wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 04:19 pm BST

PDB ID	:	3ZUW
Title	:	Photosynthetic Reaction Centre Mutant with TYR L128 replaced with HIS
Authors	:	Gibasiewicz, K.; Pajzderska, M.; Potter, J.A.; Fyfe, P.K.; Dobek, A.; Brettel, K.; Jones, M.R.
Deposited on	:	2011-07-20
Resolution	:	2.31 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:

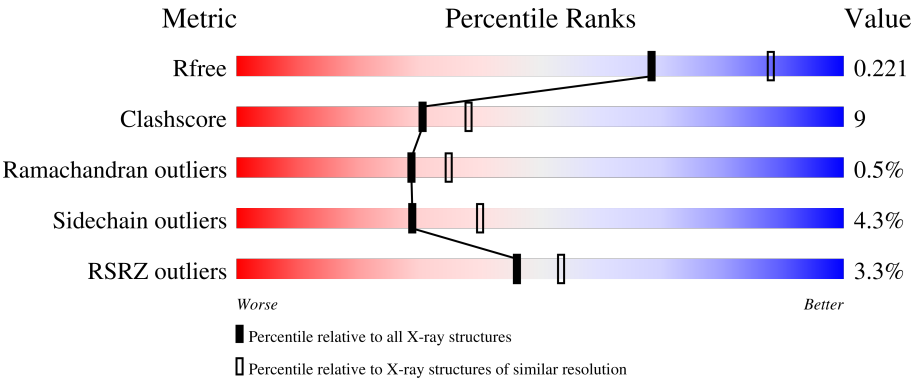
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	5% 78% 12% · 7%
2	L	281	3% 88% 9% ·
3	M	307	2% 86% 11% ··

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	LDA	L	1284	-	-	X	-
6	BPH	L	1285	X	-	-	-
6	BPH	M	1311	X	-	-	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 7456 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	0	1
			1830	1169	315	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
			2230	1504	357	361	8			

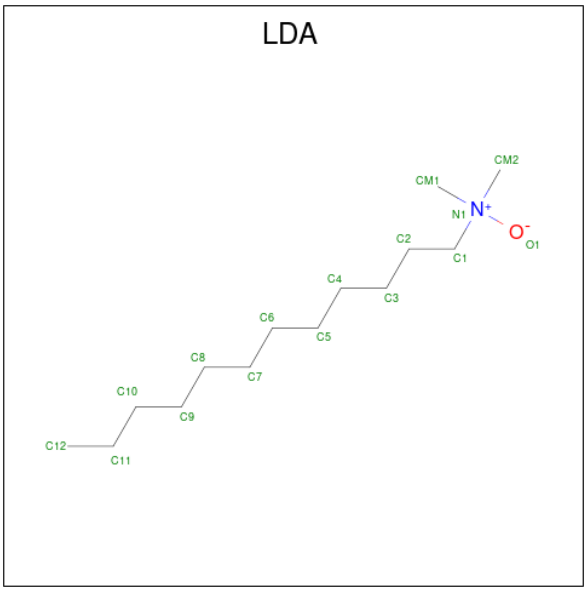
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	128	HIS	TYR	engineered mutation	UNP P0C0Y8

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

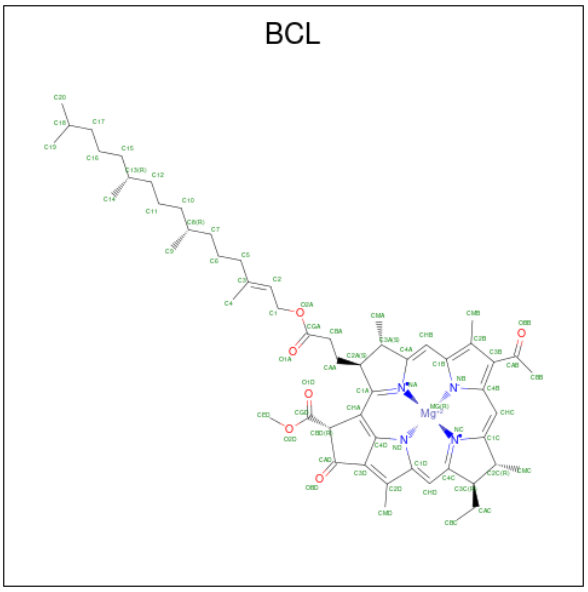
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	1	0
			2414	1610	397	397	10			

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



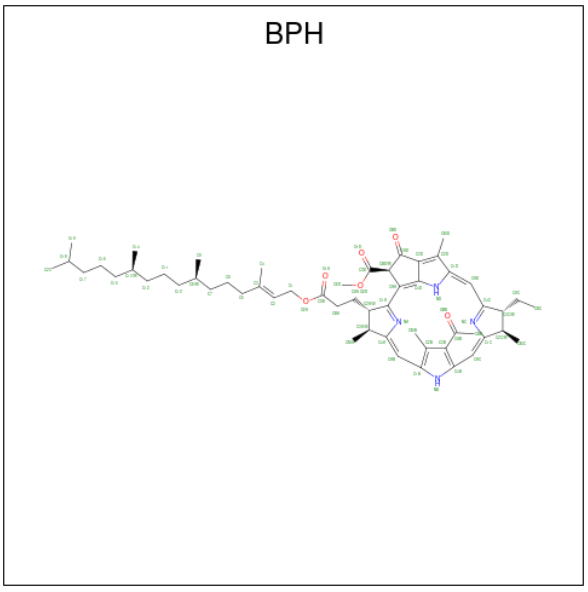
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C 12 12	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	H	1	Total C N O 16 14 1 1	0	0
4	L	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0
4	M	1	Total C N O 16 14 1 1	0	0

