



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:03 AM UTC

PDB ID : 2UWW / pdb_00002uww
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 6.5 in the neutral state
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-23
Resolution : 2.05 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

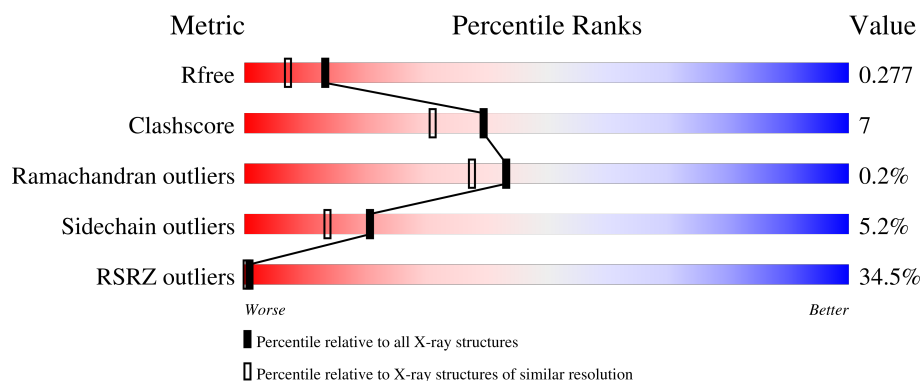
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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

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	1252	-	-	X	-
5	BCL	L	1282	X	-	-	-
5	BCL	L	1290	X	-	-	-
5	BCL	M	1304	X	-	-	-
5	BCL	M	1305	X	-	-	-
6	LDA	L	1284	-	-	-	X
6	LDA	L	1285	-	-	-	X
6	LDA	L	1286	-	-	-	X
6	LDA	M	1309	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7772 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	0	1
			1830	1169	315	337	9			

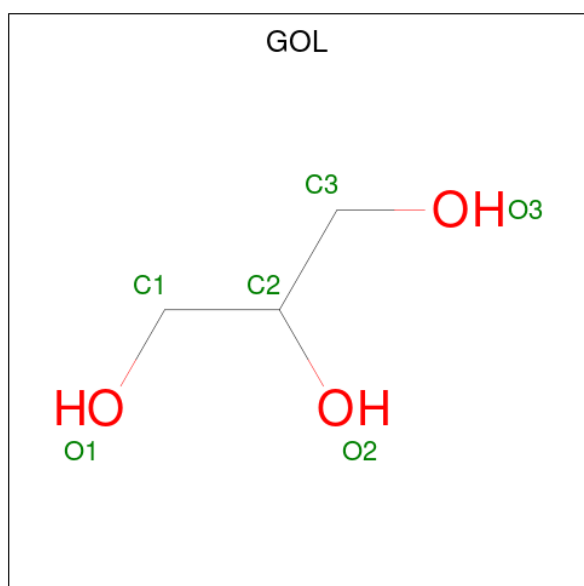
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

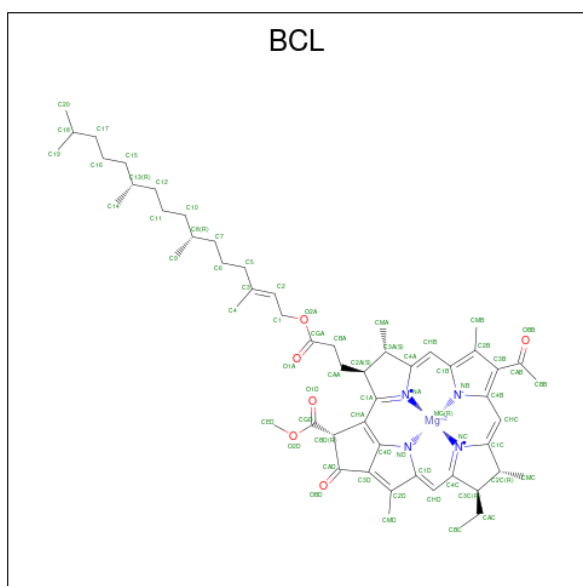
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

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



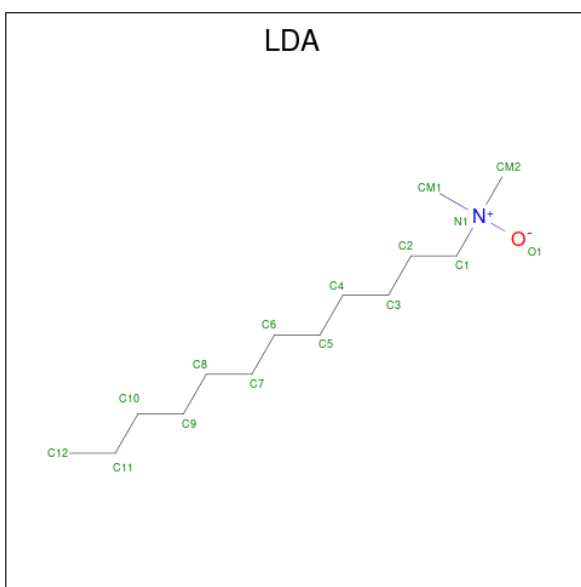
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	M	1	Total	C	O	0	0
			6	3	3		

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



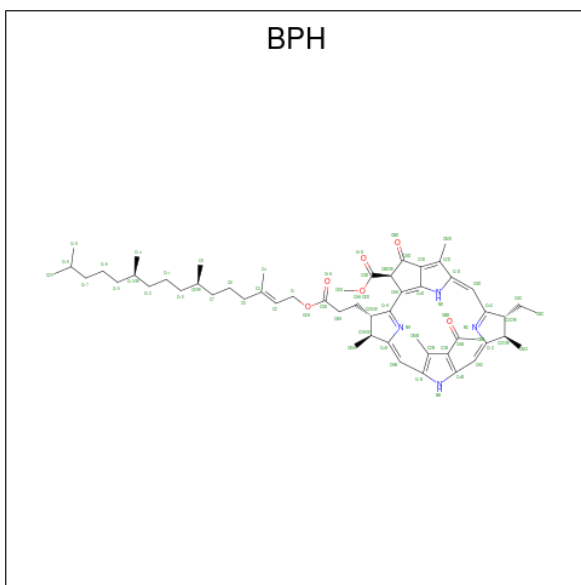
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



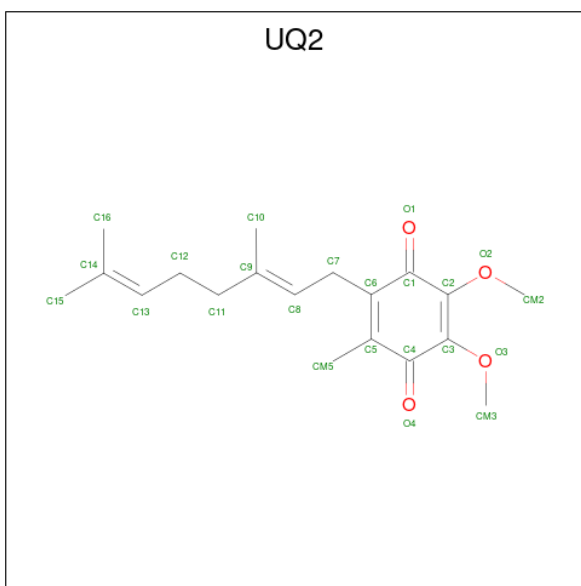
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

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



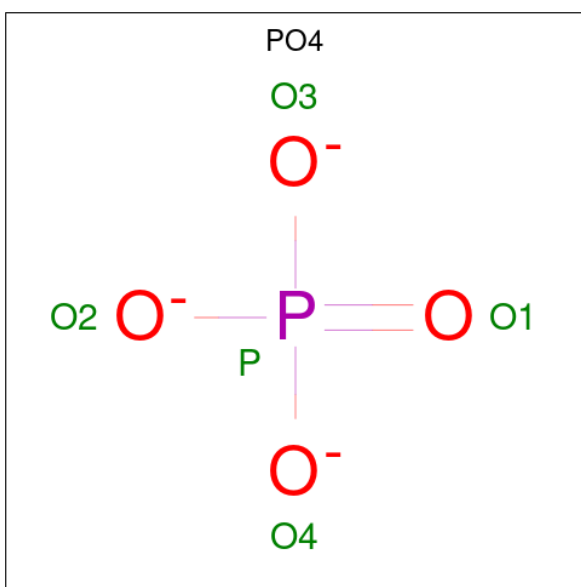
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (CCD ID: UQ2) (formula: C₁₉H₂₆O₄).



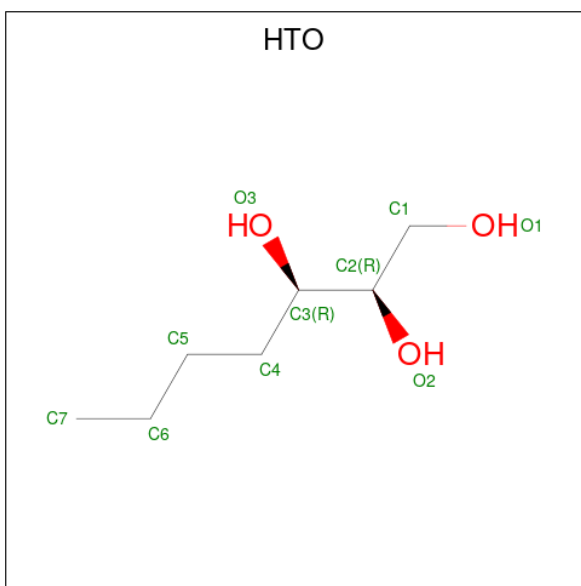
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 9 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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: $C_7H_{16}O_3$).

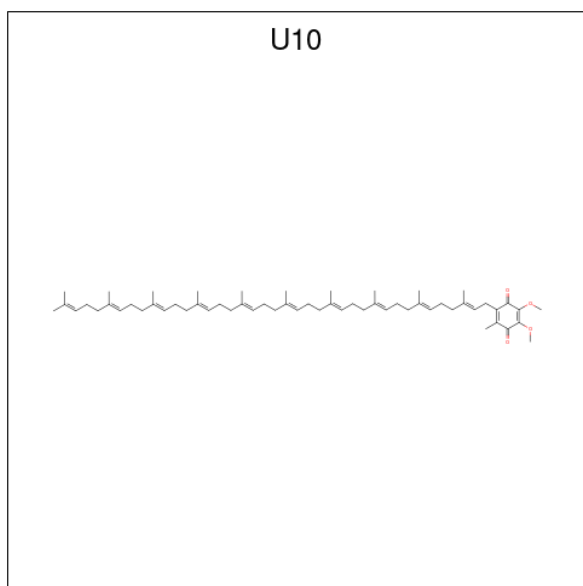


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

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

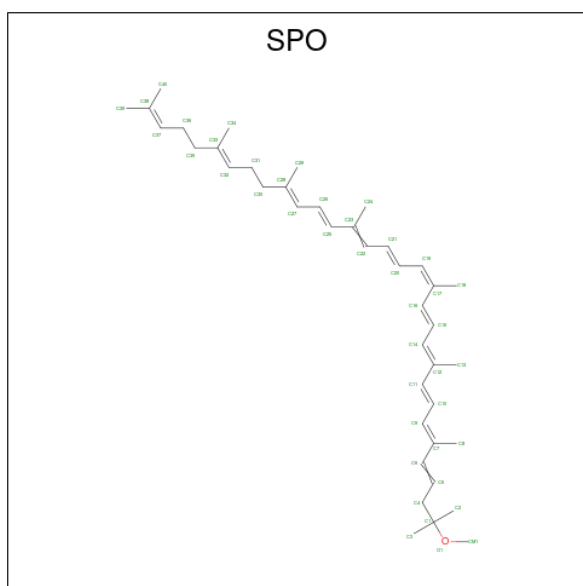
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



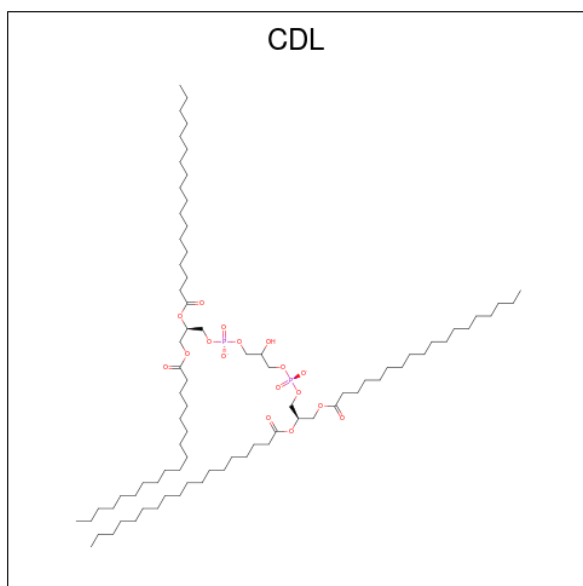
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

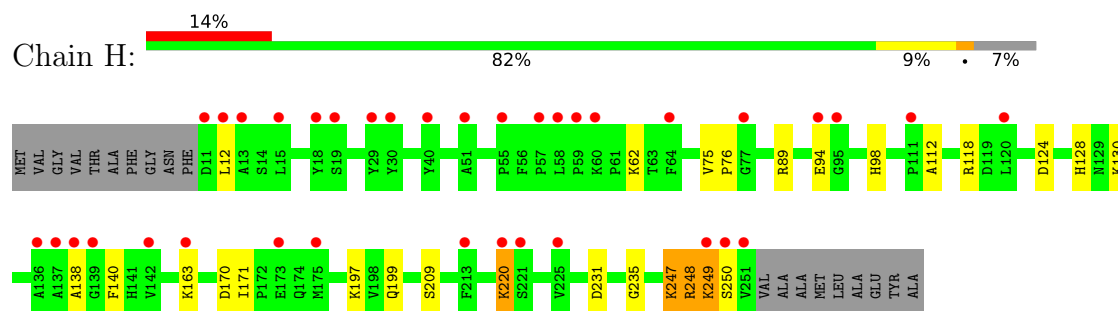
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	198	Total	O	0	0
			198	198		
15	L	132	Total	O	0	0
			132	132		
15	M	158	Total	O	0	0
			158	158		

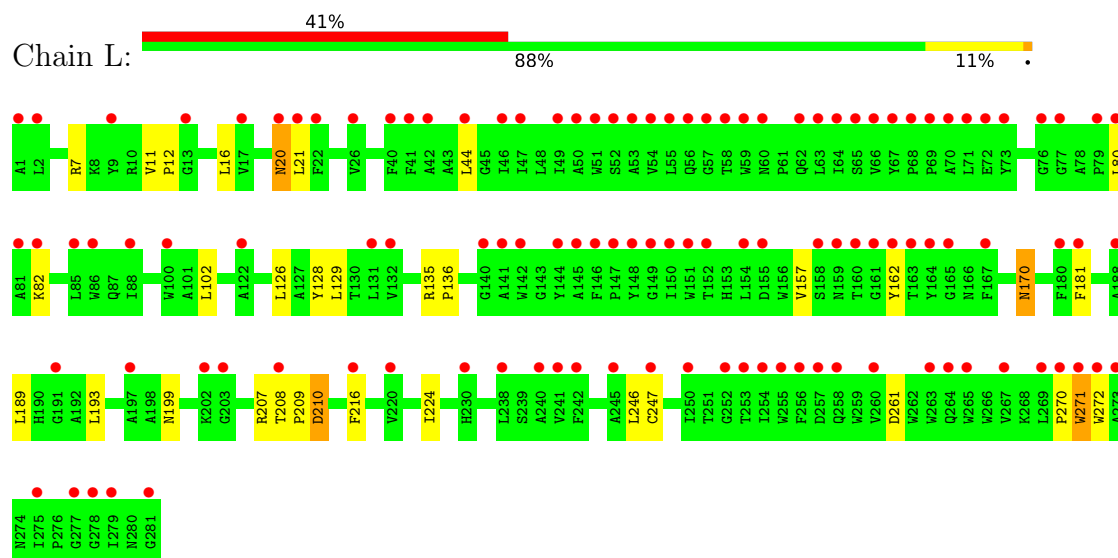
3 Residue-property plots [i](#)

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.

