



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:48 pm BST

PDB ID : 2UX4
Title : X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 9 in the charge-separated state, 2nd dataset
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.
Deposited on : 2007-03-26
Resolution : 2.51 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

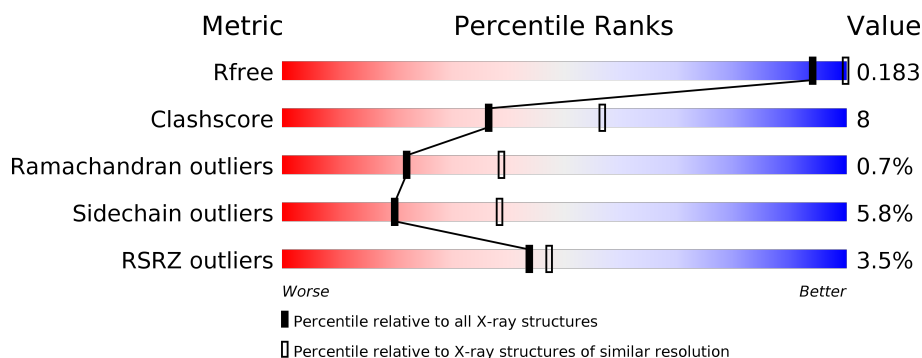
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>7%</div> </div> </div>
2	L	281	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div></div> </div> </div>
3	M	307	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div></div> </div> </div>

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
14	CDL	M	1314	-	-	-	X
4	GOL	H	1253	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	L	1283	-	-	-	X
6	LDA	L	1285	-	-	-	X
6	LDA	M	1309	-	-	-	X
6	LDA	M	1709	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7671 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			

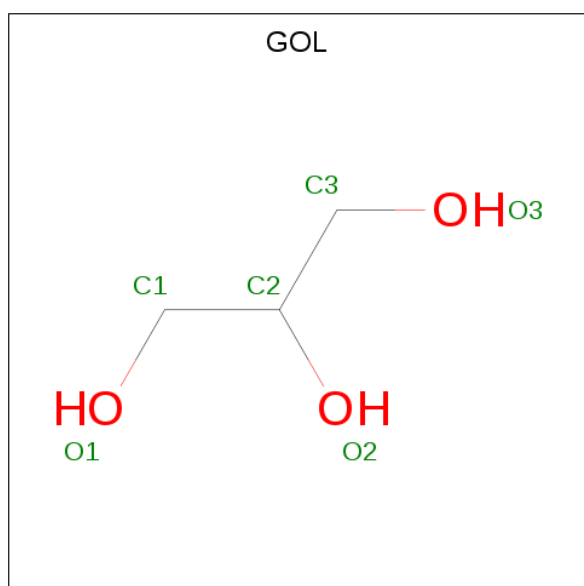
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

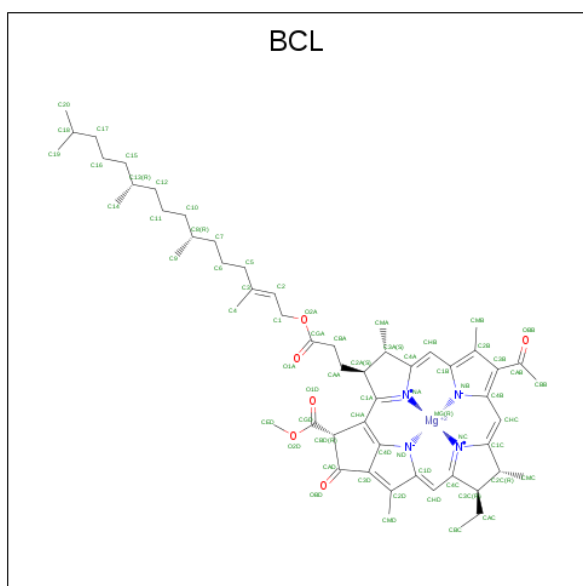
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: 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	M	1	Total	C	O	0	0
			6	3	3		

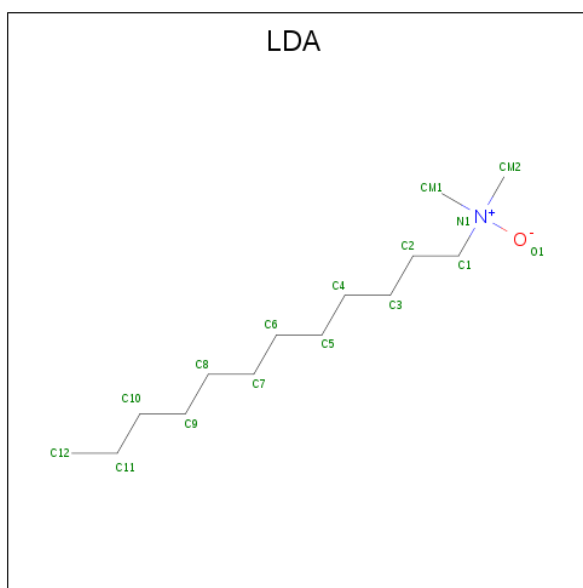
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

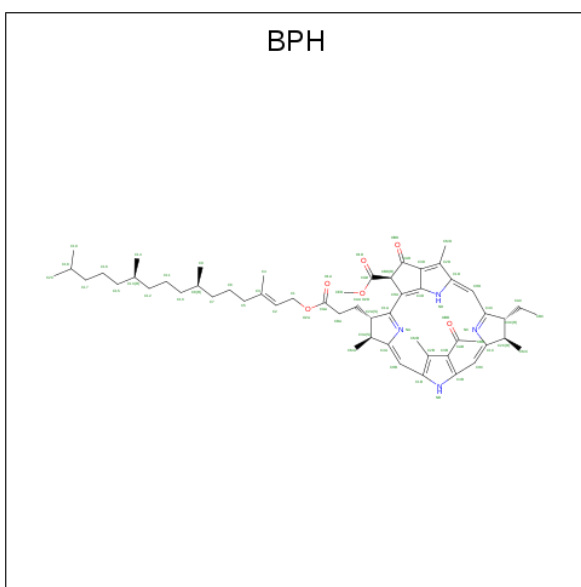
- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



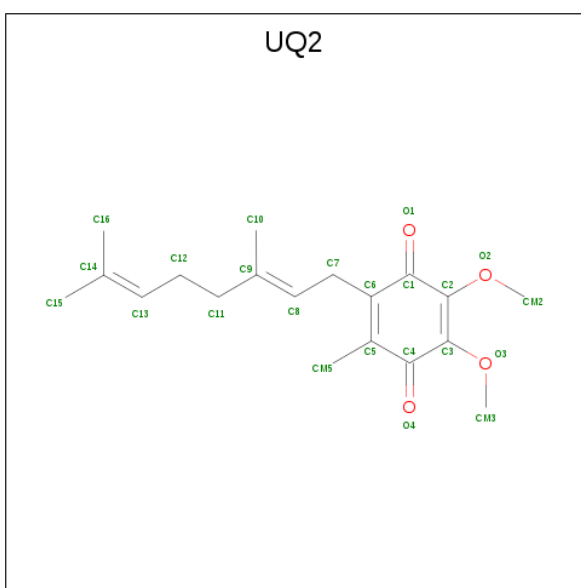
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



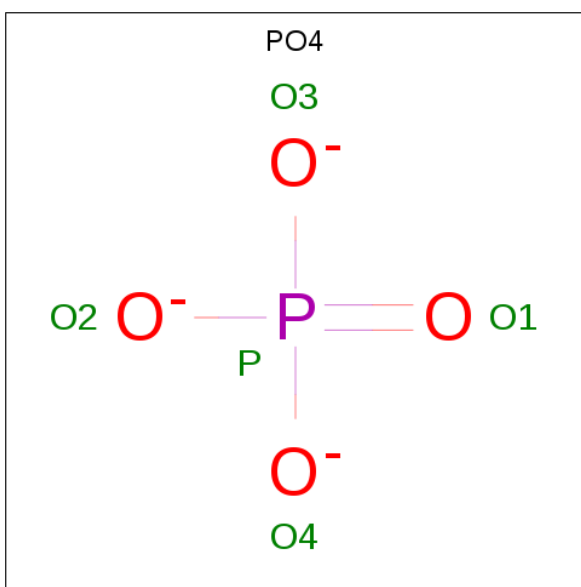
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



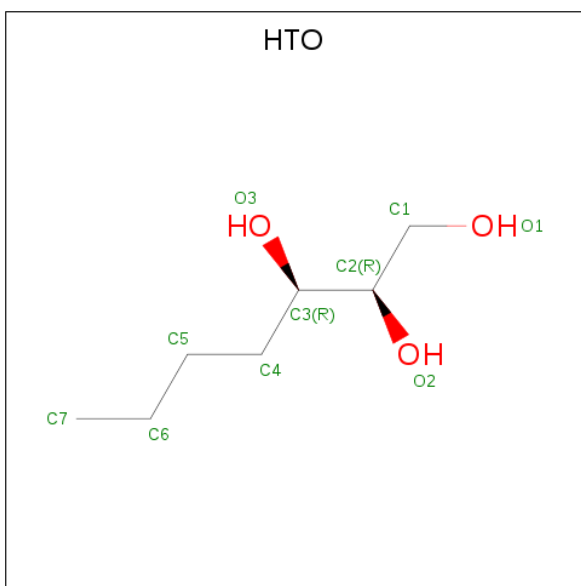
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 9 is PHOSPHATE ION (three-letter code: 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 (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

