



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:07 PM UTC

PDB ID : 2J8D / pdb_00002j8d
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 8 in the charge-separated state
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2006-10-24
Resolution : 2.07 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

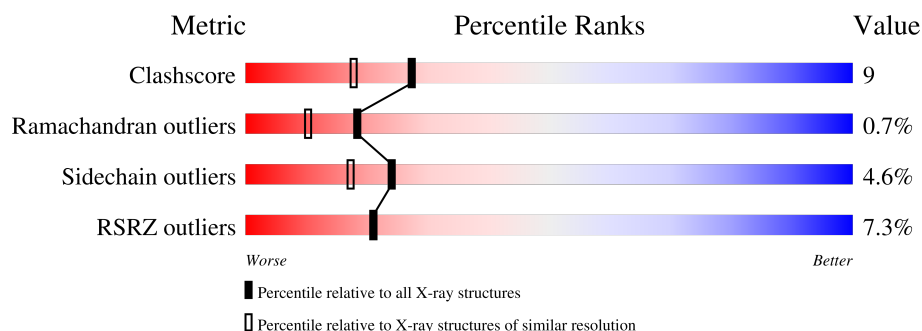
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	10% 88% 11% .
2	L	281	4% 90% 9% .
3	M	307	8% 83% 14% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	H	1261	-	-	X	-
5	BCL	L	1282	X	-	-	-
5	BCL	L	1283	X	-	-	-
5	BCL	M	1308	X	-	-	-
5	BCL	M	1309	X	-	-	-
6	LDA	L	1285	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 7895 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	260	Total	C	N	O	S	0	1	0
			1980	1271	335	363	11			

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

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

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

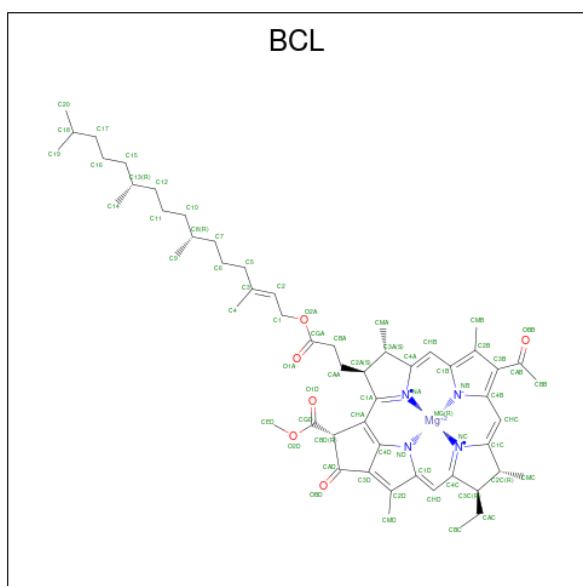
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	307	Total	C	N	O	S	0	1	0
			2451	1634	402	404	11			

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



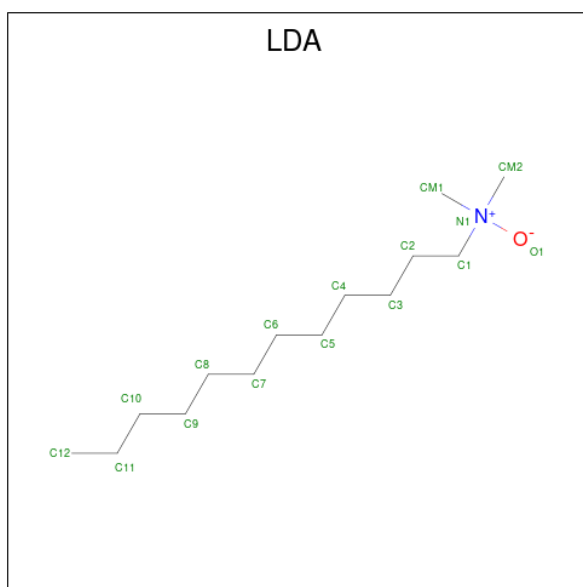
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

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



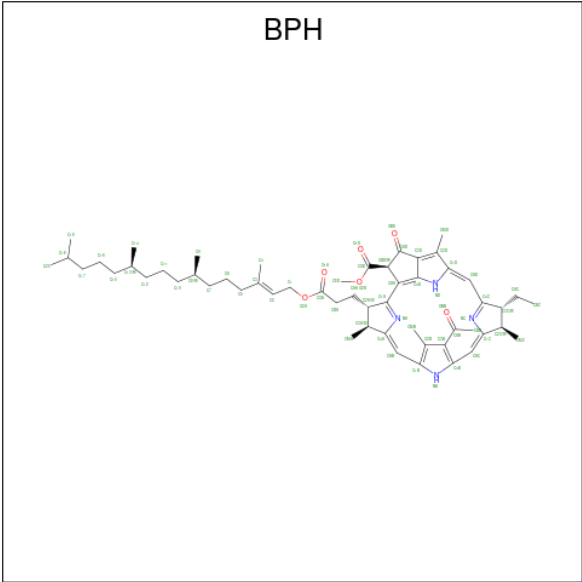
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



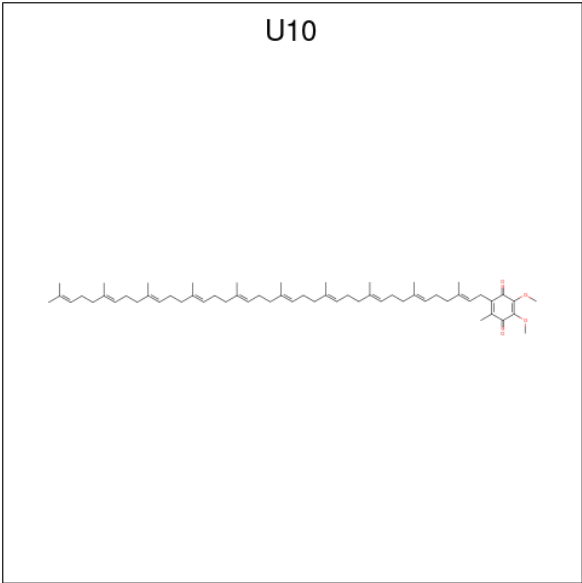
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

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



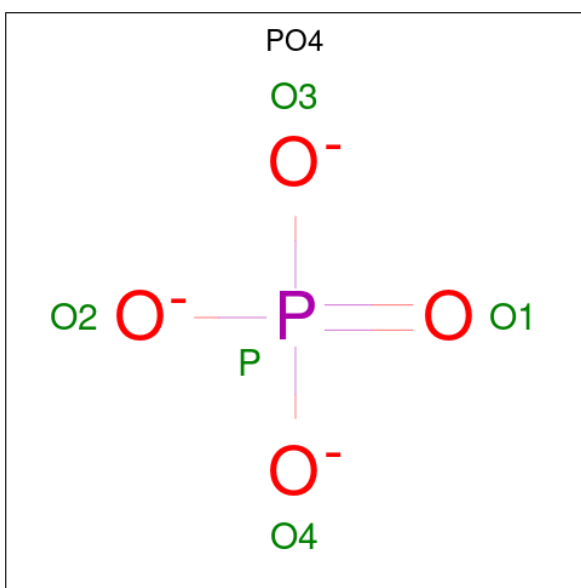
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



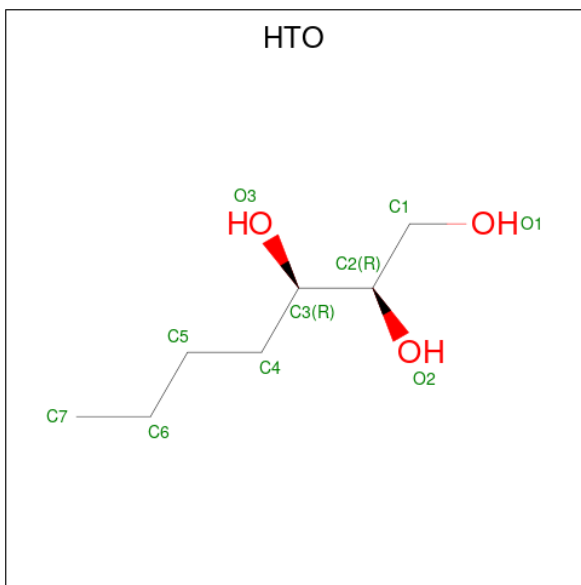
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		
8	M	1	Total	C	O	0	0
			47	44	3		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

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

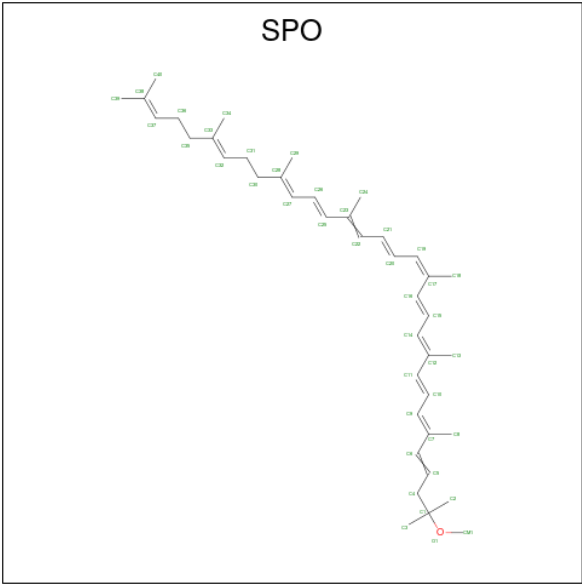


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

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

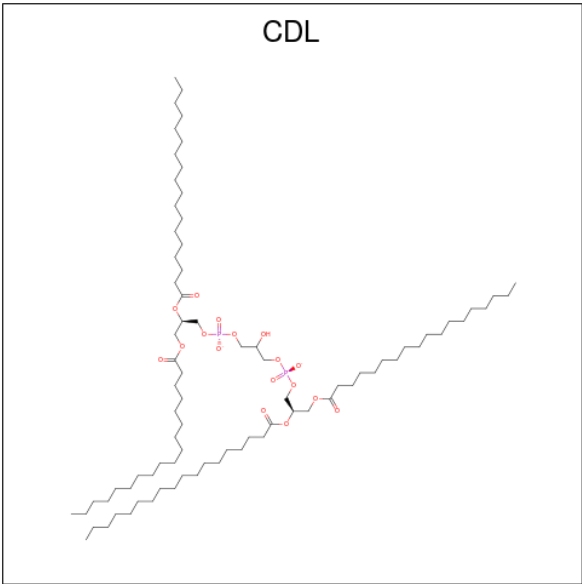
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



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

- Molecule 13 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

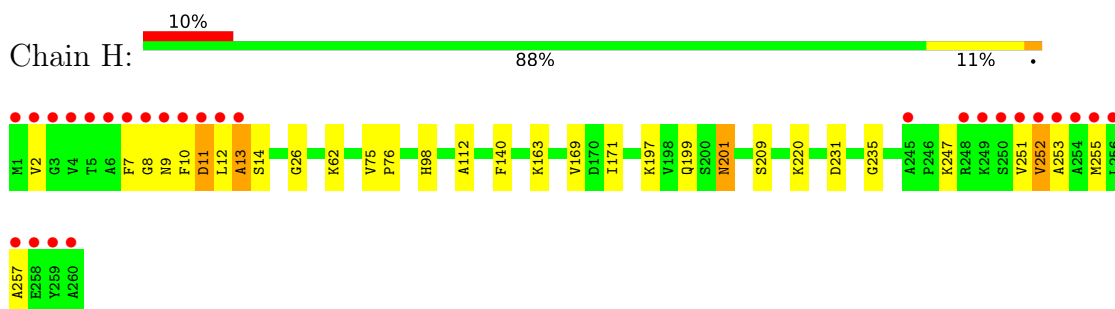
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	161	Total	O	0	0
			161	161		
14	L	121	Total	O	0	0
			121	121		
14	M	128	Total	O	0	0
			128	128		

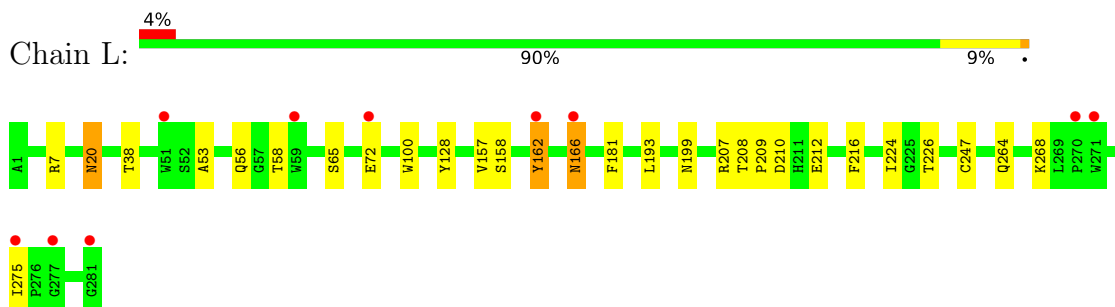
3 Residue-property plots [i](#)

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.

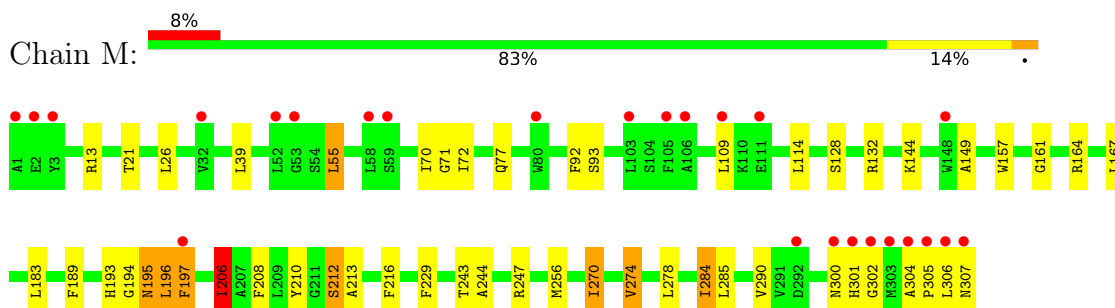
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER PROTEIN M CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.01Å 140.01Å 184.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.07 119.52 – 2.07	Depositor EDS
% Data completeness (in resolution range)	95.6 (119.52-2.07) 95.6 (119.52-2.07)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.197 , 0.218 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7895	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BCL, U10, LDA, CDL, FE, GOL, SPO, HTO, BPH, PO4

