



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:44 AM UTC

PDB ID : 2UXL / pdb_00002uxl
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 10 in the neutral state, 2nd dataset
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-28
Resolution : 2.88 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

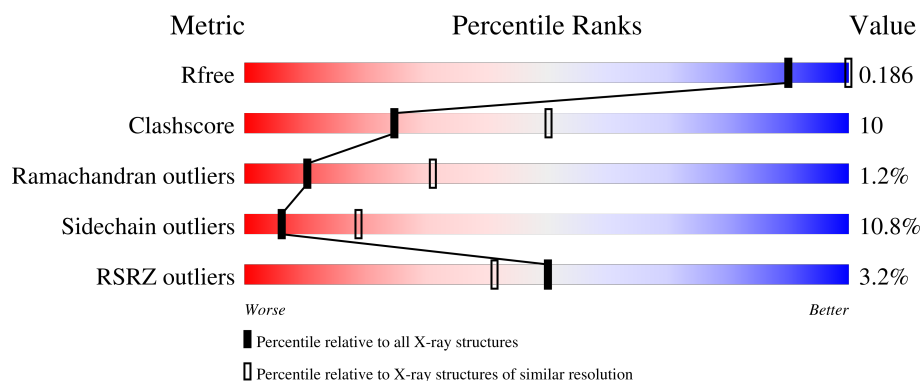
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	3% 69% 20% 7%
2	L	281	2% 80% 17% .
3	M	307	3% 73% 21% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1282	X	-	-	-
5	BCL	L	1285	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
7	UQ2	L	1284[B]	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 7302 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	241	Total	C	N	O	S	0	3	1
			1846	1181	319	337	9			

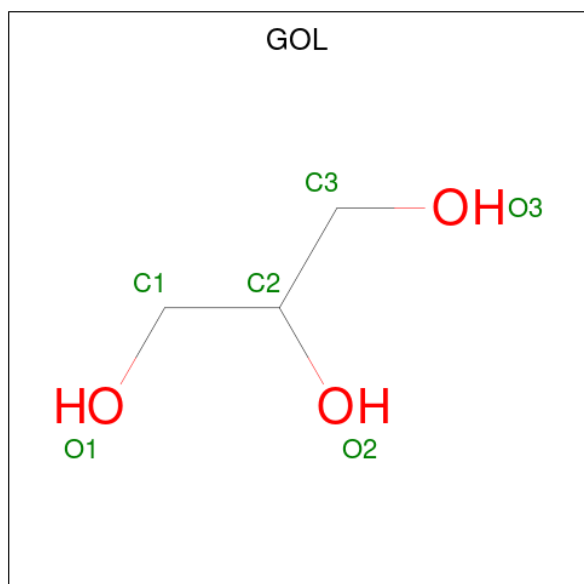
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

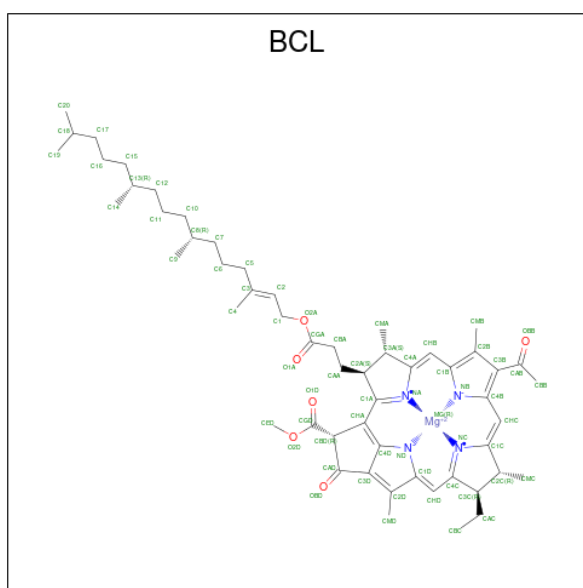
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

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



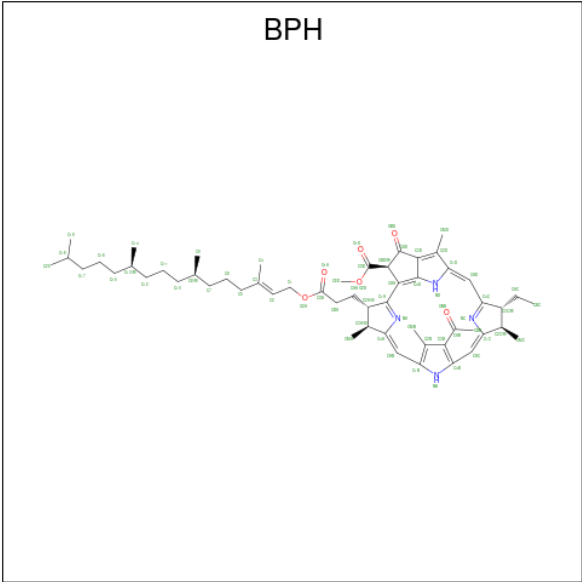
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

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



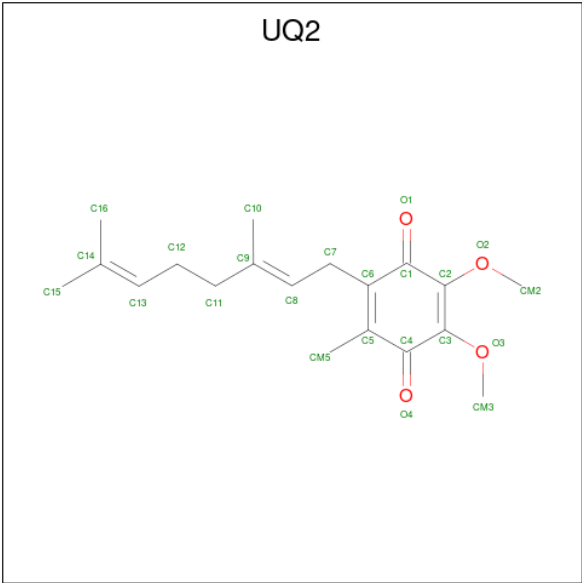
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



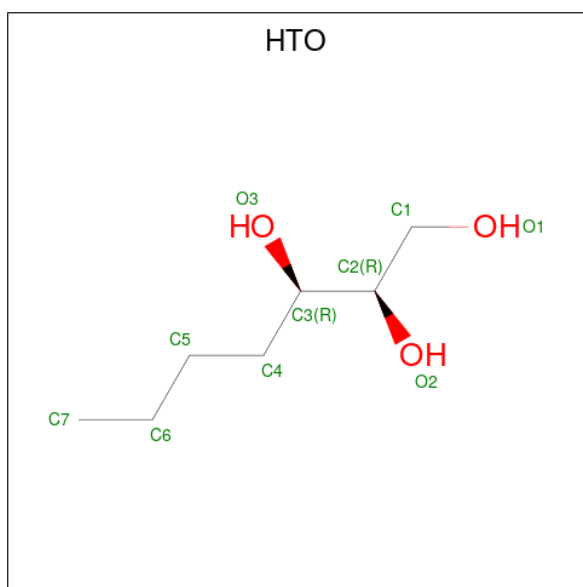
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-2 (CCD ID: UQ2) (formula: C₁₉H₂₆O₄).



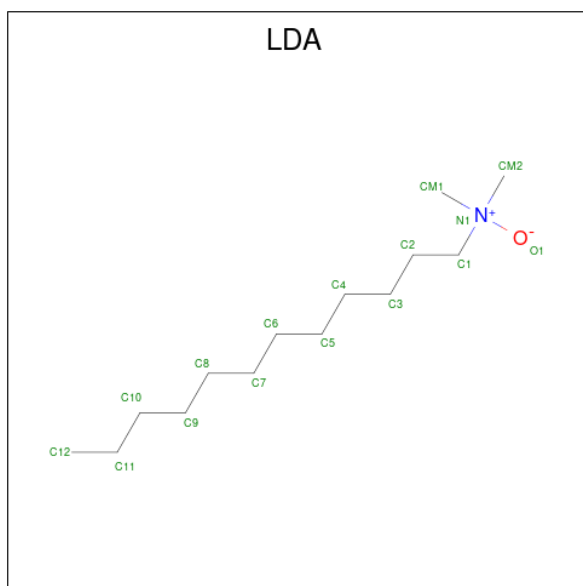
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: C₇H₁₆O₃).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).

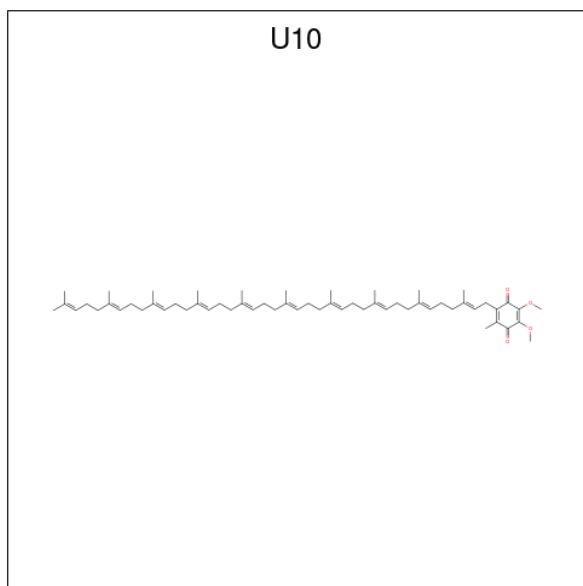


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (III) ION (CCD ID: FE) (formula: Fe).

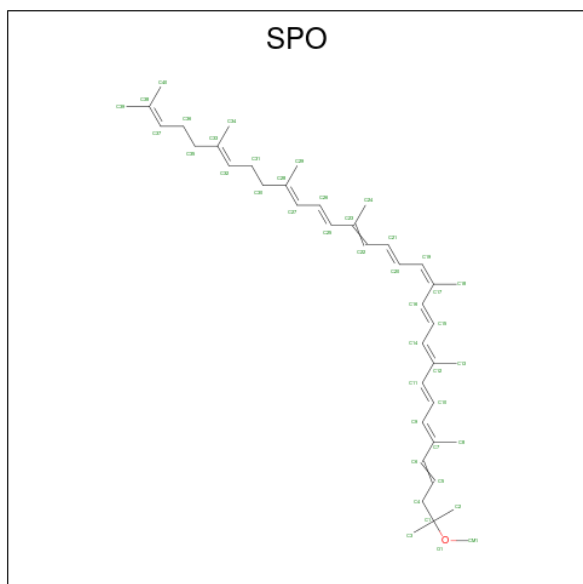
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	1	Total	Fe	0	0
			1	1		

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



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

- 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		

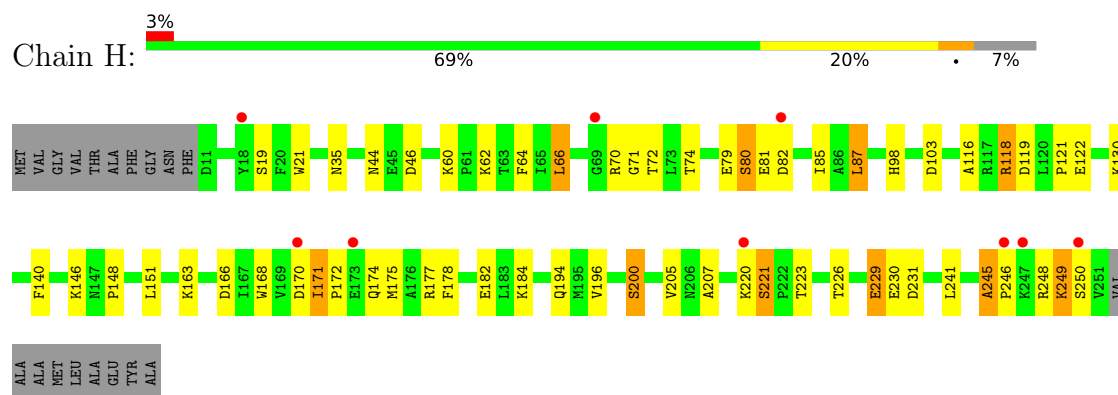
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	76	Total	O	0	0
			76	76		
13	L	68	Total	O	0	0
			68	68		
13	M	58	Total	O	0	0
			58	58		

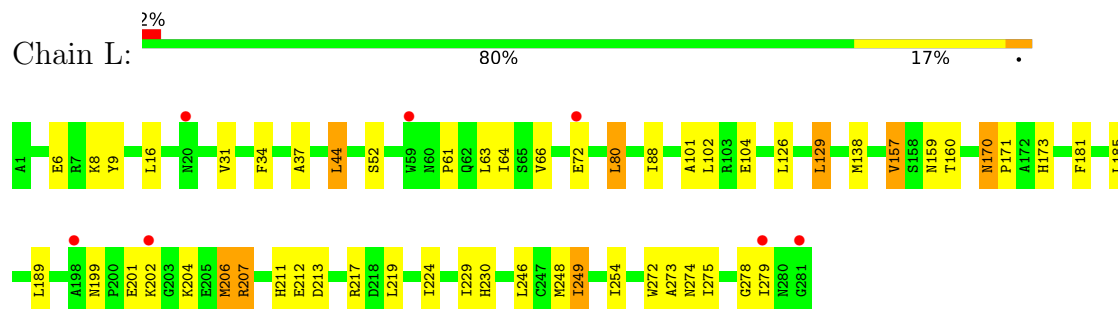
3 Residue-property plots [i](#)

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.