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



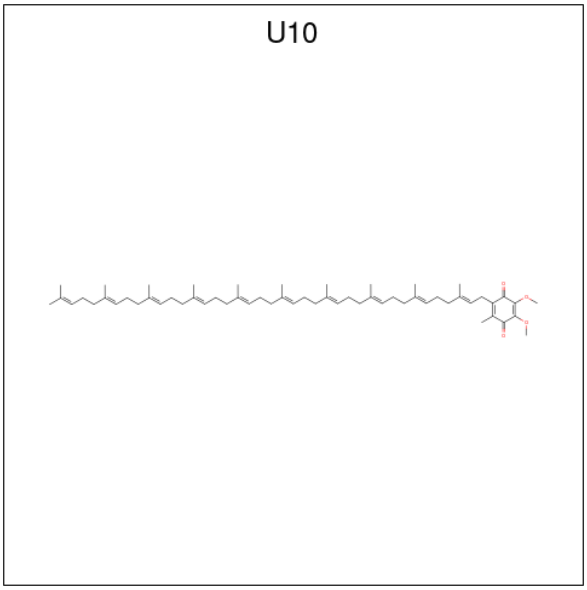
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



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

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

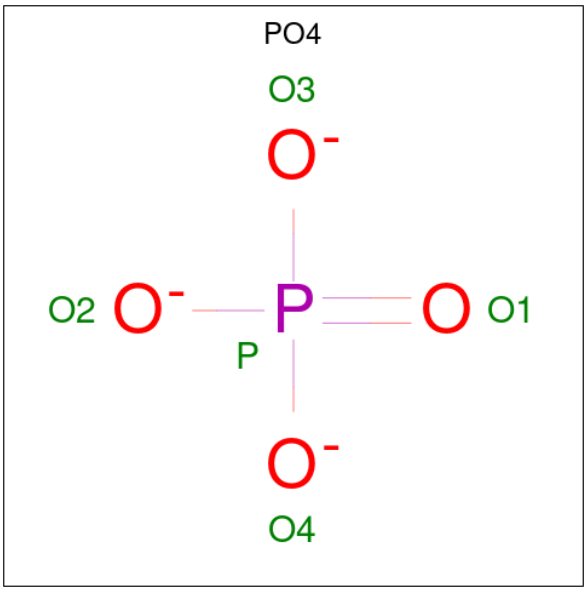


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 48 44 4	1	0
7	M	1	Total C O 48 44 4	0	0

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

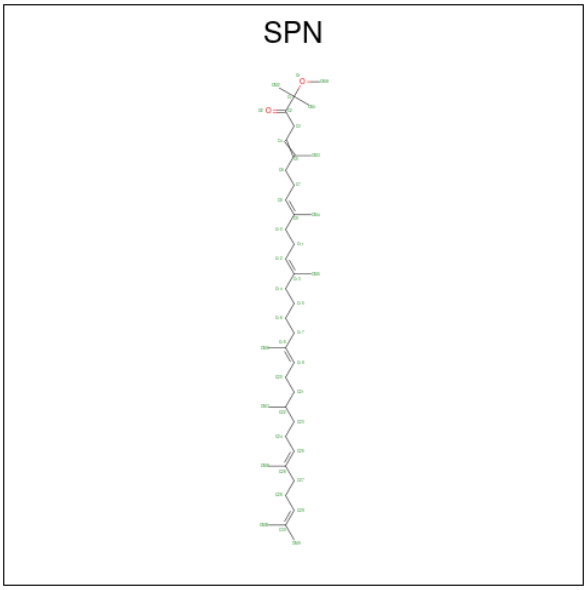
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total Fe 1 1	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C O 43 41 2	0	0

- Molecule 11 is water.

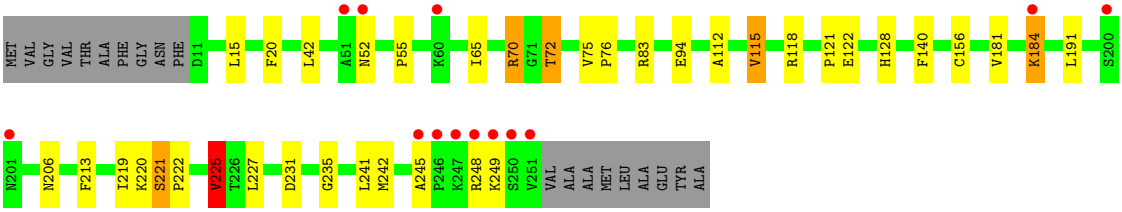
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	152	Total O 152 152	0	0
11	L	81	Total O 81 81	0	0
11	M	65	Total O 65 65	0	0

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:

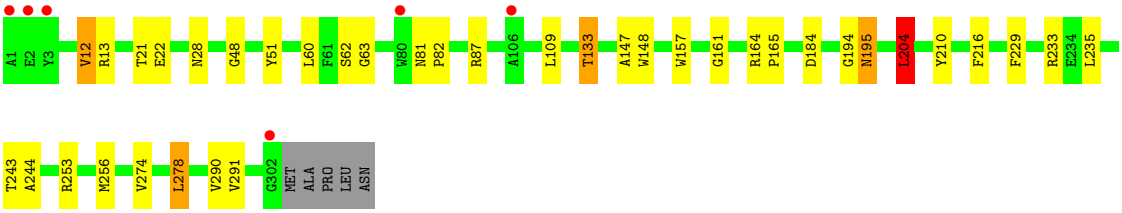


• Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:

• Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.87Å 139.87Å 184.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.87 – 2.31 14.94 – 2.31	Depositor EDS
% Data completeness (in resolution range)	98.0 (17.87-2.31) 95.2 (14.94-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.192 , 0.224 0.189 , 0.221	Depositor DCC
R_{free} test set	4341 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 61.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: FE, SPN, LDA, BCL, BPH, U10, 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	1.02	1/1878 (0.1%)	0.92	5/2555 (0.2%)
2	L	1.00	1/2318 (0.0%)	0.84	4/3172 (0.1%)
3	M	0.93	0/2511	0.79	4/3427 (0.1%)
All	All	0.98	2/6707 (0.0%)	0.84	13/9154 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	94	GLU	CG-CD	7.51	1.63	1.51
2	L	72	GLU	CG-CD	5.28	1.59	1.51