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	0.91	0/2036	0.92	0/2768
2	L	0.93	0/2320	0.95	2/3175 (0.1%)
3	M	0.96	1/2549 (0.0%)	0.95	3/3479 (0.1%)
All	All	0.94	1/6905 (0.0%)	0.94	5/9422 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	213	ALA	CA-CB	6.07	1.63	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	206	ILE	CA-CB-CG2	5.78	120.33	110.50
2	L	275	ILE	CA-C-N	-5.74	114.66	120.85
2	L	275	ILE	C-N-CA	-5.74	114.66	120.85
3	M	212	SER	CB-CA-C	5.67	121.56	110.67
3	M	70	ILE	CB-CA-C	-5.11	105.43	111.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1980	0	1986	30	0
2	L	2232	0	2187	27	0
3	M	2451	0	2362	49	0
4	H	24	0	32	5	0
4	L	18	0	24	0	0
5	L	132	0	148	4	0
5	M	132	0	148	9	0
6	L	48	0	93	1	0
6	M	96	0	186	8	0
7	L	65	0	76	6	0
7	M	65	0	76	7	0
8	L	46	0	46	9	0
8	M	47	0	63	4	0
9	L	5	0	0	0	0
10	L	20	0	32	0	0
11	M	1	0	0	0	0
12	M	42	0	60	3	0
13	M	81	0	102	18	0
14	H	161	0	0	3	0
14	L	121	0	0	2	0
14	M	128	0	0	1	0
All	All	7895	0	7621	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (137) 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)
13:M:1320:CDL:C37	13:M:1320:CDL:C36	1.80	1.57
13:M:1320:CDL:C33	13:M:1320:CDL:C34	1.74	1.56
13:M:1320:CDL:C34	13:M:1320:CDL:C35	1.83	1.55
6:M:1314:LDA:C8	6:M:1314:LDA:C9	1.78	1.55
13:M:1320:CDL:C18	13:M:1320:CDL:C17	1.83	1.53
1:H:10[B]:PHE:CD1	3:M:301[B]:HIS:NE2	1.87	1.41
1:H:10[B]:PHE:CE1	3:M:301[B]:HIS:NE2	2.04	1.25
1:H:10[B]:PHE:CE1	3:M:301[B]:HIS:CE1	2.32	1.18
1:H:201:ASN:H	1:H:201:ASN:HD22	1.08	1.00
1:H:10[B]:PHE:HD1	3:M:301[B]:HIS:NE2	1.38	0.95
2:L:162:TYR:CD2	14:L:2069:HOH:O	2.19	0.94
13:M:1320:CDL:C17	13:M:1320:CDL:C19	2.47	0.93
7:L:1287:BPH:HHC	7:L:1287:BPH:HBB3	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10[B]:PHE:HE1	3:M:301[B]:HIS:CE1	1.88	0.88
1:H:10[B]:PHE:CD1	3:M:301[B]:HIS:CE1	2.63	0.84
3:M:206:ILE:HD11	3:M:210:TYR:CE2	2.11	0.84
2:L:56:GLN:HE22	2:L:65:SER:H	1.27	0.81
13:M:1320:CDL:C18	13:M:1320:CDL:C16	2.58	0.81
7:L:1287:BPH:HHC	7:L:1287:BPH:CBB	2.10	0.80
3:M:206:ILE:CD1	3:M:210:TYR:CE2	2.63	0.80
13:M:1320:CDL:C37	13:M:1320:CDL:C35	2.60	0.78
1:H:10[B]:PHE:HD1	3:M:301[B]:HIS:HE2	0.79	0.77
2:L:158:SER:HB2	3:M:197:PHE:CE2	2.20	0.77
6:M:1314:LDA:C8	6:M:1314:LDA:C10	2.63	0.76
1:H:201:ASN:H	1:H:201:ASN:ND2	1.84	0.76
1:H:201:ASN:HD22	1:H:201:ASN:N	1.84	0.74
2:L:181:PHE:HB3	7:M:1317:BPH:HBB2	1.69	0.73
6:M:1314:LDA:C9	6:M:1314:LDA:C7	2.66	0.73
7:M:1317:BPH:HHC	7:M:1317:BPH:HBB3	1.70	0.73
3:M:189:PHE:O	3:M:193:HIS:HD2	1.71	0.73
2:L:264:GLN:NE2	14:L:2112:HOH:O	2.23	0.72
2:L:162:TYR:CD2	2:L:162:TYR:C	2.67	0.72
5:M:1309:BCL:CBB	5:M:1309:BCL:HHC	2.20	0.72
5:M:1309:BCL:HHC	5:M:1309:BCL:HBB3	1.72	0.71
5:M:1308:BCL:HHC	5:M:1308:BCL:CBB	2.22	0.70
5:M:1308:BCL:HBB3	5:M:1309:BCL:H41	1.73	0.70
3:M:157:TRP:HB2	5:M:1309:BCL:H71	1.74	0.69
13:M:1320:CDL:C36	13:M:1320:CDL:C38	2.71	0.68
4:H:1261:GOL:H32	14:H:2002:HOH:O	1.92	0.68
5:L:1283:BCL:HBB2	5:L:1283:BCL:HHC	1.77	0.67
2:L:158:SER:HB2	3:M:197:PHE:HE2	1.58	0.67
2:L:181:PHE:CD2	7:M:1317:BPH:HBB1	2.29	0.67
3:M:206:ILE:CD1	3:M:210:TYR:CZ	2.78	0.67
2:L:199:ASN:O	13:M:1320:CDL:HB22	1.96	0.66
2:L:224:ILE:H	8:L:1288[A]:U10:H8	1.61	0.65
1:H:12:LEU:O	1:H:13:ALA:CB	2.47	0.63
2:L:224:ILE:HG22	8:L:1288[A]:U10:H8	1.81	0.63
5:M:1308:BCL:HHC	5:M:1308:BCL:HBB2	1.82	0.62
7:M:1317:BPH:HHC	7:M:1317:BPH:CBB	2.31	0.61
7:L:1287:BPH:HBB3	7:L:1287:BPH:CHC	2.28	0.60
2:L:20:ASN:C	2:L:20:ASN:HD22	2.10	0.59
3:M:270:ILE:O	3:M:274:VAL:HG13	2.02	0.59
3:M:206:ILE:HD13	3:M:210:TYR:CZ	2.39	0.58
1:H:10[B]:PHE:HE1	3:M:301[B]:HIS:NE2	1.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1308:BCL:H71	5:M:1309:BCL:H202	1.85	0.58
3:M:71:GLY:HA3	12:M:1319:SPO:H6	1.86	0.57
2:L:226:THR:HG22	8:L:1288[A]:U10:H3M3	1.85	0.57
1:H:10[B]:PHE:CE1	3:M:301[B]:HIS:HE1	2.13	0.57
7:L:1287:BPH:HBB2	3:M:210:TYR:HB3	1.87	0.56
2:L:181:PHE:HB3	7:M:1317:BPH:CBB	2.36	0.56
1:H:26:GLY:HA3	13:M:1320:CDL:H171	1.87	0.55
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.87	0.55
7:M:1317:BPH:HBC2	7:M:1317:BPH:HHH	1.89	0.55
1:H:62:LYS:NZ	4:H:1261:GOL:H11	2.21	0.55
7:M:1317:BPH:HBB3	7:M:1317:BPH:CHC	2.35	0.55
3:M:208:PHE:O	3:M:212:SER:HB3	2.07	0.54
2:L:193:LEU:HD23	8:L:1288[A]:U10:C2	2.38	0.54
3:M:144:LYS:N	13:M:1320:CDL:OB3	2.31	0.54
3:M:189:PHE:O	3:M:193:HIS:CD2	2.57	0.53
8:M:1318:U10:O3	8:M:1318:U10:H4M2	2.08	0.53
3:M:149:ALA:HB2	3:M:270:ILE:HD11	1.91	0.53
1:H:209:SER:OG	1:H:247:LYS:HD3	2.09	0.53
1:H:75:VAL:HA	1:H:76:PRO:C	2.35	0.52
5:M:1309:BCL:HAA2	5:M:1309:BCL:HBD	1.92	0.52
3:M:243:THR:O	3:M:247:ARG:HG3	2.10	0.52
3:M:77:GLN:HE22	3:M:93:SER:H	1.58	0.51
2:L:166:ASN:N	2:L:166:ASN:HD22	2.08	0.51
8:M:1318:U10:H33	8:M:1318:U10:H403	1.91	0.51
7:L:1287:BPH:CBB	7:L:1287:BPH:CHC	2.81	0.51
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.29	0.50
2:L:224:ILE:HG22	8:L:1288[A]:U10:C8	2.41	0.50
3:M:195:ASN:HD22	3:M:195:ASN:C	2.18	0.50
3:M:77:GLN:NE2	3:M:92:PHE:HB3	2.26	0.50
3:M:109:LEU:O	3:M:114:LEU:HB2	2.11	0.50
1:H:112:ALA:HA	1:H:235:GLY:O	2.12	0.50
3:M:167:LEU:HD12	3:M:285:LEU:HD11	1.94	0.49
3:M:300:ASN:O	3:M:304:ALA:HB3	2.11	0.49
2:L:128:TYR:HD1	5:L:1283:BCL:HBB1	1.76	0.49
2:L:158:SER:HB2	3:M:197:PHE:CZ	2.49	0.48
2:L:212:GLU:HB3	8:L:1288[A]:U10:H4M3	1.95	0.48
6:M:1313:LDA:H51	8:M:1318:U10:H23	1.96	0.48
3:M:194:GLY:O	3:M:195:ASN:HB3	2.12	0.48
2:L:216:PHE:CE1	8:L:1288[B]:U10:H3M2	2.49	0.47
3:M:77:GLN:HE21	3:M:92:PHE:HB3	1.79	0.47
13:M:1320:CDL:C33	13:M:1320:CDL:H341	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.96	0.46
1:H:62:LYS:HZ2	4:H:1261:GOL:H11	1.79	0.46
13:M:1320:CDL:C37	13:M:1320:CDL:H351	2.44	0.46
1:H:169:VAL:HG23	1:H:171:ILE:HD13	1.97	0.46
1:H:62:LYS:HE3	4:H:1261:GOL:H12	1.98	0.46
3:M:164:ARG:HD2	3:M:284:ILE:HD12	1.98	0.46
3:M:305:PRO:C	3:M:307:ASN:H	2.21	0.46
1:H:220:LYS:NZ	14:H:2142:HOH:O	2.49	0.46
1:H:11:ASP:O	1:H:14:SER:HB2	2.16	0.45
6:M:1313:LDA:HM13	6:M:1313:LDA:H22	1.71	0.45
14:H:2002:HOH:O	13:M:1320:CDL:HA32	2.15	0.45
8:L:1288[B]:U10:H101	8:L:1288[B]:U10:H121	1.63	0.45
6:M:1312:LDA:H12	6:M:1313:LDA:HM22	1.98	0.45
2:L:208:THR:HB	2:L:209:PRO:HD2	1.99	0.44
3:M:132:ARG:HB2	14:M:2073:HOH:O	2.16	0.44
1:H:197:LYS:HE3	1:H:199:GLN:NE2	2.32	0.44
2:L:38:THR:HG21	2:L:100:TRP:HE3	1.83	0.44
5:M:1308:BCL:HHC	5:M:1308:BCL:HBB3	1.99	0.44
3:M:161:GLY:HA3	12:M:1319:SPO:H292	2.00	0.44
13:M:1320:CDL:C19	13:M:1320:CDL:H171	2.43	0.44
1:H:62:LYS:HE3	4:H:1261:GOL:C1	2.48	0.43
3:M:278:LEU:HD21	13:M:1320:CDL:H782	2.00	0.43
1:H:251:VAL:C	1:H:253:ALA:H	2.26	0.43
13:M:1320:CDL:H322	13:M:1320:CDL:H111	2.01	0.43
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.67	0.43
1:H:140:PHE:HA	3:M:13:ARG:O	2.18	0.43
5:L:1283:BCL:CAD	3:M:206:ILE:HG12	2.50	0.42
6:M:1314:LDA:C8	6:M:1314:LDA:H102	2.46	0.42
5:L:1283:BCL:HBB2	5:L:1283:BCL:CHC	2.49	0.42
3:M:196:LEU:HD12	3:M:196:LEU:HA	1.88	0.42
3:M:71:GLY:HA3	12:M:1319:SPO:C6	2.47	0.41
1:H:197:LYS:HE3	1:H:199:GLN:HE21	1.85	0.41
6:L:1286:LDA:H121	8:L:1288[A]:U10:C16	2.51	0.41
2:L:53:ALA:HB1	2:L:58:THR:O	2.20	0.41
3:M:21:THR:HG23	3:M:26:LEU:HD21	2.01	0.41
2:L:166:ASN:N	2:L:166:ASN:ND2	2.69	0.41
3:M:256:MET:CE	8:M:1318:U10:H102	2.51	0.41
6:M:1312:LDA:HM11	6:M:1312:LDA:H22	1.79	0.41
3:M:195:ASN:ND2	3:M:197:PHE:H	2.19	0.40
13:M:1320:CDL:C33	13:M:1320:CDL:H342	2.19	0.40
3:M:114:LEU:HD12	3:M:114:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1287:BPH:NC	7:L:1287:BPH:ND	2.68	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	259/260 (100%)	249 (96%)	6 (2%)	4 (2%)	8	2
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
3	M	306/307 (100%)	292 (95%)	12 (4%)	2 (1%)	18	10
All	All	844/848 (100%)	813 (96%)	25 (3%)	6 (1%)	18	10

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	13	ALA
1	H	252	VAL
1	H	257	ALA
3	M	195	ASN
1	H	8	GLY
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	209/208 (100%)	200 (96%)	9 (4%)	26	20
2	L	220/220 (100%)	211 (96%)	9 (4%)	27	21
3	M	241/240 (100%)	228 (95%)	13 (5%)	20	12
All	All	670/668 (100%)	639 (95%)	31 (5%)	24	17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	VAL
1	H	7	PHE
1	H	9	ASN
1	H	11	ASP
1	H	163	LYS
1	H	201	ASN
1	H	231	ASP
1	H	252	VAL
1	H	255	MET
2	L	20	ASN
2	L	72	GLU
2	L	157	VAL
2	L	162	TYR
2	L	166	ASN
2	L	207	ARG
2	L	210	ASP
2	L	247	CYS
2	L	268	LYS
3	M	39	LEU
3	M	55	LEU
3	M	72	ILE
3	M	183	LEU
3	M	196	LEU
3	M	197	PHE
3	M	206	ILE
3	M	216	PHE
3	M	270	ILE
3	M	274	VAL
3	M	284	ILE
3	M	290	VAL
3	M	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	44	ASN
1	H	98	HIS
1	H	201	ASN
2	L	20	ASN
2	L	56	GLN
2	L	153	HIS
2	L	159	ASN
2	L	166	ASN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	195	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 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	$\# Z > 2$
8	U10	M	1318	-	46,47,63	2.86	13 (28%)	53,59,79	1.73	13 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	L	1283	-	69,74,74	1.73	9 (13%)	79,115,115	2.11	25 (31%)
4	GOL	L	1294	-	5,5,5	0.37	0	5,5,5	0.28	0
6	LDA	L	1284	-	13,15,15	2.11	2 (15%)	14,17,17	0.51	0
4	GOL	H	1264	-	5,5,5	0.39	0	5,5,5	0.27	0
6	LDA	L	1285	-	13,15,15	2.07	2 (15%)	14,17,17	0.51	0
6	LDA	M	1312	-	13,15,15	2.01	2 (15%)	14,17,17	0.54	0
4	GOL	L	1293	-	5,5,5	0.40	0	5,5,5	0.28	0
7	BPH	L	1287	-	59,70,70	2.69	12 (20%)	59,101,101	2.58	18 (30%)
8	U10	L	1288[A]	-	23,23,63	2.61	7 (30%)	30,31,79	1.91	8 (26%)
4	GOL	H	1263	-	5,5,5	0.46	0	5,5,5	0.18	0
9	PO4	L	1289	-	4,4,4	0.89	0	6,6,6	0.83	0
6	LDA	L	1286	-	13,15,15	2.25	2 (15%)	14,17,17	0.56	0
6	LDA	M	1311	-	13,15,15	2.15	2 (15%)	14,17,17	0.54	0
6	LDA	M	1315	-	13,15,15	2.32	3 (23%)	14,17,17	0.83	0
10	HTO	L	1290	-	9,9,9	0.54	0	10,10,10	0.63	0
4	GOL	H	1262	-	5,5,5	0.53	0	5,5,5	0.53	0
10	HTO	L	1291	-	9,9,9	0.35	0	10,10,10	0.81	0
7	BPH	M	1317	-	59,70,70	2.67	12 (20%)	59,101,101	2.57	19 (32%)
5	BCL	M	1309	3	69,74,74	1.86	10 (14%)	79,115,115	1.92	20 (25%)
6	LDA	M	1314	-	13,15,15	3.04	5 (38%)	14,17,17	1.42	3 (21%)
4	GOL	H	1261	-	5,5,5	0.60	0	5,5,5	0.92	0
5	BCL	L	1282	2	69,74,74	1.85	9 (13%)	79,115,115	1.97	21 (26%)
6	LDA	M	1313	-	13,15,15	2.28	2 (15%)	14,17,17	0.65	0
13	CDL	M	1320	-	80,80,99	2.26	19 (23%)	86,92,111	1.79	18 (20%)
4	GOL	L	1292	-	5,5,5	0.43	0	5,5,5	1.00	0
5	BCL	M	1308	3	69,74,74	1.79	7 (10%)	79,115,115	1.82	14 (17%)
12	SPO	M	1319	-	41,41,41	2.61	12 (29%)	47,50,50	2.27	16 (34%)
8	U10	L	1288[B]	-	23,23,63	2.70	7 (30%)	30,31,79	1.35	4 (13%)
6	LDA	M	1310	-	13,15,15	2.02	2 (15%)	14,17,17	0.72	1 (7%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	U10	M	1318	-	-	13/45/65/87	0/1/1/1
5	BCL	L	1283	-	2/2/21/25	8/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	L	1294	-	-	2/4/4/4	-
6	LDA	L	1284	-	-	6/13/13/13	-
4	GOL	H	1264	-	-	1/4/4/4	-
6	LDA	L	1285	-	-	10/13/13/13	-
6	LDA	M	1312	-	-	8/13/13/13	-
4	GOL	L	1293	-	-	2/4/4/4	-
7	BPH	L	1287	-	-	5/37/105/105	0/5/6/6
8	U10	L	1288[A]	-	-	7/15/39/87	0/1/1/1
4	GOL	H	1263	-	-	0/4/4/4	-
6	LDA	L	1286	-	-	6/13/13/13	-
6	LDA	M	1311	-	-	9/13/13/13	-
6	LDA	M	1315	-	-	8/13/13/13	-
10	HTO	L	1290	-	-	9/10/10/10	-
4	GOL	H	1262	-	-	2/4/4/4	-
10	HTO	L	1291	-	-	7/10/10/10	-
7	BPH	M	1317	-	-	18/37/105/105	0/5/6/6
5	BCL	M	1309	3	2/2/21/25	8/41/137/137	-
6	LDA	M	1314	-	-	3/13/13/13	-
4	GOL	H	1261	-	-	2/4/4/4	-
5	BCL	L	1282	2	2/2/21/25	9/41/137/137	-
6	LDA	M	1313	-	-	7/13/13/13	-
13	CDL	M	1320	-	-	49/91/91/110	-
4	GOL	L	1292	-	-	2/4/4/4	-
5	BCL	M	1308	3	2/2/21/25	12/41/137/137	-
12	SPO	M	1319	-	-	9/47/47/47	-
8	U10	L	1288[B]	-	-	8/15/39/87	0/1/1/1
6	LDA	M	1310	-	-	5/13/13/13	-