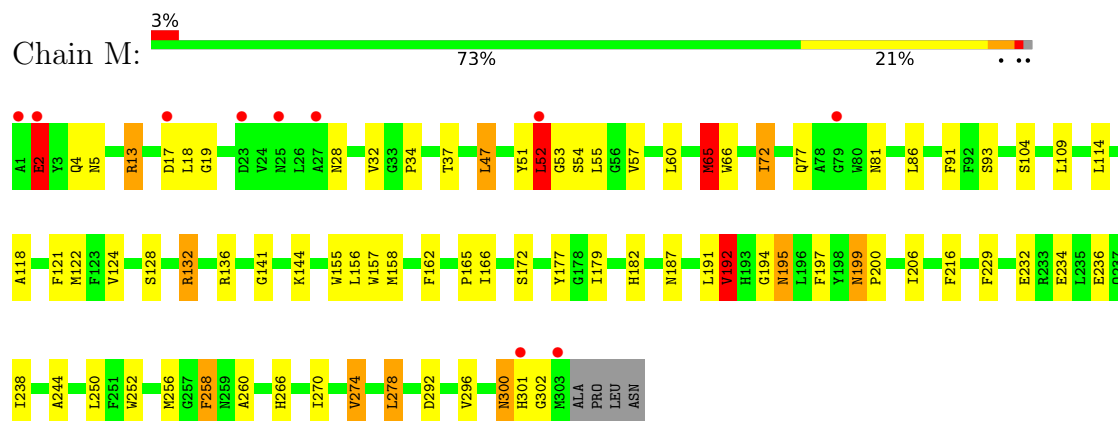
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• 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	139.00Å 139.00Å 183.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.88 119.52 – 2.88	Depositor EDS
% Data completeness (in resolution range)	81.2 (119.52-2.88) 77.9 (119.52-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.220 0.179 , 0.186	Depositor DCC
R_{free} test set	1906 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7302	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: U10, HTO, FE, LDA, BPH, UQ2, SPO, BCL, GOL

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	0.94	1/1906 (0.1%)	1.14	4/2591 (0.2%)
2	L	0.93	2/2320 (0.1%)	1.04	2/3175 (0.1%)
3	M	0.93	4/2501 (0.2%)	1.09	4/3415 (0.1%)
All	All	0.93	7/6727 (0.1%)	1.09	10/9181 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	138	MET	SD-CE	8.51	2.00	1.79
1	H	250	SER	C-N	-6.49	1.24	1.33
3	M	72	ILE	CA-CB	6.41	1.62	1.54
2	L	230	HIS	CA-C	5.95	1.60	1.52
3	M	124	VAL	CA-CB	5.90	1.62	1.54
3	M	302	GLY	C-N	-5.44	1.25	1.33
3	M	65	MET	SD-CE	5.35	1.93	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	248	ARG	CA-C-N	6.27	132.99	121.70
1	H	248	ARG	C-N-CA	6.27	132.99	121.70
3	M	5	ASN	N-CA-C	6.06	119.92	111.74
1	H	245	ALA	N-CA-C	5.65	122.29	109.81
3	M	52	LEU	CA-CB-CG	5.28	134.77	116.30
2	L	157	VAL	N-CA-C	-5.27	105.57	110.53
3	M	19	GLY	N-CA-C	5.27	120.61	112.81
2	L	230	HIS	CB-CA-C	5.27	119.81	110.85
3	M	292	ASP	CB-CA-C	-5.05	100.08	110.38
1	H	166	ASP	N-CA-C	5.03	116.17	108.42

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	1846	0	1861	33	0
2	L	2232	0	2187	37	0
3	M	2409	0	2321	46	0
4	H	18	0	24	3	0
4	L	6	0	8	2	0
5	L	132	0	148	3	0
5	M	132	0	148	12	0
6	L	65	0	76	8	0
6	M	65	0	76	11	0
7	L	46	0	52	13	0
8	L	10	0	16	0	0
9	M	48	0	93	3	0
10	M	1	0	0	0	0
11	M	48	0	63	1	0
12	M	42	0	60	1	0
13	H	76	0	0	3	0
13	L	68	0	0	1	0
13	M	58	0	0	1	0
All	All	7302	0	7133	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (139) 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)
6:L:1283:BPH:CBB	6:L:1283:BPH:HHC	1.94	0.97
6:M:1309:BPH:CBB	6:M:1309:BPH:HHC	1.94	0.95
5:M:1303:BCL:H91	5:M:1303:BCL:H151	1.53	0.89
3:M:66:TRP:CZ2	3:M:122:MET:HE3	2.07	0.88
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.55	0.85
7:L:1284[B]:UQ2:H5M3	7:L:1284[B]:UQ2:C8	2.08	0.84
6:L:1283:BPH:HHC	6:L:1283:BPH:HBB2	1.60	0.83
2:L:224:ILE:HG22	7:L:1284[B]:UQ2:C8	2.14	0.78
6:M:1309:BPH:HHC	6:M:1309:BPH:HBB3	1.64	0.78
6:M:1309:BPH:HBC3	6:M:1309:BPH:HHD	1.66	0.78
5:M:1303:BCL:HBC1	5:M:1304:BCL:HAA2	1.66	0.77
9:M:1305:LDA:H101	9:M:1306:LDA:H121	1.65	0.77
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.20	0.77
1:H:122:GLU:HG3	3:M:236:GLU:OE1	1.86	0.74
6:L:1283:BPH:CBB	6:L:1283:BPH:CHC	2.67	0.73
6:L:1283:BPH:HHC	6:L:1283:BPH:HBB3	1.70	0.72
2:L:170:ASN:HD22	2:L:170:ASN:C	1.98	0.72
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.72	0.71
6:M:1309:BPH:HHC	6:M:1309:BPH:HBB2	1.73	0.69
3:M:194:GLY:O	3:M:195:ASN:HB3	1.93	0.69
1:H:62:LYS:HE2	1:H:64:PHE:CZ	2.29	0.68
9:M:1305:LDA:C10	9:M:1306:LDA:H121	2.26	0.66
6:M:1309:BPH:CBB	6:M:1309:BPH:CHC	2.74	0.65
2:L:212:GLU:HB3	7:L:1284[B]:UQ2:H2M3	1.79	0.65
1:H:80:SER:O	13:H:2025:HOH:O	2.15	0.64
1:H:177:ARG:NH2	3:M:232:GLU:OE2	2.31	0.63
3:M:187:ASN:HD22	5:M:1304:BCL:HBC1	1.65	0.62
7:L:1284[B]:UQ2:H5M3	7:L:1284[B]:UQ2:H8	1.79	0.61
2:L:88:ILE:HD11	4:L:1287:GOL:H31	1.83	0.60
2:L:157:VAL:HG21	5:L:1282:BCL:HHD	1.83	0.59
1:H:118[B]:ARG:HH11	1:H:119:ASP:H	1.49	0.59
3:M:199:ASN:HD22	3:M:199:ASN:C	2.09	0.59
2:L:278:GLY:HA2	3:M:77:GLN:O	2.03	0.59
6:L:1283:BPH:CHC	6:L:1283:BPH:HBB3	2.32	0.58
1:H:62:LYS:HD2	4:H:1251:GOL:H31	1.84	0.57
1:H:66:LEU:HG	1:H:71:GLY:O	2.03	0.57
5:L:1282:BCL:HBB3	5:L:1285:BCL:H41	1.86	0.57
3:M:77:GLN:HE22	3:M:93:SER:H	1.53	0.57
3:M:65:MET:HB3	3:M:121:PHE:CD2	2.40	0.57
7:L:1284[B]:UQ2:C8	7:L:1284[B]:UQ2:CM5	2.83	0.57
2:L:272:TRP:HA	2:L:275:ILE:HD12	1.87	0.56
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.89	0.55
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.89	0.54
3:M:53:GLY:O	3:M:57:VAL:HG23	2.07	0.54
1:H:246:PRO:O	1:H:249:LYS:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:ALA:HA	1:H:241:LEU:HD23	1.90	0.54
5:M:1304:BCL:C2	6:M:1309:BPH:HBB3	2.39	0.53
5:L:1282:BCL:HMD2	3:M:206:ILE:HD13	1.91	0.53
2:L:101:ALA:O	2:L:104:GLU:HB2	2.10	0.52
1:H:81:GLU:HG3	1:H:85[B]:ILE:HD11	1.92	0.52
2:L:212:GLU:CB	7:L:1284[B]:UQ2:H2M3	2.39	0.52
6:M:1309:BPH:HBB3	6:M:1309:BPH:CHC	2.35	0.52
1:H:140:PHE:HA	3:M:13:ARG:O	2.10	0.51
1:H:146:LYS:HE2	1:H:200:SER:O	2.10	0.51
3:M:256:MET:HE3	3:M:258:PHE:CE1	2.45	0.51
3:M:234:GLU:O	3:M:238:ILE:HG13	2.11	0.51
3:M:162:PHE:C	3:M:165:PRO:HD2	2.36	0.50
3:M:296:VAL:O	3:M:300:ASN:ND2	2.44	0.50
2:L:229:ILE:HD13	7:L:1284[B]:UQ2:H111	1.93	0.50
1:H:62:LYS:O	1:H:74:THR:HA	2.12	0.49
1:H:171:ILE:N	1:H:172:PRO:HD2	2.28	0.49
2:L:189:LEU:HD12	7:L:1284[B]:UQ2:H163	1.94	0.49
3:M:28:ASN:HB2	3:M:51:TYR:CE2	2.47	0.49
3:M:270:ILE:O	3:M:274:VAL:HG13	2.13	0.49
3:M:300:ASN:ND2	3:M:300:ASN:N	2.61	0.48
3:M:194:GLY:O	3:M:195:ASN:CB	2.61	0.48
1:H:70:ARG:NH2	1:H:121:PRO:O	2.46	0.48
1:H:196:VAL:HG12	1:H:205:VAL:HG22	1.96	0.48
1:H:35:ASN:OD1	3:M:260:ALA:HB1	2.13	0.48
2:L:213:ASP:HB3	2:L:217:ARG:NH1	2.29	0.48
3:M:300:ASN:N	3:M:300:ASN:HD22	2.12	0.47
2:L:80:LEU:HD13	4:L:1287:GOL:H11	1.97	0.47
3:M:192:VAL:O	3:M:192:VAL:HG13	2.15	0.47
6:M:1309:BPH:H2	6:M:1309:BPH:H6C2	1.72	0.47
2:L:275:ILE:HG21	3:M:81:ASN:ND2	2.30	0.46
2:L:212:GLU:OE2	7:L:1284[B]:UQ2:O3	2.33	0.46
1:H:21:TRP:CE2	4:H:1253:GOL:H11	2.51	0.46
1:H:81:GLU:O	1:H:82:ASP:HB2	2.14	0.46
6:L:1283:BPH:HBC2	6:L:1283:BPH:HHD	1.96	0.46
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.46	0.46
3:M:66:TRP:HD1	3:M:118:ALA:O	1.99	0.46
6:M:1309:BPH:HBC3	6:M:1309:BPH:CHD	2.43	0.46
2:L:34:PHE:HA	2:L:37:ALA:HB3	1.98	0.46
4:H:1252:GOL:H31	2:L:199:ASN:HA	1.99	0.45
6:L:1283:BPH:HBC2	6:L:1283:BPH:CHD	2.47	0.45
7:L:1284[B]:UQ2:H2M2	7:L:1284[B]:UQ2:O1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:ASN:HB2	1:H:46:ASP:OD1	2.16	0.45
2:L:170:ASN:HD22	2:L:171:PRO:N	2.14	0.45
2:L:8:LYS:HZ3	2:L:9:TYR:HE2	1.64	0.44
5:M:1304:BCL:H2	6:M:1309:BPH:HBB3	1.98	0.44
1:H:175:MET:HE2	1:H:177:ARG:HG2	1.99	0.44
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.99	0.44
2:L:61:PRO:HA	2:L:64:ILE:HD12	1.99	0.44
3:M:2:GLU:H	3:M:4:GLN:HE21	1.65	0.44
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.18	0.44
6:L:1283:BPH:HED3	3:M:252:TRP:CZ3	2.53	0.44
3:M:252:TRP:CD1	11:M:1310:U10:C6	3.00	0.44
1:H:148:PRO:HA	1:H:151:LEU:CD1	2.44	0.43
1:H:194:GLN:NE2	13:H:2062:HOH:O	2.15	0.43
1:H:220[B]:LYS:HZ3	1:H:221:SER:HB3	1.83	0.43
3:M:177:TYR:HD2	12:M:1311:SPO:H19	1.83	0.43
1:H:226:THR:OG1	1:H:229:GLU:HB2	2.18	0.43
1:H:118[B]:ARG:NH1	1:H:119:ASP:H	2.16	0.43
2:L:160:THR:HG21	2:L:248:MET:HE1	2.01	0.43
3:M:157:TRP:CE3	3:M:158:MET:HG2	2.53	0.43
3:M:278:LEU:HD23	3:M:278:LEU:HA	1.89	0.43
2:L:229:ILE:HD13	7:L:1284[B]:UQ2:H8	2.01	0.43
2:L:219:LEU:O	3:M:132:ARG:NH1	2.52	0.42
2:L:44:LEU:HD23	2:L:44:LEU:HA	1.95	0.42
2:L:207:ARG:HG3	2:L:211:HIS:CD2	2.54	0.42
7:L:1284[B]:UQ2:H122	7:L:1284[B]:UQ2:H101	1.77	0.42
5:M:1303:BCL:H13	5:M:1303:BCL:H102	1.74	0.42
1:H:249:LYS:N	13:H:2076:HOH:O	2.52	0.42
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.97	0.42
2:L:129:LEU:HD12	2:L:129:LEU:HA	1.82	0.42
2:L:201:GLU:OE2	3:M:141:GLY:HA2	2.19	0.42
5:M:1303:BCL:H141	5:M:1303:BCL:H162	1.75	0.42
2:L:159:ASN:HD22	2:L:159:ASN:HA	1.70	0.42
3:M:199:ASN:HA	3:M:200:PRO:HD2	1.95	0.42
3:M:199:ASN:C	3:M:199:ASN:ND2	2.78	0.42
9:M:1307:LDA:HM13	13:M:2013:HOH:O	2.19	0.42
2:L:249:ILE:HD13	2:L:249:ILE:HA	1.87	0.41
2:L:170:ASN:HB3	2:L:173:HIS:CB	2.50	0.41
2:L:272:TRP:C	2:L:274:ASN:H	2.29	0.41
2:L:170:ASN:HA	2:L:171:PRO:HD2	1.91	0.41
1:H:220[B]:LYS:NZ	1:H:221:SER:HB3	2.35	0.41
2:L:170:ASN:C	2:L:170:ASN:ND2	2.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:279:ILE:HG21	3:M:91:PHE:HB3	2.03	0.41
13:L:2058:HOH:O	3:M:136:ARG:HD3	2.21	0.41
3:M:155:TRP:O	3:M:156:LEU:C	2.64	0.41
3:M:234:GLU:OE2	3:M:266:HIS:HE1	2.02	0.41
2:L:224:ILE:HG22	7:L:1284[B]:UQ2:H8	1.96	0.41
3:M:55:LEU:HD22	3:M:128:SER:HB2	2.03	0.40
2:L:181:PHE:CD2	6:M:1309:BPH:HBB1	2.55	0.40
3:M:34:PRO:O	3:M:47:LEU:HB2	2.20	0.40
3:M:256:MET:HE3	3:M:258:PHE:CZ	2.56	0.40
2:L:6:GLU:HA	3:M:250:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	242/260 (93%)	226 (93%)	14 (6%)	2 (1%)	16	41
2	L	279/281 (99%)	265 (95%)	11 (4%)	3 (1%)	11	33
3	M	301/307 (98%)	277 (92%)	19 (6%)	5 (2%)	7	23
All	All	822/848 (97%)	768 (93%)	44 (5%)	10 (1%)	10	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	2	GLU
3	M	52	LEU
1	H	116	ALA
2	L	273	ALA
1	H	245	ALA
2	L	206	MET
2	L	31	VAL

