wwPDB X-ray Structure Validation Summary Report (i)

Dec 7, 2023 – 07:48 am GMT

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

The following versions of software and data (see references (i)) were used in the production of this report:

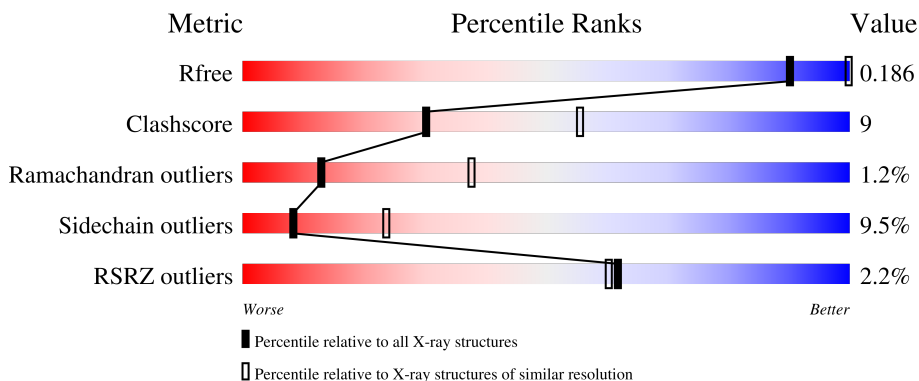|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.186
Clashscore		9
Ramachandran outliers		1.2%
Sidechain outliers		9.5%
RSRZ outliers		2.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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

Mol	Chain	Length	Quality of chain
1	H	260	2% / 70% / 19% · 7%
2	L	281	2% / 81% / 16% ·
3	M	307	3% / 75% / 20% · ··

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:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	H	1253	-	-	-	X
5	BCL	L	1282	X	-	-	-
5	BCL	L	1285	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
7	UQ2	L	1284[B]	-	-	X	-

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 7302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	3	1
			1846	1181	319	337	9			

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

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

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
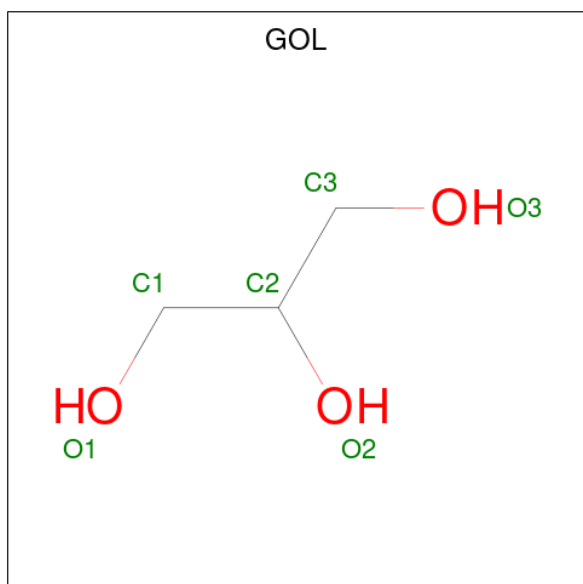
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).
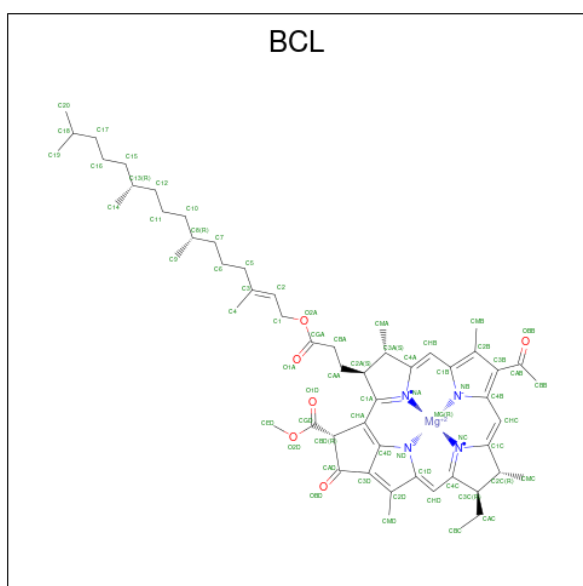
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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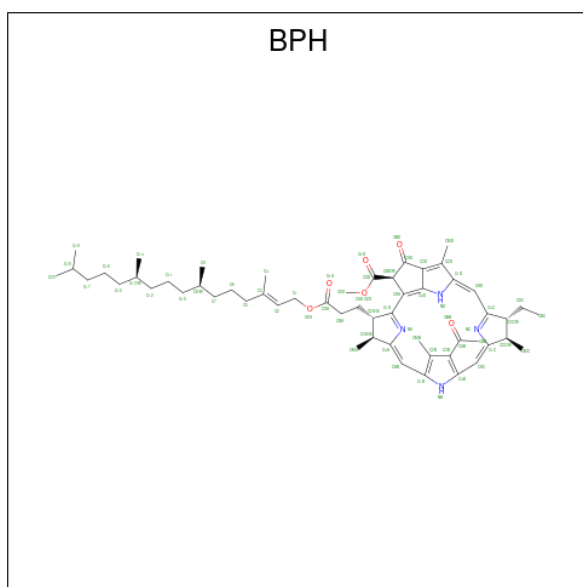
BPH

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

- Molecule 7 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).

