wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2026 – 08:38 am BST

PDB ID	:	2UWS / pdb_00002uws
Title	:	X-ray high resolution structure of the photosynthetic reaction center from Rb. sphaeroides at pH 6.5 in the charge-separated state
Authors	:	Koepke, J.; Diehm, R.; Fritzsch, G.
Deposited on	:	2007-03-23
Resolution	:	2.90 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:

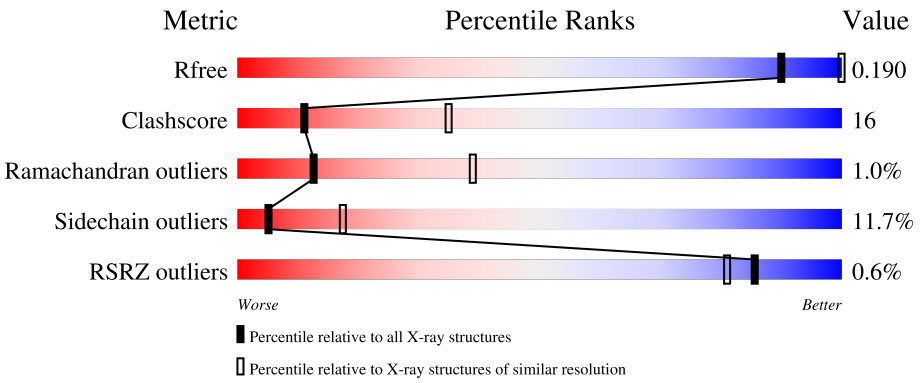
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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

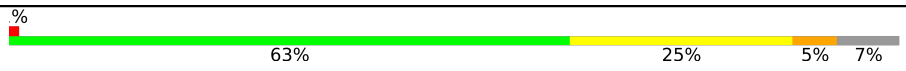
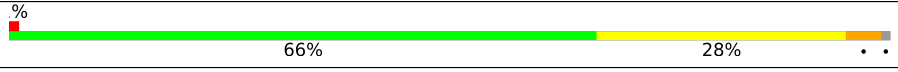
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	L	281	
3	M	307	

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
6	BCL	L	1282	X	-	-	-
6	BCL	L	1286	X	-	-	-
6	BCL	M	1303	X	-	-	-
6	BCL	M	1304	X	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 7325 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	1830	1169	315	337	9	0	0	1

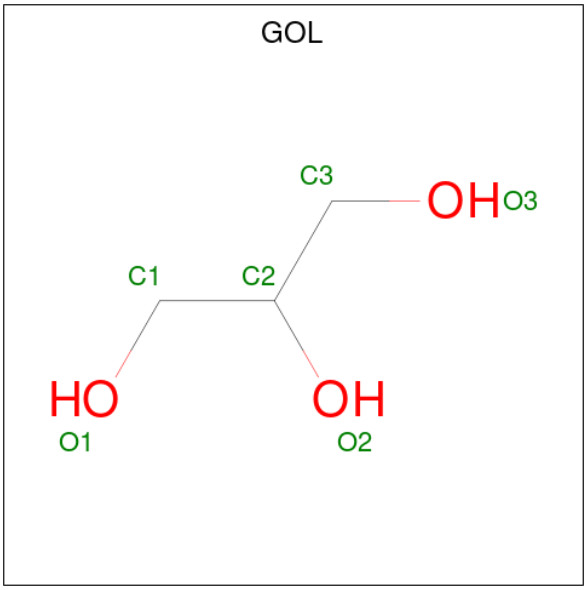
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	280	2222	1501	352	361	8	0	0	0

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

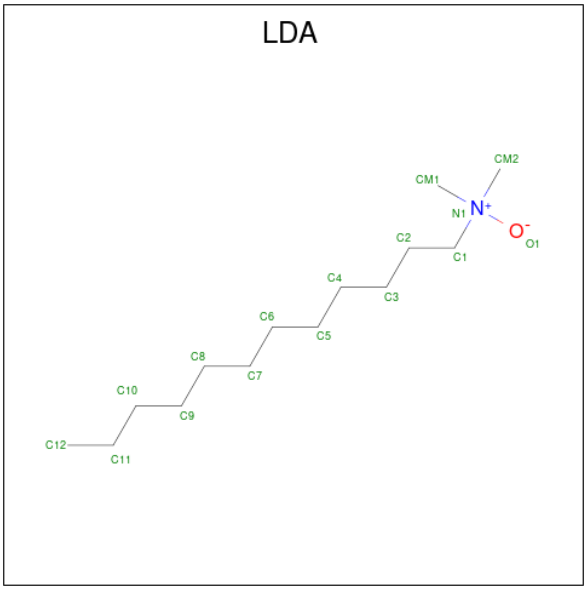
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	303	2409	1607	395	397	10	0	0	1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	O		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 LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



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

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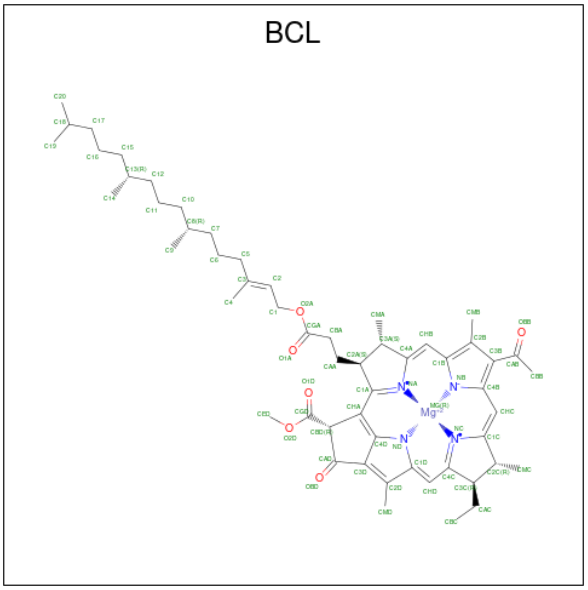
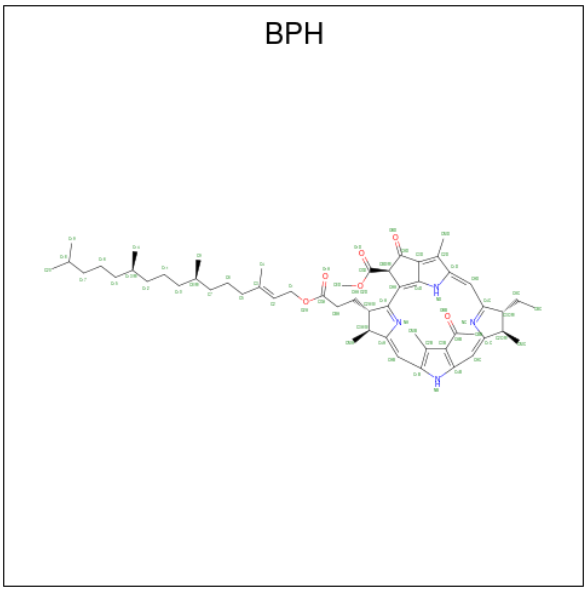
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	16	14	1	1	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



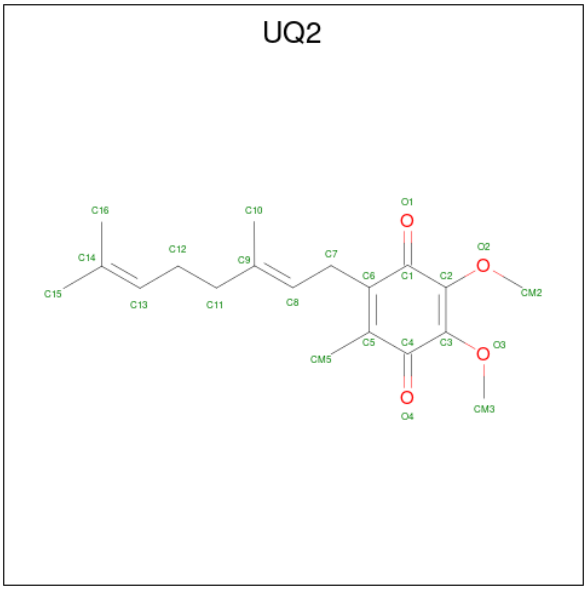
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
6	M	1	66	55	1	4	6	0	0

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



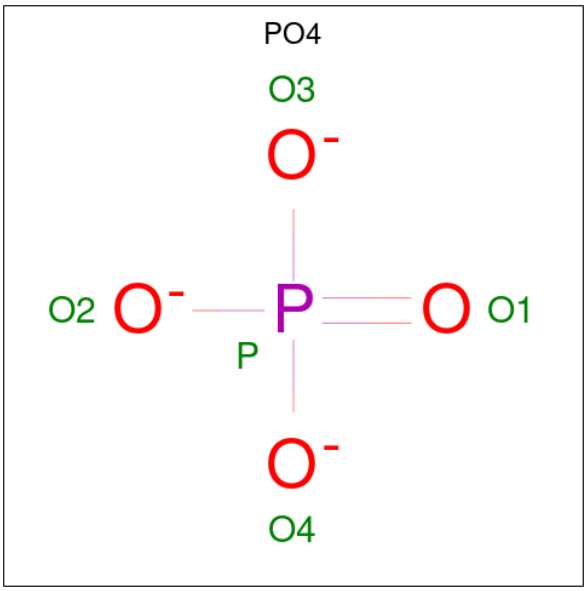
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	L	1	65	55	4	6	0	0
7	M	1	65	55	4	6	0	0

- 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).