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	217	ARG	NE-CZ-NH1	8.16	124.38	120.30
3	M	233	ARG	NE-CZ-NH1	-6.35	117.13	120.30
3	M	204	LEU	CB-CG-CD1	6.09	121.35	111.00
1	H	225	VAL	CG1-CB-CG2	6.07	120.61	110.90
1	H	225	VAL	CB-CA-C	-6.04	99.93	111.40

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	1830	0	1836	30	0
2	L	2230	0	2185	27	0
3	M	2414	0	2330	30	0
4	H	76	0	147	9	0
4	L	16	0	31	9	0
4	M	48	0	93	9	0
5	L	132	0	148	5	0
5	M	132	0	148	17	0
6	L	65	0	76	7	0
6	M	65	0	76	10	0
7	L	48	0	58	16	0
7	M	48	0	63	1	0
8	M	1	0	0	0	0
9	M	10	0	0	1	0
10	M	43	0	70	7	0
11	H	152	0	0	10	0
11	L	81	0	0	2	0
11	M	65	0	0	0	0
All	All	7456	0	7261	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)
1:H:52:ASN:HB3	11:H:2041:HOH:O	1.48	1.10
7:L:1286:U10:H351	7:L:1286:U10:C46	1.84	1.08
1:H:220:LYS:HE3	11:H:2095:HOH:O	1.62	0.99
1:H:242:MET:HE3	2:L:13:GLY:HA3	1.41	0.98
6:L:1285:BPH:HHC	6:L:1285:BPH:HBB3	1.46	0.96

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	239/260 (92%)	232 (97%)	6 (2%)	1 (0%)	34	41
2	L	279/281 (99%)	267 (96%)	12 (4%)	0	100	100
3	M	301/307 (98%)	285 (95%)	13 (4%)	3 (1%)	15	17
All	All	819/848 (97%)	784 (96%)	31 (4%)	4 (0%)	29	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
3	M	48	GLY
3	M	195	ASN
3	M	109	LEU

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%)	187 (96%)	8 (4%)	30	43
2	L	220/220 (100%)	208 (94%)	12 (6%)	21	29
3	M	237/240 (99%)	229 (97%)	8 (3%)	37	51
All	All	652/668 (98%)	624 (96%)	28 (4%)	29	40

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	185	LEU
3	M	278	LEU
2	L	247	CYS
3	M	204	LEU
2	L	210	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
3	M	301	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	LDA	L	1284	-	12,15,15	1.95	1 (8%)	14,17,17	0.39	0
4	LDA	H	1254	-	12,15,15	1.96	1 (8%)	14,17,17	0.38	0
5	BCL	L	1282	2	64,74,74	1.82	5 (7%)	78,115,115	1.96	17 (21%)
9	PO4	M	1307	-	4,4,4	2.06	2 (50%)	6,6,6	0.66	0
4	LDA	M	1309	-	12,15,15	2.14	1 (8%)	14,17,17	1.53	3 (21%)
7	U10	M	1313	-	48,48,63	2.69	12 (25%)	58,61,79	1.87	13 (22%)
7	U10	L	1286	-	47,47,63	3.05	14 (29%)	56,59,79	1.96	13 (23%)
4	LDA	H	1256	-	12,15,15	1.96	1 (8%)	14,17,17	0.54	0
4	LDA	M	1308	-	12,15,15	2.26	1 (8%)	14,17,17	1.30	1 (7%)
4	LDA	H	1253	-	11,11,15	0.28	0	10,10,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BCL	M	1303	3	64,74,74	1.73	5 (7%)	78,115,115	2.06	18 (23%)
4	LDA	M	1310	-	12,15,15	1.91	1 (8%)	14,17,17	0.72	0
4	LDA	H	1252	-	12,15,15	1.96	1 (8%)	14,17,17	0.61	0
6	BPH	L	1285	-	51,70,70	0.84	1 (1%)	52,101,101	1.40	6 (11%)
5	BCL	M	1304	3	64,74,74	1.88	6 (9%)	78,115,115	2.02	20 (25%)
6	BPH	M	1311	-	51,70,70	0.78	1 (1%)	52,101,101	1.42	12 (23%)
5	BCL	L	1283	2	64,74,74	2.00	6 (9%)	78,115,115	1.97	21 (26%)
4	LDA	H	1255	-	12,15,15	2.04	1 (8%)	14,17,17	0.55	0
9	PO4	M	1306	-	4,4,4	0.93	0	6,6,6	0.47	0
10	SPN	M	1312	-	40,42,42	0.78	0	50,52,52	1.81	11 (22%)

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	U10	L	1286	-	-	22/41/65/87	0/1/1/1
4	LDA	L	1284	-	-	3/13/13/13	-
4	LDA	H	1254	-	-	4/13/13/13	-
6	BPH	L	1285	-	2/2/18/22	13/37/105/105	0/5/6/6
4	LDA	H	1256	-	-	5/13/13/13	-
4	LDA	M	1308	-	-	3/13/13/13	-
5	BCL	L	1283	2	-	5/37/137/137	-
5	BCL	L	1282	2	-	8/37/137/137	-
4	LDA	H	1255	-	-	5/13/13/13	-
6	BPH	M	1311	-	2/2/18/22	10/37/105/105	0/5/6/6
4	LDA	H	1253	-	-	4/9/9/13	-
4	LDA	M	1310	-	-	9/13/13/13	-
5	BCL	M	1303	3	-	8/37/137/137	-
5	BCL	M	1304	3	-	1/37/137/137	-
4	LDA	M	1309	-	-	4/13/13/13	-
4	LDA	H	1252	-	-	5/13/13/13	-
7	U10	M	1313	-	-	13/45/69/87	0/1/1/1
10	SPN	M	1312	-	-	16/50/51/51	-

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1286	U10	C27-C26	-9.93	1.07	1.51
5	L	1283	BCL	C4B-NB	9.44	1.43	1.35
5	M	1303	BCL	C1B-NB	9.10	1.43	1.35
5	M	1304	BCL	C4B-NB	8.66	1.42	1.35
5	L	1282	BCL	C4B-NB	8.51	1.42	1.35