UQ2
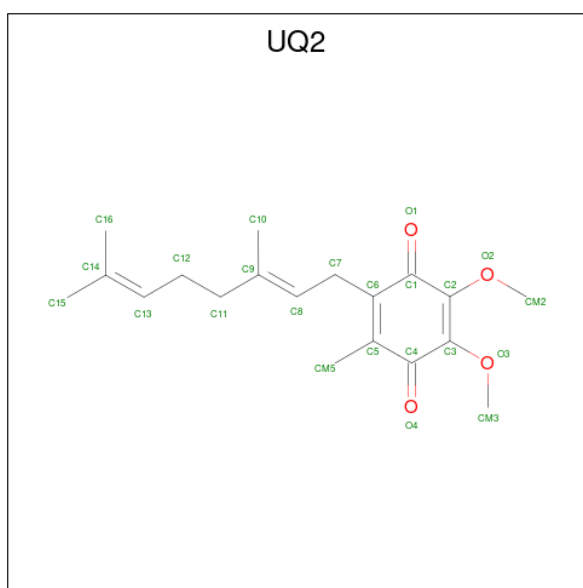
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

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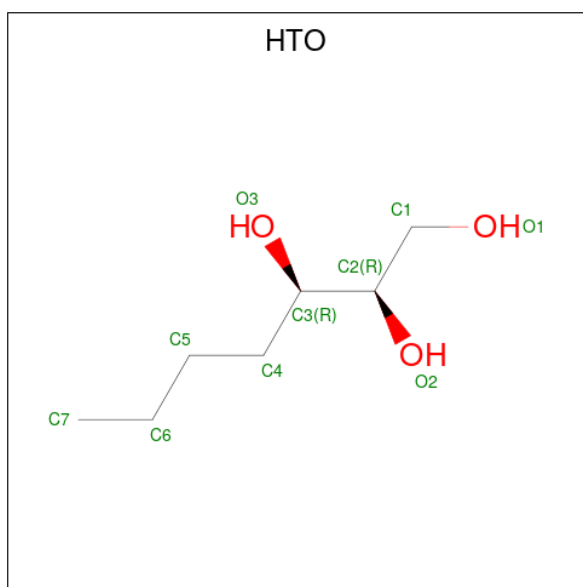
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total 10	C 7	O 3	0	0

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

LDA

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

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

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).
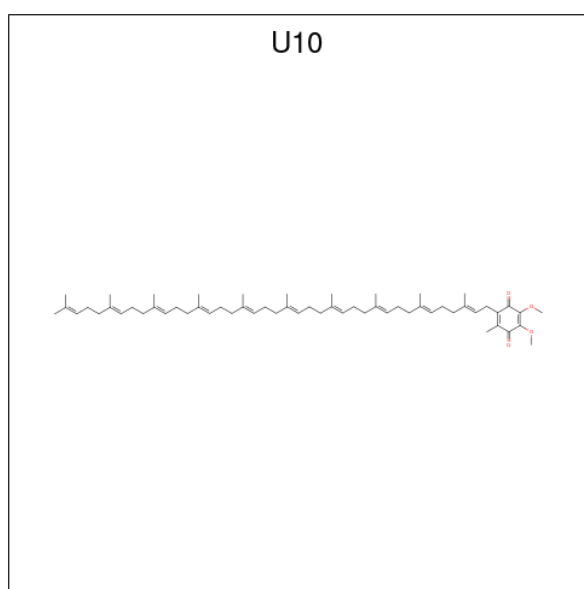
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	M	1	Total 48	C 44	O 4	0	0

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).
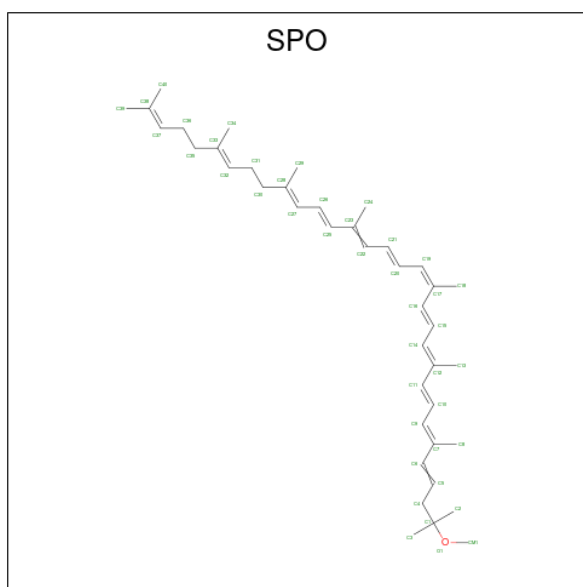
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total 42	C 41	O 1	0	0

- Molecule 13 is water.

