wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2026 – 04:46 am BST

PDB ID	:	2UX4 / pdb_00002ux4
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.; Fritzsch, 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 (i) 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 (i)) were used in the production of this report:

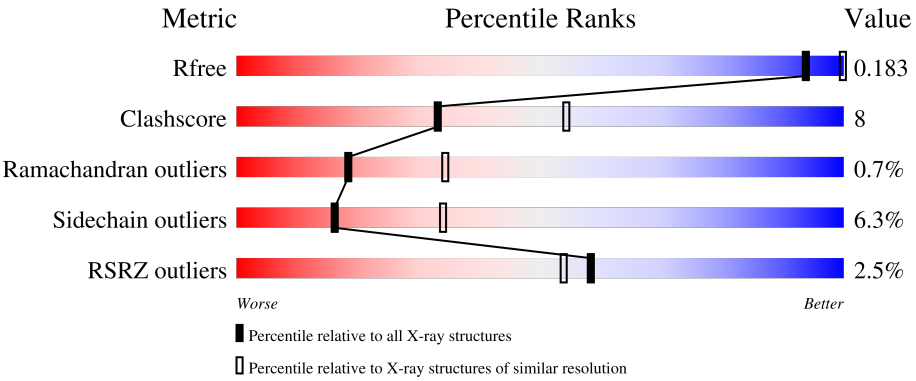
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	3% 83% 7% · 7%
2	L	281	% 87% 12% ·
3	M	307	3% 80% 16% ··

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	L	1282	X	-	-	-
5	BCL	L	1288	X	-	-	-
5	BCL	M	1303	X	-	-	-
5	BCL	M	1304	X	-	-	-
6	LDA	M	1309	-	-	-	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
			Total	C	N	O	S			
1	H	241	1846	1181	319	337	9	0	3	1

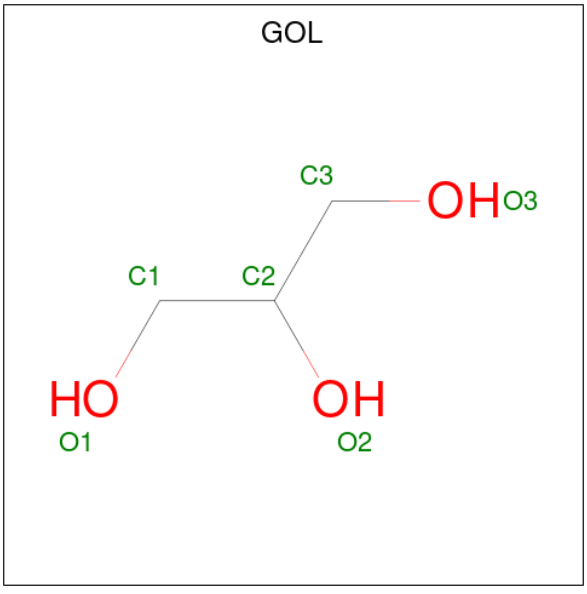
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

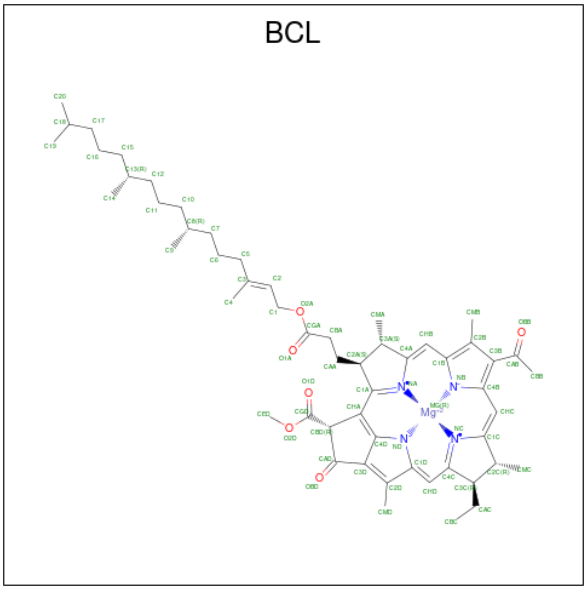
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

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



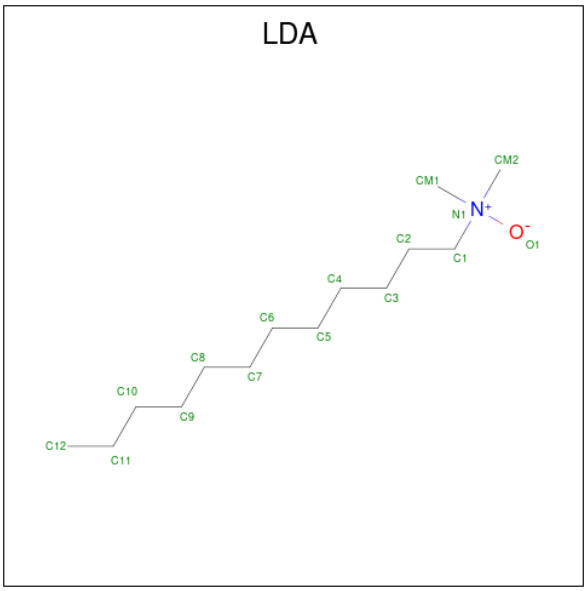
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	M	1	Total C O 6 3 3	0	0

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



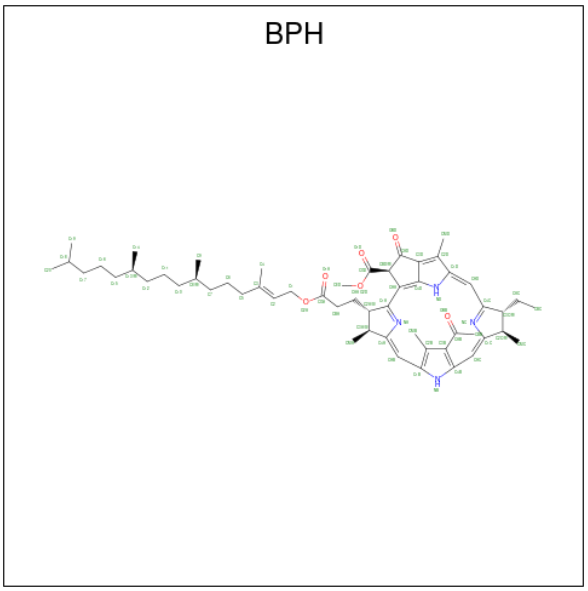
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0

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



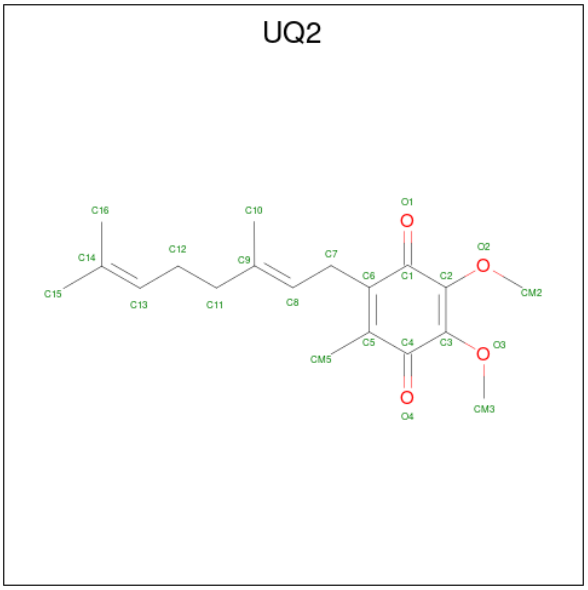
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	L	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M	1	Total C N O 16 14 1 1	0	0
6	M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

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



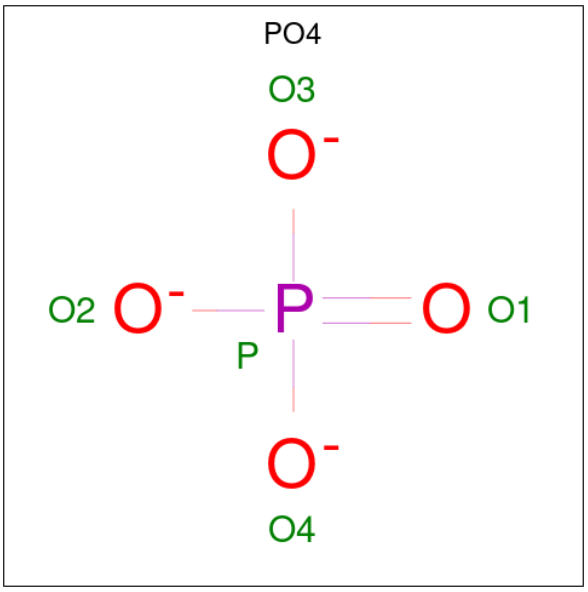
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
			Total	C	N	O		
7	M	1	65	55	4	6	0	0

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



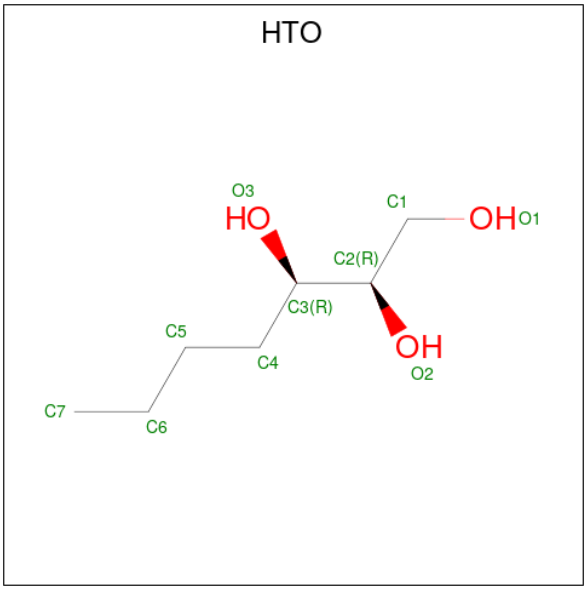
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	L	1	46	38	8	0	1

