	1311	CDL	C17-C16-C15	11.70	173.84	114.42
7	M	1308	BPH	O2D-CGD-CBD	10.24	123.98	111.00
13	M	1311	CDL	C20-C19-C18	9.40	162.17	114.42
7	M	1308	BPH	C2B-C1B-NB	8.49	115.39	109.53
7	L	1286	BPH	C2B-C1B-NB	8.39	115.32	109.53
7	L	1286	BPH	O2D-CGD-CBD	8.13	121.29	111.00
13	M	1311	CDL	C12-C11-CA5	7.55	141.08	113.62
7	M	1308	BPH	C2D-C1D-ND	6.93	114.31	109.53
7	L	1286	BPH	C2D-C1D-ND	6.68	114.14	109.53
12	M	1310	SPO	C20-C19-C17	-6.36	118.23	127.31
5	L	1282	BCL	O2D-CGD-CBD	6.05	122.01	111.27
7	M	1308	BPH	O1D-CGD-CBD	-5.94	114.84	124.74
12	M	1310	SPO	C21-C22-C23	-5.54	119.40	127.31
7	L	1286	BPH	C4D-ND-C1D	-5.50	103.23	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1308	BPH	C4D-ND-C1D	-5.43	103.31	108.83
5	M	1303	BCL	O2D-CGD-CBD	5.10	120.33	111.27
5	M	1303	BCL	CMB-C2B-C1B	-4.89	117.92	125.37
13	M	1311	CDL	C34-C33-C32	4.85	150.27	113.42
13	M	1311	CDL	OA6-CA5-C11	4.84	121.94	111.50
7	M	1308	BPH	C3D-C4D-ND	4.83	114.31	107.72
5	M	1303	BCL	C2B-C1B-NB	-4.76	107.04	110.23
5	M	1303	BCL	C2D-C1D-ND	-4.76	106.60	110.10
5	M	1304	BCL	O2D-CGD-CBD	4.75	119.71	111.27
5	L	1288	BCL	C2B-C1B-NB	-4.67	107.10	110.23
5	L	1288	BCL	CMB-C2B-C1B	-4.67	118.26	125.37
7	L	1286	BPH	CMA-C3A-C4A	-4.65	104.20	114.38
15	M	1313	GGD	OC6-CC5-C14	4.64	121.50	111.50
12	M	1310	SPO	C10-C9-C7	-4.58	120.77	127.31
5	M	1304	BCL	C1C-NC-C4C	4.58	108.76	106.71
7	L	1286	BPH	C3D-C4D-ND	4.55	113.93	107.72
5	L	1282	BCL	C2B-C1B-NB	-4.55	107.18	110.23
7	M	1308	BPH	C1B-NB-C4B	-4.54	101.80	108.83
5	L	1288	BCL	CMD-C2D-C1D	4.51	132.67	124.71
15	M	1313	GGD	OC8-CC6-CC4	4.45	121.40	108.43
5	L	1282	BCL	CMB-C2B-C1B	-4.42	118.64	125.37
14	M	1312	PC1	O21-C21-C22	4.39	120.97	111.50
7	L	1286	BPH	C1B-NB-C4B	-4.37	102.06	108.83
15	M	1313	GGD	OA1-CC3-CC4	4.35	121.39	110.90
13	M	1311	CDL	C33-C32-C31	4.31	133.09	113.44
5	M	1304	BCL	CMB-C2B-C1B	-4.30	118.81	125.37
5	L	1288	BCL	C1C-NC-C4C	-4.23	104.80	106.71
8	L	1287[A]	U10	C1M-C1-C6	-4.22	117.52	124.40
5	L	1288	BCL	CMA-C3A-C4A	-4.20	100.49	111.77
8	M	1309	U10	C25-C24-C26	4.19	122.32	115.27
5	L	1282	BCL	CMD-C2D-C1D	4.14	132.00	124.71
5	M	1304	BCL	C16-C15-C13	-4.13	102.58	115.92
13	M	1311	CDL	OB6-CB5-C51	3.96	120.03	111.50
5	M	1304	BCL	C2D-C1D-ND	-3.91	107.22	110.10
7	L	1286	BPH	O1D-CGD-CBD	-3.90	118.25	124.74
5	L	1282	BCL	C4A-NA-C1A	3.90	108.46	106.71
7	M	1308	BPH	CAC-C3C-C2C	-3.84	104.66	114.26
5	M	1303	BCL	C1D-ND-C4D	3.78	109.02	106.33
5	L	1282	BCL	C4-C3-C5	3.76	121.60	115.27
7	M	1308	BPH	C4D-CHA-CBD	-3.74	106.83	108.52
8	M	1309	U10	C10-C9-C11	3.73	121.54	115.27
5	L	1282	BCL	O1D-CGD-CBD	-3.65	117.02	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	M	1313	GGD	CC3-OA1-CA1	3.63	120.83	113.74
5	M	1304	BCL	CBB-CAB-C3B	-3.62	112.70	120.43
5	L	1288	BCL	C2D-C1D-ND	-3.58	107.47	110.10
12	M	1310	SPO	C15-C14-C12	-3.54	122.26	127.31
5	M	1304	BCL	CAB-C3B-C2B	-3.52	123.06	128.34
15	M	1313	GGD	OB1-CA3-CA2	3.51	116.62	107.28
5	M	1304	BCL	OBB-CAB-C3B	3.50	126.88	120.41
13	M	1311	CDL	CA4-OA6-CA5	-3.50	109.18	117.79
5	M	1303	BCL	O1D-CGD-CBD	-3.48	117.37	124.48
5	L	1282	BCL	O2A-CGA-CBA	3.47	122.81	111.91
5	L	1288	BCL	O2D-CGD-CBD	3.46	117.42	111.27
5	L	1288	BCL	O2A-CGA-CBA	3.42	122.66	111.91
5	M	1303	BCL	C1-O2A-CGA	3.42	125.41	116.44
5	L	1282	BCL	CMA-C3A-C4A	-3.41	102.60	111.77
15	M	1313	GGD	OC6-CC4-CC6	3.41	120.74	108.40
8	L	1287[A]	U10	C3M-O3-C3	3.40	128.51	116.47
8	L	1287[A]	U10	C7-C8-C9	-3.40	121.14	126.79
8	M	1309	U10	C15-C14-C16	3.39	120.98	115.27
5	M	1304	BCL	O2A-CGA-CBA	3.38	122.52	111.91
7	L	1286	BPH	C1-C2-C3	-3.38	120.20	126.04
5	M	1304	BCL	CED-O2D-CGD	3.38	123.58	115.94
14	M	1312	PC1	O31-C31-C32	3.31	122.29	111.91
7	M	1308	BPH	CED-O2D-CGD	3.28	123.35	115.94
12	M	1310	SPO	C5-C6-C7	-3.24	121.00	125.89
15	M	1313	GGD	OC6-CC4-CC3	3.20	120.00	108.40
15	M	1313	GGD	CC6-CC4-CC3	3.16	119.26	111.79
12	M	1310	SPO	C14-C15-C16	-3.12	113.48	123.22
8	L	1287[A]	U10	O5-C5-C6	-3.08	116.15	121.55
5	L	1288	BCL	C1D-ND-C4D	3.07	108.52	106.33
5	L	1288	BCL	C3C-C4C-CHD	-3.06	116.86	123.39
7	M	1308	BPH	CMA-C3A-C4A	-3.03	107.74	114.38
12	M	1310	SPO	C34-C33-C35	2.98	120.28	115.27
12	M	1310	SPO	C27-C26-C25	-2.96	113.98	123.22
7	M	1308	BPH	CBA-CAA-C2A	-2.95	105.20	113.81
7	L	1286	BPH	CED-O2D-CGD	2.92	122.55	115.94
7	L	1286	BPH	CMB-C2B-C3B	2.92	130.14	124.68
13	M	1311	CDL	OA8-CA7-C31	2.92	121.07	111.91
5	L	1288	BCL	C4-C3-C5	2.91	120.16	115.27
8	L	1287[A]	U10	C10-C9-C11	2.88	120.11	115.27
5	M	1304	BCL	CMD-C2D-C1D	2.86	129.76	124.71
7	L	1286	BPH	C4C-C3C-C2C	-2.82	100.15	102.84
8	M	1309	U10	C17-C18-C19	-2.80	120.93	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	1309	U10	C27-C28-C29	-2.79	120.95	127.66
13	M	1311	CDL	OA6-CA5-OA7	-2.77	117.01	123.70
5	M	1303	BCL	O2A-CGA-CBA	2.76	120.57	111.91
12	M	1310	SPO	C24-C23-C25	2.76	122.42	118.08
5	M	1303	BCL	CAB-C3B-C2B	-2.75	124.22	128.34
8	L	1287[B]	U10	C10-C9-C11	2.74	119.89	115.27
7	L	1286	BPH	O2A-CGA-CBA	2.74	120.50	111.91
7	M	1308	BPH	C4A-C3A-C2A	-2.73	100.24	102.84
12	M	1310	SPO	C10-C11-C12	-2.69	118.85	126.42
7	L	1286	BPH	CBA-CAA-C2A	-2.66	106.03	113.81
13	M	1311	CDL	OB8-CB7-C71	2.64	120.18	111.91
5	L	1288	BCL	CAA-C2A-C3A	-2.63	105.58	112.78
14	M	1312	PC1	O31-C31-O32	-2.63	116.96	123.59
7	M	1308	BPH	CMB-C2B-C3B	2.59	129.53	124.68
7	L	1286	BPH	C3B-C4B-NB	2.59	111.92	108.04
5	L	1288	BCL	CMD-C2D-C3D	-2.58	121.67	127.61
5	L	1288	BCL	CMB-C2B-C3B	2.57	132.88	125.93
7	M	1308	BPH	C3B-C4B-NB	2.57	111.89	108.04
8	M	1309	U10	C41-C39-C40	2.57	120.27	114.60
5	M	1303	BCL	CMB-C2B-C3B	2.57	132.86	125.93
15	M	1313	GGD	OC8-CC7-C31	2.55	119.92	111.91
7	M	1308	BPH	C1-O2A-CGA	2.54	123.12	116.44
5	L	1282	BCL	C2D-C1D-ND	-2.54	108.23	110.10
5	L	1288	BCL	C9-C8-C7	2.52	120.40	111.29
8	M	1309	U10	C30-C29-C31	2.51	119.50	115.27
15	M	1313	GGD	CA1-OA5-CA5	2.51	118.61	113.69
5	M	1304	BCL	C7-C6-C5	-2.50	106.58	113.36
8	M	1309	U10	C22-C23-C24	-2.50	121.65	127.66
14	M	1312	PC1	C11-C12-N	2.48	124.07	115.78
5	M	1304	BCL	C1D-ND-C4D	2.48	108.10	106.33
5	L	1282	BCL	OBB-CAB-C3B	2.48	125.00	120.41
15	M	1313	GGD	CB4-CB3-CB2	-2.47	106.50	110.82
8	M	1309	U10	C1M-C1-C6	-2.47	120.37	124.40
5	M	1303	BCL	CHC-C4B-NB	-2.47	121.64	124.26
5	L	1288	BCL	C14-C13-C15	2.47	120.24	111.29
5	L	1288	BCL	CAA-C2A-C1A	-2.46	103.92	111.97
5	L	1282	BCL	CMD-C2D-C3D	-2.45	121.97	127.61
7	L	1286	BPH	C1C-C2C-C3C	-2.45	100.50	102.84
5	L	1282	BCL	CAA-C2A-C3A	-2.44	106.10	112.78
5	L	1282	BCL	CED-O2D-CGD	2.43	121.44	115.94
5	L	1288	BCL	C1-O2A-CGA	2.43	122.83	116.44
12	M	1310	SPO	C20-C21-C22	-2.43	118.51	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1303	BCL	CMD-C2D-C1D	2.41	128.97	124.71
5	M	1304	BCL	C4A-NA-C1A	2.41	107.79	106.71
5	L	1282	BCL	C5-C3-C2	-2.40	116.26	121.12
8	L	1287[A]	U10	C7-C6-C5	2.40	121.36	118.48
7	M	1308	BPH	C4C-C3C-C2C	-2.38	100.58	102.84
15	M	1313	GGD	C21-C22-C23	-2.38	112.17	131.07
5	L	1282	BCL	C1-C2-C3	-2.37	121.95	126.04
12	M	1310	SPO	C8-C7-C6	2.37	121.81	118.08
15	M	1313	GGD	CB3-CB4-CB5	-2.37	106.02	110.24
12	M	1310	SPO	C29-C28-C30	2.36	119.25	115.27
7	L	1286	BPH	O2A-CGA-O1A	-2.36	117.64	123.59
8	L	1287[A]	U10	C16-C14-C15	2.35	119.79	114.60
5	M	1303	BCL	CHC-C4B-C3B	-2.34	124.02	132.35
5	M	1304	BCL	CHC-C4B-NB	-2.33	121.79	124.26
5	M	1304	BCL	CHD-C4C-NC	2.33	127.66	125.08
12	M	1310	SPO	C2-C1-C4	-2.33	107.28	110.86
12	M	1310	SPO	C9-C10-C11	-2.32	115.97	123.22
5	M	1304	BCL	C1D-CHD-C4C	-2.31	121.04	126.62
13	M	1311	CDL	OA8-CA7-OA9	-2.29	117.80	123.59
5	L	1282	BCL	CHC-C4B-C3B	-2.29	124.20	132.35
5	L	1288	BCL	O2A-CGA-O1A	-2.28	117.84	123.59
13	M	1311	CDL	OB8-CB7-OB9	-2.28	117.85	123.59
15	M	1313	GGD	OC6-CC5-OC7	-2.26	118.25	123.70
15	M	1313	GGD	CB1-OB5-CB5	2.25	118.10	113.69
12	M	1310	SPO	C21-C20-C19	-2.25	118.88	123.47
5	M	1303	BCL	C2A-C3A-C4A	2.24	105.49	101.87
8	M	1309	U10	C35-C34-C36	2.24	119.03	115.27
14	M	1312	PC1	C26-C25-C24	-2.23	103.12	114.42
5	M	1304	BCL	O1D-CGD-CBD	-2.22	119.94	124.48
5	M	1304	BCL	CMB-C2B-C3B	2.21	131.90	125.93
5	L	1282	BCL	CHA-C1A-NA	-2.21	121.34	126.40
10	L	1291	HTO	C5-C4-C3	-2.21	110.55	114.18
5	L	1282	BCL	C4B-C3B-C2B	-2.19	104.83	108.36
5	M	1304	BCL	C2B-C1B-NB	-2.19	108.77	110.23
8	M	1309	U10	C12-C13-C14	-2.17	122.43	127.66
12	M	1310	SPO	C6-C7-C9	-2.17	115.62	118.94
7	M	1308	BPH	CMC-C2C-C1C	-2.15	109.68	114.38
7	M	1308	BPH	OBD-CAD-CBD	-2.13	122.69	125.82
5	L	1282	BCL	C1-O2A-CGA	2.13	122.03	116.44
12	M	1310	SPO	C1-C4-C5	-2.10	107.48	113.06
8	L	1287[B]	U10	C16-C14-C15	2.10	119.23	114.60
5	L	1288	BCL	C14-C13-C12	2.10	118.88	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1304	BCL	C9-C8-C10	2.10	118.88	111.29
5	L	1288	BCL	C11-C12-C13	2.09	122.68	115.92
14	M	1312	PC1	C23-C22-C21	2.08	121.18	113.62
5	L	1282	BCL	CAA-C2A-C1A	-2.07	105.18	111.97
15	M	1313	GGD	C16-C15-C14	2.07	120.63	113.19
5	M	1303	BCL	CHA-C1A-NA	-2.07	121.67	126.40
7	M	1308	BPH	C4-C3-C5	2.06	118.73	115.27
12	M	1310	SPO	C40-C38-C39	2.06	119.14	114.60
12	M	1310	SPO	C25-C23-C22	-2.05	115.79	118.94
15	M	1313	GGD	CA3-CA4-CA5	2.05	114.02	109.66
8	L	1287[B]	U10	C1M-C1-C6	-2.03	121.09	124.40
5	L	1282	BCL	CMB-C2B-C3B	2.02	131.39	125.93
15	M	1313	GGD	OC8-CC7-OC9	-2.02	118.49	123.59
7	L	1286	BPH	C7-C6-C5	-2.02	107.88	113.36
10	L	1290	HTO	C5-C4-C3	-2.01	110.87	114.18