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

# 3 Residue-property plots ⓘ

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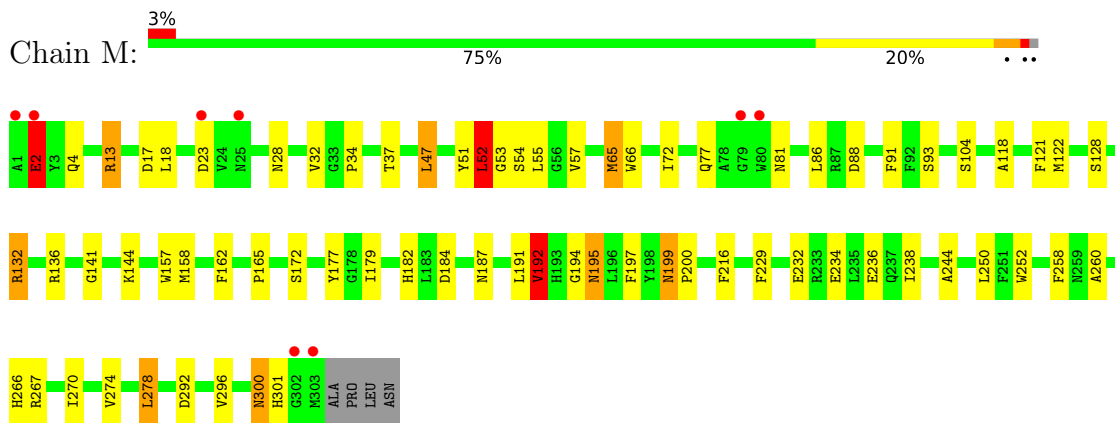
- Molecule 1: REACTION CENTER PROTEIN H CHAIN
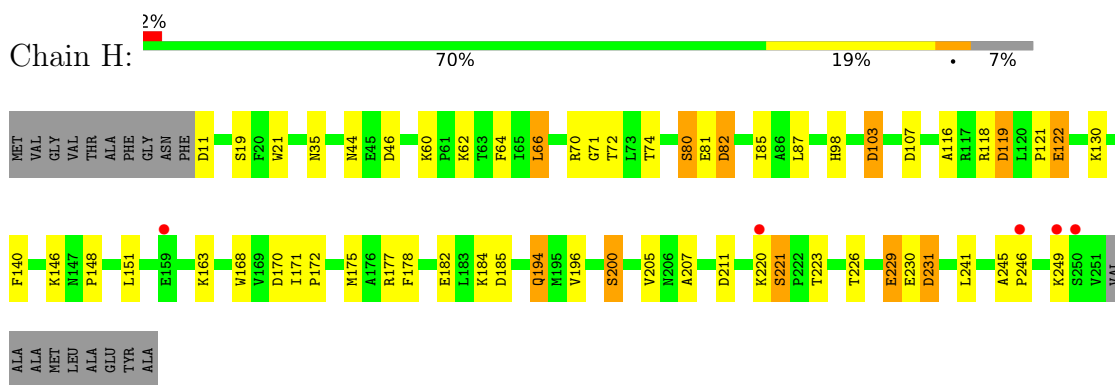
- Molecule 2: REACTION CENTER PROTEIN L CHAIN
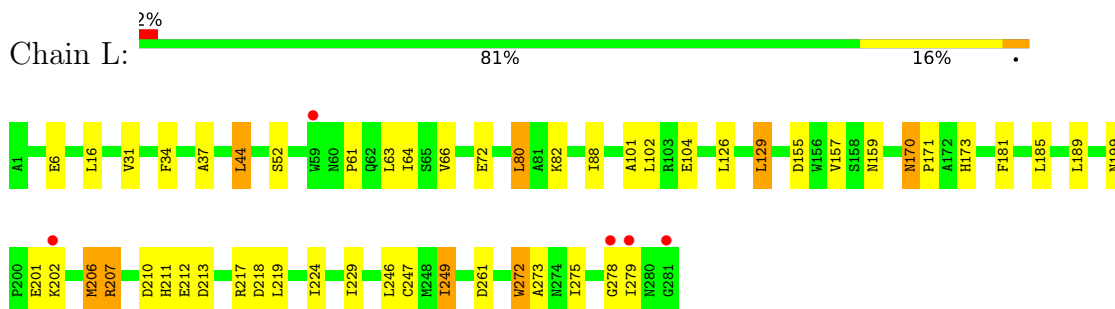
- Molecule 3: REACTION CENTER PROTEIN M CHAIN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.00Å 139.00Å 183.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.88 42.91 – 2.88	Depositor EDS
% Data completeness (in resolution range)	81.2 (119.52-2.88) 77.9 (42.91-2.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.176 , 0.220 0.179 , 0.186	Depositor DCC
R_{free} test set	1906 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 67.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7302	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, GOL, U10, LDA, BCL, HTO, BPH, FE, 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	0.83	2/1906 (0.1%)	0.92	7/2591 (0.3%)
2	L	0.80	0/2320	0.82	4/3175 (0.1%)
3	M	0.78	0/2501	0.81	5/3415 (0.1%)
All	All	0.80	2/6727 (0.0%)	0.85	16/9181 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	122	GLU	CG-CD	5.70	1.60	1.51
1	H	194	GLN	CG-CD	5.07	1.62	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	52	LEU	CA-CB-CG	8.47	134.77	115.30
2	L	261	ASP	CB-CG-OD2	7.19	124.77	118.30
1	H	107	ASP	CB-CG-OD2	5.88	123.59	118.30
3	M	23	ASP	CB-CG-OD2	5.83	123.55	118.30
1	H	103	ASP	CB-CG-OD2	5.79	123.51	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	32	0
2	L	2232	0	2187	35	0
3	M	2409	0	2321	41	0
4	H	18	0	24	3	0
4	L	6	0	8	2	0
5	L	132	0	148	3	0
5	M	132	0	148	13	0
6	L	65	0	76	8	0
6	M	65	0	76	11	0
7	L	46	0	52	14	0
8	L	10	0	16	0	0
9	M	48	0	93	3	0
10	M	1	0	0	0	0
11	M	48	0	63	1	0
12	M	42	0	60	1	0
13	H	76	0	0	3	0
13	L	68	0	0	1	0
13	M	58	0	0	2	0
All	All	7302	0	7133	133	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 133 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:1283:BPH:CBB	6:L:1283:BPH:HHC	1.94	0.97
6:M:1309:BPH:CBB	6:M:1309:BPH:HHC	1.94	0.95
5:M:1303:BCL:H91	5:M:1303:BCL:H151	1.53	0.89
7:L:1284[B]:UQ2:C8	7:L:1284[B]:UQ2:H5M1	2.02	0.88
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.86

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	242/260 (93%)	226 (93%)	14 (6%)	2 (1%)	19	48
2	L	279/281 (99%)	265 (95%)	11 (4%)	3 (1%)	14	40
3	M	301/307 (98%)	277 (92%)	19 (6%)	5 (2%)	9	28
All	All	822/848 (97%)	768 (93%)	44 (5%)	10 (1%)	13	38

5 of 10 Ramachandran outliers are listed below:

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

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%)	182 (92%)	16 (8%)	11	31
2	L	220/220 (100%)	200 (91%)	20 (9%)	9	26
3	M	236/240 (98%)	210 (89%)	26 (11%)	6	17
All	All	654/668 (98%)	592 (90%)	62 (10%)	8	24