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



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

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

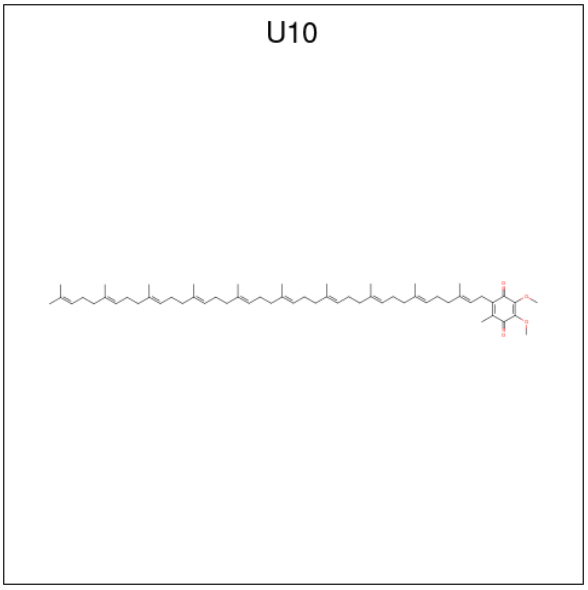


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total C O 10 7 3	0	0

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

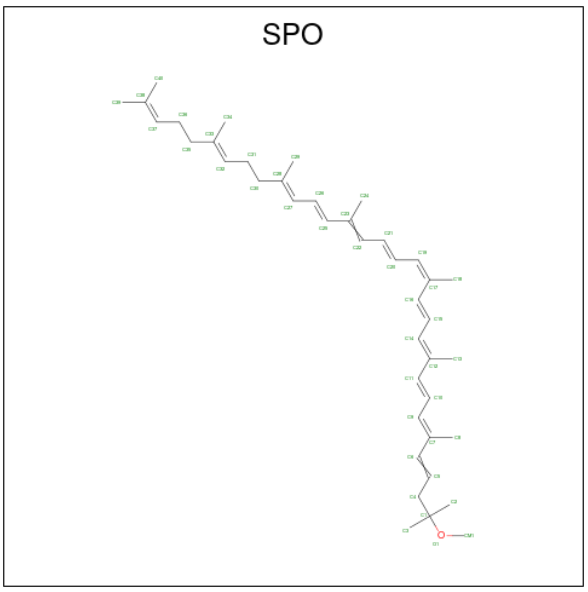
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total Fe 1 1	0	0

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



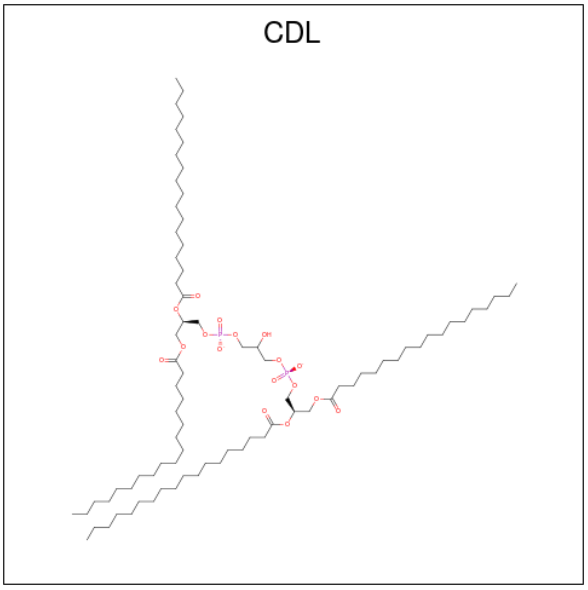
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 48 44 4	0	0

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



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

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



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

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	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		

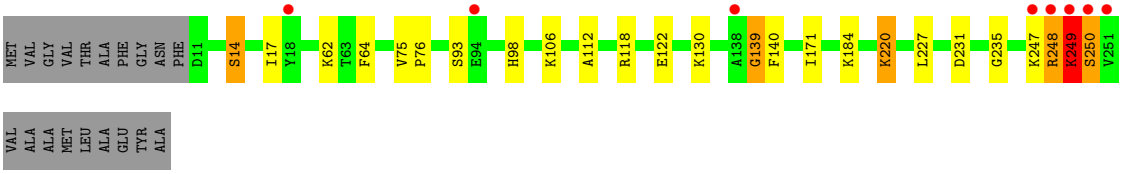
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, 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

Chain H:

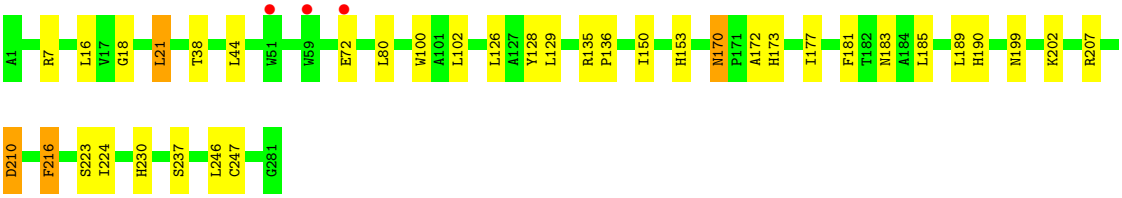




• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:

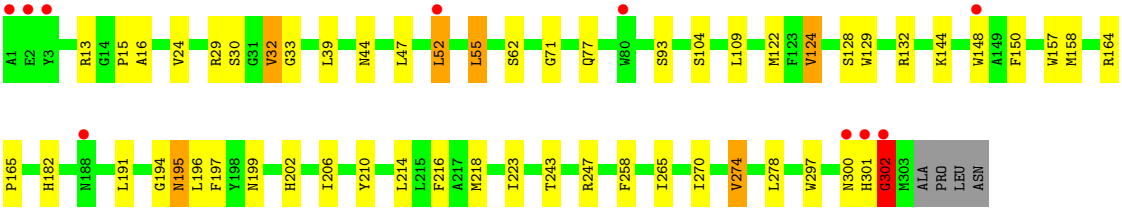




• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:





4 Data and refinement statistics (i)

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 50.00 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.51) 90.8 (50.00-2.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.211 0.185 , 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)	0.32 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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: PO4, FE, GOL, U10, HTO, UQ2, CDL, SPO, LDA, BCL, BPH

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	0.64	1/1906 (0.1%)	0.87	3/2591 (0.1%)
2	L	0.64	0/2320	0.85	0/3175
3	M	0.63	2/2501 (0.1%)	0.88	0/3415
All	All	0.64	3/6727 (0.0%)	0.87	3/9181 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	218	MET	SD-CE	6.59	1.96	1.79
3	M	302	GLY	C-N	-6.34	1.24	1.33
1	H	250	SER	C-N	-6.30	1.24	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	139	GLY	N-CA-C	-5.15	98.37	113.30
1	H	248	ARG	CA-C-N	5.07	130.82	121.70
1	H	248	ARG	C-N-CA	5.07	130.82	121.70

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	25	0
3	M	2409	0	2321	39	0
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	5	0
5	M	132	0	148	23	0
6	L	48	0	93	7	0
6	M	96	0	186	9	0
7	L	65	0	76	7	0
7	M	65	0	76	11	0
8	L	46	0	52	7	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	115	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 115 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%)	30 49
2	L	279/281 (99%)	270 (97%)	9 (3%)	0	100 100
3	M	301/307 (98%)	287 (95%)	9 (3%)	5 (2%)	7 13
All	All	822/848 (97%)	790 (96%)	26 (3%)	6 (1%)	18 34

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%)	187 (94%)	11 (6%)	19 39
2	L	220/220 (100%)	203 (92%)	17 (8%)	12 25
3	M	236/240 (98%)	222 (94%)	14 (6%)	18 37
All	All	654/668 (98%)	612 (94%)	42 (6%)	16 33

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	32	VAL
3	M	148	TRP
3	M	39	LEU
3	M	104	SER
3	M	191	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	187	ASN
3	M	193	HIS
3	M	199	ASN
2	L	170	ASN
2	L	183	ASN

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 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	$\#\|Z\|>2$
7	BPH	L	1286	-	59,70,70	2.76	10 (16%)	61,101,101	2.25	17 (27%)
8	UQ2	L	1287[B]	-	23,23,23	2.76	7 (30%)	28,31,31	1.18	1 (3%)
6	LDA	M	1306	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
6	LDA	M	1309	-	12,15,15	2.01	1 (8%)	14,17,17	0.45	0
14	CDL	M	1314	-	80,80,99	2.33	18 (22%)	86,92,111	4.01	15 (17%)
4	GOL	L	1291	-	5,5,5	0.32	0	5,5,5	0.51	0
8	UQ2	L	1287[A]	-	23,23,23	2.67	8 (34%)	28,31,31	1.61	5 (17%)
6	LDA	M	1305	-	12,15,15	2.10	1 (8%)	14,17,17	0.49	0
7	BPH	M	1311	-	59,70,70	2.70	11 (18%)	61,101,101	2.12	15 (24%)
5	BCL	M	1304	3	69,74,74	1.92	9 (13%)	83,115,115	2.10	25 (30%)
5	BCL	L	1288	2	69,74,74	1.84	8 (11%)	83,115,115	2.35	22 (26%)
6	LDA	M	1308	-	12,15,15	2.05	1 (8%)	14,17,17	0.46	0
4	GOL	H	1253	-	5,5,5	0.35	0	5,5,5	0.28	0
4	GOL	H	1251	-	5,5,5	0.52	0	5,5,5	0.73	0
9	PO4	L	1289	-	4,4,4	0.84	0	6,6,6	0.48	0
12	U10	M	1312	-	48,48,63	2.69	12 (25%)	58,61,79	1.65	12 (20%)
4	GOL	M	1315	-	5,5,5	0.33	0	5,5,5	0.31	0
6	LDA	L	1285	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
6	LDA	M	1307	-	12,15,15	2.00	1 (8%)	14,17,17	0.60	0
4	GOL	L	1292	-	5,5,5	0.36	0	5,5,5	0.23	0
5	BCL	M	1303	3	69,74,74	1.93	10 (14%)	83,115,115	2.13	19 (22%)
5	BCL	L	1282	2	69,74,74	1.85	9 (13%)	83,115,115	2.33	25 (30%)
6	LDA	L	1284	-	12,15,15	2.04	1 (8%)	14,17,17	0.50	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
13	SPO	M	1313	-	40,41,41	4.16	12 (30%)	47,50,50	1.89	11 (23%)
4	GOL	H	1252	-	5,5,5	0.38	0	5,5,5	0.22	0
6	LDA	M	1709	-	12,15,15	2.02	1 (8%)	14,17,17	0.51	0
4	GOL	H	1254	-	5,5,5	0.37	0	5,5,5	0.25	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
7	BPH	L	1286	-	-	9/37/105/105	0/5/6/6
8	UQ2	L	1287[B]	-	-	8/15/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1306	-	-	7/13/13/13	-
6	LDA	M	1309	-	-	12/13/13/13	-
14	CDL	M	1314	-	-	46/91/91/110	-
4	GOL	L	1291	-	-	2/4/4/4	-
8	UQ2	L	1287[A]	-	-	8/15/39/39	0/1/1/1
6	LDA	M	1305	-	-	5/13/13/13	-
7	BPH	M	1311	-	-	17/37/105/105	0/5/6/6
5	BCL	M	1304	3	2/2/21/25	9/41/137/137	-
5	BCL	L	1288	2	2/2/21/25	9/41/137/137	-
6	LDA	M	1308	-	-	5/13/13/13	-
4	GOL	H	1253	-	-	1/4/4/4	-
4	GOL	H	1251	-	-	4/4/4/4	-
12	U10	M	1312	-	-	13/45/69/87	0/1/1/1
4	GOL	M	1315	-	-	3/4/4/4	-
6	LDA	L	1285	-	-	9/13/13/13	-
6	LDA	M	1307	-	-	8/13/13/13	-
4	GOL	L	1292	-	-	4/4/4/4	-
5	BCL	M	1303	3	2/2/21/25	16/41/137/137	-
5	BCL	L	1282	2	2/2/21/25	10/41/137/137	-
6	LDA	L	1284	-	-	4/13/13/13	-
10	HTO	L	1290	-	-	7/10/10/10	-
6	LDA	L	1283	-	-	6/13/13/13	-
13	SPO	M	1313	-	-	24/47/47/47	-
4	GOL	H	1252	-	-	4/4/4/4	-
6	LDA	M	1709	-	-	8/13/13/13	-
4	GOL	H	1254	-	-	0/4/4/4	-