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Mol	Chain	Res	Type
3	M	195	ASN
3	M	179	ILE
3	M	192	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	198/208 (95%)	176 (89%)	22 (11%)	6	17
2	L	220/220 (100%)	201 (91%)	19 (9%)	10	28
3	M	236/240 (98%)	206 (87%)	30 (13%)	4	12
All	All	654/668 (98%)	583 (89%)	71 (11%)	6	18

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	19	SER
1	H	60	LYS
1	H	66	LEU
1	H	72	THR
1	H	79	GLU
1	H	80	SER
1	H	87	LEU
1	H	103	ASP
1	H	118[A]	ARG
1	H	118[B]	ARG
1	H	163	LYS
1	H	171	ILE
1	H	174	GLN
1	H	182	GLU
1	H	184	LYS
1	H	200	SER
1	H	221	SER
1	H	223	THR
1	H	229	GLU

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Mol	Chain	Res	Type
1	H	230	GLU
1	H	231	ASP
1	H	249	LYS
2	L	16	LEU
2	L	44	LEU
2	L	52	SER
2	L	63	LEU
2	L	66	VAL
2	L	72	GLU
2	L	80	LEU
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	170	ASN
2	L	185	LEU
2	L	202	LYS
2	L	204	LYS
2	L	206	MET
2	L	207	ARG
2	L	246	LEU
2	L	249	ILE
2	L	254	ILE
3	M	2	GLU
3	M	13	ARG
3	M	17	ASP
3	M	18	LEU
3	M	32	VAL
3	M	37	THR
3	M	47	LEU
3	M	52	LEU
3	M	54	SER
3	M	60	LEU
3	M	65	MET
3	M	72	ILE
3	M	86	LEU
3	M	104	SER
3	M	109	LEU
3	M	114	LEU
3	M	132	ARG
3	M	144	LYS
3	M	166	ILE
3	M	172	SER

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Mol	Chain	Res	Type
3	M	182	HIS
3	M	191	LEU
3	M	192	VAL
3	M	199	ASN
3	M	216	PHE
3	M	258	PHE
3	M	274	VAL
3	M	278	LEU
3	M	300	ASN
3	M	301	HIS

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

Mol	Chain	Res	Type
1	H	174	GLN
2	L	62	GLN
2	L	159	ASN
2	L	170	ASN
2	L	264	GLN
3	M	4	GLN
3	M	77	GLN
3	M	187	ASN
3	M	199	ASN
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

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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
9	LDA	M	1305	-	13,15,15	2.00	1 (7%)	14,17,17	0.73	1 (7%)
9	LDA	M	1306	-	13,15,15	2.14	2 (15%)	14,17,17	0.69	0
7	UQ2	L	1284[A]	-	23,23,23	2.87	7 (30%)	30,31,31	1.52	6 (20%)
5	BCL	L	1285	2	69,74,74	1.82	10 (14%)	79,115,115	2.48	25 (31%)
6	BPH	M	1309	-	59,70,70	2.79	10 (16%)	59,101,101	2.93	21 (35%)
7	UQ2	L	1284[B]	-	23,23,23	2.68	8 (34%)	30,31,31	1.51	5 (16%)
4	GOL	H	1251	-	5,5,5	0.62	0	5,5,5	0.72	0
4	GOL	H	1253	-	5,5,5	0.39	0	5,5,5	0.42	0
4	GOL	H	1252	-	5,5,5	0.28	0	5,5,5	0.61	0
12	SPO	M	1311	-	41,41,41	2.84	12 (29%)	47,50,50	2.00	12 (25%)
8	HTO	L	1286	-	9,9,9	0.98	1 (11%)	10,10,10	1.35	2 (20%)
4	GOL	L	1287	-	5,5,5	0.41	0	5,5,5	0.48	0
9	LDA	M	1307	-	13,15,15	2.10	2 (15%)	14,17,17	0.59	0
6	BPH	L	1283	-	59,70,70	2.98	10 (16%)	59,101,101	2.79	18 (30%)
5	BCL	M	1304	3	69,74,74	1.85	7 (10%)	79,115,115	2.10	19 (24%)
5	BCL	M	1303	3	69,74,74	1.92	9 (13%)	79,115,115	2.30	23 (29%)
11	U10	M	1310	-	48,48,63	2.82	13 (27%)	60,61,79	1.71	12 (20%)
5	BCL	L	1282	2	69,74,74	1.93	8 (11%)	79,115,115	2.27	23 (29%)

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
9	LDA	M	1305	-	-	5/13/13/13	-
9	LDA	M	1306	-	-	6/13/13/13	-
7	UQ2	L	1284[A]	-	-	7/15/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	1285	2	2/2/21/25	7/41/137/137	-
6	BPH	M	1309	-	-	14/37/105/105	0/5/6/6
7	UQ2	L	1284[B]	-	-	10/15/39/39	0/1/1/1
4	GOL	H	1251	-	-	2/4/4/4	-
4	GOL	H	1253	-	-	0/4/4/4	-
4	GOL	H	1252	-	-	2/4/4/4	-
12	SPO	M	1311	-	-	18/47/47/47	-
8	HTO	L	1286	-	-	5/10/10/10	-
4	GOL	L	1287	-	-	2/4/4/4	-
9	LDA	M	1307	-	-	5/13/13/13	-
6	BPH	L	1283	-	-	10/37/105/105	0/5/6/6
5	BCL	M	1304	3	2/2/21/25	8/41/137/137	-
5	BCL	M	1303	3	2/2/21/25	13/41/137/137	-
11	U10	M	1310	-	-	19/45/69/87	0/1/1/1
5	BCL	L	1282	2	2/2/21/25	13/41/137/137	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1283	BPH	OBD-CAD	15.13	1.42	1.22
6	M	1309	BPH	OBD-CAD	12.52	1.38	1.22
5	L	1282	BCL	OBD-CAD	11.58	1.42	1.22
5	M	1303	BCL	OBD-CAD	10.70	1.40	1.22
5	M	1304	BCL	OBD-CAD	10.60	1.40	1.22
5	L	1285	BCL	OBD-CAD	9.56	1.38	1.22
6	L	1283	BPH	O1D-CGD	8.15	1.41	1.21
6	M	1309	BPH	O1D-CGD	8.10	1.41	1.21
7	L	1284[A]	UQ2	C8-C9	7.29	1.49	1.33
11	M	1310	U10	C33-C34	7.11	1.49	1.33
7	L	1284[B]	UQ2	C8-C9	6.94	1.49	1.33
11	M	1310	U10	C28-C29	6.93	1.49	1.33
12	M	1311	SPO	C32-C33	6.87	1.48	1.33
6	M	1309	BPH	C3D-C2D	6.79	1.51	1.39
9	M	1307	LDA	O1-N1	-6.73	1.25	1.42
11	M	1310	U10	C13-C14	6.69	1.48	1.33
9	M	1305	LDA	O1-N1	-6.56	1.26	1.42
6	L	1283	BPH	C2-C3	6.54	1.48	1.33
6	M	1309	BPH	OBB-CAB	6.51	1.41	1.22
6	M	1309	BPH	O1A-CGA	6.50	1.41	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1283	BPH	O1A-CGA	6.42	1.41	1.22
11	M	1310	U10	C18-C19	6.38	1.47	1.33
6	L	1283	BPH	OBG-CAB	6.36	1.41	1.22
5	L	1282	BCL	O1A-CGA	6.29	1.41	1.22
9	M	1306	LDA	O1-N1	-6.21	1.26	1.42
11	M	1310	U10	C23-C24	6.15	1.47	1.33
11	M	1310	U10	C38-C39	6.14	1.50	1.32
11	M	1310	U10	C8-C9	6.10	1.47	1.33
6	M	1309	BPH	C2-C3	6.06	1.47	1.33
5	M	1303	BCL	O1A-CGA	6.01	1.40	1.22
6	L	1283	BPH	C3D-C2D	5.98	1.49	1.39
5	L	1285	BCL	O1A-CGA	5.80	1.39	1.22
5	M	1304	BCL	O1A-CGA	5.74	1.39	1.22
7	L	1284[A]	UQ2	C13-C14	5.70	1.49	1.32
12	M	1311	SPO	C37-C38	5.54	1.49	1.32
7	L	1284[B]	UQ2	C13-C14	5.52	1.48	1.32
12	M	1311	SPO	C6-C5	5.45	1.47	1.32
7	L	1284[A]	UQ2	O3-C3	-5.35	1.23	1.36
12	M	1311	SPO	C14-C12	5.33	1.48	1.35
12	M	1311	SPO	C22-C23	5.27	1.48	1.35
12	M	1311	SPO	C9-C7	5.13	1.47	1.35
12	M	1311	SPO	C26-C25	4.93	1.47	1.34
12	M	1311	SPO	C10-C11	4.91	1.47	1.34
11	M	1310	U10	O3-C3	-4.77	1.25	1.36
7	L	1284[B]	UQ2	O2-C2	-4.76	1.25	1.36
12	M	1311	SPO	C19-C17	4.70	1.46	1.35
7	L	1284[A]	UQ2	O2-C2	-4.69	1.25	1.36
5	M	1304	BCL	C3D-C4D	-4.57	1.33	1.44
7	L	1284[B]	UQ2	O3-C3	-4.57	1.25	1.36
12	M	1311	SPO	C15-C16	4.48	1.46	1.34
9	M	1306	LDA	C1-N1	-4.39	1.47	1.51
5	M	1303	BCL	C3D-C4D	-4.23	1.34	1.44
11	M	1310	U10	O4-C4	-4.23	1.26	1.36
12	M	1311	SPO	C27-C28	4.13	1.48	1.35
6	L	1283	BPH	C3D-CAD	-4.13	1.39	1.47
12	M	1311	SPO	C21-C20	3.97	1.47	1.36
5	L	1285	BCL	C3D-C4D	-3.95	1.35	1.44
5	M	1303	BCL	C2-C3	3.95	1.42	1.33
5	L	1285	BCL	C2-C3	3.91	1.42	1.33
7	L	1284[A]	UQ2	C6-C5	3.86	1.42	1.35
5	L	1282	BCL	C3D-C4D	-3.79	1.35	1.44
6	M	1309	BPH	O2D-CGD	-3.78	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1309	BPH	C3D-C4D	-3.58	1.36	1.41
6	M	1309	BPH	C3D-CAD	-3.51	1.41	1.47
7	L	1284[B]	UQ2	C6-C5	3.42	1.41	1.35
5	L	1282	BCL	C2-C3	3.37	1.40	1.33
5	M	1303	BCL	O2D-CGD	-3.29	1.25	1.33
5	L	1285	BCL	CHD-C4C	3.24	1.48	1.39
9	M	1307	LDA	C1-N1	-3.09	1.48	1.51
6	L	1283	BPH	O2D-CGD	-2.94	1.26	1.33
5	L	1285	BCL	C1D-ND	2.84	1.41	1.37
5	L	1285	BCL	C1D-C2D	-2.79	1.39	1.45
5	M	1304	BCL	CHD-C4C	2.78	1.47	1.39
5	M	1304	BCL	C2-C3	2.77	1.39	1.33
11	M	1310	U10	C6-C1	2.75	1.40	1.35
5	M	1303	BCL	C1D-C2D	-2.74	1.39	1.45
5	L	1282	BCL	CHD-C4C	2.66	1.46	1.39
7	L	1284[A]	UQ2	C3-C4	-2.64	1.41	1.48
6	M	1309	BPH	O2A-CGA	-2.59	1.25	1.33
7	L	1284[B]	UQ2	C3-C4	-2.56	1.41	1.48
5	L	1285	BCL	O2A-CGA	-2.53	1.26	1.33
5	L	1282	BCL	O2D-CGD	-2.50	1.27	1.33
5	M	1304	BCL	O2A-CGA	-2.47	1.26	1.33
5	M	1304	BCL	O2D-CGD	-2.45	1.27	1.33
11	M	1310	U10	C4-C5	-2.44	1.41	1.48
7	L	1284[A]	UQ2	C2-C1	-2.43	1.41	1.48
8	L	1286	HTO	C4-C3	2.42	1.56	1.52
6	L	1283	BPH	C3D-C4D	-2.35	1.38	1.41
7	L	1284[B]	UQ2	C5-C4	-2.27	1.39	1.47
7	L	1284[B]	UQ2	C2-C1	-2.26	1.42	1.48
5	M	1303	BCL	C3C-C4C	-2.25	1.48	1.51
5	L	1285	BCL	O2D-CGD	-2.23	1.27	1.33
5	L	1285	BCL	O1D-CGD	2.22	1.26	1.21
5	L	1282	BCL	O2A-CGA	-2.21	1.26	1.33
5	L	1282	BCL	OBG-CAB	2.16	1.28	1.23
11	M	1310	U10	C3-C2	-2.16	1.42	1.48
11	M	1310	U10	C6-C5	-2.16	1.40	1.46
5	M	1303	BCL	CHD-C4C	2.12	1.45	1.39
6	L	1283	BPH	C3A-C2A	-2.08	1.52	1.54
5	M	1303	BCL	MG-ND	-2.03	2.01	2.05