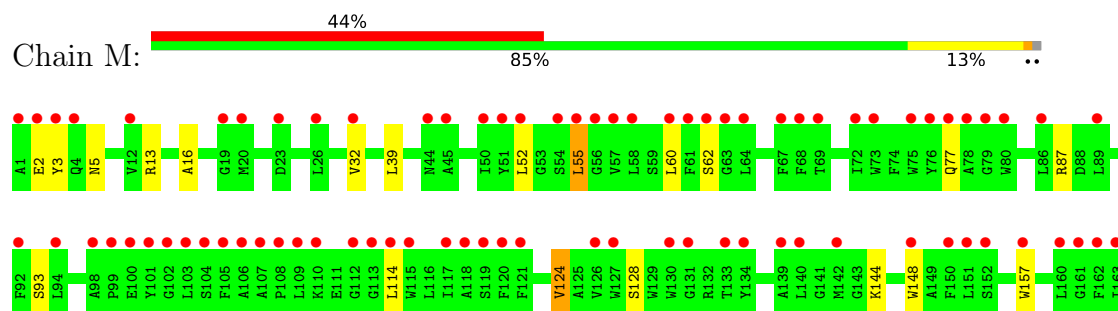
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

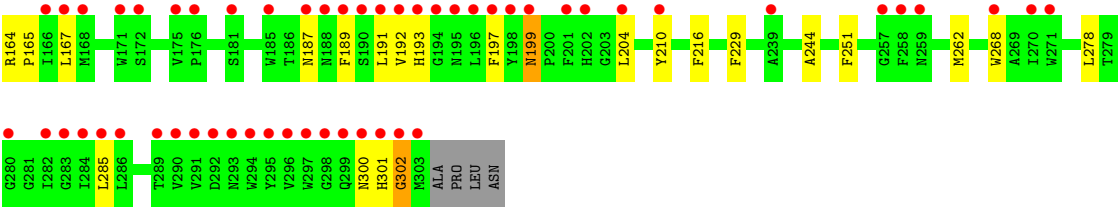


• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• 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	138.69Å 138.69Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.05 119.52 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (119.52-2.05) 89.6 (119.52-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.233 (Not available) , 0.277	Depositor DCC
R_{free} test set	2639 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.2	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	0.92	EDS
Total number of atoms	7772	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: SPO, FE, BCL, HTO, CDL, BPH, UQ2, PO4, GOL, U10, LDA

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	0.79	1/1878 (0.1%)	0.88	2/2555 (0.1%)
2	L	0.79	0/2320	0.89	0/3175
3	M	0.80	2/2501 (0.1%)	0.89	0/3415
All	All	0.80	3/6699 (0.0%)	0.89	2/9145 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	302	GLY	C-N	-6.82	1.23	1.33
1	H	250	SER	C-N	-6.28	1.24	1.33
3	M	262	MET	SD-CE	-5.05	1.67	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	248	ARG	CA-C-N	5.78	132.10	121.70
1	H	248	ARG	C-N-CA	5.78	132.10	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	138	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1830	0	1836	18	0
2	L	2232	0	2187	24	0
3	M	2409	0	2321	28	0
4	H	24	0	32	5	0
4	L	12	0	16	1	0
4	M	6	0	8	0	0
5	L	132	0	148	4	0
5	M	132	0	148	20	0
6	L	80	0	155	1	0
6	M	64	0	124	3	0
7	L	65	0	76	6	0
7	M	65	0	76	9	0
8	L	46	0	52	6	0
9	L	5	0	0	0	0
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	1	0
13	M	42	0	60	2	0
14	M	81	0	84	3	0
15	H	198	0	0	5	1
15	L	132	0	0	1	1
15	M	158	0	0	0	0
All	All	7772	0	7402	98	1

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

All (98) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1288:BPH:HBB3	7:L:1288:BPH:HHC	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:LYS:HD3	15:H:2181:HOH:O	1.75	0.86
5:L:1282:BCL:HBB2	5:L:1282:BCL:HHC	1.59	0.85
1:H:62:LYS:HE3	4:H:1252:GOL:H11	1.60	0.84
3:M:197:PHE:HZ	5:M:1305:BCL:HBB2	1.44	0.81
3:M:197:PHE:CZ	5:M:1305:BCL:HBB2	2.16	0.80
1:H:248:ARG:HA	1:H:249:LYS:CB	2.11	0.79
7:L:1288:BPH:HHC	7:L:1288:BPH:CBB	2.14	0.77
2:L:271:TRP:H	2:L:271:TRP:CD1	2.03	0.76
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.67	0.75
7:M:1311:BPH:HHC	7:M:1311:BPH:HBB3	1.69	0.74
4:H:1252:GOL:C3	15:H:2003:HOH:O	2.38	0.71
6:M:1306:LDA:H81	6:M:1308:LDA:H121	1.73	0.70
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.28	0.68
3:M:189:PHE:O	3:M:193:HIS:HD2	1.77	0.67
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.77	0.66
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.27	0.63
7:M:1311:BPH:HHC	7:M:1311:BPH:CBB	2.28	0.63
5:M:1305:BCL:CBB	5:M:1305:BCL:HHC	2.28	0.63
2:L:261:ASP:OD1	15:L:2120:HOH:O	2.16	0.62
4:H:1252:GOL:H31	15:H:2003:HOH:O	1.96	0.62
3:M:144:LYS:N	14:M:1314:CDL:OB3	2.27	0.61
7:L:1288:BPH:HBB3	7:L:1288:BPH:CHC	2.22	0.61
2:L:170:ASN:HD22	2:L:170:ASN:C	2.09	0.61
4:H:1252:GOL:H32	15:H:2003:HOH:O	1.99	0.60
2:L:199:ASN:O	14:M:1314:CDL:HB22	2.02	0.59
5:M:1304:BCL:HBB3	5:M:1305:BCL:H41	1.83	0.59
5:M:1304:BCL:CBB	5:M:1304:BCL:HHC	2.34	0.58
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.85	0.57
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.22	0.56
3:M:157:TRP:HB2	5:M:1305:BCL:H71	1.88	0.56
7:L:1288:BPH:CBB	7:L:1288:BPH:CHC	2.81	0.55
1:H:128:HIS:HE1	15:H:2125:HOH:O	1.88	0.55
1:H:75:VAL:HA	1:H:76:PRO:C	2.31	0.55
7:L:1288:BPH:HBB2	3:M:210:TYR:HB3	1.90	0.55
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.56	0.54
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.35	0.54
1:H:248:ARG:HA	1:H:249:LYS:HB3	1.91	0.53
3:M:189:PHE:O	3:M:193:HIS:CD2	2.61	0.53
3:M:77:GLN:HE22	3:M:93:SER:H	1.54	0.53
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.39	0.53
5:M:1305:BCL:HBB2	5:M:1305:BCL:HHC	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:199:ASN:HD22	3:M:199:ASN:C	2.16	0.52
1:H:197:LYS:HE3	1:H:199:GLN:NE2	2.24	0.52
1:H:209:SER:OG	1:H:247:LYS:HD3	2.10	0.52
5:M:1304:BCL:HBB2	13:M:1313:SPO:H243	1.92	0.52
3:M:300:ASN:C	3:M:302:GLY:H	2.17	0.52
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.74	0.52
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.92	0.51
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.93	0.51
2:L:189:LEU:CD1	8:L:1289[A]:UQ2:H121	2.40	0.51
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB2	1.94	0.50
6:M:1308:LDA:H52	6:M:1309:LDA:H42	1.93	0.50
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.94	0.50
5:M:1304:BCL:CBB	13:M:1313:SPO:H243	2.42	0.50
2:L:157:VAL:HG11	5:M:1305:BCL:HBB1	1.94	0.49
5:M:1305:BCL:HAA2	5:M:1305:BCL:HBD	1.95	0.49
5:M:1304:BCL:H62	7:M:1311:BPH:HMB3	1.95	0.48
3:M:167:LEU:HD12	3:M:285:LEU:HD11	1.94	0.48
1:H:62:LYS:CE	4:H:1252:GOL:H11	2.39	0.48
2:L:271:TRP:CD1	2:L:271:TRP:N	2.79	0.48
3:M:197:PHE:HZ	5:M:1305:BCL:CBB	2.19	0.48
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.47	0.47
1:H:248:ARG:CA	1:H:249:LYS:HB2	2.43	0.47
5:M:1305:BCL:HHC	5:M:1305:BCL:HBB3	1.97	0.46
2:L:199:ASN:HA	4:L:1293:GOL:H31	1.98	0.46
6:L:1287:LDA:H121	8:L:1289[A]:UQ2:H161	1.97	0.46
5:L:1282:BCL:H192	7:L:1288:BPH:H7C2	1.98	0.46
2:L:208:THR:HB	2:L:209:PRO:HD2	1.98	0.46
2:L:193:LEU:HD23	8:L:1289[A]:UQ2:C4	2.46	0.45
1:H:112:ALA:HA	1:H:235:GLY:O	2.17	0.45
3:M:60:LEU:HD11	7:M:1311:BPH:H161	1.98	0.44
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.44
2:L:11:VAL:HB	2:L:12:PRO:HD2	1.99	0.44
5:M:1305:BCL:CBB	5:M:1305:BCL:CHC	2.94	0.44
1:H:89:ARG:NH2	1:H:94:GLU:HG2	2.33	0.43
2:L:224:ILE:HG22	8:L:1289[A]:UQ2:H8	2.00	0.43
1:H:140:PHE:HA	3:M:13:ARG:O	2.19	0.43
3:M:62:SER:OG	3:M:124:VAL:HG22	2.18	0.43
3:M:300:ASN:C	3:M:302:GLY:N	2.76	0.43
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.19	0.43
2:L:272:TRP:CD1	3:M:87:ARG:HG3	2.54	0.43
5:M:1304:BCL:H102	5:M:1304:BCL:H13	1.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:ASN:N	2:L:20:ASN:HD22	2.17	0.42
5:M:1304:BCL:H71	5:M:1305:BCL:H202	2.02	0.42
3:M:251:PHE:CD1	3:M:251:PHE:C	2.98	0.42
5:M:1304:BCL:H101	5:M:1305:BCL:H171	2.02	0.41
7:M:1311:BPH:H7C2	7:M:1311:BPH:H112	1.81	0.41
8:L:1289[A]:UQ2:H101	8:L:1289[A]:UQ2:H122	1.88	0.41
1:H:124:ASP:HB2	2:L:210:ASP:OD2	2.20	0.41
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.56	0.41
3:M:278:LEU:HD21	14:M:1314:CDL:H782	2.01	0.41
3:M:268:TRP:CD1	12:M:1312:U10:H111	2.56	0.41
6:M:1308:LDA:C5	6:M:1309:LDA:H42	2.52	0.40
3:M:3:TYR:CZ	3:M:5:ASN:HA	2.57	0.40
3:M:197:PHE:CE1	5:M:1305:BCL:HBB2	2.56	0.40
2:L:270:PRO:HG2	2:L:271:TRP:CD1	2.57	0.40
8:L:1289[B]:UQ2:H121	8:L:1289[B]:UQ2:H101	1.50	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:2050:HOH:O	15:L:2077:HOH:O[6_655]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	239/260 (92%)	235 (98%)	3 (1%)	1 (0%)	30	22
2	L	279/281 (99%)	274 (98%)	5 (2%)	0	100	100
3	M	301/307 (98%)	290 (96%)	10 (3%)	1 (0%)	36	30
All	All	819/848 (97%)	799 (98%)	18 (2%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	301	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	195/208 (94%)	188 (96%)	7 (4%)	31	26
2	L	220/220 (100%)	204 (93%)	16 (7%)	13	7
3	M	236/240 (98%)	225 (95%)	11 (5%)	23	17
All	All	651/668 (98%)	617 (95%)	34 (5%)	21	14

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

Mol	Chain	Res	Type
1	H	12	LEU
1	H	118	ARG
1	H	163	LYS
1	H	171	ILE
1	H	220	LYS
1	H	231	ASP
1	H	247	LYS
2	L	16	LEU
2	L	20	ASN
2	L	21	LEU
2	L	44	LEU
2	L	80	LEU
2	L	82	LYS
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	170	ASN
2	L	207	ARG
2	L	210	ASP

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Mol	Chain	Res	Type
2	L	216	PHE
2	L	246	LEU
2	L	247	CYS
2	L	271	TRP
3	M	2	GLU
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	114	LEU
3	M	124	VAL
3	M	191	LEU
3	M	192	VAL
3	M	199	ASN
3	M	204	LEU
3	M	216	PHE

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

Mol	Chain	Res	Type
1	H	68	HIS
1	H	98	HIS
1	H	141	HIS
2	L	20	ASN
2	L	159	ASN
2	L	170	ASN
2	L	183	ASN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	UQ2	L	1289[B]	-	23,23,23	2.68	9 (39%)	30,31,31	1.27	4 (13%)
6	LDA	L	1283	-	13,15,15	2.13	2 (15%)	14,17,17	0.46	0
6	LDA	M	1307	-	13,15,15	2.19	2 (15%)	14,17,17	0.60	0
13	SPO	M	1313	-	41,41,41	2.57	12 (29%)	47,50,50	2.27	19 (40%)
14	CDL	M	1314	-	80,80,99	2.14	16 (20%)	86,92,111	2.85	13 (15%)
6	LDA	L	1284	-	13,15,15	2.23	2 (15%)	14,17,17	0.54	0
7	BPH	M	1311	-	59,70,70	2.73	11 (18%)	59,101,101	2.47	18 (30%)
4	GOL	H	1253	-	5,5,5	0.39	0	5,5,5	0.31	0
5	BCL	L	1290	2	69,74,74	1.76	7 (10%)	79,115,115	1.93	21 (26%)
6	LDA	M	1308	-	13,15,15	2.23	2 (15%)	14,17,17	0.64	0
4	GOL	H	1255	-	5,5,5	0.36	0	5,5,5	0.37	0
6	LDA	M	1309	-	13,15,15	2.23	2 (15%)	14,17,17	0.57	0
4	GOL	H	1254	-	5,5,5	0.38	0	5,5,5	0.29	0
6	LDA	L	1287	-	13,15,15	2.27	2 (15%)	14,17,17	0.59	0
6	LDA	L	1285	-	13,15,15	2.21	2 (15%)	14,17,17	0.54	0
4	GOL	M	1315	-	5,5,5	0.37	0	5,5,5	0.27	0
10	HTO	L	1292	-	9,9,9	0.39	0	10,10,10	0.65	0
5	BCL	L	1282	2	69,74,74	1.79	10 (14%)	79,115,115	1.81	18 (22%)
5	BCL	M	1304	3	69,74,74	1.77	7 (10%)	79,115,115	1.81	13 (16%)
6	LDA	L	1286	-	13,15,15	2.17	2 (15%)	14,17,17	0.67	0
12	U10	M	1312	-	48,48,63	2.71	11 (22%)	60,61,79	1.55	13 (21%)
4	GOL	H	1252	-	5,5,5	0.58	0	5,5,5	1.15	0
4	GOL	L	1294	-	5,5,5	0.37	0	5,5,5	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	M	1305	3	69,74,74	1.86	11 (15%)	79,115,115	1.89	19 (24%)
6	LDA	M	1306	-	13,15,15	2.23	2 (15%)	14,17,17	0.68	0
9	PO4	L	1291	-	4,4,4	1.01	0	6,6,6	0.70	0
4	GOL	L	1293	-	5,5,5	0.41	0	5,5,5	0.77	0
8	UQ2	L	1289[A]	-	23,23,23	2.59	8 (34%)	30,31,31	1.82	10 (33%)
7	BPH	L	1288	-	59,70,70	2.62	11 (18%)	59,101,101	2.65	21 (35%)