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1317	BPH	OBD-CAD	12.46	1.38	1.22
7	L	1287	BPH	OBD-CAD	12.24	1.38	1.22
5	M	1309	BCL	OBD-CAD	10.37	1.40	1.22
5	L	1282	BCL	OBD-CAD	9.68	1.39	1.22
5	M	1308	BCL	OBD-CAD	9.37	1.38	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	1283	BCL	OBD-CAD	9.21	1.38	1.22
7	L	1287	BPH	OBB-CAB	7.02	1.43	1.22
7	L	1287	BPH	O1D-CGD	6.96	1.38	1.21
7	M	1317	BPH	O1D-CGD	6.85	1.38	1.21
6	L	1286	LDA	O1-N1	-6.75	1.25	1.42
5	L	1282	BCL	O1A-CGA	6.70	1.42	1.22
8	L	1288[B]	U10	C8-C9	6.69	1.48	1.33
6	M	1313	LDA	O1-N1	-6.68	1.25	1.42
8	M	1318	U10	C3-C4	6.66	1.43	1.36
6	M	1315	LDA	O1-N1	-6.65	1.25	1.42
8	M	1318	U10	C33-C34	6.62	1.48	1.33
8	L	1288[A]	U10	C8-C9	6.60	1.48	1.33
6	M	1314	LDA	O1-N1	-6.58	1.26	1.42
6	L	1285	LDA	O1-N1	-6.56	1.26	1.42
6	M	1310	LDA	O1-N1	-6.56	1.26	1.42
6	L	1284	LDA	O1-N1	-6.55	1.26	1.42
7	L	1287	BPH	C2-C3	6.52	1.48	1.33
6	M	1311	LDA	O1-N1	-6.51	1.26	1.42
12	M	1319	SPO	C32-C33	6.38	1.47	1.33
13	M	1320	CDL	C18-C17	6.32	1.83	1.51
7	M	1317	BPH	C2-C3	6.31	1.47	1.33
13	M	1320	CDL	C35-C34	6.28	1.83	1.51
7	M	1317	BPH	OBB-CAB	6.23	1.41	1.22
8	M	1318	U10	C8-C9	6.13	1.47	1.33
6	M	1312	LDA	O1-N1	-6.12	1.27	1.42
8	M	1318	U10	C23-C24	6.09	1.47	1.33
7	L	1287	BPH	O1A-CGA	6.02	1.40	1.22
8	M	1318	U10	C28-C29	6.00	1.46	1.33
8	M	1318	U10	C13-C14	5.91	1.46	1.33
13	M	1320	CDL	OA6-CA5	5.87	1.50	1.34
8	M	1318	U10	C6-C1	5.77	1.42	1.34
7	M	1317	BPH	O1A-CGA	5.71	1.39	1.22
5	M	1308	BCL	O1A-CGA	5.70	1.39	1.22
13	M	1320	CDL	C37-C36	5.68	1.80	1.51
8	M	1318	U10	C18-C19	5.61	1.46	1.33
12	M	1319	SPO	C37-C38	5.60	1.49	1.32
5	M	1309	BCL	O1A-CGA	5.54	1.39	1.22
5	L	1283	BCL	O1A-CGA	5.42	1.38	1.22
8	L	1288[A]	U10	C13-C14	5.30	1.48	1.32
8	M	1318	U10	C38-C39	5.28	1.48	1.32
6	M	1314	LDA	C9-C8	5.27	1.78	1.51
12	M	1319	SPO	C9-C7	5.24	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	1288[B]	U10	O4-C4	-5.21	1.24	1.36
13	M	1320	CDL	OA8-CA7	5.20	1.48	1.33
12	M	1319	SPO	C19-C17	5.19	1.47	1.35
8	L	1288[B]	U10	O3-C3	-5.18	1.24	1.36
7	M	1317	BPH	C3D-C2D	5.13	1.48	1.39
8	L	1288[A]	U10	O4-C4	-5.12	1.24	1.36
8	L	1288[B]	U10	C13-C14	5.06	1.47	1.32
12	M	1319	SPO	C6-C5	5.02	1.46	1.32
13	M	1320	CDL	OB6-CB5	5.00	1.48	1.34
13	M	1320	CDL	OB8-CB7	4.98	1.47	1.33
13	M	1320	CDL	C11-CA5	-4.98	1.36	1.50
12	M	1319	SPO	C22-C23	4.76	1.46	1.35
13	M	1320	CDL	C20-C19	-4.70	1.28	1.51
6	M	1313	LDA	C1-N1	-4.68	1.46	1.51
7	M	1317	BPH	C3D-CAD	-4.67	1.38	1.47
13	M	1320	CDL	C34-C33	4.63	1.74	1.51
12	M	1319	SPO	C14-C12	4.61	1.46	1.35
7	L	1287	BPH	C3D-CAD	-4.61	1.38	1.47
7	L	1287	BPH	C3D-C2D	4.47	1.47	1.39
12	M	1319	SPO	C10-C11	4.44	1.46	1.34
6	M	1314	LDA	C8-C7	4.43	1.73	1.51
6	L	1286	LDA	C1-N1	-4.40	1.46	1.51
8	L	1288[A]	U10	O3-C3	-4.17	1.26	1.36
5	M	1308	BCL	C3D-C4D	-4.12	1.34	1.44
6	M	1314	LDA	C1-N1	-4.10	1.47	1.51
6	M	1311	LDA	C1-N1	-4.10	1.47	1.51
13	M	1320	CDL	C12-C11	4.00	1.66	1.52
12	M	1319	SPO	C15-C16	3.96	1.45	1.34
6	M	1312	LDA	C1-N1	-3.78	1.47	1.51
12	M	1319	SPO	C26-C25	3.77	1.44	1.34
6	L	1284	LDA	C1-N1	-3.71	1.47	1.51
6	M	1315	LDA	C1-N1	-3.65	1.47	1.51
5	M	1309	BCL	C3D-C4D	-3.61	1.36	1.44
12	M	1319	SPO	C27-C28	3.56	1.46	1.35
7	L	1287	BPH	C3D-C4D	-3.52	1.36	1.41
7	L	1287	BPH	O2D-CGD	-3.52	1.24	1.33
5	L	1282	BCL	C2-C3	3.47	1.41	1.33
12	M	1319	SPO	C21-C20	3.46	1.45	1.36
13	M	1320	CDL	C79-C78	-3.43	1.34	1.51
5	L	1282	BCL	C3D-C4D	-3.40	1.36	1.44
8	L	1288[B]	U10	C6-C1	3.39	1.41	1.35
5	L	1283	BCL	C2-C3	3.37	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1320	CDL	C22-C21	-3.36	1.35	1.51
13	M	1320	CDL	C80-C79	-3.35	1.35	1.51
6	L	1285	LDA	C1-N1	-3.31	1.48	1.51
8	M	1318	U10	O3-C3	-3.28	1.28	1.36
7	M	1317	BPH	CBD-CGD	-3.25	1.48	1.52
8	L	1288[A]	U10	C3-C2	-3.20	1.39	1.48
5	M	1308	BCL	C2-C3	3.17	1.40	1.33
5	L	1283	BCL	C3D-C4D	-3.11	1.37	1.44
5	M	1309	BCL	C2-C3	3.08	1.40	1.33
8	M	1318	U10	O4-C4	-3.08	1.27	1.36
7	M	1317	BPH	O2D-CGD	-3.07	1.25	1.33
8	L	1288[B]	U10	C3-C2	-3.00	1.40	1.48
5	M	1309	BCL	OBG-CAB	2.90	1.29	1.23
5	L	1282	BCL	O2D-CGD	-2.82	1.26	1.33
5	M	1308	BCL	O2D-CGD	-2.81	1.26	1.33
8	L	1288[B]	U10	C4-C5	-2.76	1.40	1.48
8	M	1318	U10	C1-C2	-2.74	1.37	1.47
5	M	1309	BCL	O2D-CGD	-2.74	1.26	1.33
8	M	1318	U10	C5-C6	-2.72	1.44	1.50
7	M	1317	BPH	C4D-ND	-2.64	1.34	1.38
5	L	1282	BCL	O2A-CGA	-2.64	1.25	1.33
8	L	1288[A]	U10	C6-C1	2.60	1.39	1.35
13	M	1320	CDL	C36-C35	2.59	1.64	1.51
5	M	1308	BCL	C1D-C2D	-2.58	1.40	1.45
7	L	1287	BPH	O2A-CGA	-2.56	1.25	1.33
13	M	1320	CDL	C32-C31	2.53	1.61	1.52
13	M	1320	CDL	C33-C32	2.51	1.64	1.51
7	L	1287	BPH	C3A-C2A	-2.50	1.52	1.54
5	L	1282	BCL	CHD-C4C	2.48	1.46	1.39
5	L	1283	BCL	O2D-CGD	-2.47	1.27	1.33
6	M	1315	LDA	C3-C2	2.46	1.64	1.51
8	L	1288[A]	U10	C4-C5	-2.45	1.41	1.48
13	M	1320	CDL	C13-C12	-2.43	1.39	1.51
7	M	1317	BPH	O2A-CGA	-2.38	1.26	1.33
6	M	1310	LDA	C1-N1	-2.36	1.49	1.51
5	M	1309	BCL	CHD-C4C	2.35	1.45	1.39
5	L	1283	BCL	O2A-CGA	-2.35	1.26	1.33
7	M	1317	BPH	C3D-C4D	-2.32	1.38	1.41
5	L	1283	BCL	CHD-C4C	2.28	1.45	1.39
5	M	1309	BCL	C1B-NB	2.25	1.40	1.37
5	L	1282	BCL	C1D-C2D	-2.23	1.40	1.45
5	L	1283	BCL	C1D-C2D	-2.22	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1308	BCL	CHD-C4C	2.19	1.45	1.39
6	M	1314	LDA	C12-C11	2.16	1.65	1.50
5	L	1283	BCL	O1D-CGD	2.14	1.26	1.21
5	M	1309	BCL	MG-NA	2.07	2.11	2.06
13	M	1320	CDL	C15-C14	2.05	1.62	1.51
5	L	1282	BCL	CHC-C4B	2.05	1.44	1.39
5	M	1309	BCL	O2A-CGA	-2.04	1.27	1.33
7	L	1287	BPH	CBB-CAB	-2.02	1.43	1.49