All (167) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1285	BCL	C1D-ND-C4D	10.68	113.81	106.31
6	M	1309	BPH	O2D-CGD-CBD	10.46	122.44	110.95
6	M	1309	BPH	C2B-C1B-NB	8.44	115.53	109.43
6	M	1309	BPH	OBD-CAD-CBD	-8.41	113.48	125.82
6	L	1283	BPH	C2B-C1B-NB	8.27	115.41	109.43
5	L	1285	BCL	C2D-C1D-ND	-7.63	102.57	110.13
5	M	1303	BCL	C1D-ND-C4D	7.62	111.66	106.31
5	M	1304	BCL	C1D-ND-C4D	7.12	111.31	106.31
6	L	1283	BPH	O2D-CGD-CBD	7.04	118.68	110.95
5	L	1282	BCL	O2D-CGD-CBD	6.82	123.15	111.23
6	L	1283	BPH	C2D-C1D-ND	6.61	114.21	109.43
5	L	1282	BCL	C4A-NA-C1A	6.39	109.59	106.68
5	M	1303	BCL	O2D-CGD-CBD	6.26	122.17	111.23
5	M	1303	BCL	C1C-NC-C4C	-6.21	103.85	106.68
5	M	1304	BCL	C2D-C1D-ND	-6.13	104.06	110.13
6	L	1283	BPH	C3D-C4D-ND	5.40	114.63	107.71
6	M	1309	BPH	C2D-C1D-ND	5.40	113.33	109.43
5	L	1285	BCL	CHB-C4A-NA	-5.38	116.64	124.40
5	M	1304	BCL	CMD-C2D-C1D	5.35	134.15	124.73
12	M	1311	SPO	C21-C22-C23	-5.34	119.79	127.28
5	M	1303	BCL	C1-O2A-CGA	5.28	129.43	116.65
6	L	1283	BPH	C1C-C2C-C3C	-5.14	97.95	102.84
6	M	1309	BPH	O2D-CGD-O1D	-5.12	113.87	123.85
6	M	1309	BPH	C3D-C4D-ND	5.04	114.17	107.71
5	L	1285	BCL	CMB-C2B-C1B	-5.02	117.78	125.42
5	M	1303	BCL	C2D-C1D-ND	-5.00	105.18	110.13
6	L	1283	BPH	C1B-NB-C4B	-4.95	101.59	108.82
5	L	1282	BCL	CMB-C2B-C1B	-4.89	117.98	125.42
12	M	1311	SPO	C20-C19-C17	-4.86	120.46	127.28
5	M	1304	BCL	CMB-C2B-C1B	-4.70	118.27	125.42
5	M	1303	BCL	C4A-NA-C1A	4.67	108.81	106.68
5	M	1303	BCL	C2B-C1B-NB	-4.67	105.48	110.33
12	M	1311	SPO	C10-C9-C7	-4.66	120.74	127.28
6	M	1309	BPH	CMA-C3A-C4A	-4.66	104.56	114.61
6	L	1283	BPH	C4D-ND-C1D	-4.64	103.31	108.87
5	L	1282	BCL	C1D-ND-C4D	4.59	109.53	106.31
11	M	1310	U10	C32-C33-C34	-4.58	117.15	127.62
12	M	1311	SPO	C15-C14-C12	-4.57	120.87	127.28
5	L	1282	BCL	CMD-C2D-C1D	4.56	132.76	124.73
5	L	1285	BCL	CED-O2D-CGD	4.52	126.17	115.92
5	L	1285	BCL	CHD-C1D-ND	-4.50	118.47	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	C2D-C1D-ND	-4.50	105.68	110.13
5	L	1282	BCL	C2B-C1B-NB	-4.35	105.82	110.33
6	L	1283	BPH	C1-C2-C3	-4.18	119.35	126.20
6	L	1283	BPH	CMD-C2D-C3D	-4.15	116.38	124.68
6	M	1309	BPH	C1B-NB-C4B	-4.15	102.76	108.82
5	L	1282	BCL	CHC-C4B-NB	-4.10	117.90	124.05
11	M	1310	U10	C10-C9-C11	4.09	122.32	115.23
6	M	1309	BPH	C1-C2-C3	-4.04	119.58	126.20
5	M	1304	BCL	O2D-CGD-CBD	4.04	118.29	111.23
5	L	1282	BCL	C1C-NC-C4C	4.03	108.52	106.68
5	L	1285	BCL	CMD-C2D-C1D	4.02	131.81	124.73
5	L	1282	BCL	C1D-CHD-C4C	-4.00	116.98	126.62
5	M	1303	BCL	CMB-C2B-C1B	-3.93	119.43	125.42
5	L	1285	BCL	O2A-CGA-CBA	3.92	123.80	111.83
6	L	1283	BPH	OBD-CAD-C3D	-3.90	121.81	127.89
6	L	1283	BPH	CED-O2D-CGD	3.82	124.58	115.92
6	L	1283	BPH	C4-C3-C5	3.81	121.84	115.23
11	M	1310	U10	C25-C24-C26	3.80	121.83	115.23
5	M	1304	BCL	CMD-C2D-C3D	-3.78	119.02	127.69
7	L	1284[A]	UQ2	C6-C5-C4	3.69	122.08	119.17
11	M	1310	U10	C17-C18-C19	-3.69	119.18	127.62
6	L	1283	BPH	CMC-C2C-C1C	-3.67	106.70	114.61
6	L	1283	BPH	O1D-CGD-CBD	-3.66	119.18	124.72
5	M	1303	BCL	CHD-C1D-ND	-3.59	119.75	124.80
5	L	1285	BCL	CHA-C1A-NA	-3.54	118.38	126.39
5	M	1304	BCL	C1D-CHD-C4C	-3.53	118.10	126.62
5	M	1304	BCL	O2A-CGA-CBA	3.52	122.58	111.83
5	M	1303	BCL	CMD-C2D-C1D	3.52	130.93	124.73
6	M	1309	BPH	C4D-ND-C1D	-3.49	104.69	108.87
11	M	1310	U10	C30-C29-C31	3.47	121.25	115.23
6	M	1309	BPH	C1A-C2A-C3A	-3.40	99.60	102.84
11	M	1310	U10	C22-C23-C24	-3.39	119.87	127.62
6	M	1309	BPH	OBD-CAD-C3D	-3.37	122.63	127.89
6	M	1309	BPH	CMD-C2D-C3D	-3.36	117.97	124.68
6	L	1283	BPH	OBD-CAD-CBD	-3.34	120.92	125.82
5	M	1303	BCL	O1D-CGD-CBD	-3.32	117.96	124.52
5	L	1285	BCL	CMD-C2D-C3D	-3.29	120.13	127.69
5	L	1282	BCL	CHD-C1D-ND	-3.25	120.23	124.80
5	L	1285	BCL	C2B-C1B-NB	-3.23	106.98	110.33
5	L	1285	BCL	O2D-CGD-CBD	3.22	116.86	111.23
5	M	1303	BCL	C2A-C3A-C4A	3.19	107.02	101.87
5	L	1282	BCL	O2D-CGD-O1D	-3.18	117.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	CHA-C1A-NA	-3.18	119.19	126.39
5	L	1282	BCL	CMD-C2D-C3D	-3.17	120.41	127.69
5	M	1304	BCL	C4-C3-C5	3.15	120.69	115.23
5	L	1285	BCL	C1-O2A-CGA	3.12	124.21	116.65
5	L	1282	BCL	CHC-C1C-NC	-3.11	119.90	124.40
12	M	1311	SPO	C4-C5-C6	-3.10	120.56	124.91
5	L	1285	BCL	C1D-CHD-C4C	-3.08	119.19	126.62
5	M	1303	BCL	O2A-CGA-CBA	3.06	121.18	111.83
5	L	1282	BCL	C1-O2A-CGA	3.03	123.99	116.65
6	M	1309	BPH	C4D-CHA-CBD	3.01	109.90	108.45
8	L	1286	HTO	C5-C4-C3	3.00	119.02	114.11
6	M	1309	BPH	C1C-C2C-C3C	-2.99	99.99	102.84
5	M	1303	BCL	C1D-CHD-C4C	-2.97	119.45	126.62
5	M	1304	BCL	C1-O2A-CGA	2.95	123.80	116.65
12	M	1311	SPO	C29-C28-C30	2.94	120.33	115.23
7	L	1284[B]	UQ2	C10-C9-C11	2.91	120.28	115.23
6	L	1283	BPH	C3B-C4B-NB	2.87	112.23	108.05
5	L	1285	BCL	CHA-C4D-ND	2.87	138.48	132.55
6	L	1283	BPH	O2A-CGA-CBA	2.87	120.59	111.83
8	L	1286	HTO	O3-C3-C4	2.86	115.62	109.14
5	M	1304	BCL	CHA-C1A-NA	-2.85	119.94	126.39
12	M	1311	SPO	C26-C27-C28	-2.81	123.74	127.69
11	M	1310	U10	C1M-C1-C6	-2.78	119.89	124.45
7	L	1284[A]	UQ2	C7-C6-C1	2.77	121.73	118.52
5	M	1304	BCL	C3C-C4C-CHD	-2.75	117.59	123.39
5	M	1304	BCL	C2B-C1B-NB	-2.75	107.48	110.33
5	M	1303	BCL	OBB-CAB-C3B	-2.75	115.58	120.43
5	M	1303	BCL	CHB-C4A-NA	-2.74	120.44	124.40
6	M	1309	BPH	C1-O2A-CGA	2.74	123.28	116.65
7	L	1284[B]	UQ2	CM2-O2-C2	2.73	126.07	116.47
7	L	1284[B]	UQ2	C7-C6-C5	-2.73	120.21	124.89
7	L	1284[B]	UQ2	C6-C5-C4	2.70	121.30	119.17
5	L	1282	BCL	O1D-CGD-CBD	-2.70	119.19	124.52
5	L	1282	BCL	C11-C10-C8	-2.69	107.02	115.97
5	M	1303	BCL	CAA-C2A-C3A	-2.69	105.73	113.00
5	L	1282	BCL	CHA-C1A-NA	-2.67	120.34	126.39
5	L	1285	BCL	CMA-C3A-C4A	-2.65	104.66	111.77
5	L	1282	BCL	C2A-C3A-C4A	2.64	106.13	101.87
5	M	1304	BCL	CHB-C4A-NA	-2.61	120.63	124.40
5	M	1304	BCL	CMB-C2B-C3B	2.57	133.78	125.67
5	L	1282	BCL	C4-C3-C5	2.53	119.62	115.23
5	L	1285	BCL	C3D-C4D-ND	-2.53	105.87	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1284[A]	UQ2	C7-C6-C5	-2.52	120.57	124.89
5	M	1303	BCL	CHC-C4B-NB	-2.47	120.34	124.05
5	L	1285	BCL	O2D-CGD-O1D	-2.47	119.05	123.85
6	M	1309	BPH	C4-C3-C5	2.46	119.50	115.23
5	L	1282	BCL	CMA-C3A-C4A	-2.46	105.16	111.77
7	L	1284[B]	UQ2	CM3-O3-C3	2.46	125.11	116.47
6	M	1309	BPH	O2A-CGA-CBA	2.45	119.31	111.83
11	M	1310	U10	C27-C28-C29	-2.45	122.01	127.62
5	L	1285	BCL	CMB-C2B-C3B	2.45	133.40	125.67
6	L	1283	BPH	C1A-C2A-C3A	-2.44	100.52	102.84
5	M	1304	BCL	O2A-CGA-O1A	-2.42	117.56	123.63
5	L	1285	BCL	O2A-CGA-O1A	-2.41	117.60	123.63
11	M	1310	U10	C7-C6-C1	-2.40	120.77	124.89
5	M	1303	BCL	C3C-C4C-CHD	-2.39	118.36	123.39
5	M	1304	BCL	CHC-C4B-NB	-2.37	120.49	124.05
7	L	1284[A]	UQ2	C5-C6-C1	-2.36	117.32	119.62
5	L	1285	BCL	C3C-C4C-CHD	-2.32	118.50	123.39
5	L	1285	BCL	OBb-CAB-C3B	-2.32	116.33	120.43
5	M	1303	BCL	CHC-C1C-NC	-2.30	121.08	124.40
5	L	1282	BCL	CMB-C2B-C3B	2.27	132.84	125.67
12	M	1311	SPO	C18-C17-C19	-2.27	119.14	122.82
5	L	1285	BCL	CHC-C1C-NC	-2.27	121.13	124.40
12	M	1311	SPO	C40-C38-C39	2.26	119.79	114.59
6	M	1309	BPH	O2A-CGA-O1A	-2.25	118.00	123.63
11	M	1310	U10	C7-C8-C9	-2.25	122.96	126.83
5	M	1303	BCL	CMD-C2D-C3D	-2.25	122.53	127.69
6	M	1309	BPH	CBC-CAC-C3C	-2.25	109.36	113.78
12	M	1311	SPO	C8-C7-C9	-2.24	119.19	122.82
7	L	1284[A]	UQ2	C10-C9-C11	2.22	119.09	115.23
12	M	1311	SPO	C8-C7-C6	2.19	121.43	118.09
5	M	1304	BCL	CBA-CAA-C2A	-2.17	107.33	113.79
11	M	1310	U10	C25-C24-C23	-2.16	118.07	123.63
6	M	1309	BPH	C3D-CAD-CBD	2.15	110.43	107.61
12	M	1311	SPO	C34-C33-C35	2.14	118.94	115.23
5	L	1285	BCL	C16-C15-C13	-2.13	108.89	115.97
5	L	1282	BCL	O2A-CGA-CBA	2.12	118.28	111.83
7	L	1284[A]	UQ2	CM2-O2-C2	2.06	123.72	116.47
5	M	1303	BCL	O2D-CGD-O1D	-2.05	119.87	123.85
11	M	1310	U10	C35-C34-C36	2.04	118.78	115.23
9	M	1305	LDA	CM1-N1-C1	2.01	114.47	110.23
5	M	1304	BCL	CHA-C4D-ND	2.01	136.69	132.55
5	L	1285	BCL	C4-C3-C5	2.00	118.70	115.23

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C13
5	L	1282	BCL	C8
5	L	1285	BCL	C13
5	L	1285	BCL	C8
5	M	1303	BCL	C13
5	M	1303	BCL	C8
5	M	1304	BCL	C13
5	M	1304	BCL	C8