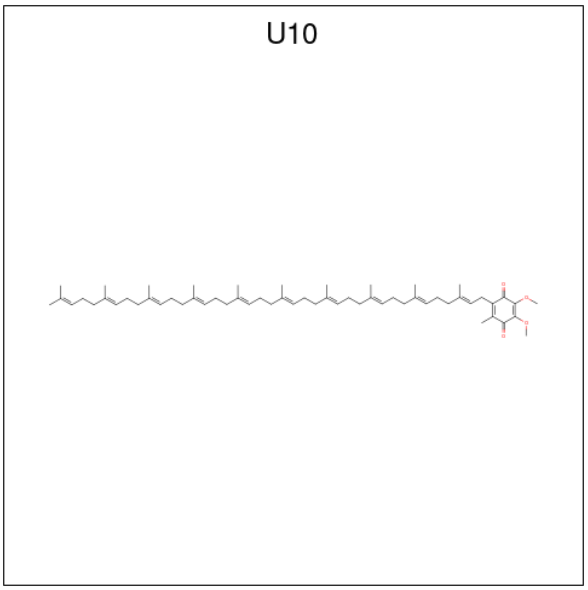


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total O P 5 4 1	0	0

- Molecule 10 is FE (III) ION (CCD ID: FE) (formula: Fe).

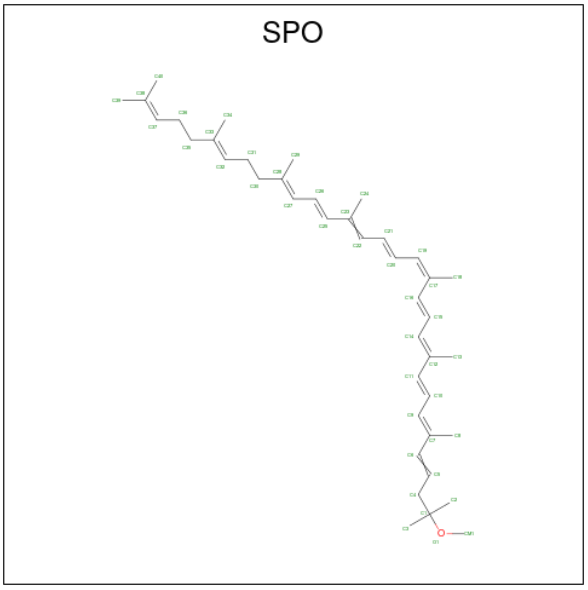
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Fe 1 1	0	0

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 12 is SPHEROIDENE (CCD ID: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 13 is water.

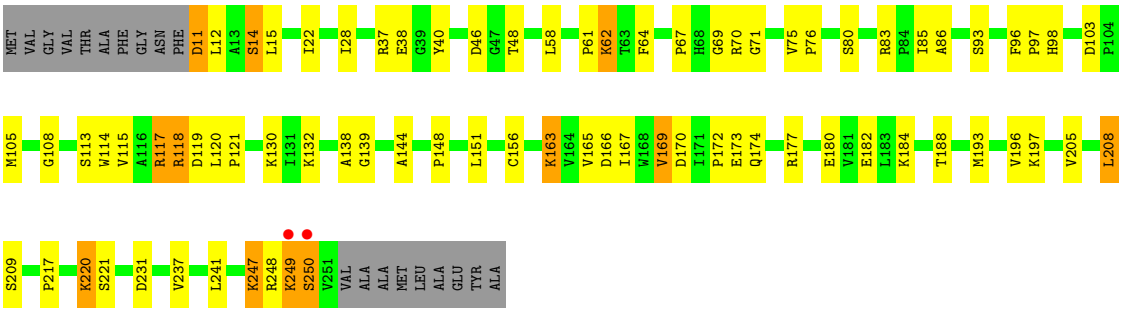
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	H	70	70	70	0	0
			Total	O		
13	L	59	59	59	0	0
			Total	O		
13	M	41	41	41	0	0

3 Residue-property plots (i)

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

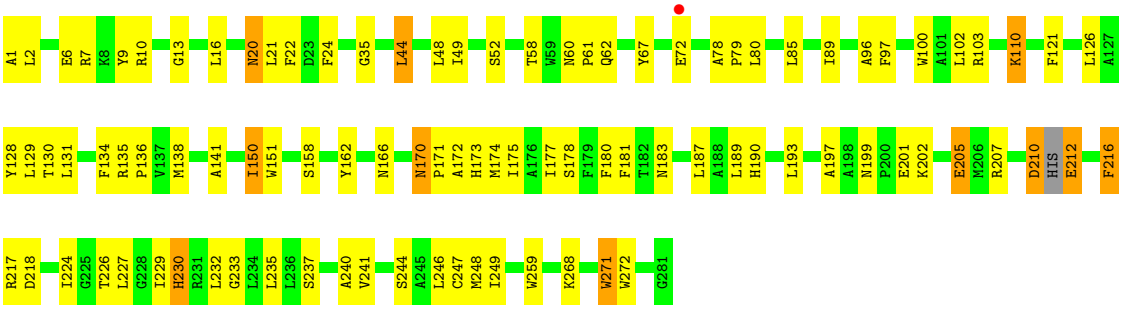
• Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



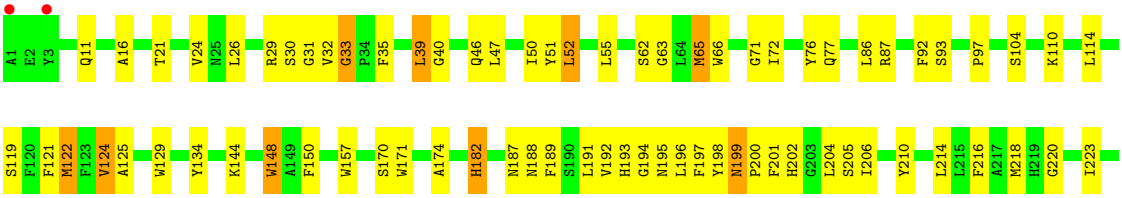
• Molecule 2: REACTION CENTER PROTEIN L CHAIN

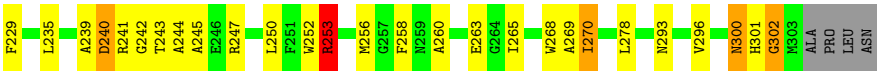
Chain L:



• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:




F229
L235
A239
D240
R241
G242
T243
A244
A245
E246
R247
L250
F251
W252
R253
M256
G257
F258
N259
A260
E263
G264
I265
W268
A269
I270
L278
N293
V296
N300
H301
G302
M303
ALA
PRO
LEU
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.31Å 139.31Å 184.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.90 119.52 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (119.52-2.90) 88.5 (119.52-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.248 0.191 , 0.190	Depositor DCC
R_{free} test set	3032 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	50.2	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7325	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	H	1.04	3/1878 (0.2%)	1.15	4/2555 (0.2%)
2	L	0.97	1/2308 (0.0%)	1.08	7/3157 (0.2%)
3	M	0.98	2/2501 (0.1%)	1.14	9/3415 (0.3%)
All	All	0.99	6/6687 (0.1%)	1.13	20/9127 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	302	GLY	C-N	-7.23	1.23	1.33
3	M	256	MET	SD-CE	-6.34	1.63	1.79
2	L	138	MET	SD-CE	6.30	1.95	1.79
1	H	250	SER	C-N	-5.83	1.25	1.33
1	H	85	ILE	CA-CB	5.45	1.59	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	302	GLY	O-C-N	-6.85	112.04	123.00
1	H	250	SER	O-C-N	-6.33	112.88	123.00
3	M	253	ARG	N-CA-C	-6.16	104.65	111.36
3	M	182	HIS	CB-CA-C	6.10	120.92	110.79
2	L	141	ALA	N-CA-C	6.07	119.41	108.48

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1830	0	1836	51	0
2	L	2222	0	2179	70	0
3	M	2409	0	2321	79	0
4	H	12	0	16	1	0
4	L	12	0	16	2	0
4	M	6	0	8	0	0
5	L	32	0	62	2	0
5	M	96	0	186	10	0
6	L	132	0	148	18	0
6	M	132	0	148	29	0
7	L	65	0	76	18	0
7	M	65	0	76	11	0
8	L	46	0	52	12	0
9	L	5	0	0	0	0
10	M	1	0	0	0	0
11	M	48	0	63	8	0
12	M	42	0	60	6	0
13	H	70	0	0	5	1
13	L	59	0	0	0	0
13	M	41	0	0	1	0
All	All	7325	0	7247	236	1

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 16.