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
8	UQ2	L	1289[B]	-	-	6/15/39/39	0/1/1/1
6	LDA	L	1283	-	-	6/13/13/13	-
6	LDA	M	1307	-	-	6/13/13/13	-
13	SPO	M	1313	-	-	13/47/47/47	-
14	CDL	M	1314	-	-	55/91/91/110	-
6	LDA	L	1284	-	-	7/13/13/13	-
7	BPH	M	1311	-	-	16/37/105/105	0/5/6/6
4	GOL	H	1253	-	-	2/4/4/4	-
5	BCL	L	1290	2	2/2/21/25	13/41/137/137	-
6	LDA	M	1308	-	-	7/13/13/13	-
4	GOL	H	1255	-	-	2/4/4/4	-
6	LDA	M	1309	-	-	7/13/13/13	-
4	GOL	H	1254	-	-	0/4/4/4	-
6	LDA	L	1287	-	-	9/13/13/13	-
6	LDA	L	1285	-	-	6/13/13/13	-
4	GOL	M	1315	-	-	2/4/4/4	-
10	HTO	L	1292	-	-	8/10/10/10	-
5	BCL	L	1282	2	2/2/21/25	14/41/137/137	-
5	BCL	M	1304	3	2/2/21/25	13/41/137/137	-
6	LDA	L	1286	-	-	5/13/13/13	-
12	U10	M	1312	-	-	7/45/69/87	0/1/1/1
4	GOL	H	1252	-	-	0/4/4/4	-
5	BCL	M	1305	3	2/2/21/25	6/41/137/137	-
4	GOL	L	1294	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1306	-	-	4/13/13/13	-
4	GOL	L	1293	-	-	2/4/4/4	-
8	UQ2	L	1289[A]	-	-	8/15/39/39	0/1/1/1
7	BPH	L	1288	-	-	4/37/105/105	0/5/6/6

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1311	BPH	OBD-CAD	13.06	1.39	1.22
7	L	1288	BPH	OBD-CAD	11.22	1.37	1.22
5	M	1305	BCL	OBD-CAD	10.16	1.40	1.22
5	L	1282	BCL	OBD-CAD	9.75	1.39	1.22
5	L	1290	BCL	OBD-CAD	9.58	1.39	1.22
5	M	1304	BCL	OBD-CAD	9.53	1.38	1.22
7	L	1288	BPH	OBB-CAB	7.63	1.45	1.22
12	M	1312	U10	C33-C34	7.10	1.49	1.33
7	M	1311	BPH	O1D-CGD	6.98	1.38	1.21
8	L	1289[B]	UQ2	C8-C9	6.84	1.48	1.33
6	L	1287	LDA	O1-N1	-6.83	1.25	1.42
14	M	1314	CDL	C11-CA5	-6.78	1.31	1.50
6	L	1285	LDA	O1-N1	-6.71	1.25	1.42
6	L	1286	LDA	O1-N1	-6.70	1.25	1.42
6	M	1309	LDA	O1-N1	-6.70	1.25	1.42
7	L	1288	BPH	O1D-CGD	6.67	1.38	1.21
6	M	1307	LDA	O1-N1	-6.66	1.25	1.42
6	L	1284	LDA	O1-N1	-6.62	1.25	1.42
6	L	1283	LDA	O1-N1	-6.60	1.26	1.42
7	M	1311	BPH	OBB-CAB	6.56	1.42	1.22
7	L	1288	BPH	C2-C3	6.55	1.48	1.33
7	M	1311	BPH	C2-C3	6.51	1.48	1.33
12	M	1312	U10	C8-C9	6.48	1.48	1.33
12	M	1312	U10	C13-C14	6.47	1.48	1.33
14	M	1314	CDL	C32-C31	-6.45	1.28	1.52
13	M	1313	SPO	C32-C33	6.40	1.47	1.33
12	M	1312	U10	C28-C29	6.33	1.47	1.33
6	M	1308	LDA	O1-N1	-6.32	1.26	1.42
8	L	1289[A]	UQ2	C8-C9	6.29	1.47	1.33
6	M	1306	LDA	O1-N1	-6.25	1.26	1.42
5	L	1290	BCL	O1A-CGA	6.25	1.41	1.22
7	L	1288	BPH	O1A-CGA	6.05	1.40	1.22
12	M	1312	U10	C18-C19	6.03	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1311	BPH	O1A-CGA	5.95	1.40	1.22
12	M	1312	U10	C23-C24	5.92	1.46	1.33
5	M	1305	BCL	O1A-CGA	5.86	1.40	1.22
5	M	1304	BCL	O1A-CGA	5.62	1.39	1.22
5	L	1282	BCL	O1A-CGA	5.44	1.38	1.22
13	M	1313	SPO	C37-C38	5.41	1.48	1.32
8	L	1289[A]	UQ2	O2-C2	-5.35	1.23	1.36
8	L	1289[A]	UQ2	C13-C14	5.28	1.48	1.32
13	M	1313	SPO	C9-C7	5.23	1.47	1.35
14	M	1314	CDL	C17-C16	-5.11	1.26	1.51
14	M	1314	CDL	C19-C18	-5.10	1.26	1.51
14	M	1314	CDL	C16-C15	-5.09	1.26	1.51
12	M	1312	U10	C38-C39	5.08	1.47	1.32
8	L	1289[B]	UQ2	O2-C2	-5.01	1.24	1.36
14	M	1314	CDL	C20-C19	-5.01	1.26	1.51
8	L	1289[B]	UQ2	C13-C14	4.98	1.47	1.32
6	M	1306	LDA	C1-N1	-4.97	1.46	1.51
6	M	1308	LDA	C1-N1	-4.92	1.46	1.51
13	M	1313	SPO	C6-C5	4.87	1.45	1.32
7	M	1311	BPH	C3D-C2D	4.85	1.47	1.39
13	M	1313	SPO	C19-C17	4.85	1.47	1.35
14	M	1314	CDL	OA6-CA5	4.84	1.48	1.34
7	L	1288	BPH	C3D-C2D	4.79	1.47	1.39
14	M	1314	CDL	OA8-CA7	4.75	1.47	1.33
8	L	1289[B]	UQ2	O3-C3	-4.74	1.25	1.36
7	L	1288	BPH	C3D-CAD	-4.66	1.38	1.47
14	M	1314	CDL	OB6-CB5	4.58	1.47	1.34
8	L	1289[A]	UQ2	O3-C3	-4.56	1.25	1.36
7	M	1311	BPH	C3D-CAD	-4.51	1.39	1.47
6	L	1284	LDA	C1-N1	-4.48	1.46	1.51
13	M	1313	SPO	C14-C12	4.45	1.46	1.35
6	L	1287	LDA	C1-N1	-4.44	1.46	1.51
14	M	1314	CDL	OB8-CB7	4.41	1.46	1.33
13	M	1313	SPO	C10-C11	4.41	1.46	1.34
13	M	1313	SPO	C22-C23	4.38	1.45	1.35
6	M	1309	LDA	C1-N1	-4.31	1.47	1.51
6	L	1285	LDA	C1-N1	-4.18	1.47	1.51
6	M	1307	LDA	C1-N1	-4.11	1.47	1.51
12	M	1312	U10	O4-C4	-4.10	1.26	1.36
13	M	1313	SPO	C26-C25	4.07	1.45	1.34
13	M	1313	SPO	C15-C16	4.02	1.45	1.34
5	M	1304	BCL	C3D-C4D	-3.99	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1312	U10	O3-C3	-3.95	1.27	1.36
6	L	1286	LDA	C1-N1	-3.90	1.47	1.51
12	M	1312	U10	C6-C1	3.88	1.42	1.35
13	M	1313	SPO	C27-C28	3.78	1.47	1.35
6	L	1283	LDA	C1-N1	-3.73	1.47	1.51
14	M	1314	CDL	C37-C36	-3.60	1.33	1.51
14	M	1314	CDL	C79-C78	-3.54	1.34	1.51
5	M	1305	BCL	C3D-C4D	-3.53	1.36	1.44
5	L	1282	BCL	C3D-C4D	-3.52	1.36	1.44
14	M	1314	CDL	C80-C79	-3.50	1.34	1.51
14	M	1314	CDL	C22-C21	-3.42	1.34	1.51
14	M	1314	CDL	C13-C12	-3.41	1.34	1.51
5	M	1304	BCL	C2-C3	3.41	1.40	1.33
5	L	1290	BCL	C2-C3	3.38	1.40	1.33
8	L	1289[B]	UQ2	C6-C5	3.33	1.41	1.35
13	M	1313	SPO	C21-C20	3.27	1.45	1.36
7	L	1288	BPH	O2D-CGD	-3.24	1.25	1.33
8	L	1289[A]	UQ2	C3-C4	-3.09	1.39	1.48
7	L	1288	BPH	C3D-C4D	-3.09	1.37	1.41
7	M	1311	BPH	O2D-CGD	-3.08	1.25	1.33
5	L	1290	BCL	O2D-CGD	-3.07	1.25	1.33
5	L	1290	BCL	C3D-C4D	-3.07	1.37	1.44
8	L	1289[B]	UQ2	C3-C4	-3.03	1.40	1.48
5	M	1305	BCL	C2-C3	2.87	1.39	1.33
7	M	1311	BPH	CBD-CGD	-2.87	1.48	1.52
7	M	1311	BPH	O2A-CGA	-2.86	1.25	1.33
8	L	1289[A]	UQ2	C6-C5	2.85	1.40	1.35
5	L	1282	BCL	O2A-CGA	-2.85	1.25	1.33
8	L	1289[B]	UQ2	C2-C1	-2.84	1.40	1.48
7	M	1311	BPH	C4D-ND	-2.76	1.34	1.38
12	M	1312	U10	C4-C5	-2.74	1.40	1.48
5	M	1305	BCL	CBB-CAB	-2.74	1.44	1.50
5	M	1305	BCL	OBG-CAB	2.66	1.29	1.23
5	M	1304	BCL	O2D-CGD	-2.62	1.26	1.33
5	L	1282	BCL	C2-C3	2.58	1.39	1.33
5	L	1282	BCL	O2D-CGD	-2.57	1.26	1.33
5	L	1290	BCL	CHD-C4C	2.56	1.46	1.39
5	L	1282	BCL	C1D-C2D	-2.52	1.40	1.45
7	L	1288	BPH	O2A-CGA	-2.50	1.26	1.33
8	L	1289[A]	UQ2	C6-C1	-2.46	1.39	1.46
5	M	1304	BCL	CHD-C4C	2.44	1.46	1.39
5	M	1305	BCL	O2D-CGD	-2.44	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	O2A-CGA	-2.36	1.26	1.33
5	M	1305	BCL	O2A-CGA	-2.29	1.26	1.33
7	L	1288	BPH	C4D-ND	-2.27	1.35	1.38
8	L	1289[A]	UQ2	C2-C1	-2.27	1.42	1.48
5	M	1305	BCL	CHD-C4C	2.24	1.45	1.39
5	L	1282	BCL	MG-ND	-2.20	2.01	2.05
5	L	1290	BCL	O2A-CGA	-2.15	1.27	1.33
5	M	1305	BCL	C1D-C2D	-2.11	1.41	1.45
5	M	1305	BCL	C3B-C2B	-2.10	1.35	1.42
5	L	1282	BCL	CHD-C4C	2.08	1.45	1.39
14	M	1314	CDL	C33-C32	-2.08	1.41	1.51
5	L	1282	BCL	O1D-CGD	2.07	1.26	1.21
8	L	1289[B]	UQ2	O2-CM2	-2.03	1.40	1.45
8	L	1289[B]	UQ2	C6-C1	-2.02	1.40	1.46