All (146) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	C1-C2-C3-O3
4	L	1287	GOL	O1-C1-C2-C3
5	L	1282	BCL	CHA-CBD-CGD-O1D
5	L	1282	BCL	CHA-CBD-CGD-O2D
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
5	M	1304	BCL	C1A-C2A-CAA-CBA
5	M	1304	BCL	C3A-C2A-CAA-CBA
7	L	1284[A]	UQ2	C7-C8-C9-C10
7	L	1284[A]	UQ2	C7-C8-C9-C11
7	L	1284[A]	UQ2	C12-C11-C9-C8
7	L	1284[A]	UQ2	C12-C13-C14-C15
7	L	1284[A]	UQ2	C12-C13-C14-C16
7	L	1284[B]	UQ2	C1-C6-C7-C8
7	L	1284[B]	UQ2	C12-C13-C14-C16
8	L	1286	HTO	O1-C1-C2-O2
8	L	1286	HTO	O1-C1-C2-C3
8	L	1286	HTO	O3-C3-C4-C5
9	M	1305	LDA	C2-C1-N1-O1
9	M	1305	LDA	C2-C1-N1-CM1
9	M	1306	LDA	N1-C1-C2-C3
11	M	1310	U10	C22-C23-C24-C25
11	M	1310	U10	C22-C23-C24-C26
11	M	1310	U10	C32-C33-C34-C35
11	M	1310	U10	C32-C33-C34-C36
12	M	1311	SPO	C6-C7-C9-C10
12	M	1311	SPO	C8-C7-C9-C10
12	M	1311	SPO	C9-C10-C11-C12
12	M	1311	SPO	C14-C15-C16-C17
12	M	1311	SPO	C15-C16-C17-C19

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Mol	Chain	Res	Type	Atoms
12	M	1311	SPO	C16-C17-C19-C20
12	M	1311	SPO	C18-C17-C19-C20
12	M	1311	SPO	C19-C20-C21-C22
12	M	1311	SPO	C21-C22-C23-C24
7	L	1284[B]	UQ2	C12-C13-C14-C15
11	M	1310	U10	C37-C38-C39-C41
7	L	1284[A]	UQ2	C12-C11-C9-C10
7	L	1284[B]	UQ2	C12-C11-C9-C10
11	M	1310	U10	C30-C29-C31-C32
11	M	1310	U10	C28-C29-C31-C32
7	L	1284[B]	UQ2	C7-C8-C9-C10
7	L	1284[B]	UQ2	C7-C8-C9-C11
11	M	1310	U10	C35-C34-C36-C37
7	L	1284[B]	UQ2	C12-C11-C9-C8
11	M	1310	U10	C14-C16-C17-C18
11	M	1310	U10	C34-C36-C37-C38
5	M	1303	BCL	C10-C11-C12-C13
11	M	1310	U10	C37-C38-C39-C40
5	L	1282	BCL	CBD-CGD-O2D-CED
5	L	1285	BCL	CBD-CGD-O2D-CED
12	M	1311	SPO	C36-C37-C38-C40
5	L	1282	BCL	C6-C7-C8-C9
5	L	1282	BCL	C14-C13-C15-C16
5	M	1303	BCL	C14-C13-C15-C16
12	M	1311	SPO	C15-C16-C17-C18
12	M	1311	SPO	C24-C23-C25-C26
12	M	1311	SPO	C22-C23-C25-C26
5	M	1303	BCL	C2-C1-O2A-CGA
11	M	1310	U10	C27-C28-C29-C30
5	M	1303	BCL	C8-C10-C11-C12
5	M	1304	BCL	C6-C7-C8-C10
7	L	1284[B]	UQ2	C9-C11-C12-C13
11	M	1310	U10	C29-C31-C32-C33
5	L	1285	BCL	C13-C15-C16-C17
6	L	1283	BPH	C8-C10-C11-C12
5	L	1282	BCL	C15-C16-C17-C18
5	L	1285	BCL	C15-C16-C17-C18
12	M	1311	SPO	C36-C37-C38-C39
5	L	1282	BCL	C8-C10-C11-C12
6	L	1283	BPH	C5-C6-C7-C8
12	M	1311	SPO	C13-C12-C14-C15
4	H	1251	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
12	M	1311	SPO	C11-C12-C14-C15
12	M	1311	SPO	C21-C22-C23-C25
5	M	1303	BCL	C13-C15-C16-C17
5	L	1285	BCL	O1D-CGD-O2D-CED
9	M	1306	LDA	C2-C3-C4-C5
4	L	1287	GOL	O1-C1-C2-O2
5	L	1282	BCL	O1D-CGD-O2D-CED
5	M	1303	BCL	C3-C5-C6-C7
9	M	1307	LDA	C4-C5-C6-C7
5	M	1304	BCL	C13-C15-C16-C17
6	M	1309	BPH	C5-C6-C7-C8
9	M	1306	LDA	C4-C5-C6-C7
9	M	1307	LDA	C1-C2-C3-C4
11	M	1310	U10	C33-C34-C36-C37
5	L	1285	BCL	C11-C12-C13-C14
9	M	1306	LDA	C5-C6-C7-C8
6	M	1309	BPH	C16-C17-C18-C19
6	M	1309	BPH	C3-C5-C6-C7
11	M	1310	U10	C19-C21-C22-C23
5	M	1304	BCL	C15-C16-C17-C18
5	L	1282	BCL	C6-C7-C8-C10
5	L	1285	BCL	C11-C10-C8-C7
5	M	1304	BCL	C16-C17-C18-C20
9	M	1305	LDA	C4-C5-C6-C7
9	M	1307	LDA	C2-C3-C4-C5
6	M	1309	BPH	O2A-C1-C2-C3
9	M	1306	LDA	C3-C4-C5-C6
5	M	1303	BCL	C4-C3-C5-C6
4	H	1252	GOL	O2-C2-C3-O3
6	M	1309	BPH	C6-C7-C8-C9
5	M	1303	BCL	C12-C13-C15-C16
6	M	1309	BPH	C6-C7-C8-C10
9	M	1305	LDA	C2-C3-C4-C5
6	M	1309	BPH	C16-C17-C18-C20
9	M	1307	LDA	C5-C6-C7-C8
11	M	1310	U10	C5-C4-O4-C4M
8	L	1286	HTO	C2-C3-C4-C5
5	M	1303	BCL	C2-C3-C5-C6
6	M	1309	BPH	C1-C2-C3-C5
5	M	1304	BCL	C6-C7-C8-C9
11	M	1310	U10	C27-C28-C29-C31
6	L	1283	BPH	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	L	1282	BCL	C13-C15-C16-C17
5	L	1282	BCL	C11-C10-C8-C7
5	L	1282	BCL	C12-C13-C15-C16
7	L	1284[B]	UQ2	C5-C6-C7-C8
11	M	1310	U10	C24-C26-C27-C28
6	M	1309	BPH	C8-C10-C11-C12
9	M	1305	LDA	C2-C1-N1-CM2
5	M	1303	BCL	C11-C10-C8-C7
6	L	1283	BPH	C16-C17-C18-C20
5	L	1282	BCL	C11-C10-C8-C9
5	M	1303	BCL	C11-C10-C8-C9
5	M	1304	BCL	C16-C17-C18-C19
9	M	1307	LDA	C9-C10-C11-C12
7	L	1284[A]	UQ2	C1-C2-O2-CM2
7	L	1284[B]	UQ2	C3-C2-O2-CM2
6	L	1283	BPH	C11-C10-C8-C9
9	M	1306	LDA	C11-C10-C9-C8
6	M	1309	BPH	C12-C13-C15-C16
6	M	1309	BPH	C14-C13-C15-C16
6	M	1309	BPH	C1-C2-C3-C4
6	L	1283	BPH	C11-C10-C8-C7
6	L	1283	BPH	C11-C12-C13-C14
11	M	1310	U10	C20-C19-C21-C22
4	H	1251	GOL	O2-C2-C3-O3
6	L	1283	BPH	C14-C13-C15-C16
6	M	1309	BPH	C11-C12-C13-C14
5	L	1285	BCL	C11-C12-C13-C15
6	M	1309	BPH	C11-C12-C13-C15
8	L	1286	HTO	C1-C2-C3-O3
6	L	1283	BPH	C4-C3-C5-C6
6	L	1283	BPH	C6-C7-C8-C10
12	M	1311	SPO	C34-C33-C35-C36

There are no ring outliers.

16 monomers are involved in 55 short contacts:

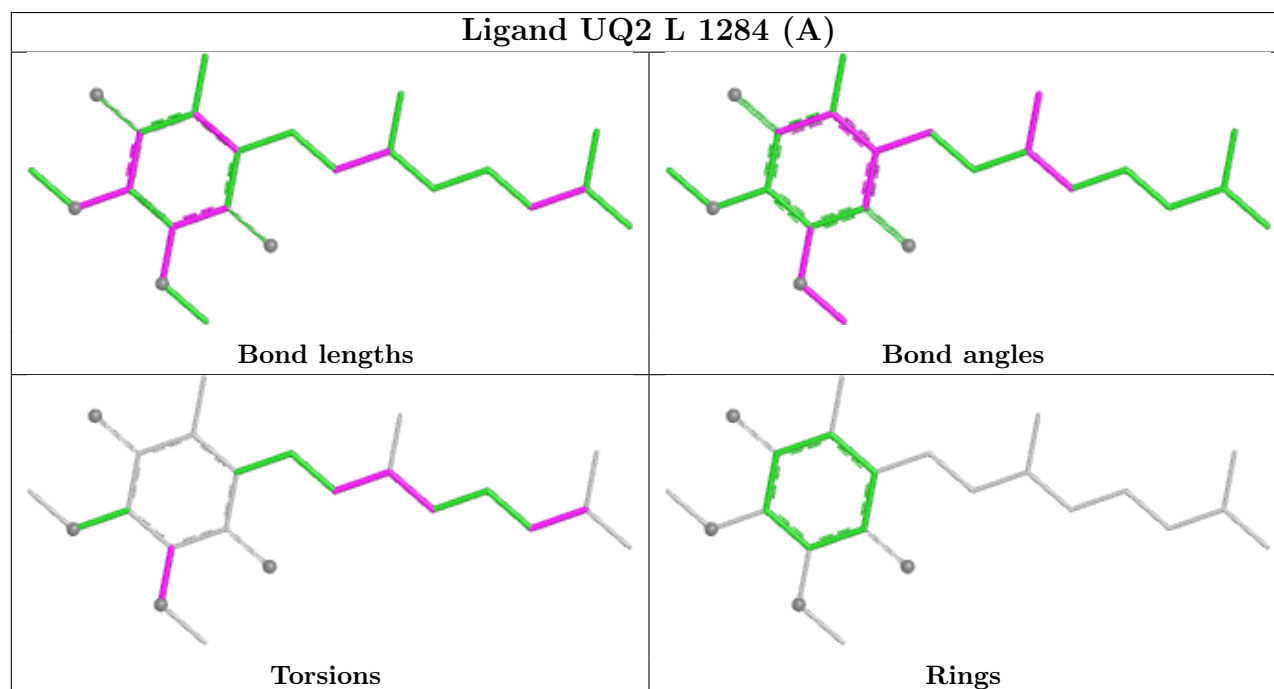
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	1305	LDA	2	0
9	M	1306	LDA	2	0
5	L	1285	BCL	1	0
6	M	1309	BPH	11	0
7	L	1284[B]	UQ2	13	0