The worst 5 of 236 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:M:1303:BCL:H71	6:M:1304:BCL:H202	1.36	1.04
7:L:1284:BPH:CBB	7:L:1284:BPH:HHC	1.95	0.96
11:M:1313:U10:H352	11:M:1313:U10:H312	1.49	0.95
3:M:197:PHE:CZ	6:M:1304:BCL:HBB2	2.07	0.89
11:M:1313:U10:H312	11:M:1313:U10:C35	2.06	0.86

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:2021:HOH:O	13:H:2021:HOH:O[4_555]	1.99	0.21

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	239/260 (92%)	222 (93%)	14 (6%)	3 (1%)	9 32
2	L	276/281 (98%)	253 (92%)	23 (8%)	0	100 100
3	M	301/307 (98%)	274 (91%)	22 (7%)	5 (2%)	7 26
All	All	816/848 (96%)	749 (92%)	59 (7%)	8 (1%)	12 39

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	30	SER
3	M	240	ASP
3	M	301	HIS
1	H	86	ALA

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	195/208 (94%)	172 (88%)	23 (12%)	5 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	219/220 (100%)	191 (87%)	28 (13%)	4	14
3	M	236/240 (98%)	211 (89%)	25 (11%)	6	22
All	All	650/668 (97%)	574 (88%)	76 (12%)	5	17

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	86	LEU
3	M	258	PHE
3	M	110	LYS
3	M	191	LEU
3	M	300	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	193	HIS
3	M	199	ASN
2	L	170	ASN
2	L	183	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	BCL	M	1304	3	69,74,74	1.87	9 (13%)	83,115,115	2.89	30 (36%)
6	BCL	L	1286	2	69,74,74	1.92	9 (13%)	83,115,115	2.71	24 (28%)
5	LDA	M	1305	-	12,15,15	1.99	1 (8%)	14,17,17	0.76	0
6	BCL	M	1303	3	69,74,74	1.97	7 (10%)	83,115,115	2.79	24 (28%)
5	LDA	L	1281	-	12,15,15	2.08	1 (8%)	14,17,17	0.62	0
8	UQ2	L	1285[B]	-	23,23,23	2.80	8 (34%)	28,31,31	1.48	5 (17%)
5	LDA	M	1308	-	12,15,15	2.14	1 (8%)	14,17,17	0.61	0
4	GOL	M	1315	-	5,5,5	0.48	0	5,5,5	0.50	0
5	LDA	M	1306	-	12,15,15	1.99	1 (8%)	14,17,17	0.59	0
5	LDA	M	1309	-	12,15,15	1.87	1 (8%)	14,17,17	0.61	0
7	BPH	M	1312	-	59,70,70	2.59	12 (20%)	61,101,101	2.72	19 (31%)
5	LDA	M	1307	-	12,15,15	1.87	1 (8%)	14,17,17	0.65	0
4	GOL	L	1289	-	5,5,5	0.37	0	5,5,5	0.39	0
5	LDA	M	1310	-	12,15,15	2.03	1 (8%)	14,17,17	0.54	0
4	GOL	L	1288	-	5,5,5	0.35	0	5,5,5	0.72	0
9	PO4	L	1287	-	4,4,4	0.82	0	6,6,6	0.61	0
6	BCL	L	1282	2	69,74,74	1.92	8 (11%)	83,115,115	2.52	29 (34%)
4	GOL	H	1252	-	5,5,5	0.49	0	5,5,5	0.57	0
12	SPO	M	1314	-	40,41,41	4.24	12 (30%)	47,50,50	2.20	14 (29%)
5	LDA	L	1283	-	12,15,15	2.03	1 (8%)	14,17,17	0.69	1 (7%)
8	UQ2	L	1285[A]	-	23,23,23	2.83	9 (39%)	28,31,31	1.31	2 (7%)
11	U10	M	1313	-	48,48,63	2.78	11 (22%)	58,61,79	1.92	15 (25%)
4	GOL	H	1251	-	5,5,5	0.50	0	5,5,5	0.35	0
7	BPH	L	1284	-	59,70,70	2.85	11 (18%)	61,101,101	2.71	23 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	M	1304	3	2/2/21/25	12/41/137/137	-
6	BCL	L	1286	2	2/2/21/25	10/41/137/137	-
5	LDA	M	1305	-	-	5/13/13/13	-
6	BCL	M	1303	3	2/2/21/25	17/41/137/137	-
5	LDA	L	1281	-	-	8/13/13/13	-
8	UQ2	L	1285[B]	-	-	8/15/39/39	0/1/1/1
5	LDA	M	1308	-	-	8/13/13/13	-
4	GOL	M	1315	-	-	2/4/4/4	-
5	LDA	M	1306	-	-	5/13/13/13	-
5	LDA	M	1309	-	-	5/13/13/13	-
7	BPH	M	1312	-	-	17/37/105/105	0/5/6/6
5	LDA	M	1307	-	-	8/13/13/13	-
4	GOL	L	1289	-	-	4/4/4/4	-
5	LDA	M	1310	-	-	5/13/13/13	-
4	GOL	L	1288	-	-	2/4/4/4	-
6	BCL	L	1282	2	2/2/21/25	14/41/137/137	-
4	GOL	H	1252	-	-	4/4/4/4	-
12	SPO	M	1314	-	-	25/47/47/47	-
5	LDA	L	1283	-	-	8/13/13/13	-
8	UQ2	L	1285[A]	-	-	8/15/39/39	0/1/1/1
11	U10	M	1313	-	-	16/45/69/87	0/1/1/1
4	GOL	H	1251	-	-	2/4/4/4	-
7	BPH	L	1284	-	-	12/37/105/105	0/5/6/6

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1284	BPH	OBD-CAD	14.21	1.42	1.22
12	M	1314	SPO	C27-C28	13.40	1.48	1.34
7	M	1312	BPH	OBD-CAD	11.80	1.38	1.22
6	L	1286	BCL	OBD-CAD	10.82	1.41	1.22
6	M	1303	BCL	OBD-CAD	10.70	1.40	1.22

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1286	BCL	C2D-C1D-ND	-11.07	101.95	110.10
7	L	1284	BPH	O2D-CGD-CBD	10.67	124.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1312	BPH	OBD-CAD-CBD	-10.28	110.73	125.82
6	L	1286	BCL	C1D-ND-C4D	10.14	113.54	106.33
6	M	1303	BCL	C2D-C1D-ND	-9.22	103.31	110.10

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	1282	BCL	C13
6	L	1282	BCL	C8
6	L	1286	BCL	C13
6	L	1286	BCL	C8
6	M	1303	BCL	C13

5 of 205 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	GOL	O1-C1-C2-C3
4	H	1252	GOL	C1-C2-C3-O3
4	L	1288	GOL	C1-C2-C3-O3
4	L	1289	GOL	O1-C1-C2-C3
5	M	1307	LDA	C2-C1-N1-O1

There are no ring outliers.

18 monomers are involved in 100 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1304	BCL	24	0
6	L	1286	BCL	13	0
5	M	1305	LDA	2	0
6	M	1303	BCL	10	0
5	L	1281	LDA	1	0
8	L	1285[B]	UQ2	4	0
5	M	1308	LDA	2	0
5	M	1309	LDA	4	0
7	M	1312	BPH	11	0
5	M	1307	LDA	6	0
4	L	1288	GOL	2	0
6	L	1282	BCL	8	0
12	M	1314	SPO	6	0
5	L	1283	LDA	1	0
8	L	1285[A]	UQ2	8	0
11	M	1313	U10	8	0

