



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 01:06 PM UTC

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

This is a wwPDB X-ray Structure Validation Summary 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

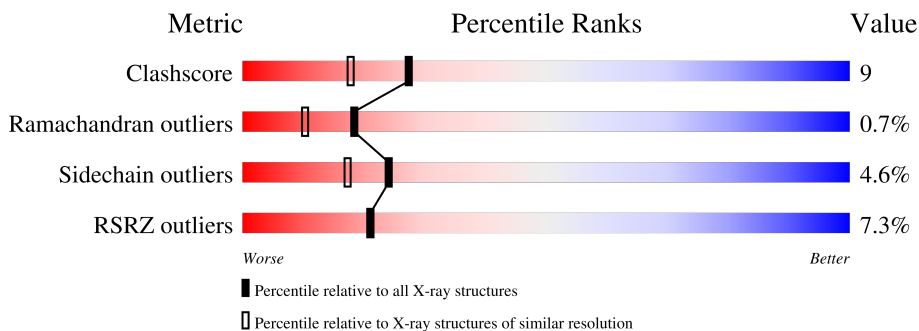
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

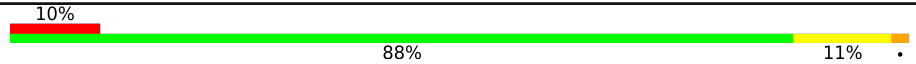
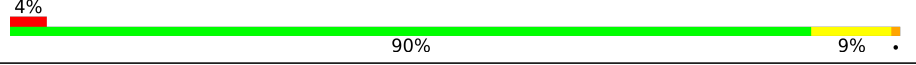

The reported resolution of this entry is 2.07 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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

Mol	Chain	Length	Quality of chain
1	H	260	 10% 88% 11% .
2	L	281	 4% 90% 9% .
3	M	307	 8% 83% 14% .

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

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

2 Entry composition [i](#)

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

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

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

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

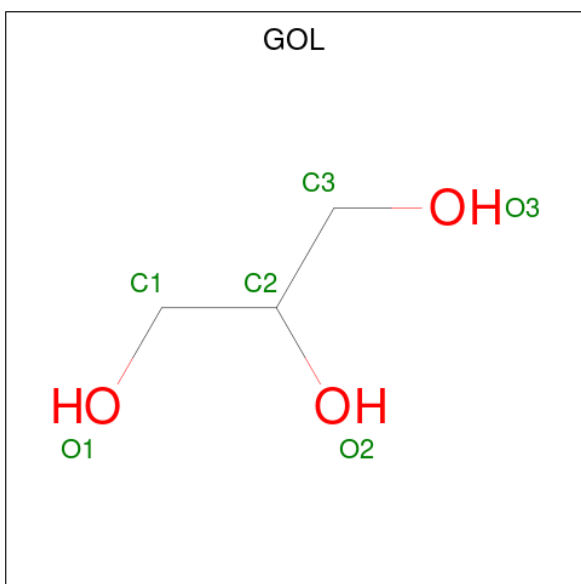
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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

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

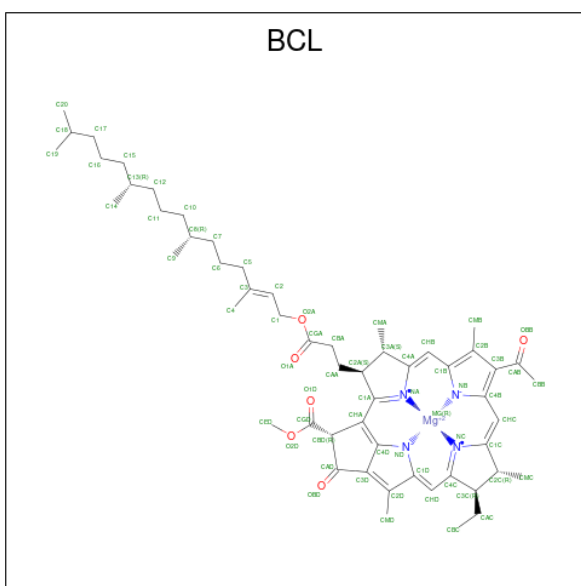
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	307	2451	1634	402	404	11	0	1	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



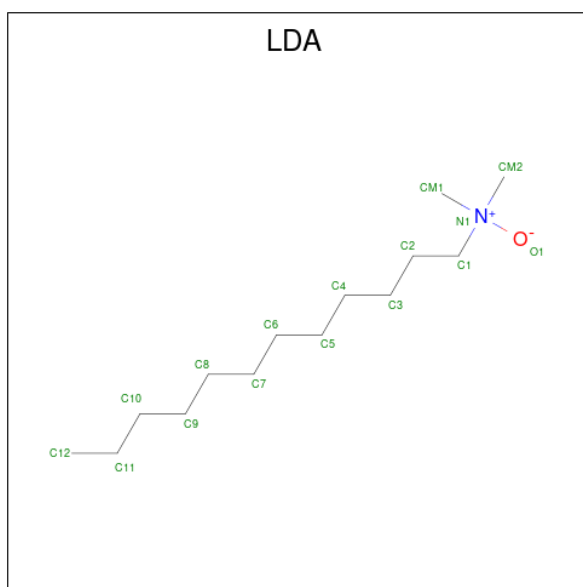
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

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



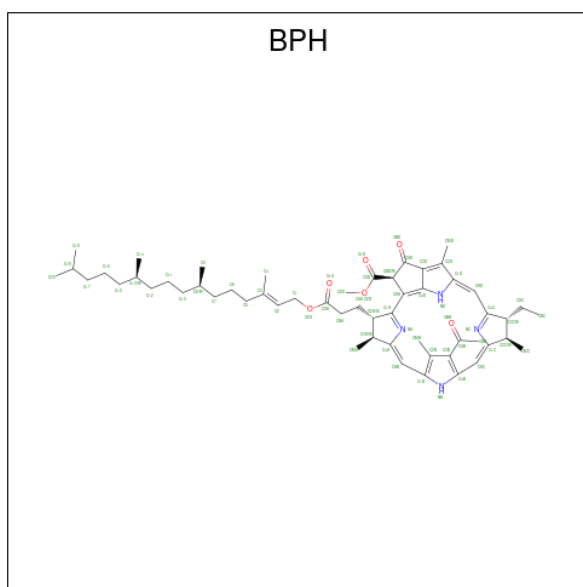
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



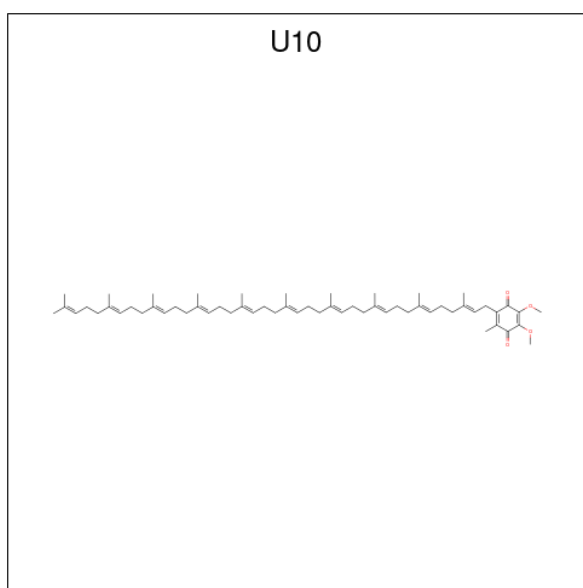
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	L	1	Total 16	C 14	N 1	O 1	0	0
6	L	1	Total 16	C 14	N 1	O 1	0	0
6	L	1	Total 16	C 14	N 1	O 1	0	0
6	M	1	Total 16	C 14	N 1	O 1	0	0
6	M	1	Total 16	C 14	N 1	O 1	0	0
6	M	1	Total 16	C 14	N 1	O 1	0	0
6	M	1	Total 16	C 14	N 1	O 1	0	0
6	M	1	Total 16	C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

- Molecule 7 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



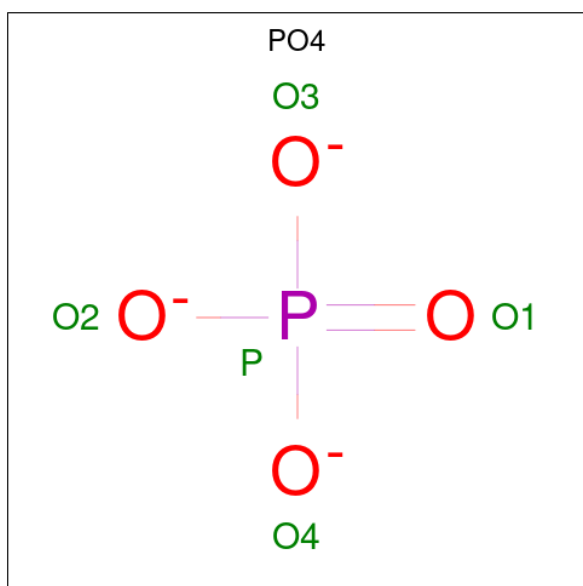
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
7	M	1	65	55	4	6	0	0

