



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:43 AM UTC

PDB ID : 2UXJ / pdb_00002uxj
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 10 in the neutral state
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-28
Resolution : 2.25 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

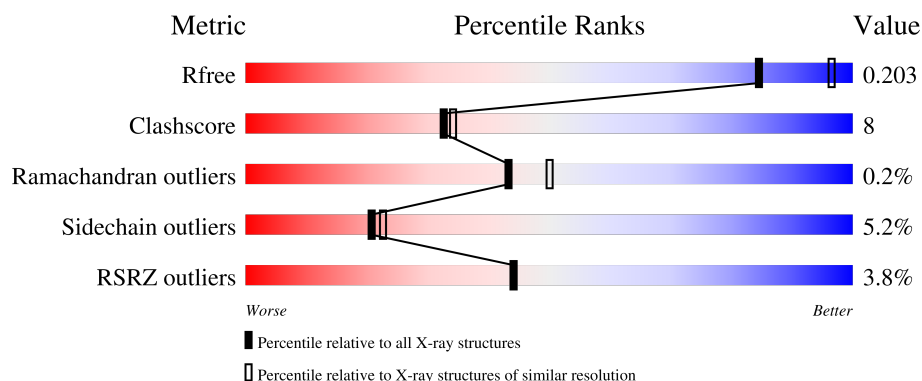
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	6% 80% 12% 7%
2	L	281	% 88% 12% .
3	M	307	4% 80% 16% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1282	X	-	-	-
5	BCL	L	1287	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
8	UQ2	L	1286[B]	-	-	X	-

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7707 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			

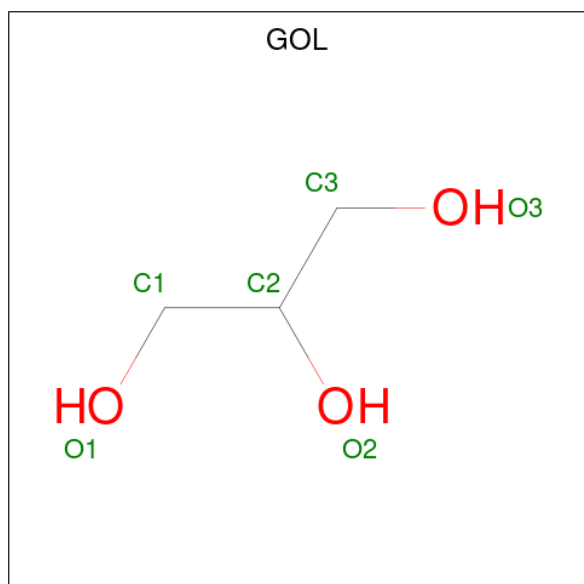
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

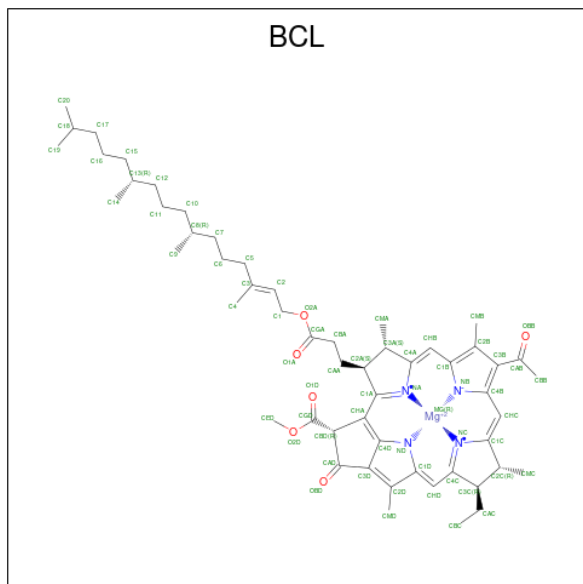
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

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



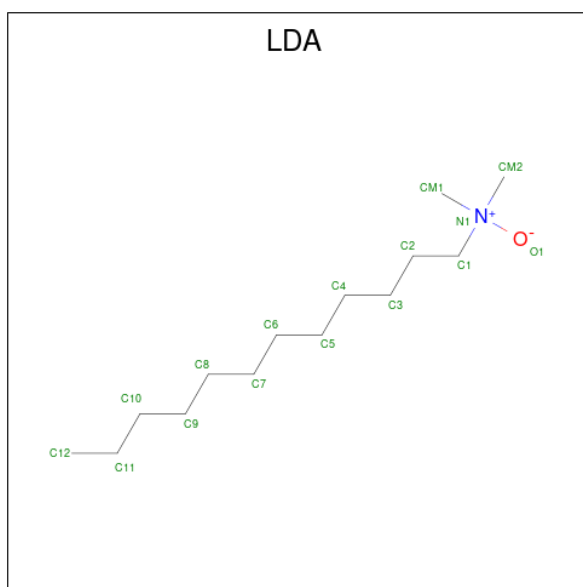
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

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



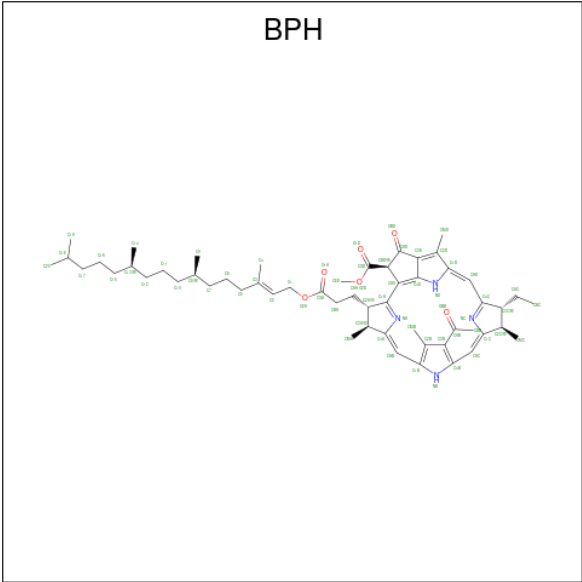
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



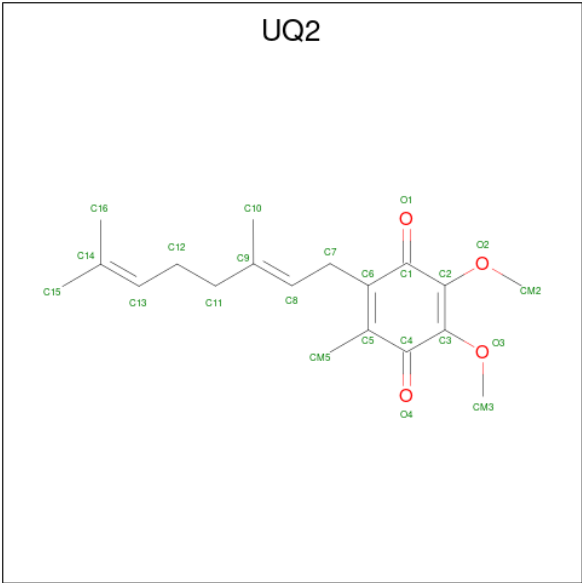
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

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



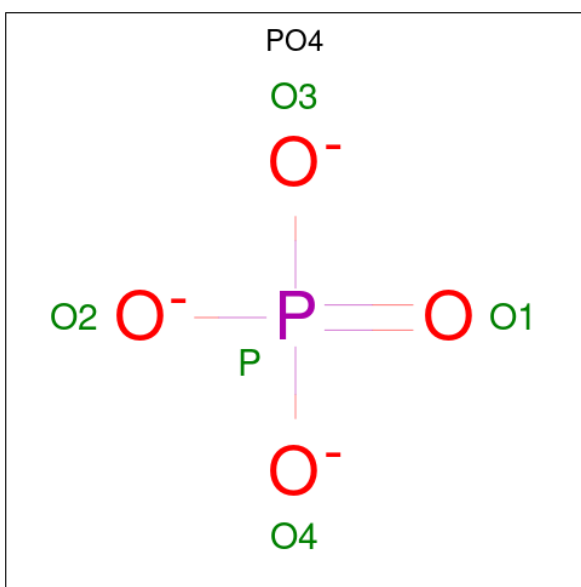
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



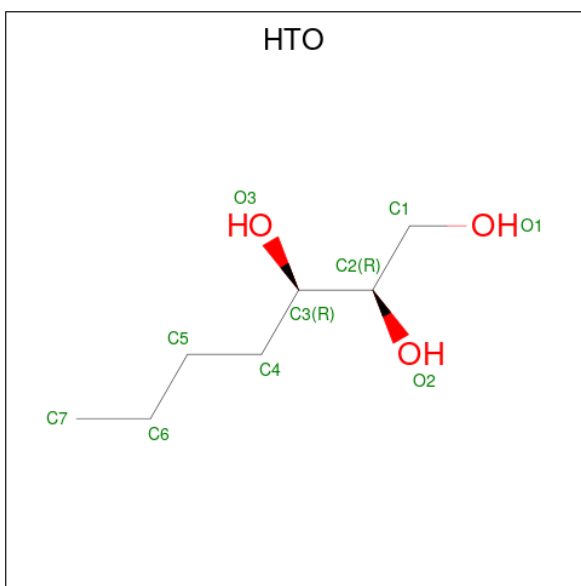
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- 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: $C_7H_{16}O_3$).

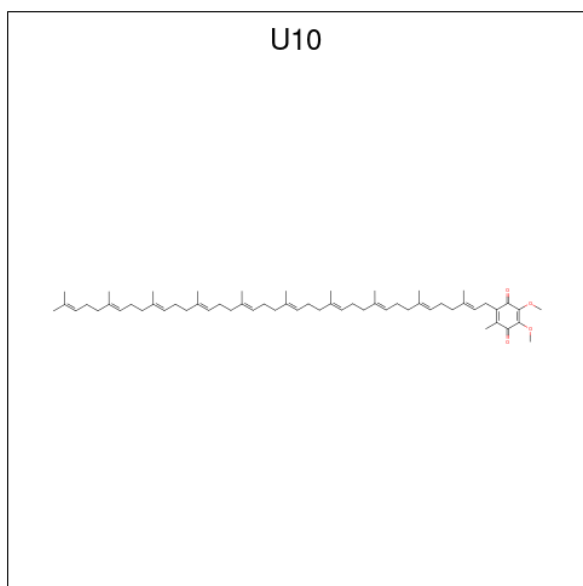


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

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

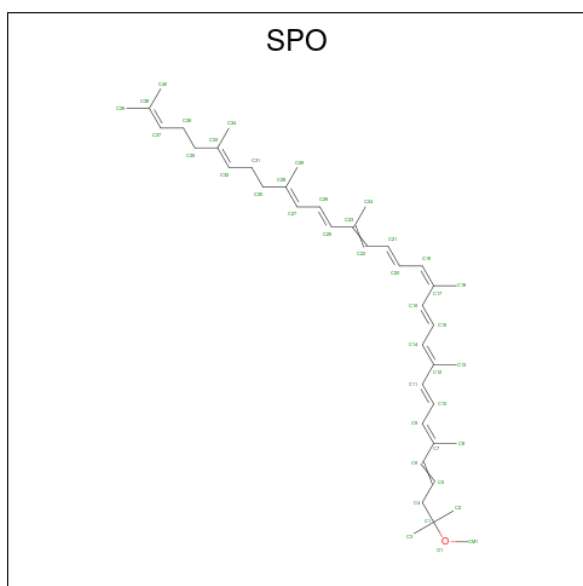
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



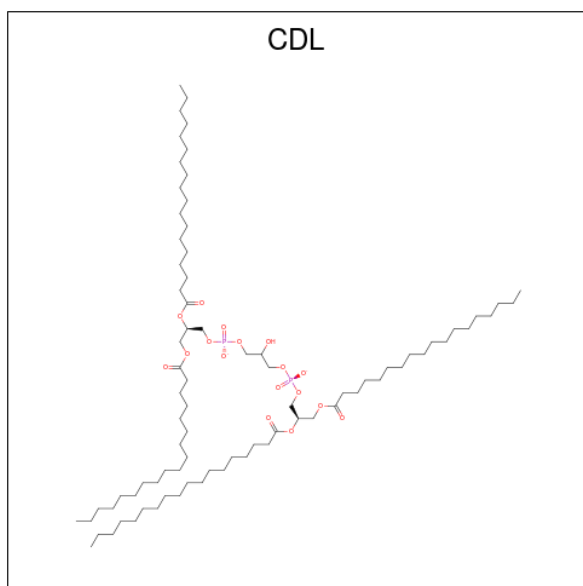
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- 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		

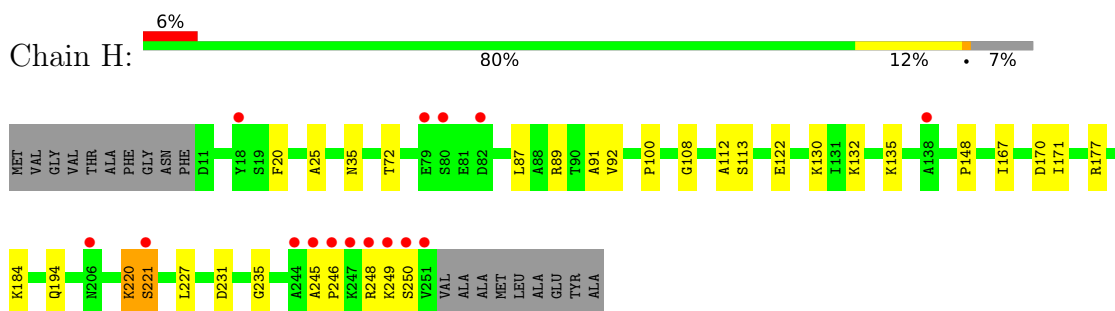
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	122	Total	O	0	0
			122	122		
15	L	134	Total	O	0	0
			134	134		
15	M	147	Total	O	0	0
			147	147		

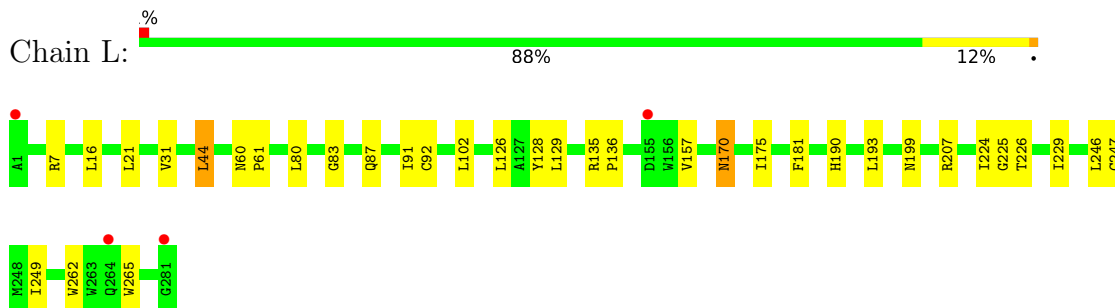
3 Residue-property plots [i](#)

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.