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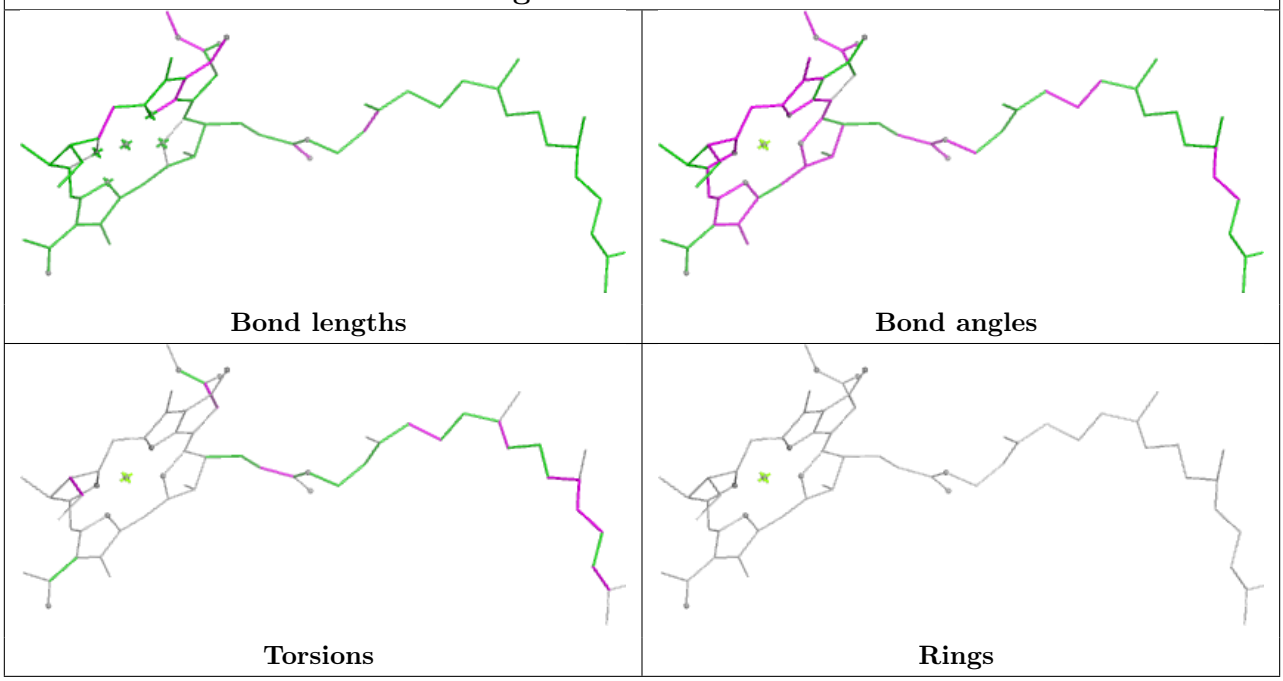
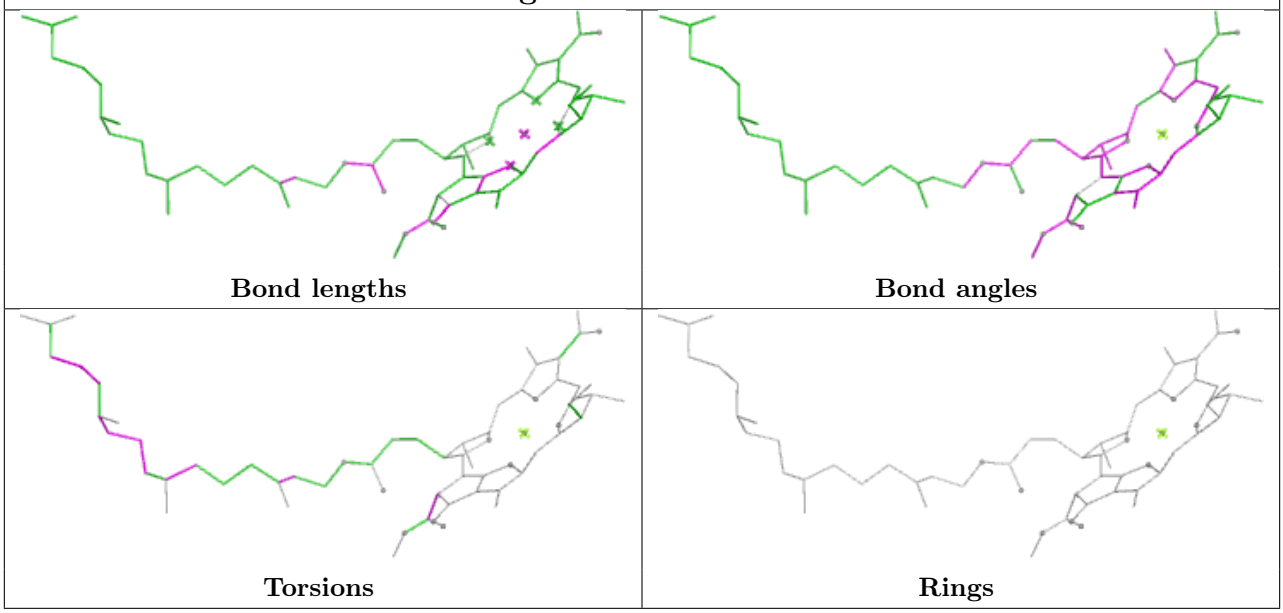
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	GOL	1	0
7	L	1284	BPH	18	0

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.

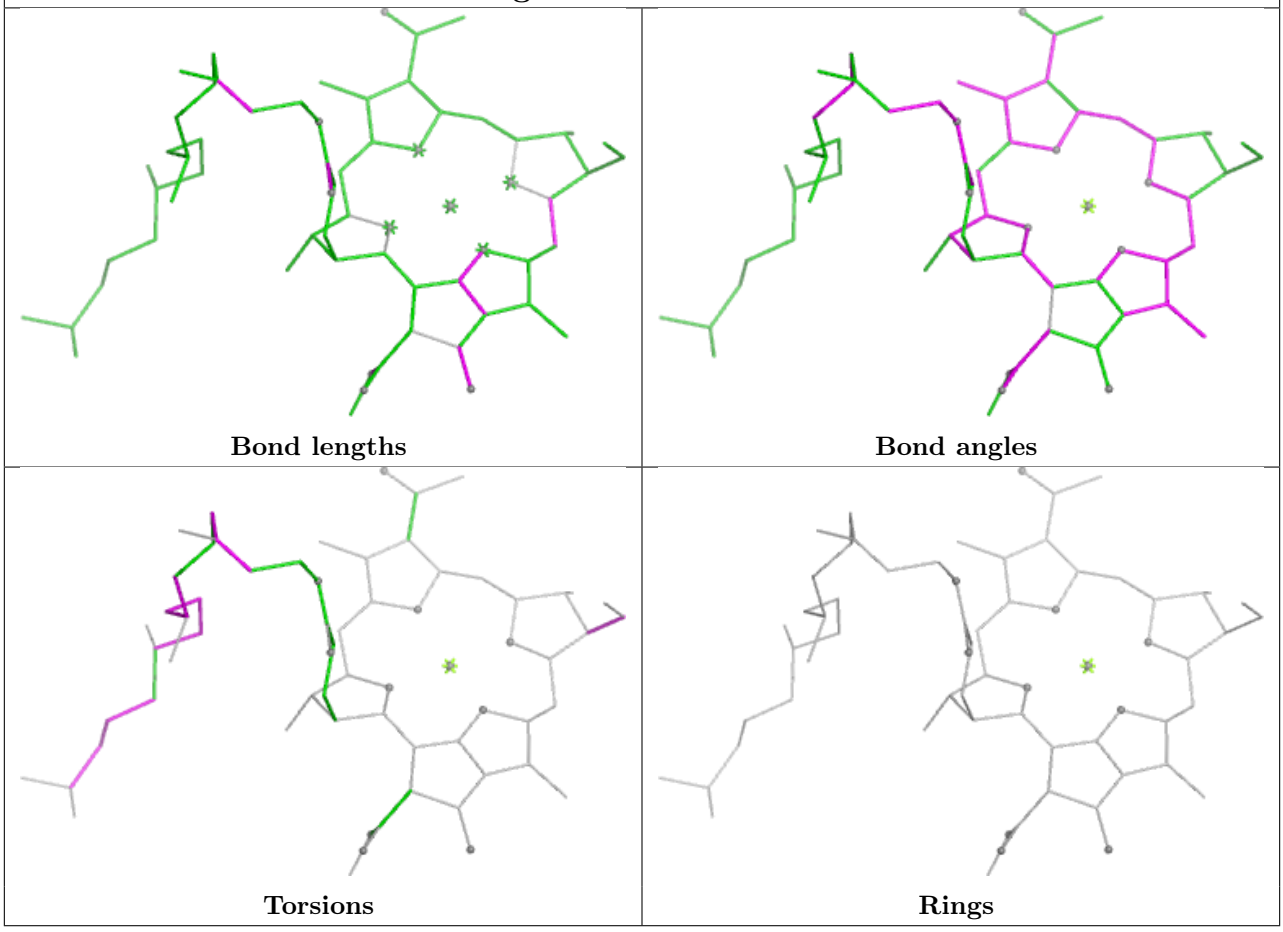
Ligand BCL M 1304



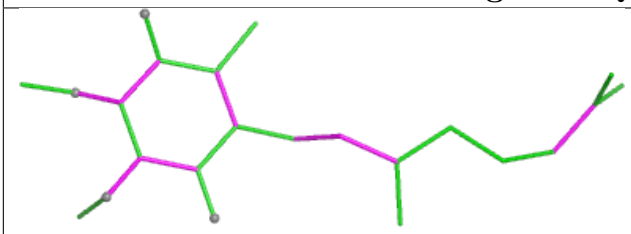
Ligand BCL L 1286



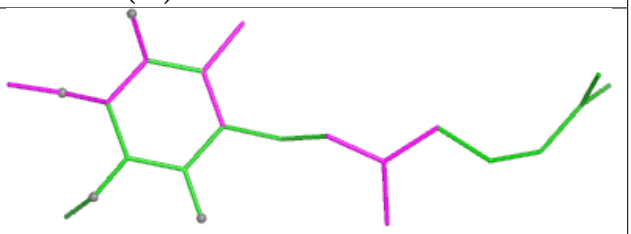
Ligand BCL M 1303



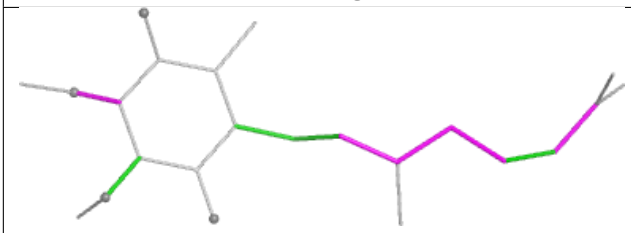
Ligand UQ2 L 1285 (B)