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



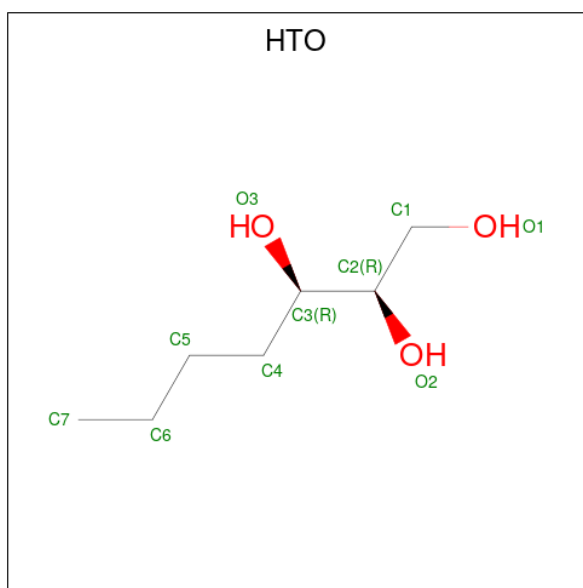
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	46	38	8	0	1
8	M	1	47	44	3	0	0

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



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

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

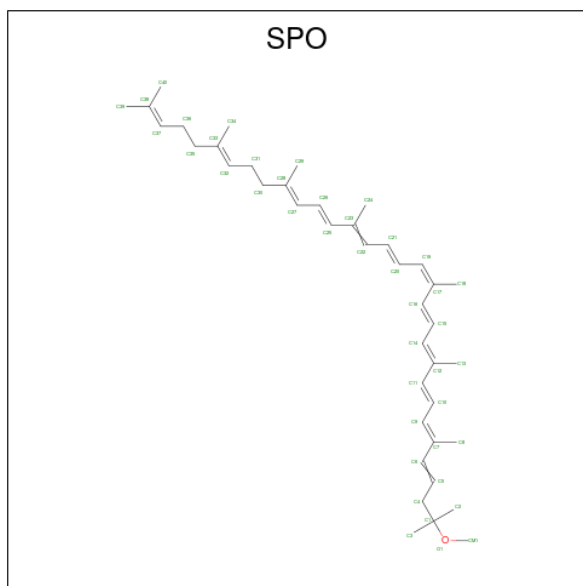


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		
10	L	1	Total	C	O	0	0
			10	7	3		

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

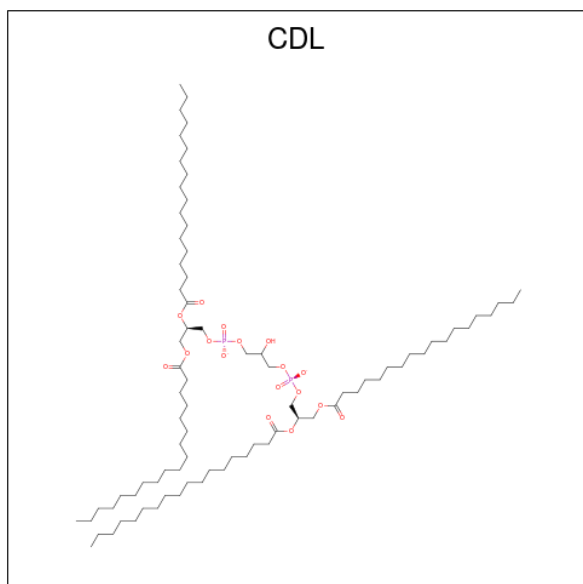
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

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



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

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



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

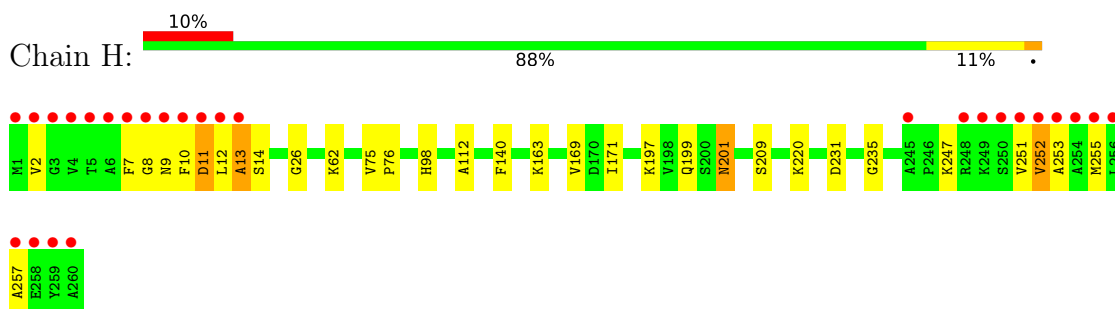
- Molecule 14 is water.

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

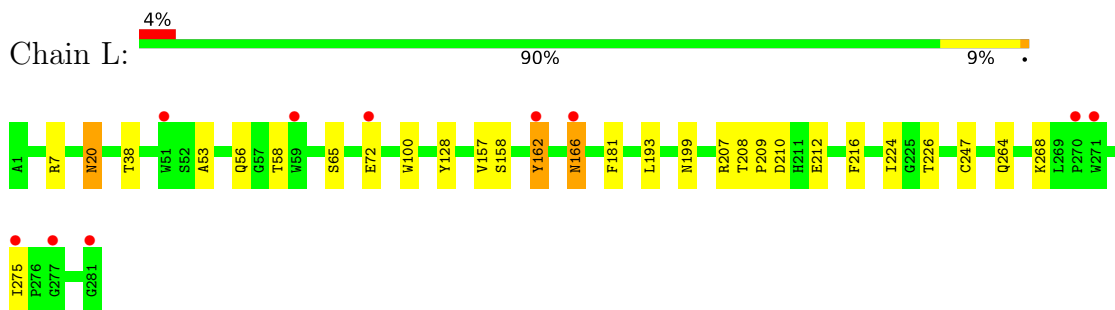
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

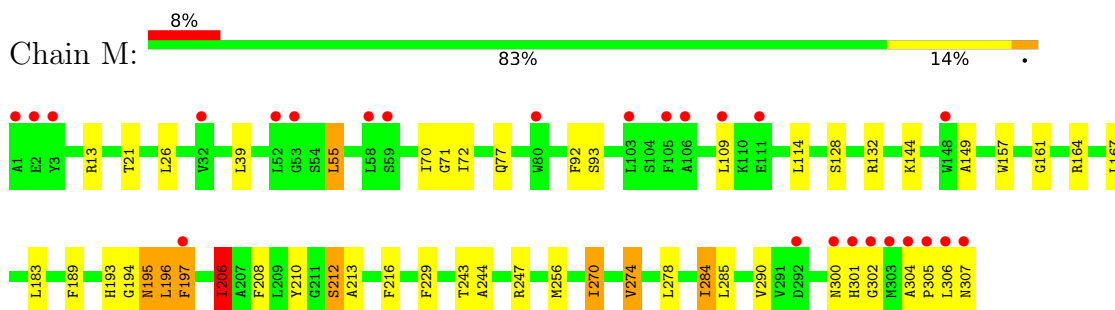
- Molecule 1: REACTION CENTER PROTEIN H CHAIN



- Molecule 2: REACTION CENTER PROTEIN L CHAIN



- Molecule 3: REACTION CENTER PROTEIN M CHAIN



4 Data and refinement statistics i

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

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, U10, LDA, CDL, FE, GOL, SPO, HTO, BPH, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	H	0.91	0/2036	0.92	0/2768
2	L	0.93	0/2320	0.95	2/3175 (0.1%)
3	M	0.96	1/2549 (0.0%)	0.95	3/3479 (0.1%)
All	All	0.94	1/6905 (0.0%)	0.94	5/9422 (0.1%)

All (1) bond length outliers are listed below:

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

All (5) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

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

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

The worst 5 of 137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:1320:CDL:C37	13:M:1320:CDL:C36	1.80	1.57
13:M:1320:CDL:C33	13:M:1320:CDL:C34	1.74	1.56
13:M:1320:CDL:C34	13:M:1320:CDL:C35	1.83	1.55
6:M:1314:LDA:C8	6:M:1314:LDA:C9	1.78	1.55
13:M:1320:CDL:C18	13:M:1320:CDL:C17	1.83	1.53

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	259/260 (100%)	249 (96%)	6 (2%)	4 (2%)	8	2
2	L	279/281 (99%)	272 (98%)	7 (2%)	0	100	100
3	M	306/307 (100%)	292 (95%)	12 (4%)	2 (1%)	18	10
All	All	844/848 (100%)	813 (96%)	25 (3%)	6 (1%)	18	10

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	13	ALA
1	H	252	VAL
1	H	257	ALA
3	M	195	ASN
1	H	8	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	209/208 (100%)	200 (96%)	9 (4%)	26	20
2	L	220/220 (100%)	211 (96%)	9 (4%)	27	21
3	M	241/240 (100%)	228 (95%)	13 (5%)	20	12
All	All	670/668 (100%)	639 (95%)	31 (5%)	24	17