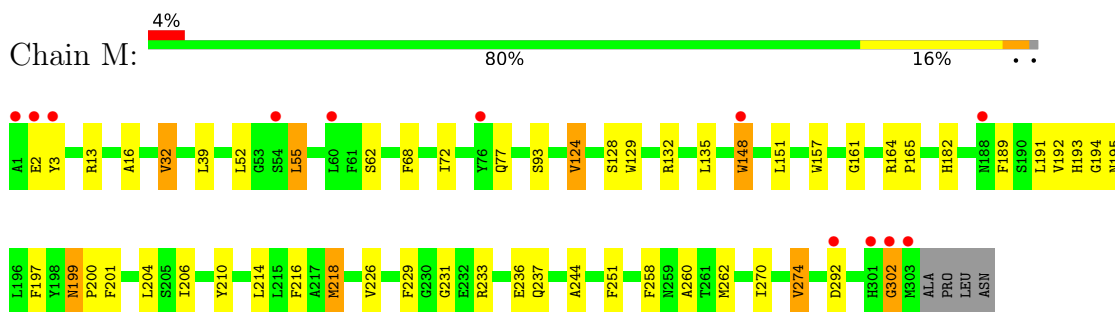
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• 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 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.38Å 139.38Å 235.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.52 – 2.25 119.52 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.0 (119.52-2.25) 90.2 (119.52-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.225 (Not available) , 0.203	Depositor DCC
R_{free} test set	5205 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7707	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, UQ2, CDL, FE, U10, PO4, BPH, HTO, GOL, SPO, 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	0.76	1/1906 (0.1%)	0.92	0/2591
2	L	0.88	0/2320	0.93	0/3175
3	M	0.84	2/2501 (0.1%)	0.92	0/3415
All	All	0.83	3/6727 (0.0%)	0.92	0/9181

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	218	MET	SD-CE	9.96	2.04	1.79
1	H	250	SER	C-N	-6.71	1.24	1.33
3	M	302	GLY	C-N	-6.19	1.24	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1846	0	1861	22	0
2	L	2232	0	2187	27	0
3	M	2409	0	2321	40	0
4	H	18	0	24	1	0
4	L	18	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	132	0	148	6	0
5	M	132	0	148	16	0
6	L	32	0	62	0	0
6	M	112	0	217	8	0
7	L	65	0	76	7	0
7	M	65	0	76	9	0
8	L	46	0	52	13	0
9	L	5	0	0	0	0
10	L	20	0	32	2	0
11	M	1	0	0	0	0
12	M	48	0	63	1	0
13	M	42	0	60	4	0
14	M	81	0	92	1	0
15	H	122	0	0	0	0
15	L	134	0	0	2	0
15	M	147	0	0	2	0
All	All	7707	0	7443	116	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 8.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:218:MET:SD	3:M:218:MET:CE	2.04	1.43
2:L:224:ILE:HG22	8:L:1286[B]:UQ2:C8	1.87	1.04
2:L:224:ILE:HG22	8:L:1286[B]:UQ2:H8	0.99	0.97
2:L:224:ILE:CG2	8:L:1286[B]:UQ2:H8	1.96	0.93
7:L:1285:BPH:HHC	7:L:1285:BPH:HBB3	1.51	0.91
2:L:229:ILE:HD13	8:L:1286[B]:UQ2:H112	1.58	0.85
2:L:7:ARG:NH1	15:L:2002:HOH:O	1.93	0.85
7:M:1313:BPH:HBB3	7:M:1313:BPH:HHC	1.61	0.83
1:H:122:GLU:HG3	3:M:236:GLU:OE1	1.80	0.81
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.44	0.81
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.16	0.79
3:M:199:ASN:HD22	3:M:199:ASN:C	1.97	0.73
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.70	0.72
5:M:1304:BCL:HHC	5:M:1304:BCL:HBB3	1.72	0.72
5:M:1303:BCL:HBB3	5:M:1304:BCL:H41	1.72	0.71
7:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.74	0.68
2:L:181:PHE:CD2	7:M:1313:BPH:HBB1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1286[B]:UQ2:CM3	15:M:2117:HOH:O	2.41	0.68
2:L:170:ASN:HD22	2:L:170:ASN:C	2.03	0.67
1:H:35:ASN:OD1	3:M:260:ALA:HB1	1.96	0.66
3:M:77:GLN:HE22	3:M:93:SER:H	1.42	0.65
2:L:7:ARG:HD3	15:L:2002:HOH:O	1.96	0.64
2:L:91:ILE:HG13	10:L:1289:HTO:H41	1.79	0.64
7:M:1313:BPH:HHC	7:M:1313:BPH:CBB	2.27	0.64
5:M:1303:BCL:HBB2	5:M:1303:BCL:HHC	1.80	0.63
2:L:181:PHE:HB3	7:M:1313:BPH:HBB2	1.79	0.62
2:L:190:HIS:HA	8:L:1286[B]:UQ2:H5M1	1.82	0.62
4:L:1292:GOL:H32	6:M:1305:LDA:H12	1.83	0.61
3:M:189:PHE:O	3:M:193:HIS:HD2	1.83	0.60
2:L:226:THR:HG22	8:L:1286[B]:UQ2:H3M3	1.84	0.60
2:L:190:HIS:ND1	8:L:1286[B]:UQ2:O4	2.25	0.59
7:L:1285:BPH:HHC	7:L:1285:BPH:CBB	2.31	0.58
6:M:1305:LDA:H101	6:M:1307:LDA:H121	1.85	0.57
2:L:175:ILE:HD11	6:M:1311:LDA:H12	1.87	0.57
3:M:68:PHE:O	3:M:72:ILE:HG12	2.05	0.56
2:L:193:LEU:HD23	8:L:1286[B]:UQ2:C4	2.34	0.56
2:L:181:PHE:HB3	7:M:1313:BPH:CBB	2.36	0.56
7:M:1313:BPH:HBB3	7:M:1313:BPH:CHC	2.34	0.56
2:L:199:ASN:HA	4:L:1290:GOL:H31	1.88	0.55
1:H:130:LYS:HE3	1:H:170:ASP:OD2	2.07	0.54
1:H:194:GLN:HA	3:M:3:TYR:HD2	1.72	0.54
2:L:157:VAL:HG11	5:M:1304:BCL:HBB1	1.89	0.53
3:M:148:TRP:HB3	14:M:1316:CDL:H741	1.90	0.53
1:H:248:ARG:HA	1:H:249:LYS:C	2.34	0.53
3:M:197:PHE:HZ	5:M:1304:BCL:CBB	2.20	0.52
1:H:248:ARG:HA	1:H:249:LYS:O	2.10	0.52
3:M:270:ILE:O	3:M:274:VAL:HG13	2.10	0.51
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.92	0.51
5:L:1282:BCL:HHC	5:L:1282:BCL:CBB	2.41	0.51
1:H:132:LYS:HD2	1:H:171:ILE:CD1	2.41	0.51
3:M:157:TRP:HB2	5:M:1304:BCL:H71	1.93	0.51
1:H:89:ARG:NH1	1:H:91:ALA:O	2.45	0.50
3:M:55:LEU:HD22	3:M:128:SER:HB2	1.93	0.50
5:M:1304:BCL:HHC	5:M:1304:BCL:CBB	2.41	0.49
1:H:87:LEU:HD23	1:H:100:PRO:HA	1.95	0.49
5:M:1303:BCL:HBB2	13:M:1315:SPO:H243	1.95	0.48
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.96	0.48
7:L:1285:BPH:ND	3:M:214:LEU:HD13	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:129:TRP:O	3:M:132:ARG:HB3	2.15	0.47
8:L:1286[A]:UQ2:H152	6:M:1309:LDA:H91	1.96	0.47
1:H:20:PHE:CD2	1:H:20:PHE:C	2.93	0.47
5:M:1303:BCL:HHC	5:M:1303:BCL:CBB	2.45	0.47
2:L:225:GLY:O	8:L:1286[B]:UQ2:O1	2.33	0.47
3:M:226:VAL:HG23	3:M:231:GLY:HA3	1.97	0.47
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.96	0.46
3:M:199:ASN:HD21	3:M:201:PHE:HB2	1.80	0.46
3:M:62:SER:OG	3:M:124:VAL:HG22	2.16	0.46
3:M:199:ASN:C	3:M:199:ASN:ND2	2.68	0.46
6:M:1307:LDA:H52	6:M:1308:LDA:H42	1.98	0.46
3:M:199:ASN:HD22	3:M:200:PRO:N	2.13	0.46
7:L:1285:BPH:HBB3	7:L:1285:BPH:CHC	2.34	0.45
3:M:55:LEU:HD12	3:M:135:LEU:HD12	1.97	0.45
3:M:161:GLY:HA3	13:M:1315:SPO:H26	1.99	0.45
1:H:194:GLN:HA	3:M:3:TYR:CD2	2.50	0.45
2:L:128:TYR:HD1	5:L:1282:BCL:HBB1	1.82	0.45
1:H:220[B]:LYS:HG2	1:H:221:SER:N	2.32	0.45
7:M:1313:BPH:H7C2	7:M:1313:BPH:H112	1.78	0.45
2:L:83:GLY:O	2:L:87:GLN:HG3	2.17	0.45
7:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.52	0.45
12:M:1314:U10:H301	12:M:1314:U10:H321	1.80	0.44
2:L:262:TRP:O	2:L:265:TRP:HD1	2.00	0.44
6:M:1307:LDA:H22	6:M:1307:LDA:HM11	1.68	0.44
5:M:1304:BCL:CBB	5:M:1304:BCL:CHC	2.95	0.44
3:M:189:PHE:O	3:M:193:HIS:CD2	2.69	0.43
7:M:1313:BPH:CBB	7:M:1313:BPH:CHC	2.96	0.43
8:L:1286[B]:UQ2:H3M1	15:M:2117:HOH:O	2.11	0.43
5:M:1303:BCL:CBB	13:M:1315:SPO:H243	2.48	0.43
1:H:108:GLY:O	1:H:113:SER:HA	2.19	0.43
2:L:157:VAL:HG21	5:L:1282:BCL:HHD	1.99	0.43
7:L:1285:BPH:CBB	7:L:1285:BPH:CHC	2.96	0.43
3:M:129:TRP:CD1	7:M:1313:BPH:HBA1	2.53	0.43
3:M:251:PHE:CD1	3:M:251:PHE:C	2.97	0.43
5:M:1303:BCL:HBB3	5:M:1304:BCL:C4	2.44	0.43
5:L:1282:BCL:HMD2	3:M:206:ILE:HD13	2.00	0.42
8:L:1286[A]:UQ2:H121	8:L:1286[A]:UQ2:H101	1.23	0.42
1:H:25:ALA:HB1	4:H:1251:GOL:H12	2.00	0.42
3:M:258:PHE:CG	6:M:1307:LDA:H51	2.54	0.42
13:M:1315:SPO:H20	13:M:1315:SPO:H181	1.94	0.42
1:H:112:ALA:HA	1:H:235:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:ASP:HB2	1:H:177:ARG:HG3	2.02	0.42
3:M:237:GLN:HB2	3:M:262:MET:HG2	2.01	0.41
3:M:194:GLY:O	3:M:195:ASN:HB3	2.20	0.41
1:H:148:PRO:HD2	1:H:167:ILE:HD11	2.03	0.41
2:L:91:ILE:CG1	10:L:1289:HTO:H41	2.49	0.41
5:M:1304:BCL:HAA2	5:M:1304:BCL:HBD	2.01	0.41
1:H:177:ARG:CZ	3:M:233:ARG:HD2	2.51	0.41
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.03	0.41
1:H:245:ALA:N	1:H:246:PRO:HD2	2.36	0.41
1:H:135:LYS:HB3	1:H:135:LYS:HE3	1.93	0.41
2:L:60:ASN:HA	2:L:61:PRO:HD3	1.90	0.41
2:L:44:LEU:HD13	2:L:92:CYS:SG	2.62	0.40
5:L:1282:BCL:H93	5:L:1282:BCL:H62	1.95	0.40
5:M:1303:BCL:CBB	5:M:1303:BCL:CHC	3.00	0.40
5:L:1282:BCL:HBB3	5:L:1287:BCL:H41	2.02	0.40
3:M:258:PHE:CB	6:M:1307:LDA:H32	2.51	0.40
1:H:20:PHE:CE2	3:M:204:LEU:HD13	2.57	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%)	235 (97%)	7 (3%)	0	100	100
2	L	279/281 (99%)	269 (96%)	9 (3%)	1 (0%)	30	31
3	M	301/307 (98%)	288 (96%)	12 (4%)	1 (0%)	36	40
All	All	822/848 (97%)	792 (96%)	28 (3%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	302	GLY
2	L	31	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%)	191 (96%)	7 (4%)	32	39
2	L	220/220 (100%)	208 (94%)	12 (6%)	19	20
3	M	236/240 (98%)	220 (93%)	16 (7%)	14	14
All	All	654/668 (98%)	619 (95%)	35 (5%)	21	21

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	72	THR
1	H	92	VAL
1	H	184	LYS
1	H	220[A]	LYS
1	H	220[B]	LYS
1	H	221	SER
1	H	231	ASP
2	L	16	LEU
2	L	21	LEU
2	L	44	LEU
2	L	80	LEU
2	L	102	LEU
2	L	126	LEU
2	L	129	LEU
2	L	170	ASN
2	L	207	ARG
2	L	246	LEU
2	L	247	CYS
2	L	249	ILE
3	M	2	GLU
3	M	13	ARG

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Mol	Chain	Res	Type
3	M	32	VAL
3	M	39	LEU
3	M	52	LEU
3	M	55	LEU
3	M	124	VAL
3	M	148	TRP
3	M	151	LEU
3	M	182	HIS
3	M	191	LEU
3	M	192	VAL
3	M	199	ASN
3	M	216	PHE
3	M	274	VAL
3	M	292	ASP

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

Mol	Chain	Res	Type
1	H	98	HIS
1	H	206	ASN
2	L	62	GLN
2	L	159	ASN
2	L	170	ASN
2	L	258	GLN
2	L	264	GLN
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN

5.3.3 RNA ⓘ

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$
6	LDA	M	1306	-	13,15,15	2.22	2 (15%)	14,17,17	0.58	0
10	HTO	L	1289	-	9,9,9	0.42	0	10,10,10	0.54	0
6	LDA	L	1283	-	13,15,15	2.14	2 (15%)	14,17,17	0.62	0
7	BPH	M	1313	-	59,70,70	2.64	12 (20%)	59,101,101	2.39	16 (27%)
5	BCL	M	1304	3	69,74,74	1.82	7 (10%)	79,115,115	1.91	18 (22%)
4	GOL	L	1290	-	5,5,5	0.18	0	5,5,5	0.63	0
9	PO4	L	1288	-	4,4,4	0.91	0	6,6,6	0.50	0
6	LDA	M	1311	-	13,15,15	2.19	2 (15%)	14,17,17	0.61	0
4	GOL	H	1252	-	5,5,5	0.39	0	5,5,5	0.33	0
6	LDA	M	1309	-	13,15,15	2.27	2 (15%)	14,17,17	0.46	0
6	LDA	M	1307	-	13,15,15	2.13	2 (15%)	14,17,17	0.55	0
6	LDA	M	1310	-	13,15,15	2.17	2 (15%)	14,17,17	0.43	0
4	GOL	L	1292	-	5,5,5	0.43	0	5,5,5	0.38	0
8	UQ2	L	1286[B]	-	23,23,23	2.61	10 (43%)	30,31,31	2.31	11 (36%)
7	BPH	L	1285	-	59,70,70	2.82	10 (16%)	59,101,101	2.81	22 (37%)
6	LDA	M	1308	-	13,15,15	2.23	2 (15%)	14,17,17	0.46	0
4	GOL	H	1251	-	5,5,5	0.46	0	5,5,5	0.25	0
10	HTO	L	1904	-	9,9,9	0.36	0	10,10,10	1.07	1 (10%)
12	U10	M	1314	-	48,48,63	2.79	13 (27%)	60,61,79	1.54	13 (21%)
13	SPO	M	1315	-	41,41,41	2.65	12 (29%)	47,50,50	2.42	17 (36%)
8	UQ2	L	1286[A]	-	23,23,23	2.76	8 (34%)	30,31,31	1.38	7 (23%)
14	CDL	M	1316	-	80,80,99	2.05	16 (20%)	86,92,111	2.95	18 (20%)
6	LDA	M	1305	-	13,15,15	2.05	2 (15%)	14,17,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LDA	L	1284	-	13,15,15	2.10	2 (15%)	14,17,17	0.47	0
4	GOL	H	1253	-	5,5,5	0.38	0	5,5,5	0.24	0
5	BCL	L	1282	2	69,74,74	1.77	7 (10%)	79,115,115	2.01	21 (26%)
5	BCL	L	1287	2	69,74,74	1.85	8 (11%)	79,115,115	1.85	20 (25%)
5	BCL	M	1303	3	69,74,74	1.83	8 (11%)	79,115,115	1.90	19 (24%)
4	GOL	L	1291	-	5,5,5	0.43	0	5,5,5	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1306	-	-	6/13/13/13	-
10	HTO	L	1289	-	-	6/10/10/10	-
6	LDA	L	1283	-	-	7/13/13/13	-
7	BPH	M	1313	-	-	13/37/105/105	0/5/6/6
5	BCL	M	1304	3	2/2/21/25	3/41/137/137	-
4	GOL	L	1290	-	-	2/4/4/4	-
6	LDA	M	1311	-	-	5/13/13/13	-
4	GOL	H	1252	-	-	2/4/4/4	-
6	LDA	M	1309	-	-	9/13/13/13	-
6	LDA	M	1307	-	-	9/13/13/13	-
6	LDA	M	1310	-	-	6/13/13/13	-
4	GOL	L	1292	-	-	4/4/4/4	-
8	UQ2	L	1286[B]	-	-	7/15/39/39	0/1/1/1
7	BPH	L	1285	-	-	5/37/105/105	0/5/6/6
6	LDA	M	1308	-	-	5/13/13/13	-
4	GOL	H	1251	-	-	2/4/4/4	-
10	HTO	L	1904	-	-	7/10/10/10	-
12	U10	M	1314	-	-	9/45/69/87	0/1/1/1
13	SPO	M	1315	-	-	8/47/47/47	-
8	UQ2	L	1286[A]	-	-	9/15/39/39	0/1/1/1
14	CDL	M	1316	-	-	43/91/91/110	-
6	LDA	M	1305	-	-	5/13/13/13	-
6	LDA	L	1284	-	-	8/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	1282	2	2/2/21/25	10/41/137/137	-
4	GOL	H	1253	-	-	3/4/4/4	-
5	BCL	L	1287	2	2/2/21/25	12/41/137/137	-
5	BCL	M	1303	3	2/2/21/25	16/41/137/137	-
4	GOL	L	1291	-	-	2/4/4/4	-