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	185	LEU
3	M	199	ASN
2	L	272	TRP
3	M	192	VAL
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	187	ASN
3	M	193	HIS
3	M	300	ASN
3	M	199	ASN
2	L	264	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
11	U10	M	1310	-	48,48,63	2.76	13 (27%)	58,61,79	1.70	11 (18%)
5	BCL	M	1304	3	64,74,74	2.02	10 (15%)	78,115,115	2.36	21 (26%)
8	HTO	L	1286	-	9,9,9	0.93	1 (11%)	10,10,10	1.36	2 (20%)
6	BPH	L	1283	-	51,70,70	2.99	7 (13%)	52,101,101	2.11	13 (25%)
7	UQ2	L	1284[B]	-	23,23,23	2.67	8 (34%)	28,31,31	1.46	4 (14%)
5	BCL	M	1303	3	64,74,74	2.18	12 (18%)	78,115,115	2.46	26 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
9	LDA	M	1305	-	12,15,15	2.08	1 (8%)	14,17,17	0.73	1 (7%)
4	GOL	H	1252	-	5,5,5	0.27	0	5,5,5	0.57	0
6	BPH	M	1309	-	51,70,70	2.80	8 (15%)	52,101,101	2.45	16 (30%)
4	GOL	L	1287	-	5,5,5	0.40	0	5,5,5	0.45	0
5	BCL	L	1285	2	64,74,74	1.98	13 (20%)	78,115,115	2.78	26 (33%)
7	UQ2	L	1284[A]	-	23,23,23	2.86	8 (34%)	28,31,31	1.49	5 (17%)
9	LDA	M	1306	-	12,15,15	1.91	1 (8%)	14,17,17	0.69	0
4	GOL	H	1253	-	5,5,5	0.39	0	5,5,5	0.40	0
12	SPO	M	1311	-	40,41,41	4.26	12 (30%)	47,50,50	1.96	10 (21%)
5	BCL	L	1282	2	64,74,74	2.09	10 (15%)	78,115,115	2.53	24 (30%)
9	LDA	M	1307	-	12,15,15	2.08	1 (8%)	14,17,17	0.60	0
4	GOL	H	1251	-	5,5,5	0.59	0	5,5,5	0.70	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
11	U10	M	1310	-	-	19/45/69/87	0/1/1/1
5	BCL	M	1304	3	2/2/21/25	12/37/137/137	-
8	HTO	L	1286	-	-	4/10/10/10	-
6	BPH	L	1283	-	-	13/37/105/105	0/5/6/6
7	UQ2	L	1284[B]	-	-	10/15/39/39	0/1/1/1
5	BCL	M	1303	3	2/2/21/25	14/37/137/137	-
9	LDA	M	1305	-	-	5/13/13/13	-
4	GOL	H	1252	-	-	2/4/4/4	-
6	BPH	M	1309	-	-	15/37/105/105	0/5/6/6
4	GOL	L	1287	-	-	2/4/4/4	-
5	BCL	L	1285	2	2/2/21/25	8/37/137/137	-
7	UQ2	L	1284[A]	-	-	7/15/39/39	0/1/1/1
9	LDA	M	1306	-	-	6/13/13/13	-
4	GOL	H	1253	-	-	0/4/4/4	-
12	SPO	M	1311	-	-	17/47/47/47	-
5	BCL	L	1282	2	2/2/21/25	14/37/137/137	-
9	LDA	M	1307	-	-	5/13/13/13	-
4	GOL	H	1251	-	-	2/4/4/4	-

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1283	BPH	OBD-CAD	14.23	1.42	1.22
12	M	1311	SPO	C27-C28	13.79	1.48	1.34
6	M	1309	BPH	OBD-CAD	11.77	1.38	1.22
5	L	1282	BCL	OBD-CAD	11.56	1.42	1.22
5	M	1303	BCL	OBD-CAD	10.67	1.40	1.22

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	1285	BCL	C1D-ND-C4D	10.52	113.81	106.33
5	L	1285	BCL	C2D-C1D-ND	-10.22	102.57	110.10
6	M	1309	BPH	O2D-CGD-CBD	9.03	122.44	111.00
6	M	1309	BPH	OBD-CAD-CBD	-8.41	113.48	125.82
5	M	1304	BCL	C2D-C1D-ND	-8.21	104.06	110.10

5 of 8 chirality outliers are listed below:

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

5 of 155 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	C1-C2-C3-O3
4	L	1287	GOL	O1-C1-C2-C3
5	M	1303	BCL	C1-C2-C3-C4
5	M	1303	BCL	C1-C2-C3-C5
5	M	1304	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

17 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	1310	U10	1	0
5	M	1304	BCL	9	0
6	L	1283	BPH	8	0
7	L	1284[B]	UQ2	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1303	BCL	6	0
9	M	1305	LDA	2	0
4	H	1252	GOL	1	0
6	M	1309	BPH	11	0
4	L	1287	GOL	2	0
5	L	1285	BCL	2	0
7	L	1284[A]	UQ2	1	0
9	M	1306	LDA	2	0
4	H	1253	GOL	1	0
12	M	1311	SPO	1	0
5	L	1282	BCL	2	0
9	M	1307	LDA	1	0
4	H	1251	GOL	1	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 then 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 U10 M 1310

Bond lengths   Bond angles

Torsions   Rings

Ligand BCL M 1304

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH L 1283

Bond lengths

Bond angles

Torsions

Rings

Ligand UQ2 L 1284 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL M 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand BPH M 1309

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 1285

Bond lengths

Bond angles

Torsions

Rings

Ligand UQ2 L 1284 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand SPO M 1311

Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 1282	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.42	5 (2%)	63	62	36, 51, 66, 102	0
2	L	281/281 (100%)	-0.65	5 (1%)	68	67	32, 44, 69, 84	0
3	M	303/307 (98%)	-0.45	8 (2%)	56	53	34, 51, 76, 104	0
All	All	825/848 (97%)	-0.51	18 (2%)	62	60	32, 49, 72, 104	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	4.1
2	L	281	GLY	3.6
1	H	249	LYS	3.4
1	H	220[A]	LYS	3.3
1	H	250	SER	3.3