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1317	BPH	O2D-CGD-CBD	9.94	121.87	110.95
7	L	1287	BPH	O2D-CGD-CBD	7.89	119.61	110.95
7	L	1287	BPH	C2B-C1B-NB	7.87	115.12	109.43
7	M	1317	BPH	C2B-C1B-NB	7.35	114.74	109.43
7	L	1287	BPH	C2D-C1D-ND	6.55	114.16	109.43
7	M	1317	BPH	C2D-C1D-ND	6.42	114.07	109.43
5	L	1283	BCL	C4A-NA-C1A	6.14	109.48	106.68
5	L	1283	BCL	O2D-CGD-CBD	5.99	121.71	111.23
5	M	1308	BCL	C1D-ND-C4D	5.96	110.50	106.31
13	M	1320	CDL	C13-C12-C11	5.78	134.38	113.13
12	M	1319	SPO	C26-C27-C28	-5.70	119.68	127.69
13	M	1320	CDL	OA6-CA5-C11	5.48	123.33	111.48
5	L	1282	BCL	C1C-NC-C4C	-5.26	104.28	106.68
5	M	1308	BCL	CMB-C2B-C1B	-5.25	117.42	125.42
5	L	1283	BCL	C1D-ND-C4D	5.23	109.98	106.31
5	M	1308	BCL	C1-O2A-CGA	5.23	129.32	116.65
5	L	1282	BCL	C1D-ND-C4D	5.19	109.96	106.31
7	L	1287	BPH	C4D-ND-C1D	-5.19	102.66	108.87
5	L	1282	BCL	CMD-C2D-C1D	5.19	133.86	124.73
7	L	1287	BPH	C3D-C4D-ND	5.10	114.25	107.71
5	M	1308	BCL	O2D-CGD-CBD	5.09	120.12	111.23
5	L	1283	BCL	CMD-C2D-C1D	5.03	133.59	124.73
7	M	1317	BPH	C3D-C4D-ND	5.02	114.15	107.71
5	M	1309	BCL	O2D-CGD-CBD	5.00	119.97	111.23
5	M	1309	BCL	CED-O2D-CGD	4.91	127.05	115.92
13	M	1320	CDL	C20-C19-C18	4.90	139.15	114.37
5	M	1309	BCL	CMB-C2B-C1B	-4.85	118.04	125.42
8	L	1288[A]	U10	C7-C6-C1	-4.81	116.65	124.89
7	L	1287	BPH	C1B-NB-C4B	-4.78	101.85	108.82
12	M	1319	SPO	C15-C14-C12	-4.74	120.63	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	CMB-C2B-C1B	-4.72	118.23	125.42
5	M	1309	BCL	CMD-C2D-C1D	4.70	133.00	124.73
12	M	1319	SPO	C10-C9-C7	-4.67	120.73	127.28
5	M	1309	BCL	C1D-ND-C4D	4.56	109.51	106.31
7	L	1287	BPH	CED-O2D-CGD	4.51	126.15	115.92
7	M	1317	BPH	OBD-CAD-CBD	-4.43	119.32	125.82
7	M	1317	BPH	C4D-ND-C1D	-4.43	103.57	108.87
12	M	1319	SPO	C21-C22-C23	-4.31	121.23	127.28
12	M	1319	SPO	C20-C19-C17	-4.30	121.24	127.28
5	M	1308	BCL	C2D-C1D-ND	-4.22	105.95	110.13
5	L	1283	BCL	CMB-C2B-C1B	-4.13	119.13	125.42
8	M	1318	U10	O4-C4-C3	-4.12	119.65	127.53
8	M	1318	U10	C10-C9-C11	3.96	122.11	115.23
13	M	1320	CDL	CA4-OA6-CA5	-3.94	108.37	117.80
5	L	1283	BCL	O2A-CGA-CBA	3.94	123.83	111.83
8	L	1288[A]	U10	C1M-C1-C6	-3.79	118.21	124.45
5	L	1282	BCL	C2B-C1B-NB	-3.76	106.43	110.33
7	L	1287	BPH	C4C-C3C-C2C	-3.73	99.29	102.84
5	M	1309	BCL	O2A-CGA-CBA	3.72	123.18	111.83
12	M	1319	SPO	C29-C28-C30	3.68	121.62	115.23
12	M	1319	SPO	C4-C5-C6	-3.66	119.78	124.91
13	M	1320	CDL	OB6-CB5-C51	3.54	119.13	111.48
8	M	1318	U10	C30-C29-C31	3.53	121.35	115.23
5	M	1309	BCL	C2D-C1D-ND	-3.52	106.65	110.13
13	M	1320	CDL	C19-C18-C17	-3.51	96.61	114.37
13	M	1320	CDL	C35-C34-C33	3.49	131.99	114.37
5	L	1282	BCL	C2D-C1D-ND	-3.43	106.73	110.13
5	L	1282	BCL	CMD-C2D-C3D	-3.41	119.87	127.69
13	M	1320	CDL	OA6-CA5-OA7	-3.40	115.76	123.70
5	L	1282	BCL	O2D-CGD-CBD	3.31	117.02	111.23
13	M	1320	CDL	C33-C32-C31	3.30	125.26	113.13
8	L	1288[A]	U10	C10-C9-C11	3.29	120.94	115.23
7	M	1317	BPH	C1B-NB-C4B	-3.26	104.06	108.82
7	L	1287	BPH	CMA-C3A-C4A	-3.25	107.61	114.61
5	M	1309	BCL	CBB-CAB-C3B	-3.25	113.56	120.40
7	M	1317	BPH	O1D-CGD-CBD	-3.25	119.80	124.72
5	L	1283	BCL	C1-C2-C3	-3.23	120.91	126.20
5	L	1283	BCL	C6-C5-C3	-3.19	105.69	113.47
8	M	1318	U10	C35-C34-C36	3.19	120.76	115.23
13	M	1320	CDL	OA8-CA7-C31	3.18	121.54	111.83
13	M	1320	CDL	C37-C36-C35	-3.17	98.35	114.37
12	M	1319	SPO	C25-C23-C22	-3.16	114.04	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1287	BPH	O1D-CGD-CBD	-3.14	119.97	124.72
5	M	1308	BCL	C2B-C1B-NB	-3.13	107.08	110.33
5	M	1308	BCL	CMA-C3A-C4A	-3.13	103.36	111.77
5	L	1282	BCL	CED-O2D-CGD	3.12	123.00	115.92
7	M	1317	BPH	CMA-C3A-C4A	-3.12	107.90	114.61
6	M	1314	LDA	C9-C8-C7	-3.11	98.62	114.37
5	L	1283	BCL	C2B-C1B-NB	-3.11	107.10	110.33
8	M	1318	U10	C27-C28-C29	-3.09	120.56	127.62
5	L	1283	BCL	C2D-C1D-ND	-3.08	107.08	110.13
5	M	1309	BCL	C16-C15-C13	-3.02	105.92	115.97
12	M	1319	SPO	C14-C15-C16	-3.02	114.46	123.20
5	L	1282	BCL	O2A-CGA-CBA	3.01	121.01	111.83
7	M	1317	BPH	OBD-CAD-C3D	-2.98	123.24	127.89
5	M	1308	BCL	O1D-CGD-CBD	-2.97	118.65	124.52
8	M	1318	U10	C22-C23-C24	-2.97	120.82	127.62
5	M	1308	BCL	O2A-CGA-CBA	2.96	120.87	111.83
8	M	1318	U10	C15-C14-C16	2.96	120.37	115.23
5	L	1283	BCL	O1D-CGD-CBD	-2.95	118.70	124.52
7	M	1317	BPH	CBA-CAA-C2A	-2.94	105.11	113.78
5	L	1282	BCL	C11-C12-C13	2.92	125.68	115.97
7	M	1317	BPH	C4D-CHA-CBD	-2.90	107.06	108.45
12	M	1319	SPO	C13-C12-C11	2.89	122.50	118.09
5	L	1283	BCL	CMD-C2D-C3D	-2.88	121.08	127.69
13	M	1320	CDL	OB8-CB7-C71	2.87	120.57	111.83
7	M	1317	BPH	O2D-CGD-O1D	-2.86	118.29	123.85
8	M	1318	U10	C12-C13-C14	-2.82	121.18	127.62
5	M	1308	BCL	C1D-CHD-C4C	-2.81	119.84	126.62
5	L	1282	BCL	CMA-C3A-C4A	-2.80	104.26	111.77
5	M	1309	BCL	CMD-C2D-C3D	-2.80	121.28	127.69
7	L	1287	BPH	O2A-CGA-O1A	-2.79	116.65	123.63
5	L	1283	BCL	CED-O2D-CGD	2.79	122.24	115.92
5	L	1283	BCL	O2A-CGA-O1A	-2.77	116.70	123.63
5	L	1282	BCL	O2A-CGA-O1A	-2.72	116.81	123.63
5	L	1282	BCL	C1-O2A-CGA	2.72	123.24	116.65
8	L	1288[A]	U10	C3M-O3-C3	2.72	126.02	116.47
8	L	1288[A]	U10	C3-C2-C1	2.71	123.45	118.10
6	M	1314	LDA	C8-C7-C6	-2.70	100.73	114.37
7	L	1287	BPH	O2A-CGA-CBA	2.69	120.03	111.83
7	L	1287	BPH	C7-C6-C5	-2.69	106.10	113.26
5	L	1282	BCL	CAA-C2A-C1A	-2.68	103.18	111.97
7	L	1287	BPH	OBD-CAD-C3D	-2.67	123.72	127.89
8	L	1288[A]	U10	O2-C2-C3	-2.67	115.37	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1317	BPH	C1-O2A-CGA	2.64	123.04	116.65
5	L	1283	BCL	CAC-C3C-C4C	-2.62	106.77	112.58
5	L	1282	BCL	O2D-CGD-O1D	-2.61	118.76	123.85
5	L	1282	BCL	C3C-C4C-CHD	-2.61	117.89	123.39
5	L	1282	BCL	CHD-C1D-C2D	2.56	130.81	125.49
7	L	1287	BPH	C1-C2-C3	-2.56	122.01	126.20
5	L	1282	BCL	C14-C13-C12	2.54	120.33	111.27
5	L	1283	BCL	CAA-C2A-C1A	-2.52	103.70	111.97
5	L	1283	BCL	C3C-C4C-CHD	-2.52	118.07	123.39
13	M	1320	CDL	C18-C17-C16	-2.51	101.70	114.37
7	M	1317	BPH	O2A-CGA-CBA	2.50	119.45	111.83
7	M	1317	BPH	CED-O2D-CGD	2.49	121.56	115.92
12	M	1319	SPO	C34-C33-C35	2.48	119.54	115.23
12	M	1319	SPO	C5-C6-C7	-2.47	122.16	125.89
5	M	1308	BCL	CMB-C2B-C3B	2.45	133.41	125.67
5	M	1309	BCL	C2B-C1B-NB	-2.44	107.80	110.33
5	L	1282	BCL	C2A-C3A-C4A	2.44	105.81	101.87
5	M	1309	BCL	C1C-NC-C4C	2.44	107.79	106.68
7	L	1287	BPH	C3B-C4B-NB	2.42	111.57	108.05
5	M	1309	BCL	C1-C2-C3	-2.42	122.23	126.20
8	L	1288[B]	U10	C7-C6-C1	-2.41	120.76	124.89
5	M	1308	BCL	CAA-C2A-C3A	-2.40	106.51	113.00
8	L	1288[A]	U10	C4-C3-C2	-2.39	116.31	120.69
7	L	1287	BPH	OB8-CAB-C3B	2.39	123.98	119.99
8	M	1318	U10	C25-C24-C26	2.38	119.36	115.23
8	L	1288[B]	U10	C10-C9-C11	2.36	119.33	115.23
12	M	1319	SPO	C40-C38-C39	2.35	119.99	114.59
5	M	1309	BCL	O1D-CGD-CBD	-2.34	119.90	124.52
5	M	1308	BCL	C3C-C4C-CHD	-2.34	118.46	123.39
5	L	1283	BCL	CHD-C1D-ND	-2.32	121.54	124.80
13	M	1320	CDL	OB8-CB7-OB9	-2.31	117.86	123.63
7	M	1317	BPH	OB8-CAB-C3B	2.30	123.84	119.99
12	M	1319	SPO	C24-C23-C25	2.30	121.60	118.09
13	M	1320	CDL	C34-C33-C32	2.30	125.97	114.37
13	M	1320	CDL	OA8-CA7-OA9	-2.28	117.92	123.63
7	M	1317	BPH	C1C-C2C-C3C	-2.27	100.68	102.84
5	L	1283	BCL	C3C-C2C-C1C	-2.25	98.24	101.87
13	M	1320	CDL	C12-C11-CA5	2.23	121.86	113.69
5	M	1309	BCL	CAB-C3B-C2B	-2.23	123.12	127.74
5	L	1283	BCL	CHA-C1A-NA	-2.22	121.36	126.39
8	M	1318	U10	C17-C18-C19	-2.22	122.55	127.62
5	M	1309	BCL	C1D-CHD-C4C	-2.22	121.27	126.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1309	BCL	C4A-NA-C1A	2.21	107.69	106.68
5	L	1282	BCL	C4A-NA-C1A	2.21	107.69	106.68
5	M	1309	BCL	CMB-C2B-C3B	2.20	132.61	125.67
13	M	1320	CDL	C80-C79-C78	2.20	125.48	114.37
5	L	1283	BCL	O2D-CGD-O1D	-2.19	119.59	123.85
8	L	1288[B]	U10	C16-C14-C15	2.17	119.59	114.59
7	L	1287	BPH	CBB-CAB-C3B	-2.17	113.84	120.34
5	M	1308	BCL	CHA-C1A-NA	-2.15	121.52	126.39
8	M	1318	U10	C22-C21-C19	-2.15	106.06	113.19
8	L	1288[A]	U10	C12-C13-C14	-2.11	120.59	127.64
5	L	1283	BCL	C2A-C3A-C4A	2.11	105.28	101.87
12	M	1319	SPO	C27-C26-C25	-2.10	117.12	123.20
8	M	1318	U10	C32-C33-C34	-2.09	122.83	127.62
5	M	1309	BCL	C3C-C4C-CHD	-2.09	119.00	123.39
5	L	1283	BCL	C4-C3-C5	2.08	118.84	115.23
6	M	1314	LDA	C10-C9-C8	-2.08	103.86	114.37
12	M	1319	SPO	C8-C7-C6	2.07	121.26	118.09
8	L	1288[B]	U10	C12-C13-C14	-2.06	120.78	127.64
5	M	1309	BCL	CAA-CBA-CGA	-2.06	107.37	113.21
5	L	1283	BCL	CHB-C4A-NA	-2.04	121.45	124.40
7	M	1317	BPH	C4A-C3A-C2A	-2.02	100.91	102.84
6	M	1310	LDA	O1-N1-C1	2.02	114.23	109.27
8	M	1318	U10	C41-C39-C40	2.02	119.23	114.59
5	L	1283	BCL	CHD-C1D-C2D	2.01	129.67	125.49

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	L	1283	BCL	C8
5	L	1283	BCL	C13
5	M	1308	BCL	C8
5	M	1308	BCL	C13
5	M	1309	BCL	C8
5	M	1309	BCL	C13