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	1303	BCL	C1D-ND-C4D	-9.47	99.61	106.33
5	L	1283	BCL	C1D-ND-C4D	-8.28	100.45	106.33
5	L	1282	BCL	C1D-ND-C4D	-8.06	100.61	106.33
5	M	1304	BCL	C1D-ND-C4D	-7.21	101.21	106.33
5	M	1304	BCL	C1C-NC-C4C	6.73	109.73	106.71

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	1285	BPH	C13
6	L	1285	BPH	C8
6	M	1311	BPH	C13
6	M	1311	BPH	C8

5 of 138 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	1252	LDA	C2-C1-N1-CM2
4	H	1254	LDA	C2-C1-N1-CM1
4	H	1254	LDA	C2-C1-N1-CM2
4	H	1256	LDA	N1-C1-C2-C3
4	M	1310	LDA	C2-C1-N1-O1

There are no ring outliers.

17 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1284	LDA	9	0
4	H	1254	LDA	2	0
5	L	1282	BCL	2	0
9	M	1307	PO4	1	0
4	M	1309	LDA	5	0
7	M	1313	U10	1	0

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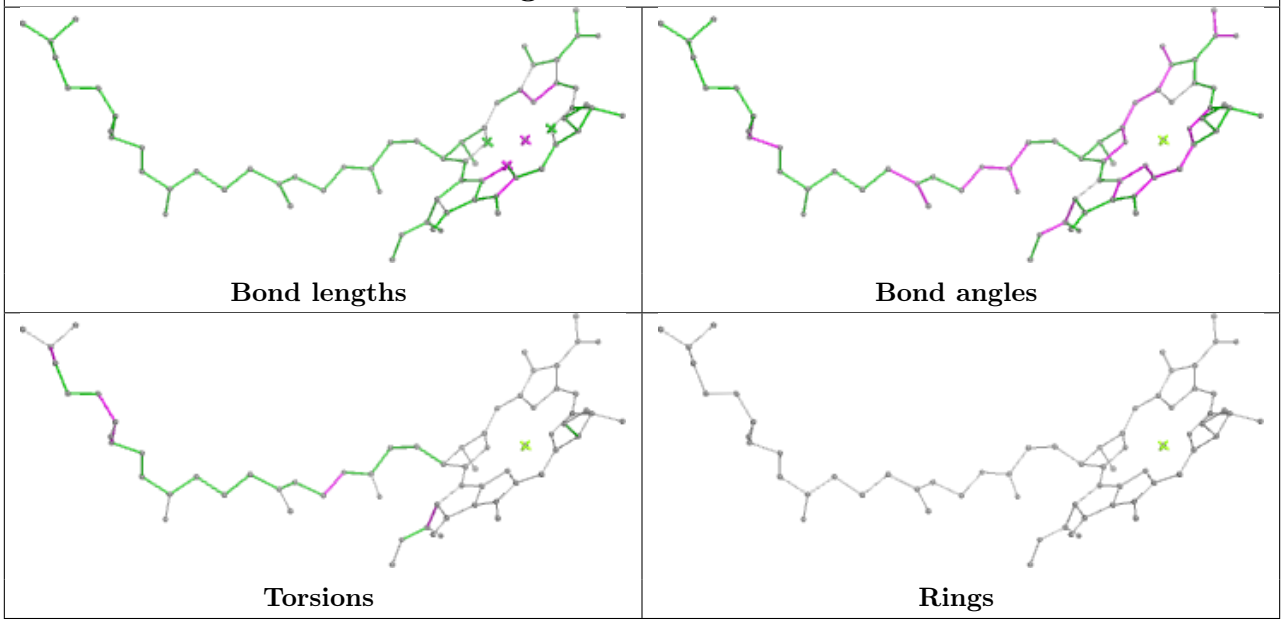
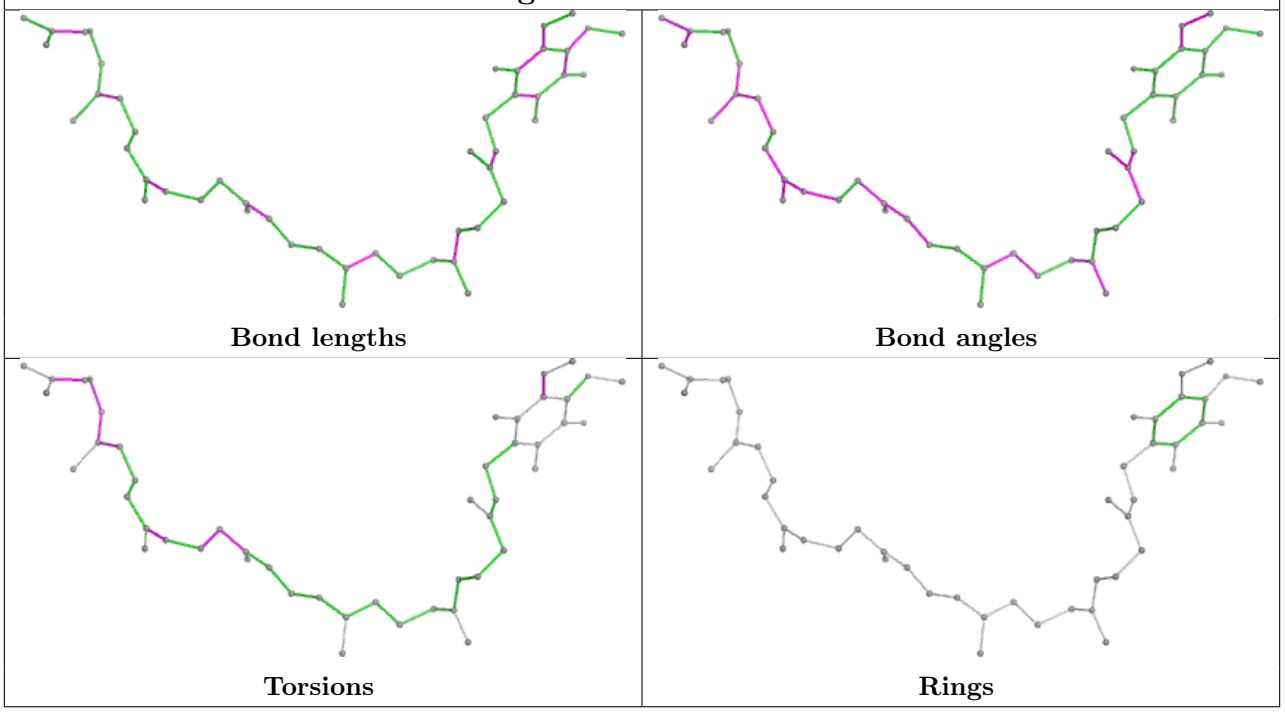
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1286	U10	16	0
4	M	1308	LDA	3	0
4	H	1253	LDA	7	0
5	M	1303	BCL	13	0
4	M	1310	LDA	3	0
4	H	1252	LDA	1	0
6	L	1285	BPH	7	0
5	M	1304	BCL	4	0
6	M	1311	BPH	10	0
5	L	1283	BCL	3	0
10	M	1312	SPN	7	0