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1285	BPH	OBD-CAD	12.52	1.38	1.22
7	M	1313	BPH	OBD-CAD	11.20	1.37	1.22
5	L	1287	BCL	OBD-CAD	10.47	1.40	1.22
5	M	1303	BCL	OBD-CAD	10.15	1.39	1.22
5	M	1304	BCL	OBD-CAD	10.06	1.39	1.22
5	L	1282	BCL	OBD-CAD	9.52	1.38	1.22
7	L	1285	BPH	OBG-CAB	7.99	1.46	1.22
8	L	1286[A]	UQ2	C8-C9	7.46	1.50	1.33
7	L	1285	BPH	O1D-CGD	7.29	1.39	1.21
7	M	1313	BPH	O1D-CGD	7.16	1.39	1.21
7	M	1313	BPH	OBG-CAB	7.06	1.43	1.22
12	M	1314	U10	C28-C29	6.97	1.49	1.33
6	M	1311	LDA	O1-N1	-6.79	1.25	1.42
6	M	1308	LDA	O1-N1	-6.77	1.25	1.42
6	M	1309	LDA	O1-N1	-6.77	1.25	1.42
7	M	1313	BPH	C2-C3	6.73	1.48	1.33
13	M	1315	SPO	C32-C33	6.69	1.48	1.33
12	M	1314	U10	C33-C34	6.67	1.48	1.33
6	M	1306	LDA	O1-N1	-6.65	1.25	1.42
6	M	1310	LDA	O1-N1	-6.63	1.25	1.42
12	M	1314	U10	C18-C19	6.61	1.48	1.33
6	M	1305	LDA	O1-N1	-6.55	1.26	1.42
12	M	1314	U10	C23-C24	6.54	1.48	1.33
7	L	1285	BPH	C2-C3	6.51	1.48	1.33
6	L	1284	LDA	O1-N1	-6.48	1.26	1.42
7	L	1285	BPH	O1A-CGA	6.43	1.41	1.22
12	M	1314	U10	C8-C9	6.41	1.47	1.33
6	L	1283	LDA	O1-N1	-6.40	1.26	1.42
5	M	1304	BCL	O1A-CGA	6.39	1.41	1.22
6	M	1307	LDA	O1-N1	-6.34	1.26	1.42
12	M	1314	U10	C13-C14	6.28	1.47	1.33
8	L	1286[B]	UQ2	C8-C9	6.05	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	1316	CDL	C32-C31	-6.00	1.30	1.52
5	L	1287	BCL	O1A-CGA	5.94	1.40	1.22
13	M	1315	SPO	C37-C38	5.89	1.50	1.32
7	L	1285	BPH	C3D-C2D	5.78	1.49	1.39
7	M	1313	BPH	O1A-CGA	5.58	1.39	1.22
5	L	1282	BCL	O1A-CGA	5.58	1.39	1.22
5	M	1303	BCL	O1A-CGA	5.56	1.39	1.22
14	M	1316	CDL	C11-CA5	-5.42	1.35	1.50
14	M	1316	CDL	C33-C32	-5.40	1.24	1.51
8	L	1286[A]	UQ2	O3-C3	-5.35	1.23	1.36
13	M	1315	SPO	C9-C7	5.33	1.48	1.35
12	M	1314	U10	C38-C39	5.32	1.48	1.32
14	M	1316	CDL	C34-C33	-5.31	1.25	1.51
7	M	1313	BPH	C3D-C2D	5.10	1.48	1.39
8	L	1286[A]	UQ2	C13-C14	5.07	1.47	1.32
13	M	1315	SPO	C14-C12	5.00	1.47	1.35
8	L	1286[B]	UQ2	C13-C14	4.95	1.47	1.32
13	M	1315	SPO	C22-C23	4.91	1.47	1.35
13	M	1315	SPO	C6-C5	4.83	1.45	1.32
14	M	1316	CDL	OA6-CA5	4.78	1.47	1.34
14	M	1316	CDL	OA8-CA7	4.78	1.47	1.33
14	M	1316	CDL	OB6-CB5	4.69	1.47	1.34
7	M	1313	BPH	C3D-CAD	-4.65	1.38	1.47
14	M	1316	CDL	C13-C12	-4.61	1.28	1.51
13	M	1315	SPO	C19-C17	4.59	1.46	1.35
7	L	1285	BPH	C3D-CAD	-4.58	1.39	1.47
8	L	1286[A]	UQ2	O2-C2	-4.58	1.25	1.36
8	L	1286[B]	UQ2	O2-C2	-4.57	1.25	1.36
6	M	1309	LDA	C1-N1	-4.47	1.46	1.51
14	M	1316	CDL	C20-C19	-4.46	1.29	1.51
12	M	1314	U10	O3-C3	-4.44	1.26	1.36
13	M	1315	SPO	C10-C11	4.33	1.46	1.34
13	M	1315	SPO	C26-C25	4.30	1.45	1.34
8	L	1286[B]	UQ2	O3-C3	-4.30	1.26	1.36
6	M	1306	LDA	C1-N1	-4.29	1.47	1.51
14	M	1316	CDL	OB8-CB7	4.25	1.45	1.33
6	M	1308	LDA	C1-N1	-4.22	1.47	1.51
6	M	1307	LDA	C1-N1	-4.22	1.47	1.51
6	L	1283	LDA	C1-N1	-4.21	1.47	1.51
8	L	1286[A]	UQ2	C6-C5	4.15	1.42	1.35
12	M	1314	U10	O4-C4	-4.11	1.26	1.36
5	L	1282	BCL	C3D-C4D	-4.03	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	1315	SPO	C15-C16	4.01	1.45	1.34
6	M	1310	LDA	C1-N1	-3.95	1.47	1.51
6	M	1311	LDA	C1-N1	-3.90	1.47	1.51
6	L	1284	LDA	C1-N1	-3.73	1.47	1.51
5	L	1287	BCL	C3D-C4D	-3.67	1.35	1.44
5	M	1303	BCL	C2-C3	3.64	1.41	1.33
12	M	1314	U10	C6-C1	3.63	1.41	1.35
5	M	1303	BCL	C3D-C4D	-3.58	1.36	1.44
7	M	1313	BPH	O2D-CGD	-3.57	1.24	1.33
7	L	1285	BPH	C3D-C4D	-3.57	1.36	1.41
14	M	1316	CDL	C37-C36	-3.56	1.34	1.51
14	M	1316	CDL	C79-C78	-3.54	1.34	1.51
5	L	1287	BCL	C2-C3	3.50	1.41	1.33
5	M	1304	BCL	C2-C3	3.48	1.41	1.33
5	M	1304	BCL	C3D-C4D	-3.48	1.36	1.44
13	M	1315	SPO	C27-C28	3.47	1.46	1.35
14	M	1316	CDL	C80-C79	-3.43	1.34	1.51
14	M	1316	CDL	C22-C21	-3.38	1.35	1.51
13	M	1315	SPO	C21-C20	3.37	1.45	1.36
8	L	1286[B]	UQ2	C6-C1	-3.20	1.37	1.46
5	L	1287	BCL	O2D-CGD	-3.14	1.25	1.33
8	L	1286[B]	UQ2	C2-C1	-3.13	1.39	1.48
7	M	1313	BPH	CBD-CGD	-3.10	1.48	1.52
5	L	1282	BCL	O2D-CGD	-3.08	1.25	1.33
5	M	1303	BCL	C1D-C2D	-3.05	1.39	1.45
5	L	1282	BCL	C2-C3	3.03	1.40	1.33
14	M	1316	CDL	C19-C18	-2.98	1.36	1.51
8	L	1286[B]	UQ2	C3-C4	-2.96	1.40	1.48
7	M	1313	BPH	C3D-C4D	-2.87	1.37	1.41
6	M	1305	LDA	C1-N1	-2.82	1.48	1.51
7	L	1285	BPH	O2D-CGD	-2.77	1.26	1.33
7	M	1313	BPH	O2A-CGA	-2.74	1.25	1.33
5	L	1282	BCL	O2A-CGA	-2.72	1.25	1.33
8	L	1286[B]	UQ2	C5-C4	-2.65	1.38	1.47
5	M	1303	BCL	O2D-CGD	-2.63	1.26	1.33
14	M	1316	CDL	C17-C16	-2.62	1.38	1.51
5	L	1287	BCL	CHD-C4C	2.51	1.46	1.39
12	M	1314	U10	C4-C5	-2.50	1.41	1.48
5	M	1304	BCL	O2D-CGD	-2.47	1.27	1.33
5	M	1303	BCL	MG-ND	-2.41	2.01	2.05
8	L	1286[B]	UQ2	O3-CM3	-2.33	1.40	1.45
8	L	1286[A]	UQ2	C3-C4	-2.31	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	CHD-C4C	2.31	1.45	1.39
5	L	1287	BCL	C1D-C2D	-2.30	1.40	1.45
8	L	1286[A]	UQ2	O2-CM2	-2.30	1.40	1.45
5	M	1303	BCL	O1D-CGD	2.29	1.27	1.21
12	M	1314	U10	C3-C2	-2.26	1.42	1.48
5	L	1282	BCL	C1D-C2D	-2.24	1.40	1.45
8	L	1286[A]	UQ2	C2-C1	-2.18	1.42	1.48
5	L	1287	BCL	O2A-CGA	-2.17	1.27	1.33
7	M	1313	BPH	C2C-C3C	-2.11	1.52	1.54
7	L	1285	BPH	C4D-ND	-2.04	1.35	1.38
8	L	1286[B]	UQ2	C6-C5	2.03	1.38	1.35
12	M	1314	U10	C1-C2	-2.03	1.40	1.47
5	M	1304	BCL	OBB-CAB	2.01	1.27	1.23