All (235) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1261	GOL	O1-C1-C2-C3
4	H	1262	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	L	1292	GOL	C1-C2-C3-O3
4	L	1293	GOL	O1-C1-C2-C3
5	M	1308	BCL	C1-C2-C3-C4
5	M	1308	BCL	C1-C2-C3-C5
6	L	1285	LDA	C2-C1-N1-O1
6	M	1310	LDA	C2-C1-N1-O1
6	M	1310	LDA	C2-C1-N1-CM1
6	M	1311	LDA	C2-C1-N1-CM1
6	M	1311	LDA	C2-C1-N1-CM2
6	M	1313	LDA	C2-C1-N1-CM1
6	M	1313	LDA	N1-C1-C2-C3
6	M	1315	LDA	C2-C1-N1-CM2
7	M	1317	BPH	C4C-C3C-CAC-CBC
7	M	1317	BPH	C2C-C3C-CAC-CBC
8	L	1288[A]	U10	C7-C8-C9-C10
8	L	1288[A]	U10	C7-C8-C9-C11
8	L	1288[B]	U10	C12-C11-C9-C10
8	M	1318	U10	C27-C28-C29-C30
8	M	1318	U10	C27-C28-C29-C31
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	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
12	M	1319	SPO	C5-C6-C7-C9
12	M	1319	SPO	C22-C23-C25-C26
12	M	1319	SPO	C36-C37-C38-C39
12	M	1319	SPO	C36-C37-C38-C40
13	M	1320	CDL	CA3-OA5-PA1-OA2
13	M	1320	CDL	CA3-OA5-PA1-OA3
13	M	1320	CDL	CA3-OA5-PA1-OA4
13	M	1320	CDL	CB3-OB5-PB2-OB2
13	M	1320	CDL	CB3-OB5-PB2-OB3
13	M	1320	CDL	CB3-OB5-PB2-OB4
13	M	1320	CDL	OA9-CA7-OA8-CA6
8	L	1288[A]	U10	C12-C13-C14-C16
8	L	1288[B]	U10	C12-C13-C14-C15
8	L	1288[B]	U10	C12-C13-C14-C16
13	M	1320	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
13	M	1320	CDL	OB9-CB7-OB8-CB6
8	L	1288[B]	U10	C12-C11-C9-C8
13	M	1320	CDL	C71-CB7-OB8-CB6
13	M	1320	CDL	C78-C79-C80-C81
8	L	1288[B]	U10	C7-C8-C9-C10
8	M	1318	U10	C32-C33-C34-C35
8	L	1288[B]	U10	C7-C8-C9-C11
8	M	1318	U10	C32-C33-C34-C36
10	L	1291	HTO	O1-C1-C2-C3
13	M	1320	CDL	C20-C21-C22-C23
8	M	1318	U10	C37-C38-C39-C41
8	M	1318	U10	C24-C26-C27-C28
8	L	1288[A]	U10	C12-C13-C14-C15
5	L	1282	BCL	C11-C12-C13-C14
5	L	1283	BCL	C6-C7-C8-C9
5	M	1309	BCL	C11-C10-C8-C9
12	M	1319	SPO	C5-C6-C7-C8
12	M	1319	SPO	C24-C23-C25-C26
13	M	1320	CDL	C11-CA5-OA6-CA4
10	L	1291	HTO	O1-C1-C2-O2
5	M	1308	BCL	C2-C1-O2A-CGA
8	M	1318	U10	C37-C38-C39-C40
4	H	1261	GOL	O1-C1-C2-O2
5	L	1282	BCL	C11-C10-C8-C7
12	M	1319	SPO	C33-C35-C36-C37
5	L	1282	BCL	C13-C15-C16-C17
5	L	1283	BCL	C13-C15-C16-C17
13	M	1320	CDL	OA7-CA5-OA6-CA4
5	L	1282	BCL	C15-C16-C17-C18
7	M	1317	BPH	C15-C16-C17-C18
7	M	1317	BPH	C10-C11-C12-C13
5	L	1283	BCL	C3-C5-C6-C7
5	M	1309	BCL	C13-C15-C16-C17
4	L	1294	GOL	C1-C2-C3-O3
7	L	1287	BPH	C8-C10-C11-C12
5	M	1309	BCL	C16-C17-C18-C20
7	M	1317	BPH	C16-C17-C18-C19
5	L	1282	BCL	C10-C11-C12-C13
5	M	1308	BCL	C8-C10-C11-C12
13	M	1320	CDL	C71-C72-C73-C74
6	L	1284	LDA	C3-C4-C5-C6
6	L	1284	LDA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	M	1320	CDL	C17-C18-C19-C20
4	L	1293	GOL	O1-C1-C2-O2
6	M	1315	LDA	C3-C4-C5-C6
6	M	1313	LDA	C2-C3-C4-C5
13	M	1320	CDL	O1-C1-CB2-OB2
6	M	1313	LDA	C3-C4-C5-C6
6	L	1286	LDA	C2-C3-C4-C5
6	M	1313	LDA	C6-C7-C8-C9
6	L	1285	LDA	C7-C8-C9-C10
6	M	1310	LDA	C2-C3-C4-C5
6	M	1312	LDA	C7-C8-C9-C10
13	M	1320	CDL	C33-C34-C35-C36
6	M	1312	LDA	C6-C7-C8-C9
13	M	1320	CDL	C16-C17-C18-C19
6	M	1311	LDA	C4-C5-C6-C7
13	M	1320	CDL	CA5-C11-C12-C13
6	L	1286	LDA	C4-C5-C6-C7
6	M	1314	LDA	C2-C3-C4-C5
6	L	1285	LDA	C1-C2-C3-C4
5	M	1309	BCL	C16-C17-C18-C19
7	M	1317	BPH	C16-C17-C18-C20
6	L	1286	LDA	C7-C8-C9-C10
6	M	1312	LDA	C4-C5-C6-C7
13	M	1320	CDL	CB5-C51-C52-C53
8	M	1318	U10	C33-C34-C36-C37
6	L	1286	LDA	C11-C10-C9-C8
13	M	1320	CDL	C54-C55-C56-C57
13	M	1320	CDL	C32-C33-C34-C35
6	M	1314	LDA	C1-C2-C3-C4
4	H	1262	GOL	O2-C2-C3-O3
5	M	1308	BCL	C5-C6-C7-C8
6	M	1315	LDA	C2-C3-C4-C5
6	L	1284	LDA	C2-C3-C4-C5
8	M	1318	U10	C5-C4-O4-C4M
5	M	1308	BCL	C6-C7-C8-C10
8	M	1318	U10	C35-C34-C36-C37
5	L	1283	BCL	C14-C13-C15-C16
5	M	1308	BCL	C6-C7-C8-C9
6	M	1312	LDA	C11-C10-C9-C8
5	M	1308	BCL	C13-C15-C16-C17
13	M	1320	CDL	CB7-C71-C72-C73
6	L	1285	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	L	1287	BPH	O2A-C1-C2-C3
7	M	1317	BPH	O2A-C1-C2-C3
13	M	1320	CDL	C80-C81-C82-C83
12	M	1319	SPO	C21-C22-C23-C25
13	M	1320	CDL	CA2-C1-CB2-OB2
13	M	1320	CDL	OA5-CA3-CA4-OA6
13	M	1320	CDL	C74-C75-C76-C77
13	M	1320	CDL	C31-C32-C33-C34
13	M	1320	CDL	C14-C15-C16-C17
13	M	1320	CDL	C19-C20-C21-C22
6	L	1285	LDA	C9-C10-C11-C12
10	L	1290	HTO	C4-C5-C6-C7
6	M	1314	LDA	C11-C10-C9-C8
13	M	1320	CDL	C36-C37-C38-C39
13	M	1320	CDL	C40-C41-C42-C43
13	M	1320	CDL	C81-C82-C83-C84
6	L	1285	LDA	C2-C3-C4-C5
6	M	1313	LDA	C1-C2-C3-C4
6	L	1286	LDA	C5-C6-C7-C8
7	M	1317	BPH	C11-C10-C8-C7
7	M	1317	BPH	C12-C13-C15-C16
13	M	1320	CDL	C55-C56-C57-C58
6	M	1311	LDA	C9-C10-C11-C12
13	M	1320	CDL	C11-C12-C13-C14
10	L	1290	HTO	C1-C2-C3-C4
13	M	1320	CDL	CA3-CA4-CA6-OA8
5	L	1283	BCL	C5-C6-C7-C8
6	M	1311	LDA	C2-C3-C4-C5
6	L	1285	LDA	C11-C10-C9-C8
6	M	1312	LDA	C3-C4-C5-C6
13	M	1320	CDL	OB5-CB3-CB4-OB6
13	M	1320	CDL	OA6-CA4-CA6-OA8
13	M	1320	CDL	C52-C53-C54-C55
10	L	1290	HTO	C2-C3-C4-C5
5	L	1283	BCL	C11-C10-C8-C9
5	M	1308	BCL	C11-C12-C13-C14
7	M	1317	BPH	C11-C10-C8-C9
5	L	1282	BCL	C5-C6-C7-C8
4	L	1294	GOL	O2-C2-C3-O3
12	M	1319	SPO	C21-C22-C23-C24
13	M	1320	CDL	OA5-CA3-CA4-CA6
5	M	1308	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
7	M	1317	BPH	C6-C7-C8-C10
6	L	1284	LDA	C9-C10-C11-C12
6	L	1284	LDA	C6-C7-C8-C9
6	M	1313	LDA	C11-C10-C9-C8
6	L	1286	LDA	C9-C10-C11-C12
13	M	1320	CDL	C51-CB5-OB6-CB4
6	L	1285	LDA	C2-C1-N1-CM1
6	M	1310	LDA	C2-C1-N1-CM2
6	M	1315	LDA	C2-C1-N1-CM1
6	L	1285	LDA	C5-C6-C7-C8
8	M	1318	U10	C34-C36-C37-C38
6	M	1315	LDA	C7-C8-C9-C10
13	M	1320	CDL	OB5-CB3-CB4-CB6
13	M	1320	CDL	OB7-CB5-OB6-CB4
7	L	1287	BPH	C4-C3-C5-C6
7	M	1317	BPH	C6-C7-C8-C9
6	M	1315	LDA	C2-C1-N1-O1
13	M	1320	CDL	C75-C76-C77-C78
6	M	1310	LDA	C11-C10-C9-C8
7	M	1317	BPH	C5-C6-C7-C8
8	L	1288[A]	U10	C2-C3-O3-C3M
6	M	1311	LDA	C6-C7-C8-C9
7	L	1287	BPH	C2-C3-C5-C6
10	L	1291	HTO	C3-C4-C5-C6
7	M	1317	BPH	C14-C13-C15-C16
8	L	1288[B]	U10	C5-C4-O4-C4M
6	M	1311	LDA	N1-C1-C2-C3
6	M	1311	LDA	C7-C8-C9-C10
5	M	1309	BCL	C6-C7-C8-C10
6	L	1285	LDA	C4-C5-C6-C7
6	M	1312	LDA	C5-C6-C7-C8
5	L	1282	BCL	C11-C10-C8-C9
5	M	1309	BCL	C11-C12-C13-C14
5	M	1308	BCL	C2-C3-C5-C6
4	L	1292	GOL	O2-C2-C3-O3
5	M	1308	BCL	C4-C3-C5-C6
5	L	1282	BCL	C11-C12-C13-C15
5	M	1309	BCL	C11-C10-C8-C7
13	M	1320	CDL	C34-C35-C36-C37
8	L	1288[A]	U10	C12-C11-C9-C10
6	L	1284	LDA	C4-C5-C6-C7
8	M	1318	U10	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
7	L	1287	BPH	CHA-CBD-CGD-O1D
7	M	1317	BPH	CHA-CBD-CGD-O1D
10	L	1290	HTO	O2-C2-C3-O3
7	M	1317	BPH	C11-C12-C13-C14
6	M	1312	LDA	C9-C10-C11-C12
6	M	1315	LDA	C11-C10-C9-C8
8	L	1288[B]	U10	C9-C11-C12-C13
4	H	1264	GOL	O2-C2-C3-O3
8	L	1288[A]	U10	C12-C11-C9-C8
5	L	1283	BCL	C12-C13-C15-C16
7	M	1317	BPH	C11-C12-C13-C15
8	M	1318	U10	C29-C31-C32-C33
5	M	1309	BCL	CAA-CBA-CGA-O2A
6	M	1315	LDA	C6-C7-C8-C9
13	M	1320	CDL	C52-C51-CB5-OB6
6	M	1312	LDA	C1-C2-C3-C4
5	L	1282	BCL	C8-C10-C11-C12
6	M	1311	LDA	C2-C1-N1-O1
10	L	1290	HTO	O2-C2-C3-C4
13	M	1320	CDL	C52-C51-CB5-OB7
5	L	1283	BCL	CAD-CBD-CGD-O2D
7	M	1317	BPH	C1-C2-C3-C4
13	M	1320	CDL	C72-C71-CB7-OB8

There are no ring outliers.

15 monomers are involved in 72 short contacts:

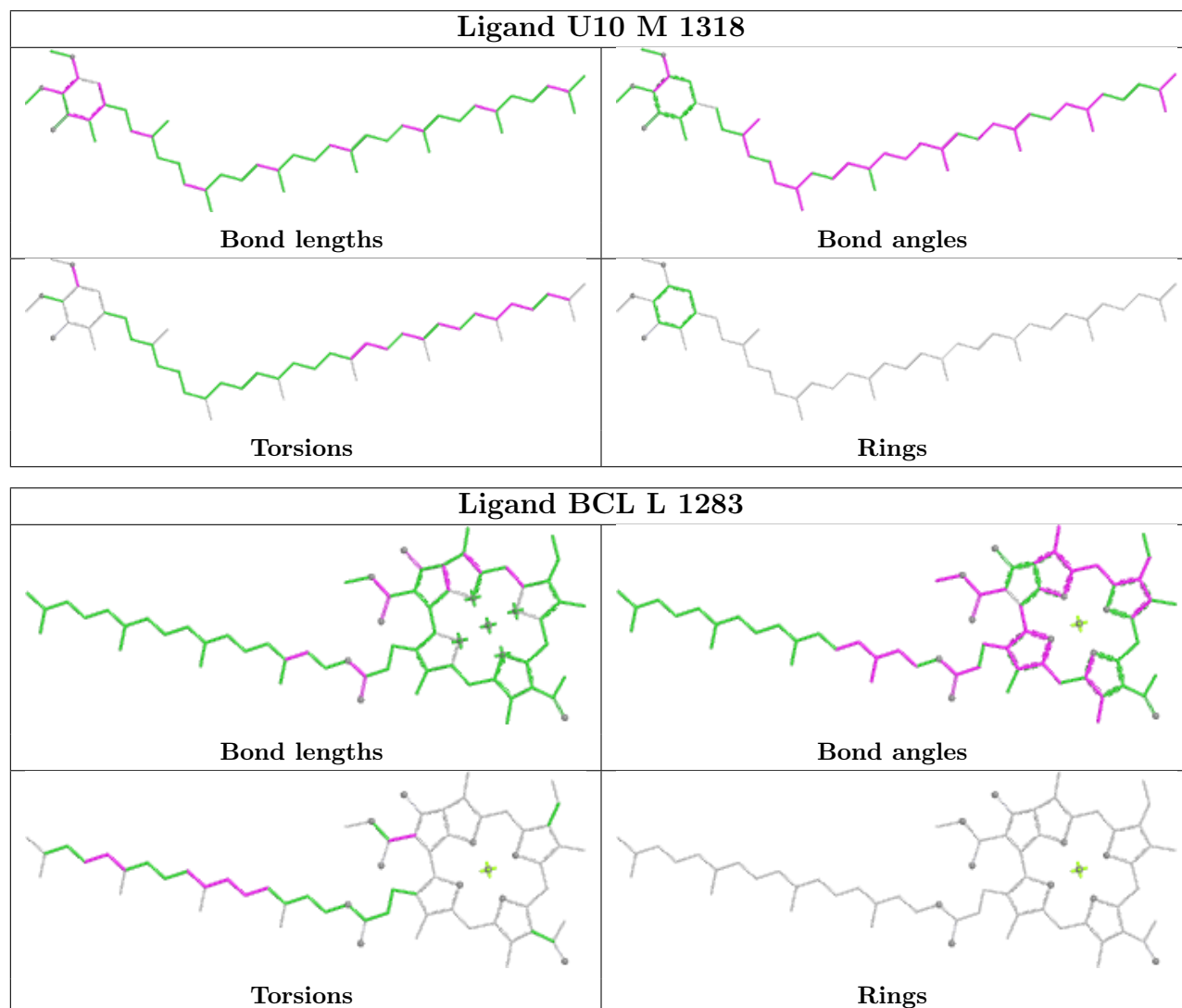
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1318	U10	4	0
5	L	1283	BCL	4	0
6	M	1312	LDA	2	0
7	L	1287	BPH	6	0
8	L	1288[A]	U10	7	0
6	L	1286	LDA	1	0
7	M	1317	BPH	7	0
5	M	1309	BCL	6	0
6	M	1314	LDA	4	0
4	H	1261	GOL	5	0
6	M	1313	LDA	3	0
13	M	1320	CDL	18	0
5	M	1308	BCL	5	0
12	M	1319	SPO	3	0

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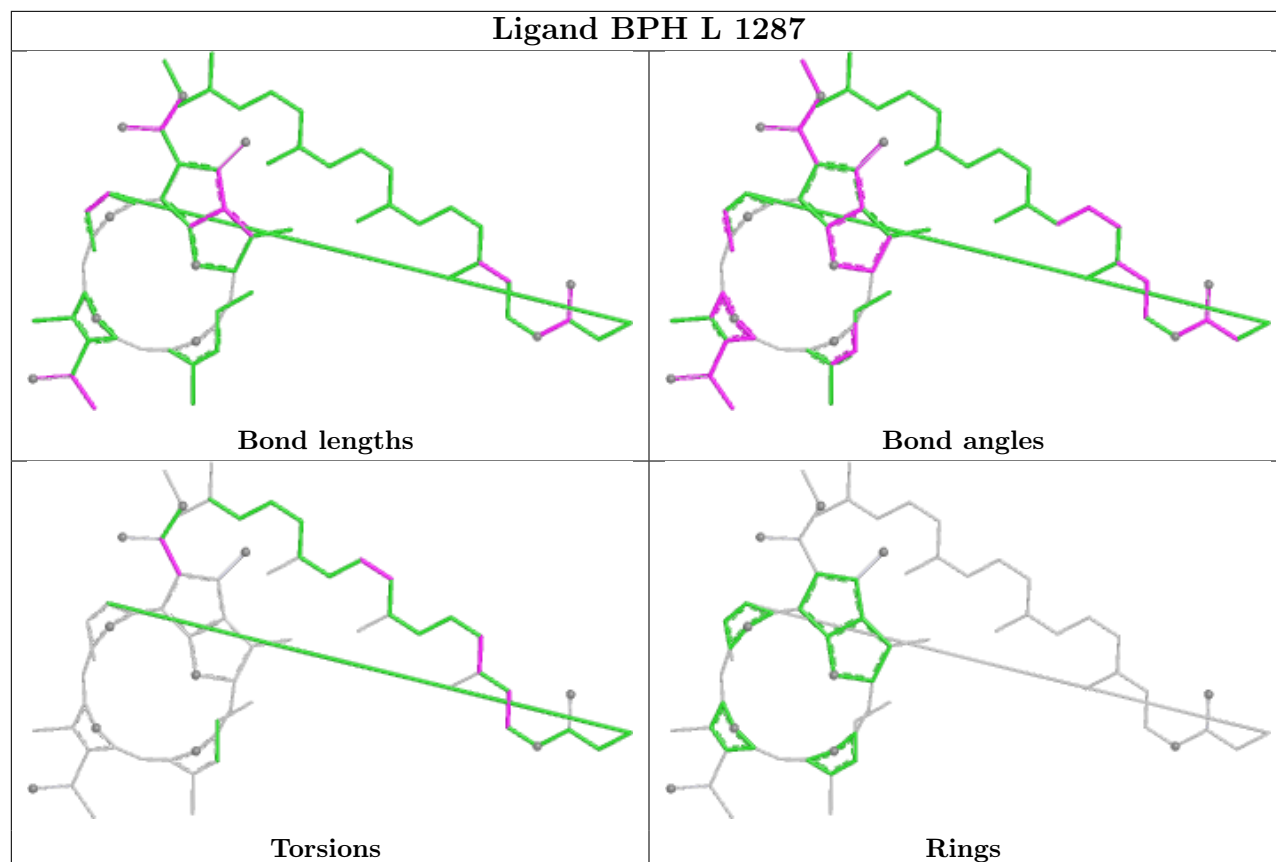
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1288[B]	U10	2	0