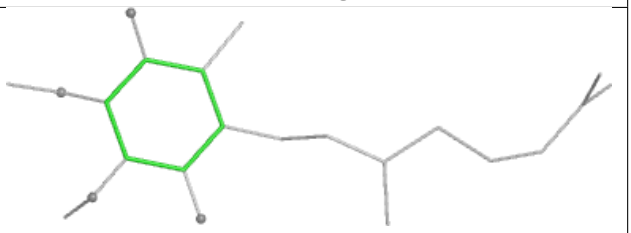
Bond lengths



Bond angles

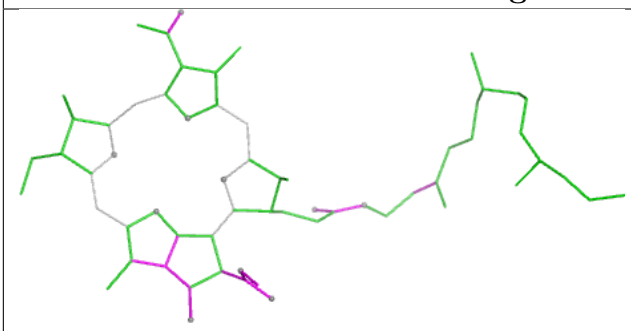


Torsions

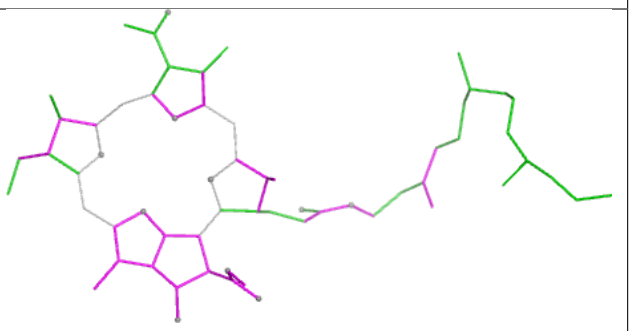


Rings

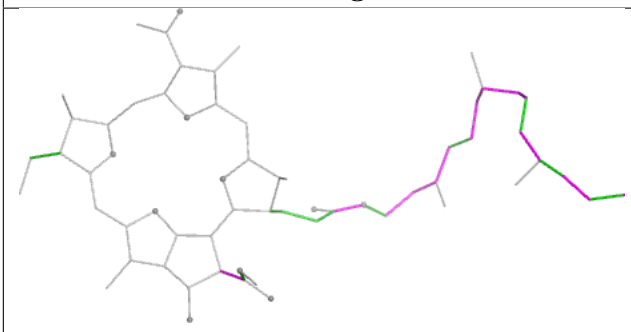
Ligand BPH M 1312



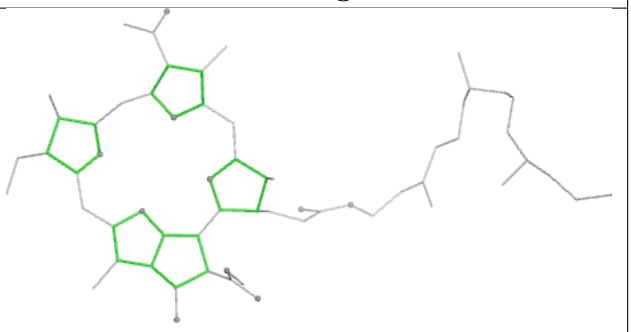
Bond lengths



Bond angles

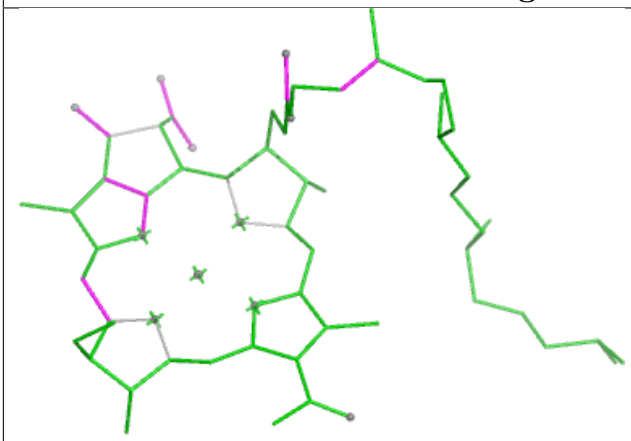


Torsions

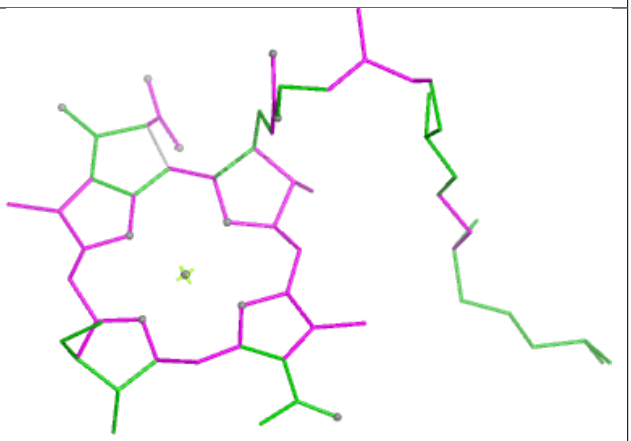


Rings

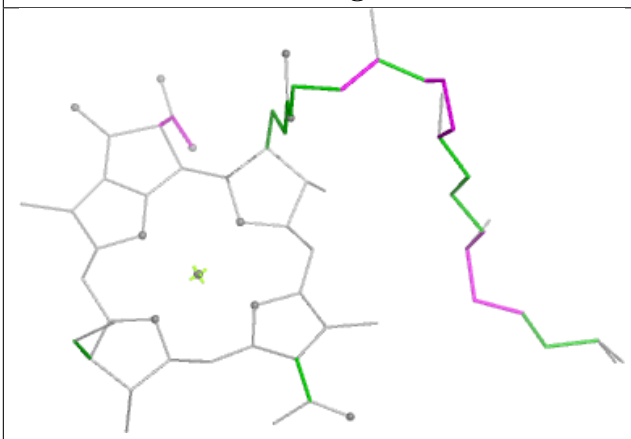
Ligand BCL L 1282



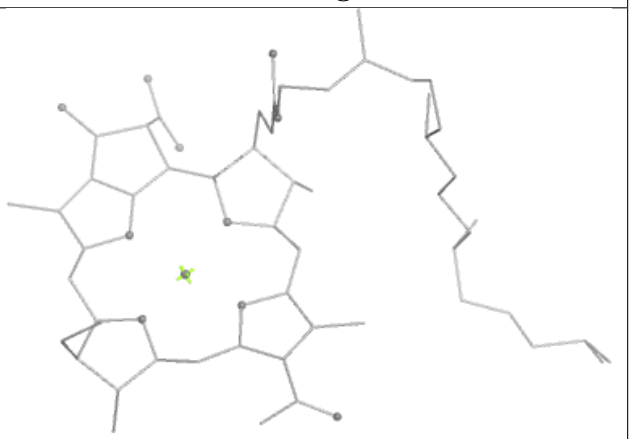
Bond lengths



Bond angles

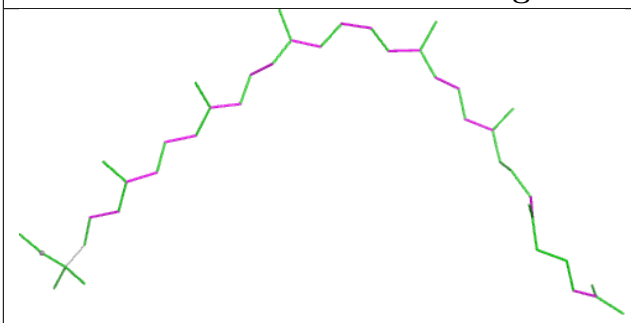


Torsions

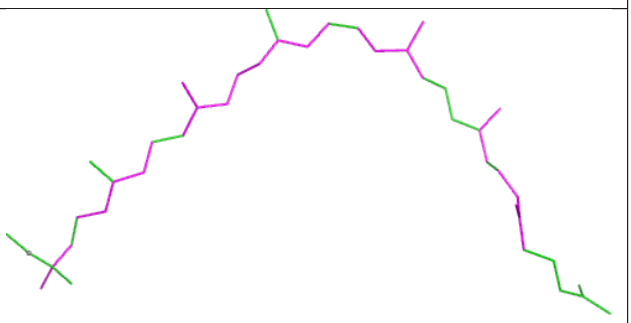


Rings

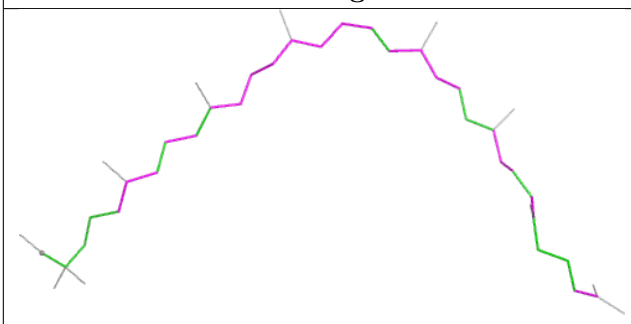
Ligand SPO M 1314



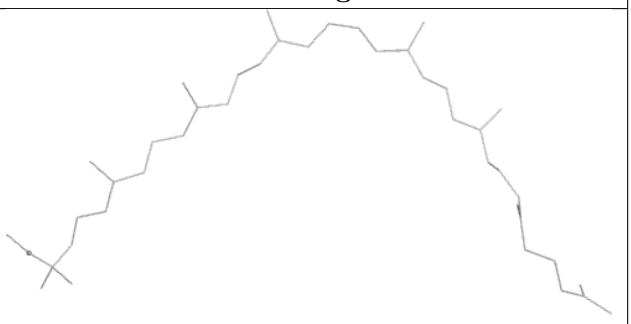
Bond lengths



Bond angles

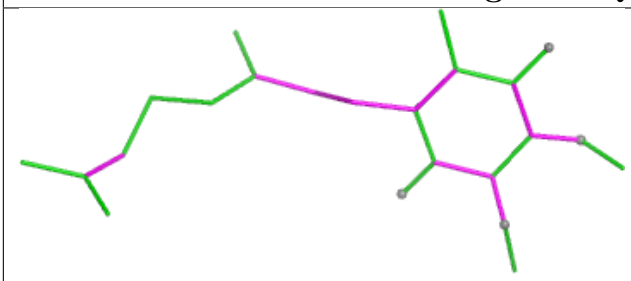


Torsions

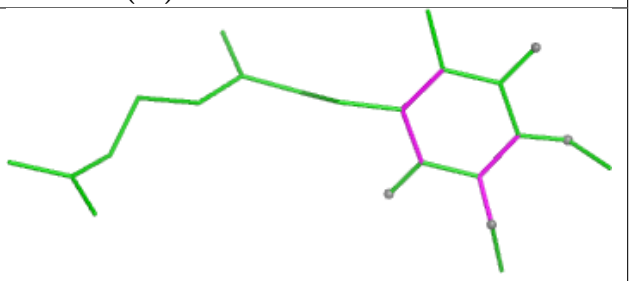


Rings