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1316	CDL	C33-C32-C31	16.95	175.40	113.13
14	M	1316	CDL	C12-C11-CA5	10.60	152.53	113.69
7	L	1285	BPH	O2D-CGD-CBD	9.72	121.63	110.95
7	M	1313	BPH	O2D-CGD-CBD	8.59	120.38	110.95
14	M	1316	CDL	C35-C34-C33	8.48	157.24	114.37
7	L	1285	BPH	C2B-C1B-NB	7.78	115.05	109.43
7	M	1313	BPH	OBD-CAD-CBD	-7.22	115.22	125.82
7	L	1285	BPH	C2D-C1D-ND	6.63	114.22	109.43
14	M	1316	CDL	C20-C19-C18	6.58	147.62	114.37
5	L	1282	BCL	C1D-ND-C4D	6.54	110.90	106.31
7	M	1313	BPH	C2B-C1B-NB	6.35	114.02	109.43
5	M	1304	BCL	C1D-ND-C4D	6.31	110.74	106.31
14	M	1316	CDL	C34-C33-C32	6.29	146.15	114.37
8	L	1286[B]	UQ2	O1-C1-C6	-6.18	109.83	121.79
14	M	1316	CDL	C17-C16-C15	6.11	145.25	114.37
7	L	1285	BPH	OBD-CAD-C3D	-5.98	118.56	127.89
5	M	1303	BCL	C1D-ND-C4D	5.92	110.47	106.31
7	L	1285	BPH	CED-O2D-CGD	5.82	129.12	115.92
5	M	1303	BCL	O2D-CGD-CBD	5.74	121.27	111.23
13	M	1315	SPO	C21-C22-C23	-5.71	119.27	127.28
5	M	1304	BCL	C1C-NC-C4C	5.65	109.26	106.68
14	M	1316	CDL	C13-C12-C11	5.51	133.39	113.13
5	L	1282	BCL	O2D-CGD-CBD	5.49	120.83	111.23
13	M	1315	SPO	C10-C9-C7	-5.45	119.64	127.28
13	M	1315	SPO	C20-C19-C17	-5.39	119.71	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1303	BCL	C1-O2A-CGA	5.17	129.17	116.65
5	L	1287	BCL	C1D-ND-C4D	5.11	109.90	106.31
5	L	1287	BCL	CMB-C2B-C1B	-5.00	117.80	125.42
5	L	1282	BCL	C2D-C1D-ND	-4.94	105.24	110.13
13	M	1315	SPO	C4-C5-C6	-4.89	118.04	124.91
7	M	1313	BPH	C3D-C4D-ND	4.77	113.82	107.71
5	M	1303	BCL	C4A-NA-C1A	4.75	108.85	106.68
7	M	1313	BPH	OBD-CAD-C3D	-4.73	120.52	127.89
14	M	1316	CDL	OA6-CA5-C11	4.69	121.62	111.48
5	M	1304	BCL	C2D-C1D-ND	-4.68	105.50	110.13
7	L	1285	BPH	C1B-NB-C4B	-4.61	102.09	108.82
5	M	1303	BCL	CMB-C2B-C1B	-4.54	118.51	125.42
8	L	1286[B]	UQ2	C7-C6-C5	-4.52	117.14	124.89
13	M	1315	SPO	C29-C28-C30	4.47	122.99	115.23
5	L	1282	BCL	CMB-C2B-C1B	-4.44	118.66	125.42
7	L	1285	BPH	O1D-CGD-CBD	-4.36	118.11	124.72
7	L	1285	BPH	C3D-C4D-ND	4.31	113.23	107.71
5	M	1304	BCL	CMB-C2B-C1B	-4.22	119.00	125.42
13	M	1315	SPO	C15-C14-C12	-4.15	121.45	127.28
5	L	1282	BCL	CMD-C2D-C1D	4.14	132.02	124.73
5	L	1282	BCL	C1C-NC-C4C	4.14	108.57	106.68
5	L	1287	BCL	CMD-C2D-C1D	4.09	131.94	124.73
5	L	1287	BCL	C1C-NC-C4C	-4.07	104.82	106.68
8	L	1286[B]	UQ2	O1-C1-C2	-4.01	112.53	121.03
5	L	1282	BCL	C1-C2-C3	-3.85	119.88	126.20
5	L	1287	BCL	C2D-C1D-ND	-3.82	106.34	110.13
14	M	1316	CDL	OB6-CB5-C51	3.78	119.67	111.48
7	L	1285	BPH	C4D-ND-C1D	-3.76	104.37	108.87
5	M	1304	BCL	O2D-CGD-CBD	3.73	117.76	111.23
12	M	1314	U10	C10-C9-C11	3.73	121.70	115.23
12	M	1314	U10	C15-C14-C16	3.69	121.64	115.23
7	L	1285	BPH	CMA-C3A-C4A	-3.64	106.76	114.61
5	M	1304	BCL	CED-O2D-CGD	3.64	124.17	115.92
13	M	1315	SPO	C26-C27-C28	-3.58	122.65	127.69
5	M	1304	BCL	O2A-CGA-CBA	3.57	122.73	111.83
8	L	1286[B]	UQ2	C10-C9-C11	3.57	121.42	115.23
5	M	1303	BCL	C2D-C1D-ND	-3.54	106.62	110.13
5	L	1287	BCL	C1-O2A-CGA	3.54	125.21	116.65
5	M	1303	BCL	O2A-CGA-CBA	3.49	122.49	111.83
5	L	1287	BCL	CMA-C3A-C4A	-3.45	102.50	111.77
7	M	1313	BPH	C1-O2A-CGA	3.45	125.00	116.65
7	M	1313	BPH	O1D-CGD-CBD	-3.43	119.53	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	1315	SPO	C34-C33-C35	3.36	121.06	115.23
5	L	1287	BCL	C4A-NA-C1A	3.34	108.20	106.68
5	M	1303	BCL	O2D-CGD-O1D	-3.34	117.35	123.85
5	M	1304	BCL	CMD-C2D-C1D	3.32	130.57	124.73
5	L	1282	BCL	C1D-CHD-C4C	-3.32	118.62	126.62
5	L	1287	BCL	O2A-CGA-CBA	3.26	121.79	111.83
13	M	1315	SPO	C13-C12-C11	3.23	123.02	118.09
5	M	1304	BCL	CHC-C1C-NC	-3.22	119.75	124.40
12	M	1314	U10	C30-C29-C31	3.13	120.66	115.23
5	L	1287	BCL	C3C-C4C-CHD	-3.09	116.88	123.39
5	L	1282	BCL	O1D-CGD-CBD	-3.07	118.45	124.52
5	L	1287	BCL	C1D-CHD-C4C	-3.02	119.33	126.62
7	M	1313	BPH	C4D-ND-C1D	-3.02	105.25	108.87
5	L	1282	BCL	O2A-CGA-CBA	3.01	121.02	111.83
8	L	1286[B]	UQ2	CM5-C5-C6	-3.01	119.50	124.45
7	L	1285	BPH	OBD-CAD-CBD	-2.99	121.43	125.82
7	L	1285	BPH	C1C-C2C-C3C	-2.99	99.99	102.84
13	M	1315	SPO	C5-C6-C7	-2.97	121.41	125.89
7	M	1313	BPH	C1B-NB-C4B	-2.94	104.53	108.82
8	L	1286[B]	UQ2	C7-C6-C1	-2.94	115.10	118.52
12	M	1314	U10	C7-C6-C1	-2.94	119.86	124.89
14	M	1316	CDL	OA8-CA7-C31	2.93	120.78	111.83
13	M	1315	SPO	C21-C20-C19	-2.93	117.52	123.52
5	M	1303	BCL	C2B-C1B-NB	-2.92	107.30	110.33
12	M	1314	U10	C22-C23-C24	-2.91	120.96	127.62
14	M	1316	CDL	OA6-CA5-OA7	-2.91	116.91	123.70
5	L	1287	BCL	O2D-CGD-CBD	2.87	116.25	111.23
7	L	1285	BPH	OBB-CAB-C3B	2.85	124.75	119.99
7	L	1285	BPH	C4C-C3C-C2C	-2.83	100.15	102.84
5	M	1303	BCL	CMD-C2D-C1D	2.82	129.69	124.73
5	L	1287	BCL	O2A-CGA-O1A	-2.82	116.59	123.63
13	M	1315	SPO	C27-C26-C25	-2.81	115.05	123.20
7	L	1285	BPH	C3B-C4B-NB	2.81	112.14	108.05
8	L	1286[B]	UQ2	O4-C4-C5	-2.81	112.88	120.73
5	L	1282	BCL	CMD-C2D-C3D	-2.80	121.27	127.69
5	M	1303	BCL	C3C-C4C-CHD	-2.80	117.49	123.39
13	M	1315	SPO	C14-C15-C16	-2.79	115.12	123.20
8	L	1286[A]	UQ2	C7-C6-C5	-2.75	120.17	124.89
7	M	1313	BPH	O2A-CGA-CBA	2.75	120.23	111.83
14	M	1316	CDL	OB8-CB7-C71	2.74	120.19	111.83
5	L	1282	BCL	C2A-C3A-C4A	2.74	106.29	101.87
7	M	1313	BPH	CED-O2D-CGD	2.72	122.08	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1282	BCL	C4-C3-C5	2.70	119.91	115.23
12	M	1314	U10	C17-C18-C19	-2.68	121.50	127.62
5	L	1287	BCL	CHB-C4A-NA	-2.67	120.55	124.40
7	M	1313	BPH	C1-C2-C3	-2.63	121.88	126.20
5	M	1303	BCL	CMA-C3A-C4A	-2.63	104.70	111.77
5	M	1303	BCL	C1D-CHD-C4C	-2.63	120.28	126.62
7	M	1313	BPH	CMB-C2B-C3B	2.62	129.92	124.68
5	L	1287	BCL	CMD-C2D-C3D	-2.61	121.71	127.69
7	L	1285	BPH	C1-C2-C3	-2.58	121.96	126.20
5	L	1282	BCL	C2B-C1B-NB	-2.57	107.66	110.33
8	L	1286[B]	UQ2	C7-C8-C9	-2.57	122.41	126.83
12	M	1314	U10	C12-C13-C14	-2.56	121.75	127.62
13	M	1315	SPO	C20-C21-C22	-2.56	118.29	123.52
7	L	1285	BPH	C7-C6-C5	-2.54	106.48	113.26
5	L	1282	BCL	C4A-NA-C1A	2.47	107.81	106.68
5	M	1304	BCL	CAC-C3C-C4C	-2.47	107.10	112.58
5	L	1282	BCL	C6-C5-C3	-2.45	107.49	113.47
5	L	1287	BCL	CMB-C2B-C3B	2.44	133.38	125.67
7	L	1285	BPH	CMD-C2D-C3D	-2.44	119.81	124.68
5	M	1304	BCL	C3C-C4C-CHD	-2.42	118.29	123.39
12	M	1314	U10	C25-C24-C26	2.41	119.41	115.23
13	M	1315	SPO	C18-C17-C16	2.39	121.73	118.09
7	L	1285	BPH	C1-O2A-CGA	2.37	122.39	116.65
5	M	1303	BCL	CMB-C2B-C3B	2.36	133.12	125.67
13	M	1315	SPO	C24-C23-C25	2.36	121.69	118.09
5	L	1282	BCL	CHA-C1A-NA	-2.36	121.05	126.39
5	M	1303	BCL	CAA-C2A-C3A	-2.36	106.64	113.00
7	M	1313	BPH	C2D-C1D-ND	2.35	111.13	109.43
5	M	1304	BCL	C16-C15-C13	-2.33	108.21	115.97
5	L	1282	BCL	CMA-C3A-C2A	-2.32	105.02	113.98
8	L	1286[A]	UQ2	CM2-O2-C2	2.31	124.59	116.47
14	M	1316	CDL	C22-C21-C20	2.30	126.00	114.37
8	L	1286[A]	UQ2	C16-C14-C15	2.28	119.83	114.59
8	L	1286[A]	UQ2	C6-C5-C4	2.27	120.96	119.17
5	M	1304	BCL	CMD-C2D-C3D	-2.27	122.48	127.69
5	L	1282	BCL	C3C-C4C-CHD	-2.27	118.61	123.39
12	M	1314	U10	C20-C19-C21	2.26	119.16	115.23
5	L	1287	BCL	CHA-C1A-NA	-2.25	121.29	126.39
7	L	1285	BPH	O2A-CGA-CBA	2.25	118.70	111.83
8	L	1286[B]	UQ2	C8-C7-C6	-2.25	106.54	112.08
5	L	1287	BCL	O2D-CGD-O1D	-2.24	119.49	123.85
7	L	1285	BPH	CBB-CAB-C3B	-2.23	113.65	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1304	BCL	C2B-C1B-NB	-2.23	108.01	110.33
5	M	1303	BCL	C2A-C3A-C4A	2.23	105.47	101.87
5	M	1304	BCL	C7-C6-C5	-2.22	107.34	113.26
12	M	1314	U10	C41-C39-C40	2.22	119.69	114.59
12	M	1314	U10	C35-C34-C36	2.22	119.07	115.23
14	M	1316	CDL	OB8-CB7-OB9	-2.21	118.09	123.63
8	L	1286[B]	UQ2	C16-C14-C15	2.21	119.67	114.59
5	M	1303	BCL	O2A-C1-C2	2.21	116.60	108.11
7	L	1285	BPH	CMC-C2C-C1C	-2.19	109.89	114.61
5	L	1287	BCL	C2A-C3A-C4A	2.19	105.41	101.87
5	M	1304	BCL	CBB-CAB-C3B	-2.18	115.81	120.40
5	M	1303	BCL	O2A-CGA-O1A	-2.17	118.19	123.63
14	M	1316	CDL	C32-C31-CA7	2.17	121.65	113.69
8	L	1286[B]	UQ2	C3-C4-C5	2.17	122.39	118.10
5	M	1304	BCL	CHA-C1A-NA	-2.16	121.49	126.39
5	L	1282	BCL	CMA-C3A-C4A	-2.16	105.96	111.77
13	M	1315	SPO	C25-C23-C22	-2.16	115.62	119.01
7	M	1313	BPH	OB8-CAB-C3B	2.15	123.59	119.99
12	M	1314	U10	C30-C29-C28	-2.15	118.11	123.63
5	M	1303	BCL	CHC-C4B-C3B	-2.14	123.22	131.72
10	L	1904	HTO	C5-C4-C3	-2.14	110.61	114.11
5	M	1304	BCL	CMB-C2B-C3B	2.12	132.37	125.67
8	L	1286[A]	UQ2	O2-C2-C3	-2.12	115.61	123.64
5	L	1282	BCL	CMB-C2B-C3B	2.11	132.33	125.67
14	M	1316	CDL	OA8-CA7-OA9	-2.08	118.42	123.63
14	M	1316	CDL	C80-C79-C78	2.07	124.85	114.37
12	M	1314	U10	C32-C33-C34	-2.07	122.88	127.62
8	L	1286[A]	UQ2	C7-C6-C1	2.06	120.91	118.52
7	M	1313	BPH	CMD-C2D-C3D	-2.05	120.59	124.68
8	L	1286[A]	UQ2	O1-C1-C2	-2.03	116.72	121.03
5	L	1287	BCL	CBA-CAA-C2A	2.01	119.76	113.79
14	M	1316	CDL	C81-C80-C79	2.00	124.49	114.37

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	L	1287	BCL	C8
5	L	1287	BCL	C13
5	M	1303	BCL	C8
5	M	1303	BCL	C13

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Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C8
5	M	1304	BCL	C13