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C13
5	L	1282	BCL	C8
5	L	1288	BCL	C13
5	L	1288	BCL	C8
5	M	1303	BCL	C13
5	M	1303	BCL	C8
5	M	1304	BCL	C13
5	M	1304	BCL	C8
14	M	1312	PC1	C2

All (257) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	C1-C2-C3-O3
4	L	1292	GOL	C1-C2-C3-O3
4	L	1293	GOL	O1-C1-C2-C3
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
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	N1-C1-C2-C3
8	L	1287[A]	U10	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	L	1287[A]	U10	C5-C6-C7-C8
8	L	1287[A]	U10	C7-C8-C9-C10
8	L	1287[A]	U10	C7-C8-C9-C11
8	L	1287[B]	U10	C12-C11-C9-C8
8	L	1287[B]	U10	C12-C11-C9-C10
8	L	1287[B]	U10	C12-C13-C14-C15
8	M	1309	U10	C27-C28-C29-C30
8	M	1309	U10	C31-C32-C33-C34
10	L	1290	HTO	O1-C1-C2-O2
10	L	1290	HTO	O1-C1-C2-C3
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
10	L	1291	HTO	C1-C2-C3-O3
10	L	1291	HTO	C1-C2-C3-C4
10	L	1291	HTO	O2-C2-C3-O3
10	L	1291	HTO	O2-C2-C3-C4
13	M	1311	CDL	CA3-OA5-PA1-OA2
13	M	1311	CDL	CA3-OA5-PA1-OA3
13	M	1311	CDL	CA3-OA5-PA1-OA4
14	M	1312	PC1	C1-O11-P-O12
14	M	1312	PC1	O13-C11-C12-N
14	M	1312	PC1	C2-C1-O11-P
15	M	1313	GGD	C14-CC5-OC6-CC4
15	M	1313	GGD	CA2-CA3-OB1-CB1
14	M	1312	PC1	O32-C31-O31-C3
14	M	1312	PC1	C32-C31-O31-C3
15	M	1313	GGD	OC7-CC5-OC6-CC4
13	M	1311	CDL	C31-CA7-OA8-CA6
13	M	1311	CDL	C20-C21-C22-C23
13	M	1311	CDL	C78-C79-C80-C81
8	L	1287[B]	U10	C7-C8-C9-C10
8	L	1287[B]	U10	C7-C8-C9-C11
8	M	1309	U10	C27-C28-C29-C31
13	M	1311	CDL	OA9-CA7-OA8-CA6
13	M	1311	CDL	OB9-CB7-OB8-CB6
8	L	1287[B]	U10	C12-C13-C14-C16
15	M	1313	GGD	OB5-CB5-CB6-OB6
5	M	1303	BCL	C3-C5-C6-C7
13	M	1311	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
8	M	1309	U10	C24-C26-C27-C28
8	M	1309	U10	C29-C31-C32-C33
13	M	1311	CDL	C11-CA5-OA6-CA4
10	L	1291	HTO	O1-C1-C2-C3
8	L	1287[A]	U10	C12-C13-C14-C16
5	L	1282	BCL	C6-C7-C8-C9
5	L	1282	BCL	C11-C10-C8-C9
5	L	1282	BCL	C14-C13-C15-C16
5	L	1288	BCL	C6-C7-C8-C9
5	L	1288	BCL	C11-C12-C13-C14
5	M	1304	BCL	C11-C10-C8-C9
7	M	1308	BPH	C5-C6-C7-C8
7	M	1308	BPH	C13-C15-C16-C17
5	L	1282	BCL	C13-C15-C16-C17
13	M	1311	CDL	CB5-C51-C52-C53
5	L	1288	BCL	C13-C15-C16-C17
5	L	1288	BCL	C11-C10-C8-C7
5	M	1304	BCL	C6-C7-C8-C10
13	M	1311	CDL	CB3-OB5-PB2-OB2
14	M	1312	PC1	C1-O11-P-O13
10	L	1291	HTO	O1-C1-C2-O2
13	M	1311	CDL	OA7-CA5-OA6-CA4
7	M	1308	BPH	C8-C10-C11-C12
12	M	1310	SPO	C8-C7-C9-C10
6	L	1285	LDA	C11-C10-C9-C8
6	M	1305	LDA	C2-C3-C4-C5
8	L	1287[A]	U10	C12-C13-C14-C15
6	L	1283	LDA	C2-C3-C4-C5
6	L	1284	LDA	C6-C7-C8-C9
6	L	1285	LDA	C5-C6-C7-C8
14	M	1312	PC1	C29-C2A-C2B-C2C
13	M	1311	CDL	O1-C1-CB2-OB2
14	M	1312	PC1	C27-C28-C29-C2A
12	M	1310	SPO	C6-C7-C9-C10
14	M	1312	PC1	C37-C38-C39-C3A
7	M	1308	BPH	C4-C3-C5-C6
6	L	1283	LDA	C3-C4-C5-C6
6	L	1284	LDA	C7-C8-C9-C10
15	M	1313	GGD	C32-C33-C34-C35
4	H	1251	GOL	O1-C1-C2-C3
15	M	1313	GGD	CB4-CB5-CB6-OB6
13	M	1311	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
7	M	1308	BPH	C16-C17-C18-C20
5	M	1303	BCL	C15-C16-C17-C18
13	M	1311	CDL	C11-C12-C13-C14
14	M	1312	PC1	C22-C23-C24-C25
6	L	1283	LDA	C5-C6-C7-C8
14	M	1312	PC1	C28-C29-C2A-C2B
13	M	1311	CDL	C71-C72-C73-C74
7	L	1286	BPH	C4-C3-C5-C6
7	L	1286	BPH	C2-C3-C5-C6
7	M	1308	BPH	C2-C3-C5-C6
4	L	1292	GOL	O2-C2-C3-O3
4	L	1293	GOL	O1-C1-C2-O2
7	M	1308	BPH	C16-C17-C18-C19
13	M	1311	CDL	C80-C81-C82-C83
6	L	1284	LDA	C5-C6-C7-C8
5	M	1303	BCL	C2-C1-O2A-CGA
13	M	1311	CDL	C74-C75-C76-C77
6	L	1284	LDA	C1-C2-C3-C4
6	L	1285	LDA	C2-C3-C4-C5
6	M	1306	LDA	C1-C2-C3-C4
5	M	1303	BCL	C4-C3-C5-C6
5	M	1303	BCL	C2-C3-C5-C6
15	M	1313	GGD	C19-C20-C21-C22
15	M	1313	GGD	C39-C40-C41-C42
8	L	1287[A]	U10	C4-C3-O3-C3M
13	M	1311	CDL	OB7-CB5-OB6-CB4
6	L	1284	LDA	C11-C10-C9-C8
8	L	1287[B]	U10	C9-C11-C12-C13
13	M	1311	CDL	C51-CB5-OB6-CB4
14	M	1312	PC1	C22-C21-O21-C2
6	L	1284	LDA	C4-C5-C6-C7
14	M	1312	PC1	C33-C34-C35-C36
15	M	1313	GGD	OA5-CA5-CA6-OA6
15	M	1313	GGD	CB2-CB1-OB1-CA3
14	M	1312	PC1	O22-C21-O21-C2
12	M	1310	SPO	C4-C5-C6-C7
6	L	1285	LDA	C4-C5-C6-C7
15	M	1313	GGD	OB5-CB1-OB1-CA3
13	M	1311	CDL	CA3-CA4-CA6-OA8
15	M	1313	GGD	CC3-CC4-CC6-OC8
6	L	1283	LDA	C9-C10-C11-C12
4	H	1251	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	M	1306	LDA	C9-C10-C11-C12
6	L	1284	LDA	C9-C10-C11-C12
13	M	1311	CDL	C54-C55-C56-C57
5	L	1288	BCL	C15-C16-C17-C18
13	M	1311	CDL	C81-C82-C83-C84
13	M	1311	CDL	C41-C42-C43-C44
13	M	1311	CDL	CA5-C11-C12-C13
6	M	1306	LDA	C3-C4-C5-C6
12	M	1310	SPO	C3-C1-O1-CM1
5	L	1282	BCL	C12-C13-C15-C16
5	M	1303	BCL	C6-C7-C8-C9
7	M	1308	BPH	C11-C12-C13-C14
6	L	1285	LDA	N1-C1-C2-C3
6	L	1285	LDA	C9-C10-C11-C12
6	M	1306	LDA	C6-C7-C8-C9
13	M	1311	CDL	OA5-CA3-CA4-CA6
10	L	1290	HTO	C4-C5-C6-C7
13	M	1311	CDL	C17-C18-C19-C20
14	M	1312	PC1	C1-C2-C3-O31
7	L	1286	BPH	O2A-C1-C2-C3
14	M	1312	PC1	C2A-C2B-C2C-C2D
4	H	1252	GOL	O2-C2-C3-O3
4	H	1253	GOL	O1-C1-C2-O2
7	M	1308	BPH	C10-C11-C12-C13
13	M	1311	CDL	OA5-CA3-CA4-OA6
14	M	1312	PC1	C36-C37-C38-C39
7	L	1286	BPH	C8-C10-C11-C12
14	M	1312	PC1	O21-C2-C3-O31
15	M	1313	GGD	OC6-CC4-CC6-OC8
13	M	1311	CDL	CA2-C1-CB2-OB2
5	M	1304	BCL	C11-C12-C13-C14
5	L	1288	BCL	C11-C12-C13-C15
5	M	1303	BCL	C6-C7-C8-C10
5	M	1303	BCL	C11-C12-C13-C15
5	M	1304	BCL	C12-C13-C15-C16
7	M	1308	BPH	C6-C7-C8-C10
7	M	1308	BPH	C11-C10-C8-C7
7	M	1308	BPH	C11-C12-C13-C15
13	M	1311	CDL	C51-C52-C53-C54
13	M	1311	CDL	C40-C41-C42-C43
13	M	1311	CDL	C15-C16-C17-C18
5	L	1282	BCL	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	CAD-CBD-CGD-O2D
7	L	1286	BPH	CAD-CBD-CGD-O2D
15	M	1313	GGD	OA1-CC3-CC4-CC6
13	M	1311	CDL	OB5-CB3-CB4-OB6
6	L	1283	LDA	C2-C1-N1-CM2
6	L	1285	LDA	C2-C1-N1-CM1
13	M	1311	CDL	C31-C32-C33-C34
5	L	1282	BCL	C11-C12-C13-C14
7	M	1308	BPH	C11-C10-C8-C9
10	L	1290	HTO	C2-C3-C4-C5
6	L	1285	LDA	C6-C7-C8-C9
15	M	1313	GGD	C41-C42-C43-C44
4	L	1294	GOL	C1-C2-C3-O3
14	M	1312	PC1	C11-O13-P-O11
13	M	1311	CDL	CB3-OB5-PB2-OB3
14	M	1312	PC1	C1-O11-P-O14
13	M	1311	CDL	OB5-CB3-CB4-CB6
7	M	1308	BPH	C3-C5-C6-C7
6	M	1305	LDA	C11-C10-C9-C8
14	M	1312	PC1	C12-C11-O13-P
5	M	1303	BCL	C13-C15-C16-C17
13	M	1311	CDL	OA6-CA4-CA6-OA8
13	M	1311	CDL	C55-C56-C57-C58
5	M	1303	BCL	C11-C12-C13-C14
5	M	1304	BCL	C14-C13-C15-C16
7	M	1308	BPH	C6-C7-C8-C9
13	M	1311	CDL	C38-C39-C40-C41
12	M	1310	SPO	C4-C1-O1-CM1
6	M	1306	LDA	C2-C3-C4-C5
8	L	1287[B]	U10	C5-C4-O4-C4M
14	M	1312	PC1	C2B-C2C-C2D-C2E
5	M	1304	BCL	C15-C16-C17-C18
14	M	1312	PC1	C38-C39-C3A-C3B
12	M	1310	SPO	C2-C1-O1-CM1
13	M	1311	CDL	C13-C14-C15-C16
5	M	1303	BCL	C10-C11-C12-C13
8	M	1309	U10	C5-C4-O4-C4M
6	M	1306	LDA	C7-C8-C9-C10
5	L	1282	BCL	C6-C7-C8-C10
13	M	1311	CDL	CB7-C71-C72-C73
10	L	1290	HTO	C3-C4-C5-C6
5	L	1288	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	C8-C10-C11-C12
13	M	1311	CDL	C21-C22-C23-C24
5	L	1282	BCL	C5-C6-C7-C8
10	L	1291	HTO	C2-C3-C4-C5
6	L	1283	LDA	C7-C8-C9-C10
5	M	1304	BCL	CAA-CBA-CGA-O2A
4	H	1253	GOL	O1-C1-C2-C3
15	M	1313	GGD	CC5-C14-C15-C16
10	L	1291	HTO	C3-C4-C5-C6
5	L	1288	BCL	C16-C17-C18-C19
13	M	1311	CDL	C75-C76-C77-C78
13	M	1311	CDL	C16-C17-C18-C19
5	L	1288	BCL	CAD-CBD-CGD-O2D
5	M	1304	BCL	CAD-CBD-CGD-O2D
7	M	1308	BPH	CAD-CBD-CGD-O2D
5	L	1288	BCL	C2-C1-O2A-CGA
6	L	1285	LDA	C7-C8-C9-C10
7	M	1308	BPH	O2A-C1-C2-C3
5	M	1304	BCL	CHA-CBD-CGD-O2D
15	M	1313	GGD	OA1-CC3-CC4-OC6
7	L	1286	BPH	CHA-CBD-CGD-O2D
13	M	1311	CDL	C72-C71-CB7-OB8
10	L	1291	HTO	C4-C5-C6-C7
5	M	1304	BCL	C6-C7-C8-C9
5	M	1303	BCL	C16-C17-C18-C19
5	M	1303	BCL	C16-C17-C18-C20
14	M	1312	PC1	C23-C24-C25-C26
15	M	1313	GGD	C34-C35-C36-C37
14	M	1312	PC1	C11-O13-P-O14
13	M	1311	CDL	C72-C71-CB7-OB9
13	M	1311	CDL	C18-C19-C20-C21
6	L	1283	LDA	C2-C1-N1-O1
6	L	1285	LDA	C2-C1-N1-O1
15	M	1313	GGD	C32-C31-CC7-OC8
13	M	1311	CDL	C12-C11-CA5-OA6
5	M	1303	BCL	C5-C6-C7-C8
13	M	1311	CDL	C12-C11-CA5-OA7