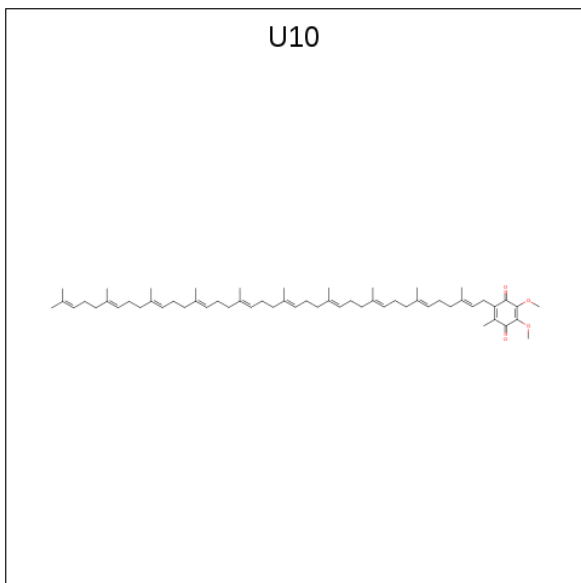


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

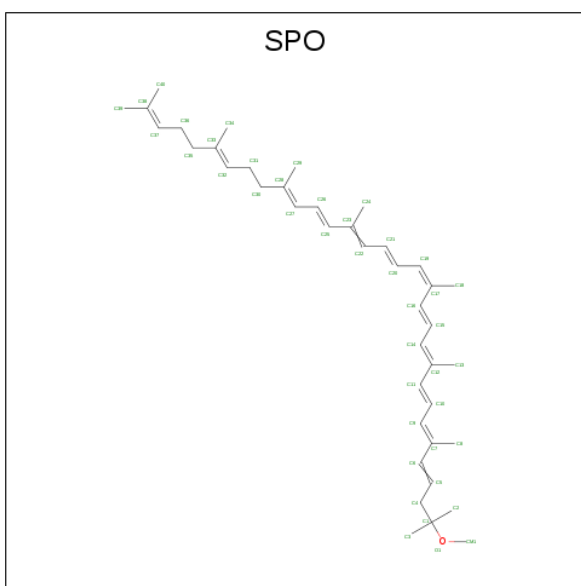
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

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



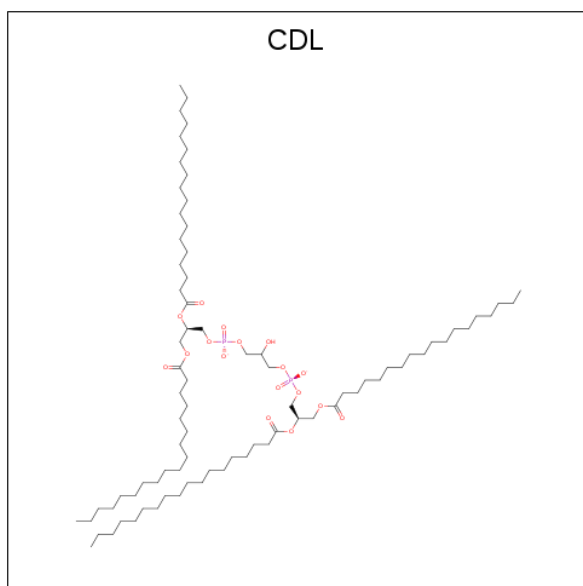
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 13 is SPHEROIDENE (three-letter code: 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 (three-letter code: 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		

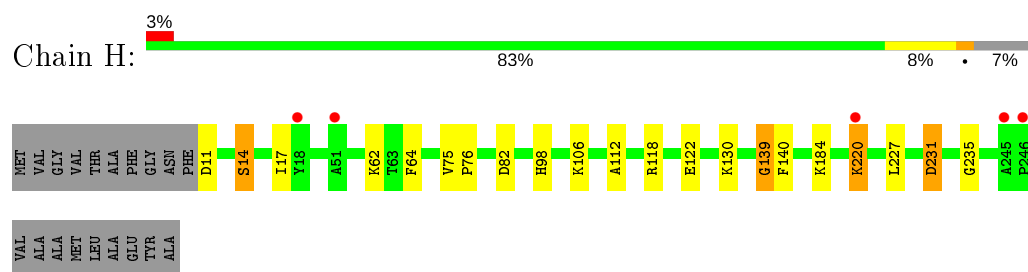
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	149	Total	O	0	0
			149	149		
15	L	111	Total	O	0	0
			111	111		
15	M	111	Total	O	0	0
			111	111		

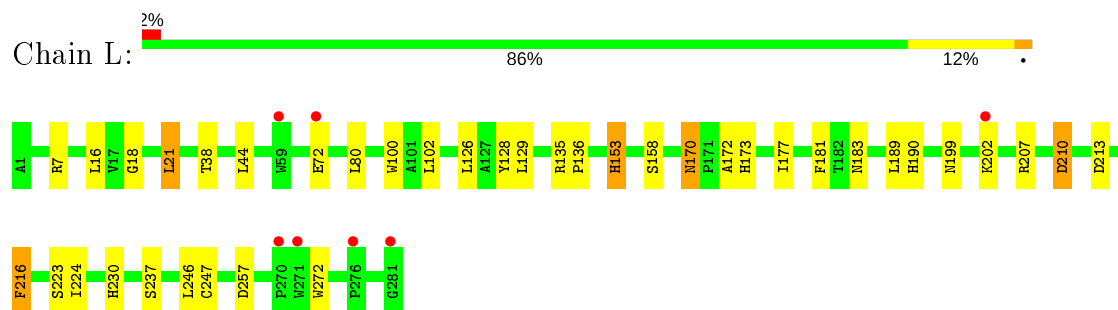
3 Residue-property plots [i](#)

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

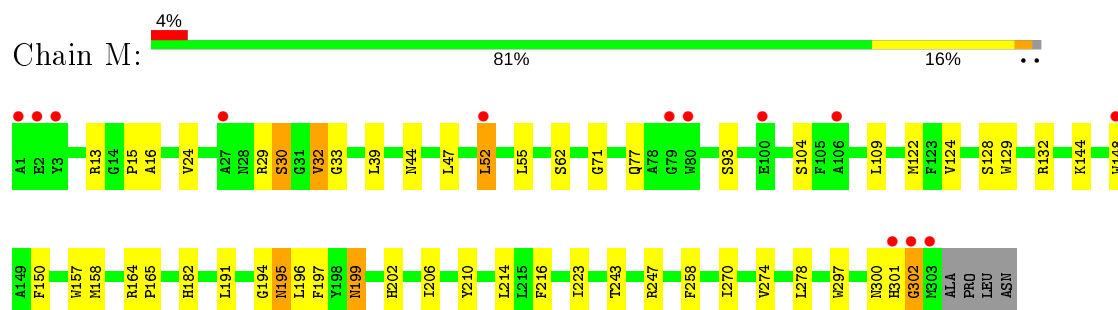
• Molecule 1: REACTION CENTER PROTEIN H CHAIN



• Molecule 2: REACTION CENTER PROTEIN L CHAIN



• Molecule 3: REACTION CENTER PROTEIN M CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.58Å 139.58Å 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.51 29.45 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.51) 90.9 (29.45-2.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.211 0.184 , 0.183	Depositor DCC
R_{free} test set	3493 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7671	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, FE, SPO, U10, UQ2

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	0.53	0/1906	0.74	4/2591 (0.2%)
2	L	0.56	0/2320	0.64	2/3175 (0.1%)
3	M	0.54	0/2501	0.63	0/3415
All	All	0.54	0/6727	0.66	6/9181 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	213	ASP	CB-CG-OD2	6.87	124.49	118.30
1	H	82	ASP	CB-CG-OD2	6.09	123.78	118.30
1	H	11	ASP	CB-CG-OD2	5.91	123.62	118.30
1	H	139	GLY	N-CA-C	-5.89	98.37	113.10
1	H	231	ASP	CB-CG-OD2	5.67	123.40	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1846	0	1861	16	0
2	L	2232	0	2187	26	0
3	M	2409	0	2321	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	24	0	32	1	0
4	L	12	0	16	1	0
4	M	6	0	8	2	0
5	L	132	0	148	7	0
5	M	132	0	148	24	0
6	L	48	0	93	7	0
6	M	96	0	186	10	0
7	L	65	0	76	7	0
7	M	65	0	76	12	0
8	L	46	0	52	6	0
9	L	5	0	0	0	0
10	L	10	0	16	0	0
11	M	1	0	0	0	0
12	M	48	0	63	0	0
13	M	42	0	60	4	0
14	M	81	0	82	2	0
15	H	149	0	0	3	0
15	L	111	0	0	1	0
15	M	111	0	0	1	0
All	All	7671	0	7425	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.

The worst 5 of 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)
1:H:248:ARG:HA	1:H:249:LYS:HB2	1.25	1.10
1:H:248:ARG:HA	1:H:249:LYS:CB	1.95	0.96
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.87
3:M:197:PHE:CZ	5:M:1304:BCL:HBB2	2.15	0.80
7:L:1286:BPH:HBB2	3:M:210:TYR:HB3	1.66	0.77

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	242/260 (93%)	233 (96%)	8 (3%)	1 (0%)	34	54
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100	100
3	M	301/307 (98%)	287 (95%)	9 (3%)	5 (2%)	9	16
All	All	822/848 (97%)	790 (96%)	26 (3%)	6 (1%)	22	39

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	301	HIS
3	M	52	LEU
3	M	195	ASN
3	M	30	SER

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	198/208 (95%)	189 (96%)	9 (4%)	27	51
2	L	220/220 (100%)	202 (92%)	18 (8%)	11	22
3	M	236/240 (98%)	224 (95%)	12 (5%)	24	45
All	All	654/668 (98%)	615 (94%)	39 (6%)	20	37

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	153	HIS
2	L	207	ARG
3	M	199	ASN
2	L	158	SER
2	L	170	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
3	M	199	ASN
3	M	187	ASN
2	L	170	ASN
3	M	77	GLN