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1314	CDL	C20-C19-C18	12.04	175.25	114.37
14	M	1314	CDL	C17-C16-C15	11.93	174.65	114.37
7	L	1288	BPH	O2D-CGD-CBD	10.11	122.05	110.95
14	M	1314	CDL	C13-C12-C11	9.48	147.97	113.13
14	M	1314	CDL	C34-C33-C32	9.24	161.05	114.37
7	M	1311	BPH	O2D-CGD-CBD	8.63	120.43	110.95
7	L	1288	BPH	C2B-C1B-NB	8.00	115.21	109.43
14	M	1314	CDL	C33-C32-C31	7.21	139.63	113.13
7	M	1311	BPH	C2B-C1B-NB	6.93	114.44	109.43
5	M	1304	BCL	C1D-ND-C4D	6.68	111.00	106.31
7	L	1288	BPH	C2D-C1D-ND	6.55	114.16	109.43
5	M	1304	BCL	CMB-C2B-C1B	-5.96	116.34	125.42
5	L	1282	BCL	O2D-CGD-CBD	5.91	121.57	111.23
5	L	1290	BCL	C1C-NC-C4C	-5.64	104.11	106.68
14	M	1314	CDL	C12-C11-CA5	5.61	134.27	113.69
13	M	1313	SPO	C4-C5-C6	-5.55	117.11	124.91
7	M	1311	BPH	C3D-C4D-ND	5.31	114.52	107.71
7	M	1311	BPH	C2D-C1D-ND	5.23	113.21	109.43
5	L	1282	BCL	C1D-ND-C4D	5.19	109.95	106.31
14	M	1314	CDL	OA6-CA5-C11	5.13	122.57	111.48
5	L	1290	BCL	CMD-C2D-C1D	5.05	133.62	124.73
7	L	1288	BPH	C1B-NB-C4B	-4.99	101.55	108.82
5	L	1290	BCL	C4A-NA-C1A	4.97	108.95	106.68
13	M	1313	SPO	C10-C9-C7	-4.77	120.59	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1305	BCL	C1C-NC-C4C	4.67	108.81	106.68
7	L	1288	BPH	O1D-CGD-CBD	-4.63	117.70	124.72
5	L	1290	BCL	C1D-ND-C4D	4.49	109.46	106.31
5	M	1304	BCL	C2D-C1D-ND	-4.49	105.68	110.13
7	M	1311	BPH	O1D-CGD-CBD	-4.46	117.96	124.72
13	M	1313	SPO	C20-C19-C17	-4.42	121.07	127.28
7	L	1288	BPH	C3D-C4D-ND	4.40	113.35	107.71
12	M	1312	U10	C30-C29-C31	4.38	122.84	115.23
5	M	1305	BCL	O2D-CGD-CBD	4.38	118.89	111.23
5	L	1290	BCL	CMB-C2B-C1B	-4.38	118.75	125.42
5	M	1305	BCL	CMD-C2D-C1D	4.32	132.34	124.73
5	L	1282	BCL	CMD-C2D-C1D	4.31	132.32	124.73
5	M	1305	BCL	C1D-ND-C4D	4.31	109.34	106.31
7	M	1311	BPH	C4D-CHA-CBD	-4.28	106.40	108.45
5	M	1304	BCL	O2D-CGD-CBD	4.27	118.70	111.23
7	M	1311	BPH	OBD-CAD-CBD	-4.23	119.62	125.82
13	M	1313	SPO	C21-C22-C23	-4.16	121.44	127.28
7	M	1311	BPH	C4D-ND-C1D	-4.09	103.97	108.87
7	L	1288	BPH	C4D-ND-C1D	-4.08	103.99	108.87
14	M	1314	CDL	OB6-CB5-C51	4.07	120.30	111.48
14	M	1314	CDL	C35-C34-C33	3.94	134.30	114.37
8	L	1289[A]	UQ2	CM5-C5-C6	-3.89	118.06	124.45
5	L	1290	BCL	O2D-CGD-CBD	3.89	118.02	111.23
5	M	1304	BCL	C1-O2A-CGA	3.87	126.03	116.65
8	L	1289[A]	UQ2	C10-C9-C11	3.83	121.87	115.23
13	M	1313	SPO	C15-C14-C12	-3.67	122.13	127.28
13	M	1313	SPO	C29-C28-C30	3.62	121.52	115.23
5	M	1305	BCL	C2D-C1D-ND	-3.61	106.55	110.13
5	M	1305	BCL	O2A-CGA-CBA	3.61	122.83	111.83
5	M	1305	BCL	C4A-NA-C1A	3.59	108.32	106.68
5	M	1305	BCL	CMB-C2B-C1B	-3.56	120.00	125.42
7	M	1311	BPH	C1B-NB-C4B	-3.52	103.69	108.82
5	L	1282	BCL	C2D-C1D-ND	-3.51	106.65	110.13
12	M	1312	U10	C25-C24-C26	3.50	121.30	115.23
5	L	1282	BCL	CMB-C2B-C1B	-3.49	120.10	125.42
13	M	1313	SPO	C26-C27-C28	-3.47	122.81	127.69
7	M	1311	BPH	CED-O2D-CGD	3.42	123.67	115.92
5	M	1305	BCL	CBB-CAB-C3B	-3.42	113.20	120.40
7	L	1288	BPH	OBD-CAD-CBD	-3.41	120.82	125.82
5	M	1304	BCL	O2A-CGA-CBA	3.40	122.20	111.83
5	M	1305	BCL	OBG-CAB-C3B	3.34	126.34	120.43
5	L	1290	BCL	CMA-C3A-C4A	-3.34	102.80	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	1289[A]	UQ2	CM3-O3-C3	3.31	128.11	116.47
5	M	1305	BCL	C16-C15-C13	-3.30	104.98	115.97
5	M	1304	BCL	C2B-C1B-NB	-3.25	106.96	110.33
12	M	1312	U10	C10-C9-C11	3.17	120.74	115.23
5	L	1282	BCL	C4-C3-C5	3.17	120.73	115.23
5	M	1304	BCL	CMD-C2D-C1D	3.17	130.30	124.73
8	L	1289[A]	UQ2	O1-C1-C6	-3.16	115.69	121.79
5	L	1282	BCL	O2A-CGA-CBA	3.15	121.44	111.83
14	M	1314	CDL	OA8-CA7-C31	3.12	121.33	111.83
5	L	1290	BCL	C2D-C1D-ND	-3.11	107.04	110.13
5	L	1290	BCL	CMD-C2D-C3D	-3.10	120.57	127.69
5	L	1290	BCL	O2A-CGA-CBA	3.07	121.20	111.83
5	M	1304	BCL	O1D-CGD-CBD	-3.06	118.48	124.52
12	M	1312	U10	C15-C14-C16	3.06	120.53	115.23
5	M	1305	BCL	CED-O2D-CGD	3.04	122.81	115.92
5	L	1282	BCL	C2B-C1B-NB	-3.01	107.20	110.33
7	L	1288	BPH	CED-O2D-CGD	2.99	122.70	115.92
7	L	1288	BPH	C3B-C4B-NB	2.95	112.34	108.05
12	M	1312	U10	C22-C23-C24	-2.94	120.90	127.62
14	M	1314	CDL	OB8-CB7-C71	2.91	120.70	111.83
13	M	1313	SPO	C14-C15-C16	-2.88	114.86	123.20
5	L	1290	BCL	C1-O2A-CGA	2.83	123.49	116.65
13	M	1313	SPO	C20-C21-C22	-2.82	117.75	123.52
5	M	1305	BCL	C1D-CHD-C4C	-2.82	119.82	126.62
7	M	1311	BPH	CMB-C2B-C3B	2.80	130.28	124.68
12	M	1312	U10	C12-C13-C14	-2.80	121.22	127.62
5	L	1282	BCL	C4A-NA-C1A	2.77	107.94	106.68
7	L	1288	BPH	O2A-CGA-CBA	2.77	120.27	111.83
7	M	1311	BPH	CMA-C3A-C4A	-2.76	108.65	114.61
5	M	1305	BCL	C7-C6-C5	-2.76	105.90	113.26
5	M	1304	BCL	CED-O2D-CGD	2.76	122.18	115.92
5	L	1290	BCL	CED-O2D-CGD	2.74	122.14	115.92
5	L	1282	BCL	C1-O2A-CGA	2.71	123.20	116.65
14	M	1314	CDL	OA6-CA5-OA7	-2.67	117.45	123.70
5	L	1282	BCL	O1D-CGD-CBD	-2.66	119.26	124.52
5	L	1282	BCL	CAA-C2A-C3A	-2.63	105.88	113.00
5	L	1282	BCL	CMD-C2D-C3D	-2.63	121.66	127.69
5	L	1290	BCL	C3C-C4C-CHD	-2.62	117.87	123.39
8	L	1289[A]	UQ2	C7-C8-C9	-2.61	122.33	126.83
13	M	1313	SPO	C40-C38-C39	2.60	120.58	114.59
13	M	1313	SPO	C34-C33-C35	2.60	119.73	115.23
5	M	1305	BCL	CMD-C2D-C3D	-2.59	121.75	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1311	BPH	CBA-CAA-C2A	-2.56	106.25	113.78
13	M	1313	SPO	C13-C12-C11	2.56	121.99	118.09
5	M	1305	BCL	O2D-CGD-O1D	-2.55	118.88	123.85
7	L	1288	BPH	C4C-C3C-C2C	-2.55	100.41	102.84
7	L	1288	BPH	O2A-CGA-O1A	-2.53	117.29	123.63
5	L	1290	BCL	O2A-CGA-O1A	-2.51	117.35	123.63
12	M	1312	U10	C30-C29-C28	-2.50	117.20	123.63
7	L	1288	BPH	OB B-CAB-C3B	2.50	124.17	119.99
7	M	1311	BPH	C1-C2-C3	-2.48	122.13	126.20
5	L	1290	BCL	C2A-C3A-C4A	2.48	105.87	101.87
5	M	1304	BCL	CMB-C2B-C3B	2.48	133.48	125.67
13	M	1313	SPO	C27-C26-C25	-2.46	116.07	123.20
5	L	1282	BCL	C1D-CHD-C4C	-2.44	120.74	126.62
13	M	1313	SPO	C8-C7-C6	2.42	121.78	118.09
7	L	1288	BPH	OB D-CAD-C3D	-2.42	124.12	127.89
5	L	1282	BCL	O2D-CGD-O1D	-2.41	119.16	123.85
13	M	1313	SPO	C25-C23-C22	-2.40	115.23	119.01
7	L	1288	BPH	C1-C2-C3	-2.39	122.28	126.20
13	M	1313	SPO	C24-C23-C25	2.39	121.74	118.09
7	M	1311	BPH	C1-O2A-CGA	2.38	122.42	116.65
8	L	1289[A]	UQ2	C7-C6-C5	-2.37	120.83	124.89
5	M	1305	BCL	C3C-C4C-CHD	-2.37	118.40	123.39
5	M	1304	BCL	O2A-CGA-O1A	-2.35	117.75	123.63
12	M	1312	U10	O5-C5-C4	-2.34	116.06	121.03
12	M	1312	U10	C27-C28-C29	-2.32	122.31	127.62
5	M	1304	BCL	CHA-C1A-NA	-2.32	121.15	126.39
13	M	1313	SPO	C16-C17-C19	-2.31	115.37	119.01
5	M	1305	BCL	CAB-C3B-C2B	-2.30	122.96	127.74
5	L	1282	BCL	C1-C2-C3	-2.30	122.43	126.20
7	M	1311	BPH	OB D-CAD-C3D	-2.30	124.31	127.89
12	M	1312	U10	C35-C34-C36	2.29	119.21	115.23
5	L	1290	BCL	C2B-C1B-NB	-2.29	107.95	110.33
13	M	1313	SPO	C31-C32-C33	-2.29	122.38	127.62
5	L	1290	BCL	C14-C13-C12	2.29	119.42	111.27
7	M	1311	BPH	CBC-CAC-C3C	2.24	118.19	113.78
8	L	1289[B]	UQ2	C10-C9-C11	2.24	119.11	115.23
8	L	1289[B]	UQ2	C16-C14-C15	2.23	119.73	114.59
8	L	1289[A]	UQ2	C16-C14-C15	2.22	119.69	114.59
5	L	1282	BCL	O2A-CGA-O1A	-2.21	118.11	123.63
14	M	1314	CDL	CA4-OA6-CA5	-2.18	112.57	117.80
5	L	1290	BCL	CMB-C2B-C3B	2.17	132.53	125.67
5	L	1290	BCL	CHD-C1D-C2D	2.17	130.00	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1290	BCL	O2D-CGD-O1D	-2.17	119.63	123.85
7	L	1288	BPH	CBB-CAB-C3B	-2.16	113.86	120.34
7	L	1288	BPH	C4A-C3A-C2A	-2.15	100.79	102.84
5	L	1290	BCL	C1D-CHD-C4C	-2.15	121.45	126.62
12	M	1312	U10	C20-C19-C21	2.13	118.92	115.23
7	M	1311	BPH	O2A-CGA-CBA	2.13	118.32	111.83
5	L	1282	BCL	CMA-C3A-C2A	-2.12	105.80	113.98
12	M	1312	U10	C41-C39-C40	2.11	119.45	114.59
13	M	1313	SPO	C10-C11-C12	-2.09	120.62	126.36
8	L	1289[B]	UQ2	C12-C13-C14	-2.09	120.66	127.64
7	L	1288	BPH	C4D-CHA-CBD	-2.07	107.46	108.45
8	L	1289[A]	UQ2	CM2-O2-C2	2.07	123.74	116.47
7	L	1288	BPH	CMA-C3A-C4A	-2.07	110.16	114.61
12	M	1312	U10	C7-C6-C1	-2.06	121.36	124.89
8	L	1289[A]	UQ2	O4-C4-C3	-2.06	116.67	121.03
5	M	1305	BCL	O2A-CGA-O1A	-2.04	118.52	123.63
8	L	1289[B]	UQ2	CM2-O2-C2	2.03	123.60	116.47
7	L	1288	BPH	C1C-C2C-C3C	-2.02	100.91	102.84
8	L	1289[A]	UQ2	C12-C13-C14	-2.01	120.95	127.64

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	L	1290	BCL	C8
5	L	1290	BCL	C13
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	M	1305	BCL	C8
5	M	1305	BCL	C13

All (232) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1253	GOL	O1-C1-C2-C3
4	L	1293	GOL	C1-C2-C3-O3
4	L	1294	GOL	C1-C2-C3-O3
4	L	1294	GOL	O2-C2-C3-O3
5	L	1290	BCL	C14-C13-C15-C16
5	M	1304	BCL	C1-C2-C3-C5
6	L	1287	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
7	M	1311	BPH	C4C-C3C-CAC-CBC
7	M	1311	BPH	C2C-C3C-CAC-CBC
8	L	1289[A]	UQ2	C7-C8-C9-C10
8	L	1289[A]	UQ2	C7-C8-C9-C11
10	L	1292	HTO	C1-C2-C3-O3
10	L	1292	HTO	C1-C2-C3-C4
10	L	1292	HTO	O2-C2-C3-O3
10	L	1292	HTO	O2-C2-C3-C4
12	M	1312	U10	C27-C28-C29-C30
12	M	1312	U10	C27-C28-C29-C31
13	M	1313	SPO	C3-C1-O1-CM1
13	M	1313	SPO	C4-C1-O1-CM1
13	M	1313	SPO	C4-C5-C6-C7
13	M	1313	SPO	C8-C7-C9-C10
13	M	1313	SPO	C36-C37-C38-C39
13	M	1313	SPO	C36-C37-C38-C40
14	M	1314	CDL	CA3-OA5-PA1-OA2
14	M	1314	CDL	CA3-OA5-PA1-OA3
14	M	1314	CDL	CB3-OB5-PB2-OB2
14	M	1314	CDL	CB3-OB5-PB2-OB4
14	M	1314	CDL	OB7-CB5-OB6-CB4
5	M	1304	BCL	C10-C11-C12-C13
8	L	1289[A]	UQ2	C12-C13-C14-C16
14	M	1314	CDL	OA9-CA7-OA8-CA6
8	L	1289[B]	UQ2	C12-C13-C14-C15
14	M	1314	CDL	C31-CA7-OA8-CA6
14	M	1314	CDL	C51-CB5-OB6-CB4
8	L	1289[A]	UQ2	C12-C11-C9-C10
8	L	1289[B]	UQ2	C12-C11-C9-C10
12	M	1312	U10	C30-C29-C31-C32
8	L	1289[A]	UQ2	C12-C11-C9-C8
8	L	1289[B]	UQ2	C12-C11-C9-C8
8	L	1289[B]	UQ2	C12-C13-C14-C16
14	M	1314	CDL	C78-C79-C80-C81
14	M	1314	CDL	C20-C21-C22-C23
8	L	1289[A]	UQ2	C12-C13-C14-C15
14	M	1314	CDL	OB9-CB7-OB8-CB6
13	M	1313	SPO	C19-C20-C21-C22
5	M	1304	BCL	C3-C5-C6-C7
14	M	1314	CDL	C71-CB7-OB8-CB6
8	L	1289[A]	UQ2	C9-C11-C12-C13
12	M	1312	U10	C29-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
14	M	1314	CDL	C15-C16-C17-C18
12	M	1312	U10	C28-C29-C31-C32
5	L	1282	BCL	C6-C7-C8-C9
5	L	1290	BCL	C6-C7-C8-C9
5	M	1305	BCL	C11-C10-C8-C9
14	M	1314	CDL	O1-C1-CB2-OB2
7	M	1311	BPH	C5-C6-C7-C8
5	L	1290	BCL	C11-C10-C8-C7
5	M	1305	BCL	C6-C7-C8-C10
7	M	1311	BPH	C11-C10-C8-C7
13	M	1313	SPO	C33-C35-C36-C37
5	L	1290	BCL	C10-C11-C12-C13
5	M	1304	BCL	C8-C10-C11-C12
12	M	1312	U10	C31-C32-C33-C34
5	L	1290	BCL	C15-C16-C17-C18
4	L	1294	GOL	O1-C1-C2-C3
4	M	1315	GOL	O1-C1-C2-C3
13	M	1313	SPO	C6-C7-C9-C10
10	L	1292	HTO	O1-C1-C2-O2
5	M	1304	BCL	C2-C1-O2A-CGA
7	M	1311	BPH	C16-C17-C18-C20
6	M	1308	LDA	C4-C5-C6-C7
4	H	1253	GOL	O1-C1-C2-O2
4	L	1294	GOL	O1-C1-C2-O2
4	M	1315	GOL	O1-C1-C2-O2
6	L	1284	LDA	C6-C7-C8-C9
7	M	1311	BPH	C13-C15-C16-C17
14	M	1314	CDL	C11-CA5-OA6-CA4
6	M	1307	LDA	C6-C7-C8-C9
6	M	1309	LDA	C5-C6-C7-C8
14	M	1314	CDL	C71-C72-C73-C74
6	L	1285	LDA	C7-C8-C9-C10
14	M	1314	CDL	CA2-C1-CB2-OB2
6	L	1287	LDA	C7-C8-C9-C10
6	M	1309	LDA	C2-C3-C4-C5
6	M	1309	LDA	C7-C8-C9-C10
6	L	1284	LDA	C7-C8-C9-C10
6	M	1308	LDA	C2-C3-C4-C5
14	M	1314	CDL	C53-C54-C55-C56
14	M	1314	CDL	OA7-CA5-OA6-CA4
14	M	1314	CDL	C11-C12-C13-C14
6	M	1308	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
6	L	1287	LDA	C4-C5-C6-C7
7	M	1311	BPH	C16-C17-C18-C19
6	M	1308	LDA	C7-C8-C9-C10
6	L	1283	LDA	C5-C6-C7-C8
7	M	1311	BPH	C10-C11-C12-C13
13	M	1313	SPO	C1-C4-C5-C6
6	L	1284	LDA	C2-C3-C4-C5
5	L	1282	BCL	C16-C17-C18-C19
5	L	1282	BCL	C16-C17-C18-C20
14	M	1314	CDL	C80-C81-C82-C83
14	M	1314	CDL	C17-C18-C19-C20
6	L	1286	LDA	C4-C5-C6-C7
6	L	1287	LDA	C11-C10-C9-C8
14	M	1314	CDL	C19-C20-C21-C22
6	L	1287	LDA	C3-C4-C5-C6
6	L	1283	LDA	C3-C4-C5-C6
14	M	1314	CDL	C52-C53-C54-C55
6	M	1306	LDA	C7-C8-C9-C10
14	M	1314	CDL	C16-C17-C18-C19
14	M	1314	CDL	CA5-C11-C12-C13
6	L	1286	LDA	C3-C4-C5-C6
6	L	1287	LDA	C5-C6-C7-C8
6	M	1306	LDA	C3-C4-C5-C6
6	M	1308	LDA	C5-C6-C7-C8
14	M	1314	CDL	C74-C75-C76-C77
6	L	1287	LDA	C2-C3-C4-C5
6	L	1285	LDA	C11-C10-C9-C8
14	M	1314	CDL	C32-C33-C34-C35
14	M	1314	CDL	OA5-CA3-CA4-CA6
5	M	1304	BCL	C11-C12-C13-C15
5	M	1305	BCL	C12-C13-C15-C16
7	M	1311	BPH	C11-C12-C13-C15
7	M	1311	BPH	C11-C12-C13-C14
14	M	1314	CDL	CA3-CA4-CA6-OA8
6	L	1285	LDA	C1-C2-C3-C4
13	M	1313	SPO	C21-C22-C23-C24
5	L	1282	BCL	C13-C15-C16-C17
6	L	1286	LDA	C6-C7-C8-C9
6	L	1284	LDA	C1-C2-C3-C4
6	M	1307	LDA	C1-C2-C3-C4
7	L	1288	BPH	C2-C3-C5-C6
7	M	1311	BPH	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	M	1314	CDL	C12-C13-C14-C15
6	L	1287	LDA	C9-C10-C11-C12
6	M	1308	LDA	N1-C1-C2-C3
6	M	1307	LDA	C3-C4-C5-C6
14	M	1314	CDL	C54-C55-C56-C57
6	L	1283	LDA	C9-C10-C11-C12
14	M	1314	CDL	C40-C41-C42-C43
5	L	1290	BCL	C8-C10-C11-C12
13	M	1313	SPO	C2-C1-O1-CM1
6	L	1285	LDA	C9-C10-C11-C12
14	M	1314	CDL	C81-C82-C83-C84
7	L	1288	BPH	C8-C10-C11-C12
5	L	1282	BCL	C14-C13-C15-C16
5	M	1304	BCL	C11-C10-C8-C9
5	M	1304	BCL	C11-C12-C13-C14
5	M	1305	BCL	C14-C13-C15-C16
14	M	1314	CDL	C14-C15-C16-C17
5	M	1304	BCL	C11-C10-C8-C7
14	M	1314	CDL	CB7-C71-C72-C73
7	L	1288	BPH	C4-C3-C5-C6
7	M	1311	BPH	C8-C10-C11-C12
10	L	1292	HTO	O3-C3-C4-C5
10	L	1292	HTO	C4-C5-C6-C7
6	M	1307	LDA	C2-C3-C4-C5
6	M	1309	LDA	C11-C10-C9-C8
7	M	1311	BPH	C4-C3-C5-C6
14	M	1314	CDL	OA5-CA3-CA4-OA6
14	M	1314	CDL	OB5-CB3-CB4-OB6
5	M	1304	BCL	C4-C3-C5-C6
7	M	1311	BPH	C1-C2-C3-C5
8	L	1289[B]	UQ2	C9-C11-C12-C13
5	M	1304	BCL	C4C-C3C-CAC-CBC
4	L	1293	GOL	O2-C2-C3-O3
5	L	1282	BCL	C6-C7-C8-C10
5	L	1290	BCL	C12-C13-C15-C16
14	M	1314	CDL	C72-C73-C74-C75
14	M	1314	CDL	C39-C40-C41-C42
4	H	1255	GOL	O1-C1-C2-C3
7	M	1311	BPH	O2A-C1-C2-C3
8	L	1289[B]	UQ2	C1-C2-O2-CM2
13	M	1313	SPO	C21-C22-C23-C25
5	L	1290	BCL	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
5	L	1290	BCL	C16-C17-C18-C19
14	M	1314	CDL	OA6-CA4-CA6-OA8
6	M	1306	LDA	C2-C3-C4-C5
6	M	1309	LDA	C2-C1-N1-CM1
6	M	1309	LDA	C2-C1-N1-CM2
5	L	1282	BCL	C3-C5-C6-C7
6	L	1287	LDA	C1-C2-C3-C4
6	L	1283	LDA	C11-C10-C9-C8
14	M	1314	CDL	OB5-CB3-CB4-CB6
6	L	1286	LDA	C9-C10-C11-C12
14	M	1314	CDL	C55-C56-C57-C58
14	M	1314	CDL	CB2-C1-CA2-OA2
5	M	1304	BCL	C2-C3-C5-C6
6	L	1283	LDA	C6-C7-C8-C9
5	L	1282	BCL	CHA-CBD-CGD-O1D
5	L	1282	BCL	CHA-CBD-CGD-O2D
14	M	1314	CDL	CA3-OA5-PA1-OA4
14	M	1314	CDL	CB3-OB5-PB2-OB3
6	L	1284	LDA	C11-C10-C9-C8
4	H	1255	GOL	O1-C1-C2-O2
5	L	1282	BCL	C8-C10-C11-C12
14	M	1314	CDL	CA7-C31-C32-C33
6	L	1286	LDA	C2-C3-C4-C5
6	M	1308	LDA	C6-C7-C8-C9
6	L	1285	LDA	N1-C1-C2-C3
6	M	1307	LDA	N1-C1-C2-C3
6	M	1307	LDA	C7-C8-C9-C10
5	L	1290	BCL	C11-C12-C13-C14
6	L	1284	LDA	C4-C5-C6-C7
6	L	1285	LDA	C4-C5-C6-C7
14	M	1314	CDL	C31-C32-C33-C34
5	L	1290	BCL	C11-C10-C8-C9
5	M	1304	BCL	C1-C2-C3-C4
7	M	1311	BPH	C1-C2-C3-C4
14	M	1314	CDL	C75-C76-C77-C78
8	L	1289[A]	UQ2	C3-C2-O2-CM2
14	M	1314	CDL	C1-CB2-OB2-PB2
5	M	1305	BCL	C11-C10-C8-C7
12	M	1312	U10	C5-C4-O4-C4M
5	L	1282	BCL	C5-C6-C7-C8
6	L	1283	LDA	C2-C3-C4-C5
6	L	1284	LDA	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
6	M	1306	LDA	C11-C10-C9-C8
14	M	1314	CDL	C13-C14-C15-C16
7	L	1288	BPH	O2A-C1-C2-C3
14	M	1314	CDL	O1-C1-CA2-OA2
14	M	1314	CDL	C21-C22-C23-C24
5	L	1282	BCL	C11-C12-C13-C14
5	L	1282	BCL	C12-C13-C15-C16
14	M	1314	CDL	C72-C71-CB7-OB8
5	M	1305	BCL	CAA-CBA-CGA-O2A
5	L	1290	BCL	C2-C1-O2A-CGA
5	L	1290	BCL	C5-C6-C7-C8
5	L	1282	BCL	C2B-C3B-CAB-CBB
10	L	1292	HTO	O1-C1-C2-C3
14	M	1314	CDL	C72-C71-CB7-OB9
6	M	1309	LDA	C2-C1-N1-O1