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

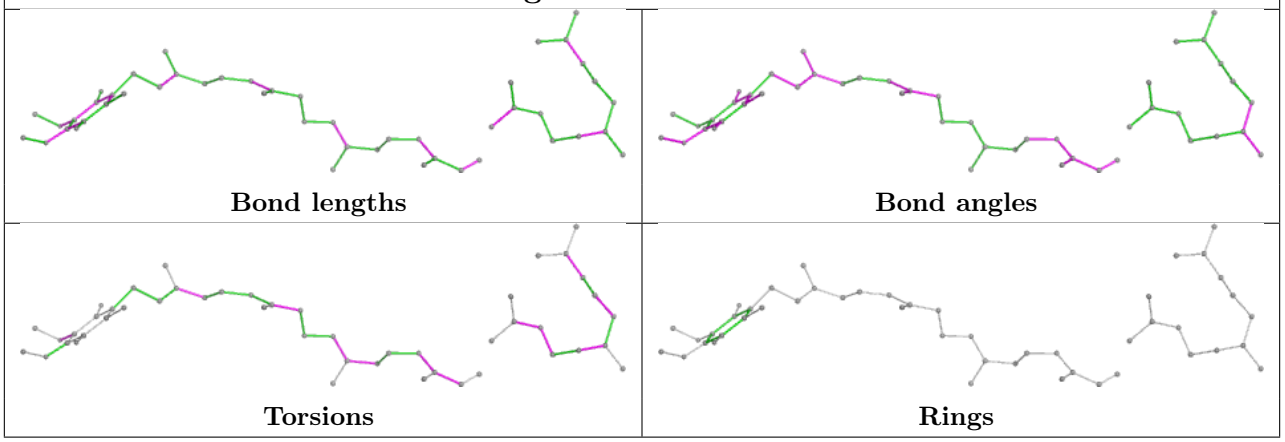
Ligand BCL L 1282



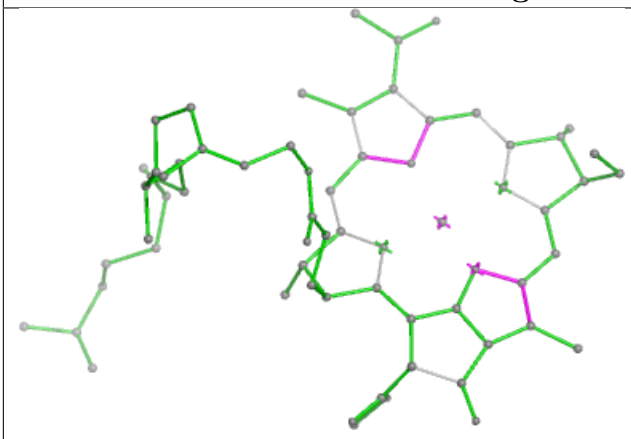
Ligand U10 M 1313



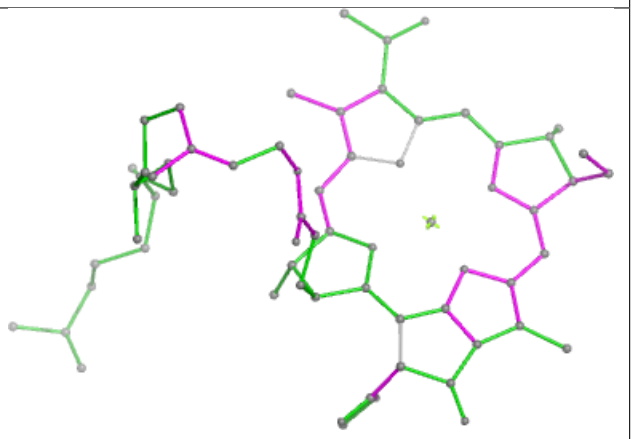
Ligand U10 L 1286



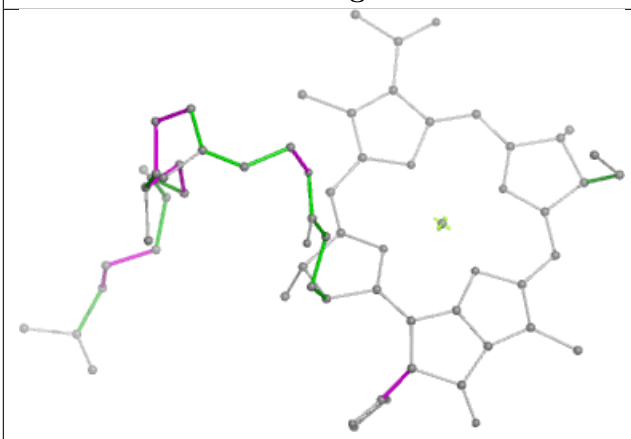
Ligand BCL M 1303



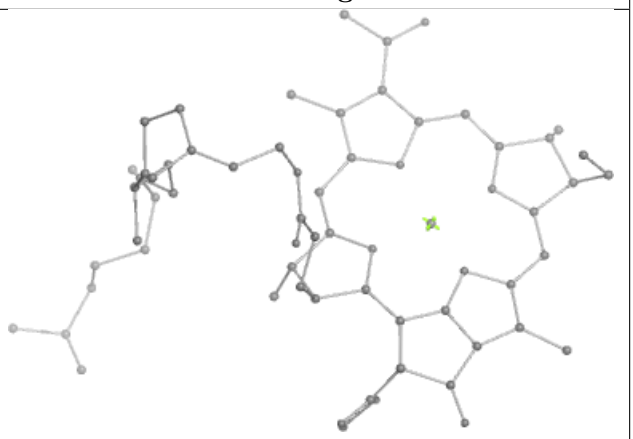
Bond lengths



Bond angles

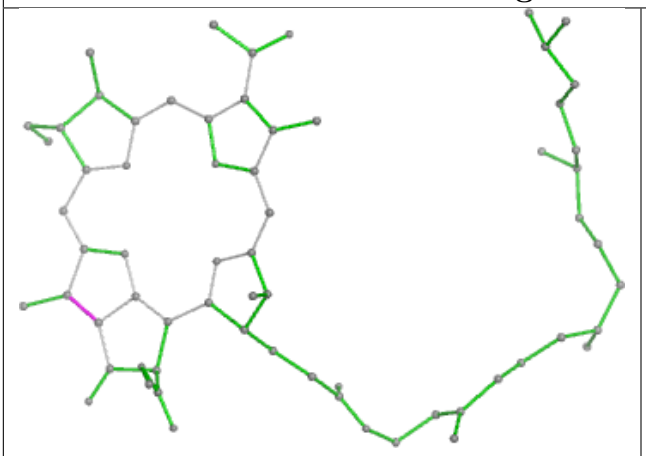