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	207	ARG
3	M	274	VAL
2	L	268	LYS
3	M	290	VAL
3	M	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	166	ASN
2	L	264	GLN
3	M	195	ASN
3	M	187	ASN
3	M	193	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	U10	M	1318	-	46,47,63	2.86	13 (28%)	53,59,79	1.73	13 (24%)
5	BCL	L	1283	-	69,74,74	1.73	9 (13%)	79,115,115	2.11	25 (31%)
4	GOL	L	1294	-	5,5,5	0.37	0	5,5,5	0.28	0
6	LDA	L	1284	-	13,15,15	2.11	2 (15%)	14,17,17	0.51	0
4	GOL	H	1264	-	5,5,5	0.39	0	5,5,5	0.27	0
6	LDA	L	1285	-	13,15,15	2.07	2 (15%)	14,17,17	0.51	0
6	LDA	M	1312	-	13,15,15	2.01	2 (15%)	14,17,17	0.54	0
4	GOL	L	1293	-	5,5,5	0.40	0	5,5,5	0.28	0
7	BPH	L	1287	-	59,70,70	2.69	12 (20%)	59,101,101	2.58	18 (30%)
8	U10	L	1288[A]	-	23,23,63	2.61	7 (30%)	30,31,79	1.91	8 (26%)
4	GOL	H	1263	-	5,5,5	0.46	0	5,5,5	0.18	0
9	PO4	L	1289	-	4,4,4	0.89	0	6,6,6	0.83	0
6	LDA	L	1286	-	13,15,15	2.25	2 (15%)	14,17,17	0.56	0
6	LDA	M	1311	-	13,15,15	2.15	2 (15%)	14,17,17	0.54	0
6	LDA	M	1315	-	13,15,15	2.32	3 (23%)	14,17,17	0.83	0
10	HTO	L	1290	-	9,9,9	0.54	0	10,10,10	0.63	0
4	GOL	H	1262	-	5,5,5	0.53	0	5,5,5	0.53	0
10	HTO	L	1291	-	9,9,9	0.35	0	10,10,10	0.81	0
7	BPH	M	1317	-	59,70,70	2.67	12 (20%)	59,101,101	2.57	19 (32%)
5	BCL	M	1309	3	69,74,74	1.86	10 (14%)	79,115,115	1.92	20 (25%)
6	LDA	M	1314	-	13,15,15	3.04	5 (38%)	14,17,17	1.42	3 (21%)
4	GOL	H	1261	-	5,5,5	0.60	0	5,5,5	0.92	0
5	BCL	L	1282	2	69,74,74	1.85	9 (13%)	79,115,115	1.97	21 (26%)
6	LDA	M	1313	-	13,15,15	2.28	2 (15%)	14,17,17	0.65	0
13	CDL	M	1320	-	80,80,99	2.26	19 (23%)	86,92,111	1.79	18 (20%)
4	GOL	L	1292	-	5,5,5	0.43	0	5,5,5	1.00	0
5	BCL	M	1308	3	69,74,74	1.79	7 (10%)	79,115,115	1.82	14 (17%)
12	SPO	M	1319	-	41,41,41	2.61	12 (29%)	47,50,50	2.27	16 (34%)
8	U10	L	1288[B]	-	23,23,63	2.70	7 (30%)	30,31,79	1.35	4 (13%)
6	LDA	M	1310	-	13,15,15	2.02	2 (15%)	14,17,17	0.72	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	U10	M	1318	-	-	13/45/65/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	1283	-	2/2/21/25	8/41/137/137	-
4	GOL	L	1294	-	-	2/4/4/4	-
6	LDA	L	1284	-	-	6/13/13/13	-
4	GOL	H	1264	-	-	1/4/4/4	-
6	LDA	L	1285	-	-	10/13/13/13	-
6	LDA	M	1312	-	-	8/13/13/13	-
4	GOL	L	1293	-	-	2/4/4/4	-
7	BPH	L	1287	-	-	5/37/105/105	0/5/6/6
8	U10	L	1288[A]	-	-	7/15/39/87	0/1/1/1
4	GOL	H	1263	-	-	0/4/4/4	-
6	LDA	L	1286	-	-	6/13/13/13	-
6	LDA	M	1311	-	-	9/13/13/13	-
6	LDA	M	1315	-	-	8/13/13/13	-
10	HTO	L	1290	-	-	9/10/10/10	-
4	GOL	H	1262	-	-	2/4/4/4	-
10	HTO	L	1291	-	-	7/10/10/10	-
7	BPH	M	1317	-	-	18/37/105/105	0/5/6/6
5	BCL	M	1309	3	2/2/21/25	8/41/137/137	-
6	LDA	M	1314	-	-	3/13/13/13	-
4	GOL	H	1261	-	-	2/4/4/4	-
5	BCL	L	1282	2	2/2/21/25	9/41/137/137	-
6	LDA	M	1313	-	-	7/13/13/13	-
13	CDL	M	1320	-	-	49/91/91/110	-
4	GOL	L	1292	-	-	2/4/4/4	-
5	BCL	M	1308	3	2/2/21/25	12/41/137/137	-
12	SPO	M	1319	-	-	9/47/47/47	-
8	U10	L	1288[B]	-	-	8/15/39/87	0/1/1/1
6	LDA	M	1310	-	-	5/13/13/13	-

The worst 5 of 139 bond length outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1308	BCL	OBD-CAD	9.37	1.38	1.22

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	1317	BPH	O2D-CGD-CBD	9.94	121.87	110.95
7	L	1287	BPH	O2D-CGD-CBD	7.89	119.61	110.95
7	L	1287	BPH	C2B-C1B-NB	7.87	115.12	109.43
7	M	1317	BPH	C2B-C1B-NB	7.35	114.74	109.43
7	L	1287	BPH	C2D-C1D-ND	6.55	114.16	109.43

5 of 8 chirality outliers are listed below:

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

5 of 235 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1261	GOL	O1-C1-C2-C3
4	H	1262	GOL	C1-C2-C3-O3
4	L	1292	GOL	C1-C2-C3-O3
4	L	1293	GOL	O1-C1-C2-C3
5	M	1308	BCL	C1-C2-C3-C4

There are no ring outliers.

15 monomers are involved in 72 short contacts:

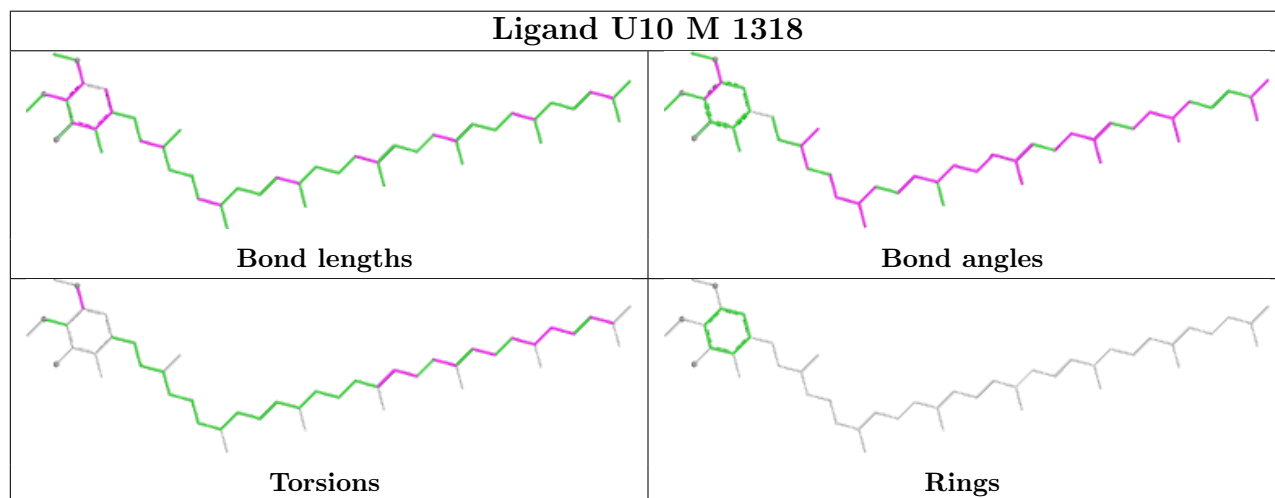
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	1318	U10	4	0
5	L	1283	BCL	4	0
6	M	1312	LDA	2	0
7	L	1287	BPH	6	0
8	L	1288[A]	U10	7	0
6	L	1286	LDA	1	0
7	M	1317	BPH	7	0
5	M	1309	BCL	6	0