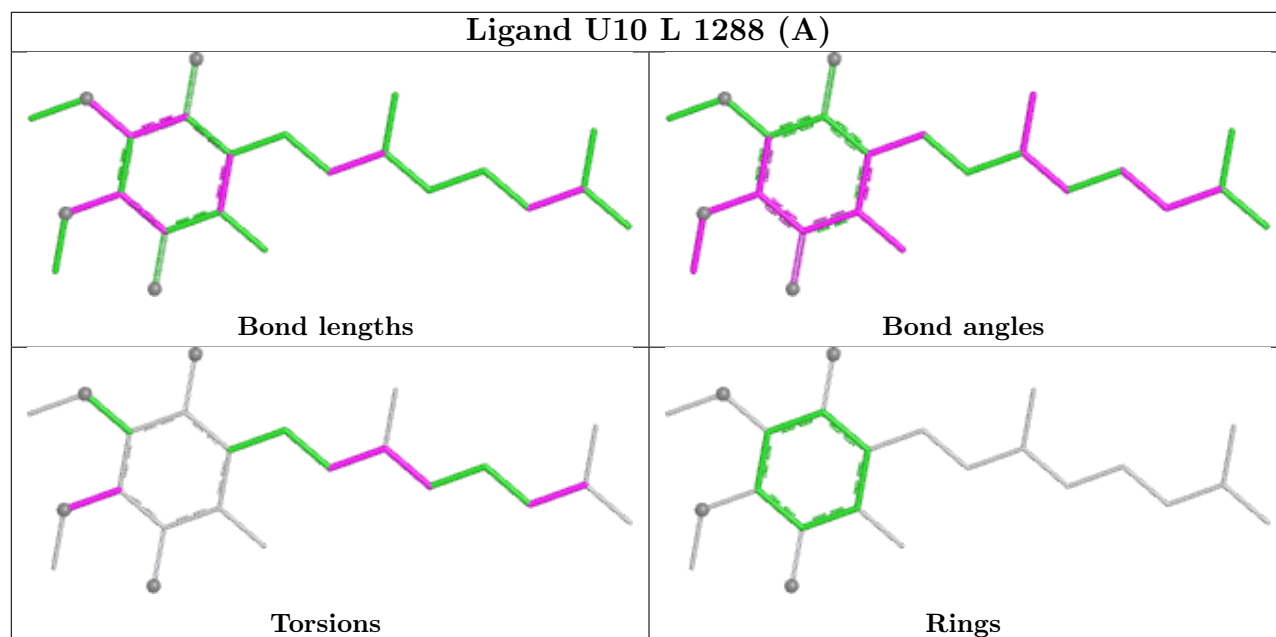
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



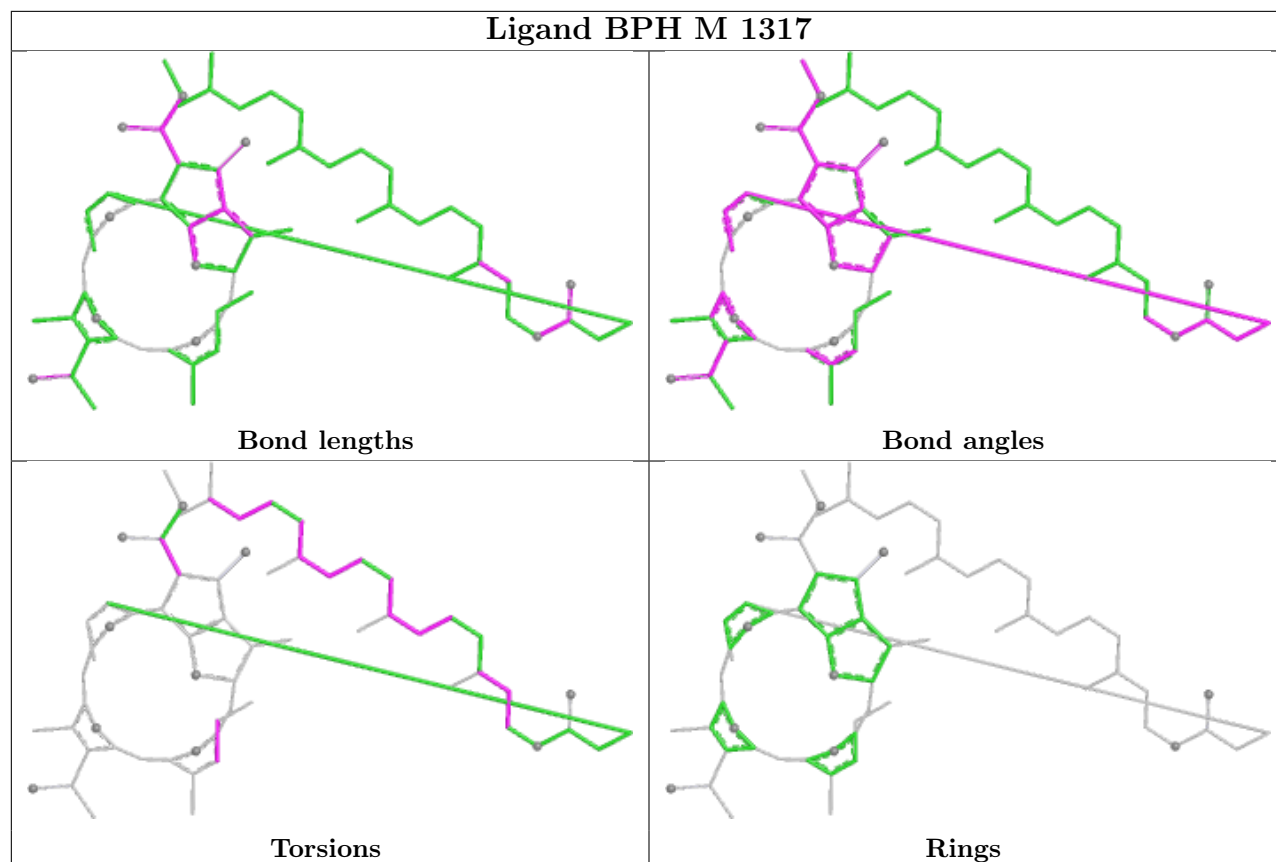
Ligand BPH L 1287



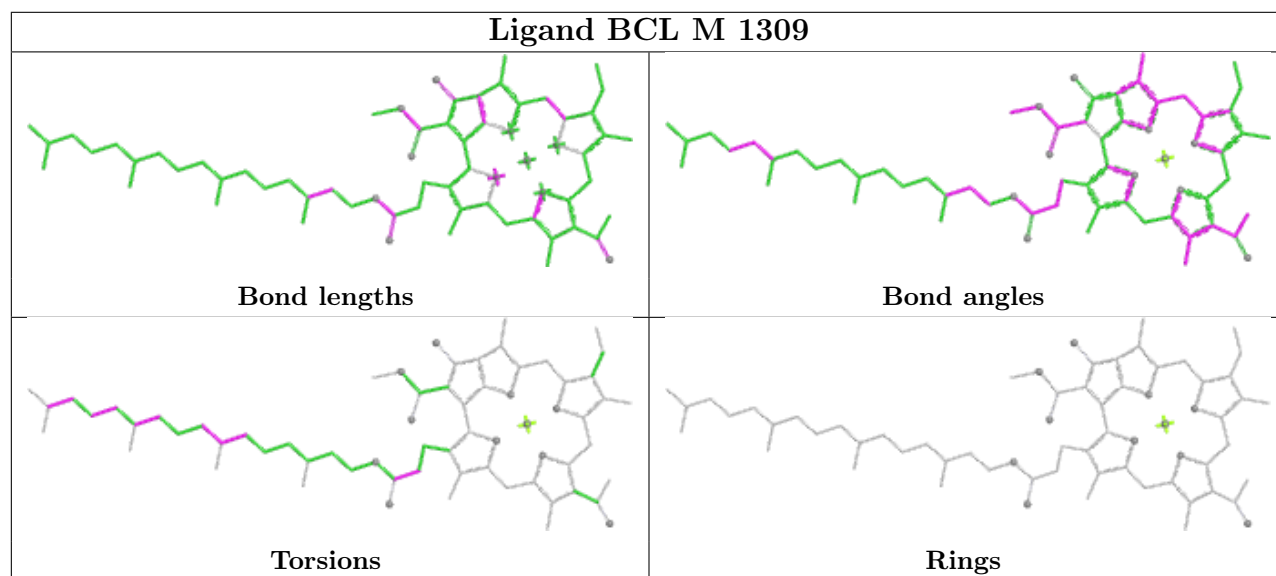
Ligand U10 L 1288 (A)

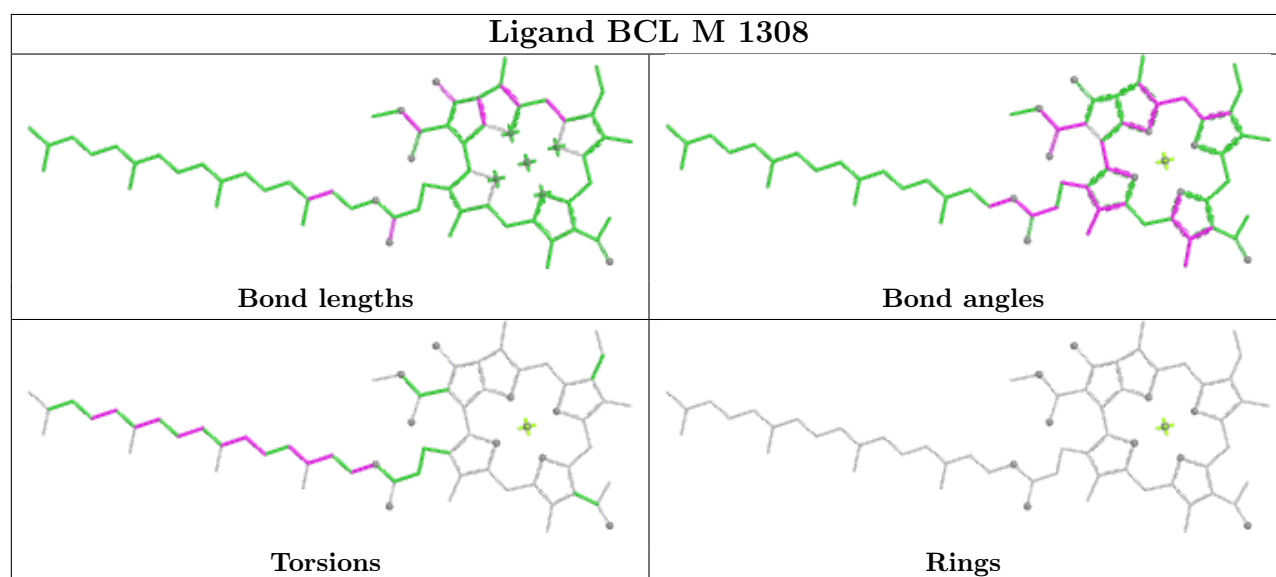
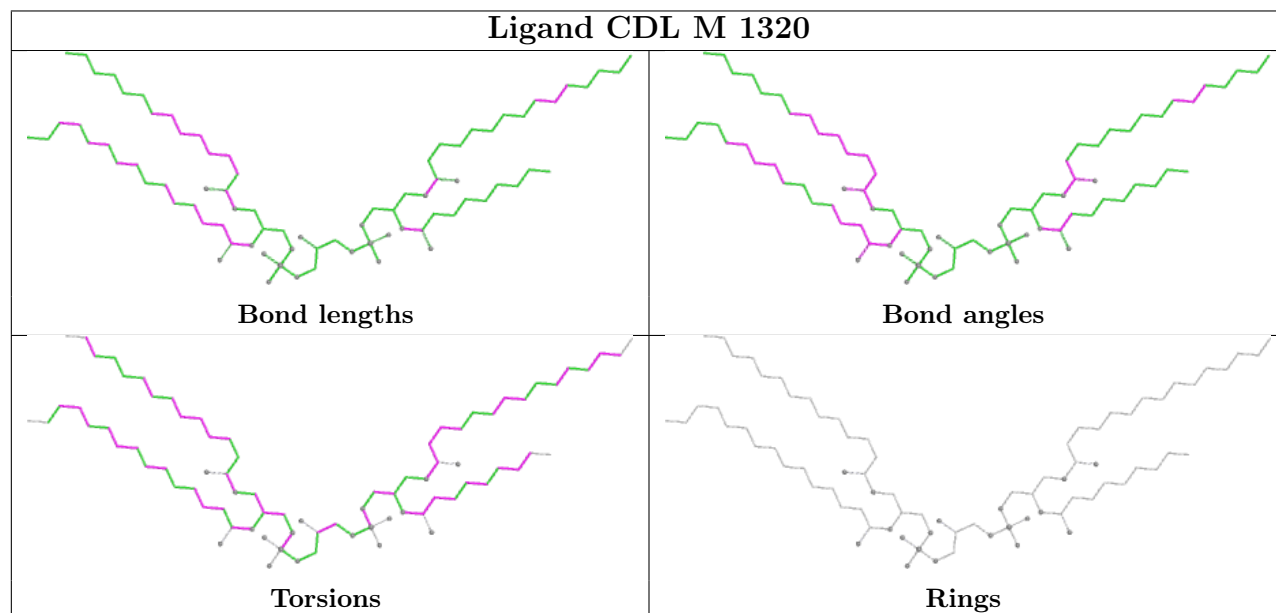
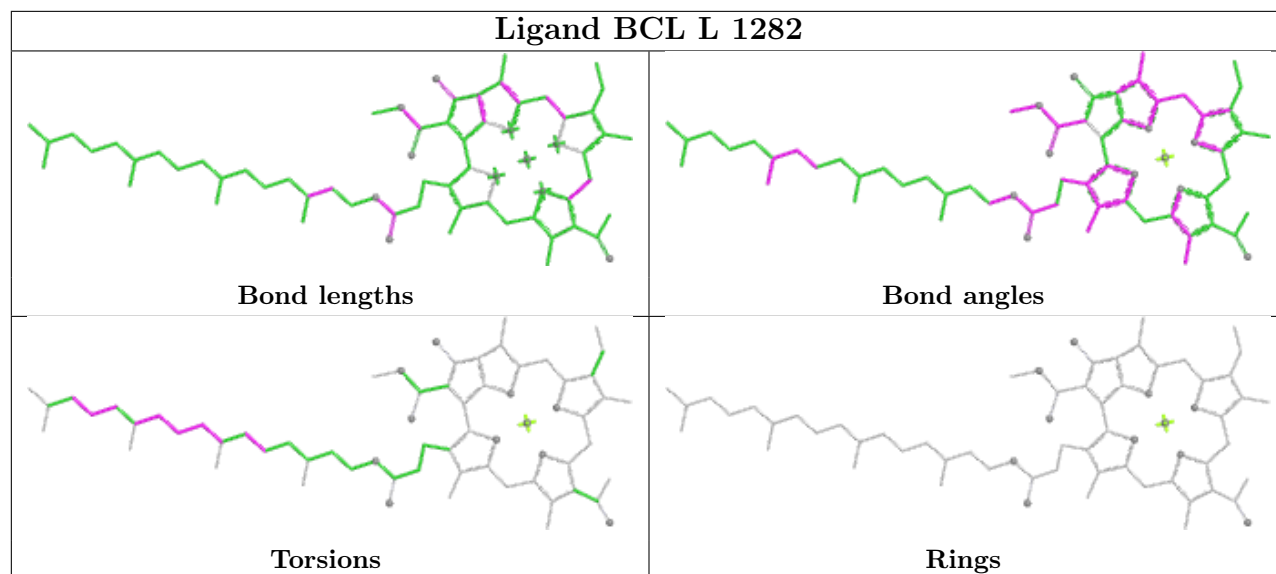