All (223) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1251	GOL	O1-C1-C2-C3
4	H	1252	GOL	C1-C2-C3-O3
4	H	1253	GOL	O1-C1-C2-C3
4	L	1290	GOL	C1-C2-C3-O3
4	L	1290	GOL	O2-C2-C3-O3
4	L	1291	GOL	C1-C2-C3-O3
4	L	1292	GOL	O1-C1-C2-C3
4	L	1292	GOL	C1-C2-C3-O3
5	L	1287	BCL	C11-C12-C13-C14
5	M	1303	BCL	C1-C2-C3-C5
6	M	1305	LDA	C2-C1-N1-O1
6	M	1305	LDA	C2-C1-N1-CM1
6	M	1305	LDA	C2-C1-N1-CM2
6	M	1309	LDA	C2-C1-N1-CM1
8	L	1286[A]	UQ2	C9-C11-C12-C13
8	L	1286[A]	UQ2	C12-C13-C14-C15
8	L	1286[A]	UQ2	C12-C13-C14-C16
8	L	1286[B]	UQ2	C7-C8-C9-C10
8	L	1286[B]	UQ2	C7-C8-C9-C11
8	L	1286[B]	UQ2	C12-C13-C14-C15
10	L	1289	HTO	C1-C2-C3-O3
10	L	1289	HTO	C1-C2-C3-C4
10	L	1289	HTO	O2-C2-C3-O3
10	L	1289	HTO	O2-C2-C3-C4
10	L	1904	HTO	C1-C2-C3-O3
10	L	1904	HTO	C1-C2-C3-C4
10	L	1904	HTO	O2-C2-C3-C4
12	M	1314	U10	C27-C28-C29-C30
12	M	1314	U10	C27-C28-C29-C31
12	M	1314	U10	C28-C29-C31-C32
12	M	1314	U10	C30-C29-C31-C32
12	M	1314	U10	C32-C33-C34-C35
12	M	1314	U10	C32-C33-C34-C36
13	M	1315	SPO	C26-C27-C28-C29
13	M	1315	SPO	C36-C37-C38-C40
14	M	1316	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
14	M	1316	CDL	CA2-OA2-PA1-OA5
14	M	1316	CDL	CA3-OA5-PA1-OA3
14	M	1316	CDL	C11-CA5-OA6-CA4
14	M	1316	CDL	OA9-CA7-OA8-CA6
14	M	1316	CDL	OB9-CB7-OB8-CB6
8	L	1286[B]	UQ2	C12-C13-C14-C16
13	M	1315	SPO	C36-C37-C38-C39
5	M	1303	BCL	C10-C11-C12-C13
14	M	1316	CDL	OA7-CA5-OA6-CA4
5	M	1303	BCL	C3-C5-C6-C7
14	M	1316	CDL	C31-CA7-OA8-CA6
14	M	1316	CDL	C71-CB7-OB8-CB6
8	L	1286[A]	UQ2	C12-C11-C9-C10
10	L	1289	HTO	O1-C1-C2-O2
8	L	1286[A]	UQ2	C7-C8-C9-C10
8	L	1286[A]	UQ2	C7-C8-C9-C11
14	M	1316	CDL	C78-C79-C80-C81
14	M	1316	CDL	C20-C21-C22-C23
5	L	1282	BCL	C3-C5-C6-C7
8	L	1286[A]	UQ2	C12-C11-C9-C8
8	L	1286[B]	UQ2	C9-C11-C12-C13
12	M	1314	U10	C29-C31-C32-C33
12	M	1314	U10	C34-C36-C37-C38
5	L	1282	BCL	C6-C7-C8-C9
5	M	1304	BCL	C11-C10-C8-C9
7	M	1313	BPH	C13-C15-C16-C17
5	M	1303	BCL	C2-C1-O2A-CGA
7	M	1313	BPH	C8-C10-C11-C12
4	H	1252	GOL	O2-C2-C3-O3
5	L	1287	BCL	C11-C10-C8-C7
5	M	1304	BCL	C6-C7-C8-C10
7	M	1313	BPH	C11-C10-C8-C7
10	L	1289	HTO	O1-C1-C2-C3
10	L	1904	HTO	O1-C1-C2-C3
13	M	1315	SPO	C33-C35-C36-C37
5	L	1287	BCL	C13-C15-C16-C17
5	M	1303	BCL	C13-C15-C16-C17
7	M	1313	BPH	C10-C11-C12-C13
5	L	1287	BCL	C15-C16-C17-C18
5	M	1303	BCL	C15-C16-C17-C18
7	M	1313	BPH	C16-C17-C18-C19
14	M	1316	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
6	M	1307	LDA	C4-C5-C6-C7
6	M	1309	LDA	C5-C6-C7-C8
6	M	1311	LDA	C11-C10-C9-C8
6	M	1306	LDA	C7-C8-C9-C10
6	M	1310	LDA	C7-C8-C9-C10
6	M	1311	LDA	C3-C4-C5-C6
4	L	1291	GOL	O2-C2-C3-O3
4	L	1292	GOL	O1-C1-C2-O2
4	L	1292	GOL	O2-C2-C3-O3
14	M	1316	CDL	C52-C53-C54-C55
14	M	1316	CDL	C79-C80-C81-C82
7	M	1313	BPH	C16-C17-C18-C20
14	M	1316	CDL	C74-C75-C76-C77
6	L	1283	LDA	C6-C7-C8-C9
6	L	1284	LDA	C4-C5-C6-C7
14	M	1316	CDL	C71-C72-C73-C74
14	M	1316	CDL	C72-C73-C74-C75
6	L	1283	LDA	C5-C6-C7-C8
6	M	1310	LDA	C3-C4-C5-C6
6	M	1305	LDA	C2-C3-C4-C5
6	L	1284	LDA	C11-C10-C9-C8
6	M	1307	LDA	C3-C4-C5-C6
6	M	1307	LDA	C7-C8-C9-C10
14	M	1316	CDL	C12-C13-C14-C15
6	L	1284	LDA	C3-C4-C5-C6
6	M	1306	LDA	C3-C4-C5-C6
7	L	1285	BPH	C8-C10-C11-C12
14	M	1316	CDL	C36-C37-C38-C39
6	M	1308	LDA	C2-C3-C4-C5
6	M	1309	LDA	C1-C2-C3-C4
6	M	1308	LDA	C1-C2-C3-C4
6	L	1283	LDA	C1-C2-C3-C4
6	M	1310	LDA	C1-C2-C3-C4
5	L	1282	BCL	C5-C6-C7-C8
14	M	1316	CDL	C15-C16-C17-C18
6	M	1308	LDA	C6-C7-C8-C9
5	L	1282	BCL	C13-C15-C16-C17
6	L	1284	LDA	C5-C6-C7-C8
6	M	1309	LDA	C3-C4-C5-C6
4	H	1251	GOL	O1-C1-C2-O2
6	L	1283	LDA	C11-C10-C9-C8
6	M	1306	LDA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
5	M	1303	BCL	C11-C12-C13-C14
7	M	1313	BPH	C11-C10-C8-C9
6	M	1309	LDA	C2-C3-C4-C5
6	M	1310	LDA	C11-C10-C9-C8
6	L	1284	LDA	C1-C2-C3-C4
7	L	1285	BPH	O2A-C1-C2-C3
6	L	1283	LDA	C3-C4-C5-C6
6	M	1308	LDA	C4-C5-C6-C7
5	L	1282	BCL	C16-C17-C18-C19
6	M	1307	LDA	N1-C1-C2-C3
6	M	1310	LDA	C9-C10-C11-C12
14	M	1316	CDL	C18-C19-C20-C21
6	L	1284	LDA	C9-C10-C11-C12
5	L	1287	BCL	C10-C11-C12-C13
5	M	1303	BCL	C8-C10-C11-C12
5	M	1303	BCL	C11-C12-C13-C15
7	M	1313	BPH	C11-C12-C13-C15
6	M	1306	LDA	C1-C2-C3-C4
14	M	1316	CDL	CA3-CA4-CA6-OA8
6	L	1283	LDA	C4-C5-C6-C7
7	L	1285	BPH	C4-C3-C5-C6
13	M	1315	SPO	C9-C10-C11-C12
6	M	1311	LDA	C6-C7-C8-C9
5	L	1282	BCL	C4C-C3C-CAC-CBC
4	H	1253	GOL	O1-C1-C2-O2
5	M	1303	BCL	C4-C3-C5-C6
7	L	1285	BPH	C2-C3-C5-C6
6	M	1309	LDA	C4-C5-C6-C7
5	L	1287	BCL	C11-C12-C13-C15
6	M	1307	LDA	C2-C3-C4-C5
8	L	1286[B]	UQ2	C4-C3-O3-CM3
5	L	1287	BCL	C5-C6-C7-C8
14	M	1316	CDL	CA5-C11-C12-C13
6	M	1308	LDA	C7-C8-C9-C10
6	M	1309	LDA	C2-C1-N1-CM2
14	M	1316	CDL	OA5-CA3-CA4-CA6
7	M	1313	BPH	C12-C13-C15-C16
14	M	1316	CDL	O1-C1-CB2-OB2
6	M	1305	LDA	C4-C5-C6-C7
13	M	1315	SPO	C2-C1-C4-C5
7	M	1313	BPH	C5-C6-C7-C8
5	L	1282	BCL	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
5	L	1287	BCL	C16-C17-C18-C20
14	M	1316	CDL	OA5-CA3-CA4-OA6
6	M	1309	LDA	C2-C1-N1-O1
6	L	1284	LDA	C2-C3-C4-C5
14	M	1316	CDL	OA6-CA4-CA6-OA8
10	L	1904	HTO	O1-C1-C2-O2
5	L	1282	BCL	CHA-CBD-CGD-O1D
5	L	1282	BCL	CHA-CBD-CGD-O2D
13	M	1315	SPO	C26-C27-C28-C30
14	M	1316	CDL	CA2-OA2-PA1-OA4
14	M	1316	CDL	CA3-OA5-PA1-OA2
14	M	1316	CDL	CA3-OA5-PA1-OA4
14	M	1316	CDL	CB2-OB2-PB2-OB3
6	M	1307	LDA	C6-C7-C8-C9
4	H	1253	GOL	C1-C2-C3-O3
7	M	1313	BPH	C15-C16-C17-C18
6	L	1283	LDA	N1-C1-C2-C3
6	L	1284	LDA	N1-C1-C2-C3
6	M	1311	LDA	N1-C1-C2-C3
10	L	1904	HTO	C2-C3-C4-C5
7	M	1313	BPH	C11-C12-C13-C14
5	M	1303	BCL	C11-C10-C8-C7
5	L	1287	BCL	C16-C17-C18-C19
6	M	1306	LDA	C5-C6-C7-C8
5	L	1287	BCL	C2-C1-O2A-CGA
12	M	1314	U10	C5-C4-O4-C4M
14	M	1316	CDL	C17-C18-C19-C20
5	L	1287	BCL	C11-C10-C8-C9
5	M	1303	BCL	C6-C7-C8-C9
5	M	1303	BCL	C1-C2-C3-C4
6	M	1309	LDA	C9-C10-C11-C12
6	M	1307	LDA	C1-C2-C3-C4
5	L	1282	BCL	C11-C12-C13-C15
5	M	1303	BCL	C6-C7-C8-C10
13	M	1315	SPO	C3-C1-C4-C5
14	M	1316	CDL	C34-C35-C36-C37
5	M	1303	BCL	C11-C10-C8-C9
6	M	1310	LDA	C2-C3-C4-C5
8	L	1286[B]	UQ2	C1-C2-O2-CM2
14	M	1316	CDL	CA2-C1-CB2-OB2
7	L	1285	BPH	CHA-CBD-CGD-O1D
5	M	1303	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	M	1307	LDA	C5-C6-C7-C8
14	M	1316	CDL	C81-C82-C83-C84
14	M	1316	CDL	C73-C74-C75-C76
7	M	1313	BPH	C14-C13-C15-C16
14	M	1316	CDL	C52-C51-CB5-OB6
14	M	1316	CDL	C21-C22-C23-C24
14	M	1316	CDL	C38-C39-C40-C41
14	M	1316	CDL	C72-C71-CB7-OB8
5	L	1287	BCL	C2A-CAA-CBA-CGA
6	M	1311	LDA	C4-C5-C6-C7
10	L	1904	HTO	C3-C4-C5-C6
14	M	1316	CDL	C40-C41-C42-C43
8	L	1286[A]	UQ2	C6-C7-C8-C9
14	M	1316	CDL	C52-C51-CB5-OB7
8	L	1286[A]	UQ2	C1-C2-O2-CM2
14	M	1316	CDL	C72-C71-CB7-OB9
6	M	1306	LDA	C4-C5-C6-C7
6	M	1307	LDA	C9-C10-C11-C12
5	M	1304	BCL	CAA-CBA-CGA-O2A

There are no ring outliers.

20 monomers are involved in 66 short contacts:

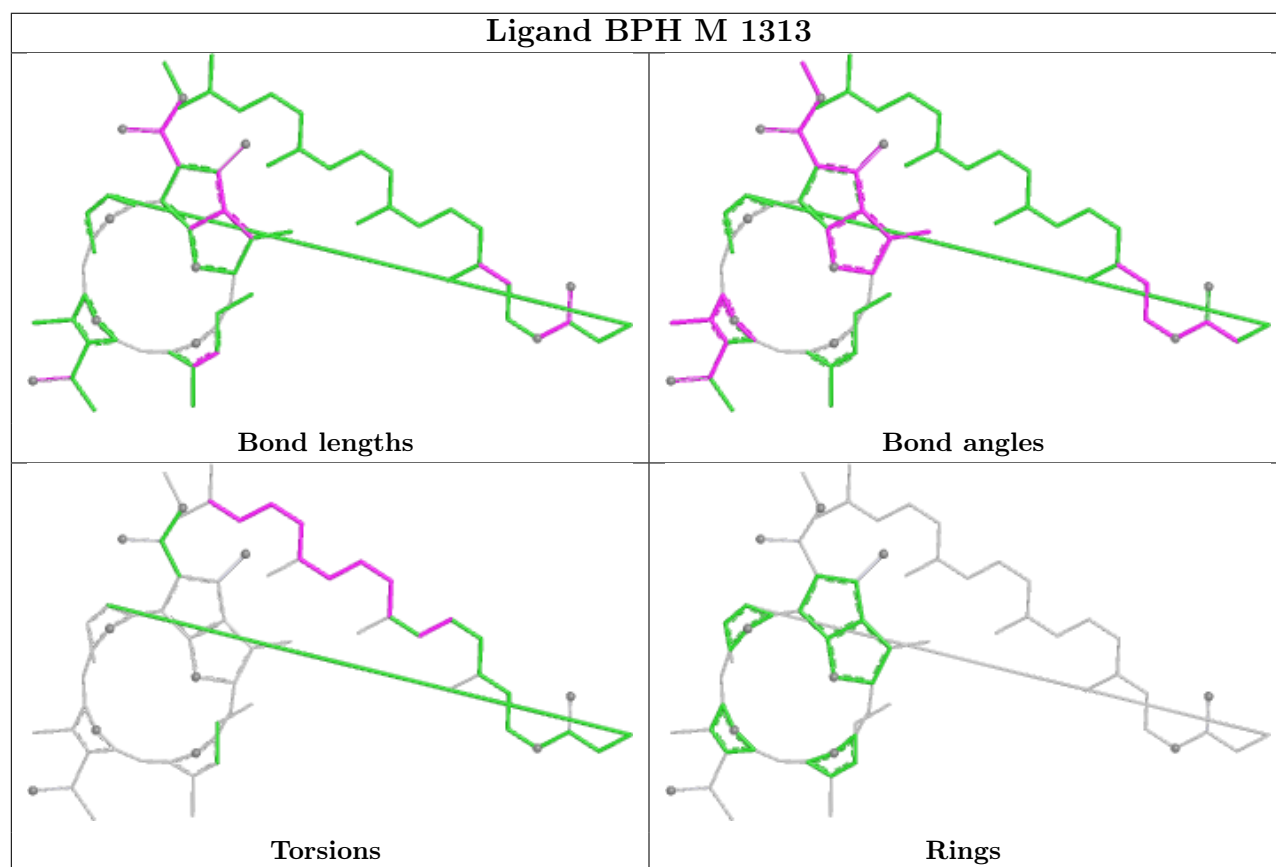
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	L	1289	HTO	2	0
7	M	1313	BPH	9	0
5	M	1304	BCL	11	0
4	L	1290	GOL	1	0
6	M	1311	LDA	1	0
6	M	1309	LDA	1	0
6	M	1307	LDA	5	0
4	L	1292	GOL	1	0
8	L	1286[B]	UQ2	11	0
7	L	1285	BPH	7	0
6	M	1308	LDA	1	0
4	H	1251	GOL	1	0
12	M	1314	U10	1	0
13	M	1315	SPO	4	0
8	L	1286[A]	UQ2	2	0
14	M	1316	CDL	1	0
6	M	1305	LDA	2	0
5	L	1282	BCL	6	0