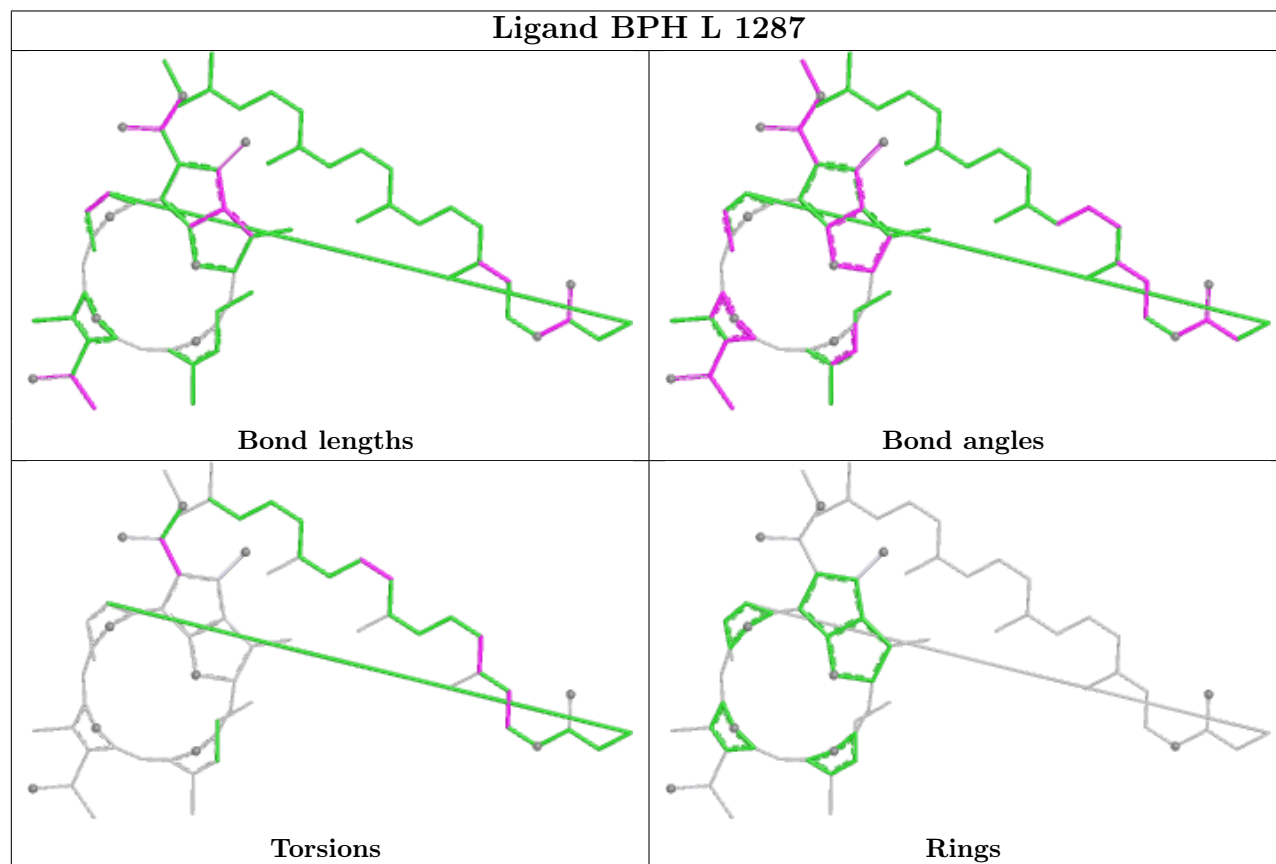
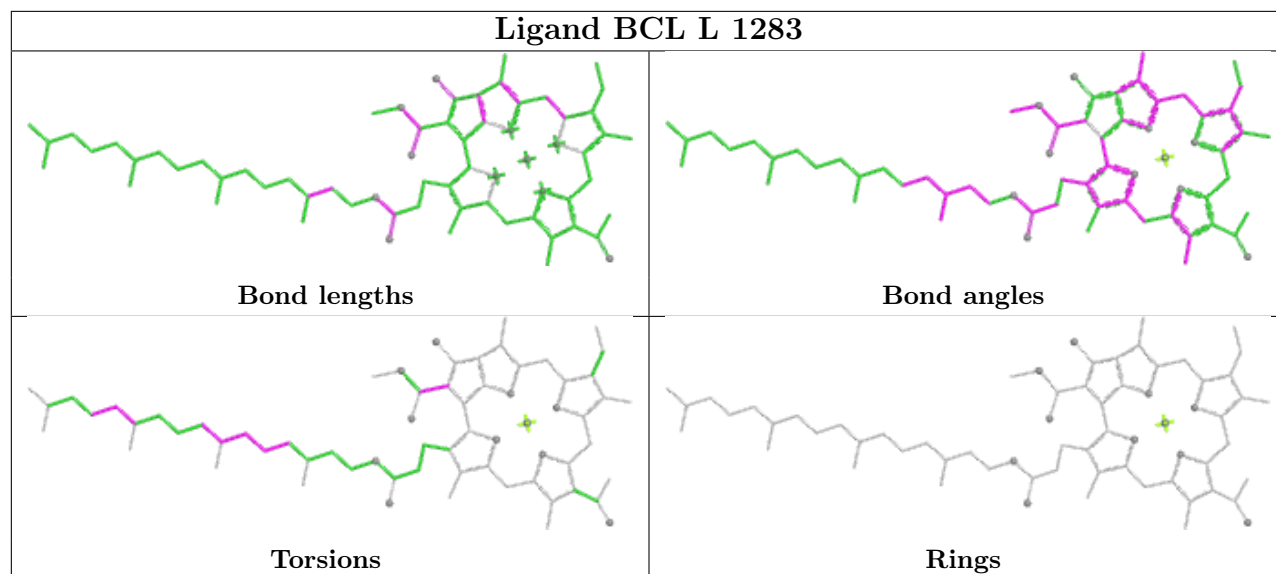
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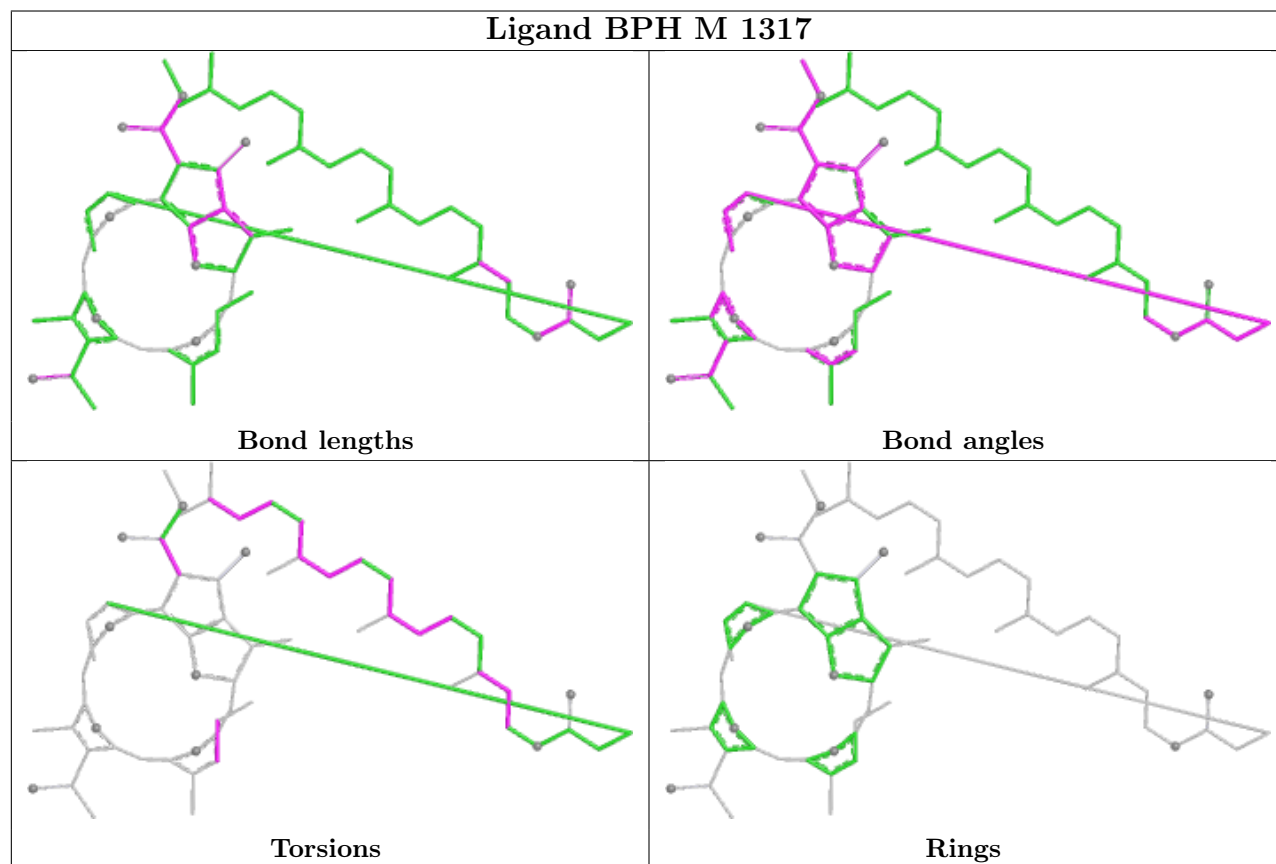
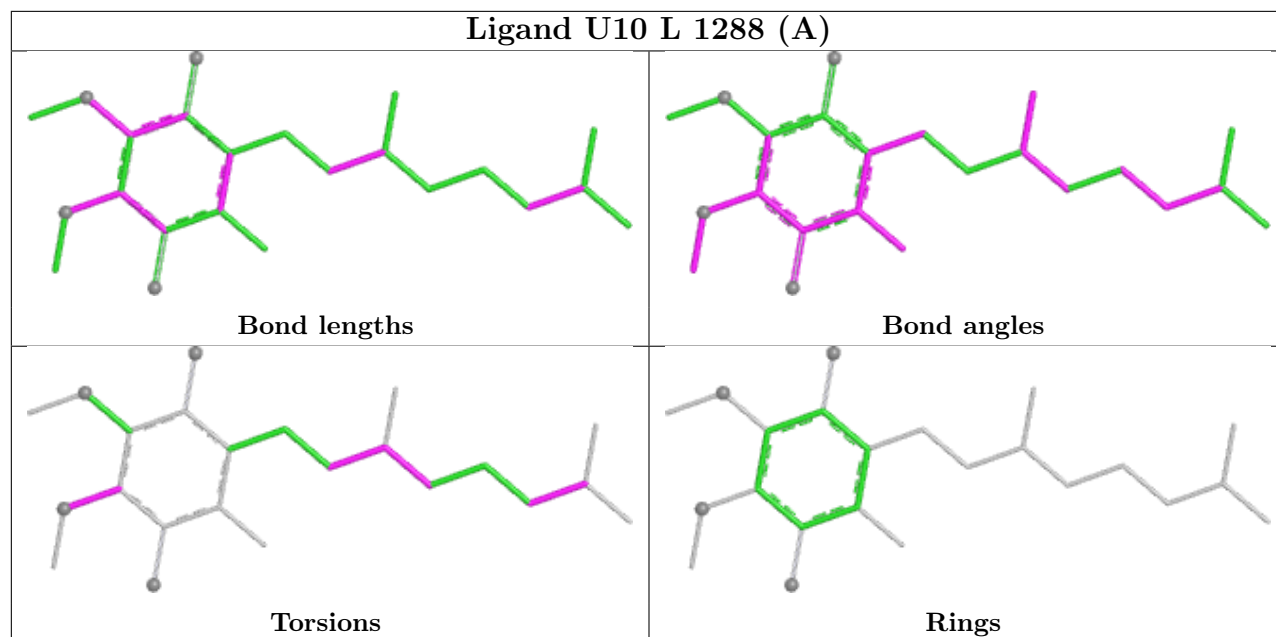
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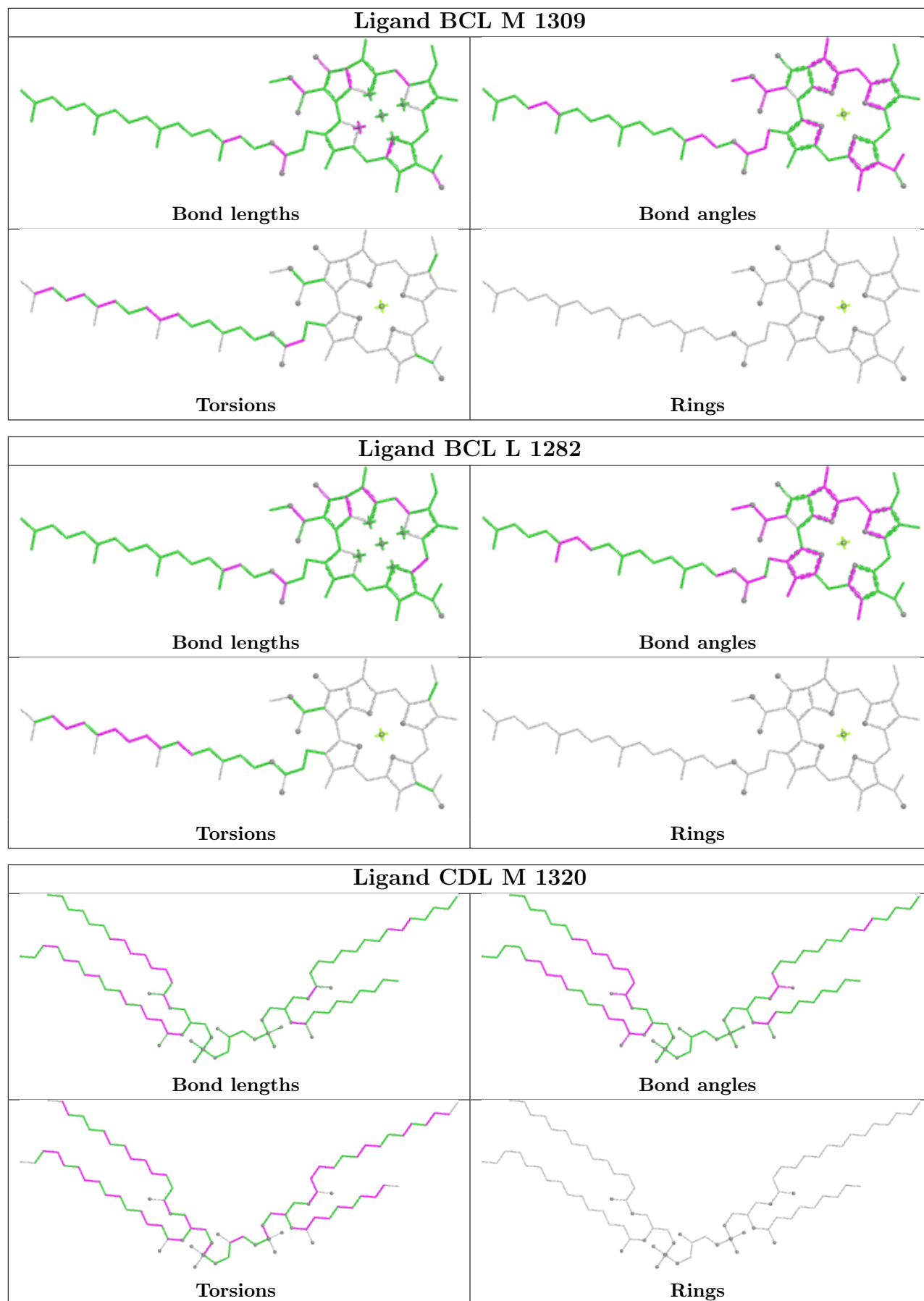
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1314	LDA	4	0
4	H	1261	GOL	5	0
6	M	1313	LDA	3	0
13	M	1320	CDL	18	0
5	M	1308	BCL	5	0
12	M	1319	SPO	3	0
8	L	1288[B]	U10	2	0