Torsions

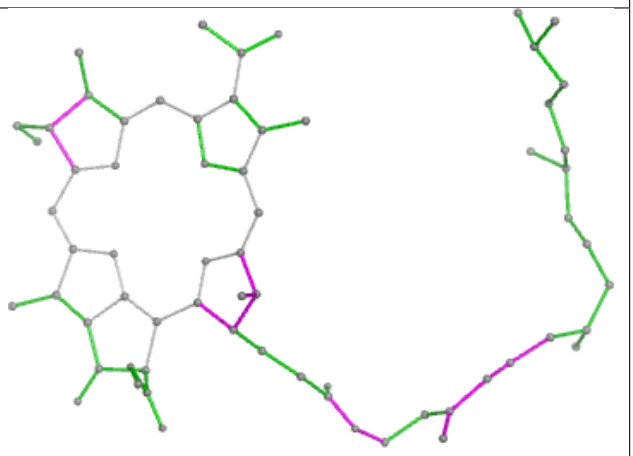


Rings

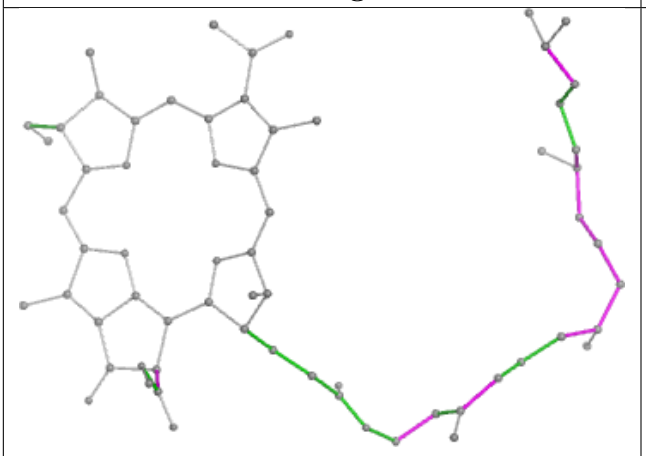
Ligand BPH L 1285



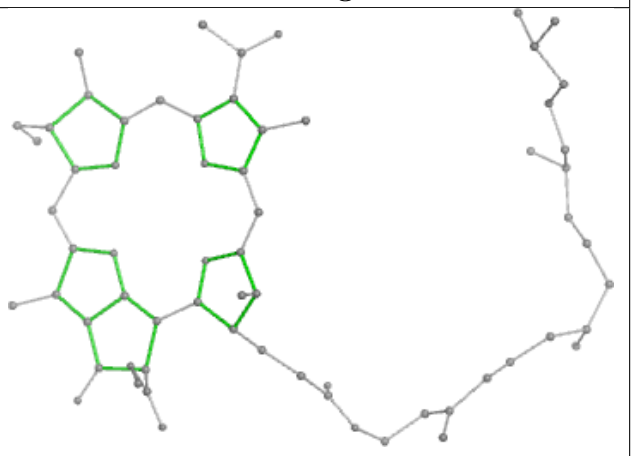
Bond lengths



Bond angles

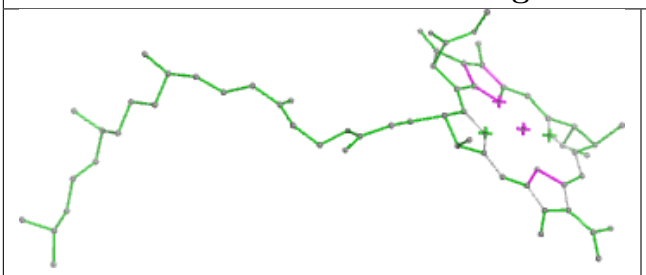


Torsions

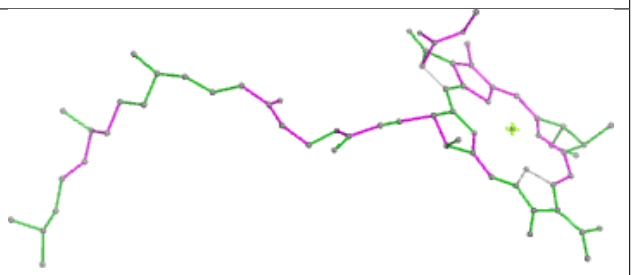


Rings

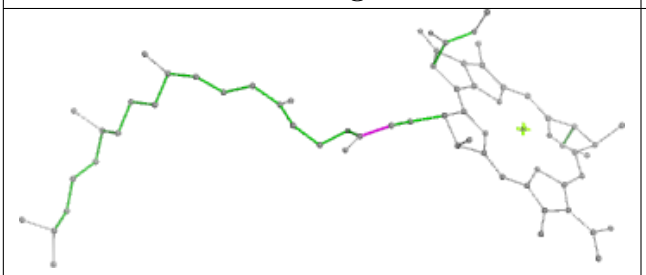
Ligand BCL M 1304



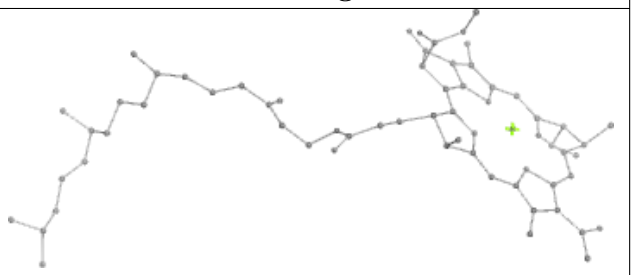