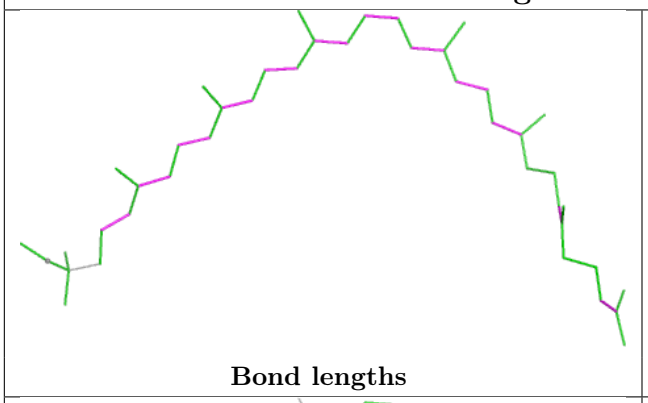
There are no ring outliers.

16 monomers are involved in 62 short contacts:

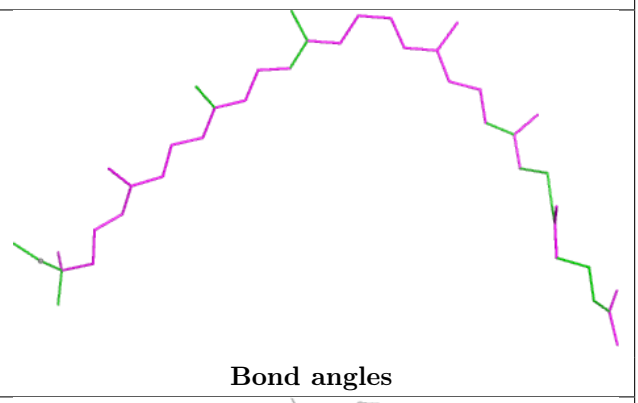
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1310	SPO	4	0
6	M	1305	LDA	1	0
4	L	1294	GOL	1	0
5	M	1304	BCL	11	0
7	M	1308	BPH	12	0
15	M	1313	GGD	2	0
5	M	1303	BCL	7	0
8	L	1287[A]	U10	5	0
13	M	1311	CDL	8	0
4	H	1252	GOL	1	0
4	H	1251	GOL	7	0
4	L	1292	GOL	1	0
8	M	1309	U10	1	0
6	M	1306	LDA	1	0
5	L	1282	BCL	4	0
7	L	1286	BPH	4	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.