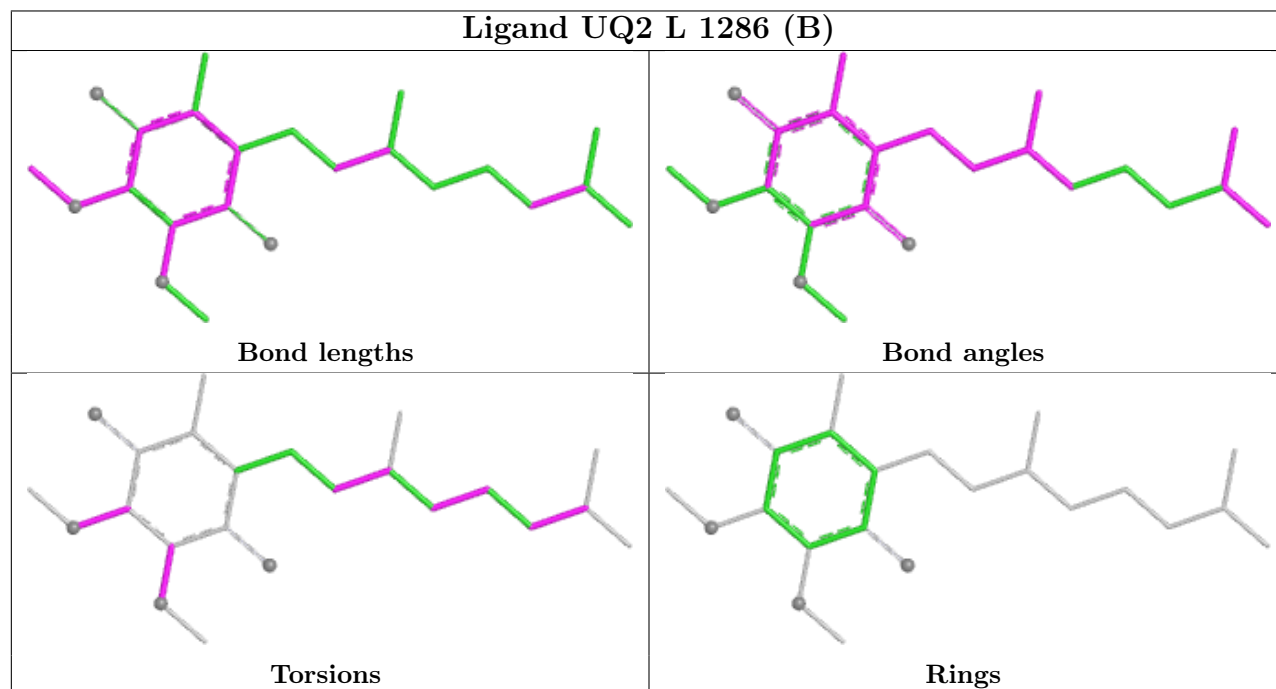
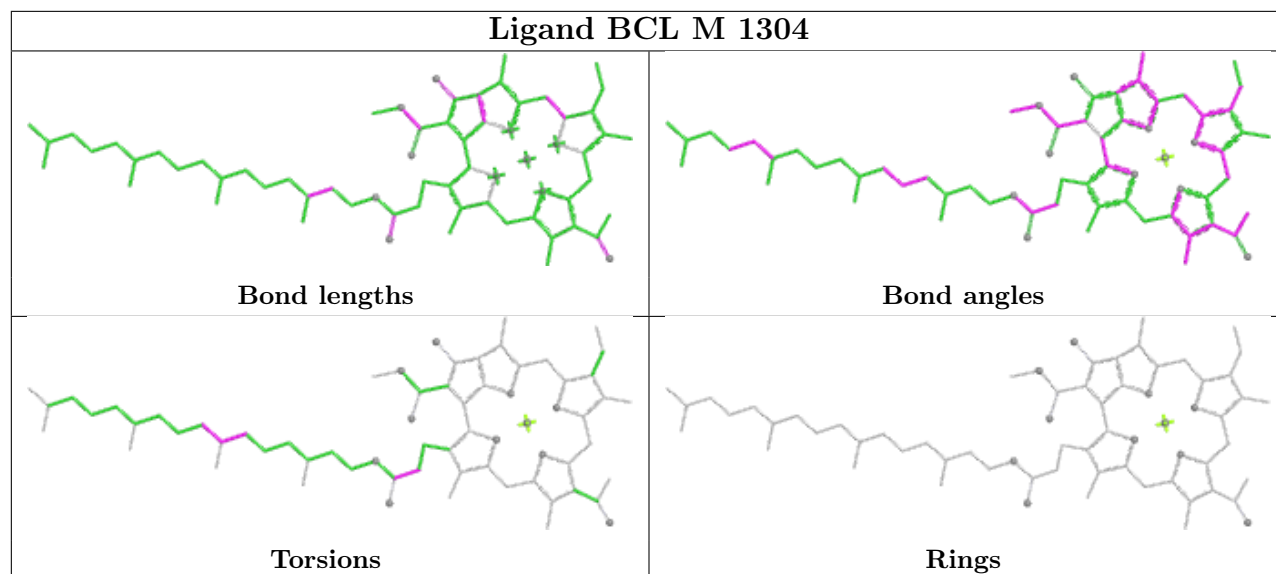
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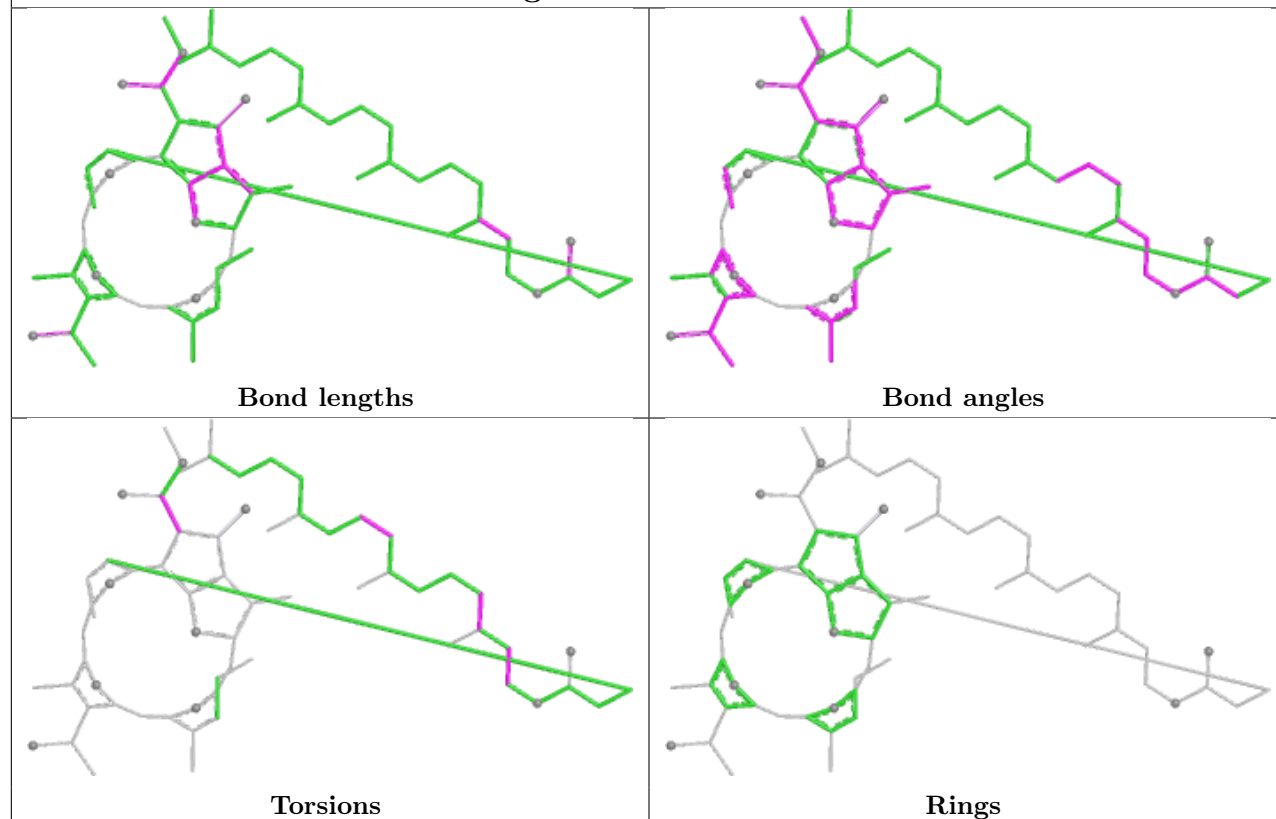
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	1287	BCL	1	0
5	M	1303	BCL	7	0

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

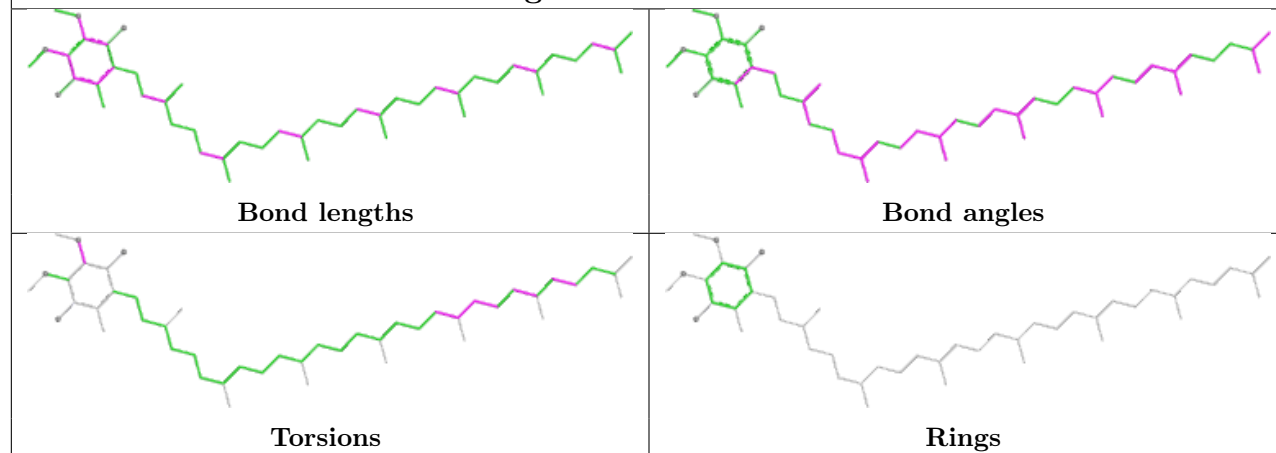


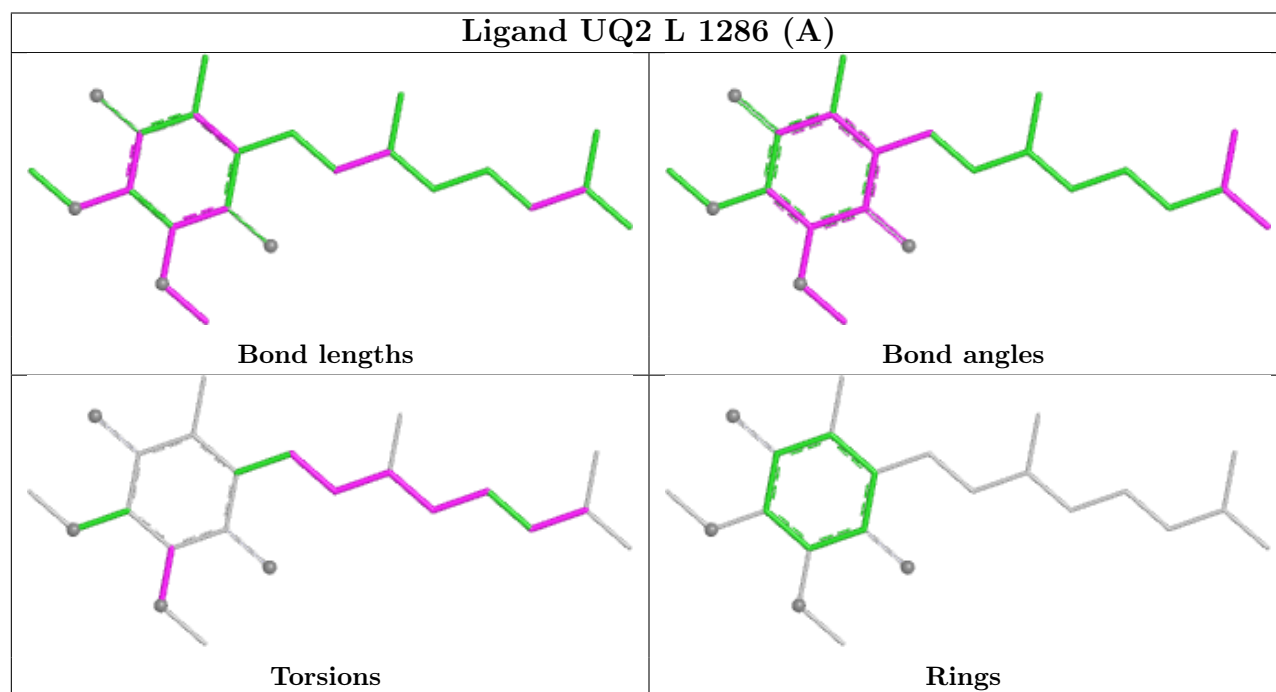
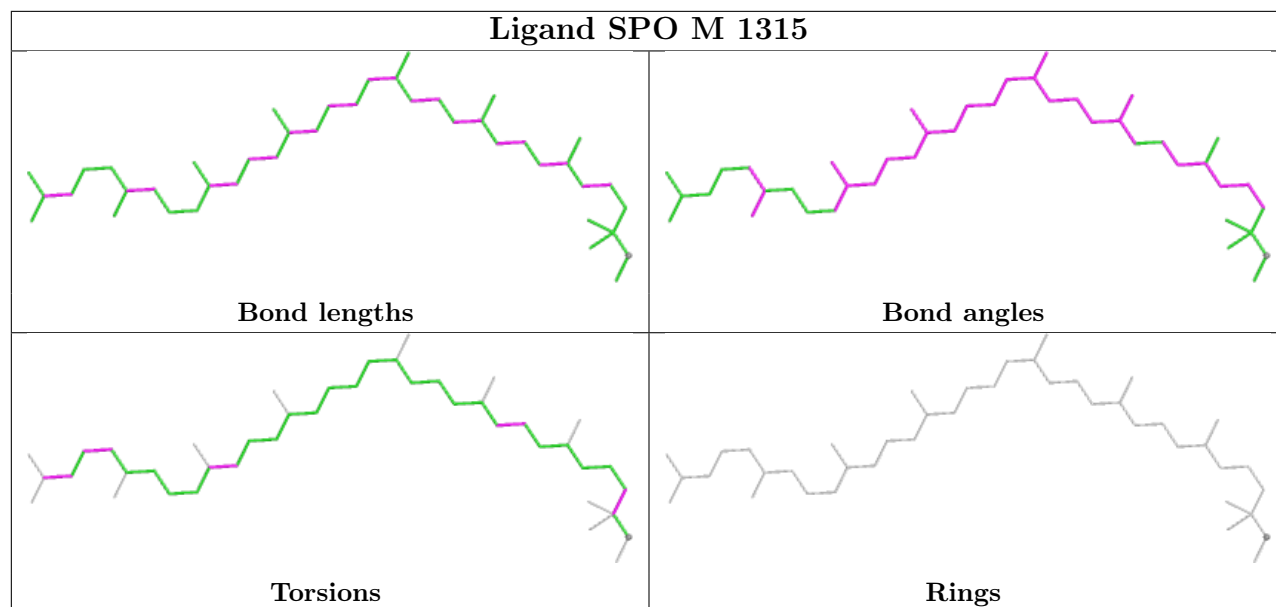