Bond lengths



Bond angles

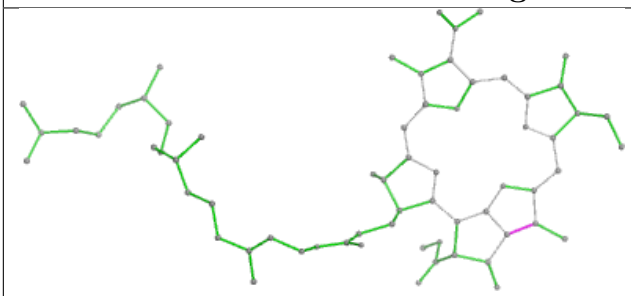


Torsions

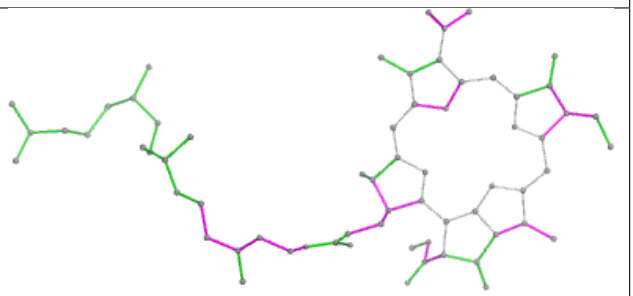


Rings

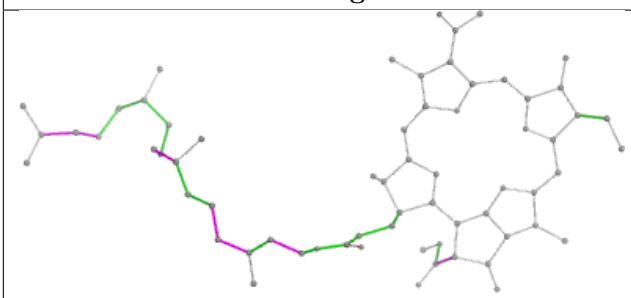
Ligand BPH M 1311



Bond lengths



Bond angles



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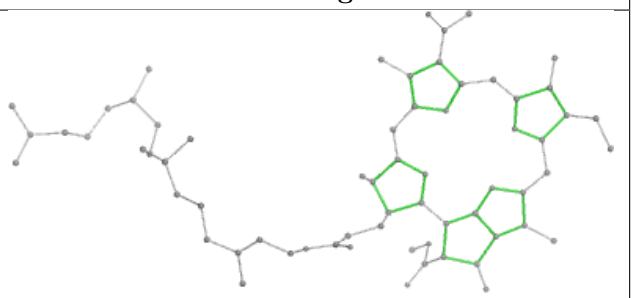
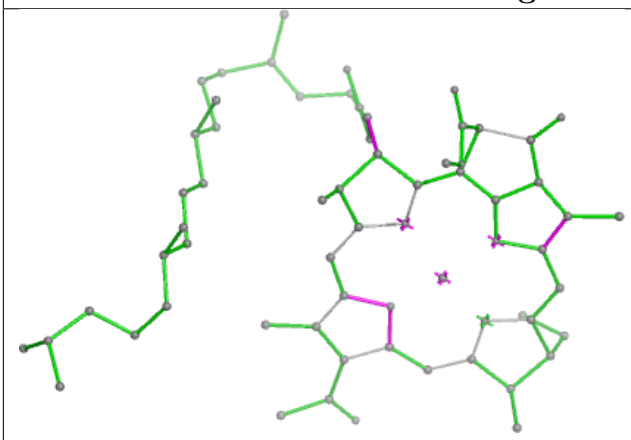
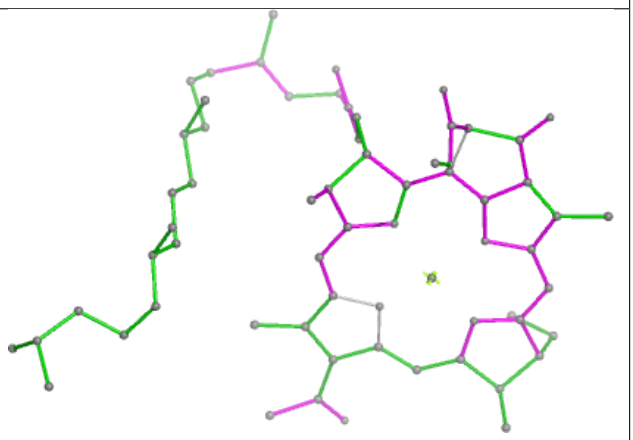