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 carbohydrates 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
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.25	0
6	LDA	L	1285	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
14	CDL	M	1314	-	80,80,99	2.33	18 (22%)	86,92,111	4.01	15 (17%)
4	GOL	H	1251	-	5,5,5	0.52	0	5,5,5	0.73	0
6	LDA	M	1309	-	12,15,15	2.01	1 (8%)	14,17,17	0.45	0
4	GOL	H	1253	-	5,5,5	0.35	0	5,5,5	0.28	0
6	LDA	L	1284	-	12,15,15	2.04	1 (8%)	14,17,17	0.50	0
13	SPO	M	1313	-	40,41,41	4.16	12 (30%)	47,50,50	1.89	11 (23%)
12	U10	M	1312	-	48,48,63	2.69	12 (25%)	58,61,79	1.65	12 (20%)
9	PO4	L	1289	-	4,4,4	0.84	0	6,6,6	0.48	0
6	LDA	M	1308	-	12,15,15	2.05	1 (8%)	14,17,17	0.46	0
5	BCL	M	1304	3	58,74,74	2.21	8 (13%)	69,115,115	1.95	18 (26%)
4	GOL	L	1292	-	5,5,5	0.36	0	5,5,5	0.23	0
4	GOL	L	1291	-	5,5,5	0.32	0	5,5,5	0.51	0
5	BCL	L	1282	2	58,74,74	2.17	8 (13%)	69,115,115	2.21	20 (28%)
5	BCL	M	1303	3	58,74,74	2.26	9 (15%)	69,115,115	1.98	14 (20%)
4	GOL	M	1315	-	5,5,5	0.33	0	5,5,5	0.31	0
10	HTO	L	1290	-	9,9,9	0.43	0	10,10,10	0.57	0
6	LDA	L	1283	-	12,15,15	2.03	1 (8%)	14,17,17	0.49	0
6	LDA	M	1307	-	12,15,15	2.00	1 (8%)	14,17,17	0.60	0
8	UQ2	L	1287[A]	-	23,23,23	2.67	8 (34%)	28,31,31	1.61	5 (17%)
6	LDA	M	1306	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
8	UQ2	L	1287[B]	-	23,23,23	2.76	7 (30%)	28,31,31	1.18	1 (3%)
4	GOL	H	1252	-	5,5,5	0.38	0	5,5,5	0.22	0
6	LDA	M	1305	-	12,15,15	2.10	1 (8%)	14,17,17	0.49	0
7	BPH	M	1311	-	64,70,70	3.01	17 (26%)	76,101,101	1.66	15 (19%)
6	LDA	M	1709	-	12,15,15	2.02	1 (8%)	14,17,17	0.51	0
5	BCL	L	1288	2	58,74,74	2.18	8 (13%)	69,115,115	2.00	17 (24%)
7	BPH	L	1286	-	64,70,70	3.02	17 (26%)	76,101,101	1.67	13 (17%)

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
4	GOL	H	1254	-	-	0/4/4/4	-
6	LDA	L	1285	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	M	1314	-	-	46/91/91/110	-
4	GOL	H	1251	-	-	4/4/4/4	-
6	LDA	M	1309	-	-	12/13/13/13	-
4	GOL	H	1253	-	-	1/4/4/4	-
6	LDA	L	1284	-	-	4/13/13/13	-
13	SPO	M	1313	-	-	24/47/47/47	-
12	U10	M	1312	-	-	13/45/69/87	0/1/1/1
6	LDA	M	1308	-	-	5/13/13/13	-
5	BCL	M	1304	3	2/2/21/25	9/37/137/137	-
4	GOL	L	1292	-	-	4/4/4/4	-
4	GOL	L	1291	-	-	2/4/4/4	-
5	BCL	L	1282	2	2/2/21/25	9/37/137/137	-
5	BCL	M	1303	3	2/2/21/25	16/37/137/137	-
4	GOL	M	1315	-	-	3/4/4/4	-
10	HTO	L	1290	-	-	7/10/10/10	-
6	LDA	L	1283	-	-	6/13/13/13	-
6	LDA	M	1307	-	-	8/13/13/13	-
8	UQ2	L	1287[A]	-	-	8/15/39/39	0/1/1/1
6	LDA	M	1306	-	-	7/13/13/13	-
8	UQ2	L	1287[B]	-	-	8/15/39/39	0/1/1/1
4	GOL	H	1252	-	-	4/4/4/4	-
6	LDA	M	1305	-	-	5/13/13/13	-
7	BPH	M	1311	-	-	24/54/105/105	0/5/6/6
6	LDA	M	1709	-	-	8/13/13/13	-
5	BCL	L	1288	2	2/2/21/25	9/37/137/137	-
7	BPH	L	1286	-	-	14/54/105/105	0/5/6/6

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1304	BCL	OBD-CAD	13.41	1.41	1.22
5	M	1303	BCL	OBD-CAD	13.35	1.41	1.22
7	L	1286	BPH	OBD-CAD	12.97	1.40	1.22
5	L	1282	BCL	OBD-CAD	12.89	1.40	1.22
7	M	1311	BPH	OBD-CAD	12.82	1.40	1.22

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	1314	CDL	C33-C32-C31	18.27	178.87	113.19
14	M	1314	CDL	C13-C12-C11	12.79	159.15	113.19
14	M	1314	CDL	C17-C16-C15	12.53	178.05	114.42
14	M	1314	CDL	C35-C34-C33	12.51	177.91	114.42
14	M	1314	CDL	C34-C33-C32	12.33	177.02	114.42

5 of 8 chirality outliers are listed below:

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

5 of 269 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	M	1314	CDL	CA3-OA5-PA1-OA3
14	M	1314	CDL	CB3-OB5-PB2-OB2
14	M	1314	CDL	CB3-OB5-PB2-OB3
4	H	1251	GOL	O1-C1-C2-O2
4	H	1251	GOL	O1-C1-C2-C3

There are no ring outliers.

20 monomers are involved in 72 short contacts:

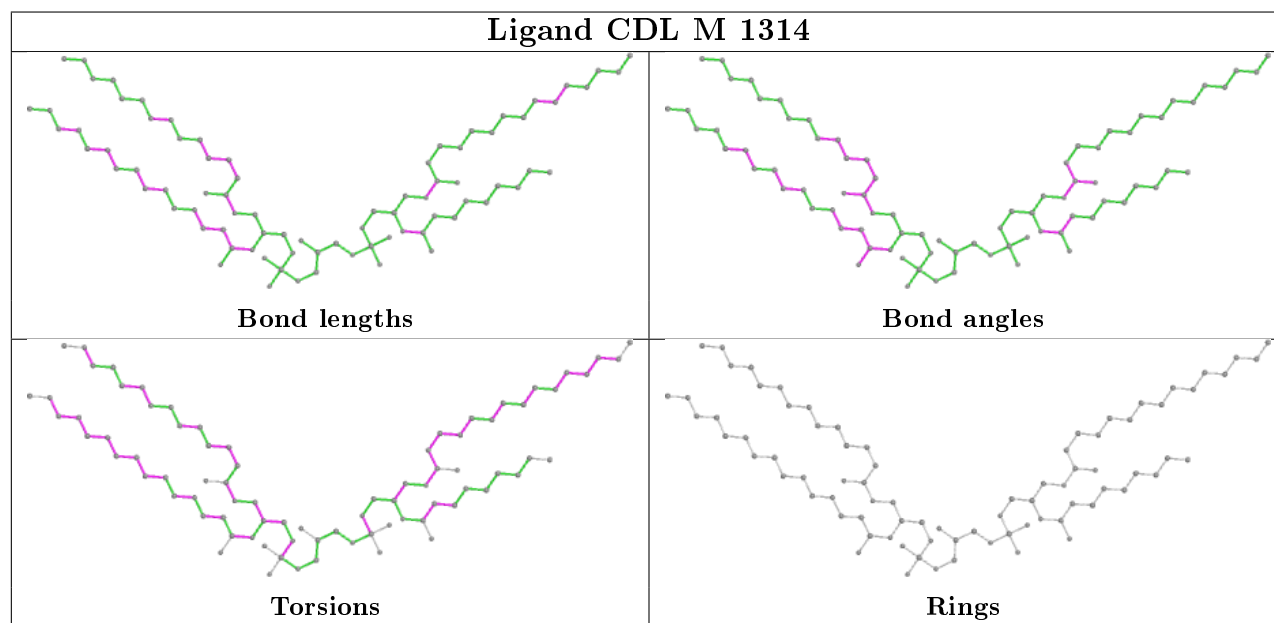
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1285	LDA	4	0
14	M	1314	CDL	2	0
4	H	1251	GOL	1	0
6	M	1309	LDA	3	0
6	L	1284	LDA	2	0
13	M	1313	SPO	4	0
6	M	1308	LDA	2	0
5	M	1304	BCL	15	0
4	L	1291	GOL	1	0
5	L	1282	BCL	4	0
5	M	1303	BCL	11	0
4	M	1315	GOL	2	0
6	L	1283	LDA	1	0
6	M	1307	LDA	5	0
8	L	1287[A]	UQ2	5	0