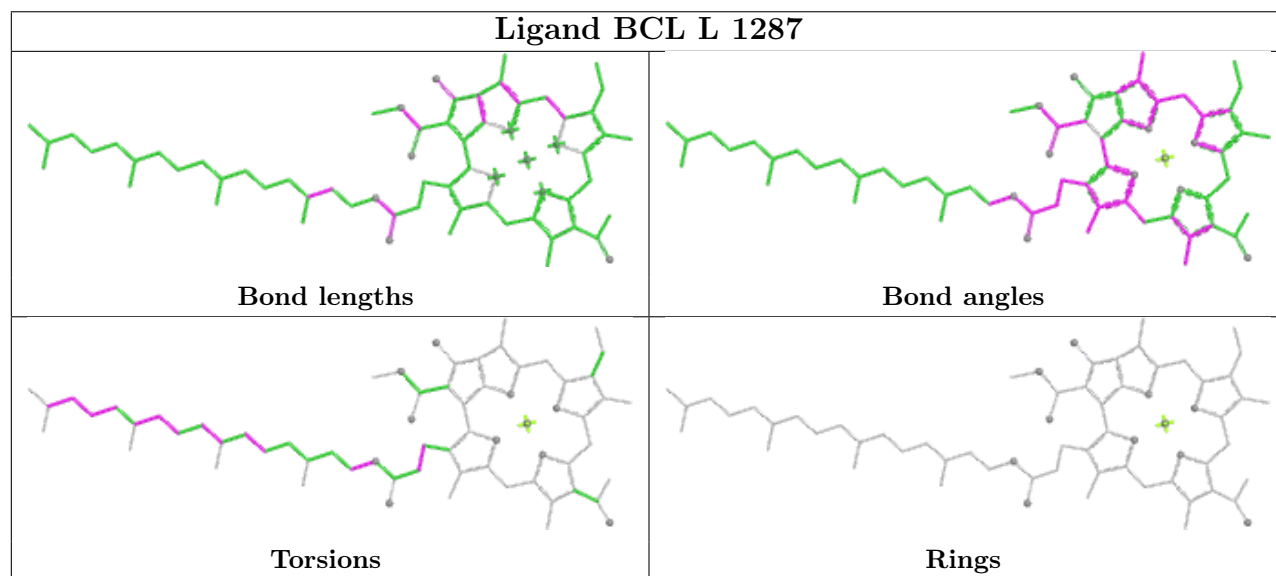
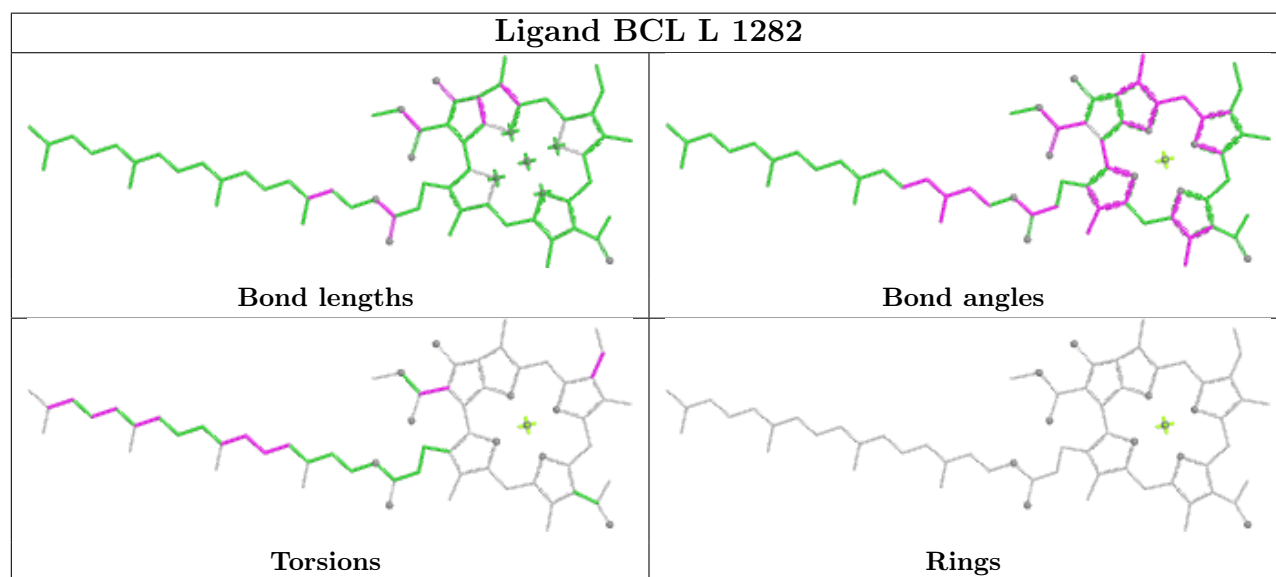
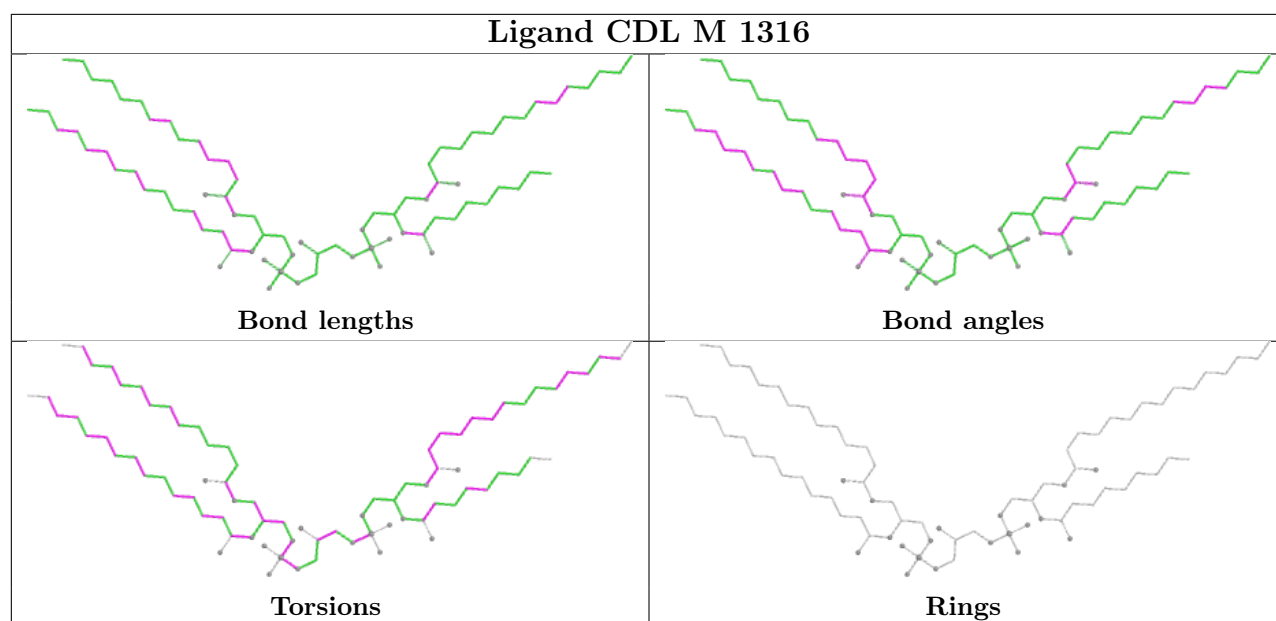
Ligand BPH L 1285

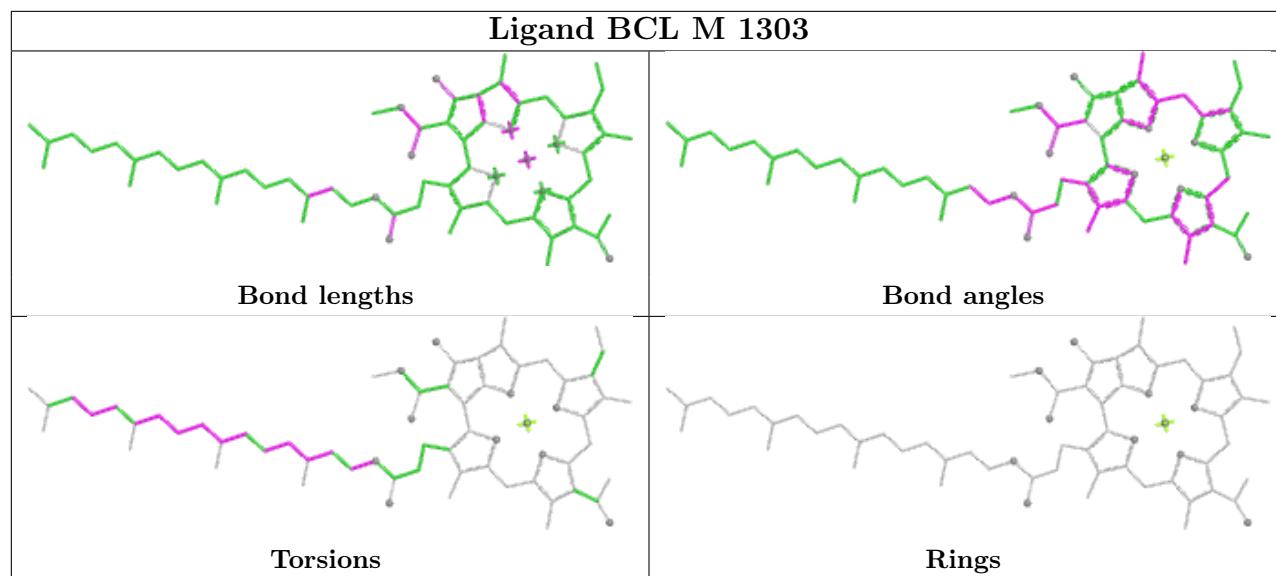


Ligand U10 M 1314









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%)	0.59	15 (6%) 26 24	32, 51, 64, 110	3 (1%)
2	L	281/281 (100%)	0.09	4 (1%) 73 74	32, 42, 56, 65	0
3	M	303/307 (98%)	0.16	12 (3%) 42 42	31, 43, 58, 88	0
All	All	825/848 (97%)	0.26	31 (3%) 44 44	31, 45, 60, 110	3 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	11.3
1	H	246	PRO	8.3
3	M	3	TYR	7.2
1	H	247	LYS	7.1
1	H	245	ALA	7.1
1	H	249	LYS	6.2
1	H	251	VAL	6.1
3	M	148	TRP	5.1
3	M	301	HIS	4.0
1	H	18	TYR	4.0
2	L	264	GLN	4.0
1	H	250	SER	4.0
2	L	281	GLY	3.7
3	M	2	GLU	3.6
1	H	244	ALA	3.6
2	L	1	ALA	3.6
1	H	248	ARG	3.5
3	M	303	MET	3.3
1	H	82	ASP	3.1
2	L	155	ASP	3.1
3	M	54	SER	2.9
3	M	302	GLY	2.6
1	H	138	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	M	188	ASN	2.5
1	H	221	SER	2.4
1	H	206	ASN	2.4
3	M	60	LEU	2.4
1	H	80	SER	2.3
3	M	76	TYR	2.1
1	H	79	GLU	2.1
3	M	292	ASP	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	1311	16/16	0.59	0.39	95,99,106,106	0
10	HTO	L	1904	10/10	0.67	0.31	107,110,111,112	0
14	CDL	M	1316	81/100	0.67	0.38	102,120,128,129	0
6	LDA	M	1308	16/16	0.73	0.36	124,125,128,128	0
6	LDA	L	1284	16/16	0.74	0.34	100,108,118,118	0
9	PO4	L	1288	5/5	0.77	0.28	166,166,167,167	0
4	GOL	L	1292	6/6	0.79	0.19	118,119,119,119	0
6	LDA	M	1310	16/16	0.80	0.30	107,113,120,120	0
6	LDA	M	1309	16/16	0.82	0.33	103,105,111,112	0
6	LDA	M	1305	16/16	0.84	0.19	59,75,80,81	0
6	LDA	M	1306	16/16	0.85	0.25	86,90,94,94	0
10	HTO	L	1289	10/10	0.85	0.20	70,73,73,74	0
6	LDA	L	1283	16/16	0.86	0.23	76,102,115,115	0
8	UQ2	L	1286[A]	23/23	0.87	0.16	24,38,57,59	23
8	UQ2	L	1286[B]	23/23	0.87	0.16	24,31,41,42	23

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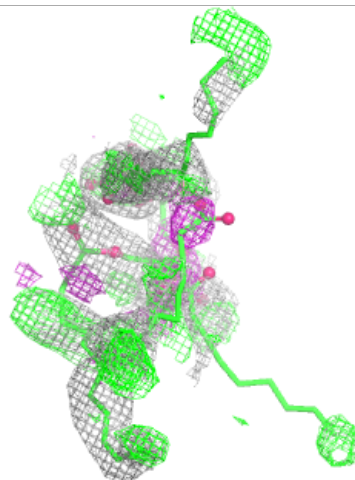
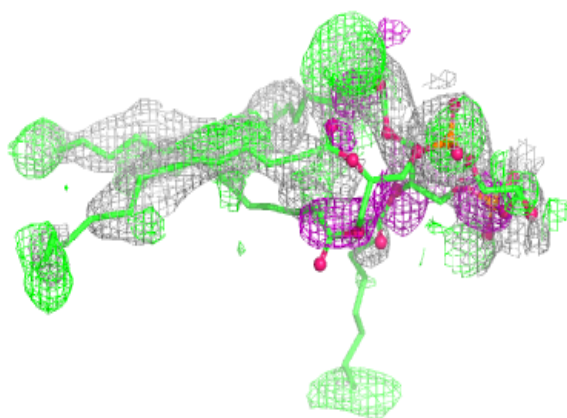
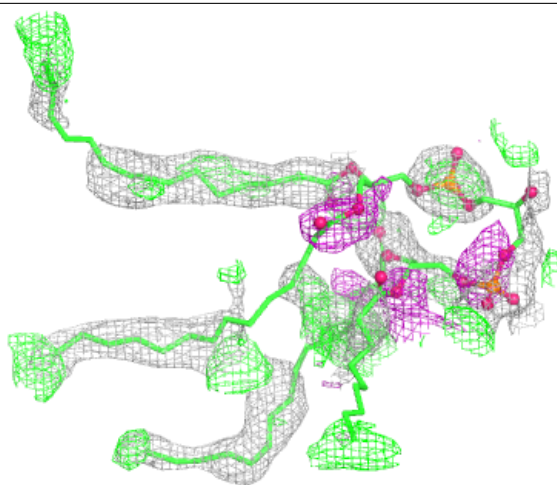
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	LDA	M	1307	16/16	0.87	0.21	75,76,81,82	0
4	GOL	H	1252	6/6	0.88	0.14	92,93,94,94	0
4	GOL	L	1291	6/6	0.88	0.17	80,81,82,83	0
4	GOL	H	1251	6/6	0.88	0.18	100,101,102,103	0
4	GOL	L	1290	6/6	0.90	0.20	66,70,72,73	0
4	GOL	H	1253	6/6	0.92	0.26	119,120,120,120	0
12	U10	M	1314	48/63	0.93	0.11	36,50,76,77	0
13	SPO	M	1315	42/42	0.94	0.11	35,44,66,71	0
7	BPH	M	1313	65/65	0.94	0.11	35,41,98,101	0
5	BCL	M	1303	66/66	0.96	0.10	28,34,79,80	0
5	BCL	L	1282	66/66	0.97	0.07	31,35,62,67	0
5	BCL	M	1304	66/66	0.97	0.08	25,34,58,64	0
7	BPH	L	1285	65/65	0.97	0.06	25,37,46,48	0
5	BCL	L	1287	66/66	0.97	0.07	27,34,54,64	0
11	FE	M	1312	1/1	1.00	0.04	35,35,35,35	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.

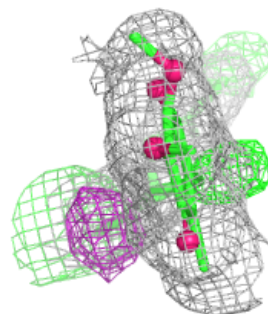
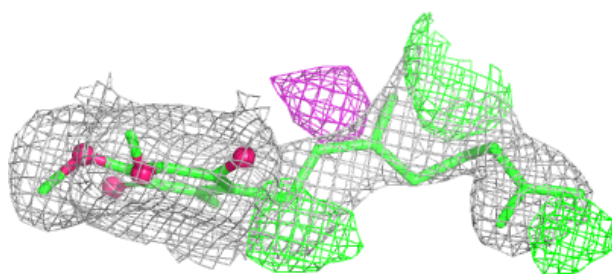
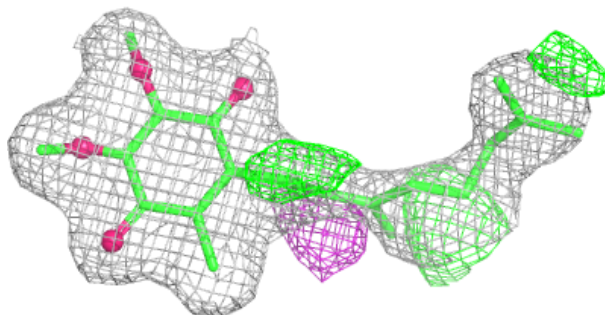
Electron density around CDL M 1316:

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

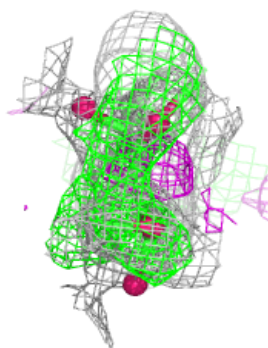
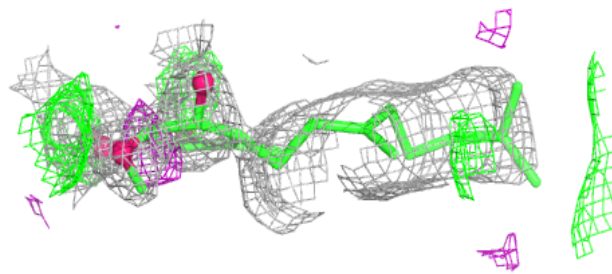
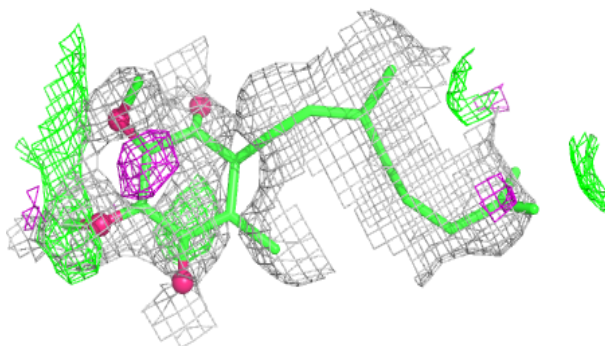