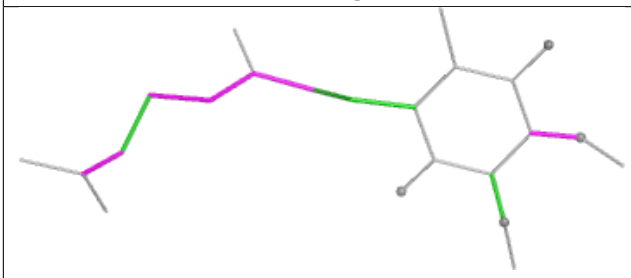
Ligand UQ2 L 1285 (A)



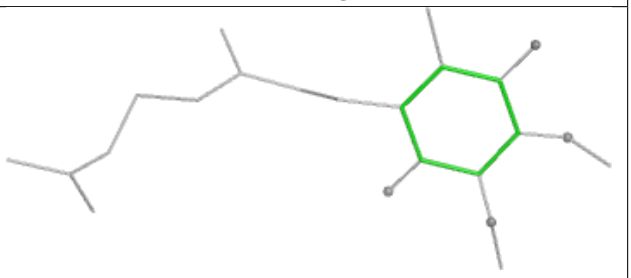
Bond lengths



Bond angles

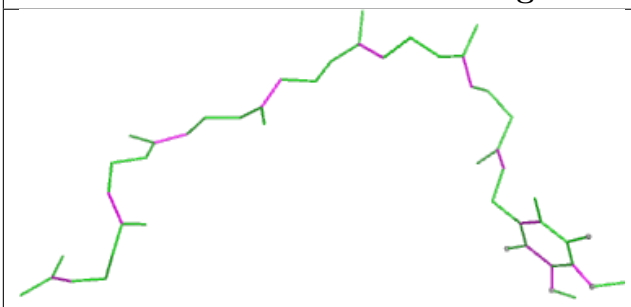


Torsions

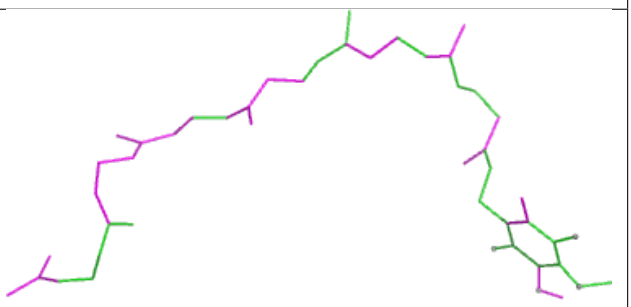


Rings

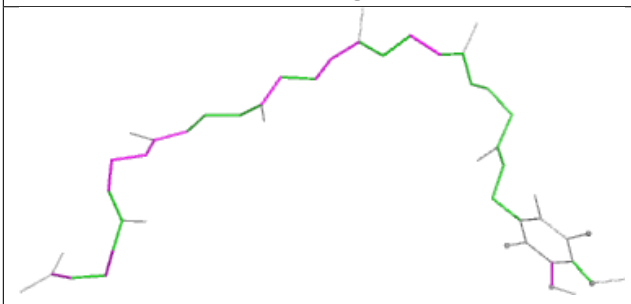
Ligand U10 M 1313



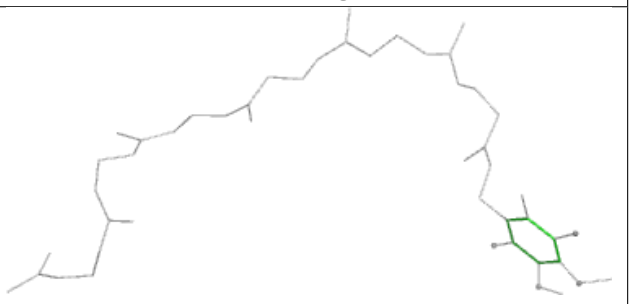
Bond lengths



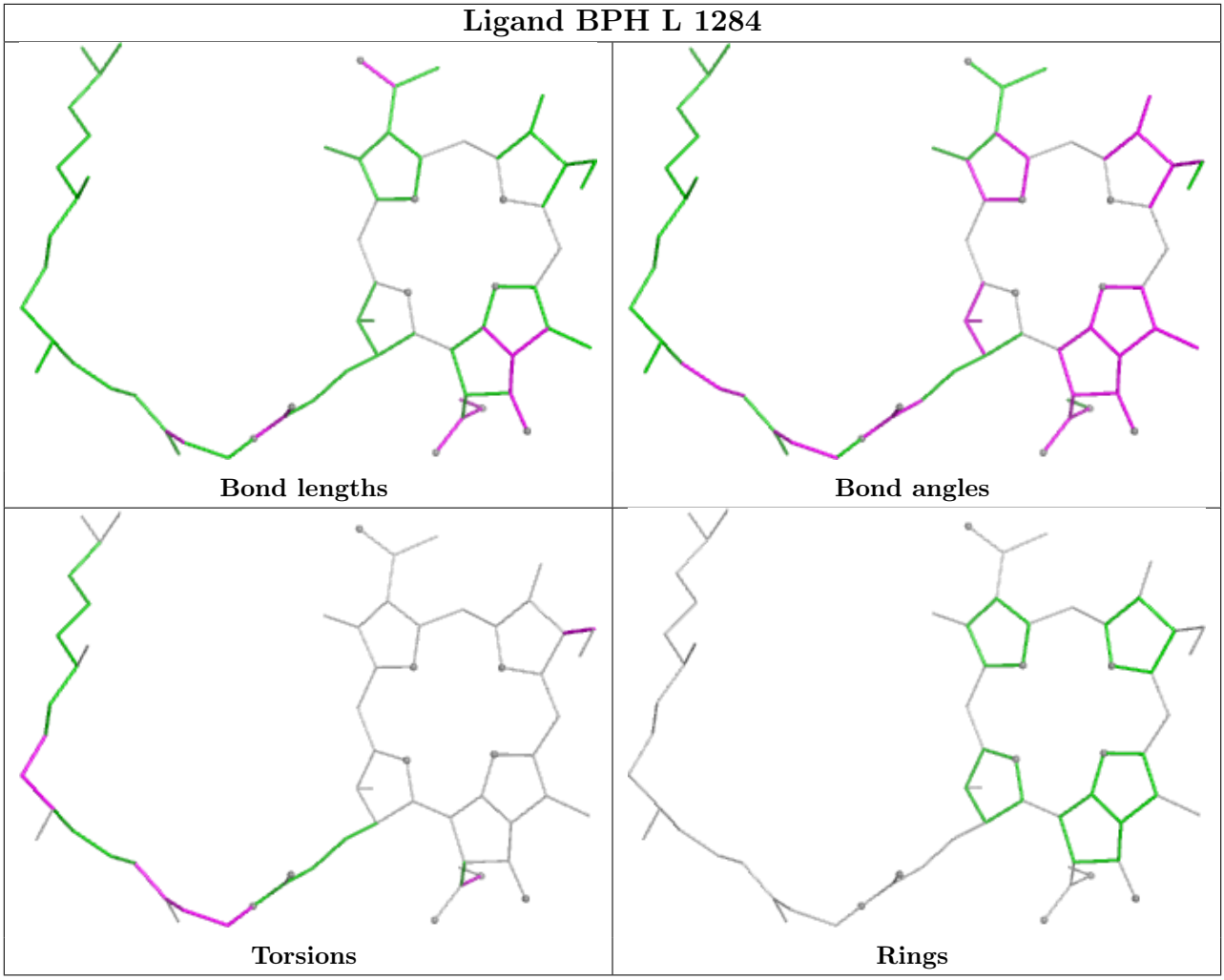
Bond angles



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 (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%)	-0.41	2 (0%)	82	77	35, 48, 61, 97	0
2	L	280/281 (99%)	-0.37	1 (0%)	88	85	32, 45, 72, 82	0
3	M	303/307 (98%)	-0.33	2 (0%)	84	79	31, 50, 75, 92	0
All	All	824/848 (97%)	-0.37	5 (0%)	85	81	31, 48, 72, 97	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	3.0
3	M	3	TYR	2.8
1	H	249	LYS	2.4
3	M	1	ALA	2.1
2	L	72	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