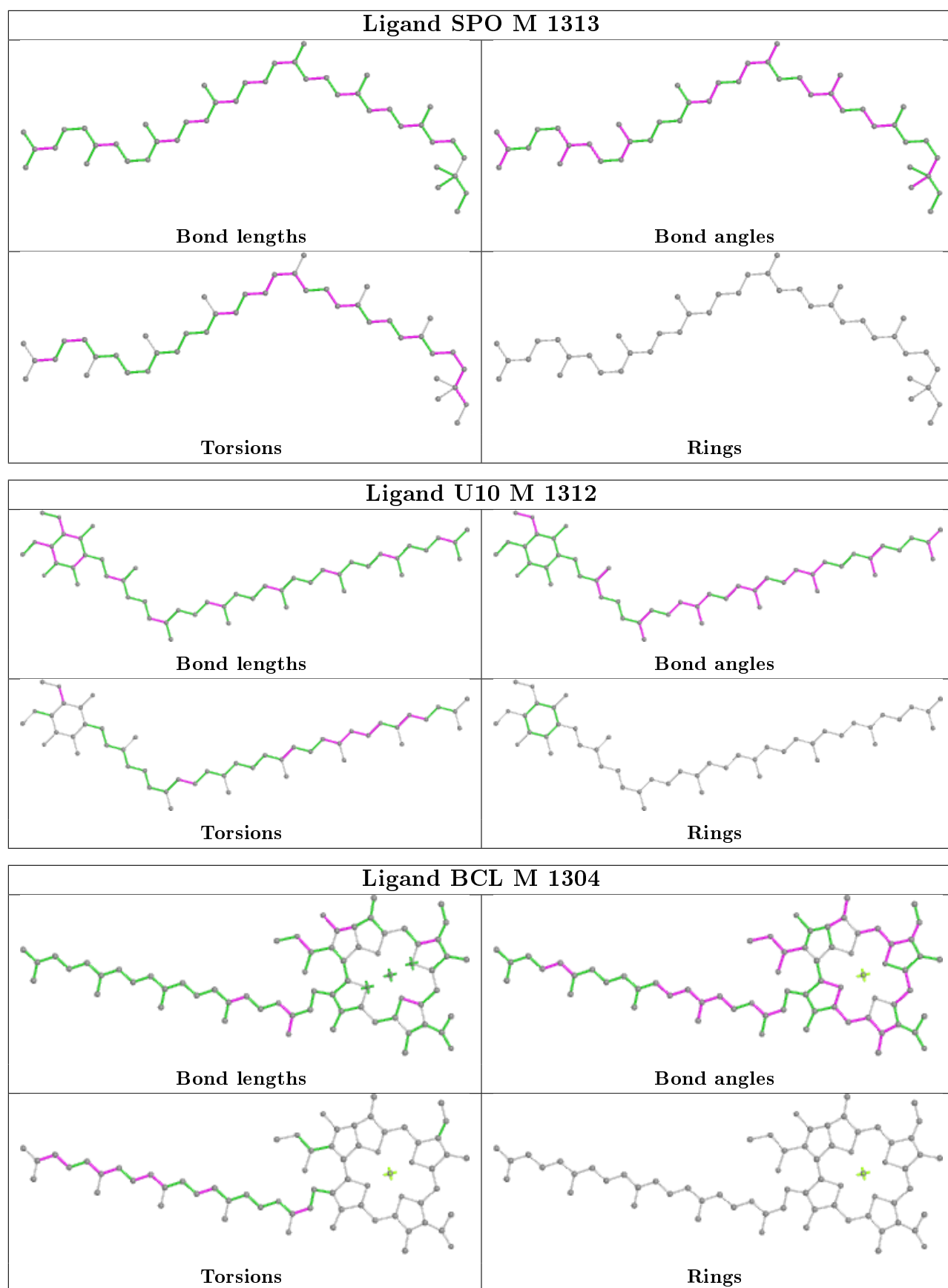
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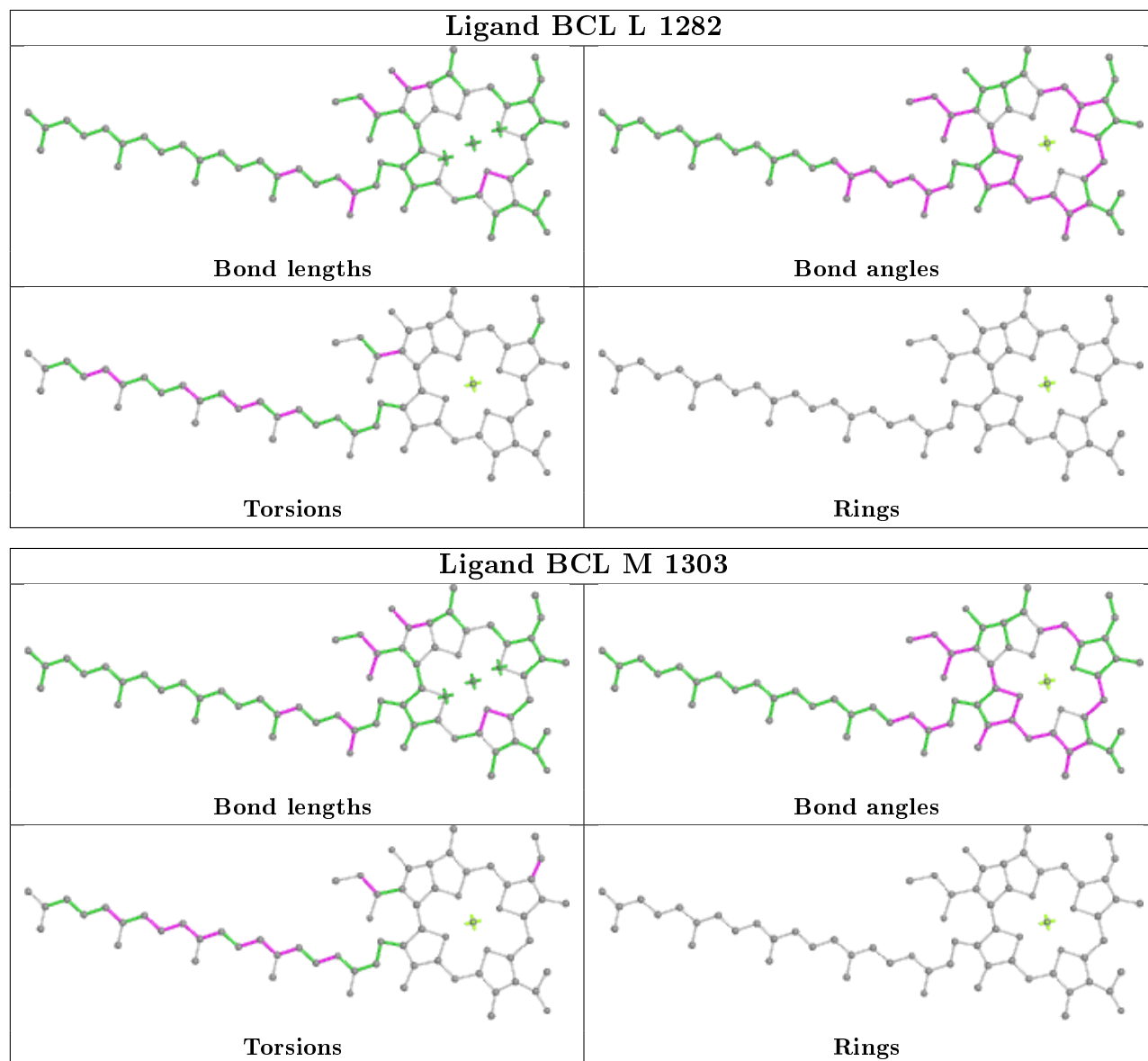
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1287[B]	UQ2	1	0
6	M	1305	LDA	3	0
7	M	1311	BPH	12	0
5	L	1288	BCL	5	0
7	L	1286	BPH	7	0

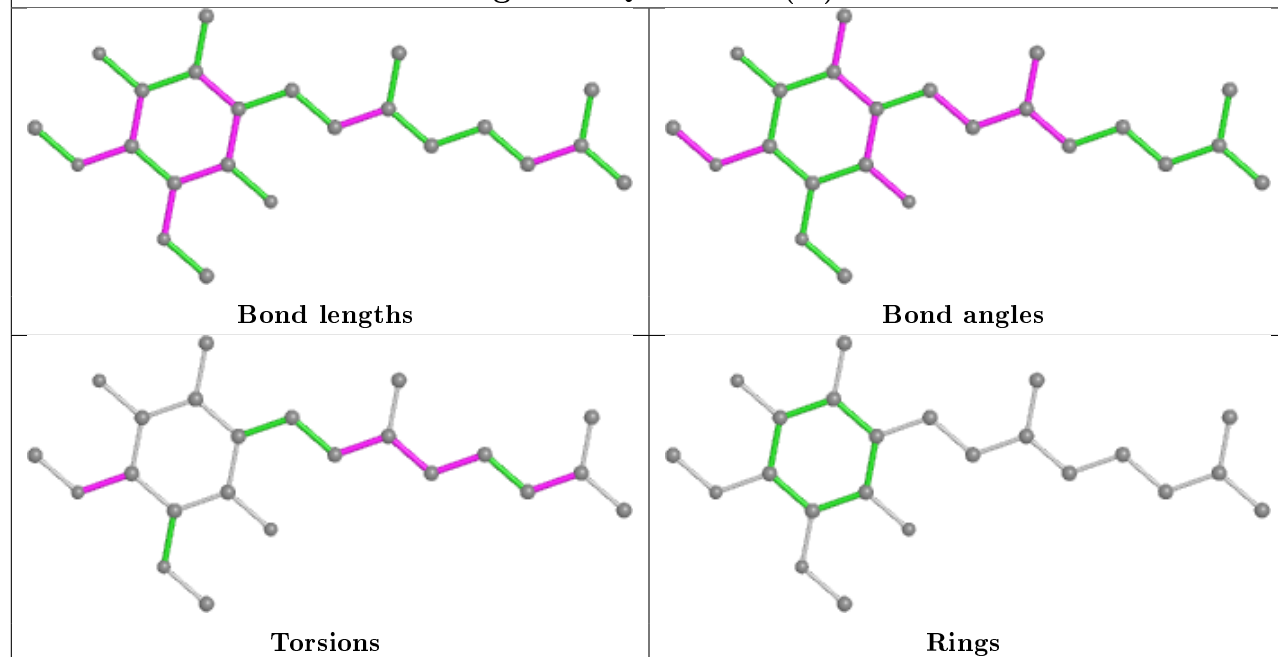
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