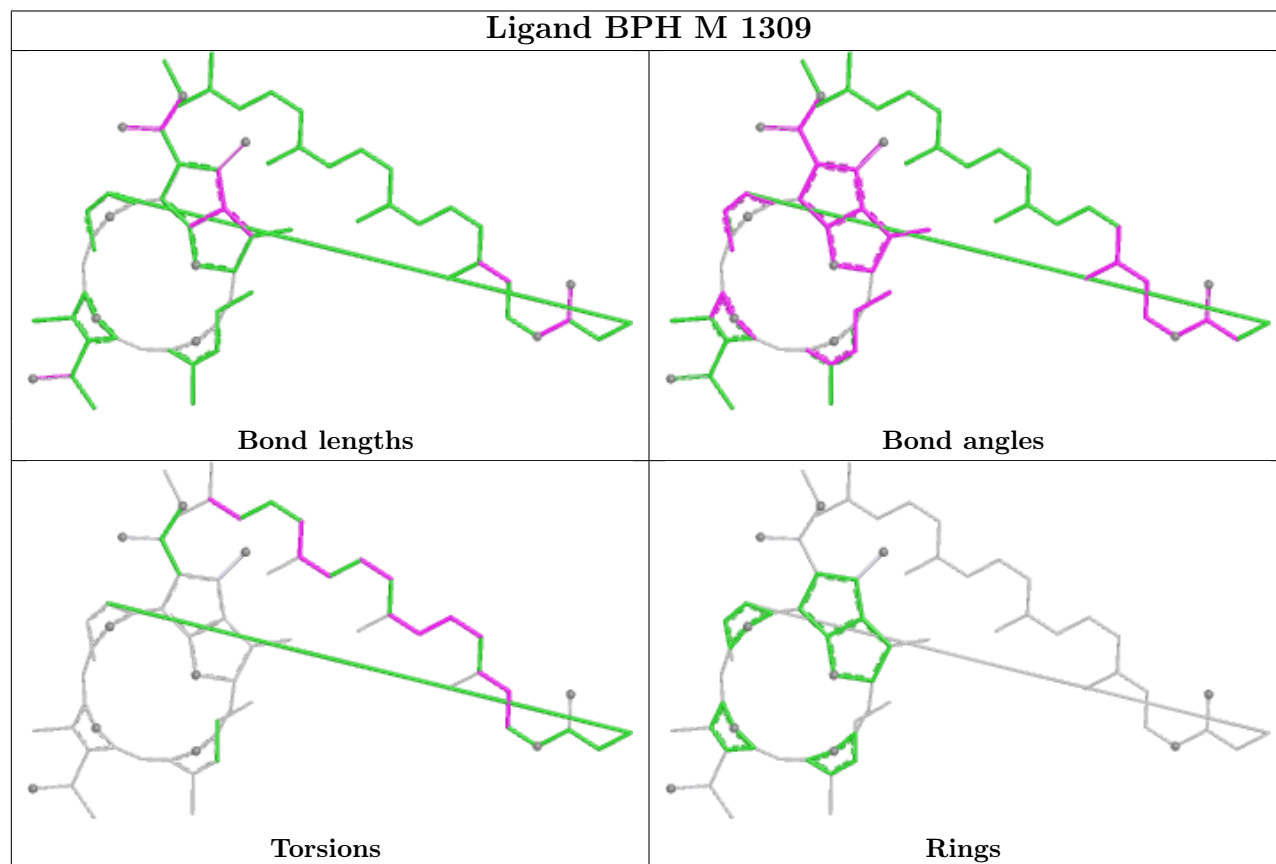
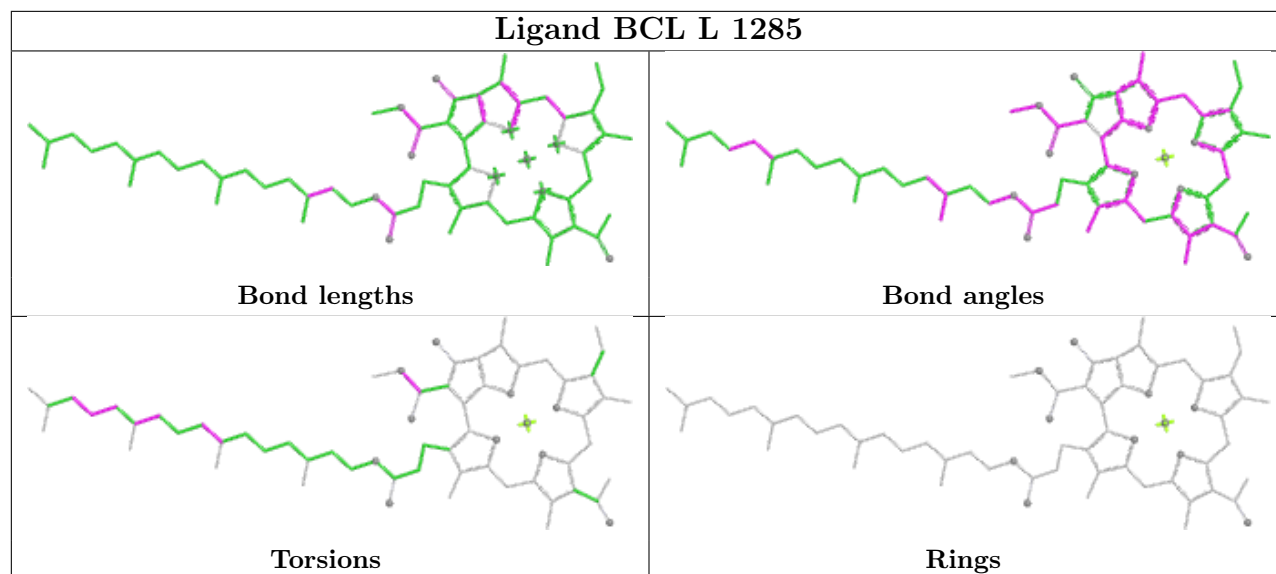
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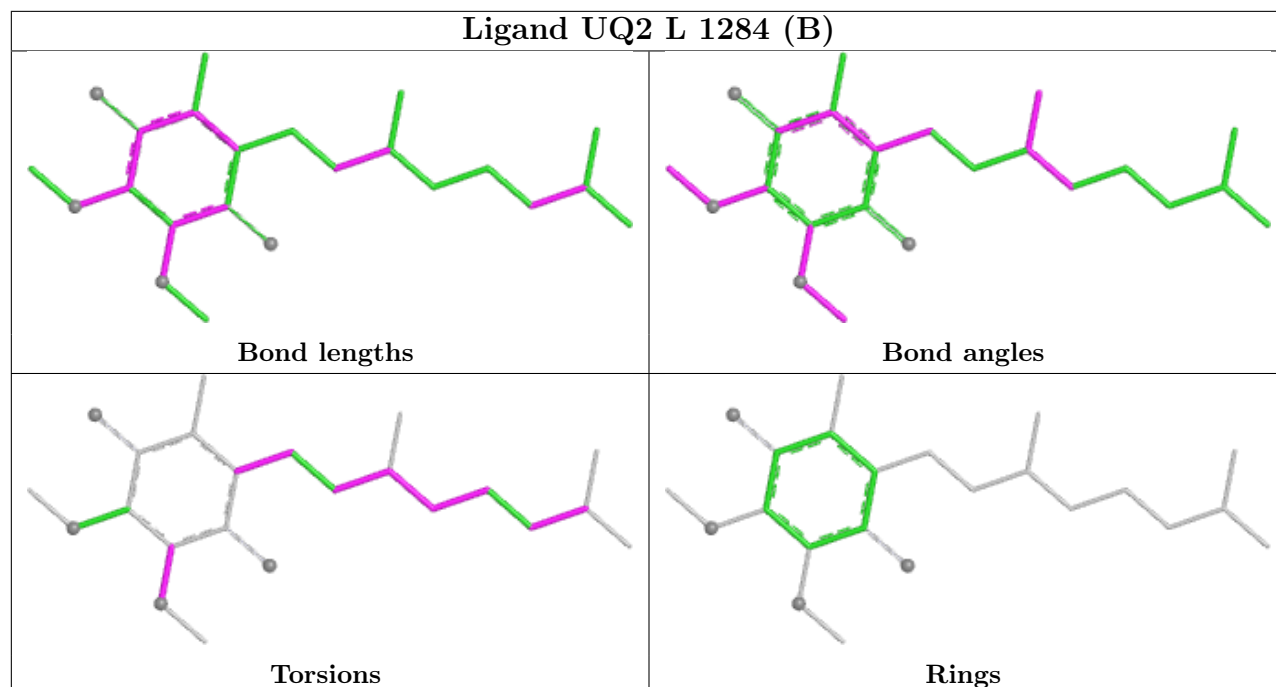
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	1	0
4	H	1253	GOL	1	0
4	H	1252	GOL	1	0
12	M	1311	SPO	1	0
4	L	1287	GOL	2	0
9	M	1307	LDA	1	0
6	L	1283	BPH	8	0
5	M	1304	BCL	9	0
5	M	1303	BCL	5	0
11	M	1310	U10	1	0
5	L	1282	BCL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

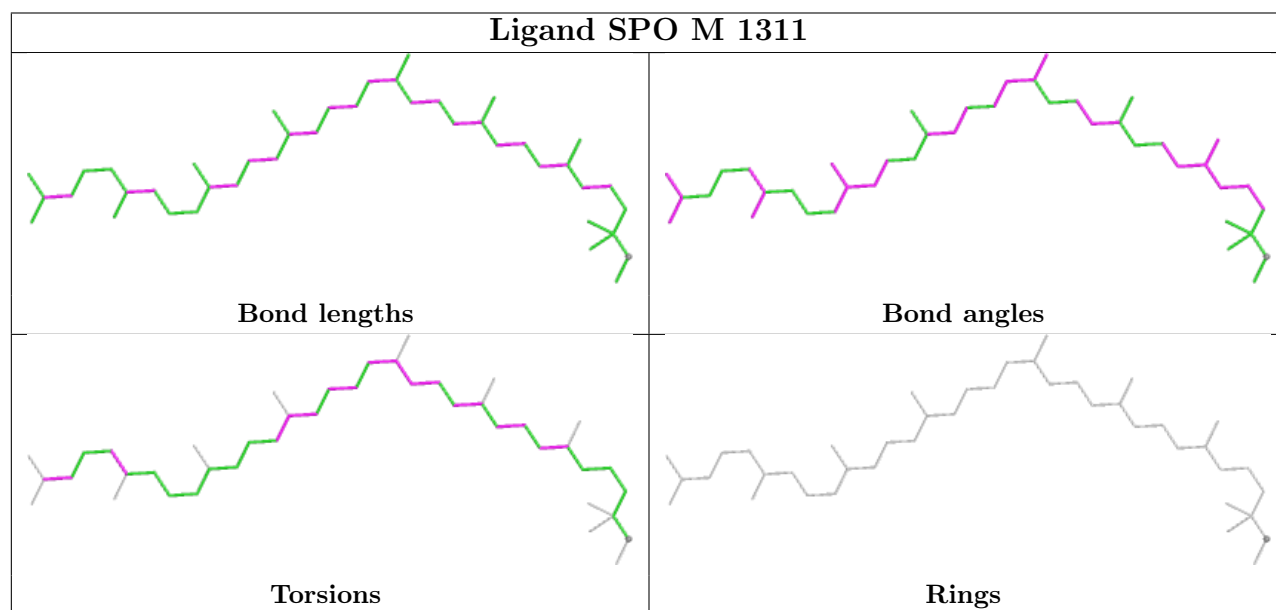


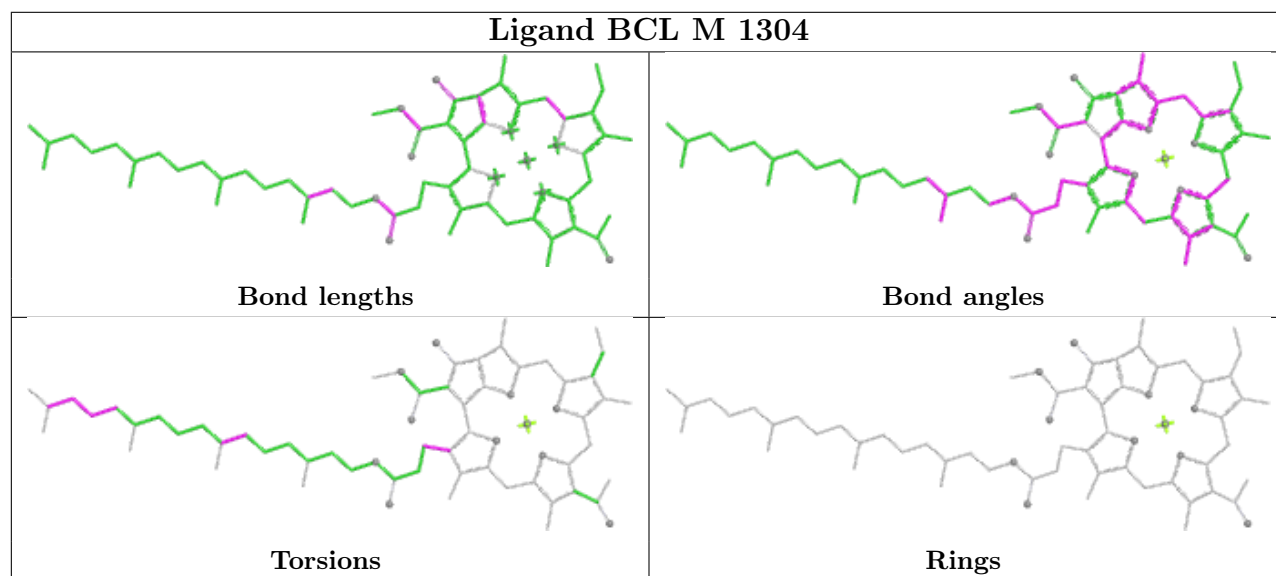
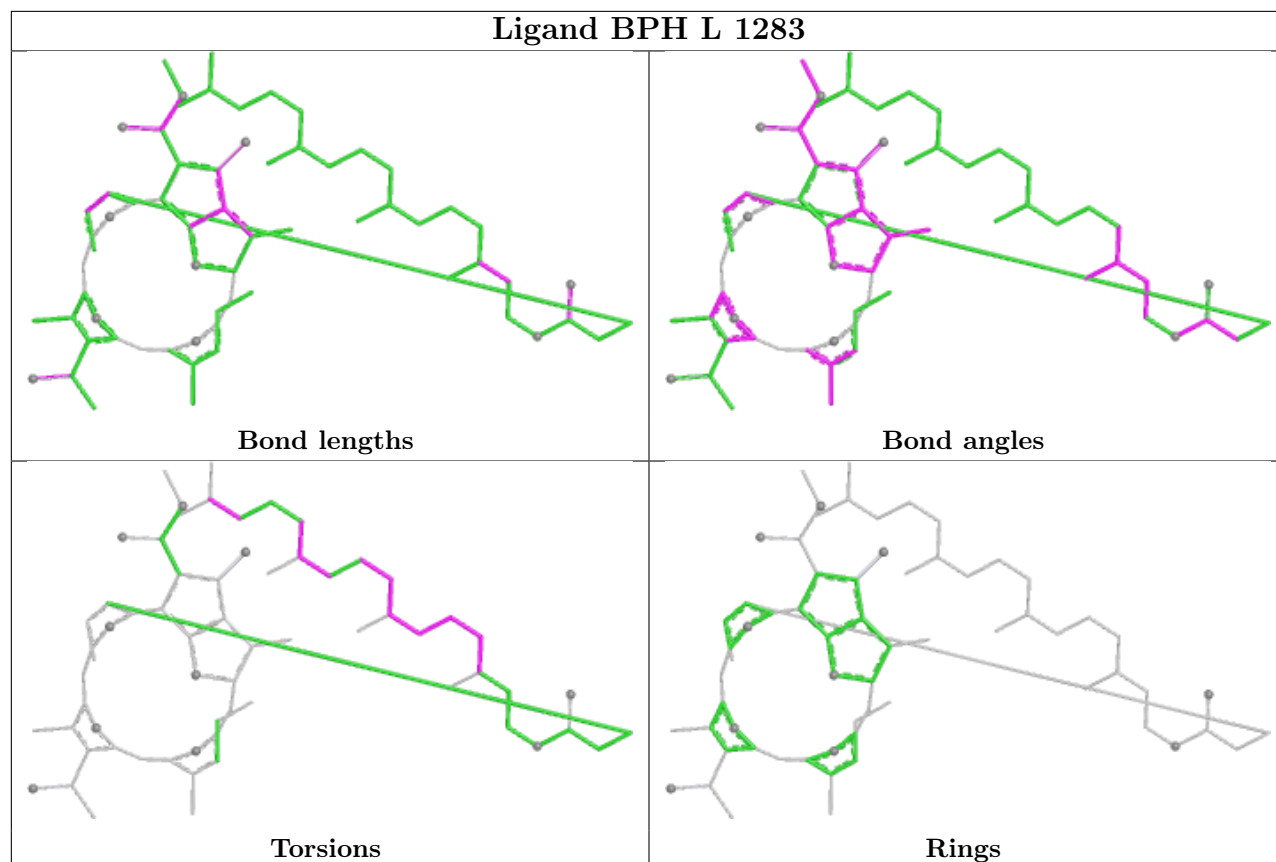