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

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

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	H	1253	6/6	0.67	0.45	113,114,115,116	0
4	GOL	H	1251	6/6	0.82	0.39	69,77,81,82	0
9	LDA	M	1307	16/16	0.83	0.32	98,102,114,115	0
7	UQ2	L	1284[B]	23/23	0.84	0.32	31,35,43,45	23
7	UQ2	L	1284[A]	23/23	0.84	0.32	51,59,74,74	23
4	GOL	L	1287	6/6	0.86	0.48	85,86,86,87	0
9	LDA	M	1305	16/16	0.87	0.26	74,83,86,87	0
4	GOL	H	1252	6/6	0.88	0.41	81,84,85,87	0
8	HTO	L	1286	10/10	0.88	0.48	71,83,83,84	0
9	LDA	M	1306	16/16	0.91	0.26	49,62,72,72	0
11	U10	M	1310	48/63	0.92	0.22	42,52,81,82	0
6	BPH	M	1309	65/65	0.94	0.21	39,48,109,110	0
12	SPO	M	1311	42/42	0.96	0.26	47,59,82,85	0
6	BPH	L	1283	65/65	0.97	0.15	25,35,53,55	0
5	BCL	M	1303	66/66	0.98	0.15	29,41,93,96	0
5	BCL	M	1304	66/66	0.98	0.16	32,40,59,68	0
5	BCL	L	1282	66/66	0.98	0.13	31,40,64,75	0
5	BCL	L	1285	66/66	0.98	0.14	30,37,55,60	0
10	FE	M	1308	1/1	0.99	0.07	41,41,41,41	0

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

Electron density around UQ2 L 1284 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
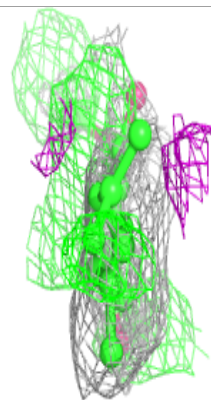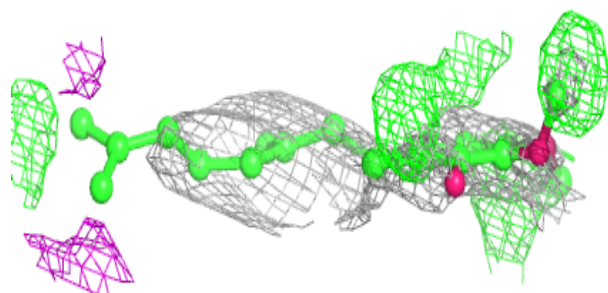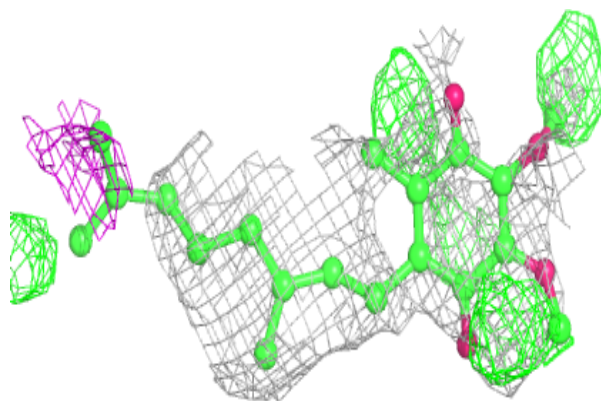
Electron density around UQ2 L 1284 (A):

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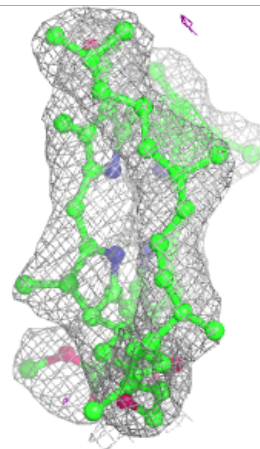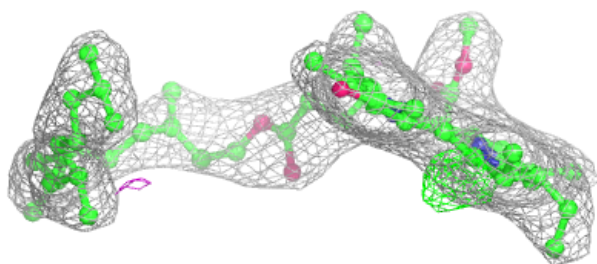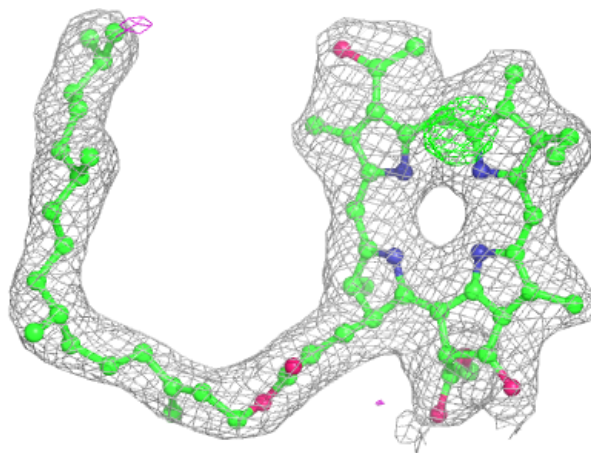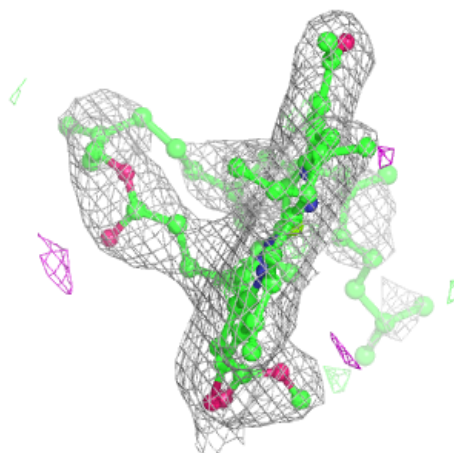$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around U10 M 1310:

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

Electron density around BPH M 1309:

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

Electron density around SPO M 1311:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
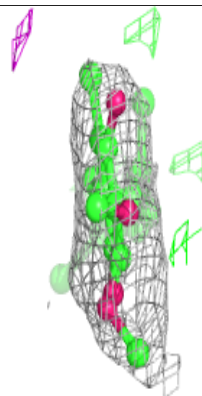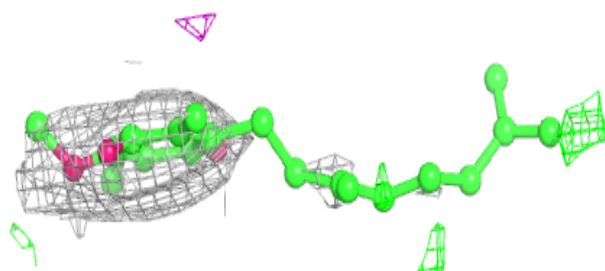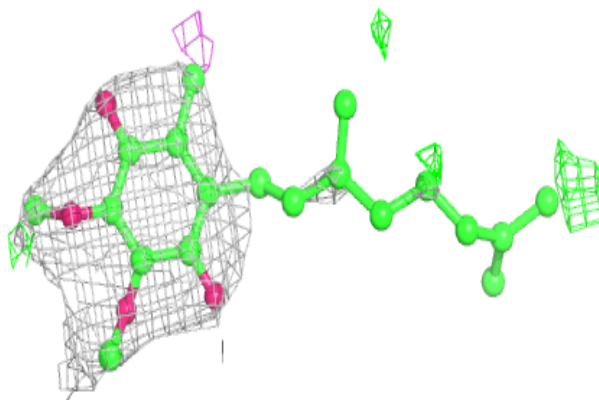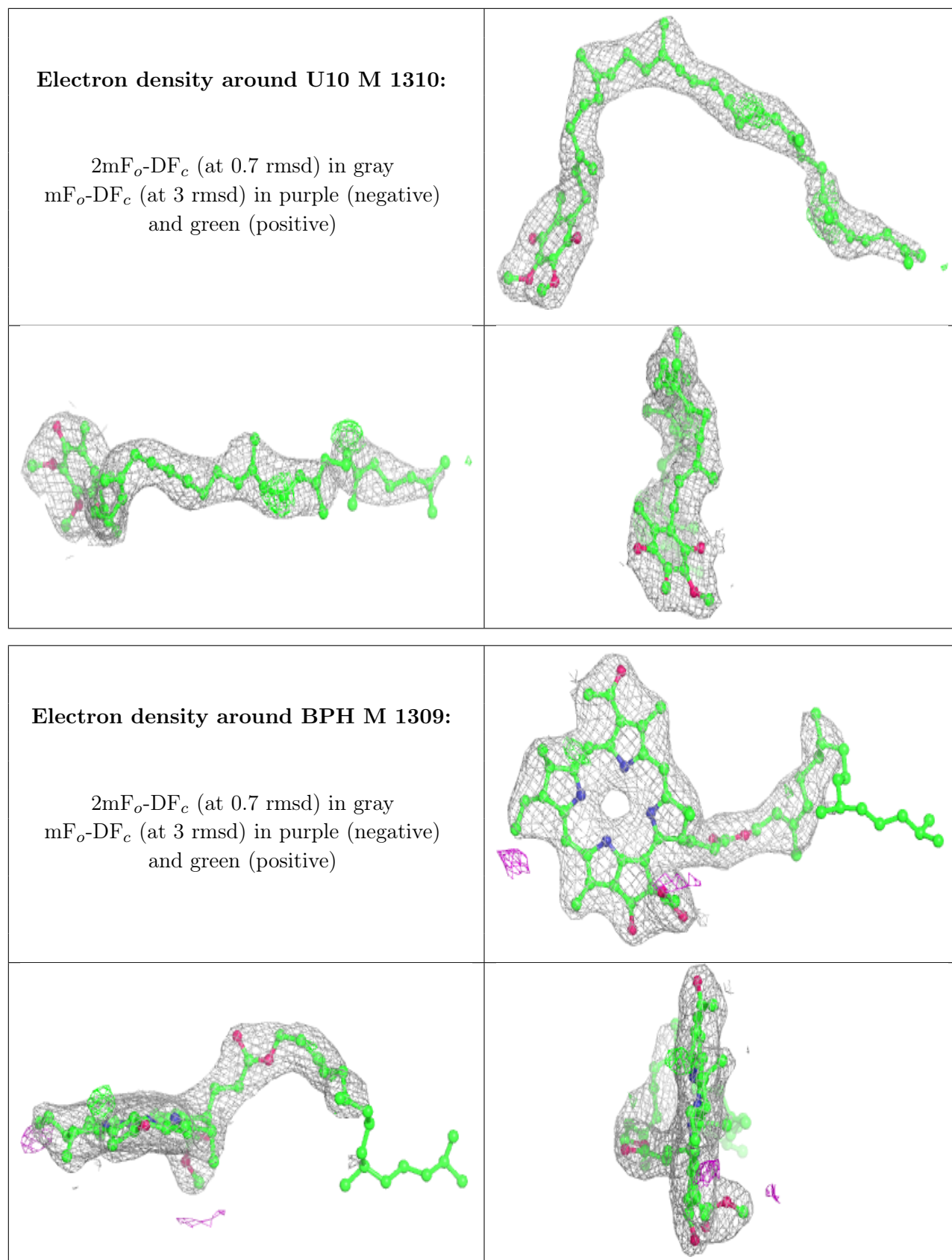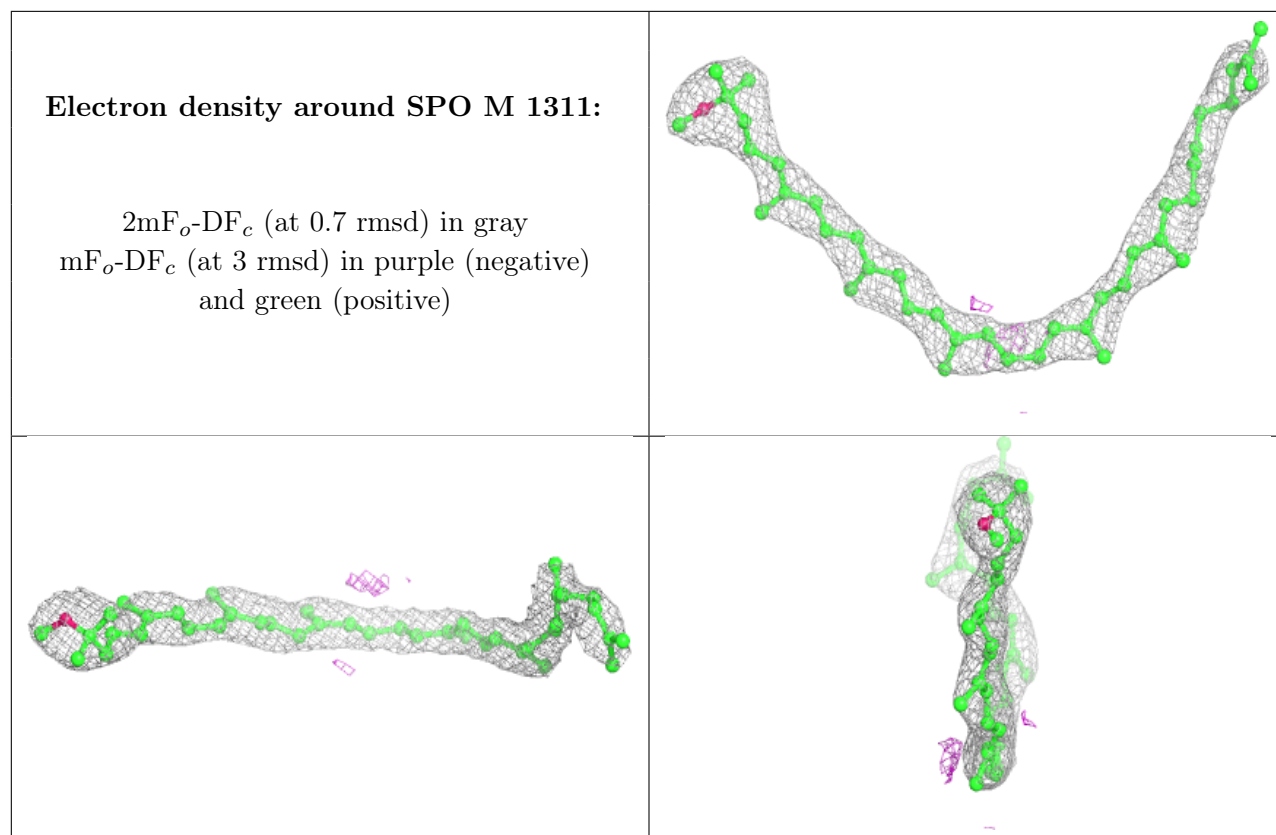
Electron density around BPH L 1283:

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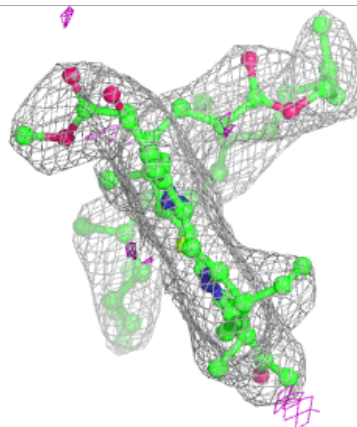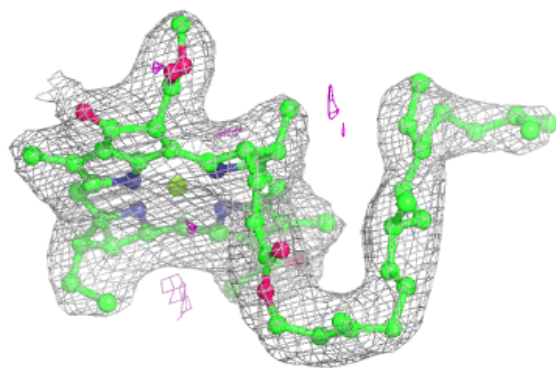mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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)
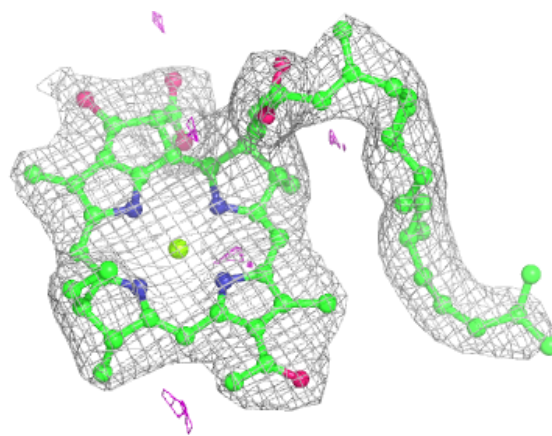and green (positive)
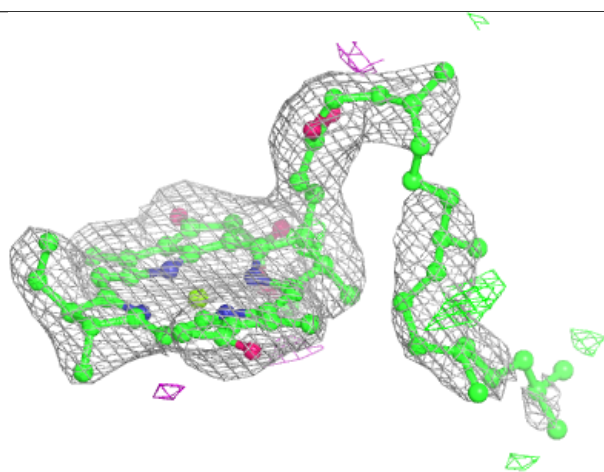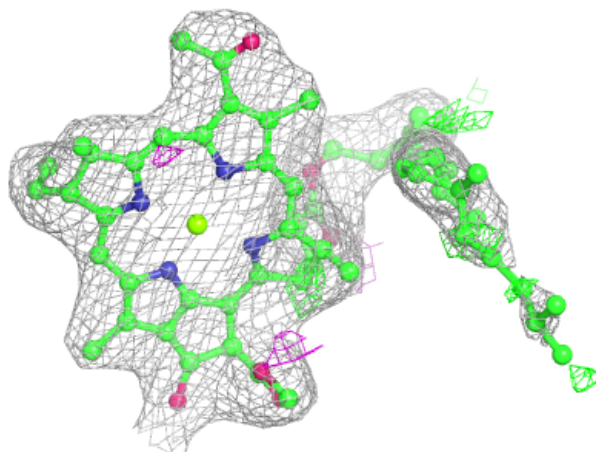
Electron density around BCL M 1304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