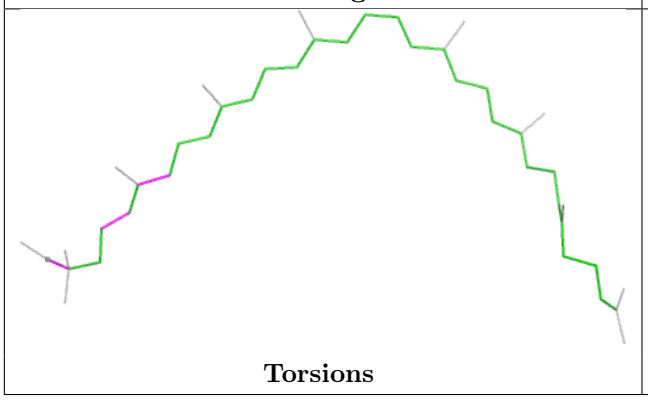
Ligand SPO M 1310



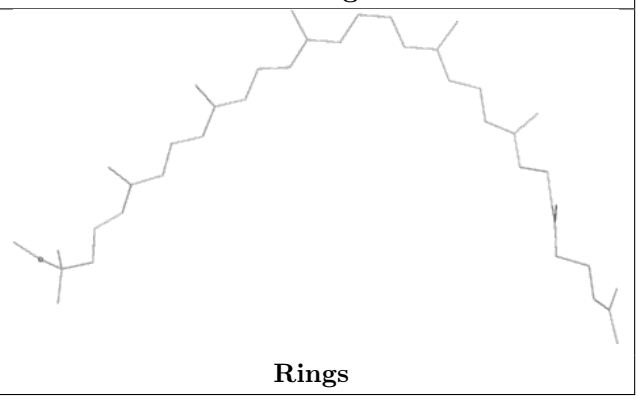
Bond lengths



Bond angles

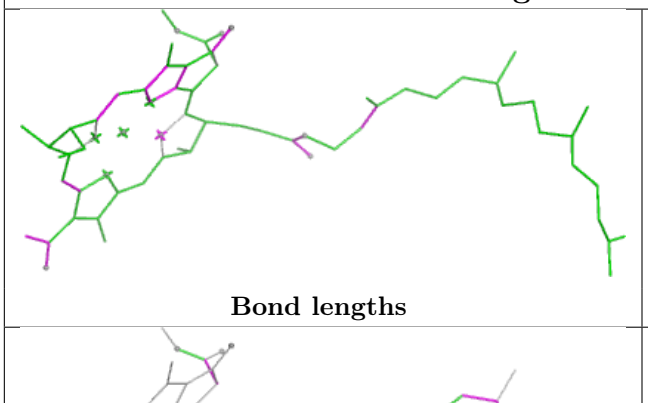


Torsions

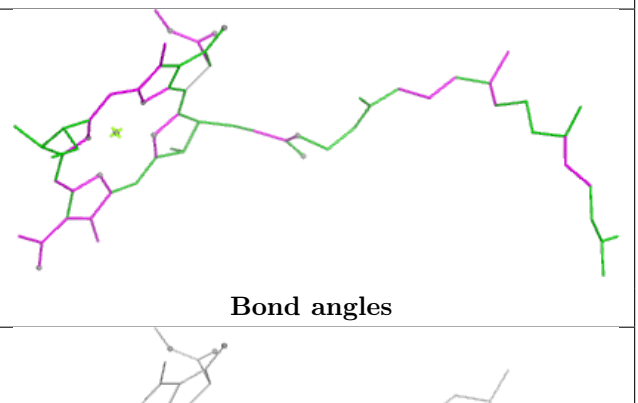


Rings

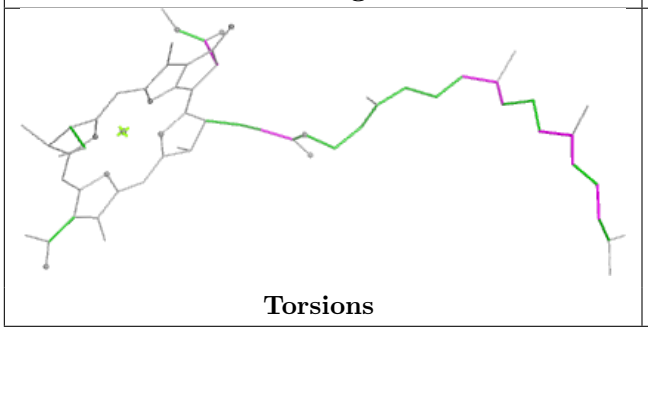
Ligand BCL M 1304



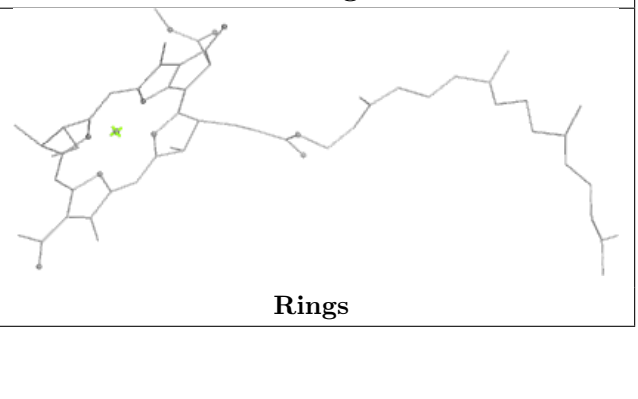
Bond lengths



Bond angles

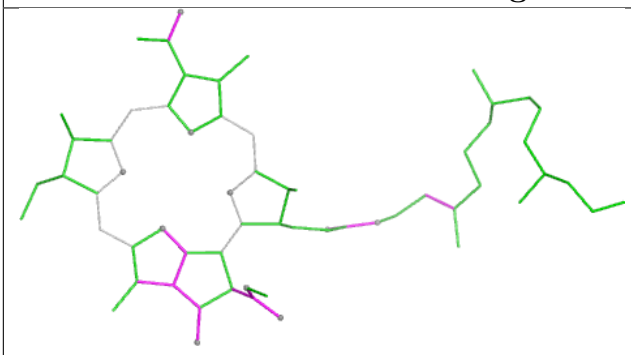


Torsions

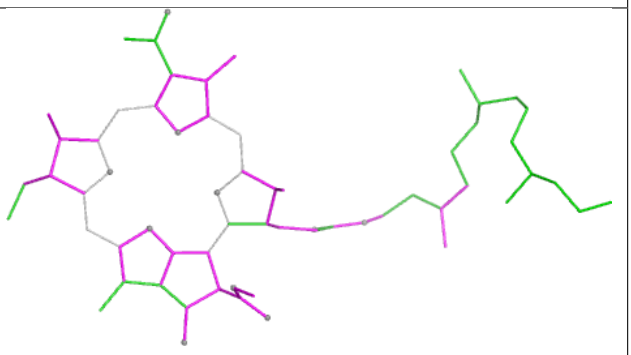


Rings

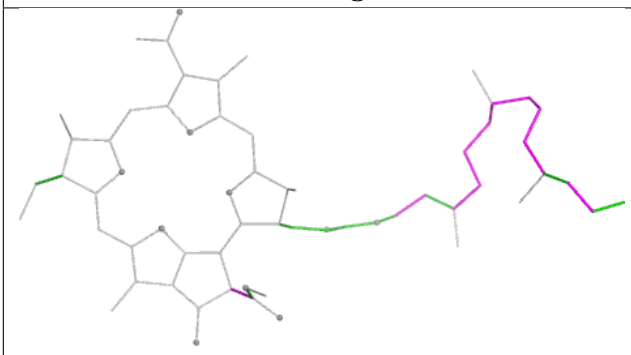
Ligand BPH M 1308



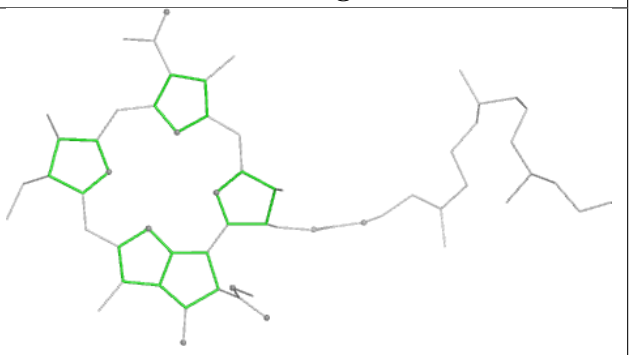
Bond lengths



Bond angles

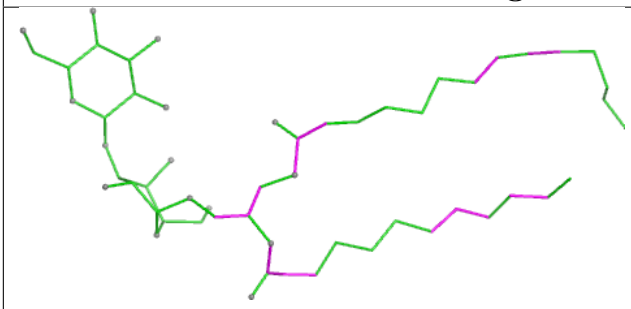


Torsions

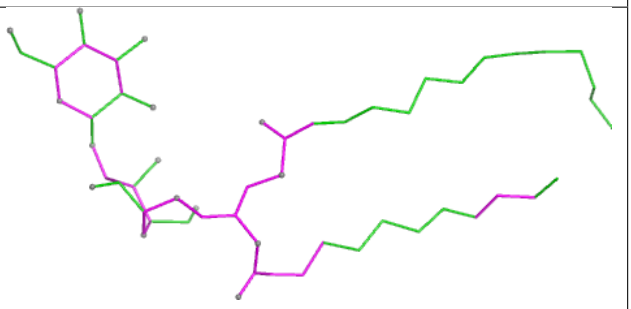


Rings

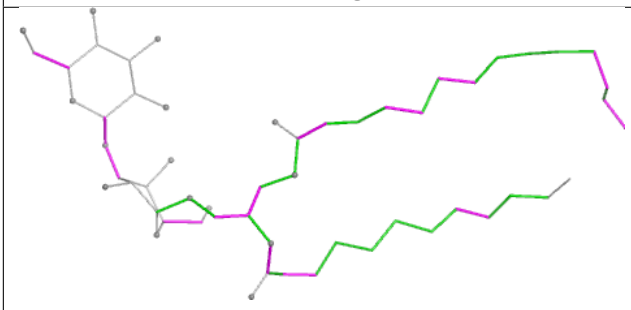
Ligand GGD M 1313



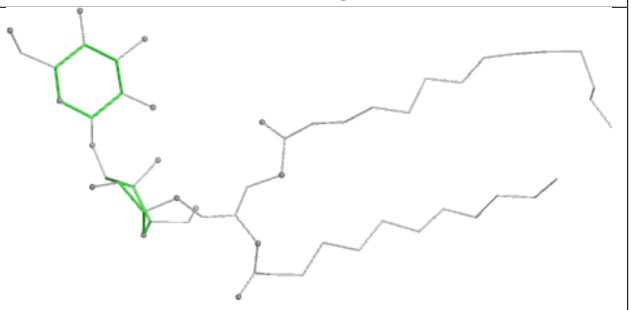
Bond lengths



Bond angles

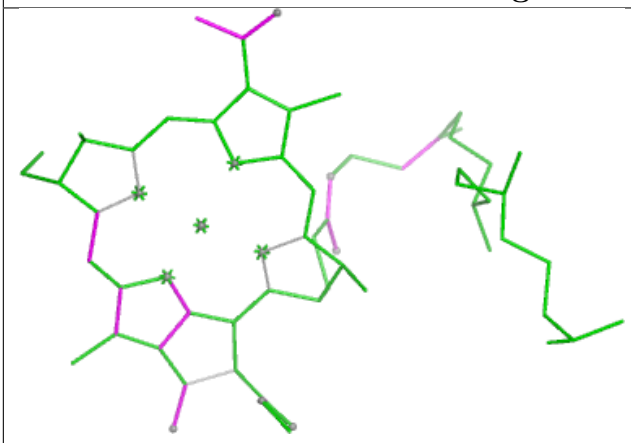


Torsions

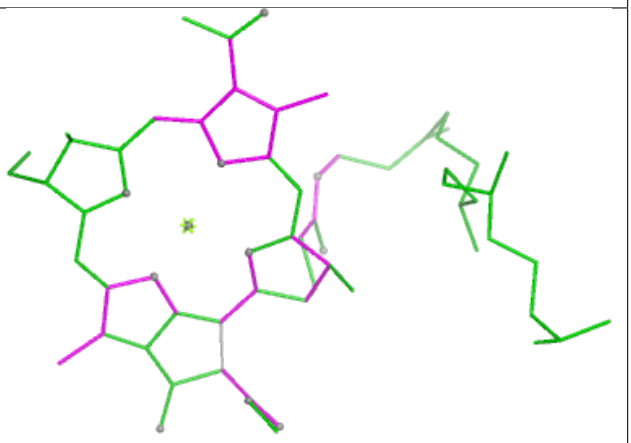


Rings

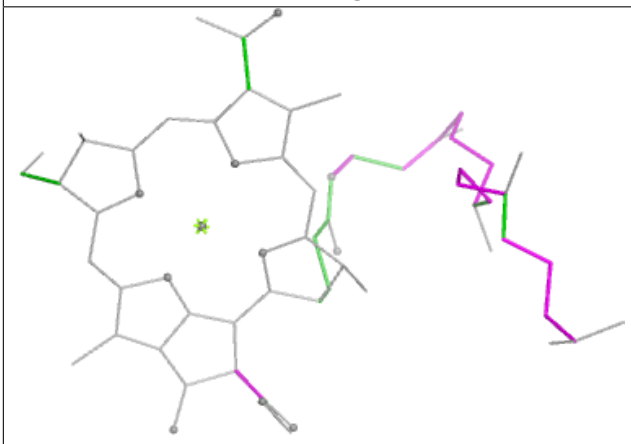
Ligand BCL M 1303



Bond lengths



Bond angles

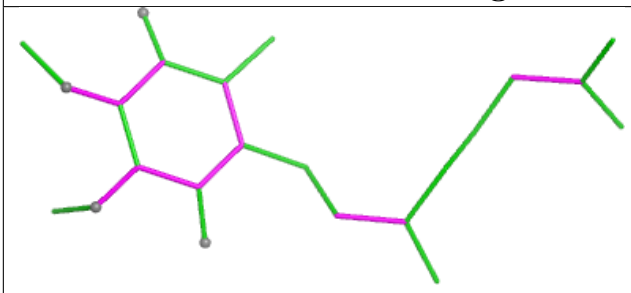


Torsions

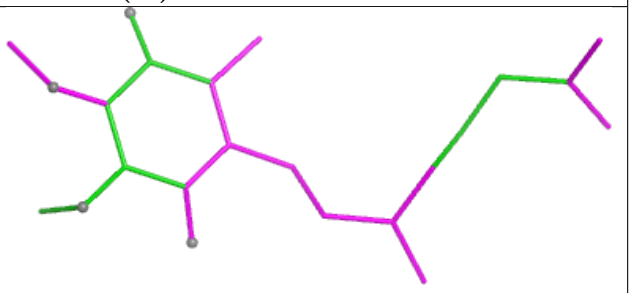


Rings

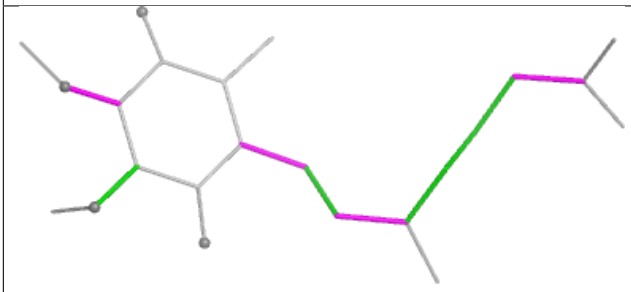
Ligand U10 L 1287 (A)