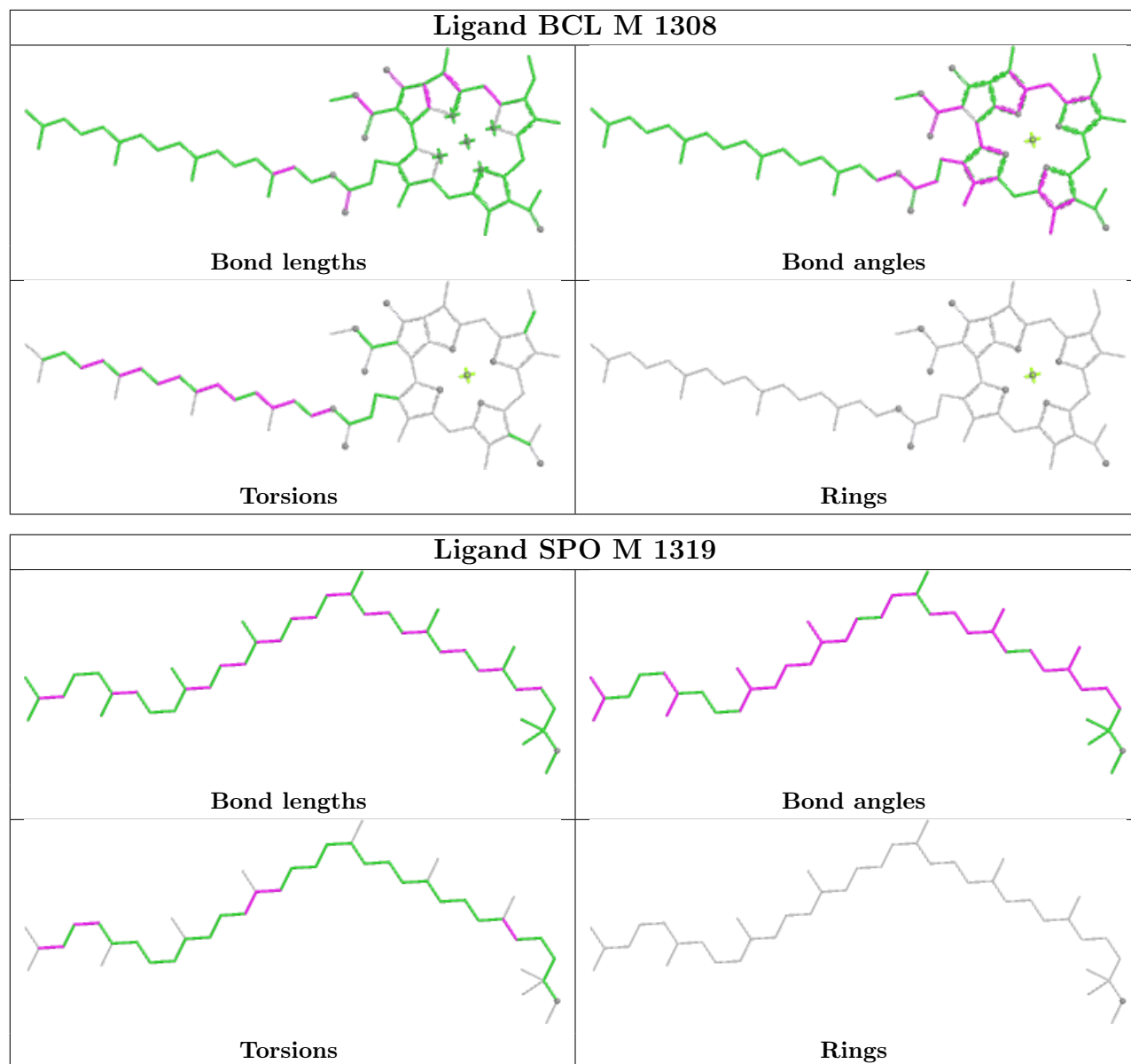
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