The worst 5 of 123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1286	BPH	OBD-CAD	12.97	1.40	1.22
7	M	1311	BPH	OBD-CAD	12.82	1.40	1.22
13	M	1313	SPO	C27-C28	12.67	1.47	1.34
5	M	1304	BCL	OBD-CAD	10.78	1.41	1.22
5	M	1303	BCL	OBD-CAD	10.72	1.41	1.22

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	L	1282	BCL	C13
5	L	1282	BCL	C8
5	L	1288	BCL	C13
5	L	1288	BCL	C8
5	M	1303	BCL	C13

5 of 258 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1251	GOL	O1-C1-C2-O2
4	H	1251	GOL	O1-C1-C2-C3
4	H	1252	GOL	O1-C1-C2-C3
4	L	1291	GOL	C1-C2-C3-O3
4	L	1292	GOL	O1-C1-C2-C3

There are no ring outliers.

20 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1286	BPH	7	0
8	L	1287[B]	UQ2	1	0
6	M	1309	LDA	2	0
14	M	1314	CDL	2	0
4	L	1291	GOL	1	0
8	L	1287[A]	UQ2	6	0
6	M	1305	LDA	3	0
7	M	1311	BPH	11	0
5	M	1304	BCL	14	0
5	L	1288	BCL	2	0
6	M	1308	LDA	2	0
4	H	1251	GOL	1	0
4	M	1315	GOL	2	0
6	L	1285	LDA	4	0
6	M	1307	LDA	5	0

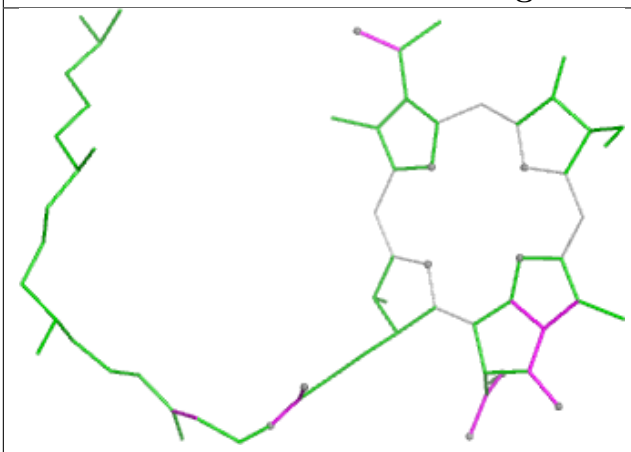
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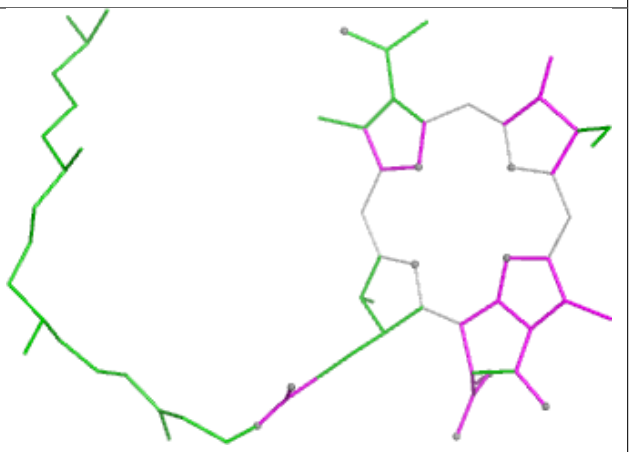
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1303	BCL	11	0
5	L	1282	BCL	4	0
6	L	1284	LDA	2	0
6	L	1283	LDA	1	0
13	M	1313	SPO	4	0

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.

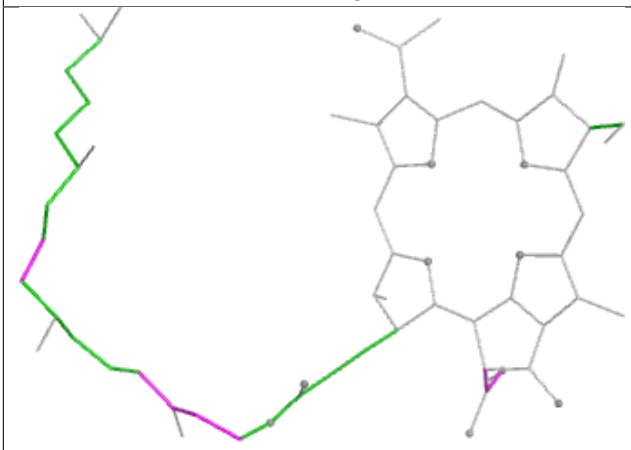
Ligand BPH L 1286



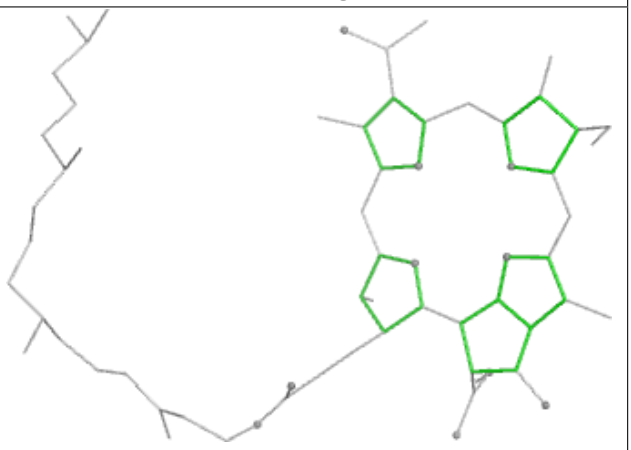
Bond lengths



Bond angles

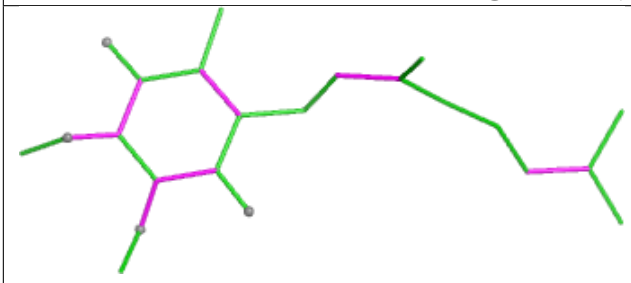


Torsions

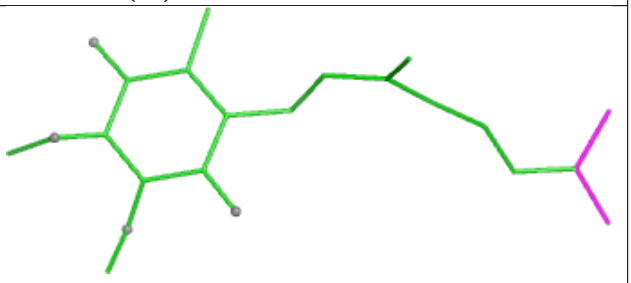


Rings

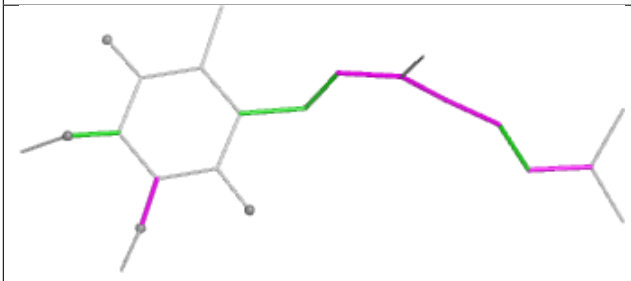
Ligand UQ2 L 1287 (B)