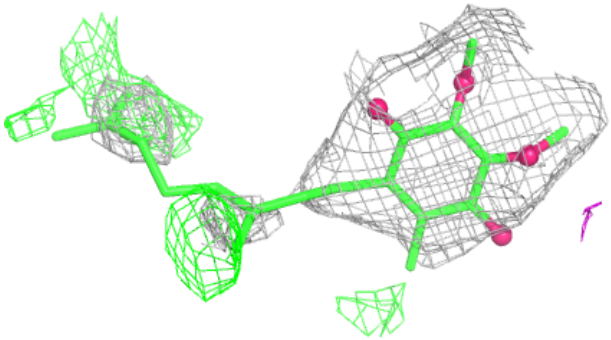
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

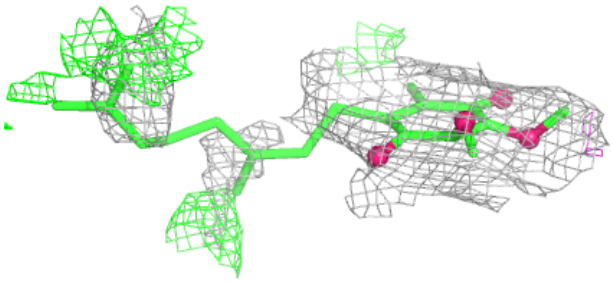
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LDA	L	1283	16/16	0.70	0.28	51,105,127,128	0
4	GOL	M	1315	6/6	0.73	0.20	98,100,101,101	0
5	LDA	L	1281	16/16	0.80	0.26	102,111,115,115	0
5	LDA	M	1308	16/16	0.80	0.29	114,120,127,128	0
5	LDA	M	1309	16/16	0.80	0.24	97,102,115,115	0
4	GOL	H	1251	6/6	0.81	0.21	98,99,100,100	0
5	LDA	M	1310	16/16	0.82	0.25	91,109,117,117	0
5	LDA	M	1306	16/16	0.83	0.23	70,77,91,91	0
5	LDA	M	1307	16/16	0.85	0.18	62,66,80,80	0
5	LDA	M	1305	16/16	0.85	0.19	55,70,79,80	0
8	UQ2	L	1285[A]	23/23	0.86	0.20	40,45,49,49	23
8	UQ2	L	1285[B]	23/23	0.86	0.20	44,46,51,51	23
4	GOL	H	1252	6/6	0.89	0.10	80,83,83,85	0
4	GOL	L	1289	6/6	0.91	0.16	95,96,97,97	0
12	SPO	M	1314	42/42	0.91	0.15	42,60,83,86	0
11	U10	M	1313	48/63	0.92	0.14	44,53,79,81	0
7	BPH	M	1312	65/65	0.93	0.11	30,50,109,112	0
4	GOL	L	1288	6/6	0.95	0.21	58,62,63,65	0
9	PO4	L	1287	5/5	0.95	0.07	91,91,92,92	0
6	BCL	L	1282	66/66	0.96	0.07	28,36,56,59	0
6	BCL	M	1303	66/66	0.96	0.09	26,37,86,87	0
7	BPH	L	1284	65/65	0.96	0.08	29,39,44,50	0
6	BCL	M	1304	66/66	0.97	0.07	32,37,58,66	0
6	BCL	L	1286	66/66	0.97	0.07	29,38,49,51	0
10	FE	M	1311	1/1	1.00	0.04	41,41,41,41	0

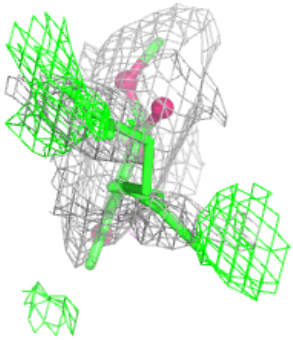
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UQ2 L 1285 (A):

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

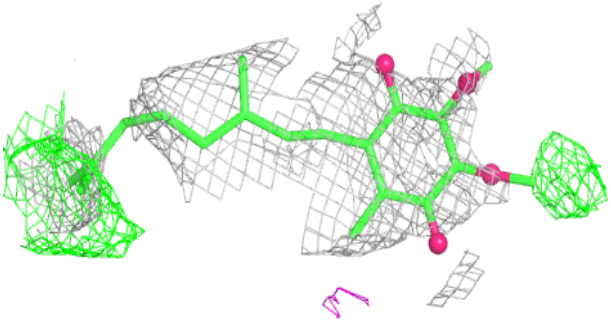


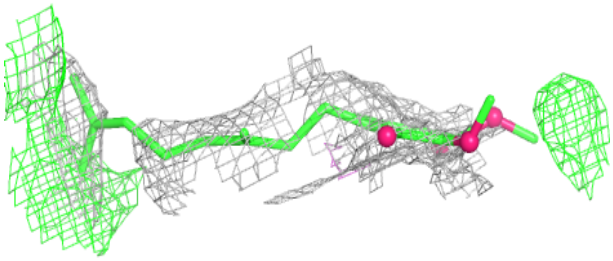


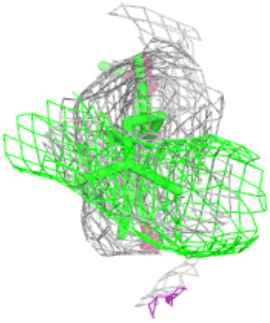


Electron density around UQ2 L 1285 (B):

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

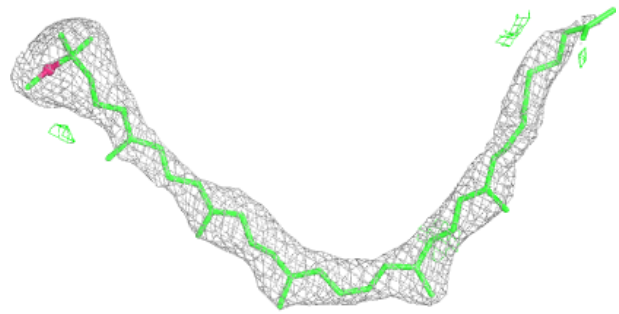


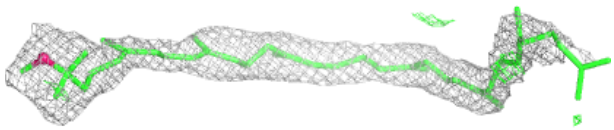


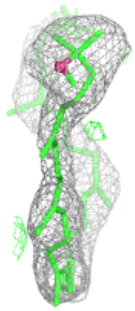


Electron density around SPO M 1314:

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

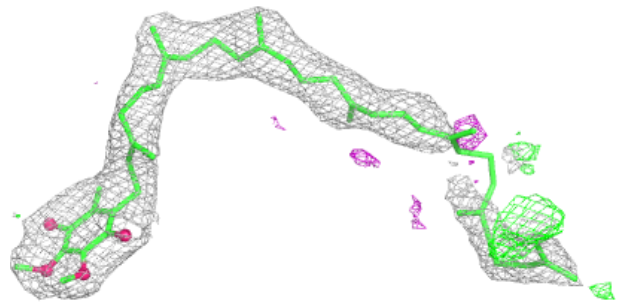


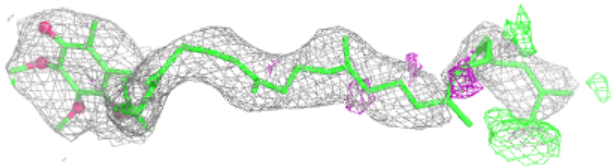




Electron density around U10 M 1313:

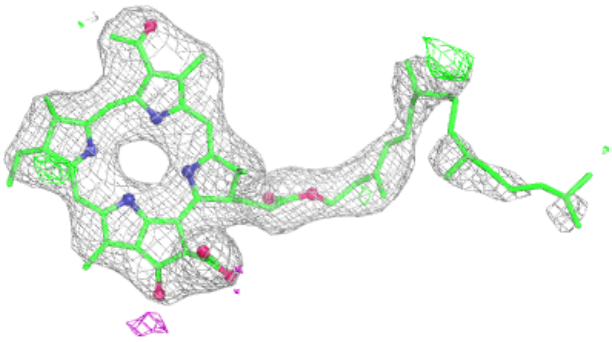
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