Electron density around UQ2 L 1286 (A):

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

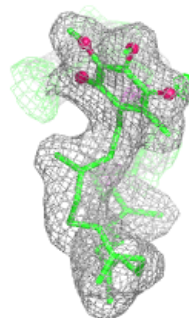
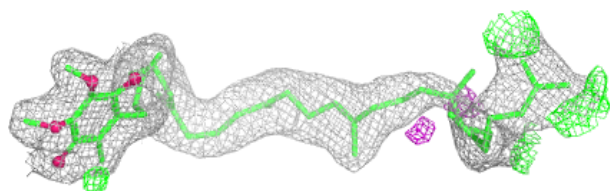
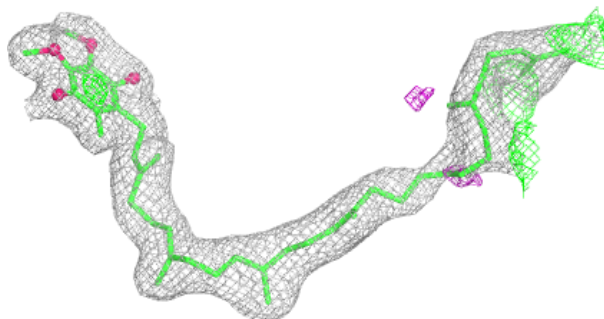
**Electron density around UQ2 L 1286 (B):**

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

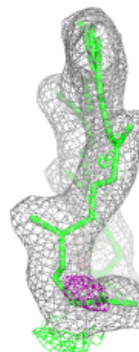
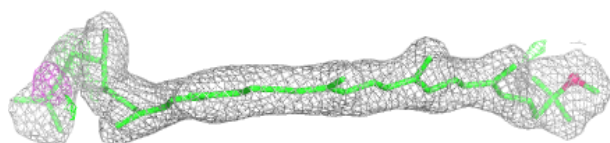
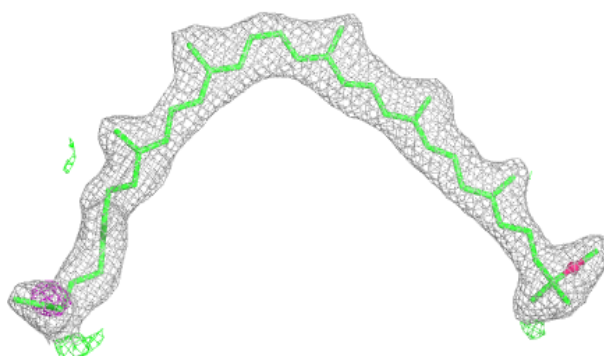


Electron density around U10 M 1314:

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

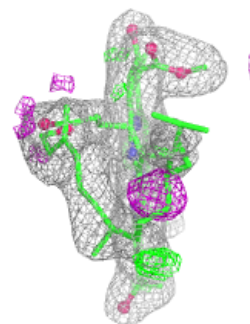
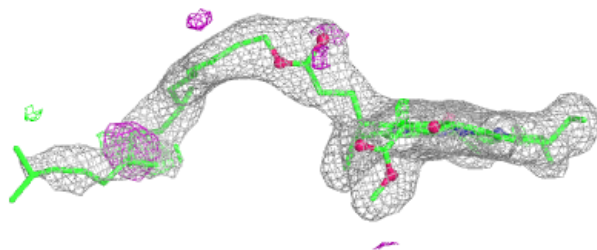
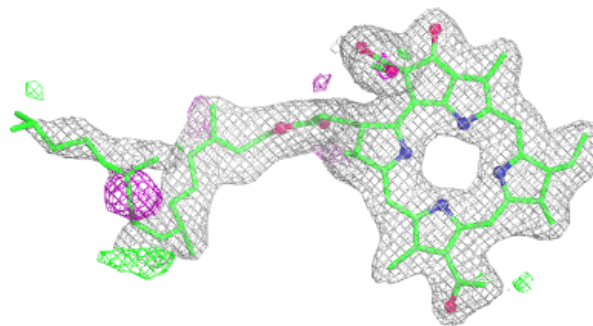
**Electron density around SPO M 1315:**

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



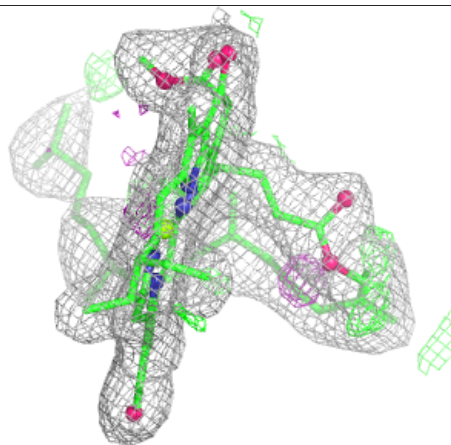
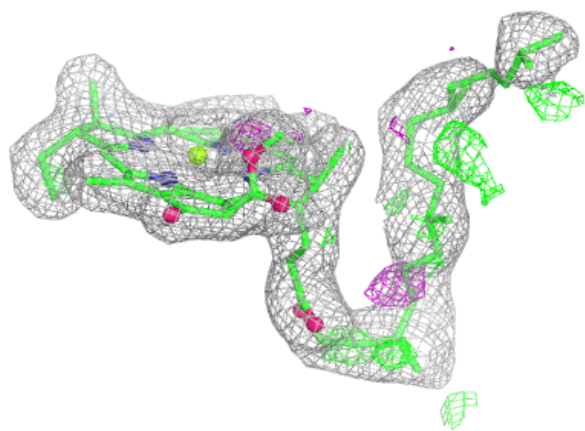
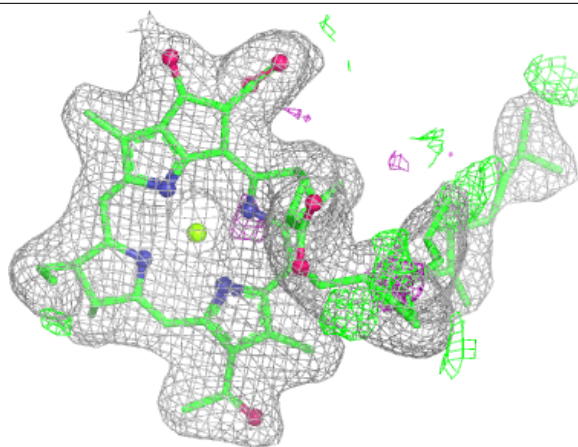
Electron density around BPH M 1313:

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



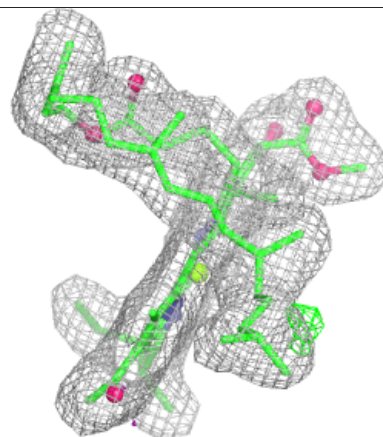
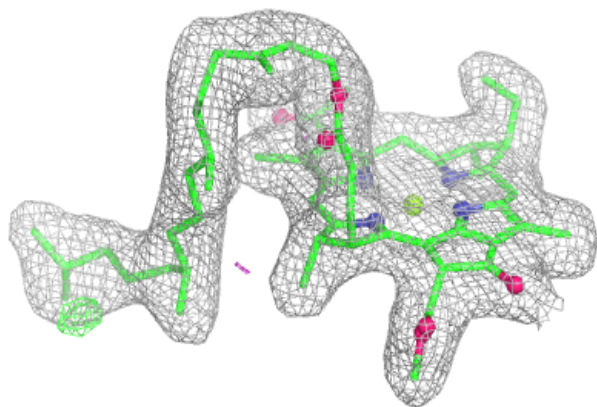
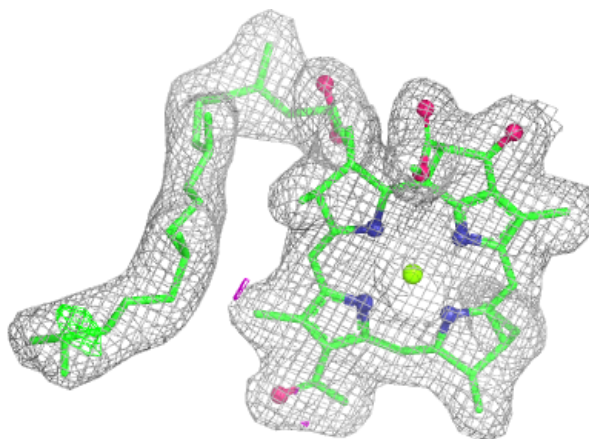
Electron density around BCL M 1303:

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



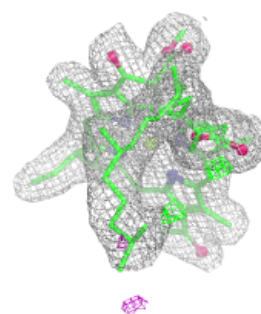
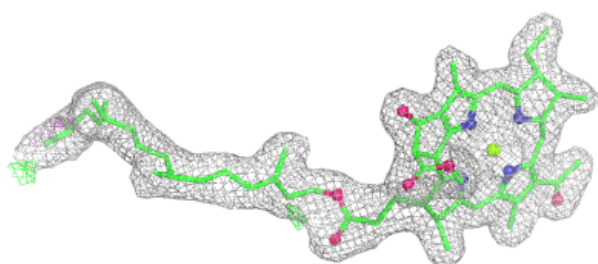
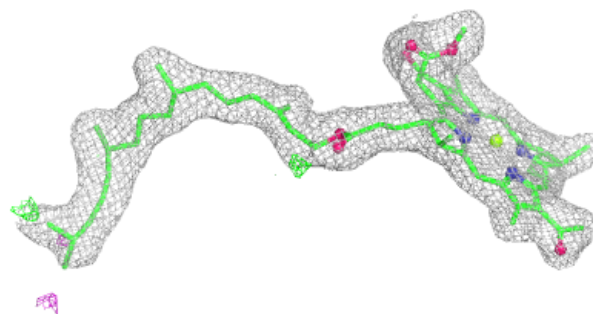
Electron density around BCL L 1282:

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



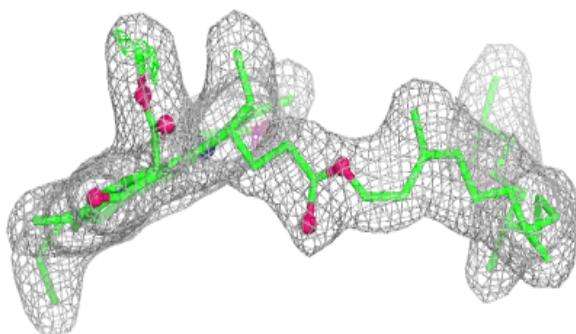
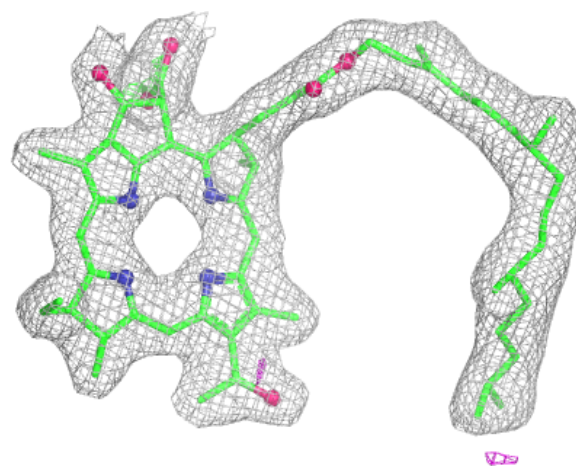
Electron density around BCL M 1304:

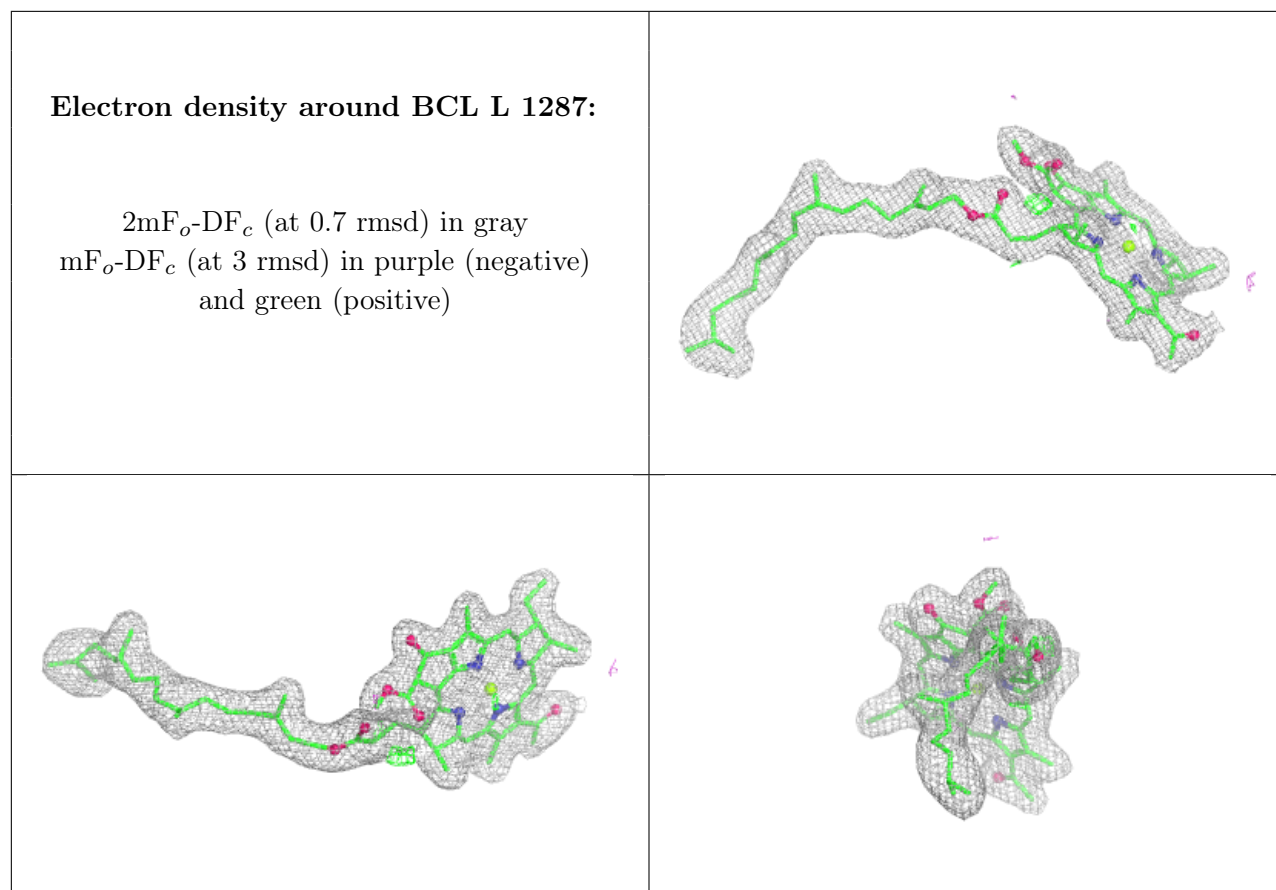
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BPH L 1285:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.