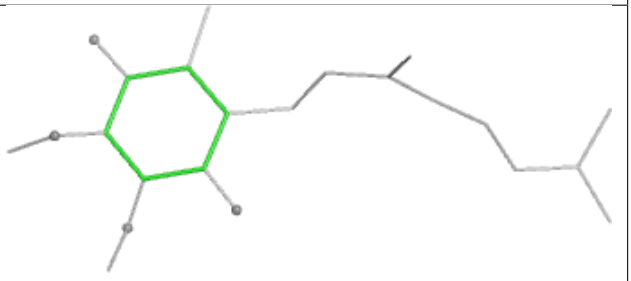
Bond lengths



Bond angles

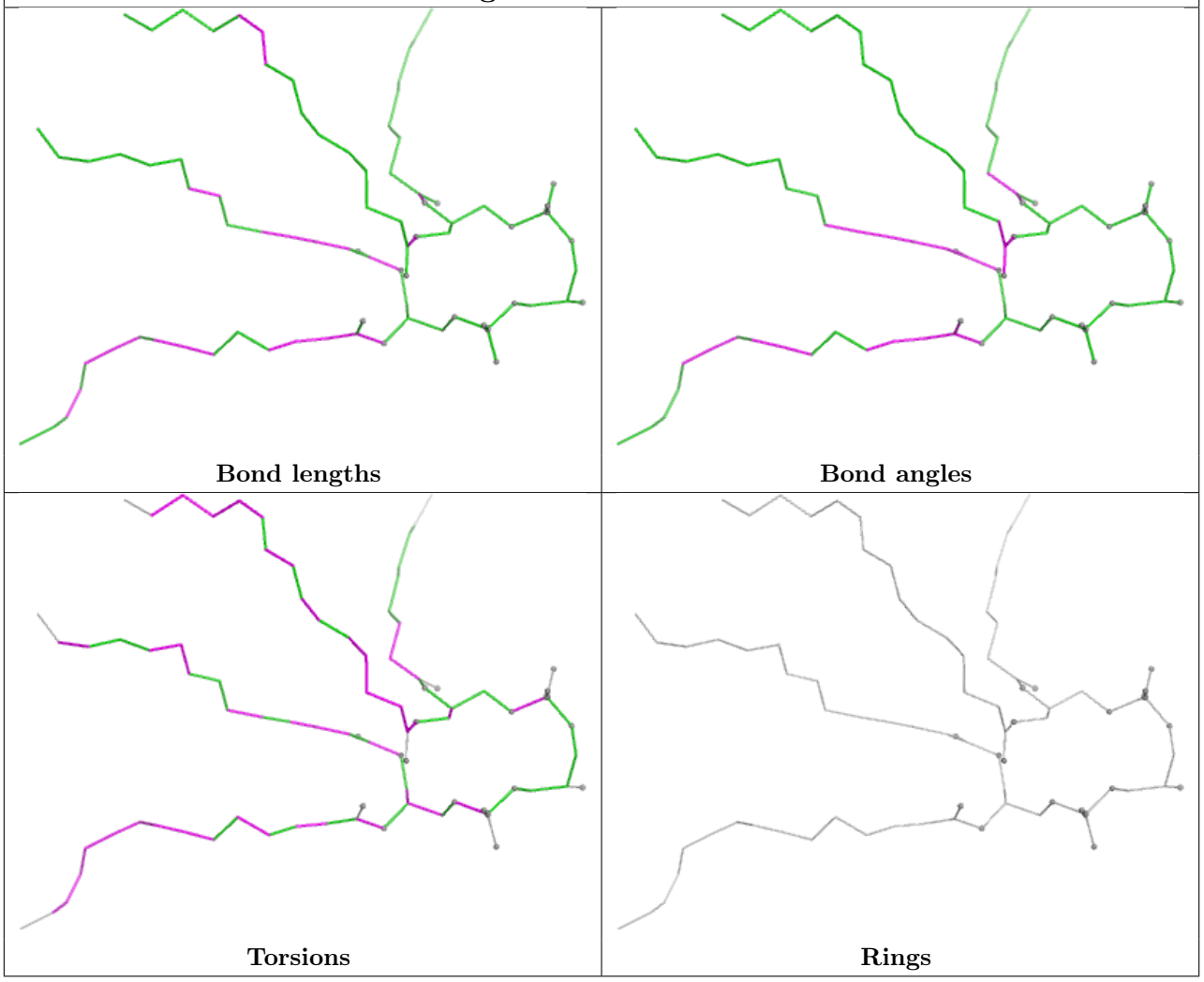


Torsions

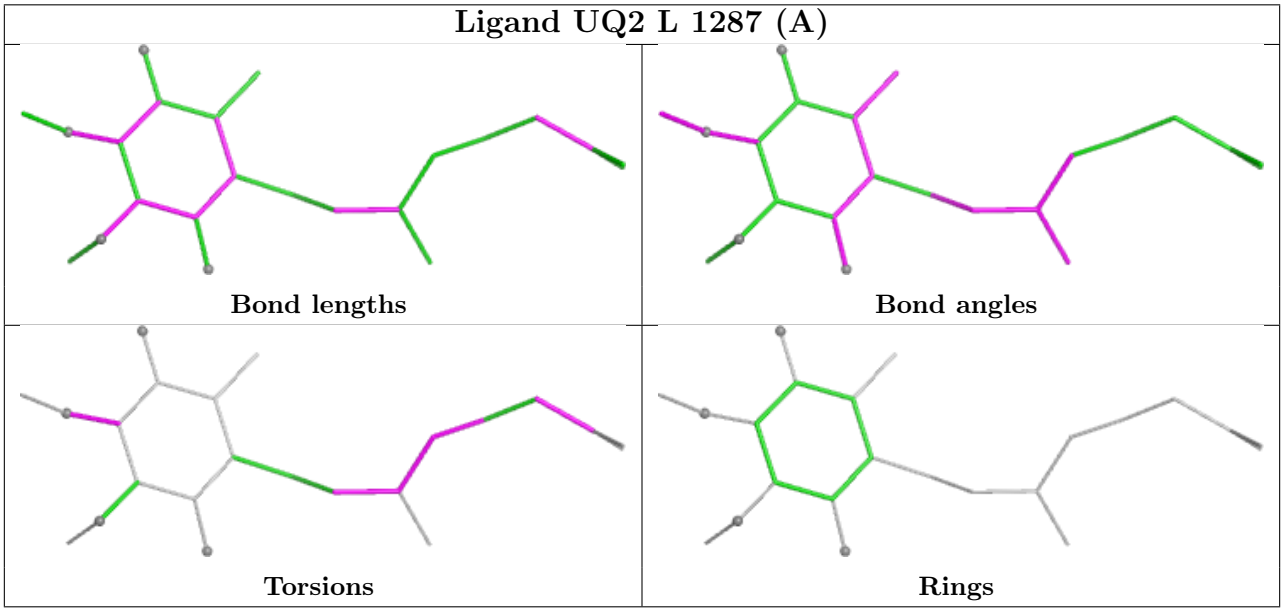


Rings

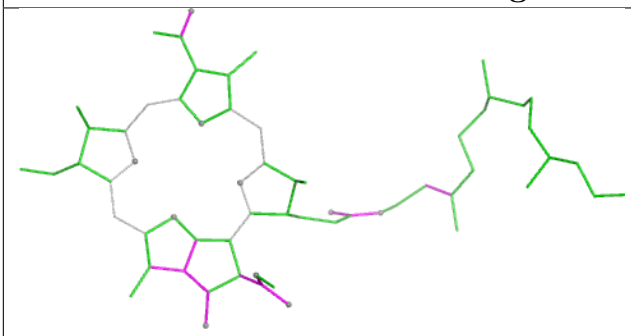
Ligand CDL M 1314



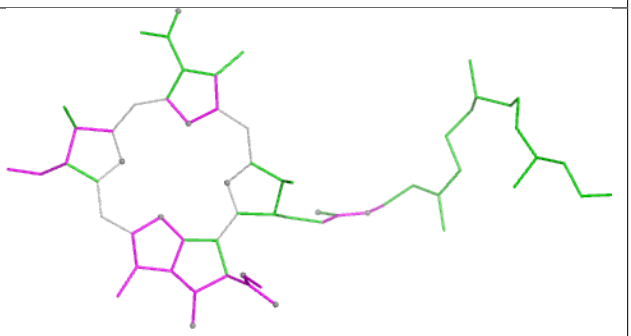
Ligand UQ2 L 1287 (A)