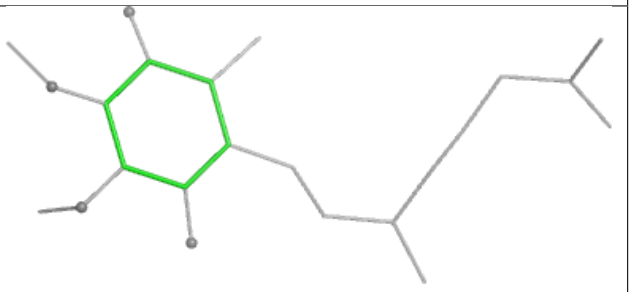
Bond lengths



Bond angles

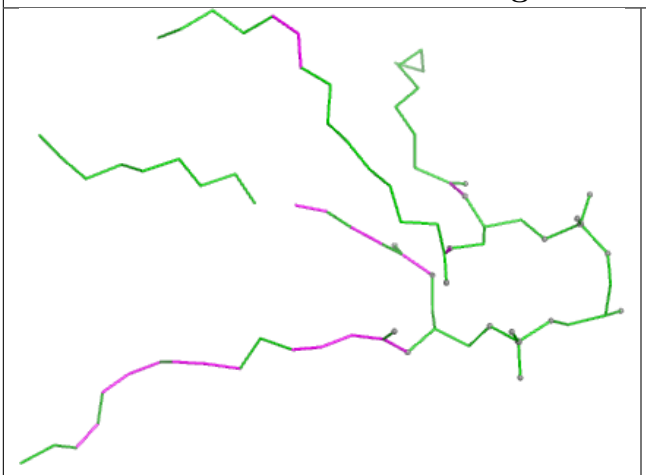


Torsions

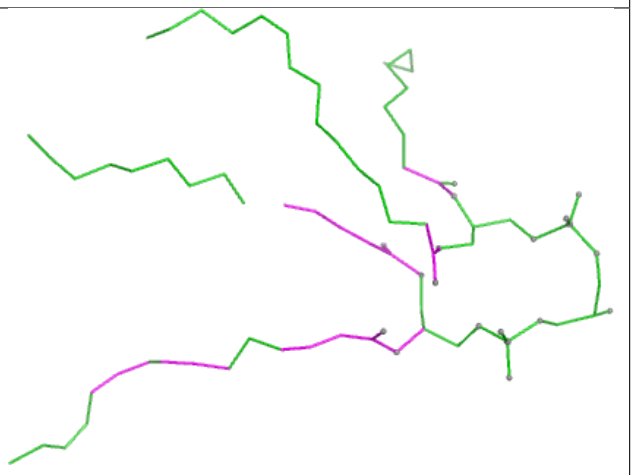


Rings

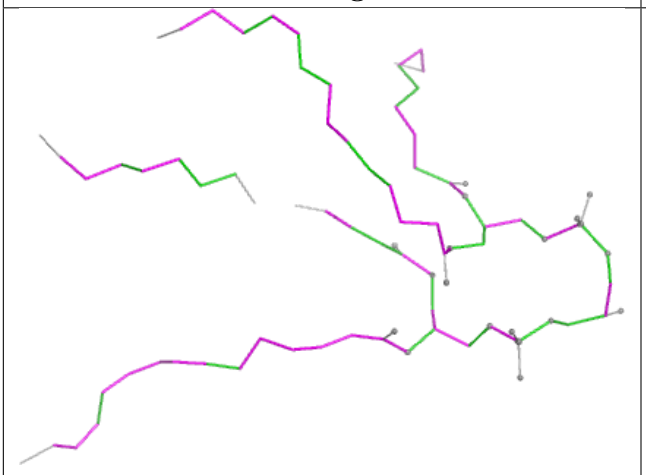
Ligand CDL M 1311



Bond lengths



Bond angles

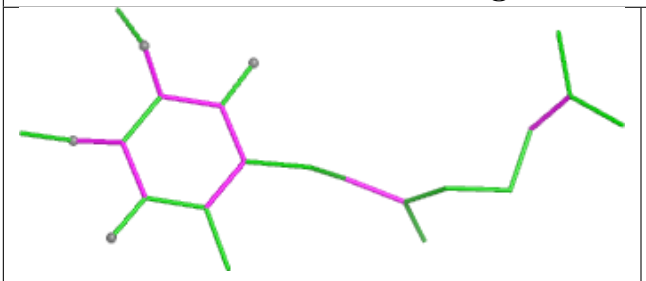


Torsions

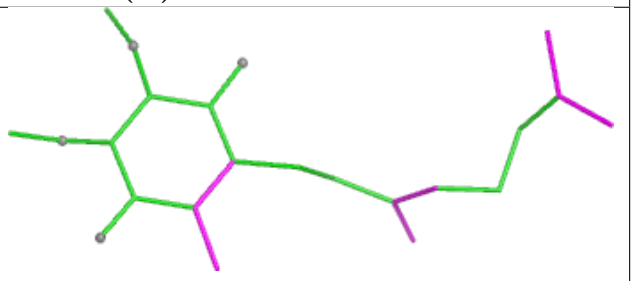


Rings

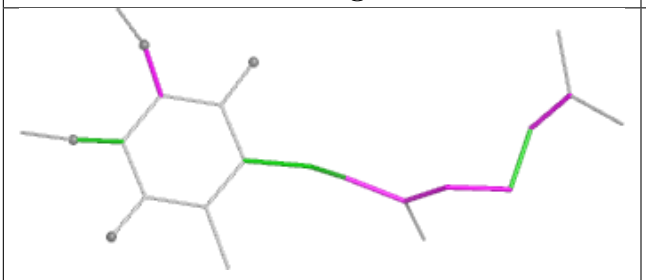
Ligand U10 L 1287 (B)