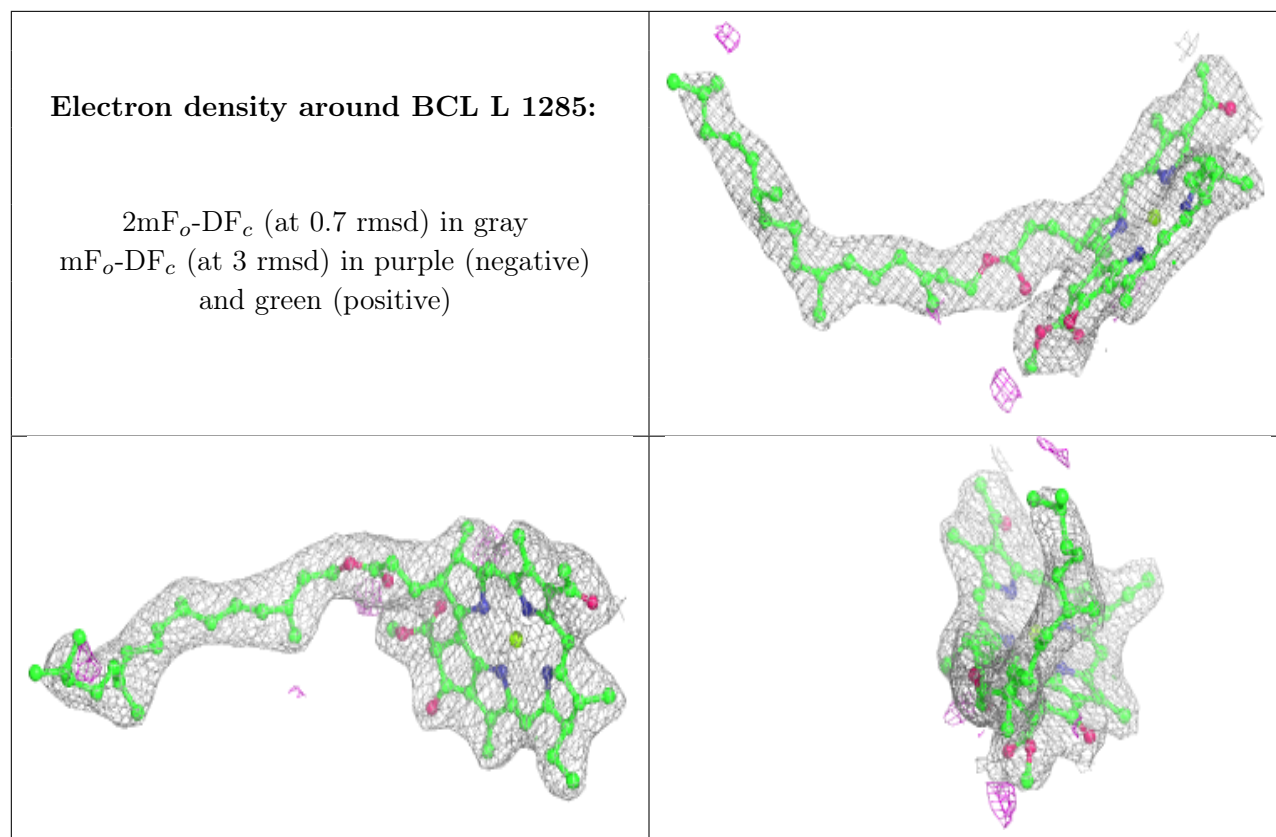mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
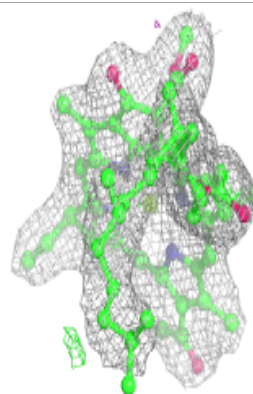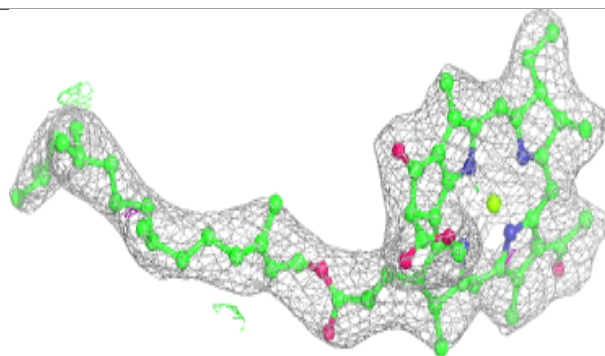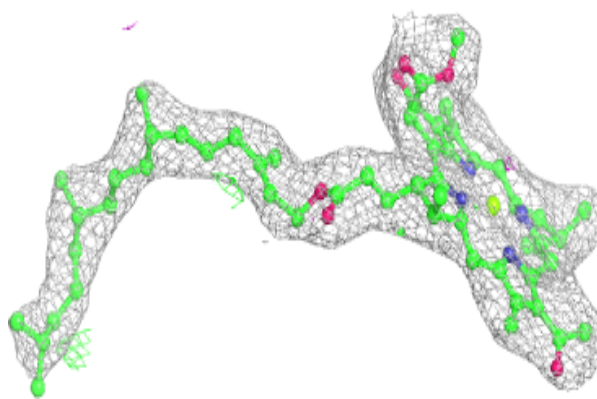
Electron density around BCL L 1282:

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

Electron density around BCL L 1285:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.