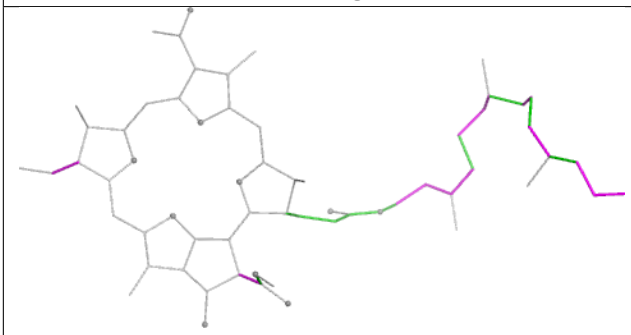
Ligand BPH M 1311



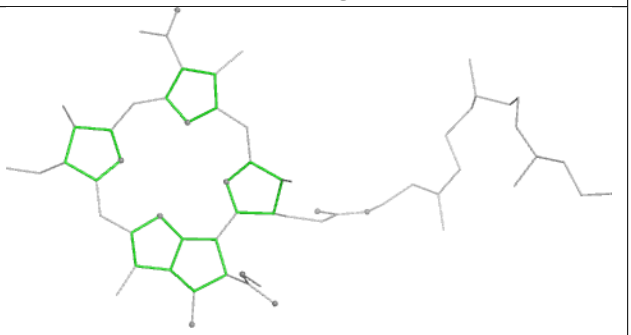
Bond lengths



Bond angles

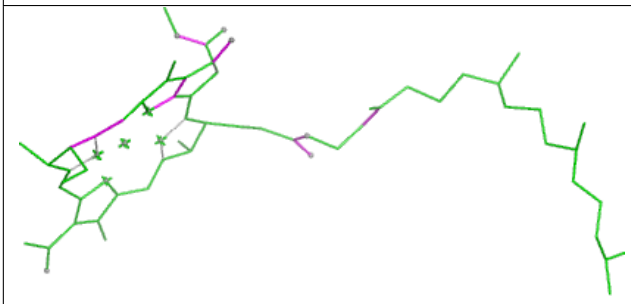


Torsions

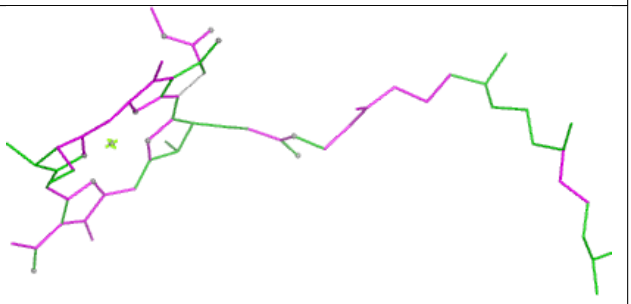


Rings

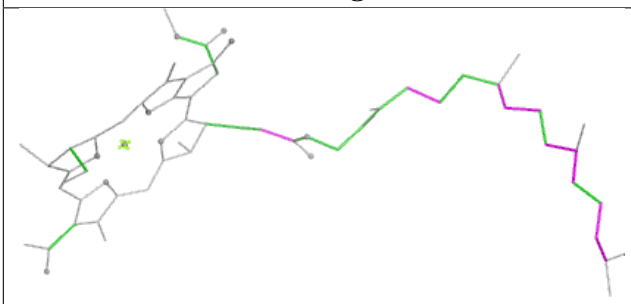
Ligand BCL M 1304



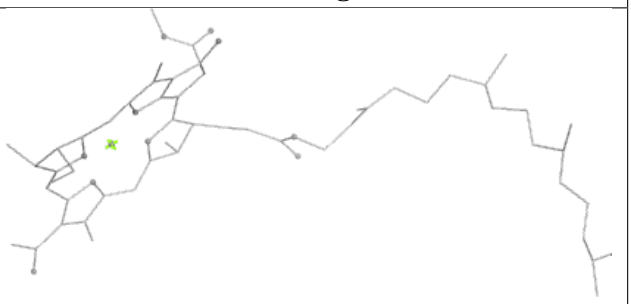
Bond lengths



Bond angles

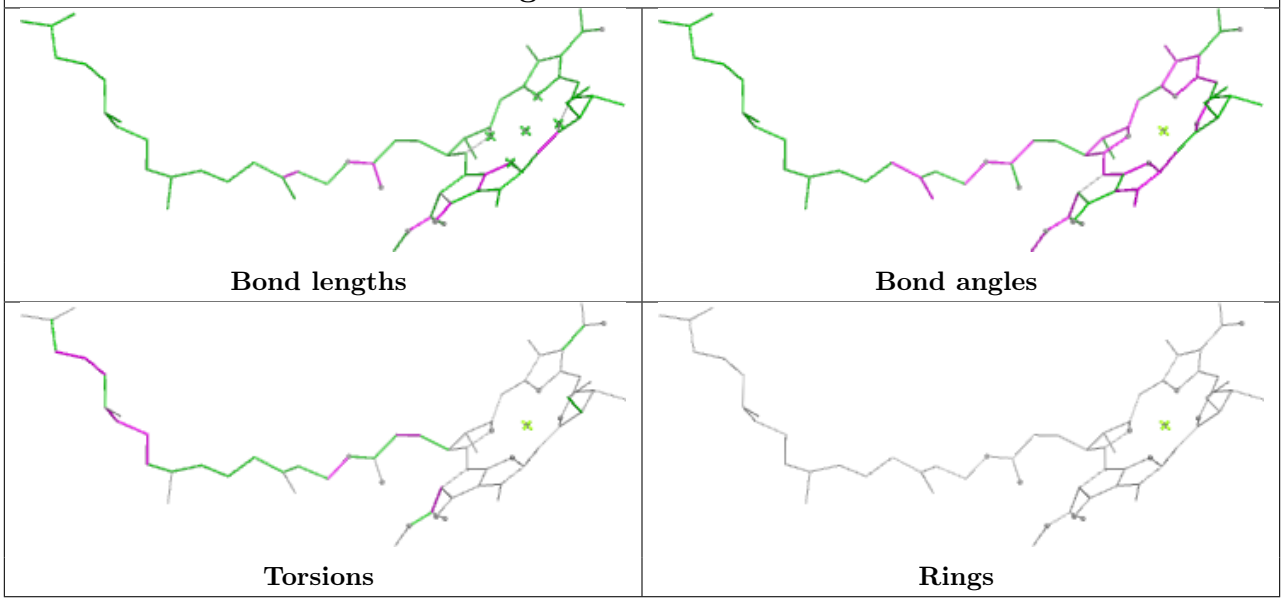


Torsions

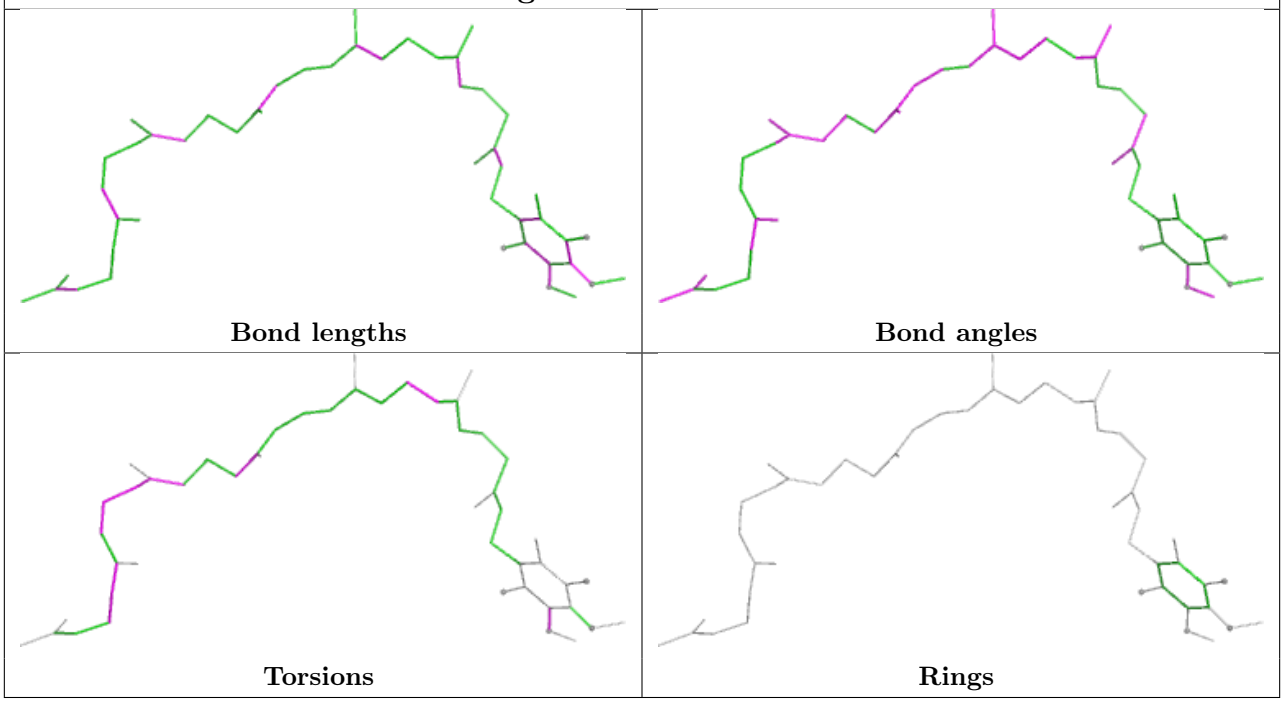


Rings

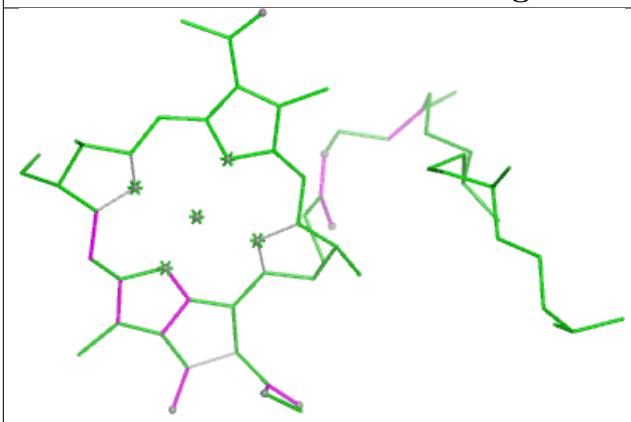
Ligand BCL L 1288



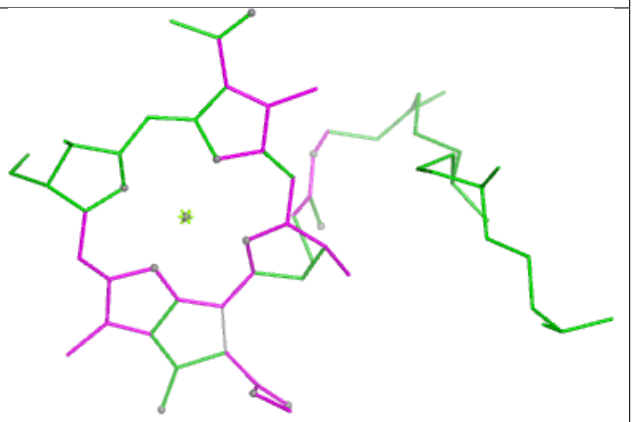
Ligand U10 M 1312



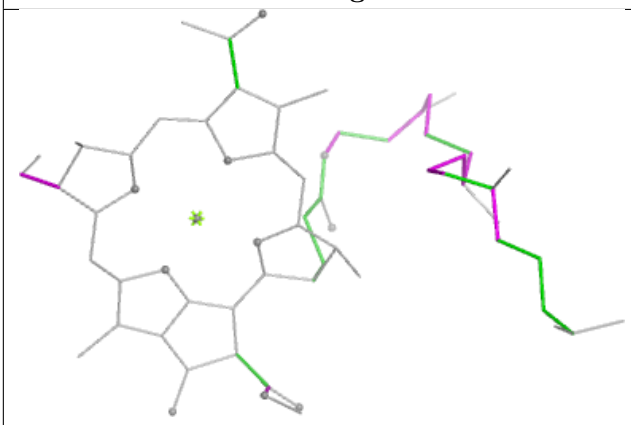
Ligand BCL M 1303



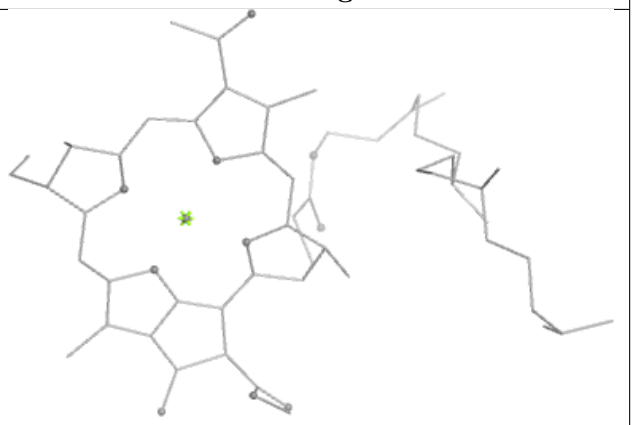
Bond lengths



Bond angles



Torsions

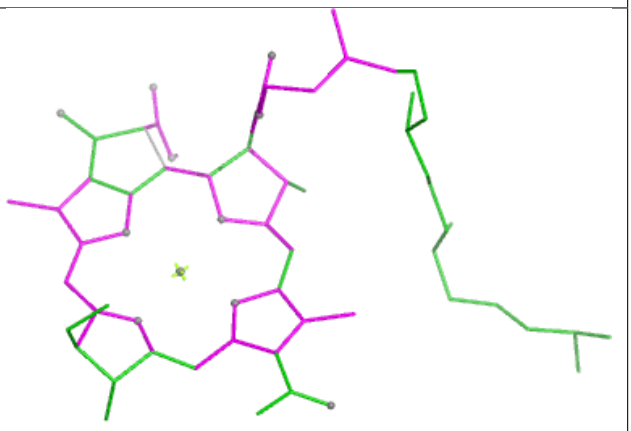


Rings

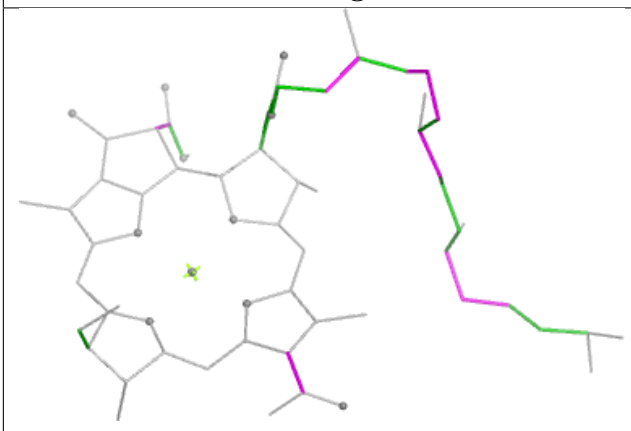
Ligand BCL L 1282



Bond lengths



Bond angles

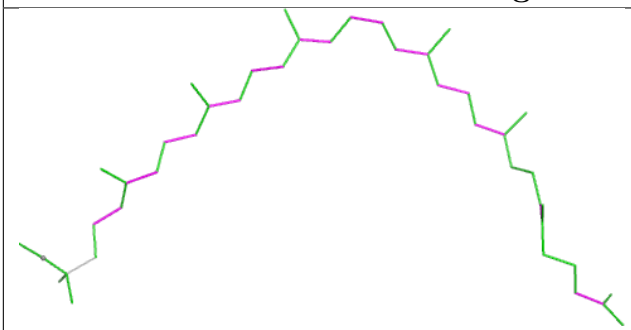


Torsions

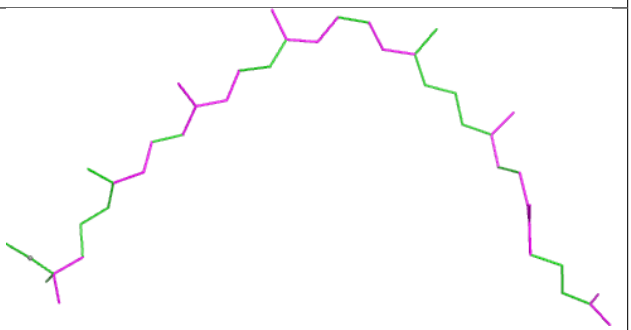


Rings

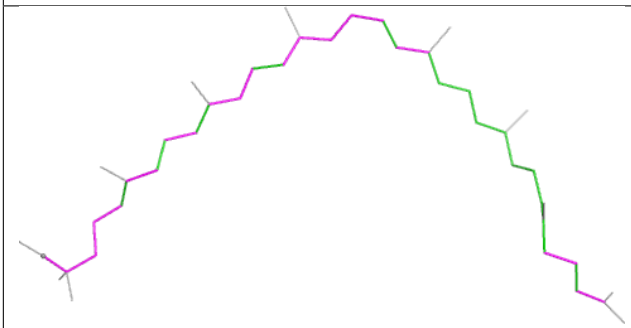
Ligand SPO M 1313



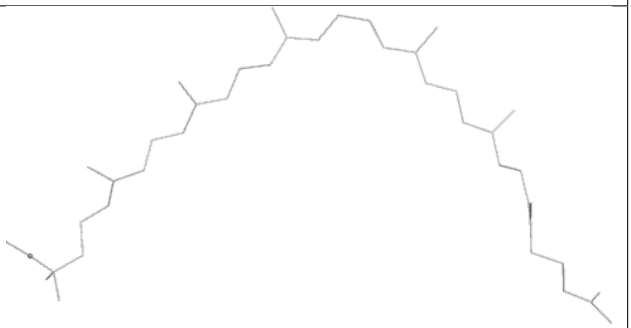
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.21	8 (3%)	49	45	25, 42, 53, 84	3 (1%)
2	L	281/281 (100%)	-0.16	3 (1%)	78	75	30, 39, 61, 68	0
3	M	303/307 (98%)	-0.03	10 (3%)	49	45	29, 44, 69, 76	0
All	All	825/848 (97%)	-0.13	21 (2%)	58	54	25, 42, 63, 84	3 (0%)

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	148	TRP	5.4
3	M	1	ALA	5.1
3	M	52	LEU	5.1
3	M	2	GLU	5.0
1	H	249	LYS	4.3

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 oligosaccharides in this entry.

6.4 Ligands

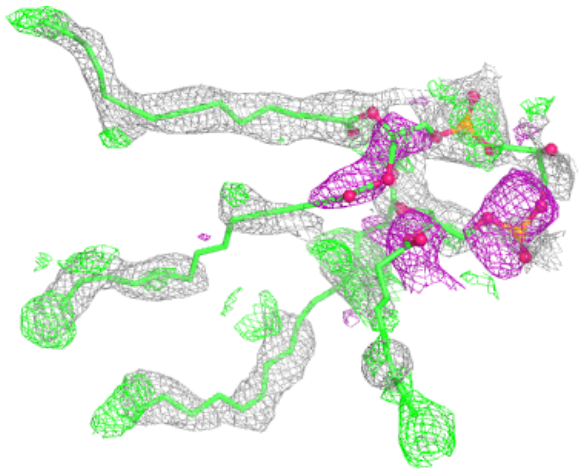
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

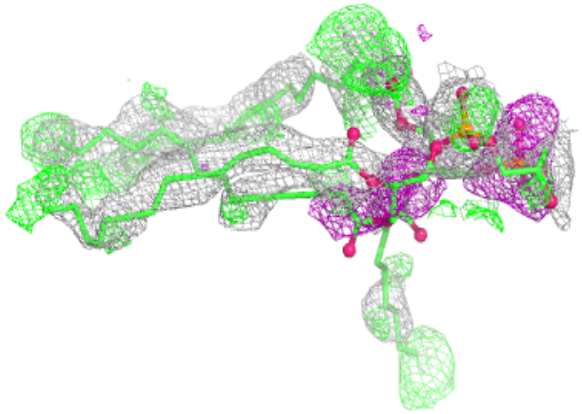