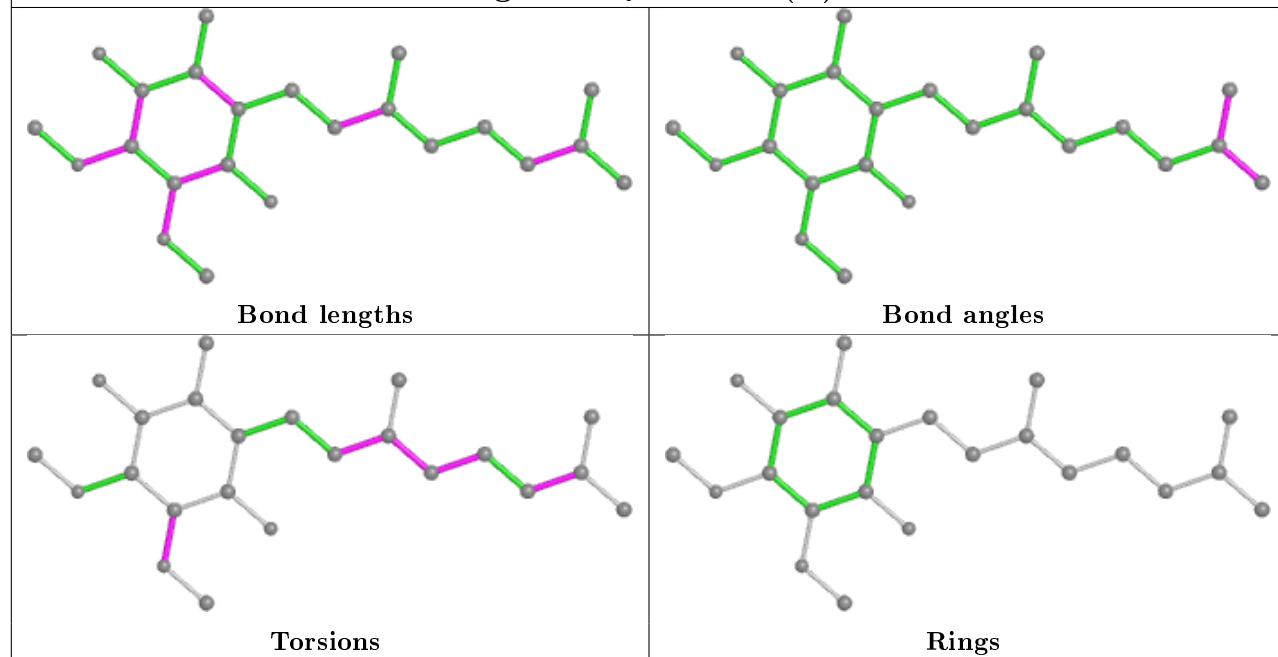




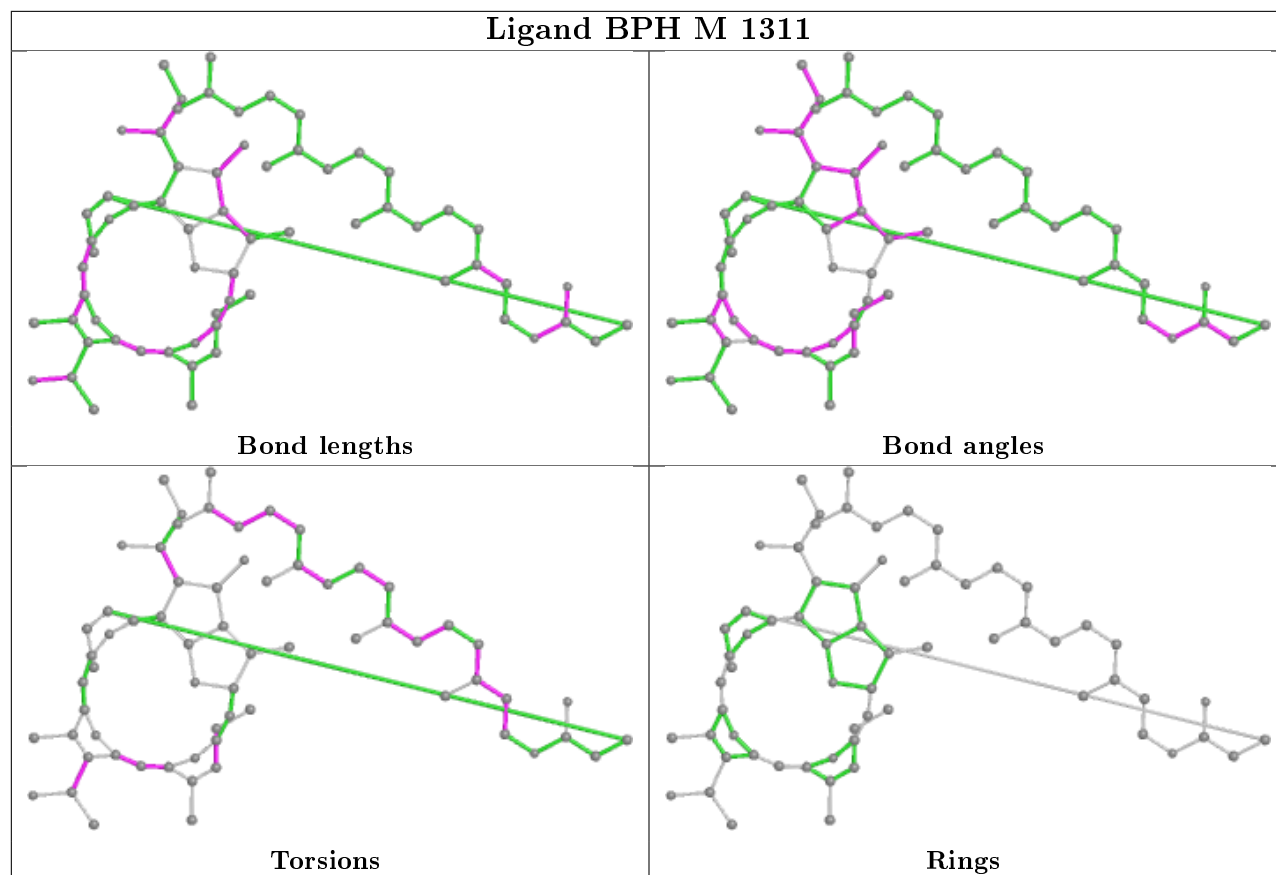
Ligand UQ2 L 1287 (A)



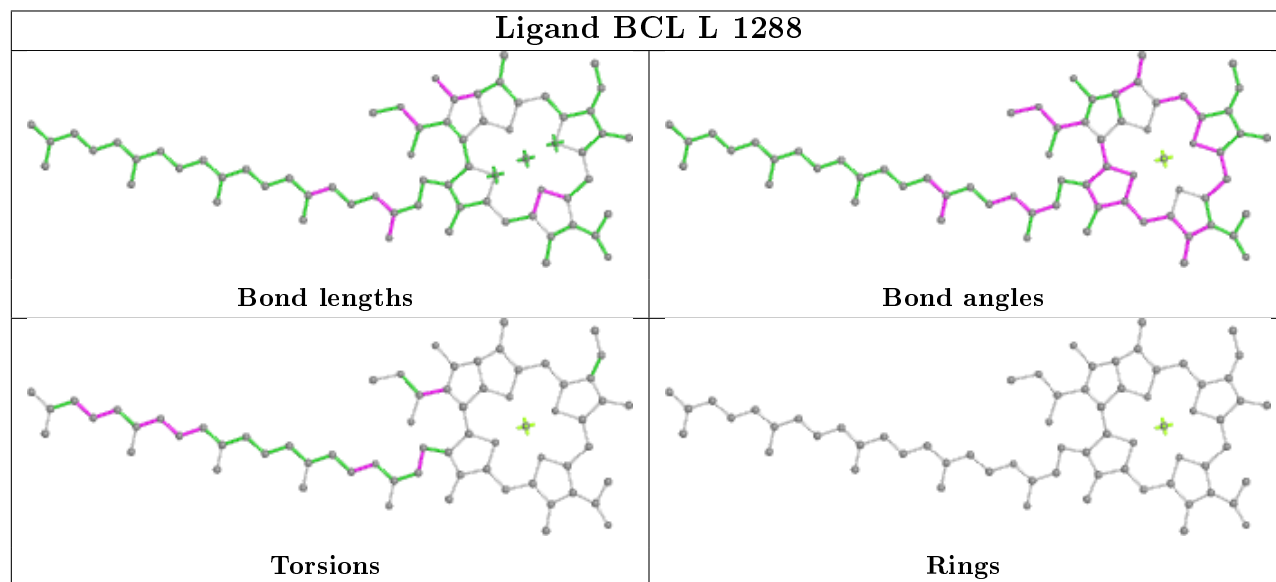
Ligand UQ2 L 1287 (B)