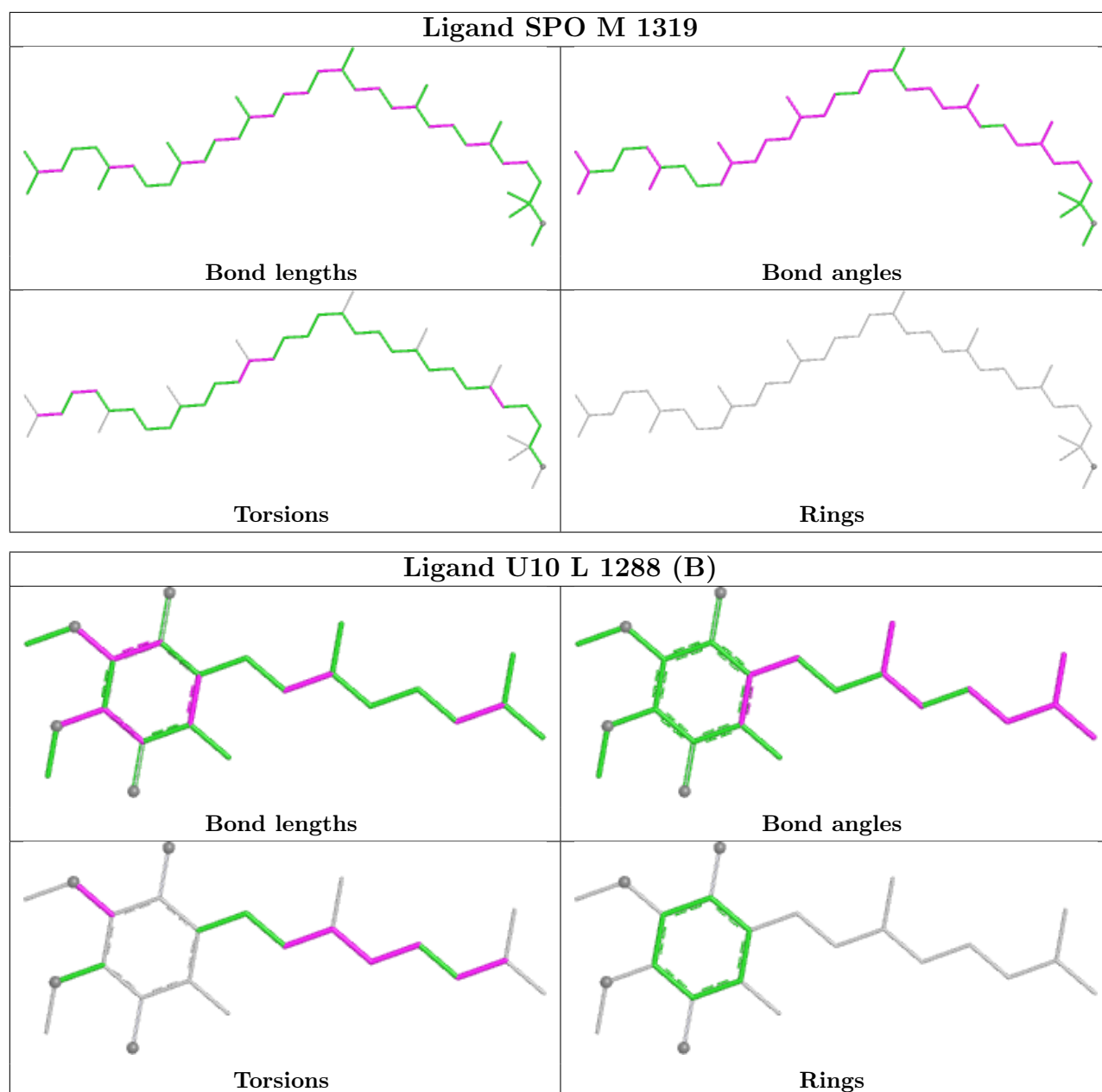
Ligand BPH M 1317



Ligand BCL M 1309







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	260/260 (100%)	0.56	27 (10%)	11 11	17, 26, 108, 129	1 (0%)
2	L	281/281 (100%)	0.16	10 (3%)	46 47	16, 24, 45, 56	0
3	M	307/307 (100%)	0.50	25 (8%)	18 18	14, 28, 52, 100	1 (0%)
All	All	848/848 (100%)	0.40	62 (7%)	21 21	14, 26, 52, 129	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	10[A]	PHE	15.8
3	M	306	LEU	13.7
1	H	4	VAL	12.8
1	H	6	ALA	10.6
3	M	304	ALA	10.1
1	H	252	VAL	9.9
1	H	256	LEU	9.8
1	H	251	VAL	9.4
3	M	305	PRO	9.1
1	H	2	VAL	8.8
2	L	162	TYR	8.8
3	M	1	ALA	8.4
3	M	197	PHE	8.0
1	H	5	THR	7.8
1	H	7	PHE	7.7
3	M	303	MET	7.4
1	H	257	ALA	6.8
3	M	301[A]	HIS	6.4
1	H	1	MET	6.4
1	H	254	ALA	6.1
1	H	260	ALA	6.0
1	H	9	ASN	5.9
3	M	302	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
3	M	3	TYR	5.7
1	H	259	TYR	5.7
2	L	166	ASN	5.6
1	H	3	GLY	5.4
1	H	255	MET	5.0
1	H	8	GLY	5.0
1	H	253	ALA	4.4
1	H	12	LEU	4.1
3	M	307	ASN	4.1
3	M	2	GLU	4.0
3	M	148	TRP	3.7
3	M	300	ASN	3.6
1	H	249	LYS	3.5
3	M	32	VAL	3.4
1	H	13	ALA	3.4
2	L	281	GLY	3.4
3	M	52	LEU	3.4
1	H	245	ALA	3.3
2	L	72	GLU	3.3
1	H	250	SER	2.9
1	H	11	ASP	2.9
2	L	277	GLY	2.9
1	H	258	GLU	2.8
2	L	51	TRP	2.8
3	M	58	LEU	2.7
3	M	105	PHE	2.7
3	M	106	ALA	2.7
2	L	59	TRP	2.7
2	L	270	PRO	2.6
3	M	292	ASP	2.5
3	M	109	LEU	2.5
2	L	275	ILE	2.4
3	M	111	GLU	2.4
3	M	53	GLY	2.3
1	H	248	ARG	2.1
2	L	271	TRP	2.1
3	M	80	TRP	2.1
3	M	59	SER	2.1
3	M	103	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
6	LDA	L	1285	16/16	0.70	0.42	88,89,95,95	0
6	LDA	M	1315	16/16	0.73	0.34	77,85,92,92	0
13	CDL	M	1320	81/100	0.73	0.35	49,79,102,105	0
10	HTO	L	1291	10/10	0.74	0.36	100,101,102,102	0
4	GOL	L	1294	6/6	0.76	0.25	94,95,95,95	0
6	LDA	L	1286	16/16	0.76	0.38	96,98,102,102	0
6	LDA	M	1314	16/16	0.76	0.34	66,72,84,85	0
8	U10	L	1288[B]	23/63	0.80	0.24	32,34,35,35	23
4	GOL	H	1263	6/6	0.80	0.19	72,74,74,75	0
8	U10	L	1288[A]	23/63	0.80	0.24	33,42,54,55	23
6	LDA	M	1311	16/16	0.81	0.25	55,60,71,72	0
10	HTO	L	1290	10/10	0.81	0.21	55,59,60,61	0
6	LDA	L	1284	16/16	0.84	0.26	55,79,92,92	0
6	LDA	M	1313	16/16	0.85	0.23	68,71,72,72	0
4	GOL	H	1261	6/6	0.85	0.22	35,46,50,52	0
4	GOL	L	1292	6/6	0.86	0.17	34,38,39,45	0
4	GOL	H	1264	6/6	0.86	0.15	71,74,74,76	0
4	GOL	L	1293	6/6	0.87	0.18	75,76,76,77	0
4	GOL	H	1262	6/6	0.87	0.17	66,67,67,68	0
6	LDA	M	1312	16/16	0.88	0.17	47,52,54,55	0
9	PO4	L	1289	5/5	0.90	0.10	58,60,60,61	0
6	LDA	M	1310	16/16	0.90	0.15	29,47,53,54	0
7	BPH	M	1317	65/65	0.93	0.14	16,26,84,85	0
8	U10	M	1318	47/63	0.93	0.12	15,26,55,57	0
12	SPO	M	1319	42/42	0.94	0.11	19,33,53,58	0
5	BCL	L	1283	66/66	0.95	0.08	14,19,45,50	0
5	BCL	M	1308	66/66	0.96	0.11	13,21,67,68	0

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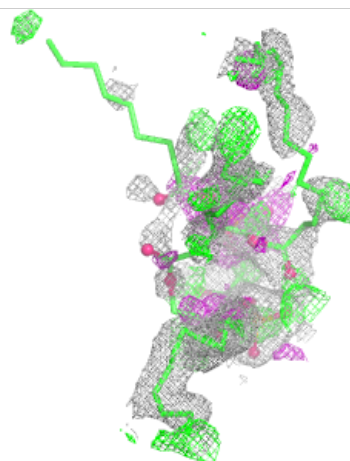
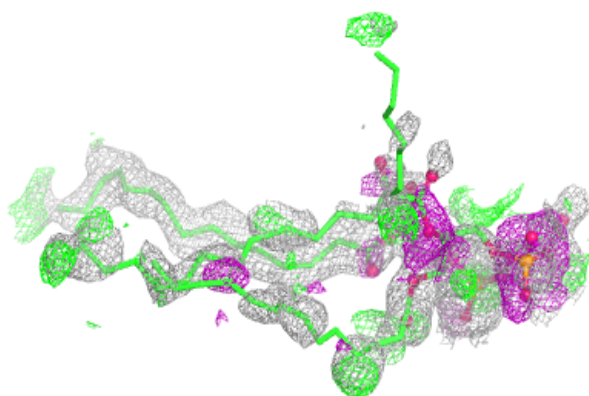
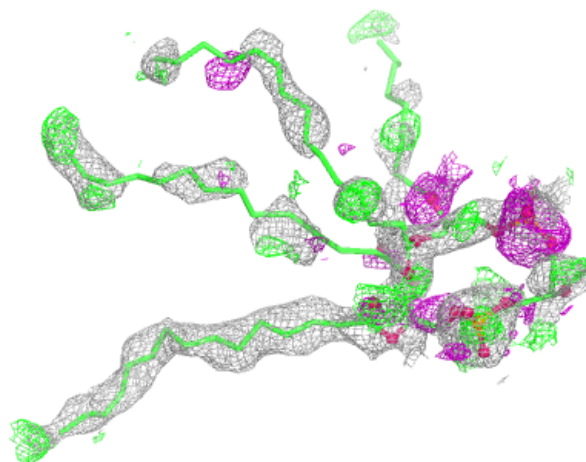
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BCL	M	1309	66/66	0.96	0.08	13,18,39,47	0
7	BPH	L	1287	65/65	0.96	0.07	10,17,31,34	0
5	BCL	L	1282	66/66	0.96	0.07	15,18,32,37	0
11	FE	M	1316	1/1	0.99	0.02	16,16,16,16	0

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.

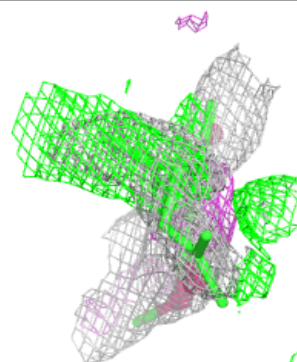
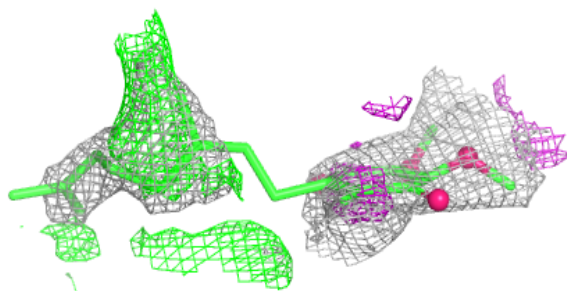
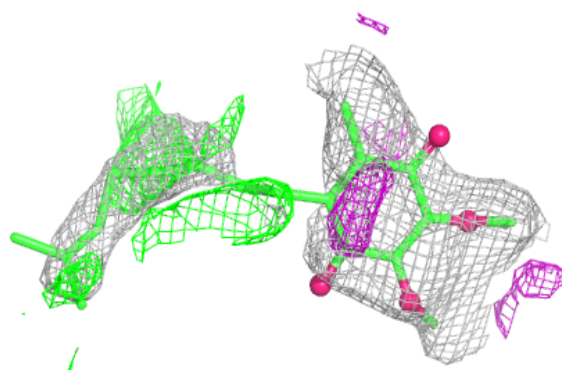
Electron density around CDL M 1320:

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

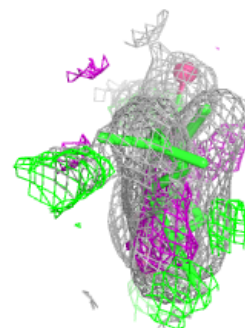
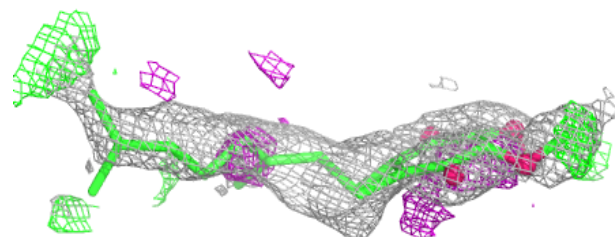
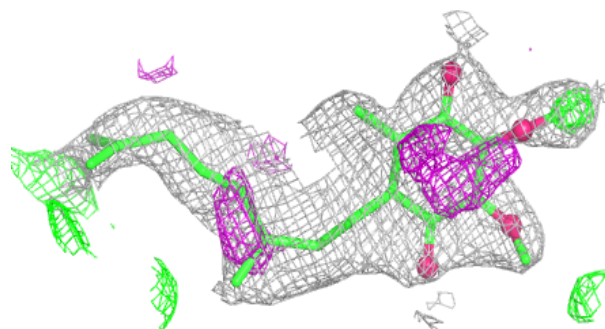


Electron density around U10 L 1288 (B):