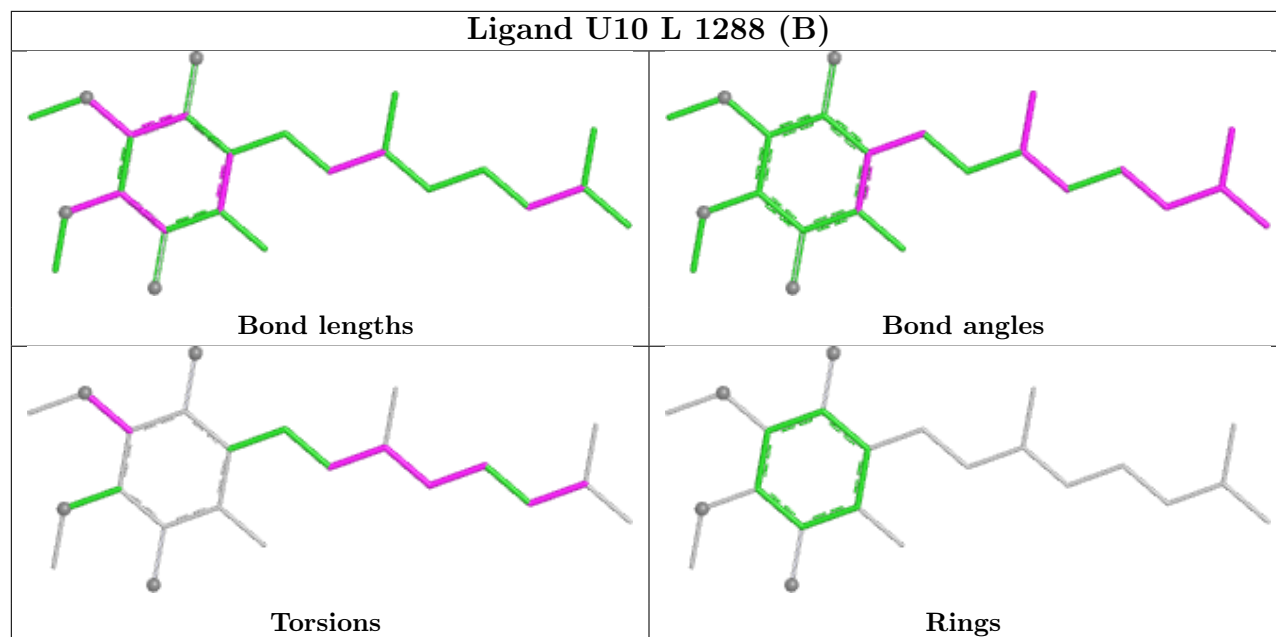












5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	H	260/260 (100%)	0.56	27 (10%)	11 11	17, 26, 108, 129	1 (0%)
2	L	281/281 (100%)	0.16	10 (3%)	46 47	16, 24, 45, 56	0
3	M	307/307 (100%)	0.50	25 (8%)	18 18	14, 28, 52, 100	1 (0%)
All	All	848/848 (100%)	0.40	62 (7%)	21 21	14, 26, 52, 129	2 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	10[A]	PHE	15.8
3	M	306	LEU	13.7
1	H	4	VAL	12.8
1	H	6	ALA	10.6
3	M	304	ALA	10.1

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](#)

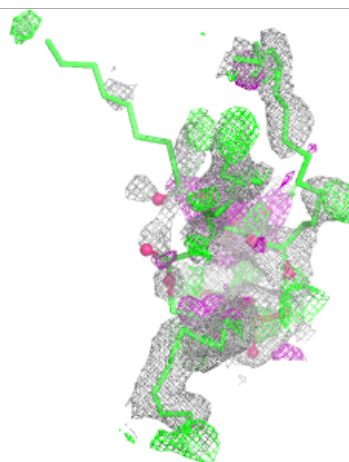
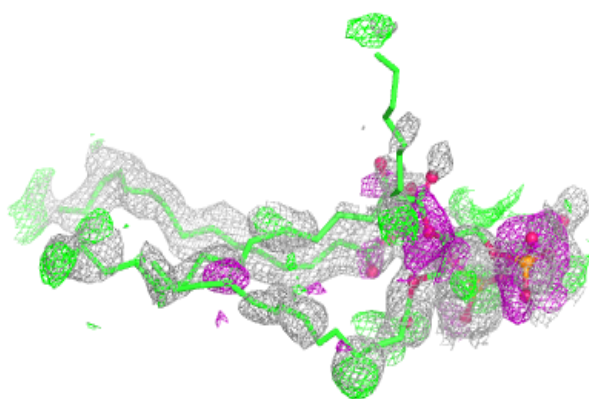
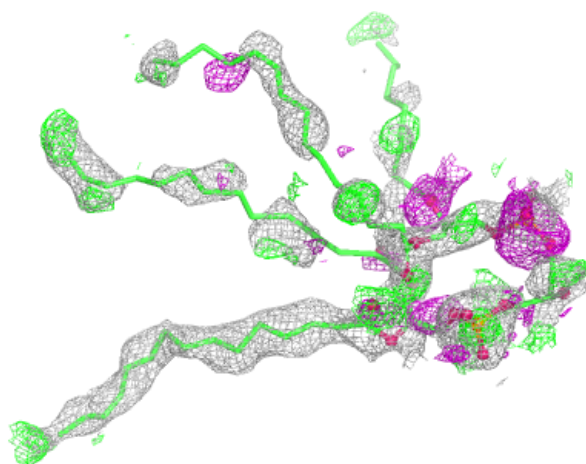
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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	L	1285	16/16	0.70	0.42	88,89,95,95	0
6	LDA	M	1315	16/16	0.73	0.34	77,85,92,92	0
13	CDL	M	1320	81/100	0.73	0.35	49,79,102,105	0
10	HTO	L	1291	10/10	0.74	0.36	100,101,102,102	0
4	GOL	L	1294	6/6	0.76	0.25	94,95,95,95	0
6	LDA	L	1286	16/16	0.76	0.38	96,98,102,102	0
6	LDA	M	1314	16/16	0.76	0.34	66,72,84,85	0
8	U10	L	1288[B]	23/63	0.80	0.24	32,34,35,35	23
4	GOL	H	1263	6/6	0.80	0.19	72,74,74,75	0
8	U10	L	1288[A]	23/63	0.80	0.24	33,42,54,55	23
6	LDA	M	1311	16/16	0.81	0.25	55,60,71,72	0
10	HTO	L	1290	10/10	0.81	0.21	55,59,60,61	0
6	LDA	L	1284	16/16	0.84	0.26	55,79,92,92	0
6	LDA	M	1313	16/16	0.85	0.23	68,71,72,72	0
4	GOL	H	1261	6/6	0.85	0.22	35,46,50,52	0
4	GOL	L	1292	6/6	0.86	0.17	34,38,39,45	0
4	GOL	H	1264	6/6	0.86	0.15	71,74,74,76	0
4	GOL	L	1293	6/6	0.87	0.18	75,76,76,77	0
4	GOL	H	1262	6/6	0.87	0.17	66,67,67,68	0
6	LDA	M	1312	16/16	0.88	0.17	47,52,54,55	0
9	PO4	L	1289	5/5	0.90	0.10	58,60,60,61	0
6	LDA	M	1310	16/16	0.90	0.15	29,47,53,54	0
7	BPH	M	1317	65/65	0.93	0.14	16,26,84,85	0
8	U10	M	1318	47/63	0.93	0.12	15,26,55,57	0
12	SPO	M	1319	42/42	0.94	0.11	19,33,53,58	0
5	BCL	L	1283	66/66	0.95	0.08	14,19,45,50	0
5	BCL	M	1308	66/66	0.96	0.11	13,21,67,68	0
5	BCL	M	1309	66/66	0.96	0.08	13,18,39,47	0
7	BPH	L	1287	65/65	0.96	0.07	10,17,31,34	0
5	BCL	L	1282	66/66	0.96	0.07	15,18,32,37	0
11	FE	M	1316	1/1	0.99	0.02	16,16,16,16	0

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

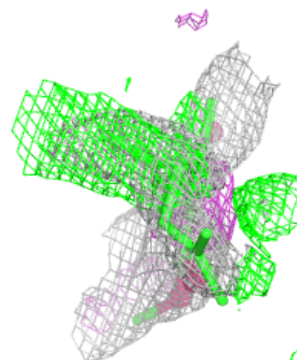
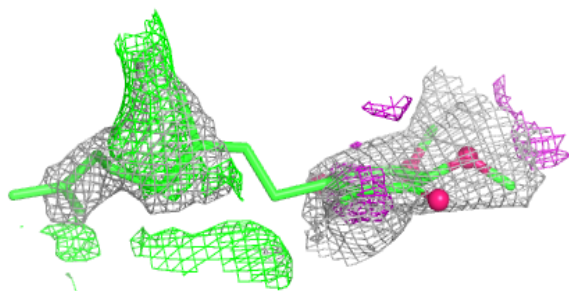
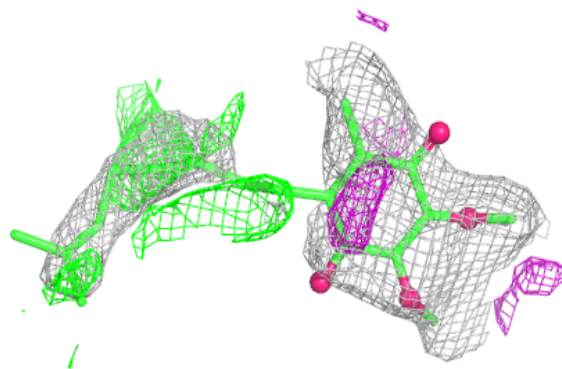
Electron density around CDL M 1320:

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

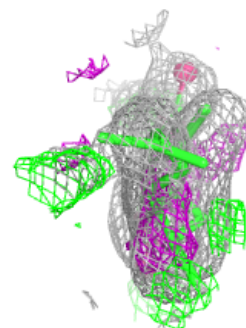
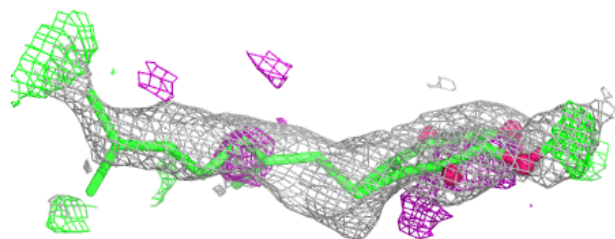
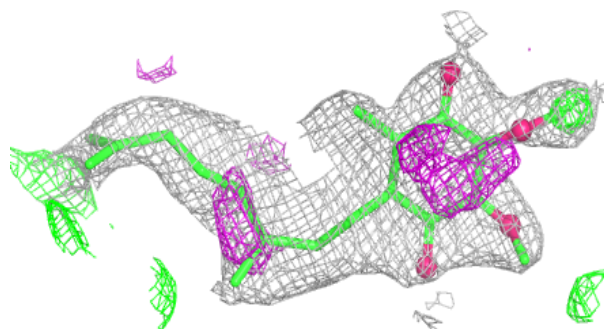


Electron density around U10 L 1288 (B):

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

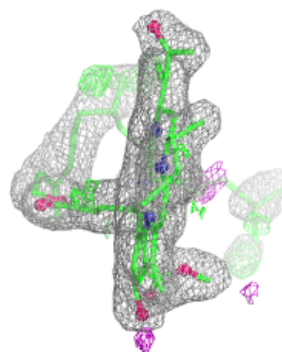
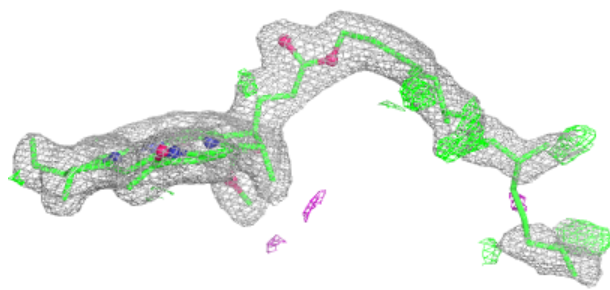
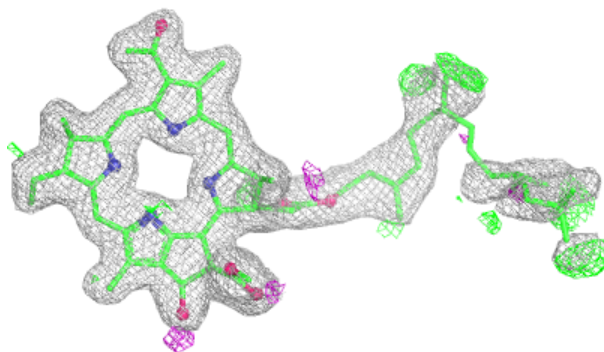
**Electron density around U10 L 1288 (A):**

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and green (positive)

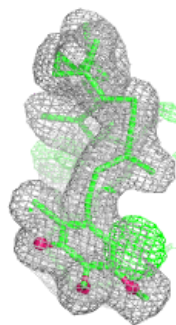
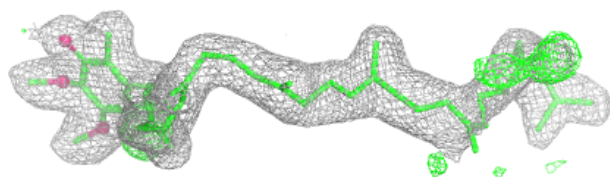
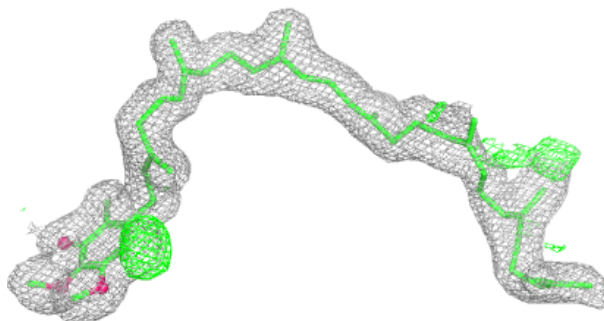


Electron density around BPH M 1317:

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and green (positive)

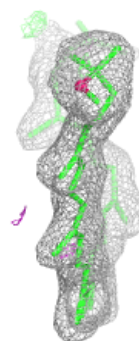
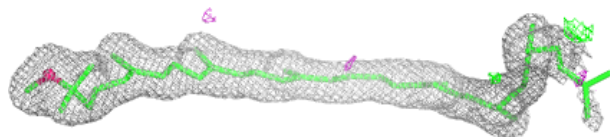
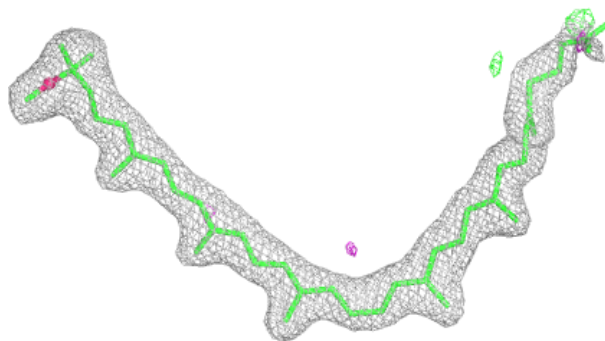
**Electron density around U10 M 1318:**

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and green (positive)

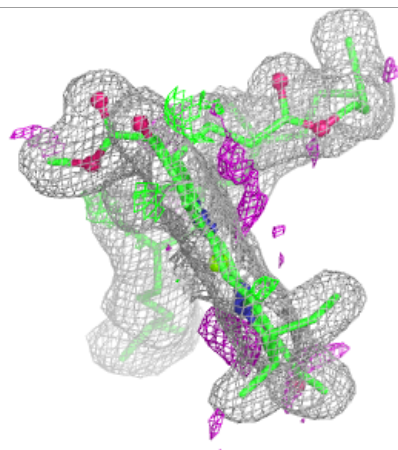
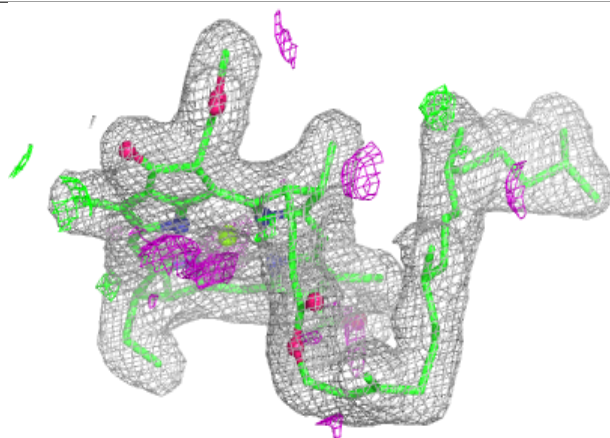
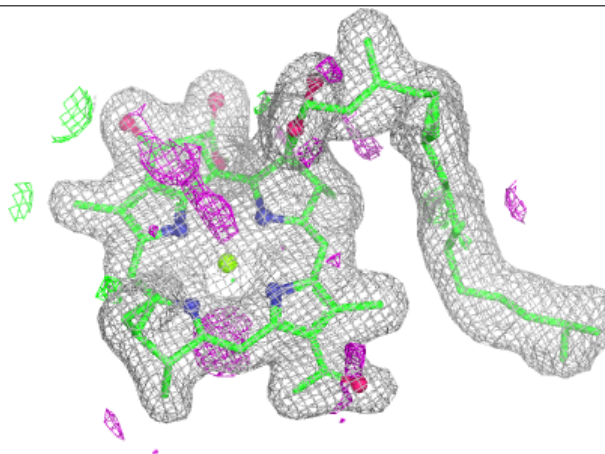


Electron density around SPO M 1319:

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and green (positive)