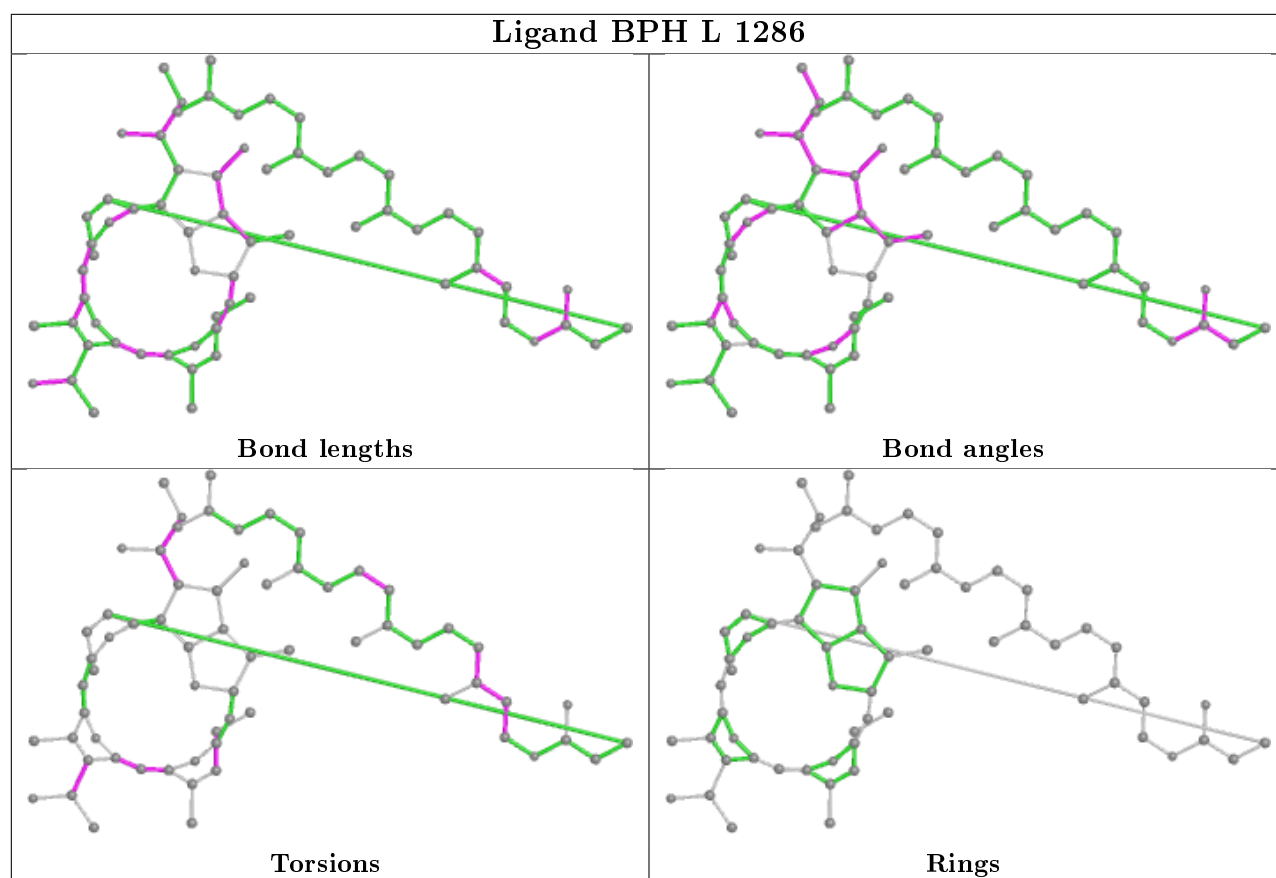


Ligand BPH M 1311



Ligand BCL L 1288





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	241/260 (92%)	-0.39	9 (3%) 41 45	33, 43, 53, 85	0
2	L	281/281 (100%)	-0.53	7 (2%) 57 61	30, 39, 61, 68	0
3	M	303/307 (98%)	-0.38	13 (4%) 35 38	29, 44, 69, 76	0
All	All	825/848 (97%)	-0.43	29 (3%) 44 47	29, 42, 63, 85	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	6.3
3	M	1	ALA	5.4
1	H	249	LYS	4.6
1	H	251	VAL	4.4
3	M	148	TRP	4.4

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 carbohydrates in this entry.

6.4 Ligands [i](#)

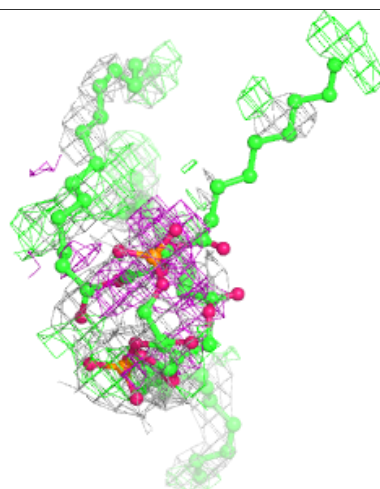
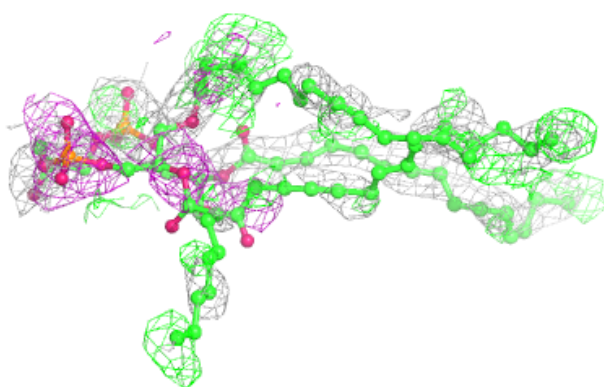
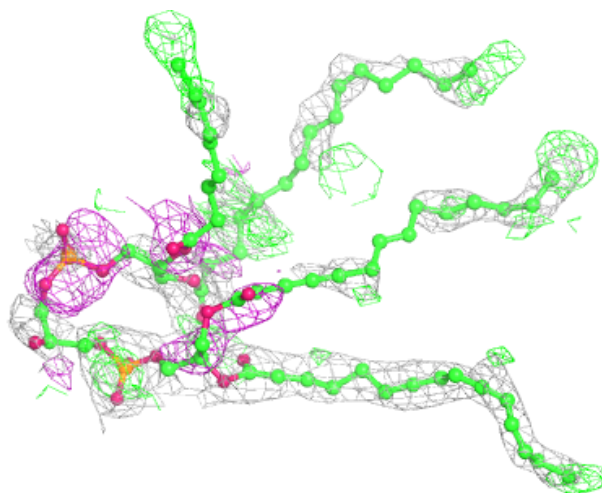
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	LDA	M	1309	16/16	0.12	0.55	94,102,110,110	0
6	LDA	L	1283	16/16	0.27	0.48	86,103,111,111	0
6	LDA	M	1709	16/16	0.40	0.49	92,100,107,107	0
14	CDL	M	1314	81/100	0.50	0.50	96,107,120,121	0
6	LDA	M	1308	16/16	0.53	0.39	90,97,105,105	0
6	LDA	L	1284	16/16	0.59	0.32	98,102,109,109	0
6	LDA	L	1285	16/16	0.67	0.41	106,109,111,111	0
4	GOL	H	1253	6/6	0.74	0.41	102,103,104,104	0
10	HTO	L	1290	10/10	0.74	0.36	74,77,77,78	0
4	GOL	L	1292	6/6	0.79	0.25	85,87,87,87	0
4	GOL	H	1254	6/6	0.79	0.21	102,102,103,103	0
6	LDA	M	1307	16/16	0.80	0.24	64,68,77,77	0
6	LDA	M	1306	16/16	0.80	0.33	72,74,84,84	0
6	LDA	M	1305	16/16	0.80	0.28	50,63,70,71	0
4	GOL	M	1315	6/6	0.80	0.22	85,86,86,87	0
4	GOL	H	1251	6/6	0.83	0.23	65,68,70,71	0
8	UQ2	L	1287[A]	23/23	0.84	0.31	39,42,51,52	23
8	UQ2	L	1287[B]	23/23	0.84	0.31	40,43,47,48	23
13	SPO	M	1313	42/42	0.86	0.21	38,51,68,71	0
4	GOL	H	1252	6/6	0.88	0.31	88,89,89,89	0
4	GOL	L	1291	6/6	0.89	0.19	47,52,53,54	0
7	BPH	M	1311	65/65	0.91	0.17	35,42,94,95	0
12	U10	M	1312	48/63	0.93	0.15	30,39,68,69	0
9	PO4	L	1289	5/5	0.95	0.26	103,103,103,103	0
5	BCL	M	1303	66/66	0.96	0.14	26,31,80,81	0
5	BCL	L	1282	66/66	0.97	0.12	30,34,51,54	0
5	BCL	M	1304	66/66	0.97	0.16	25,31,53,59	0
5	BCL	L	1288	66/66	0.97	0.13	25,30,48,52	0
7	BPH	L	1286	65/65	0.98	0.13	25,30,39,40	0
11	FE	M	1310	1/1	0.99	0.02	32,32,32,32	0

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

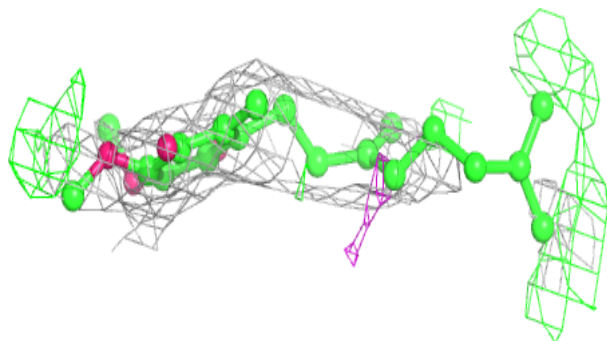
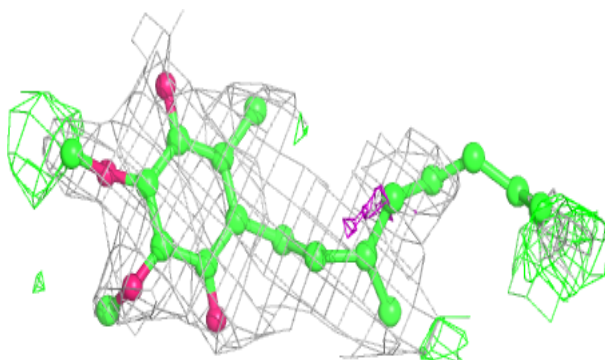
Electron density around CDL M 1314:

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

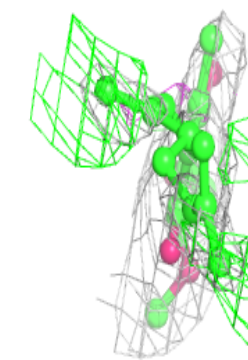
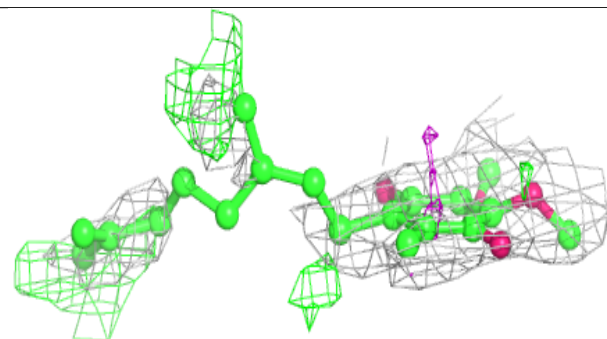
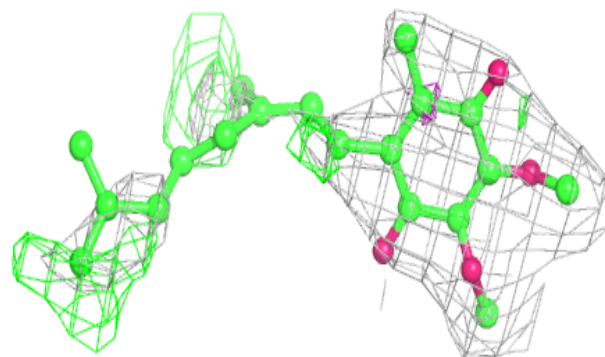


Electron density around UQ2 L 1287 (A):

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

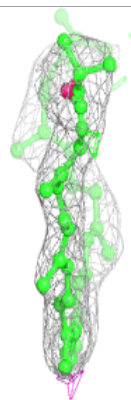
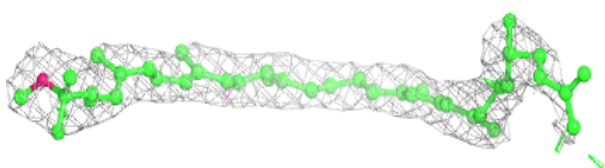
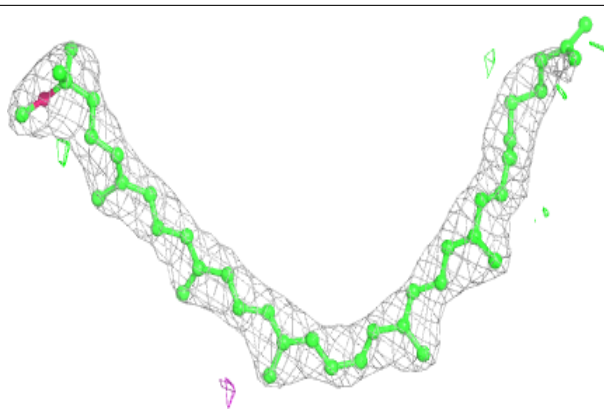
**Electron density around UQ2 L 1287 (B):**

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

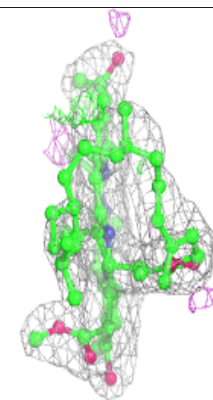
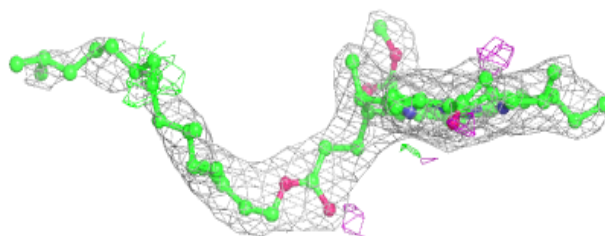
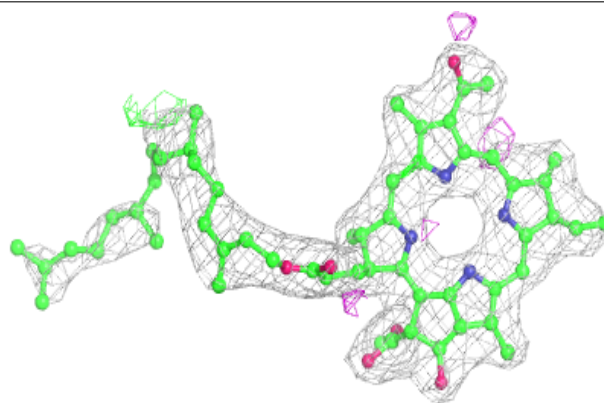


Electron density around SPO M 1313:

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

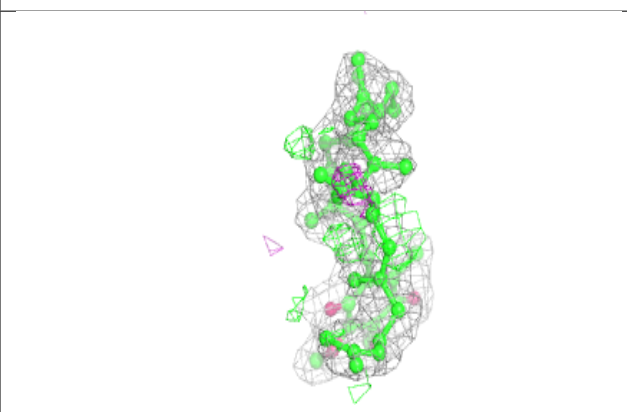
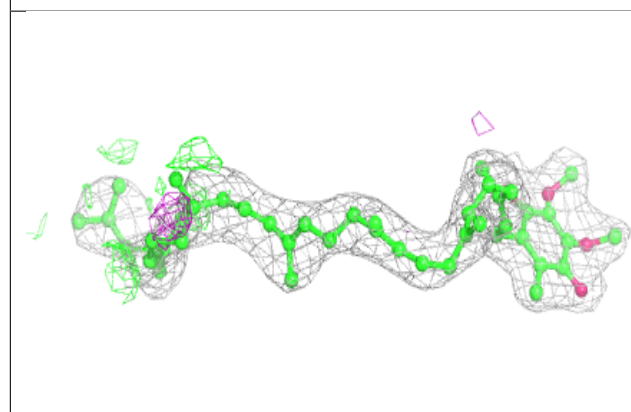
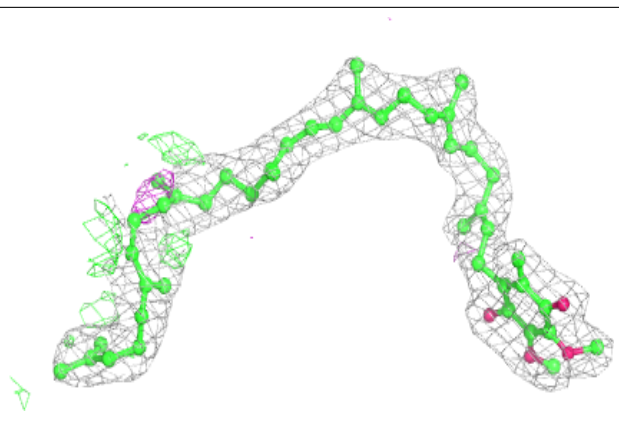
**Electron density around BPH M 1311:**

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



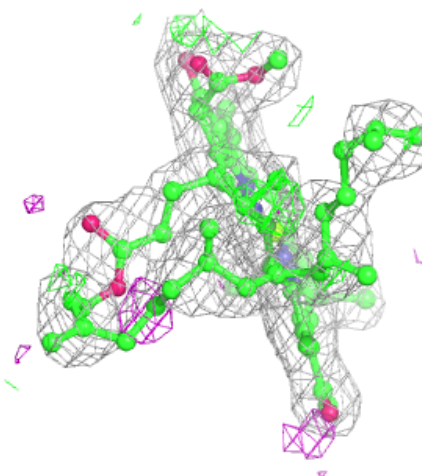
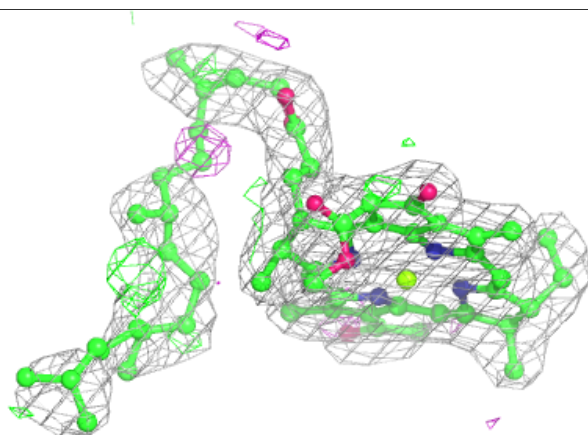
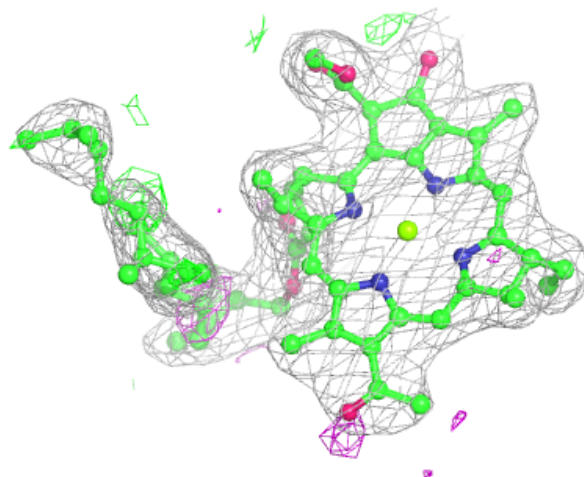
Electron density around U10 M 1312:

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



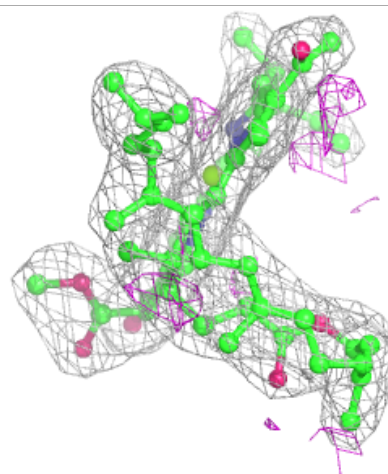
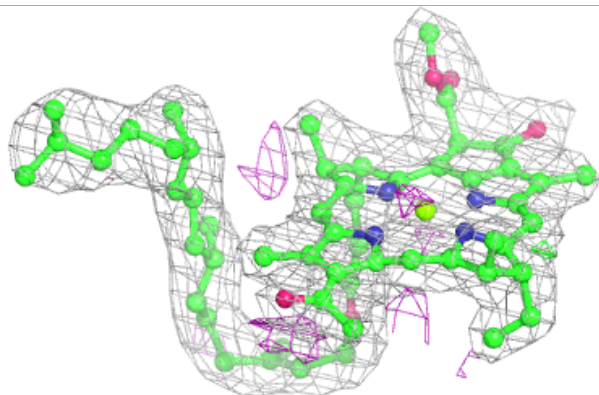
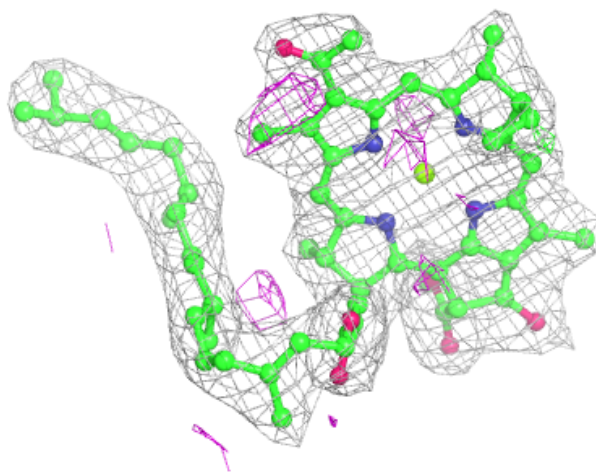
Electron density around BCL M 1303:

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



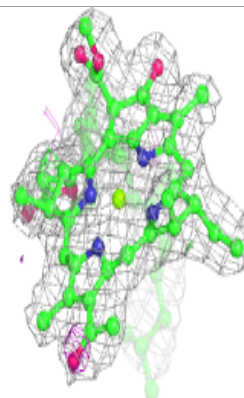
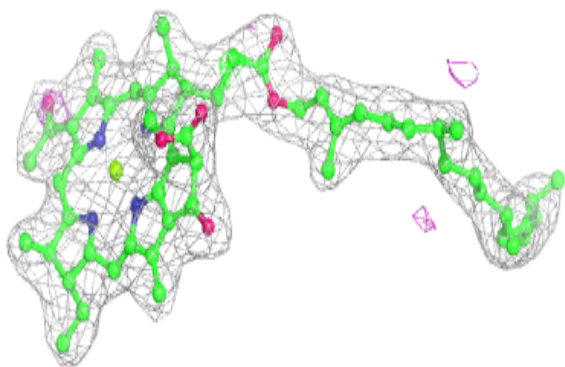
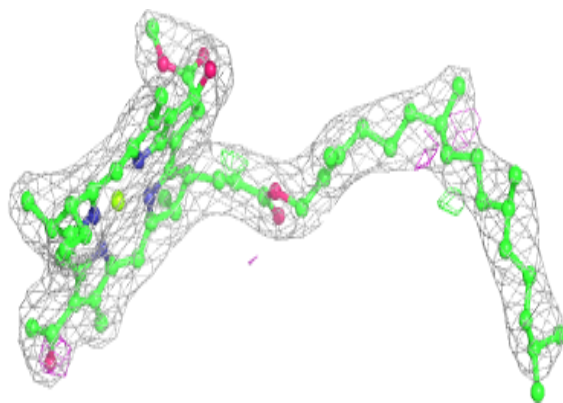
Electron density around BCL L 1282:

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

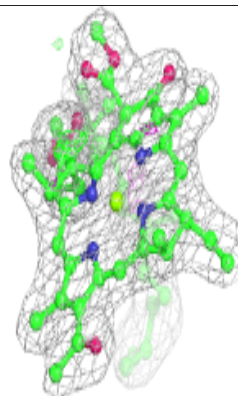
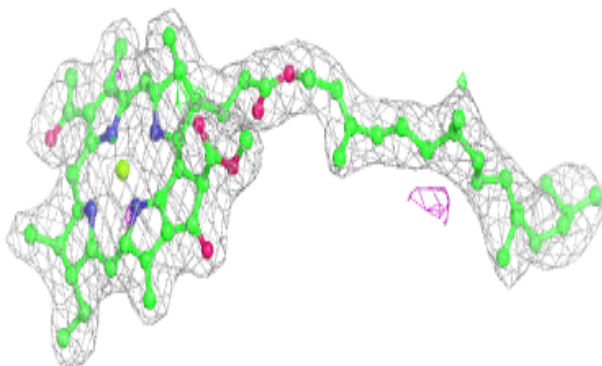
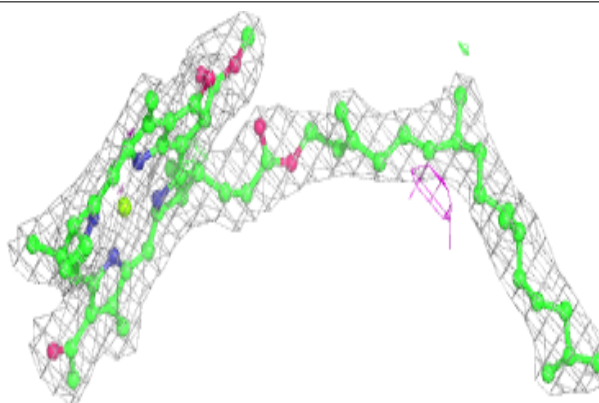


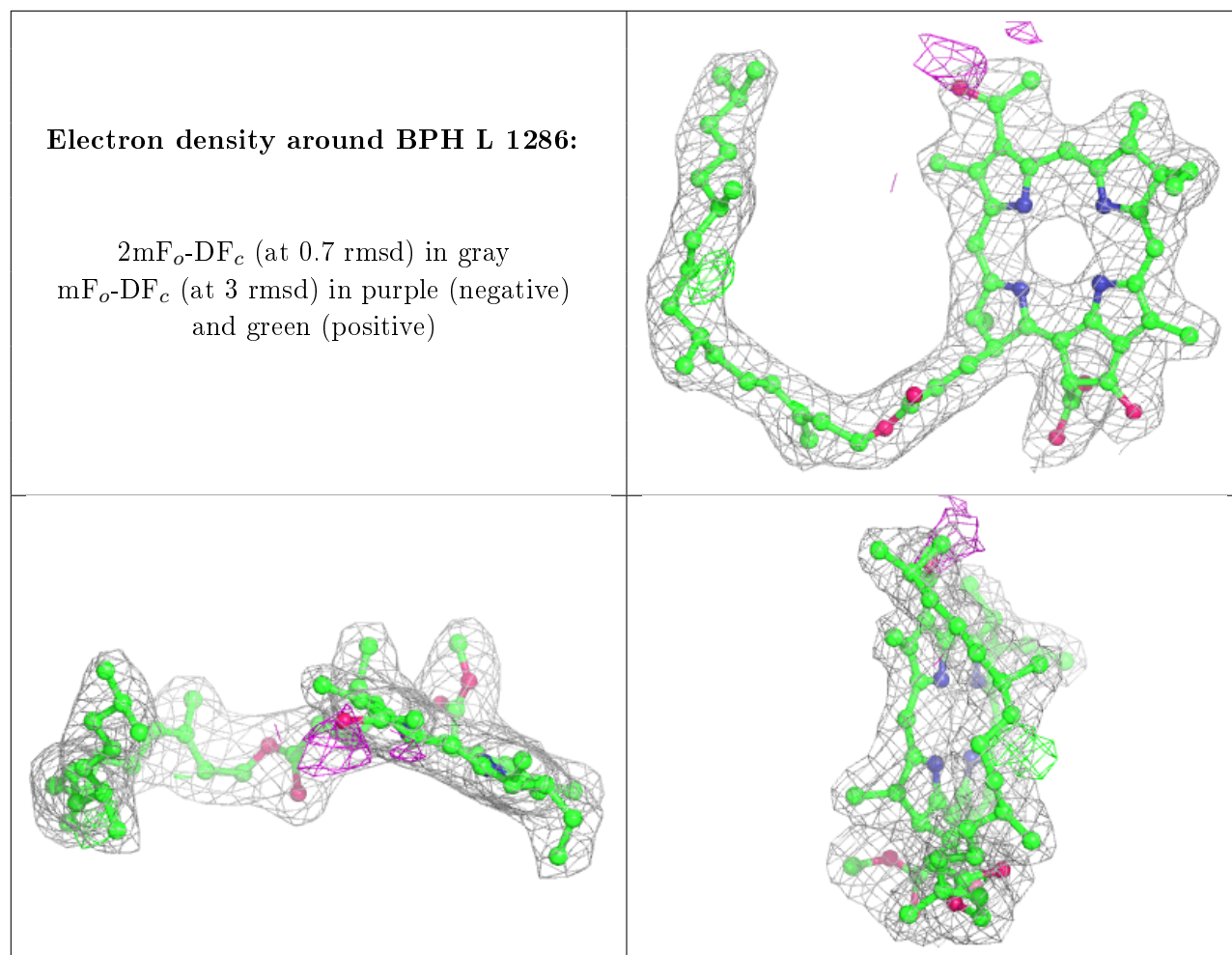
Electron density around BCL M 1304:

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

**Electron density around BCL L 1288:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.