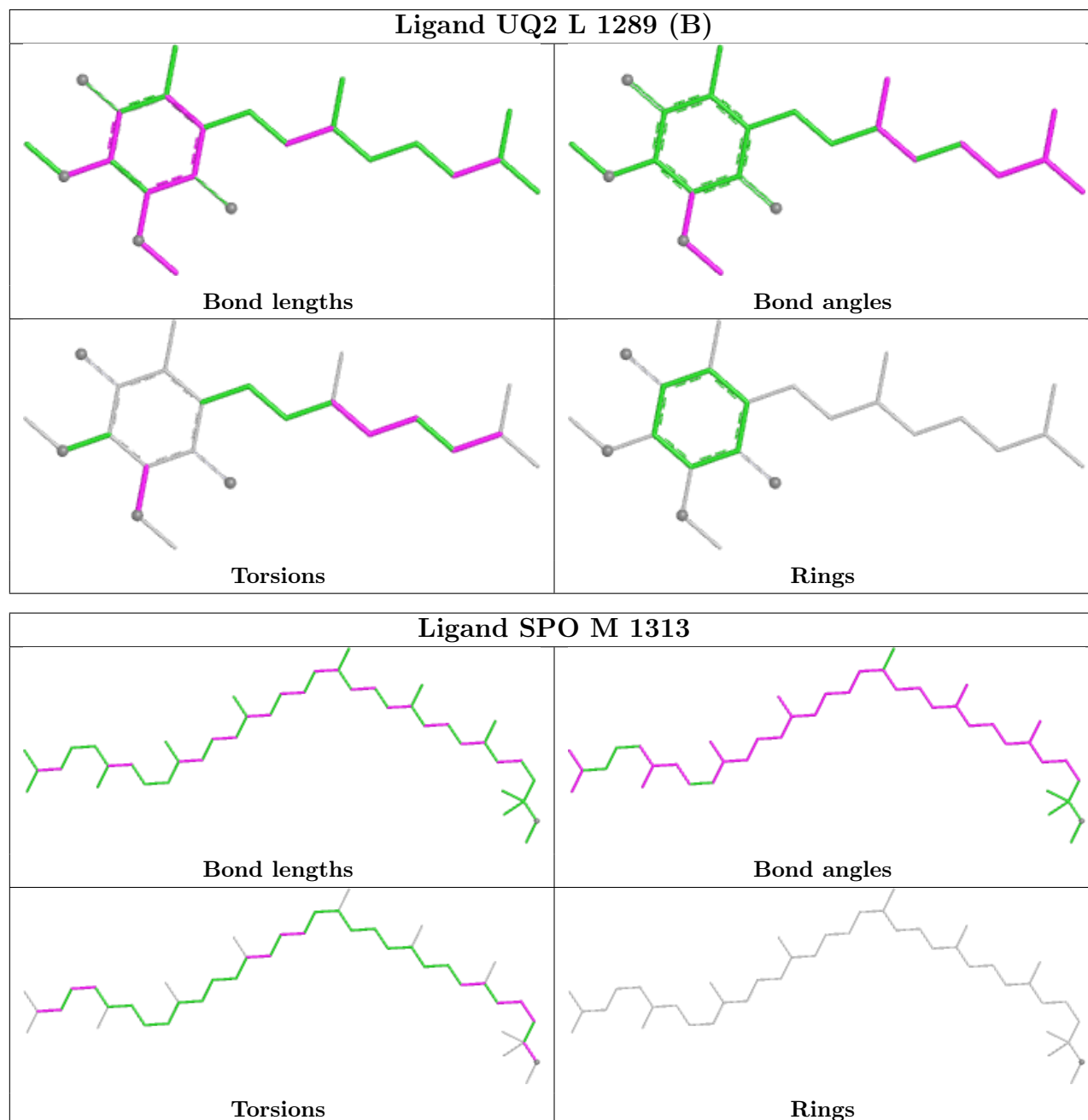
There are no ring outliers.

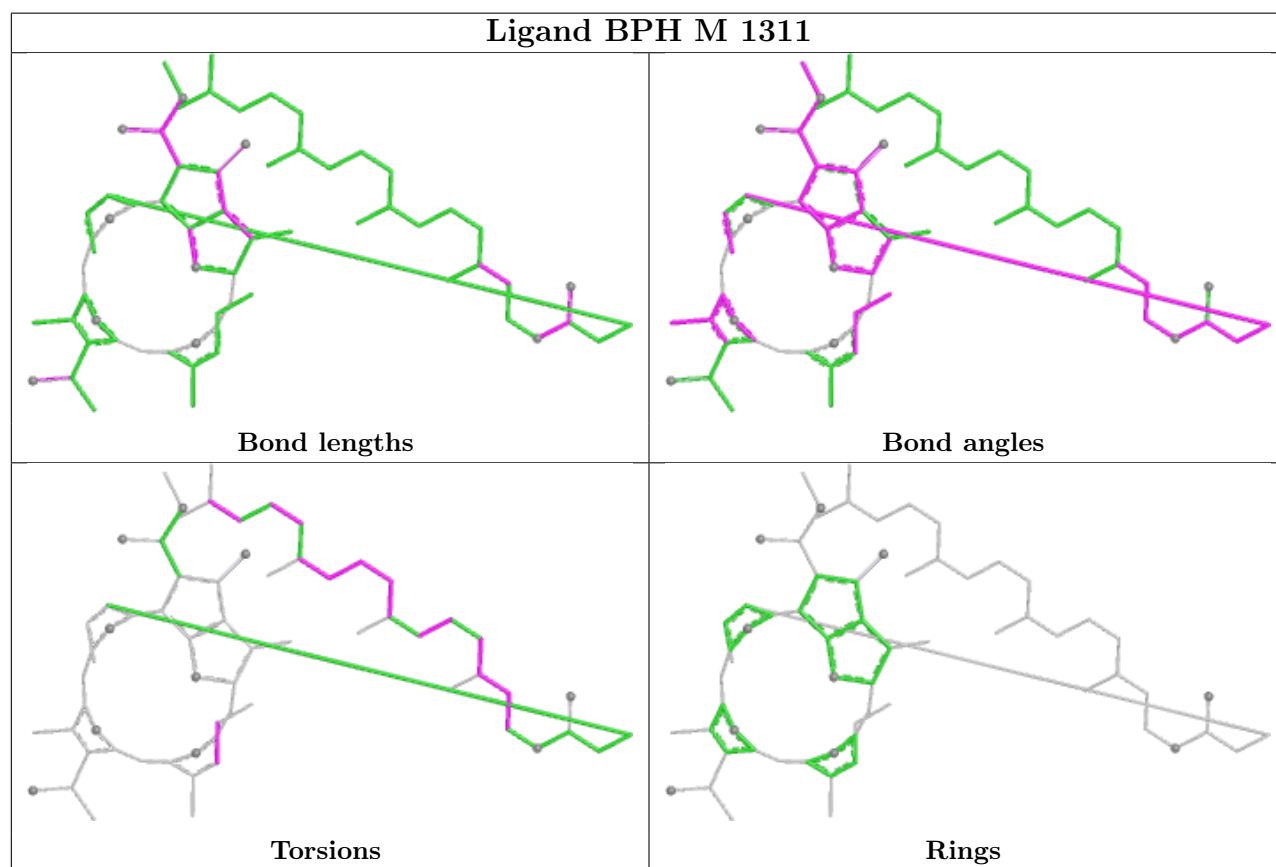
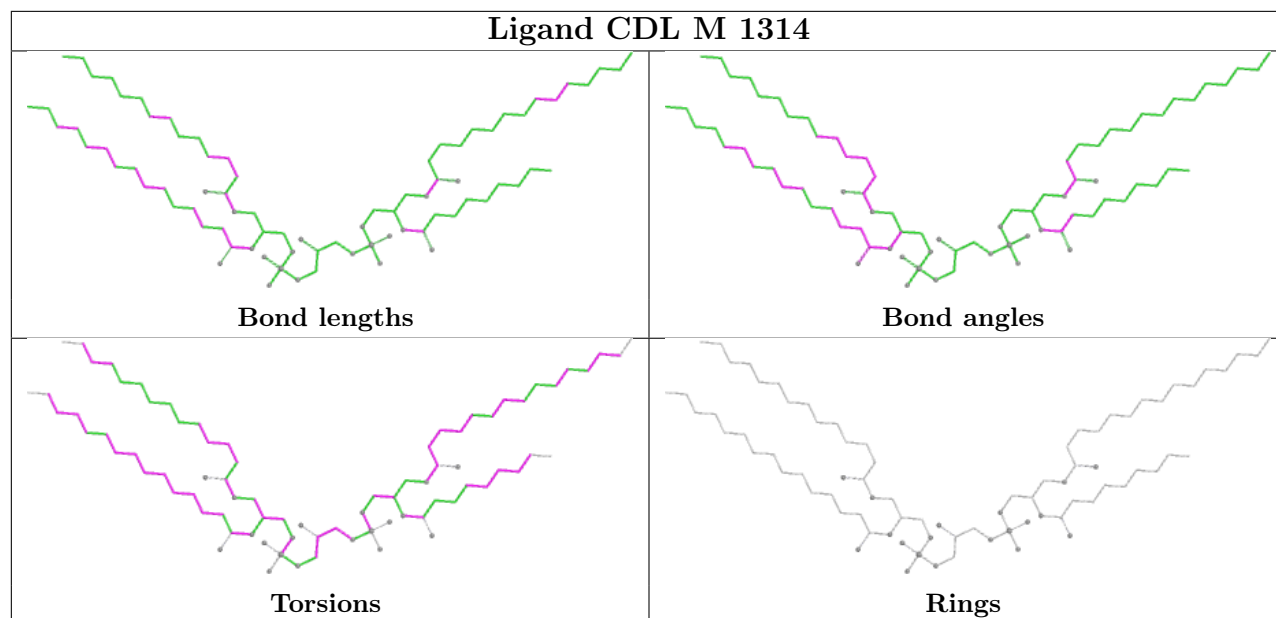
16 monomers are involved in 56 short contacts:

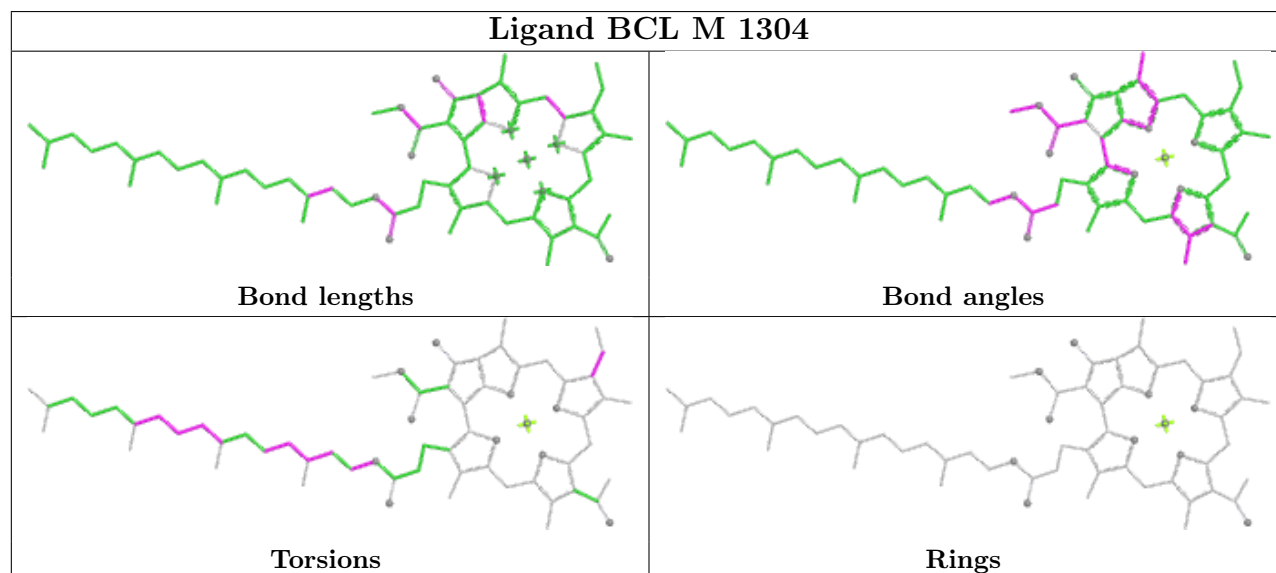
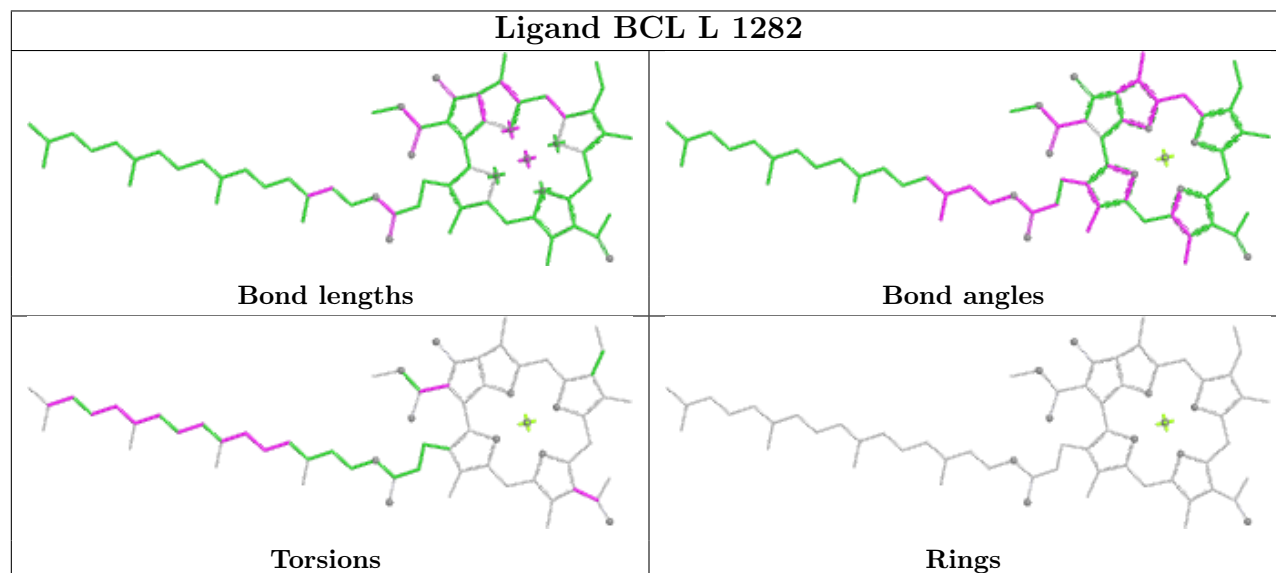
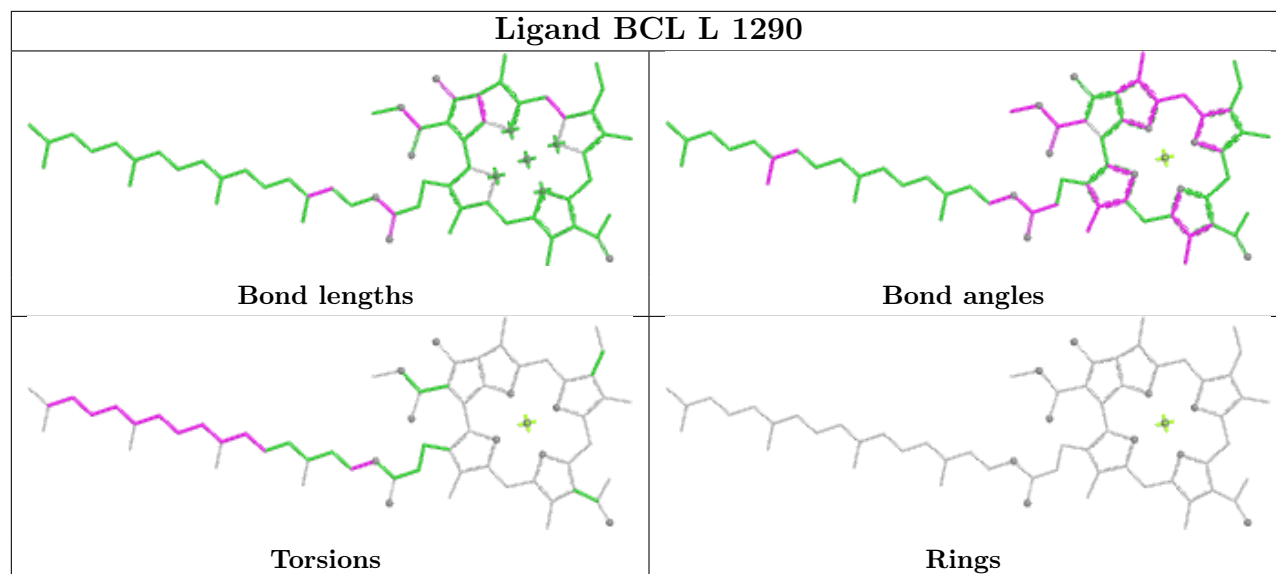
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1289[B]	UQ2	1	0
13	M	1313	SPO	2	0
14	M	1314	CDL	3	0
7	M	1311	BPH	9	0
6	M	1308	LDA	3	0
6	M	1309	LDA	2	0
6	L	1287	LDA	1	0
5	L	1282	BCL	4	0
5	M	1304	BCL	9	0
12	M	1312	U10	1	0
4	H	1252	GOL	5	0
5	M	1305	BCL	14	0
6	M	1306	LDA	1	0
4	L	1293	GOL	1	0
8	L	1289[A]	UQ2	5	0
7	L	1288	BPH	6	0

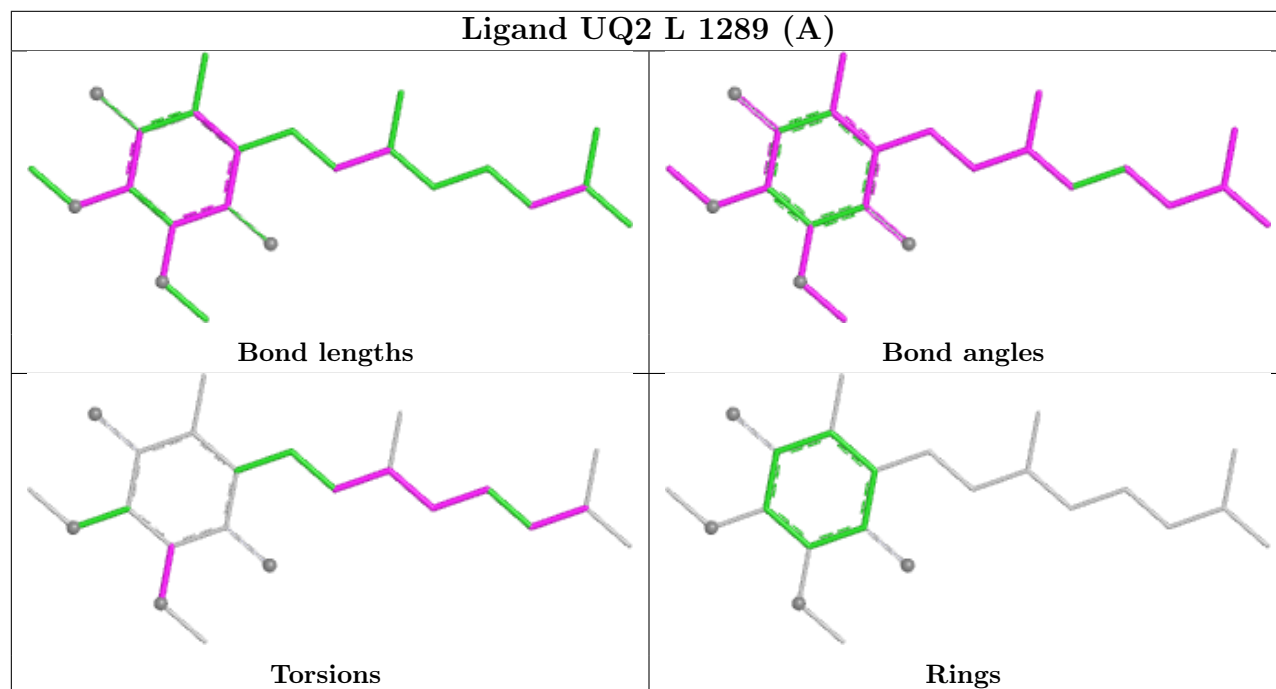
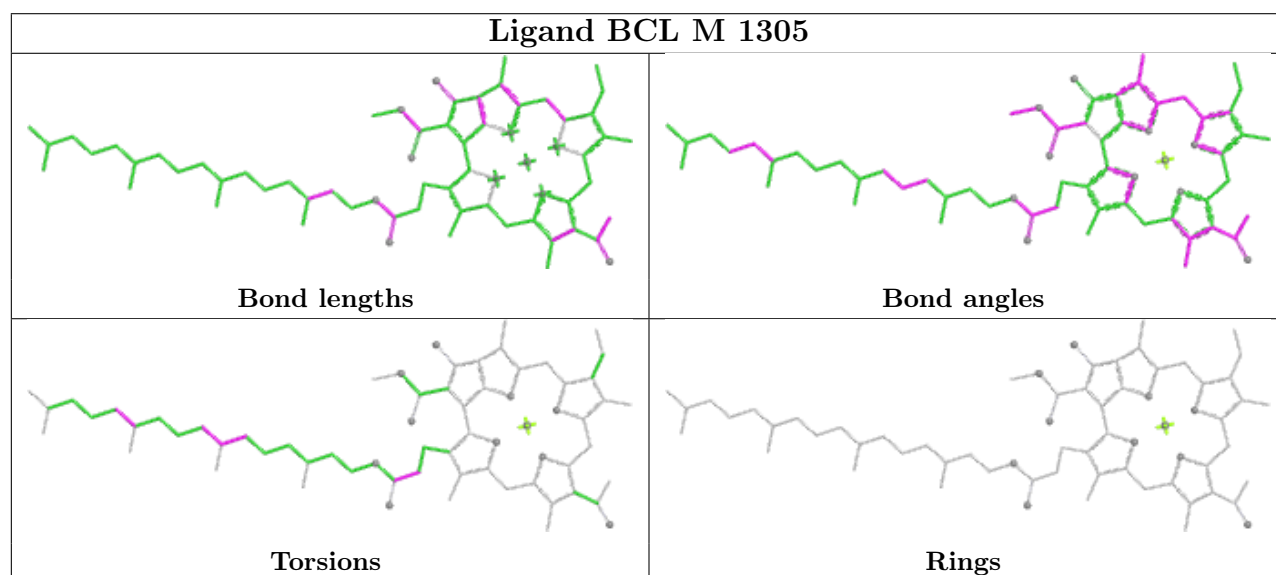
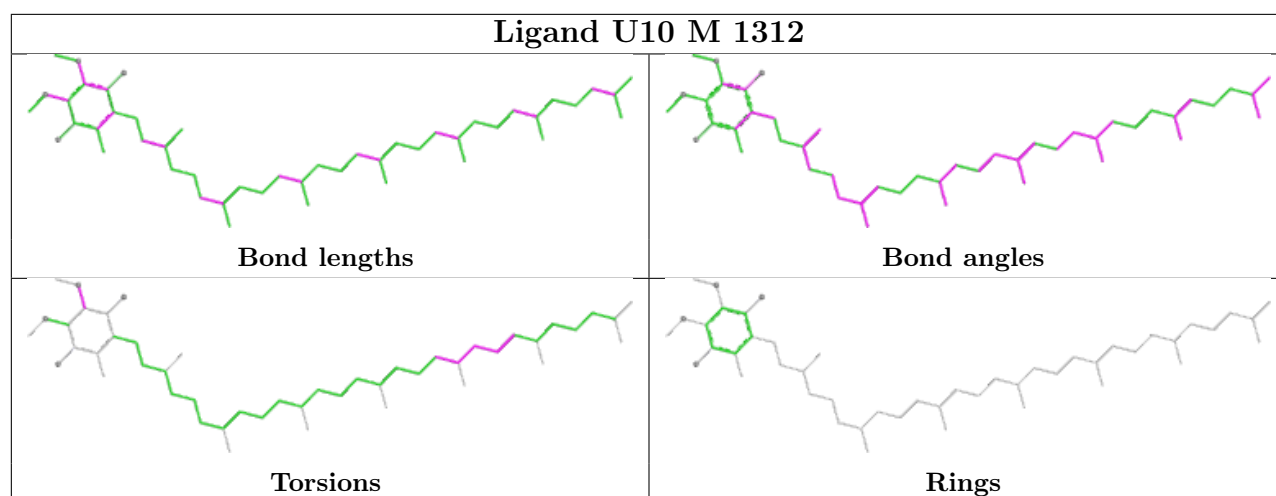
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

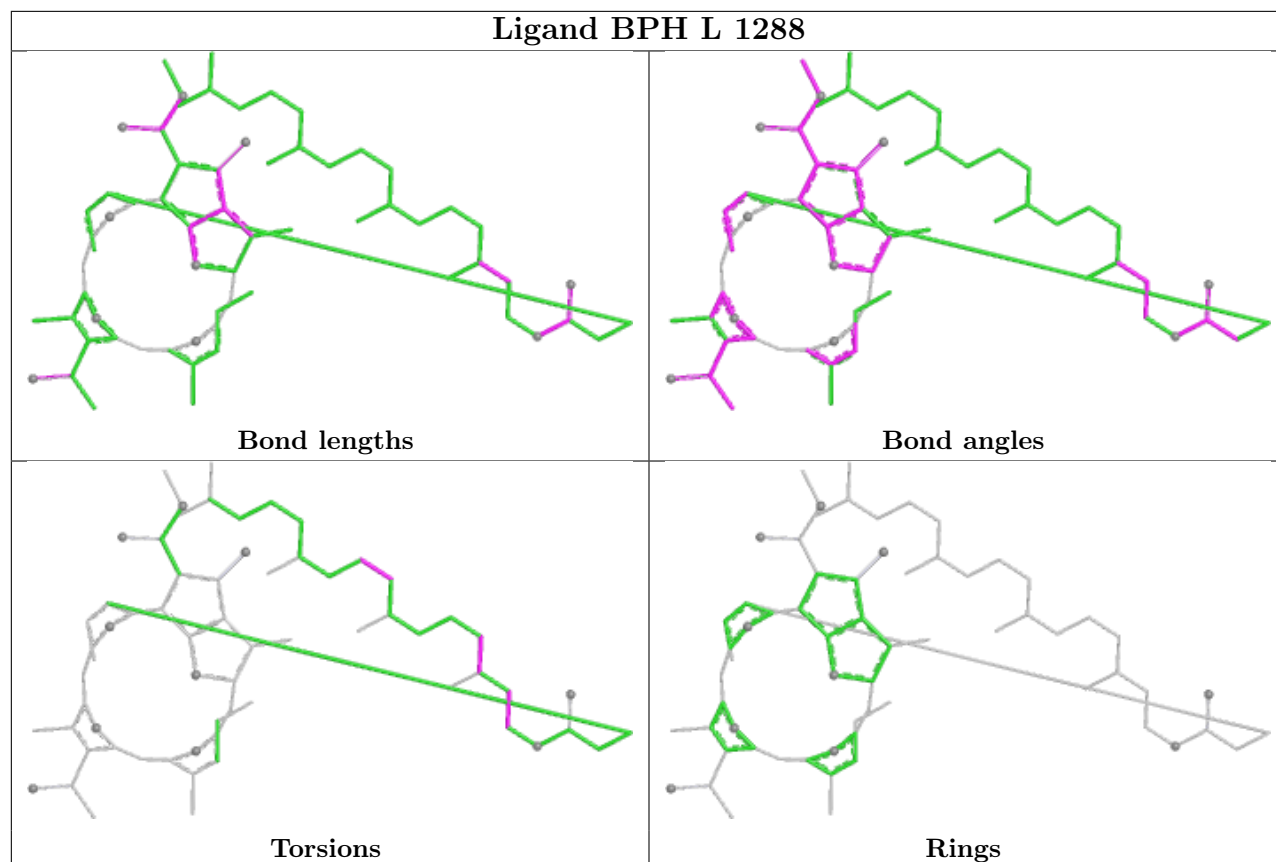
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.