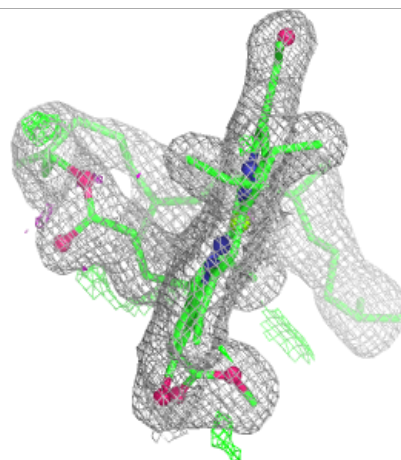
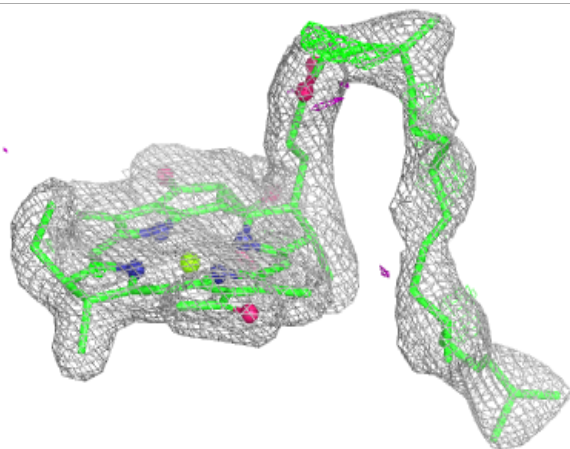
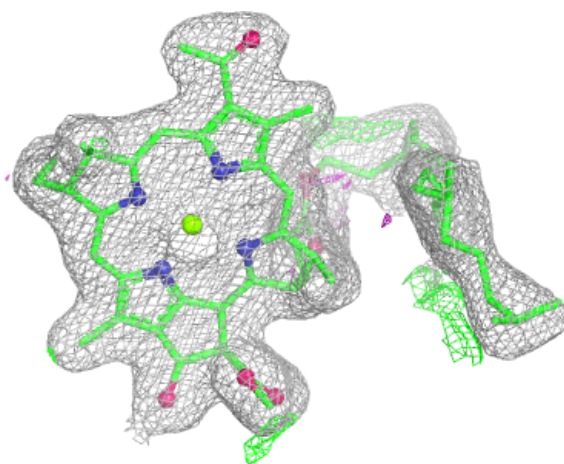
**Electron density around BCL L 1283:**

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



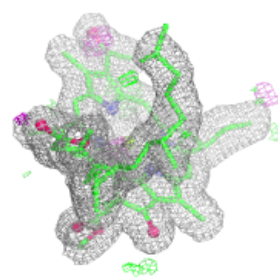
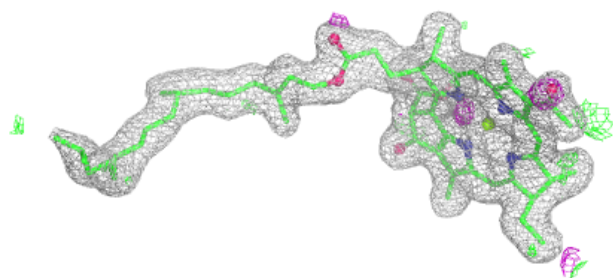
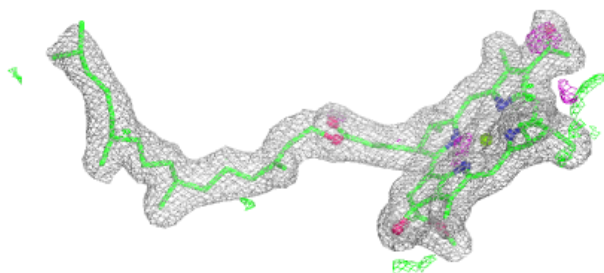
Electron density around BCL M 1308:

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and green (positive)

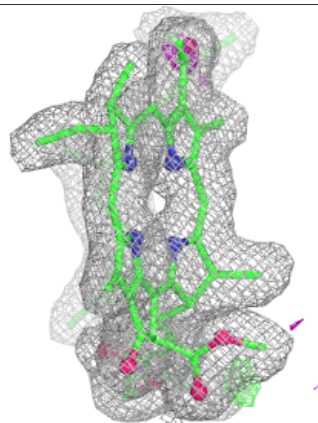
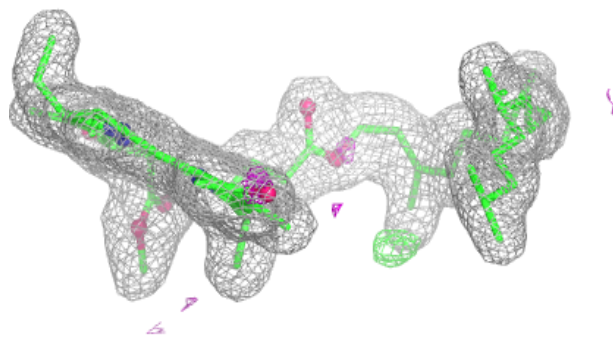
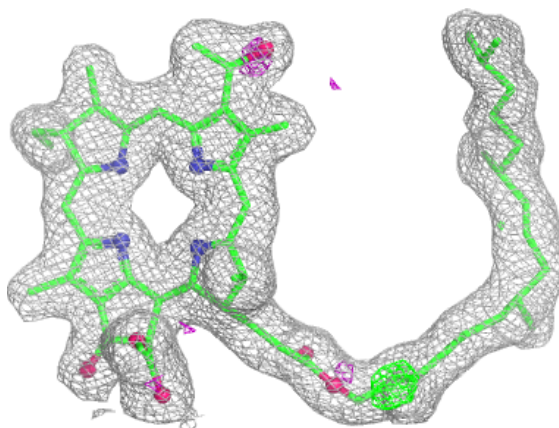


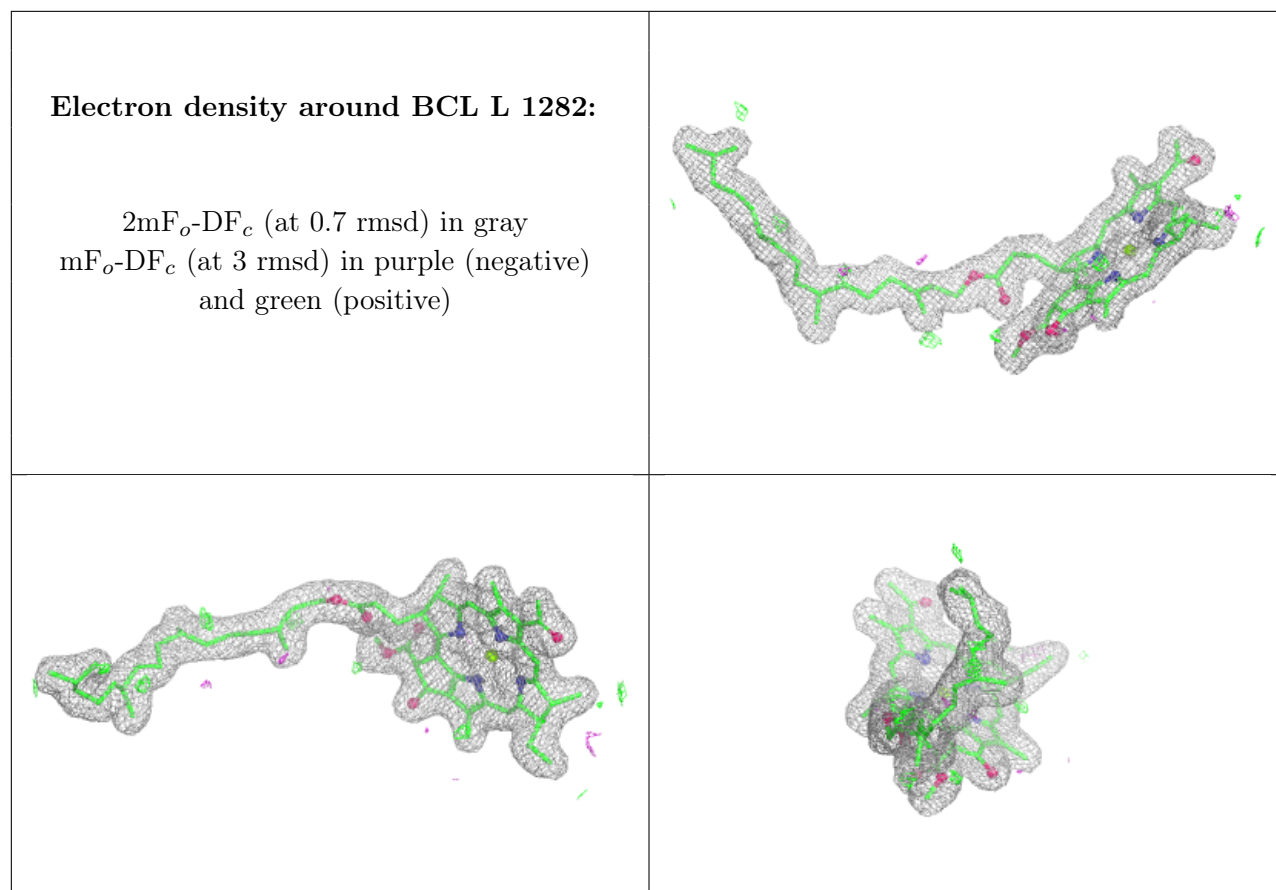
Electron density around BCL M 1309:

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

**Electron density around BPH L 1287:**

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





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.