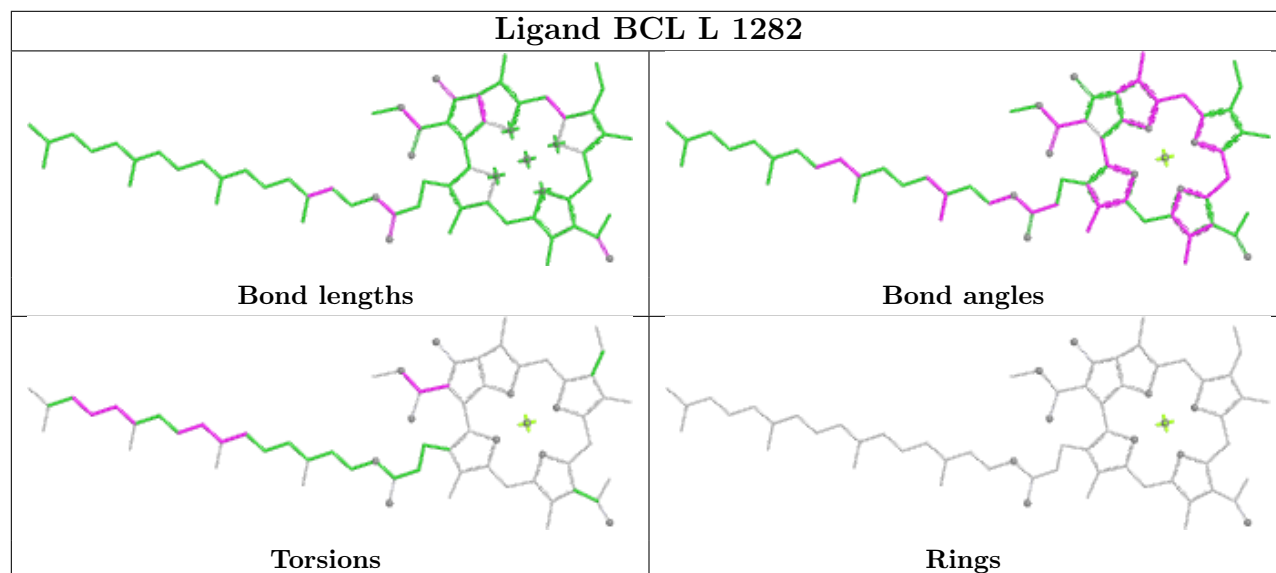
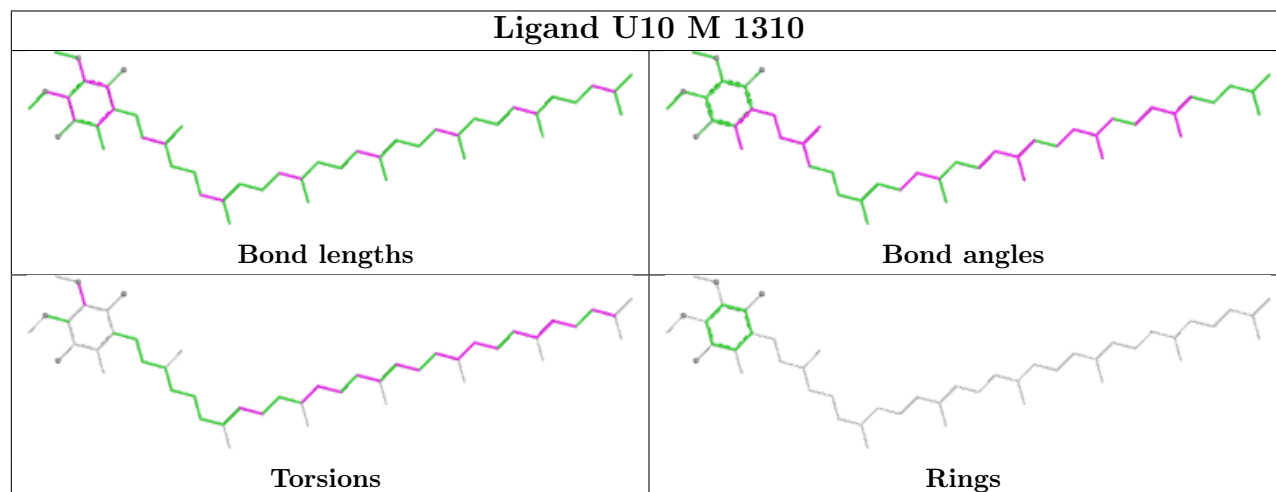
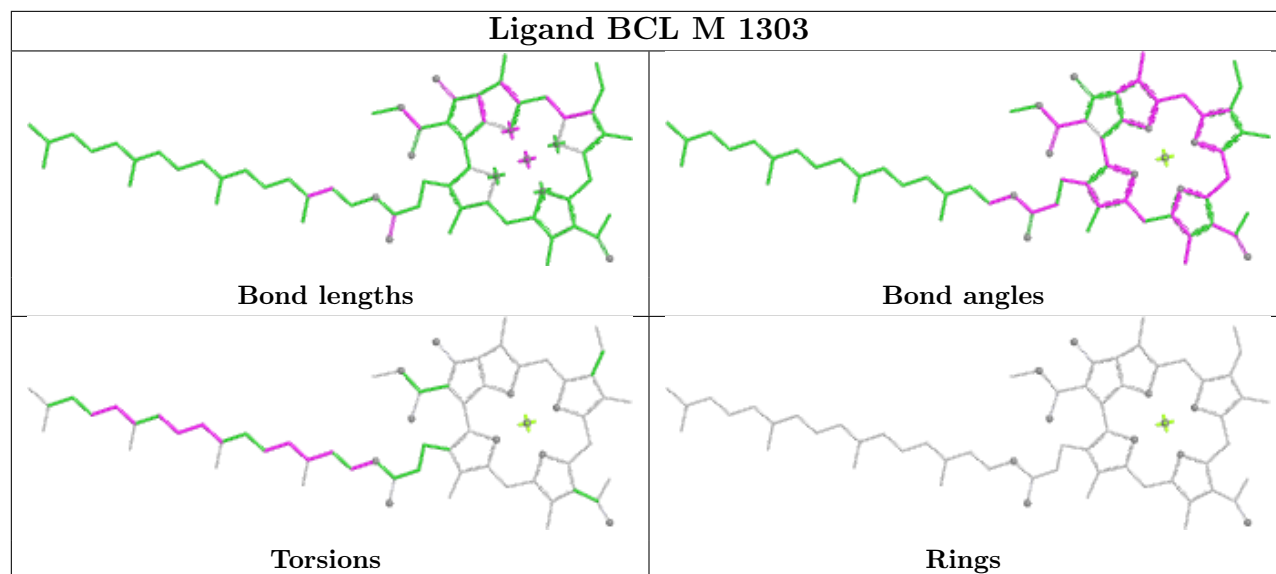
Ligand UQ2 L 1284 (B)



Ligand SPO M 1311







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%)	-0.10	9 (3%)	45	37	28, 51, 66, 102	3 (1%)
2	L	281/281 (100%)	-0.31	7 (2%)	58	49	32, 44, 69, 84	0
3	M	303/307 (98%)	-0.14	10 (3%)	49	40	34, 51, 76, 104	0
All	All	825/848 (97%)	-0.19	26 (3%)	50	41	28, 49, 72, 104	3 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	79	GLY	4.5
3	M	52	LEU	3.6
3	M	1	ALA	3.5
1	H	170	ASP	3.3
1	H	247	LYS	3.1
3	M	303	MET	3.0
3	M	23	ASP	2.9
2	L	281	GLY	2.8
1	H	173	GLU	2.8
3	M	17	ASP	2.8
2	L	279	ILE	2.5
2	L	72	GLU	2.5
3	M	301	HIS	2.5
1	H	69	GLY	2.5
1	H	18	TYR	2.5
2	L	20	ASN	2.4
3	M	25	ASN	2.4
3	M	2	GLU	2.4
1	H	220[A]	LYS	2.3
1	H	82	ASP	2.3
3	M	27	ALA	2.2
1	H	246	PRO	2.2
1	H	250	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	2.1
2	L	198	ALA	2.0
2	L	202	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

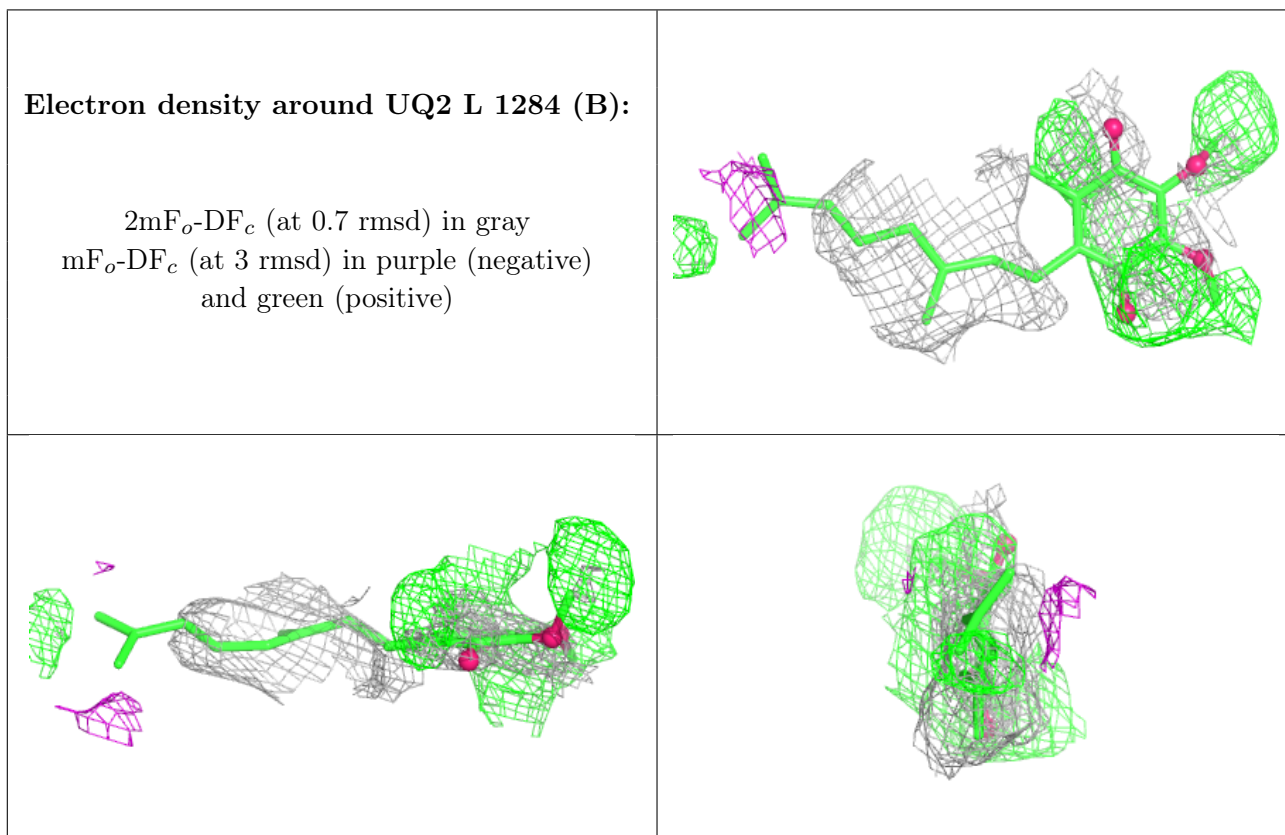
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

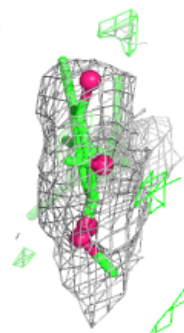
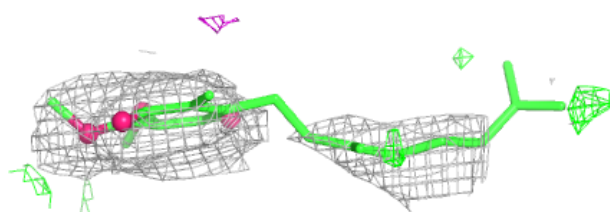
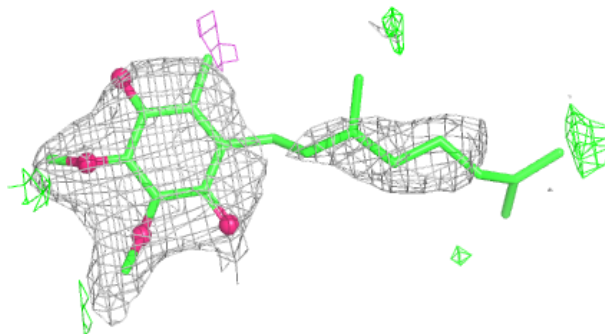
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	H	1251	6/6	0.81	0.21	69,77,81,82	0
4	GOL	H	1253	6/6	0.86	0.12	113,114,115,116	0
9	LDA	M	1307	16/16	0.86	0.31	98,102,114,115	0
7	UQ2	L	1284[B]	23/23	0.89	0.21	31,35,43,45	23
7	UQ2	L	1284[A]	23/23	0.89	0.21	51,59,74,74	23
9	LDA	M	1306	16/16	0.91	0.16	49,62,72,72	0
9	LDA	M	1305	16/16	0.92	0.19	74,83,86,87	0
4	GOL	H	1252	6/6	0.92	0.18	81,84,85,87	0
8	HTO	L	1286	10/10	0.92	0.17	71,83,83,84	0
11	U10	M	1310	48/63	0.94	0.13	42,52,81,82	0
5	BCL	M	1303	66/66	0.95	0.10	29,41,93,96	0
6	BPH	M	1309	65/65	0.95	0.12	39,48,109,110	0
4	GOL	L	1287	6/6	0.95	0.14	85,86,86,87	0
12	SPO	M	1311	42/42	0.95	0.14	47,59,82,85	0
5	BCL	M	1304	66/66	0.97	0.07	32,40,59,68	0
5	BCL	L	1282	66/66	0.97	0.07	31,40,64,75	0
6	BPH	L	1283	65/65	0.98	0.07	25,35,53,55	0
5	BCL	L	1285	66/66	0.98	0.07	30,37,55,60	0
10	FE	M	1308	1/1	1.00	0.05	41,41,41,41	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.