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%)	1.18	36 (14%) 5 5	25, 33, 45, 72	0
2	L	281/281 (100%)	1.92	115 (40%) 0 0	24, 31, 52, 61	0
3	M	303/307 (98%)	2.01	134 (44%) 0 0	22, 35, 56, 67	0
All	All	825/848 (97%)	1.73	285 (34%) 1 0	22, 33, 52, 72	0

All (285) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	105	PHE	7.1
3	M	148	TRP	6.6
3	M	1	ALA	6.0
3	M	302	GLY	5.8
2	L	57	GLY	5.4
3	M	3	TYR	5.4
3	M	106	ALA	5.4
3	M	104	SER	5.3
3	M	101	TYR	5.3
1	H	18	TYR	5.2
2	L	76	GLY	5.2
2	L	277	GLY	5.2
2	L	67	TYR	5.1
2	L	70	ALA	5.0
3	M	300	ASN	4.9
2	L	54	VAL	4.9
2	L	151	TRP	4.8
3	M	303	MET	4.8
2	L	278	GLY	4.7
3	M	103	LEU	4.7
2	L	51	TRP	4.6
3	M	80	TRP	4.6
2	L	55	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	4.4
2	L	56	GLN	4.4
3	M	301	HIS	4.4
3	M	192	VAL	4.4
2	L	279	ILE	4.4
2	L	73	TYR	4.3
3	M	292	ASP	4.3
2	L	281	GLY	4.3
3	M	296	VAL	4.3
2	L	145	ALA	4.2
2	L	1	ALA	4.2
3	M	294	TRP	4.0
3	M	109	LEU	4.0
2	L	271	TRP	3.9
3	M	297	TRP	3.9
3	M	196	LEU	3.9
3	M	134	TYR	3.9
2	L	65	SER	3.9
1	H	249	LYS	3.8
3	M	107	ALA	3.8
3	M	290	VAL	3.8
3	M	102	GLY	3.8
3	M	131	GLY	3.8
3	M	99	PRO	3.7
2	L	140	GLY	3.7
2	L	252	GLY	3.7
2	L	164	TYR	3.7
3	M	188	ASN	3.7
2	L	81	ALA	3.7
3	M	167	LEU	3.7
3	M	197	PHE	3.6
2	L	269	LEU	3.6
3	M	54	SER	3.6
1	H	12	LEU	3.6
3	M	293	ASN	3.6
3	M	130	TRP	3.5
1	H	60	LYS	3.5
2	L	275	ILE	3.5
3	M	198	TYR	3.5
3	M	166	ILE	3.5
1	H	138	ALA	3.5
3	M	23	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	58	THR	3.5
2	L	162	TYR	3.4
1	H	173	GLU	3.4
3	M	52	LEU	3.4
3	M	120	PHE	3.4
2	L	132	VAL	3.4
3	M	191	LEU	3.4
2	L	163	THR	3.3
2	L	79	PRO	3.3
3	M	117	ILE	3.3
2	L	80	LEU	3.3
2	L	216	PHE	3.3
3	M	133	THR	3.2
3	M	157	TRP	3.2
2	L	72	GLU	3.2
2	L	85	LEU	3.2
1	H	58	LEU	3.2
3	M	98	ALA	3.1
3	M	289	THR	3.1
2	L	66	VAL	3.1
3	M	291	VAL	3.1
3	M	127	TRP	3.1
2	L	40	PHE	3.1
3	M	2	GLU	3.1
3	M	78	ALA	3.1
3	M	152	SER	3.1
2	L	149	GLY	3.0
3	M	115	TRP	3.0
2	L	63	LEU	3.0
3	M	193	HIS	3.0
3	M	176	PRO	3.0
2	L	144	TYR	3.0
3	M	171	TRP	3.0
2	L	131	LEU	2.9
3	M	285	LEU	2.9
3	M	189	PHE	2.9
3	M	185	TRP	2.9
2	L	50	ALA	2.9
2	L	68	PRO	2.9
3	M	150	PHE	2.9
1	H	250	SER	2.9
1	H	77	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	M	299	GLN	2.9
1	H	29	TYR	2.9
2	L	253	THR	2.8
2	L	64	ILE	2.8
3	M	172	SER	2.8
3	M	295	TYR	2.8
3	M	283	GLY	2.8
3	M	55	LEU	2.8
2	L	247	CYS	2.8
3	M	194	GLY	2.8
1	H	15	LEU	2.8
2	L	2	LEU	2.8
1	H	220	LYS	2.8
2	L	88	ILE	2.8
2	L	62	GLN	2.7
1	H	213	PHE	2.7
3	M	162	PHE	2.7
1	H	51	ALA	2.7
2	L	273	ALA	2.7
3	M	190	SER	2.7
2	L	42	ALA	2.7
2	L	154	LEU	2.7
1	H	251	VAL	2.7
2	L	254	ILE	2.7
3	M	271	TRP	2.7
2	L	122	ALA	2.7
2	L	197	ALA	2.7
3	M	61	PHE	2.7
3	M	139	ALA	2.7
2	L	71	LEU	2.7
3	M	114	LEU	2.7
2	L	158	SER	2.7
2	L	256	PHE	2.6
3	M	108	PRO	2.6
2	L	150	ILE	2.6
3	M	168	MET	2.6
2	L	141	ALA	2.6
2	L	159	ASN	2.6
2	L	53	ALA	2.6
3	M	72	ILE	2.6
1	H	139	GLY	2.6
2	L	77	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	73	TRP	2.6
3	M	119	SER	2.6
3	M	280	GLY	2.5
2	L	152	THR	2.5
3	M	45	ALA	2.5
2	L	272	TRP	2.5
1	H	40	TYR	2.5
1	H	94	GLU	2.5
2	L	21	LEU	2.5
2	L	44	LEU	2.5
3	M	58	LEU	2.5
3	M	151	LEU	2.5
3	M	75	TRP	2.5
3	M	79	GLY	2.5
2	L	26	VAL	2.5
3	M	32	VAL	2.5
2	L	264	GLN	2.5
3	M	121	PHE	2.5
3	M	161	GLY	2.5
2	L	47	ILE	2.5
2	L	240	ALA	2.4
2	L	202	LYS	2.4
2	L	60	ASN	2.4
2	L	257	ASP	2.4
2	L	260	VAL	2.4
3	M	181	SER	2.4
1	H	55	PRO	2.4
3	M	77	GLN	2.4
2	L	86	TRP	2.4
3	M	239	ALA	2.4
1	H	120	LEU	2.4
3	M	160	LEU	2.4
3	M	100	GLU	2.4
3	M	19	GLY	2.4
3	M	257	GLY	2.4
1	H	64	PHE	2.4
3	M	67	PHE	2.4
2	L	46	ILE	2.4
3	M	163	ILE	2.4
3	M	175	VAL	2.4
1	H	163	LYS	2.4
3	M	210	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	59	PRO	2.3
1	H	136	ALA	2.3
2	L	245	ALA	2.3
3	M	187	ASN	2.3
3	M	56	GLY	2.3
3	M	140	LEU	2.3
3	M	298	GLY	2.3
1	H	175	MET	2.3
3	M	62	SER	2.3
2	L	160	THR	2.3
3	M	286	LEU	2.3
3	M	110	LYS	2.3
2	L	146	PHE	2.3
3	M	284	ILE	2.3
3	M	57	VAL	2.3
3	M	60	LEU	2.3
3	M	64	LEU	2.3
2	L	142	TRP	2.3
2	L	41	PHE	2.2
2	L	242	PHE	2.2
3	M	258	PHE	2.2
2	L	241	VAL	2.2
3	M	199	ASN	2.2
3	M	51	TYR	2.2
3	M	76	TYR	2.2
2	L	208	THR	2.2
3	M	195	ASN	2.2
2	L	17	VAL	2.2
1	H	11	ASP	2.2
2	L	203	GLY	2.2
3	M	89	LEU	2.2
3	M	94	LEU	2.2
1	H	30	TYR	2.2
1	H	221	SER	2.2
2	L	100	TRP	2.2
3	M	268	TRP	2.2
1	H	57	PRO	2.2
2	L	22	PHE	2.2
3	M	68	PHE	2.2
2	L	155	ASP	2.2
2	L	267	VAL	2.2
2	L	161	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	191	GLY	2.2
1	H	137	ALA	2.2
3	M	26	LEU	2.2
2	L	9	TYR	2.2
2	L	263	TRP	2.2
2	L	265	TRP	2.2
3	M	20	MET	2.2
2	L	250	ILE	2.1
3	M	12	VAL	2.1
1	H	19	SER	2.1
2	L	20	ASN	2.1
2	L	148	TYR	2.1
3	M	142	MET	2.1
3	M	259	ASN	2.1
2	L	69	PRO	2.1
2	L	147	PRO	2.1
2	L	270	PRO	2.1
3	M	69	THR	2.1
2	L	167	PHE	2.1
2	L	181	PHE	2.1
3	M	92	PHE	2.1
2	L	165	GLY	2.1
2	L	188	ALA	2.1
2	L	238	LEU	2.1
3	M	282	ILE	2.1
2	L	180	PHE	2.1
2	L	255	TRP	2.1
1	H	142	VAL	2.1
1	H	13	ALA	2.1
3	M	118	ALA	2.1
2	L	52	SER	2.1
3	M	86	LEU	2.1
2	L	230	HIS	2.1
3	M	113	GLY	2.1
2	L	82	LYS	2.1
3	M	50	ILE	2.1
3	M	270	ILE	2.1
2	L	220	VAL	2.1
3	M	44	ASN	2.0
2	L	258	GLN	2.0
3	M	4	GLN	2.0
3	M	202	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	111	PRO	2.0
2	L	13	GLY	2.0
3	M	63	GLY	2.0
2	L	49	ILE	2.0
1	H	225	VAL	2.0
3	M	126	VAL	2.0
3	M	201	PHE	2.0
3	M	204	LEU	2.0
1	H	95	GLY	2.0
3	M	112	GLY	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
6	LDA	M	1309	16/16	0.50	0.56	94,97,101,102	0
6	LDA	L	1286	16/16	0.56	0.54	81,90,97,97	0
4	GOL	H	1255	6/6	0.56	0.22	96,98,98,98	0
6	LDA	L	1284	16/16	0.61	0.49	94,97,103,103	0
4	GOL	H	1254	6/6	0.63	0.37	111,111,111,111	0
6	LDA	L	1285	16/16	0.68	0.42	85,91,98,98	0
14	CDL	M	1314	81/100	0.68	0.38	62,95,106,107	0
4	GOL	H	1253	6/6	0.69	0.27	74,75,75,76	0
4	GOL	H	1252	6/6	0.69	0.19	41,54,57,59	0
6	LDA	L	1283	16/16	0.70	0.34	73,92,102,102	0
6	LDA	M	1308	16/16	0.70	0.32	51,55,57,58	0
6	LDA	L	1287	16/16	0.71	0.40	107,108,111,111	0
6	LDA	M	1306	16/16	0.73	0.30	44,66,71,72	0

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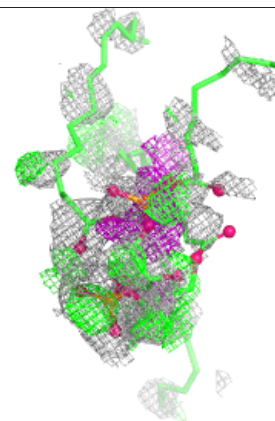
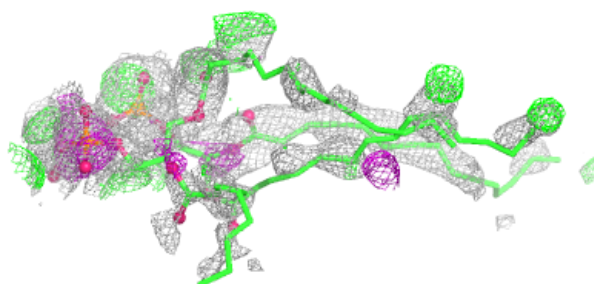
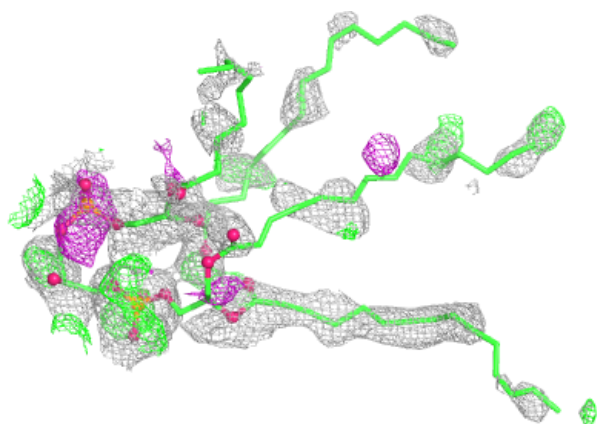
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	HTO	L	1292	10/10	0.74	0.29	78,80,80,81	0
8	UQ2	L	1289[B]	23/23	0.76	0.33	26,33,46,47	23
6	LDA	M	1307	16/16	0.76	0.33	66,71,80,81	0
8	UQ2	L	1289[A]	23/23	0.76	0.33	22,32,49,49	23
13	SPO	M	1313	42/42	0.77	0.26	34,41,62,66	0
4	GOL	M	1315	6/6	0.77	0.32	113,114,114,115	0
9	PO4	L	1291	5/5	0.79	0.21	55,56,56,57	0
4	GOL	L	1293	6/6	0.84	0.18	45,52,53,56	0
7	BPH	M	1311	65/65	0.84	0.20	23,32,86,89	0
12	U10	M	1312	48/63	0.86	0.20	24,38,63,64	0
7	BPH	L	1288	65/65	0.86	0.14	18,25,36,37	0
4	GOL	L	1294	6/6	0.86	0.22	88,89,89,89	0
5	BCL	L	1282	66/66	0.88	0.15	22,26,53,55	0
5	BCL	L	1290	66/66	0.88	0.15	23,26,43,50	0
5	BCL	M	1305	66/66	0.88	0.15	20,26,51,58	0
5	BCL	M	1304	66/66	0.90	0.17	24,29,74,76	0
11	FE	M	1310	1/1	0.94	0.06	22,22,22,22	0