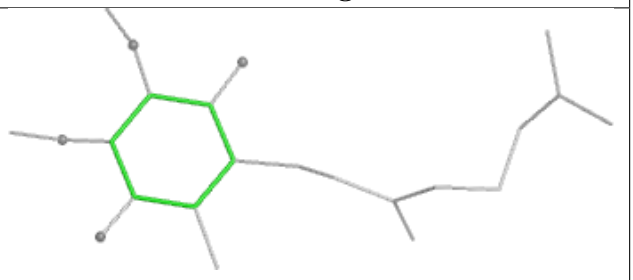
Bond lengths



Bond angles

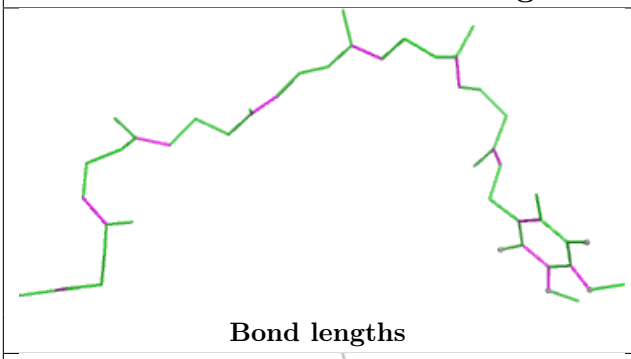


Torsions

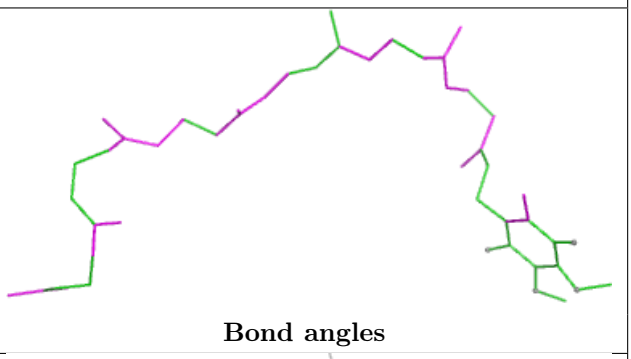


Rings

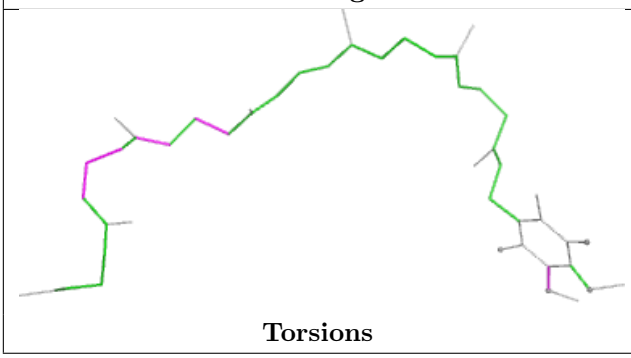
Ligand U10 M 1309



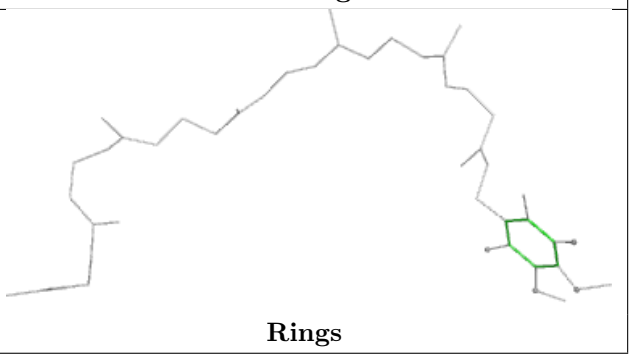
Bond lengths



Bond angles

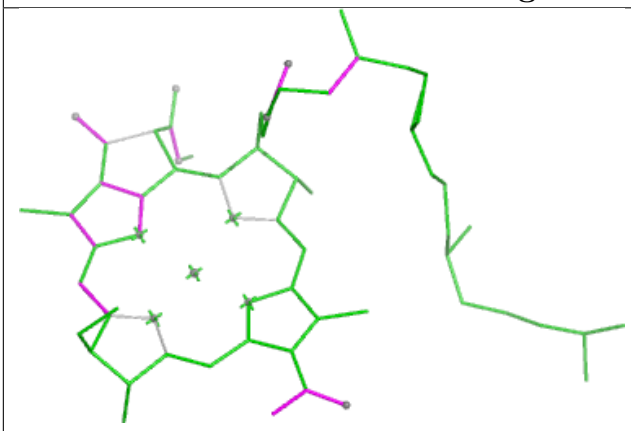


Torsions

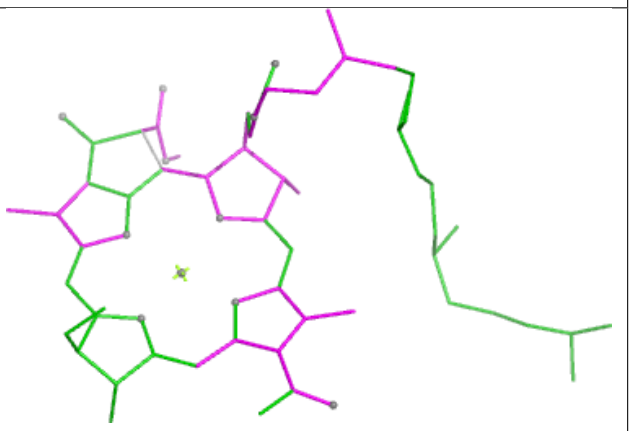


Rings

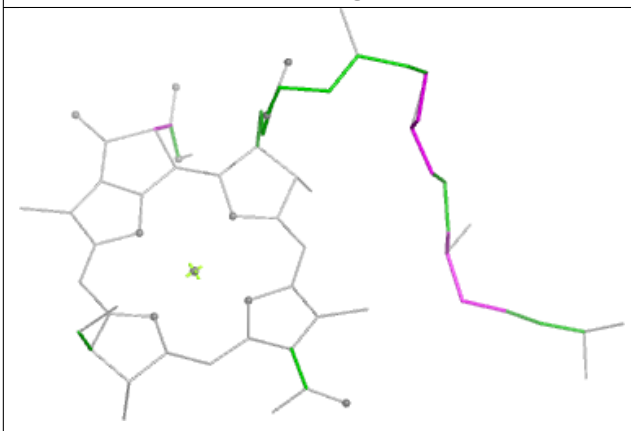
Ligand BCL L 1282



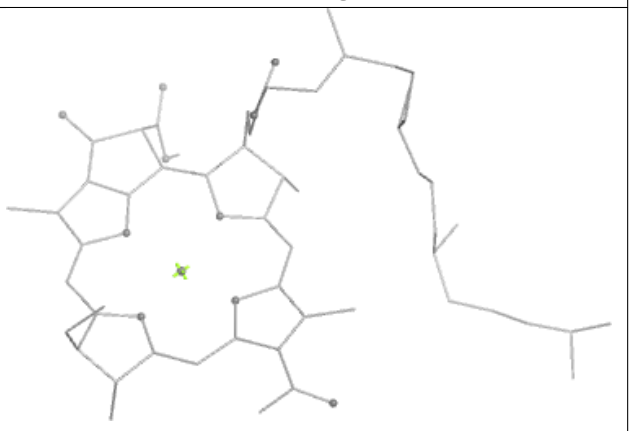
Bond lengths



Bond angles

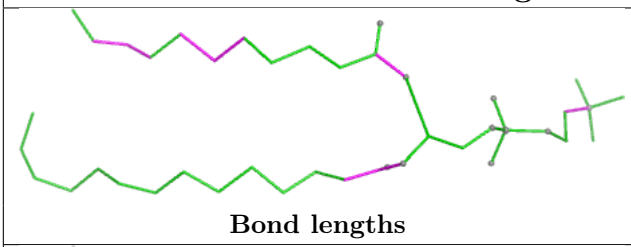


Torsions

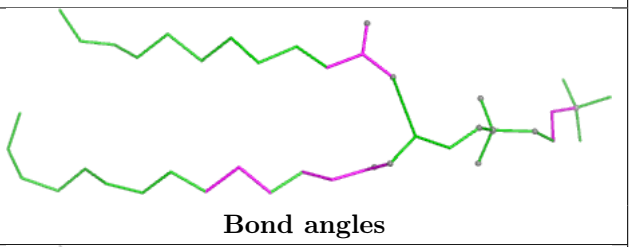


Rings

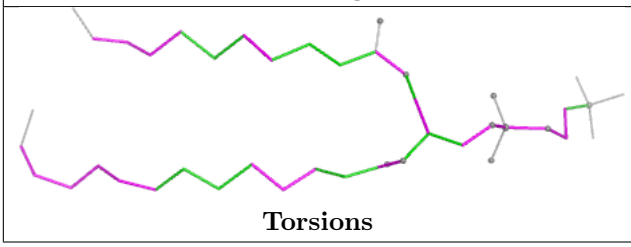
Ligand PC1 M 1312



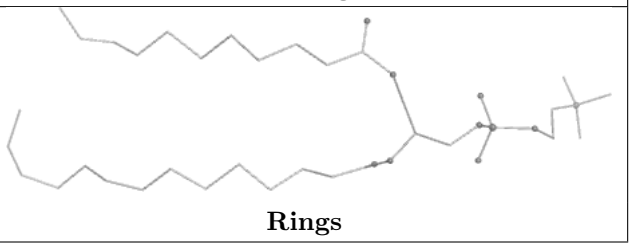
Bond lengths



Bond angles

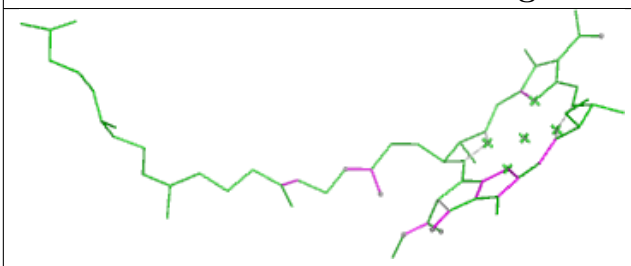


Torsions

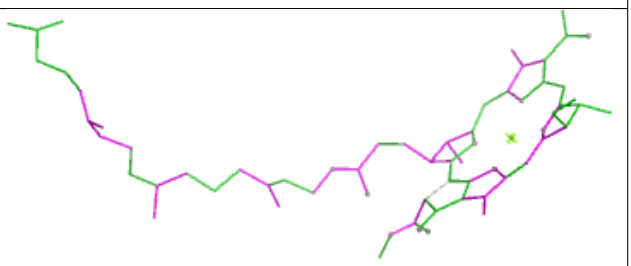


Rings

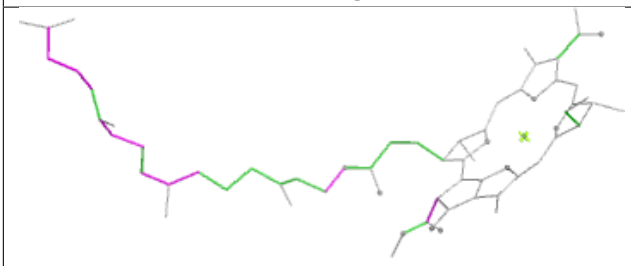
Ligand BCL L 1288



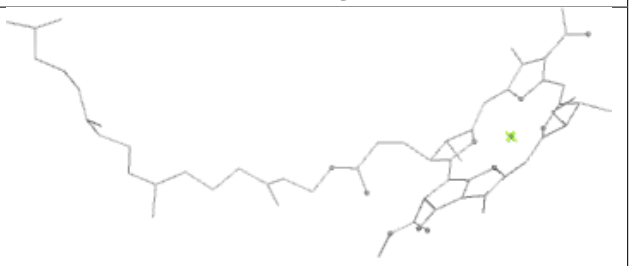
Bond lengths



Bond angles

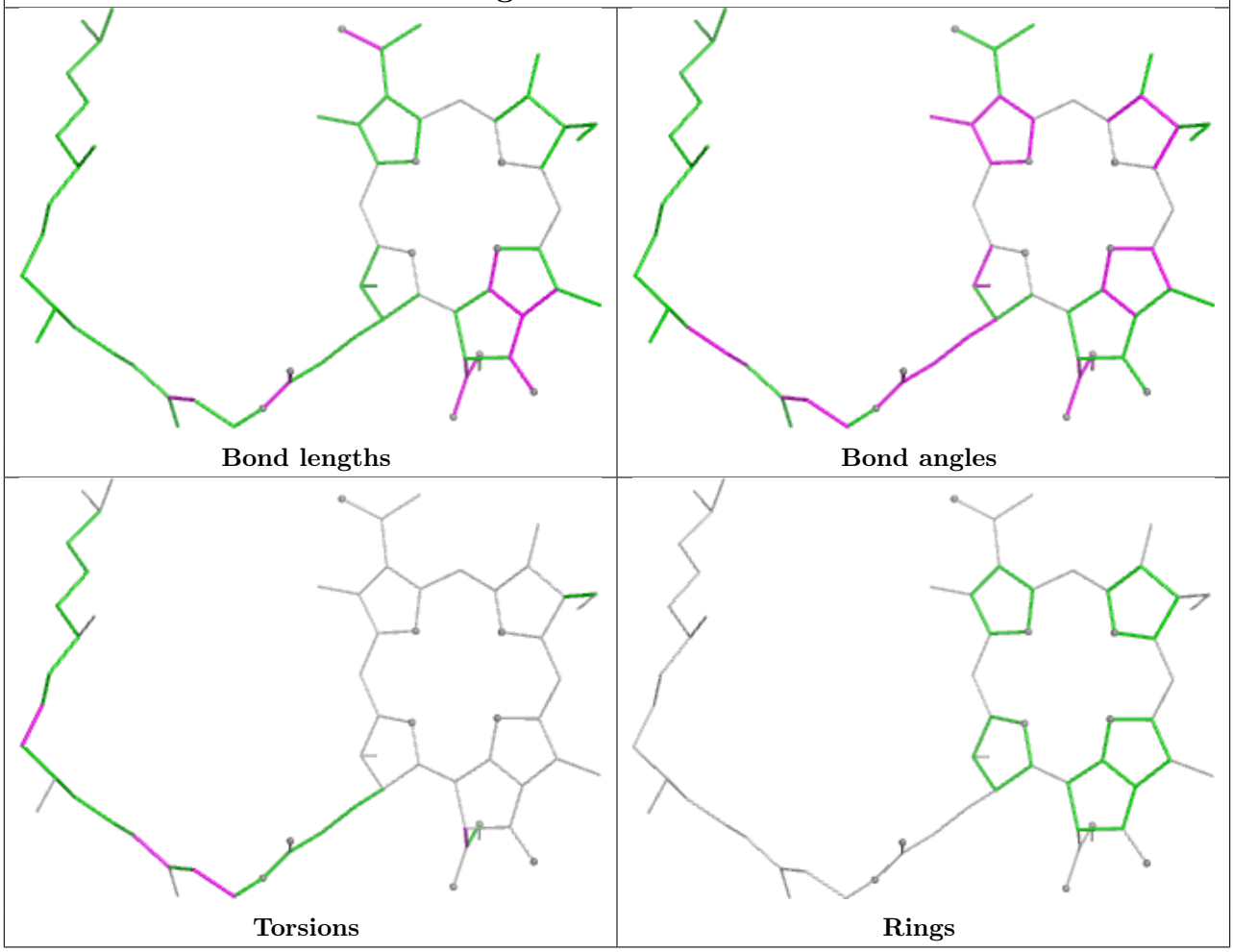


Torsions



Rings

Ligand BPH L 1286



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, 95th 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	9 (3%)	45	49	13, 24, 33, 61	8 (3%)
2	L	281/281 (100%)	-0.03	10 (3%)	46	50	14, 21, 37, 50	2 (0%)
3	M	303/307 (98%)	0.24	15 (4%)	34	36	14, 25, 42, 56	7 (2%)
All	All	825/848 (97%)	0.09	34 (4%)	41	45	13, 23, 38, 61	17 (2%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	11.0
3	M	3	TYR	6.7
1	H	249[A]	LYS	6.6
3	M	301	HIS	5.5
1	H	250	SER	5.3
2	L	281	GLY	5.2
1	H	251	VAL	5.1
3	M	2	GLU	5.1
3	M	303	MET	4.2
1	H	184	LYS	4.1
3	M	148	TRP	3.9
2	L	271[A]	TRP	3.8
2	L	275	ILE	3.7
2	L	277	GLY	3.7
3	M	106	ALA	3.3
2	L	270	PRO	3.1
3	M	302	GLY	3.0
3	M	52	LEU	2.9
3	M	105	PHE	2.9
2	L	273	ALA	2.9
3	M	300	ASN	2.7
1	H	247	LYS	2.6
1	H	139	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	138	ALA	2.5
3	M	100	GLU	2.5
1	H	175	MET	2.5
1	H	18	TYR	2.4
2	L	59	TRP	2.4
2	L	56	GLN	2.4
3	M	32	VAL	2.3
3	M	298	GLY	2.2
3	M	80	TRP	2.1
2	L	72	GLU	2.1
2	L	274	ASN	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, 95th 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	0.51	0.43	78,80,81,82	0
14	PC1	M	1312	43/54	0.56	0.39	66,82,95,96	0
6	LDA	L	1284	16/16	0.64	0.34	72,73,77,77	0
8	U10	L	1287[A]	23/63	0.68	0.29	24,40,48,49	23
8	U10	L	1287[B]	23/63	0.68	0.29	34,42,44,44	23
15	GGD	M	1313	57/67	0.69	0.28	47,73,90,90	0
4	GOL	H	1253	6/6	0.70	0.27	65,66,67,68	0
13	CDL	M	1311	81/100	0.72	0.33	42,69,83,83	0
6	LDA	L	1285	16/16	0.75	0.29	72,76,80,81	0
4	GOL	H	1251	6/6	0.77	0.20	32,46,47,49	0
4	GOL	L	1292	6/6	0.77	0.25	29,42,44,45	0
4	GOL	L	1294	6/6	0.80	0.22	80,81,81,81	0

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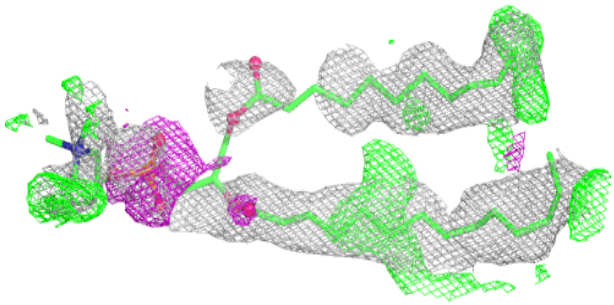
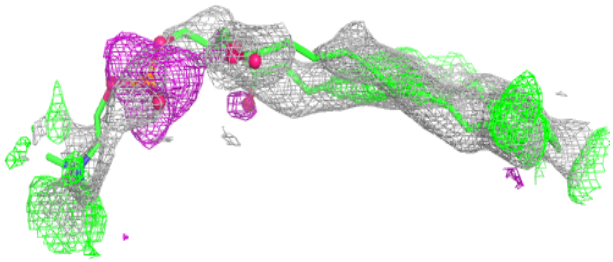
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LDA	L	1283	16/16	0.81	0.23	41,64,73,74	0
6	LDA	M	1305	16/16	0.83	0.20	31,45,51,51	0
6	LDA	M	1306	16/16	0.83	0.24	54,58,63,64	0
10	HTO	L	1290	10/10	0.86	0.22	60,62,63,64	0
4	GOL	H	1252	6/6	0.87	0.14	63,63,63,64	0
4	GOL	H	1254	6/6	0.88	0.14	63,64,64,65	0
4	GOL	L	1293	6/6	0.92	0.16	66,68,68,69	0
12	SPO	M	1310	42/42	0.94	0.11	21,26,48,51	0
8	U10	M	1309	48/63	0.94	0.12	15,25,45,48	0
5	BCL	L	1282	66/66	0.95	0.08	13,18,41,43	0
5	BCL	M	1304	66/66	0.96	0.07	12,19,38,46	0
5	BCL	L	1288	66/66	0.96	0.07	14,17,31,37	0
5	BCL	M	1303	66/66	0.96	0.10	16,21,58,58	0
7	BPH	M	1308	65/65	0.97	0.10	17,22,69,71	0
7	BPH	L	1286	65/65	0.97	0.06	10,16,26,28	0
9	PO4	L	1289	5/5	0.97	0.11	33,35,36,36	0
11	FE	M	1307	1/1	0.99	0.02	15,15,15,15	0

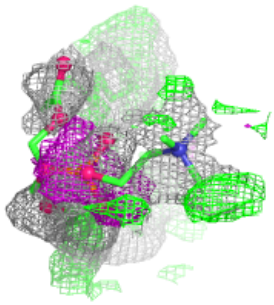
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 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)

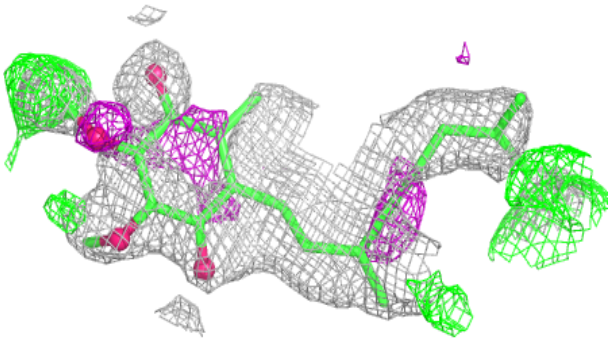


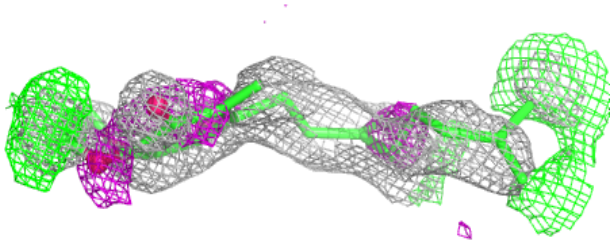


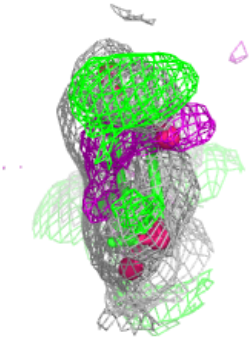


Electron density around U10 L 1287 (A):

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

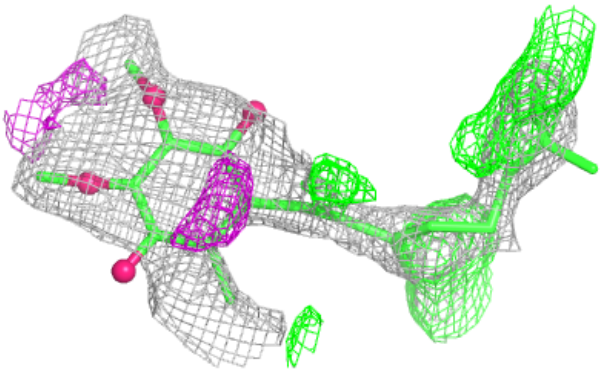


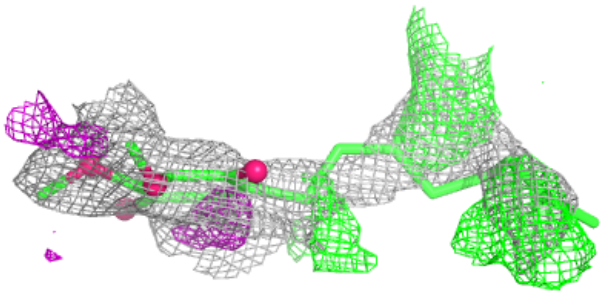


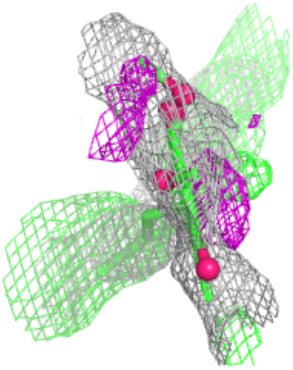


Electron density around U10 L 1287 (B):