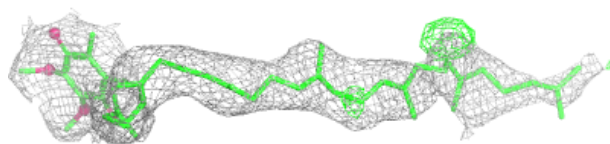
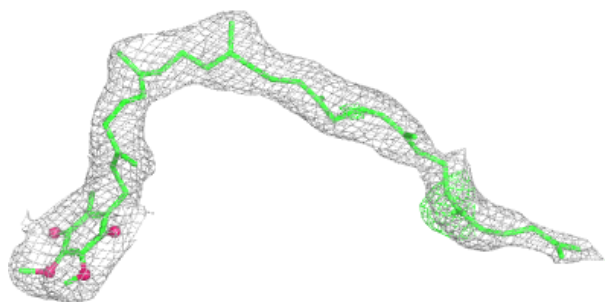


Electron density around UQ2 L 1284 (A):

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

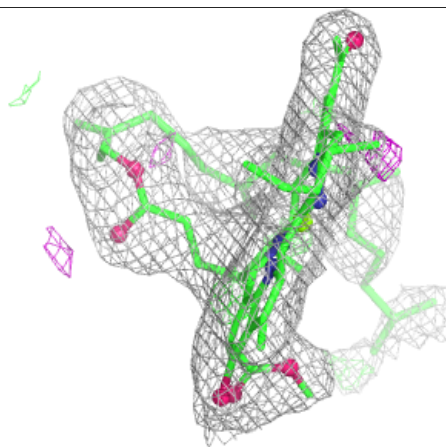
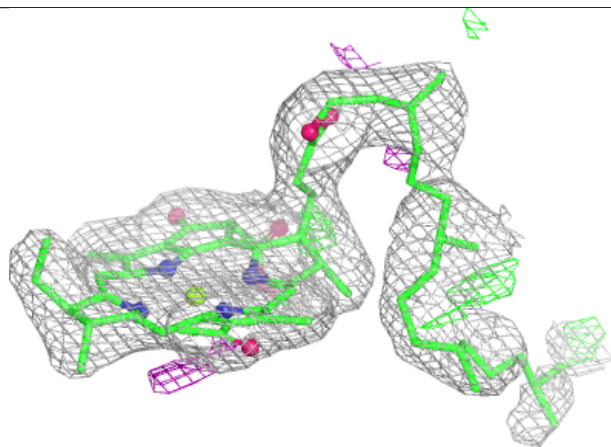
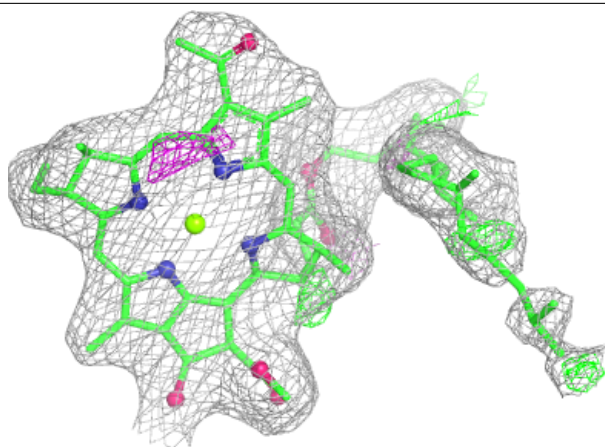
**Electron density around U10 M 1310:**

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



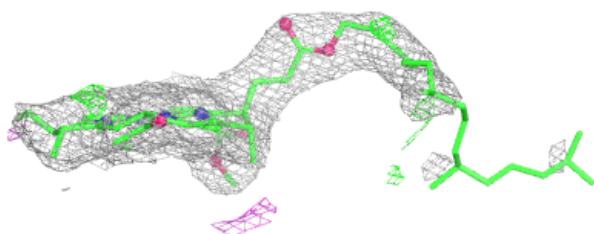
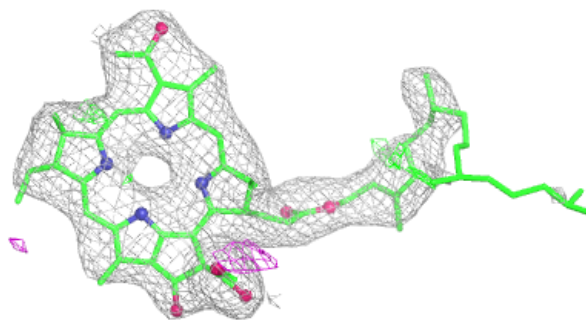
Electron density around BCL M 1303:

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

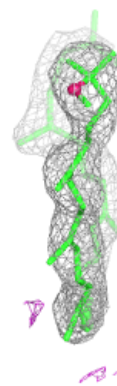
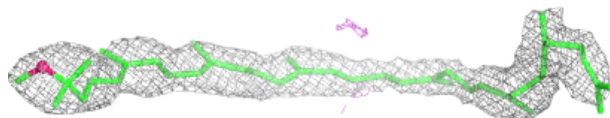
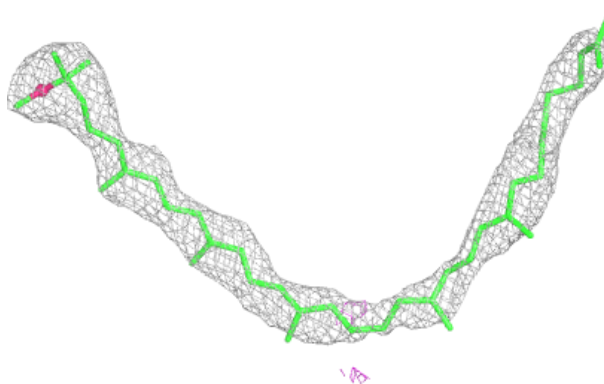


Electron density around BPH M 1309:

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

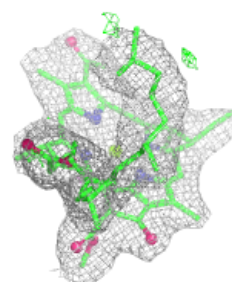
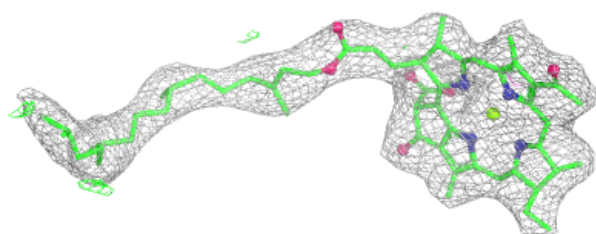
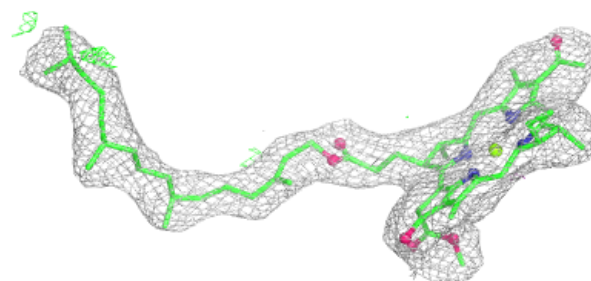
**Electron density around SPO M 1311:**

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

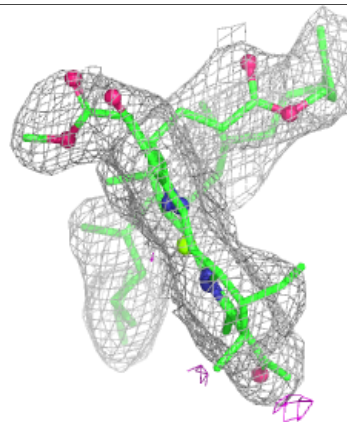
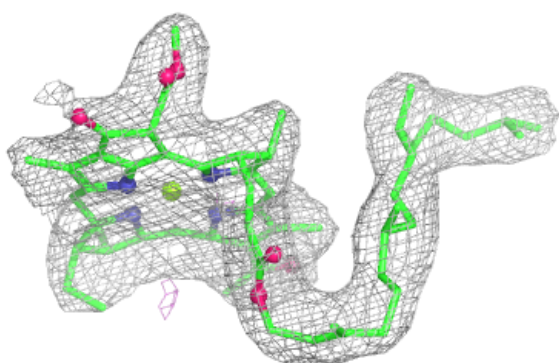
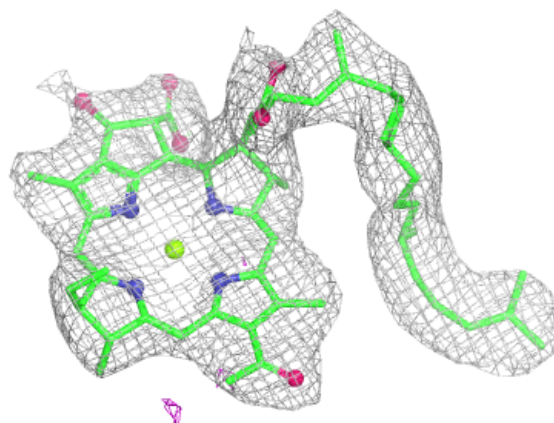


Electron density around BCL M 1304:

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and green (positive)

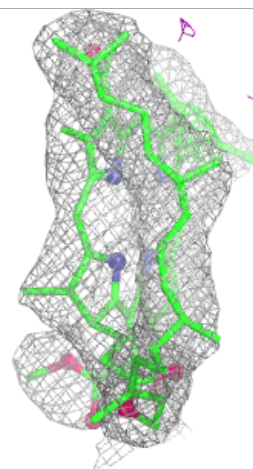
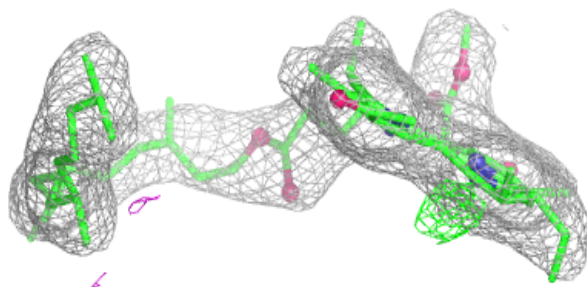
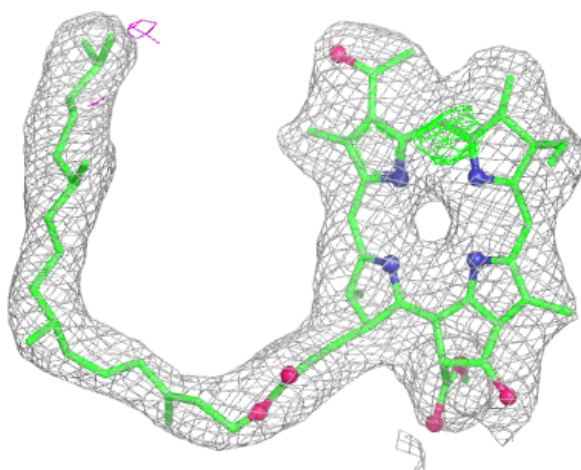
**Electron density around BCL L 1282:**

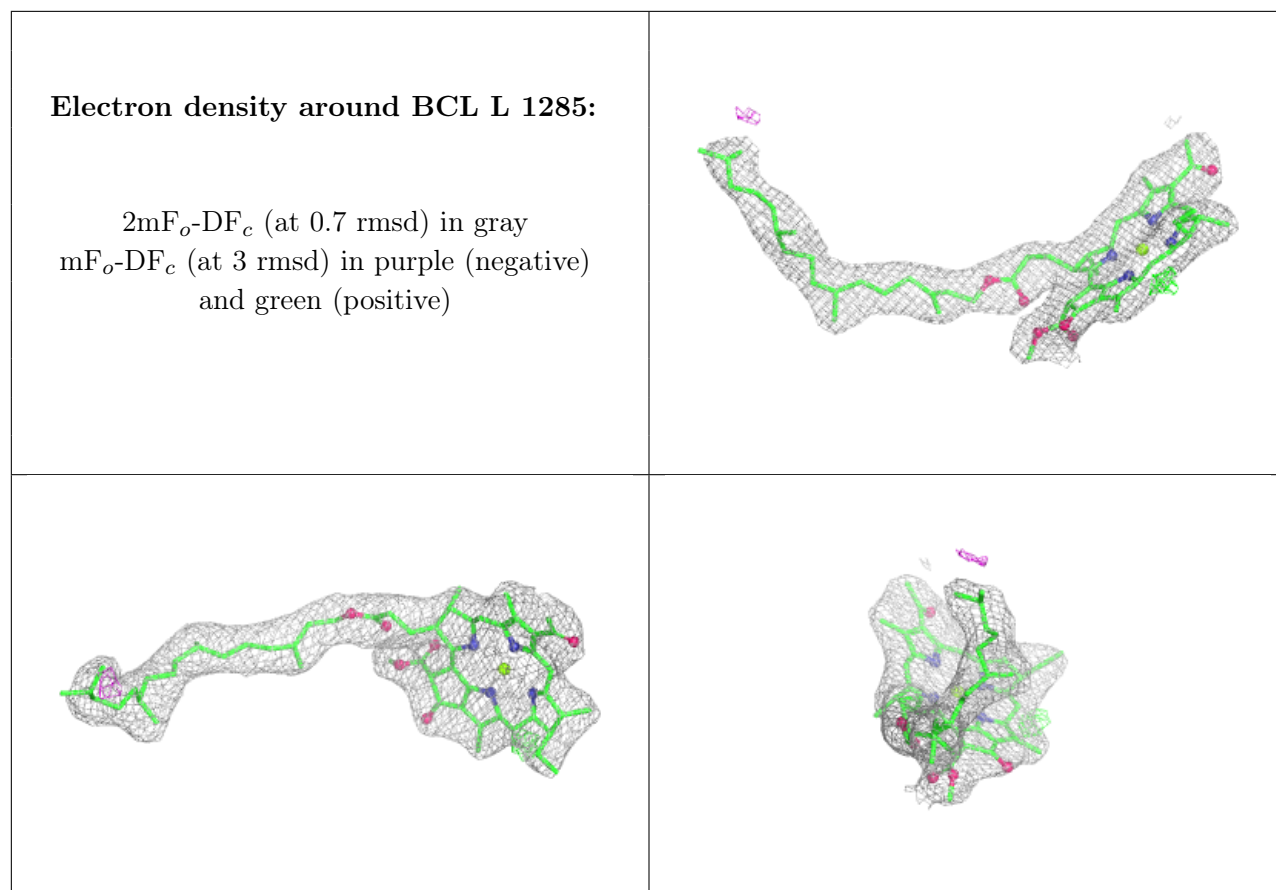
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BPH 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.