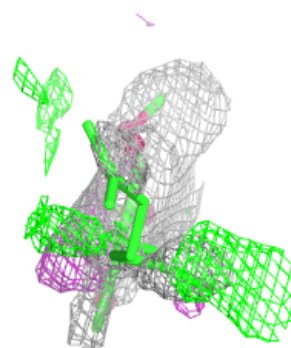
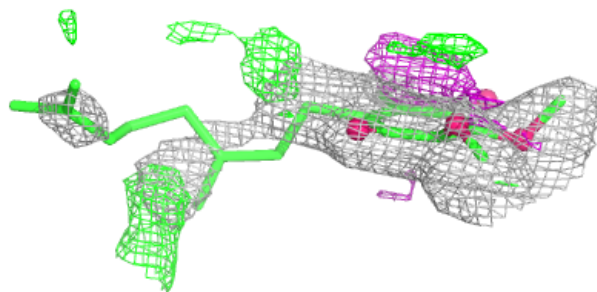
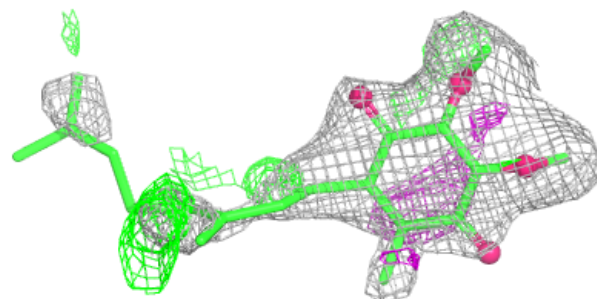
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDL M 1314:

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

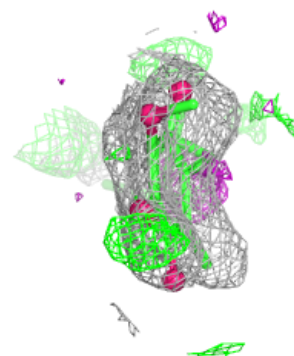
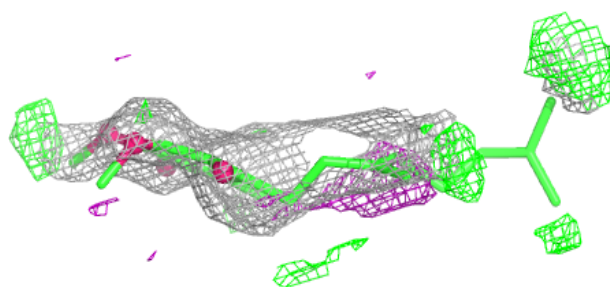
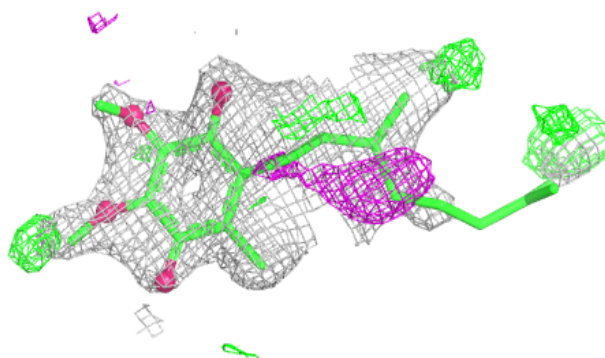
**Electron density around UQ2 L 1289 (B):**

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

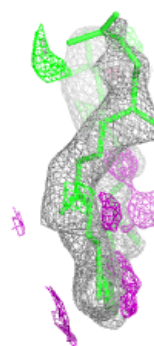
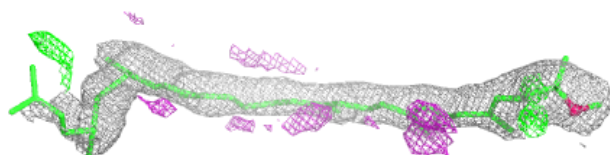
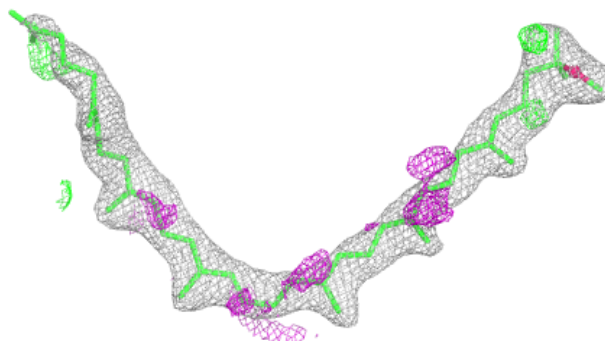


Electron density around UQ2 L 1289 (A):

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

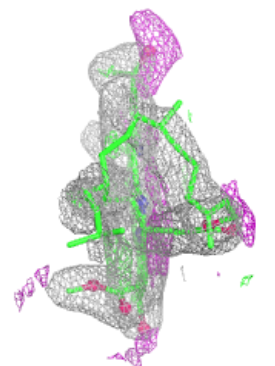
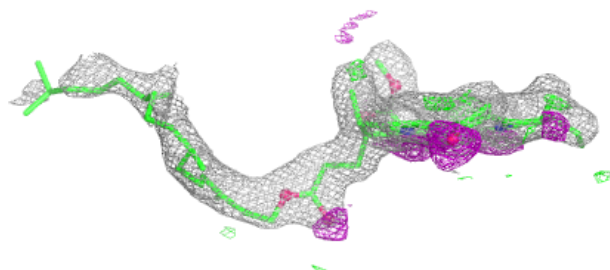
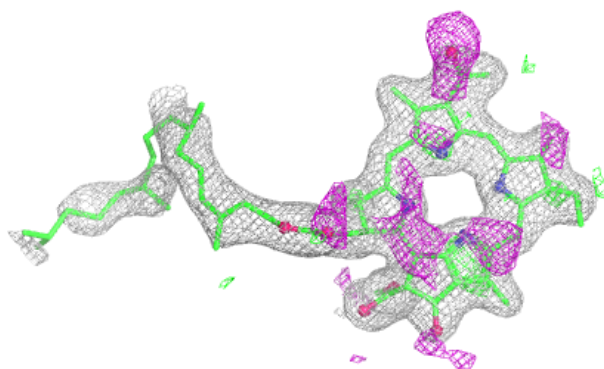
**Electron density around SPO M 1313:**

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

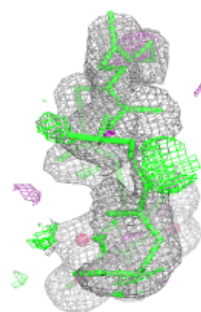
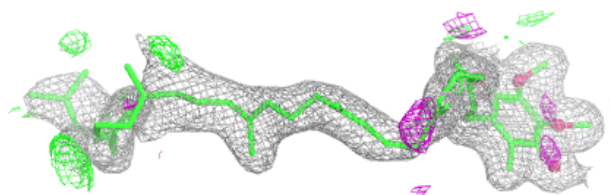
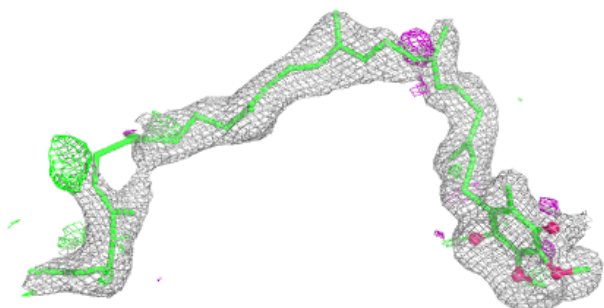


Electron density around BPH M 1311:

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

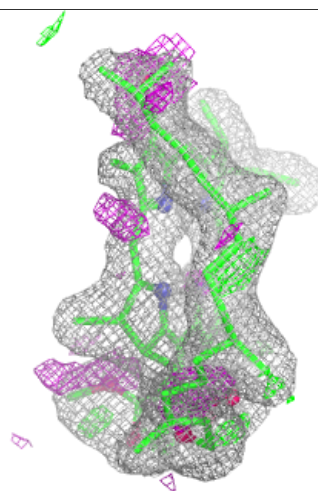
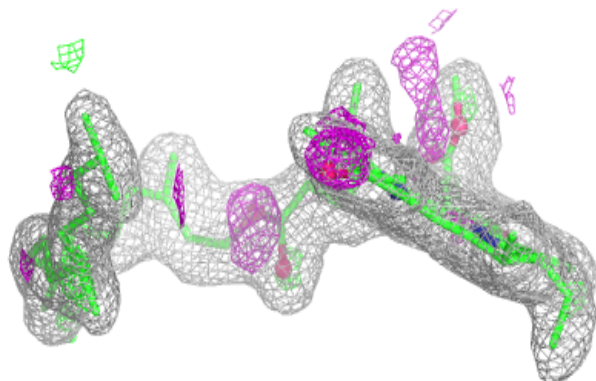
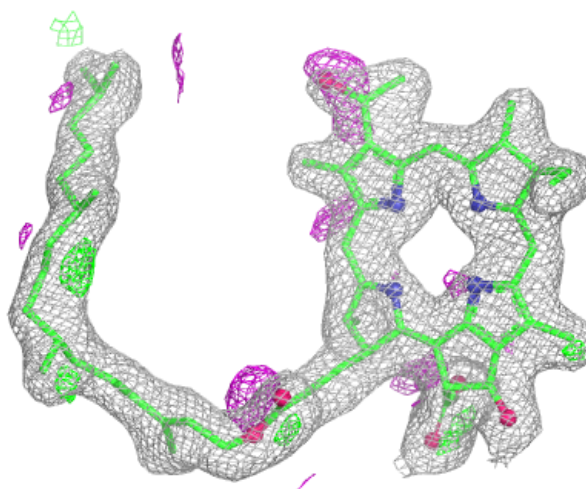
**Electron density around U10 M 1312:**

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



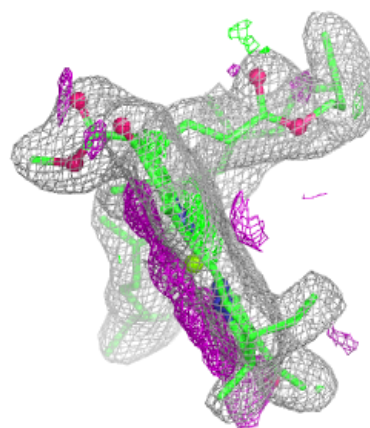
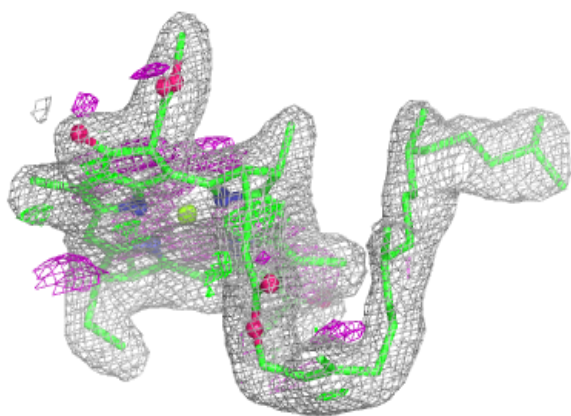
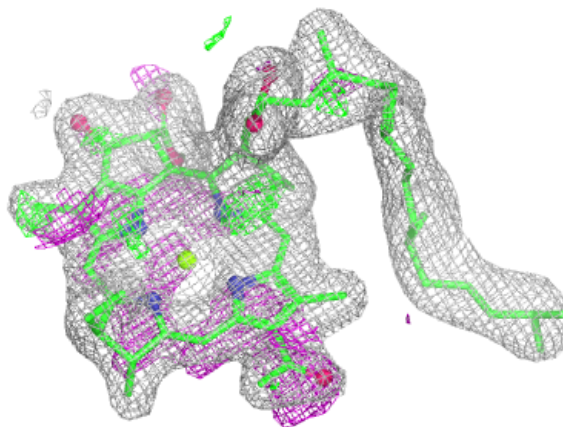
Electron density around BPH L 1288:

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



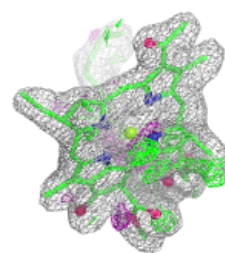
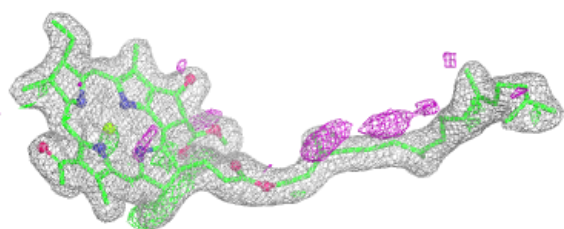
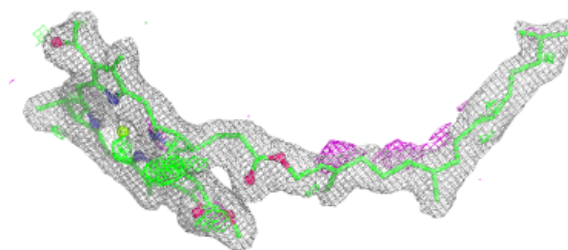
Electron density around BCL L 1282:

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

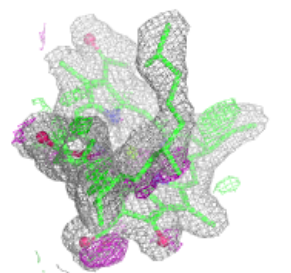
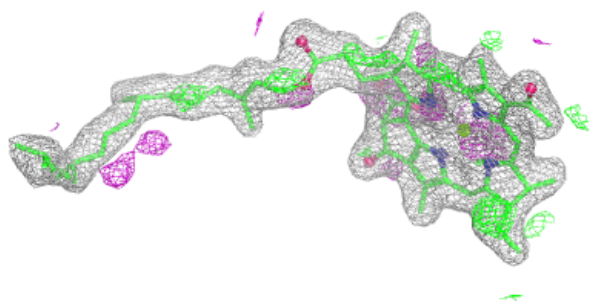
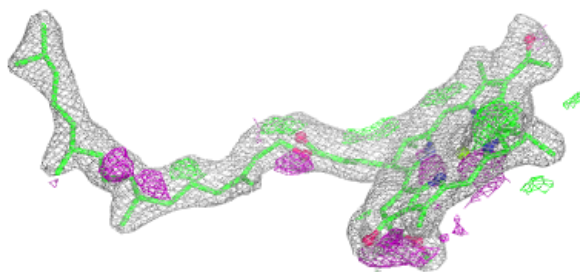


Electron density around BCL L 1290:

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

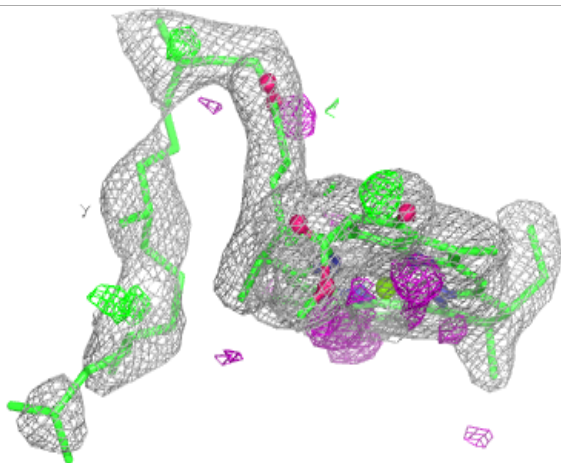
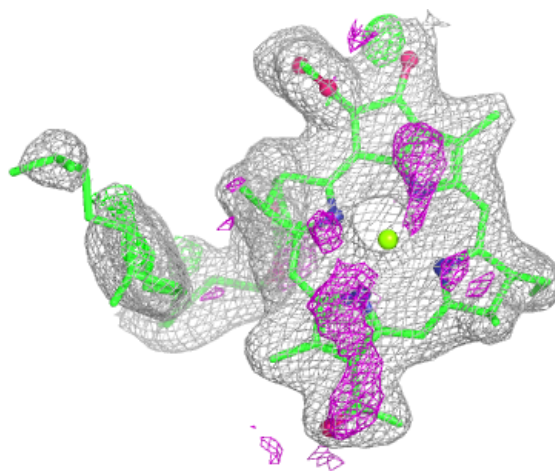
**Electron density around BCL M 1305:**

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



Electron density around BCL M 1304:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.