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

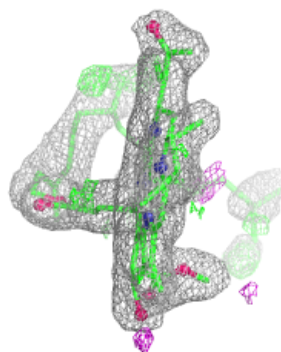
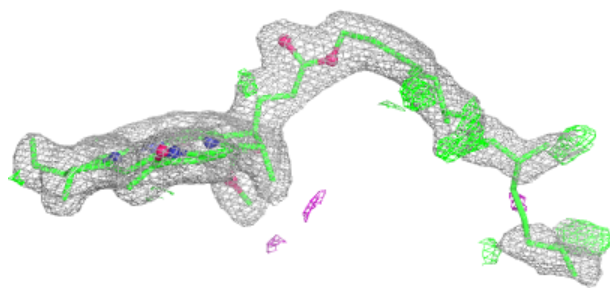
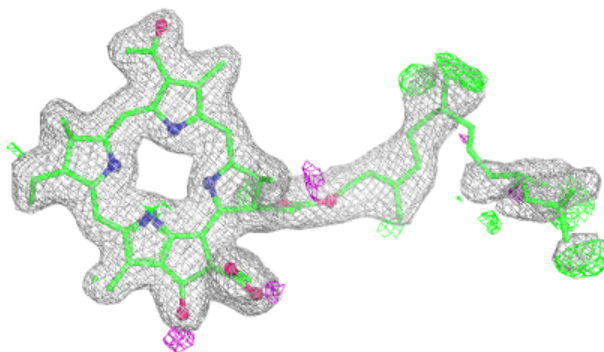
**Electron density around U10 L 1288 (A):**

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and green (positive)

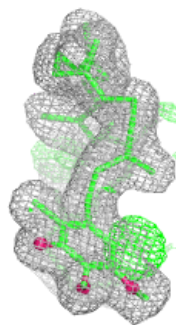
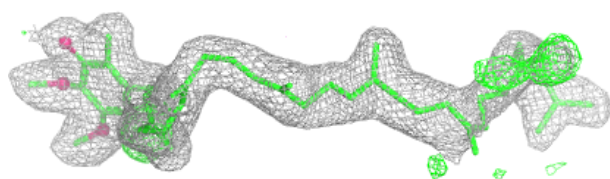
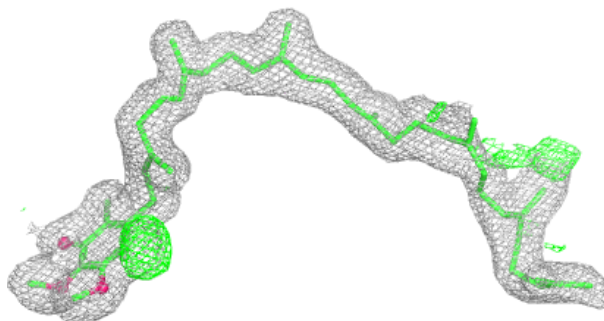


Electron density around BPH M 1317:

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

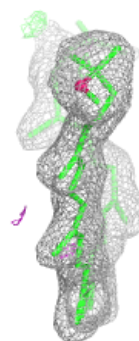
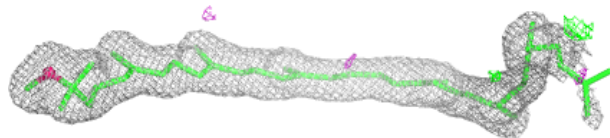
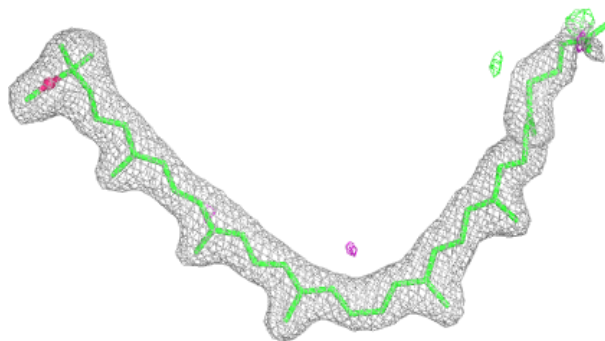
**Electron density around U10 M 1318:**

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

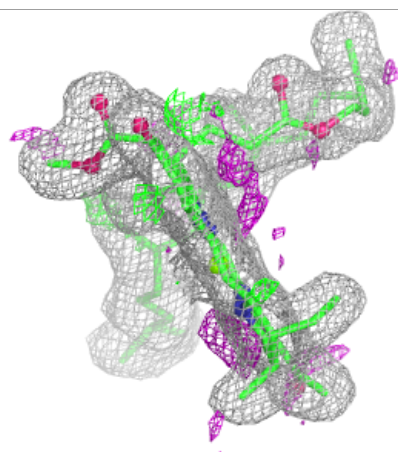
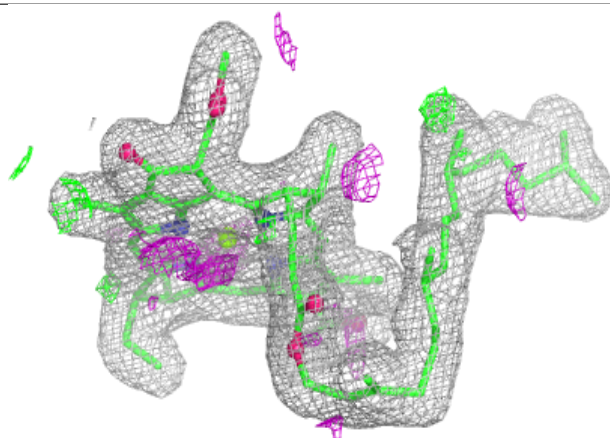
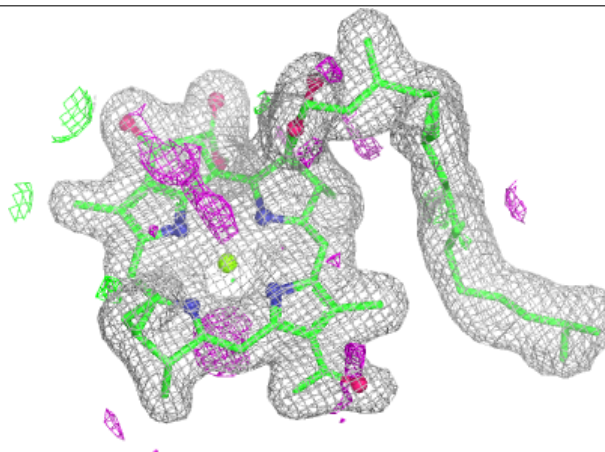


Electron density around SPO M 1319:

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

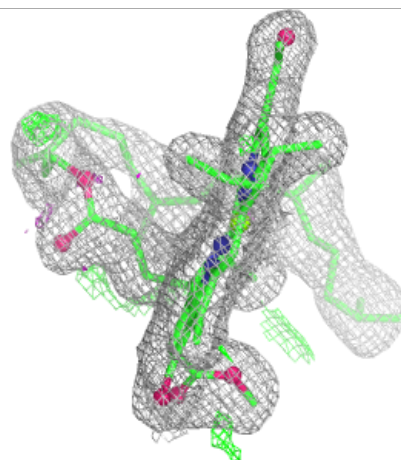
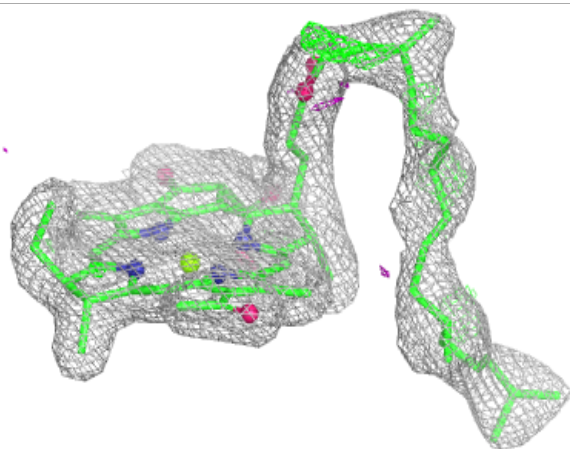
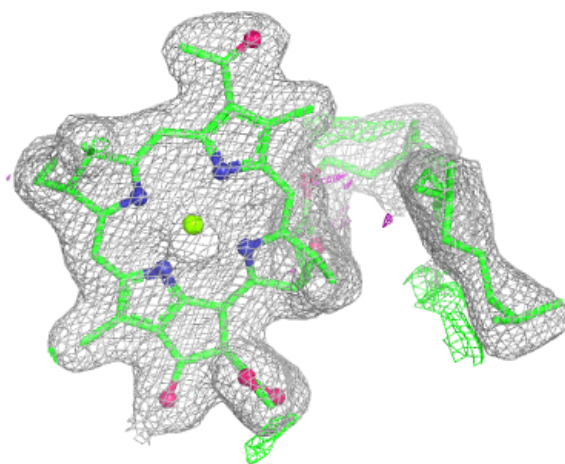
**Electron density around BCL L 1283:**

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



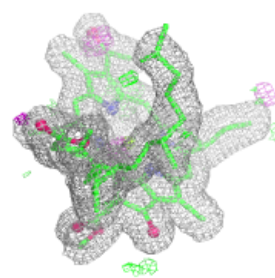
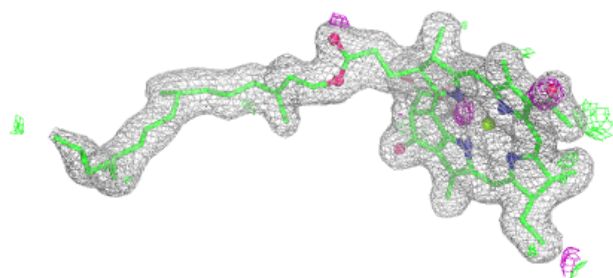
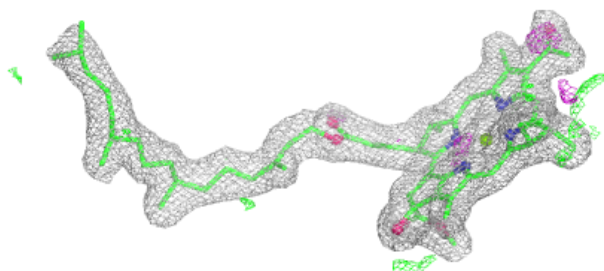
Electron density around BCL M 1308:

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

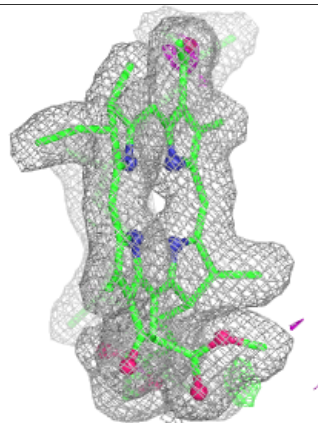
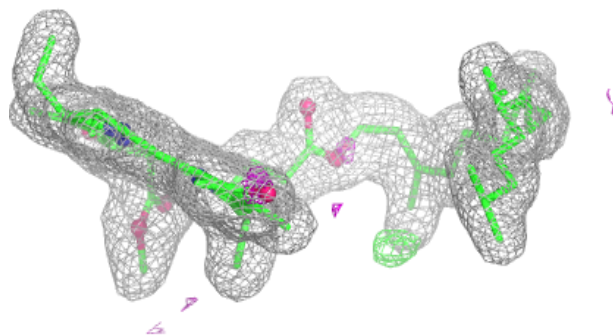
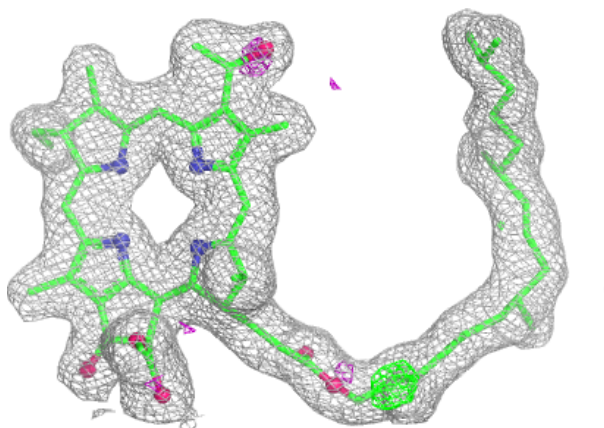


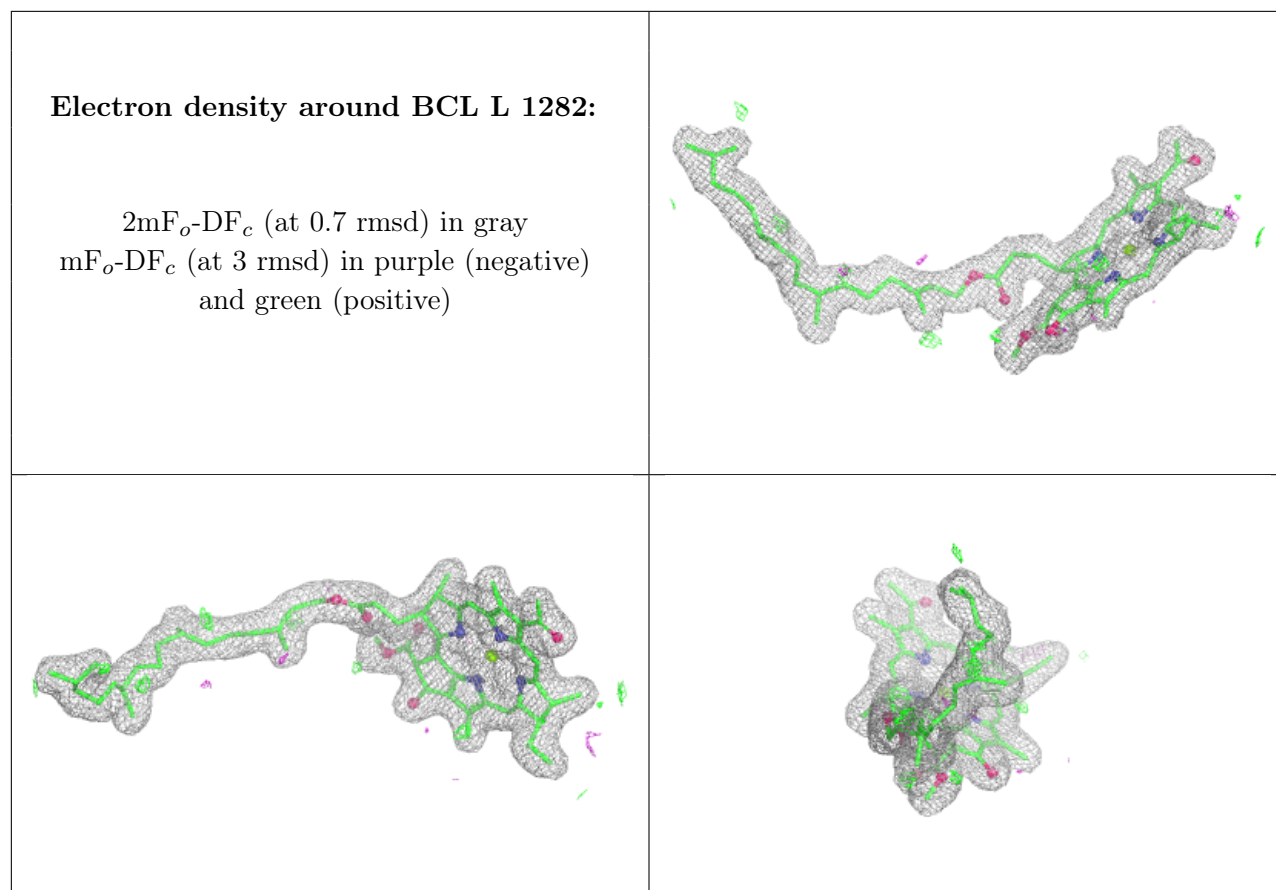
Electron density around BCL M 1309:

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

**Electron density around BPH 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 ⓘ

There are no such residues in this entry.