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

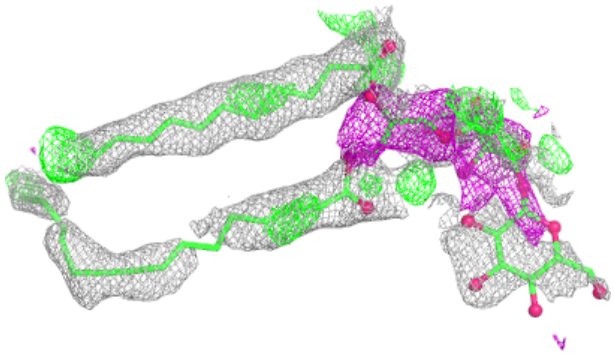


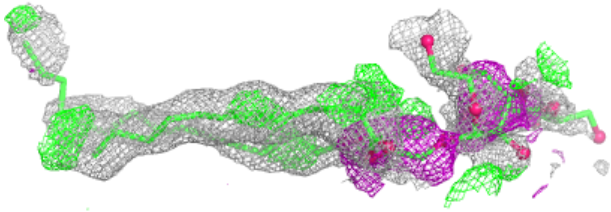


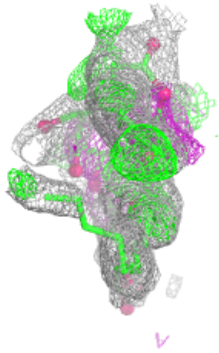


Electron density around GGD M 1313:

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

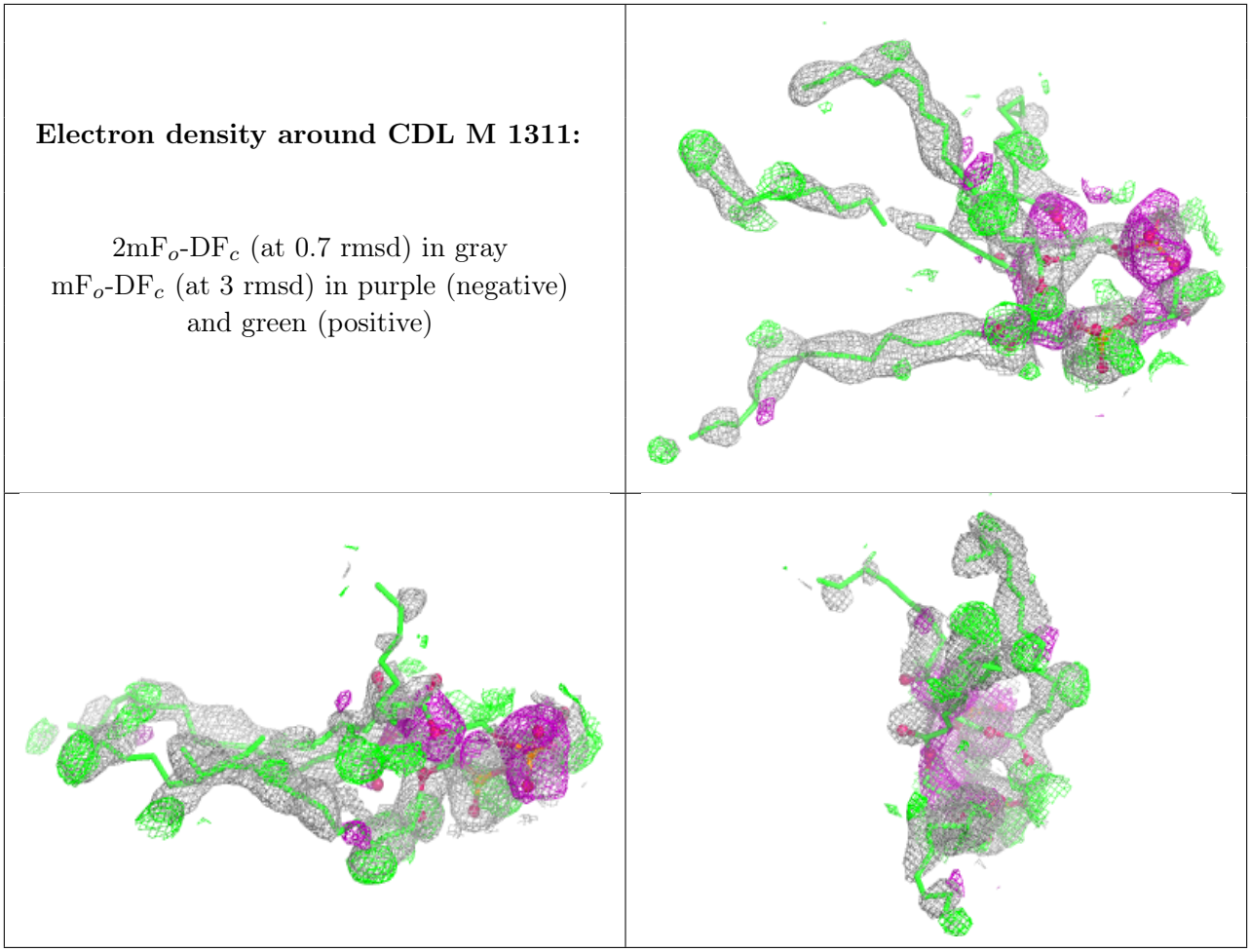






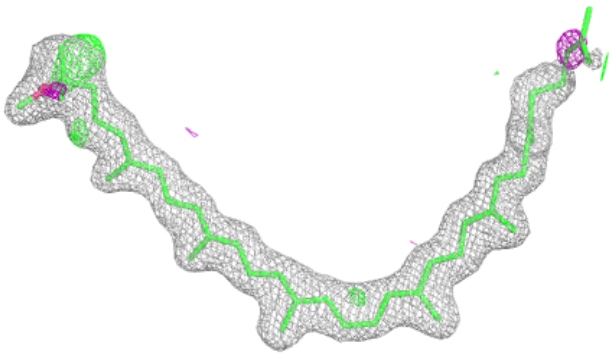
Electron density around CDL M 1311:

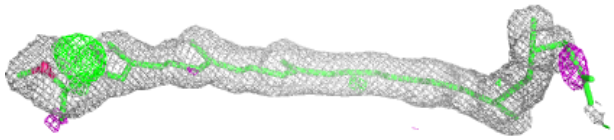
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

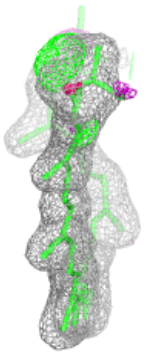


Electron density around SPO M 1310:

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

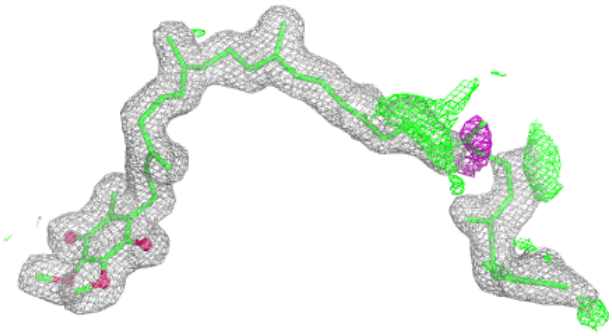


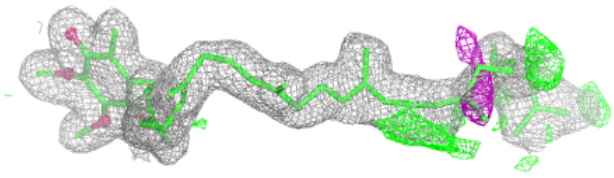


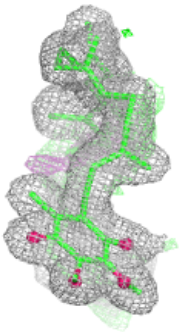


Electron density around U10 M 1309:

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

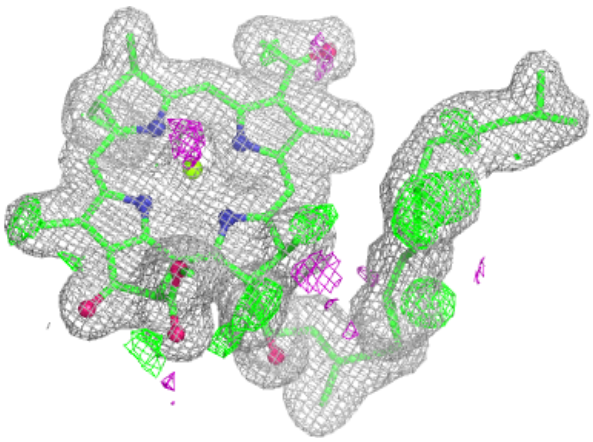


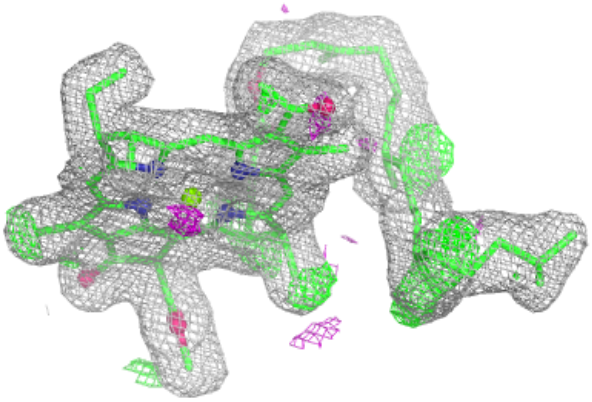


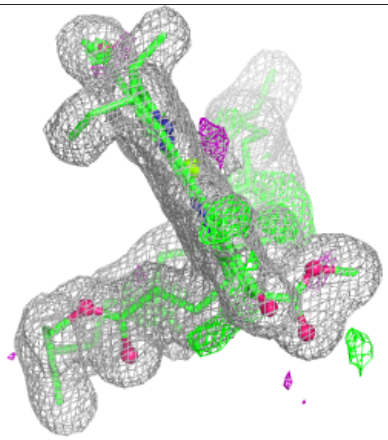


Electron density around BCL L 1282:

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

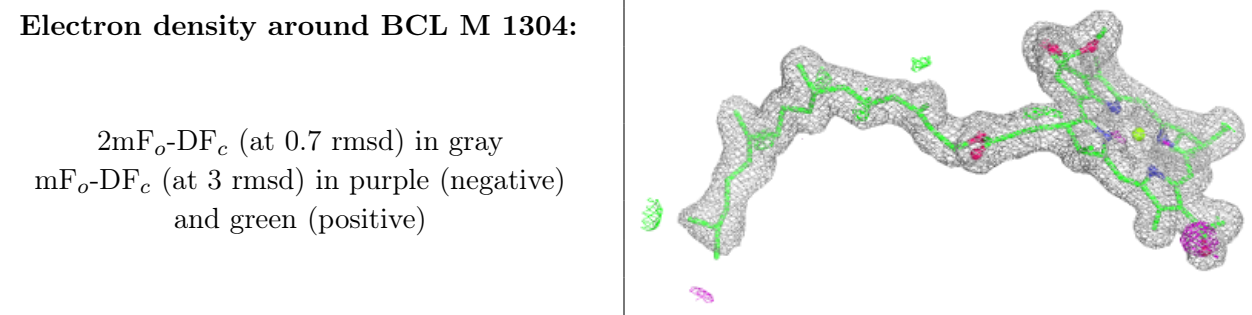


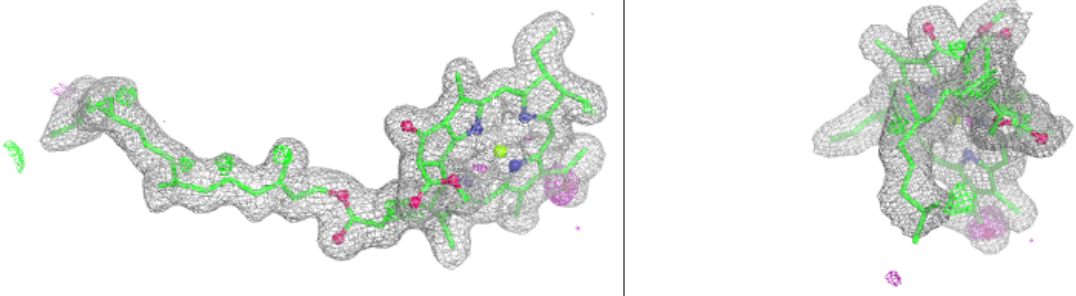




Electron density around BCL M 1304:

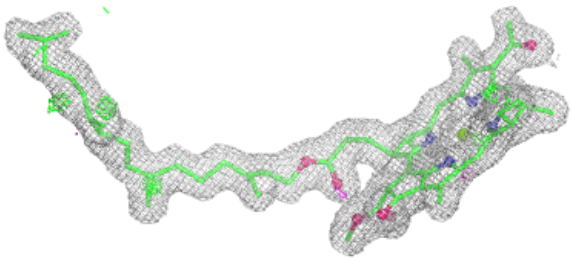
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

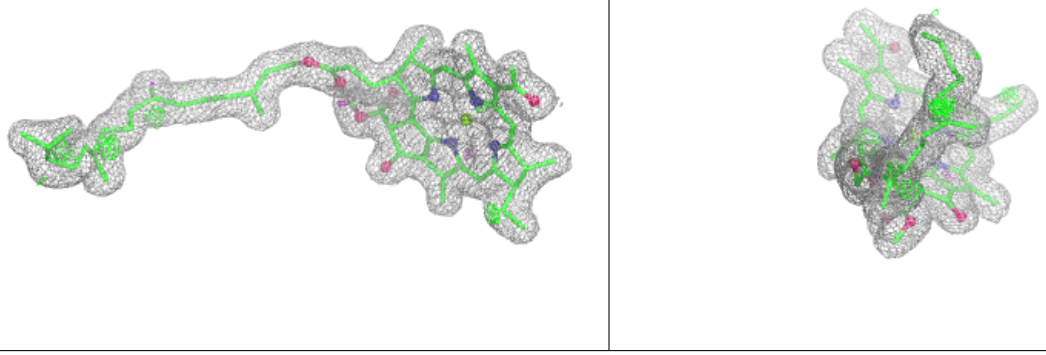




Electron density around BCL L 1288:

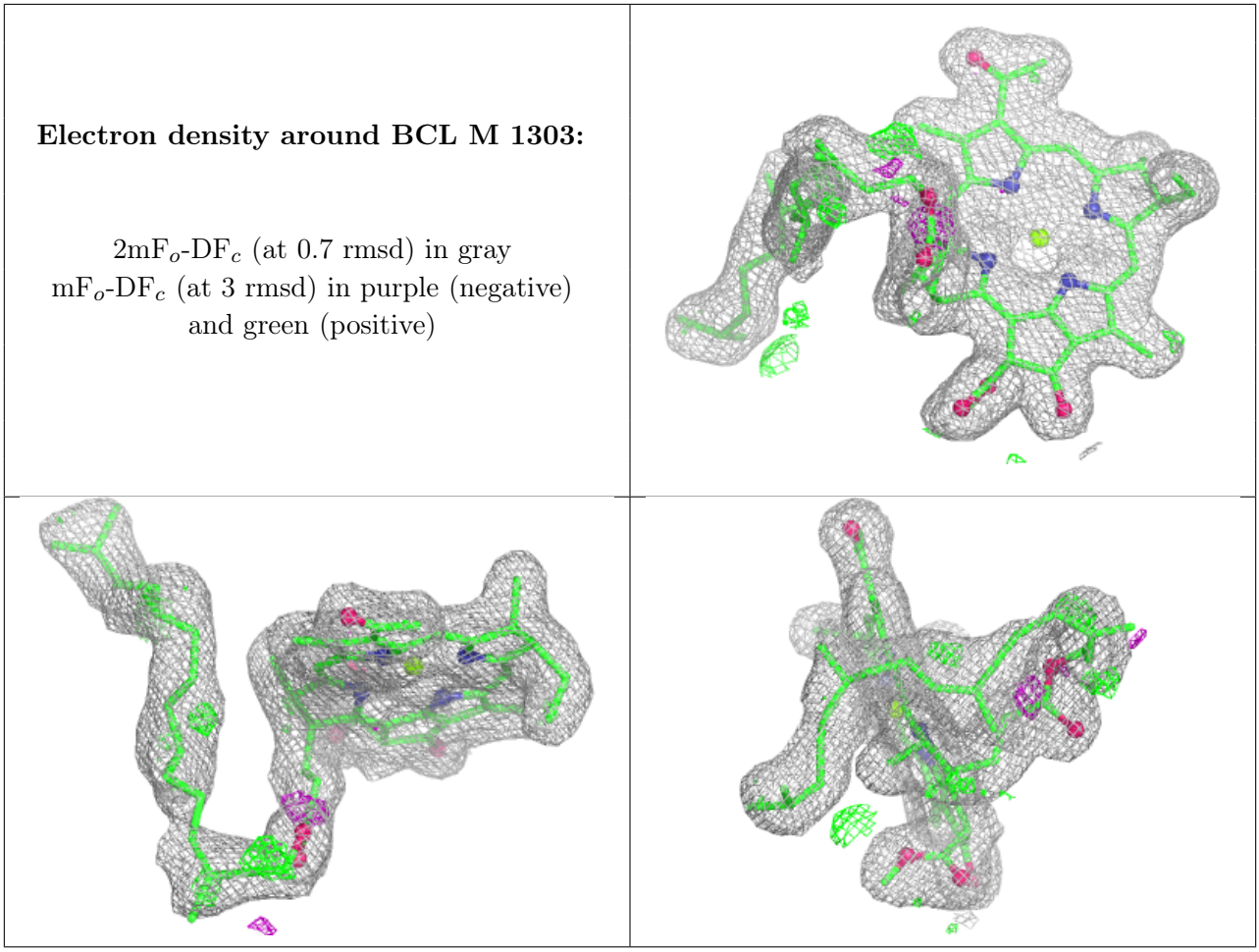
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





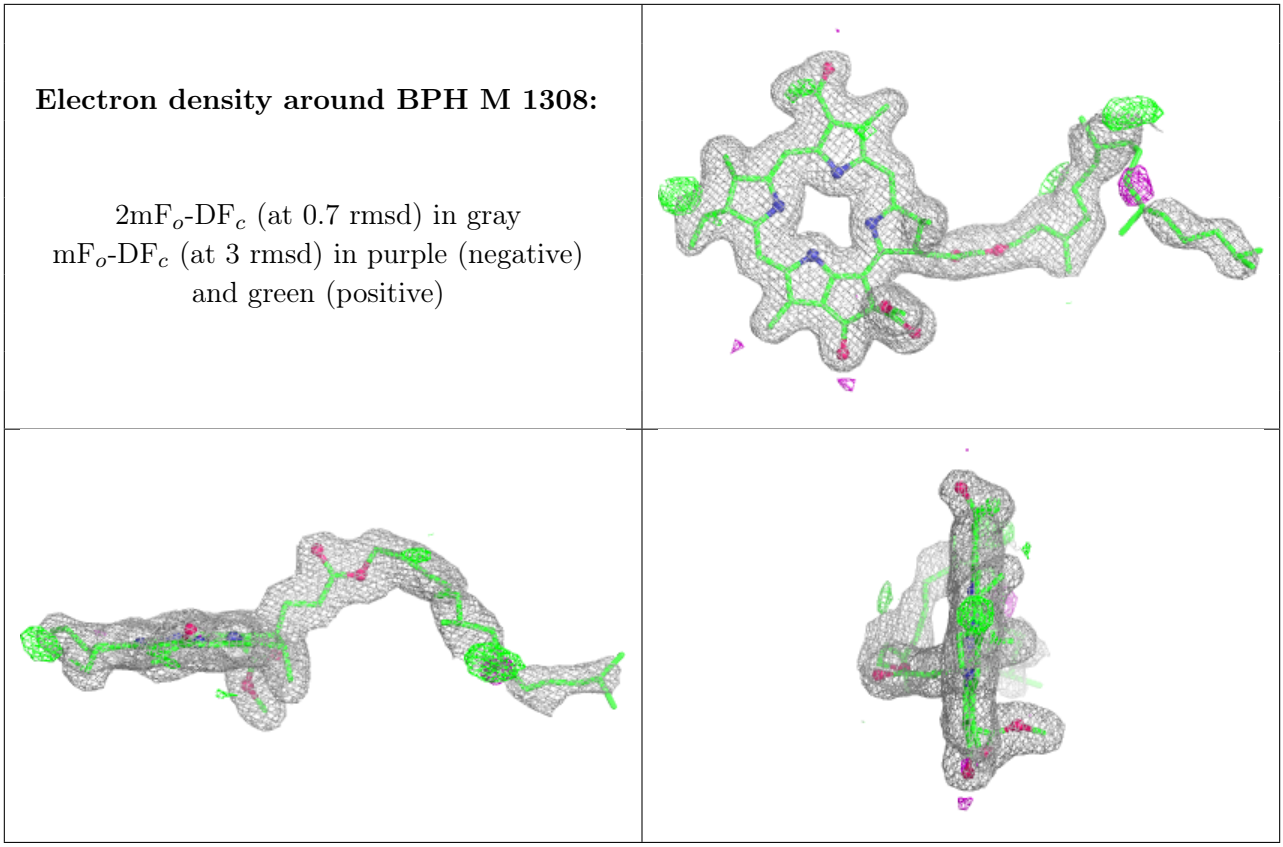
Electron density around BCL M 1303:

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



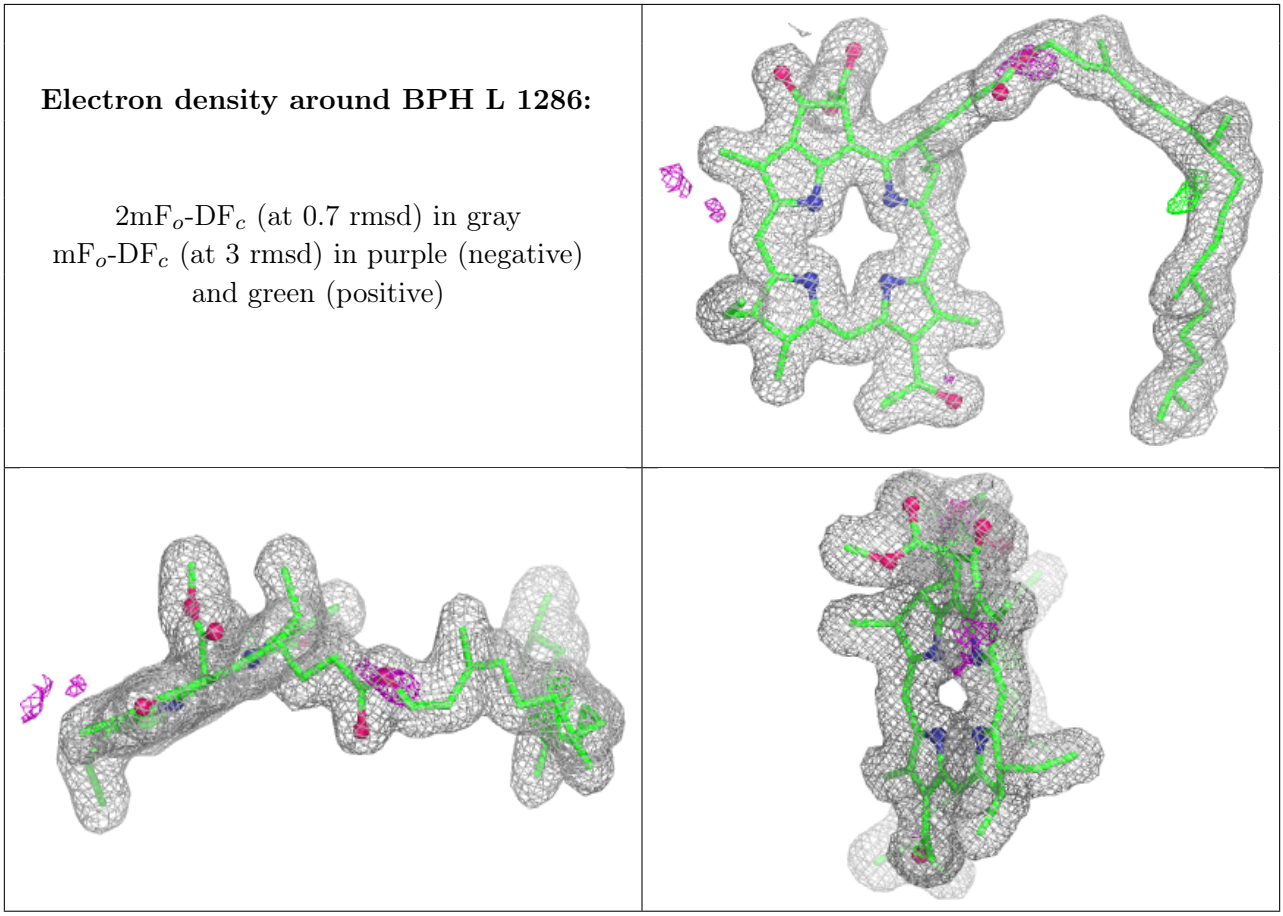
Electron density around BPH M 1308:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.