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LDA	M	1309	16/16	0.62	0.43	94,102,110,110	0
14	CDL	M	1314	81/100	0.62	0.39	96,107,120,121	0
6	LDA	M	1308	16/16	0.69	0.37	90,97,105,105	0
6	LDA	L	1284	16/16	0.73	0.35	98,102,109,109	0
6	LDA	M	1709	16/16	0.76	0.32	92,100,107,107	0
6	LDA	L	1285	16/16	0.76	0.29	106,109,111,111	0
6	LDA	L	1283	16/16	0.77	0.33	86,103,111,111	0
4	GOL	M	1315	6/6	0.81	0.18	85,86,86,87	0
6	LDA	M	1305	16/16	0.81	0.24	50,63,70,71	0
6	LDA	M	1307	16/16	0.84	0.23	64,68,77,77	0
10	HTO	L	1290	10/10	0.85	0.27	74,77,77,78	0
4	GOL	H	1251	6/6	0.85	0.19	65,68,70,71	0
4	GOL	H	1254	6/6	0.86	0.18	102,102,103,103	0
8	UQ2	L	1287[A]	23/23	0.86	0.21	39,42,51,52	23
8	UQ2	L	1287[B]	23/23	0.86	0.21	40,43,47,48	23
4	GOL	H	1253	6/6	0.86	0.15	102,103,104,104	0
6	LDA	M	1306	16/16	0.86	0.24	72,74,84,84	0
4	GOL	L	1291	6/6	0.89	0.16	47,52,53,54	0
4	GOL	L	1292	6/6	0.91	0.17	85,87,87,87	0
9	PO4	L	1289	5/5	0.91	0.17	103,103,103,103	0
12	U10	M	1312	48/63	0.92	0.13	30,39,68,69	0
4	GOL	H	1252	6/6	0.93	0.15	88,89,89,89	0
5	BCL	M	1303	66/66	0.94	0.11	26,31,80,81	0
13	SPO	M	1313	42/42	0.94	0.13	38,51,68,71	0
7	BPH	M	1311	65/65	0.94	0.12	35,42,94,95	0
7	BPH	L	1286	65/65	0.96	0.07	25,30,39,40	0
5	BCL	M	1304	66/66	0.96	0.08	25,31,53,59	0
5	BCL	L	1282	66/66	0.96	0.08	30,34,51,54	0
5	BCL	L	1288	66/66	0.97	0.07	25,30,48,52	0
11	FE	M	1310	1/1	1.00	0.05	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)

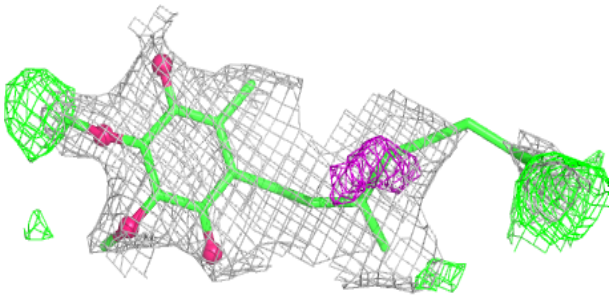


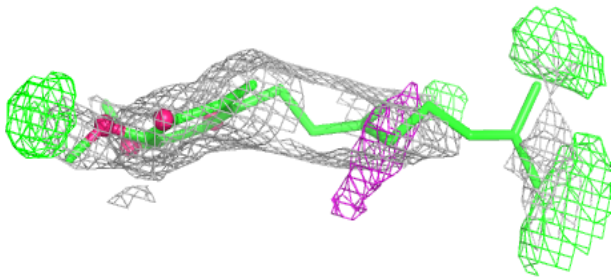


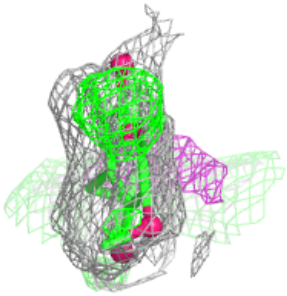


Electron density around UQ2 L 1287 (A):

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

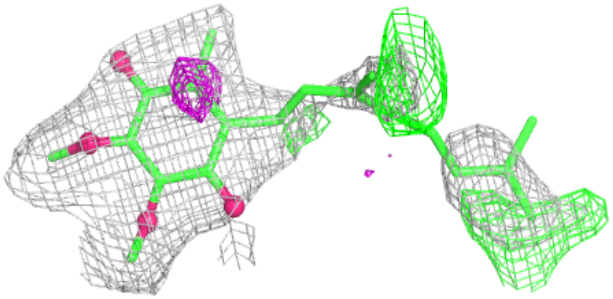


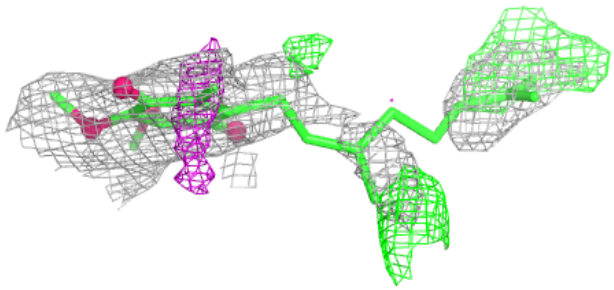


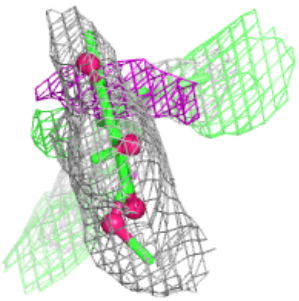


Electron density around UQ2 L 1287 (B):