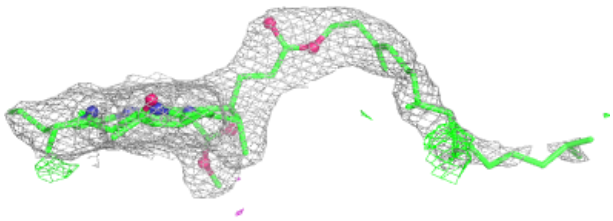




Electron density around BPH M 1312:

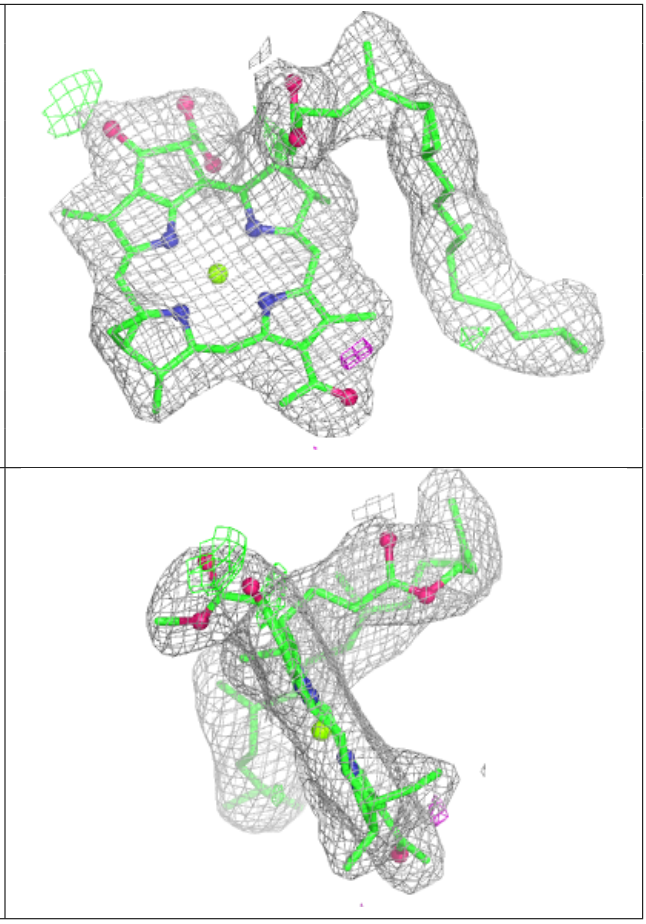
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





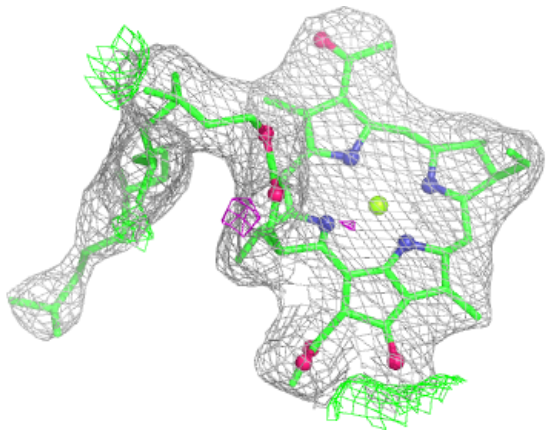
Electron density around BCL L 1282:

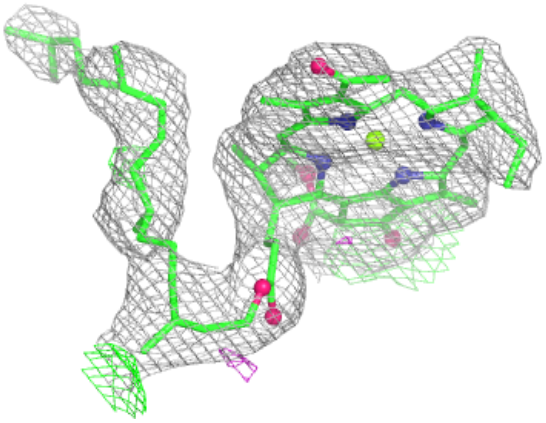
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

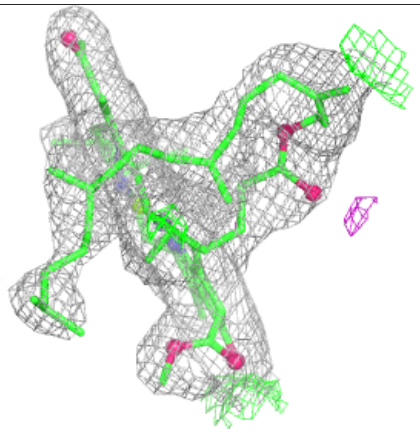


Electron density around BCL M 1303:

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

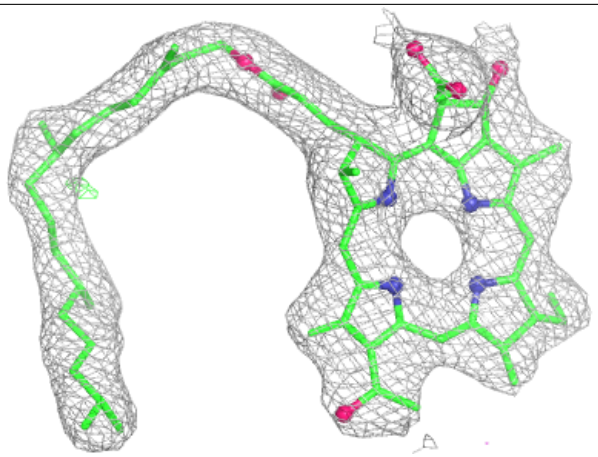


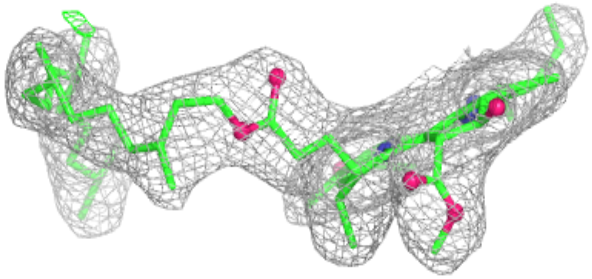


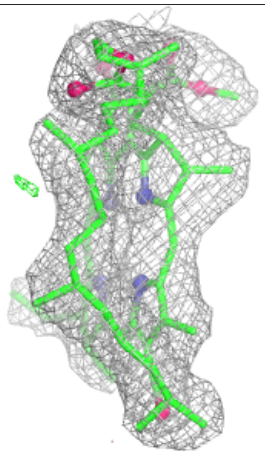


Electron density around BPH L 1284:

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

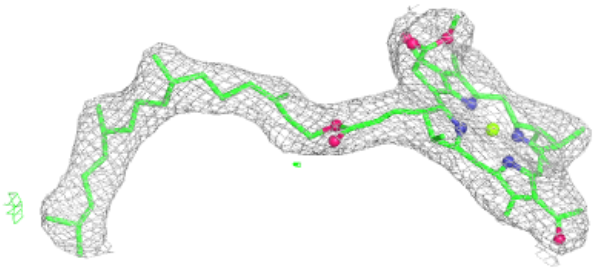


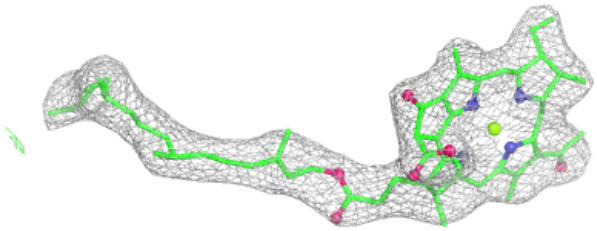


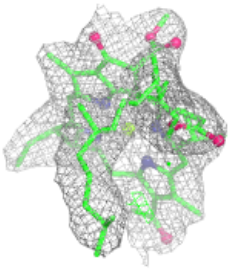


Electron density around BCL M 1304:

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

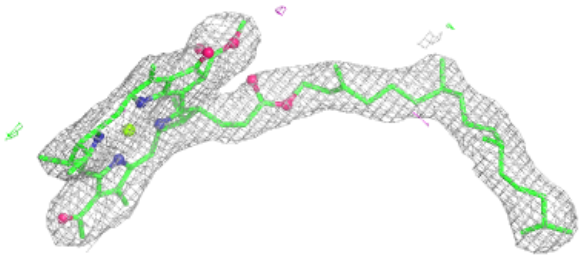


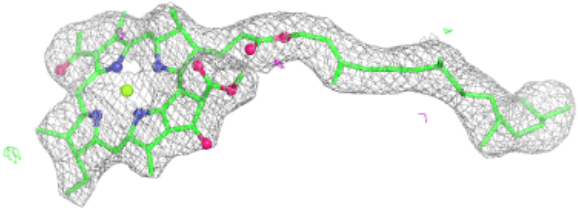


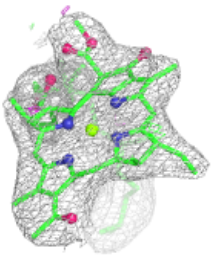


Electron density around BCL L 1286:

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







6.5 Other polymers (i)

There are no such residues in this entry.