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

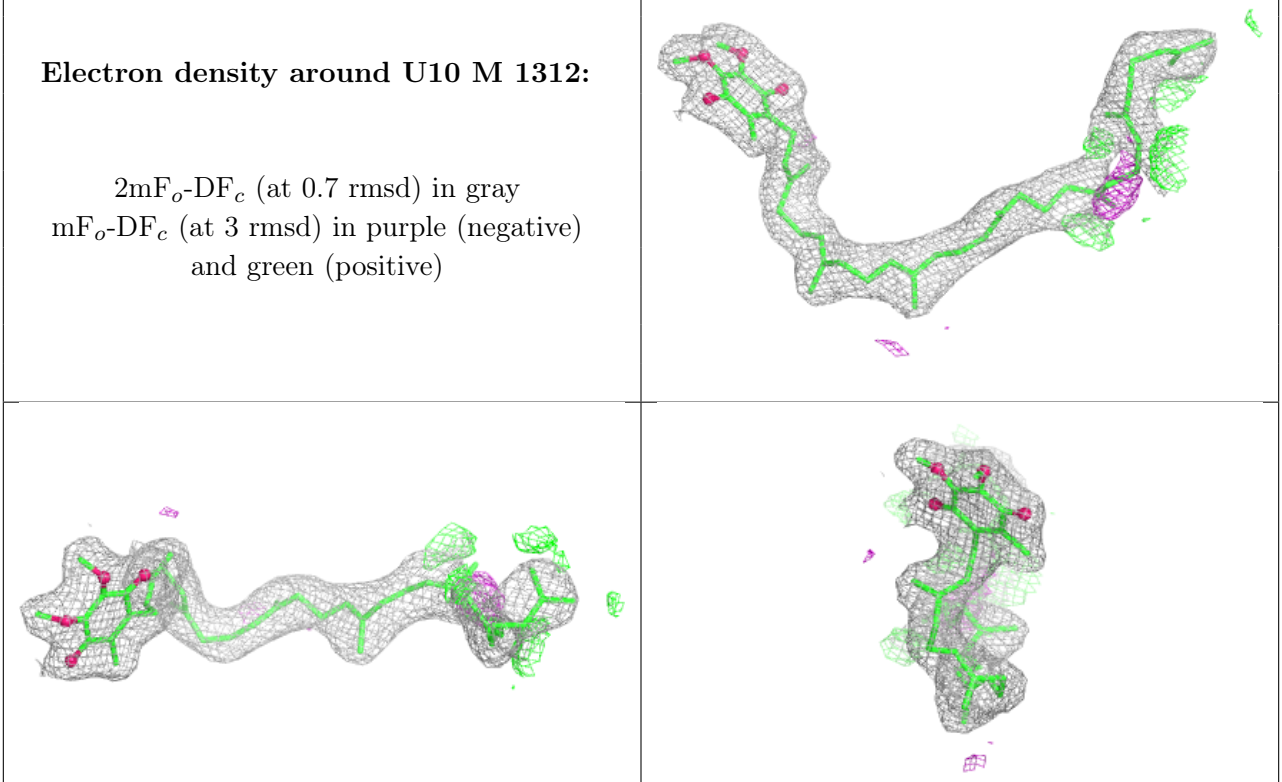






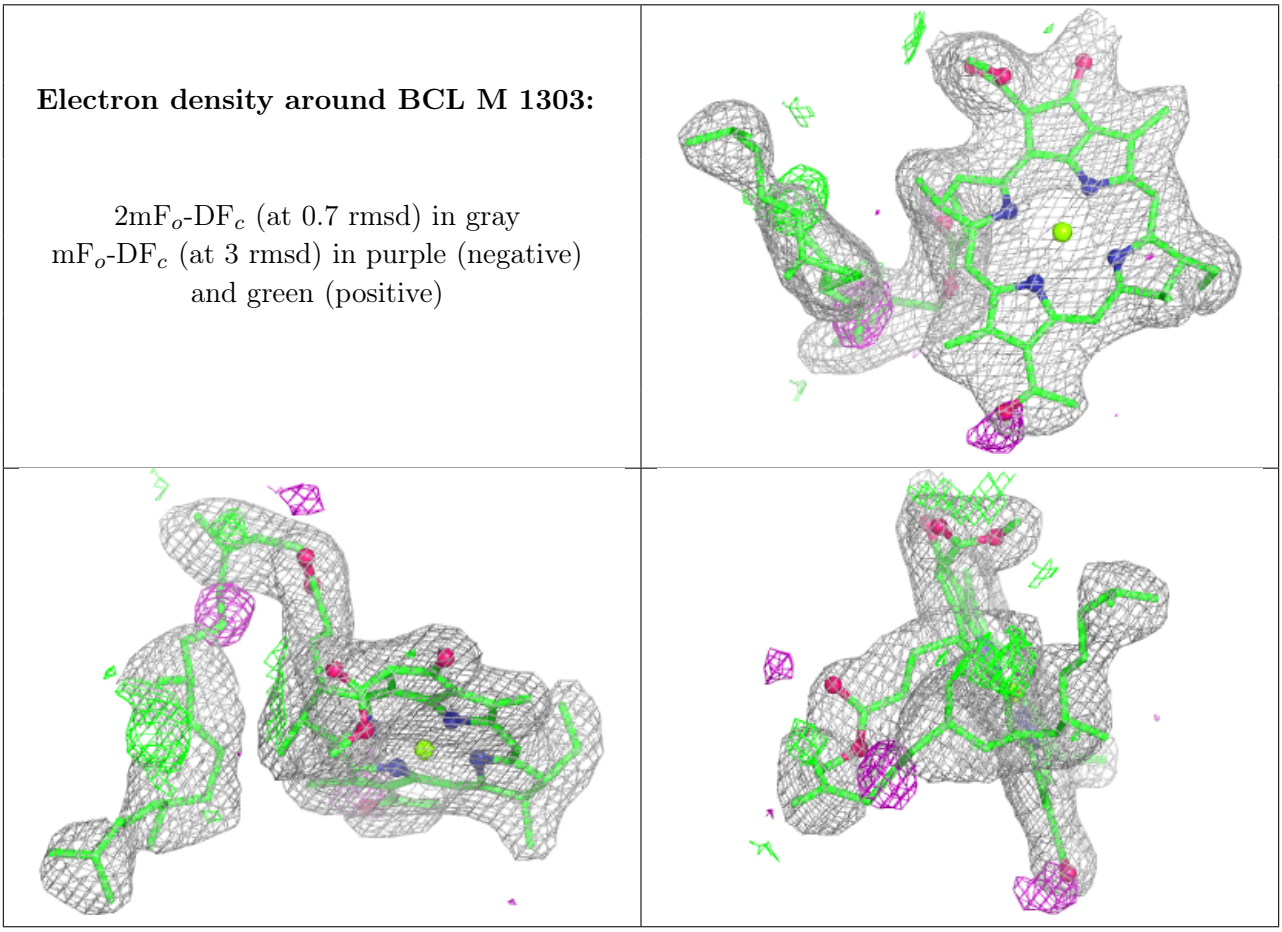
Electron density around U10 M 1312:

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



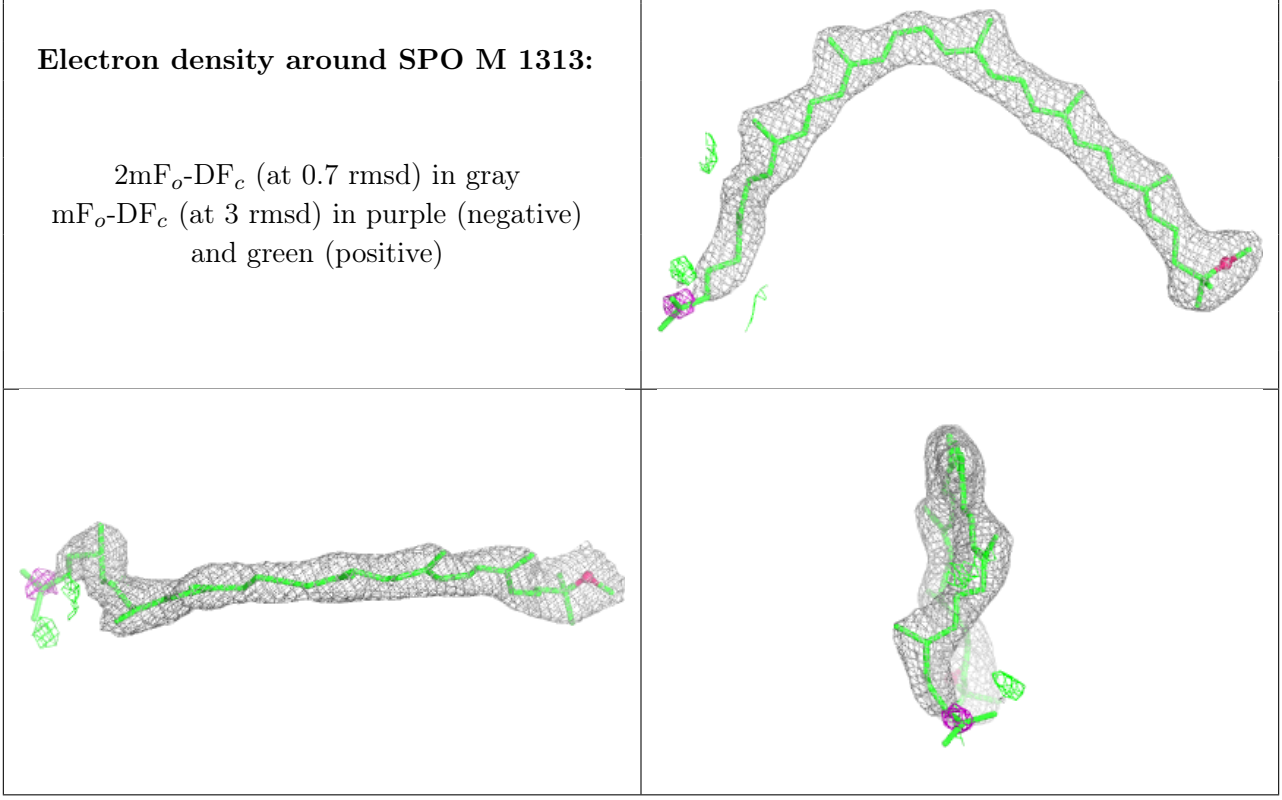
Electron density around BCL M 1303:

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



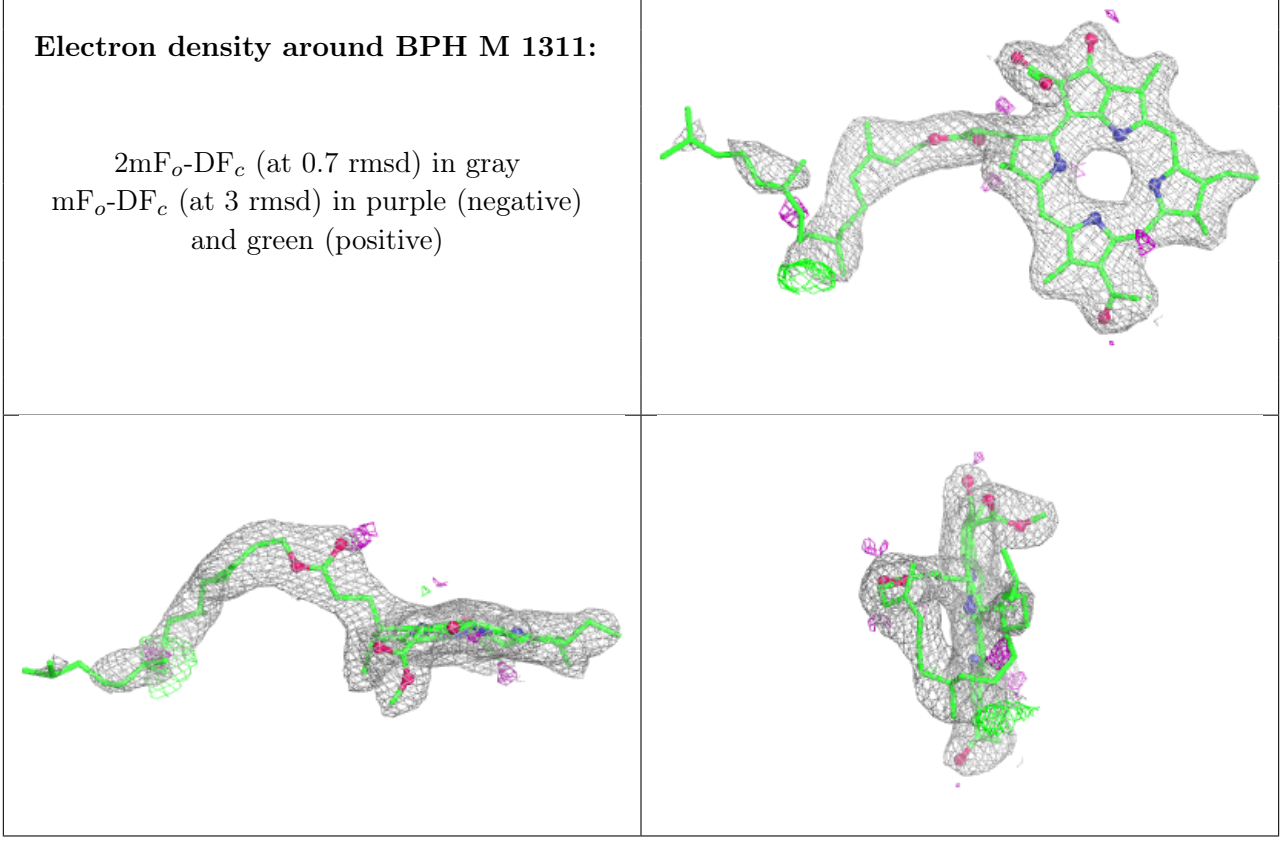
Electron density around SPO M 1313:

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



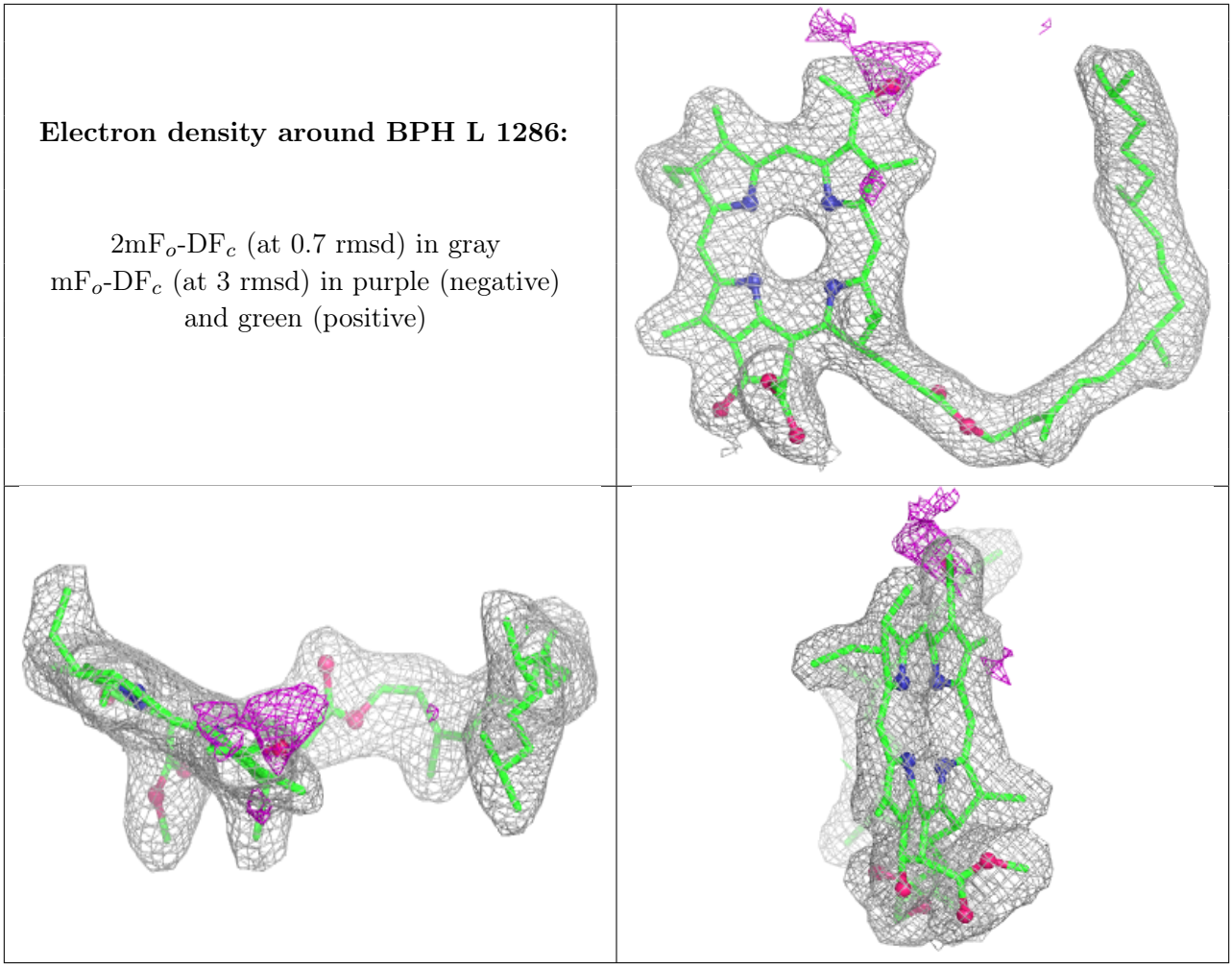
Electron density around BPH M 1311:

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



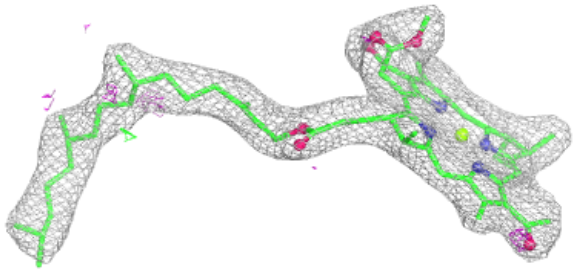
Electron density around BPH L 1286:

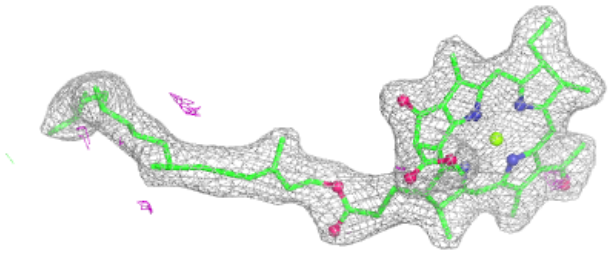
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

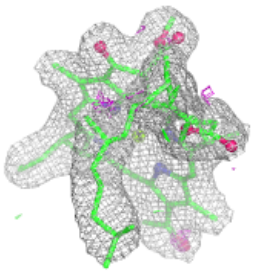


Electron density around BCL M 1304:

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

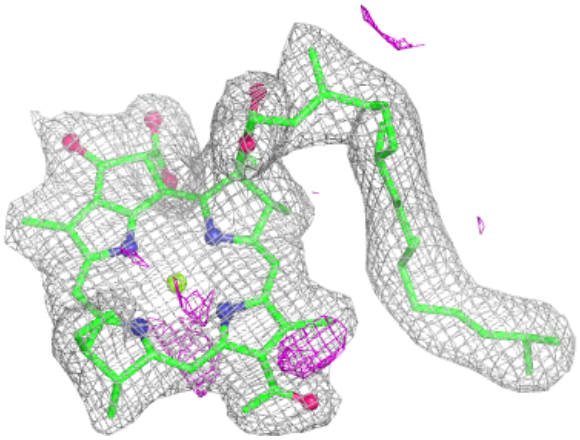


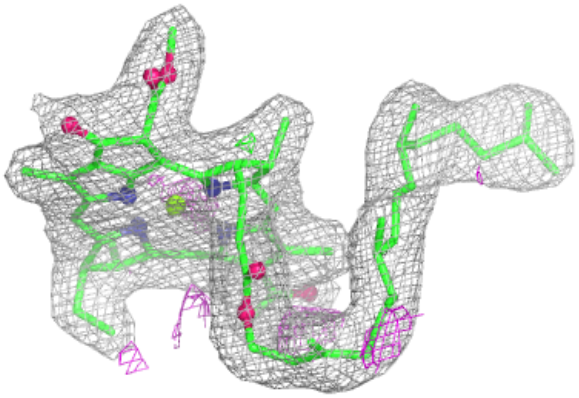




Electron density around BCL L 1282:

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

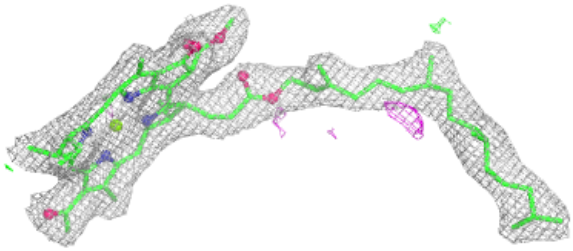


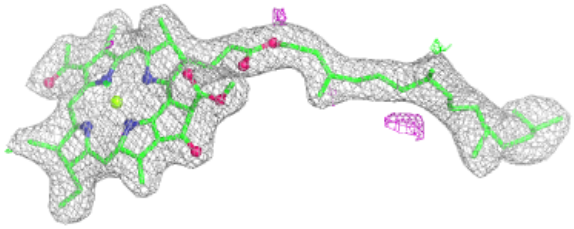


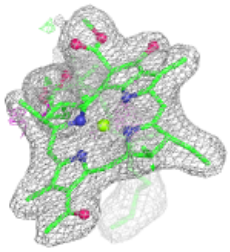


Electron density around BCL L 1288:

$2mF_o$-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.