Rings

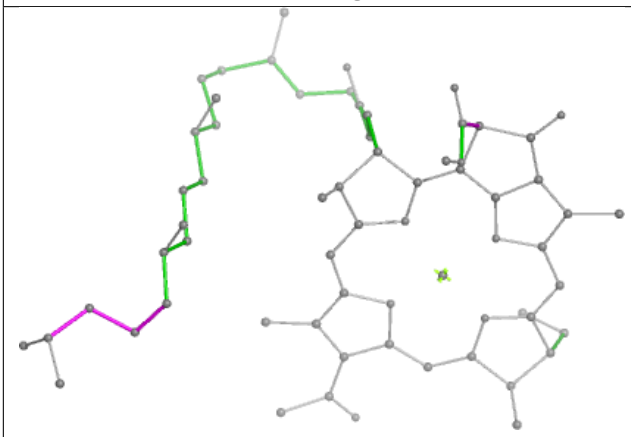
Ligand BCL L 1283



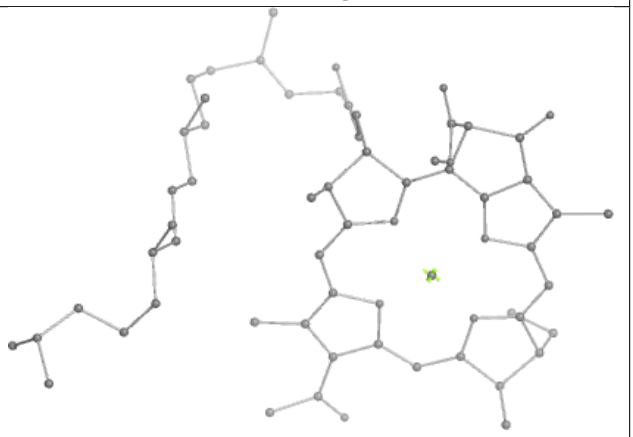
Bond lengths



Bond angles

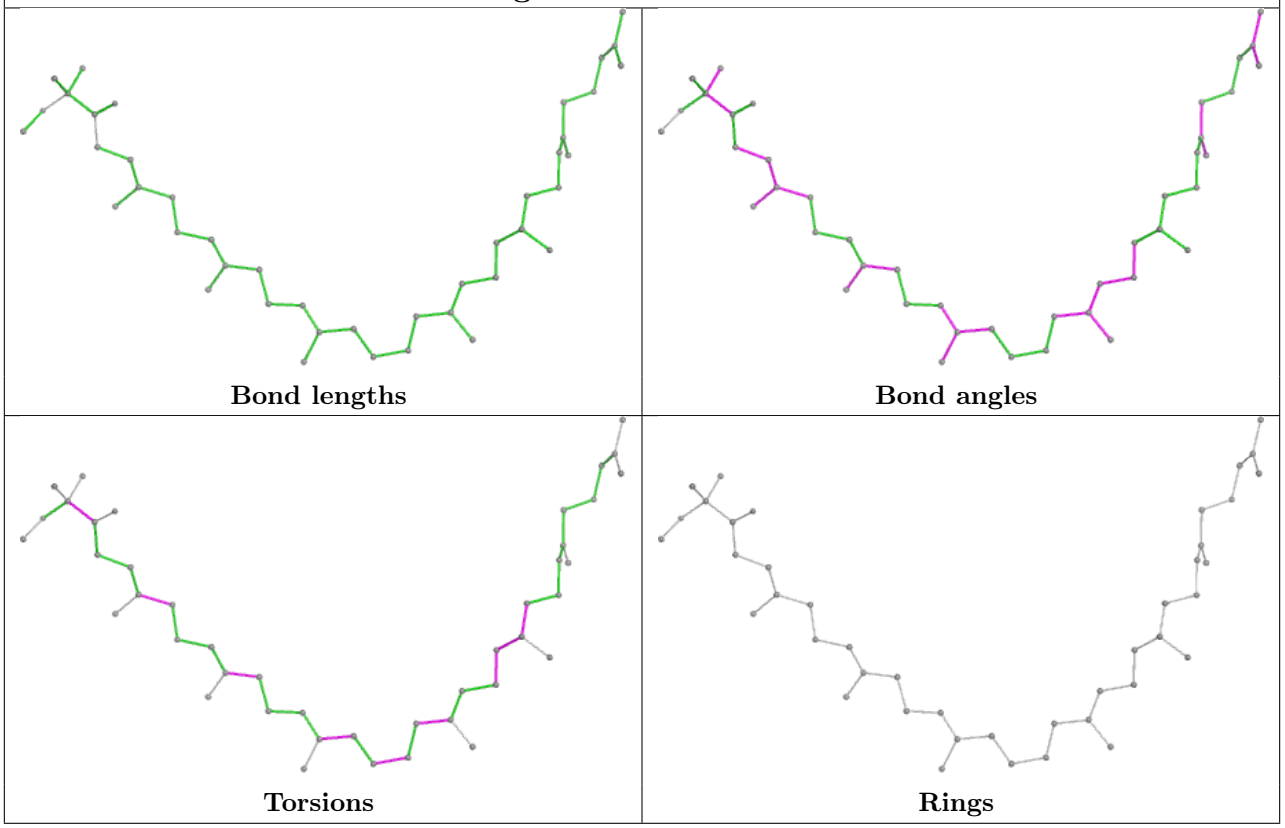


Torsions



Rings

Ligand SPN M 1312



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%)	-0.44	13 (5%)	25	32	26, 35, 52, 113	0
2	L	281/281 (100%)	-0.51	8 (2%)	53	60	24, 34, 64, 86	0
3	M	302/307 (98%)	-0.56	6 (1%)	65	72	22, 37, 61, 84	0
All	All	824/848 (97%)	-0.50	27 (3%)	46	53	22, 35, 61, 113	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	9.0
3	M	1	ALA	8.7
1	H	250	SER	8.3
1	H	245	ALA	5.3
1	H	249	LYS	5.2

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

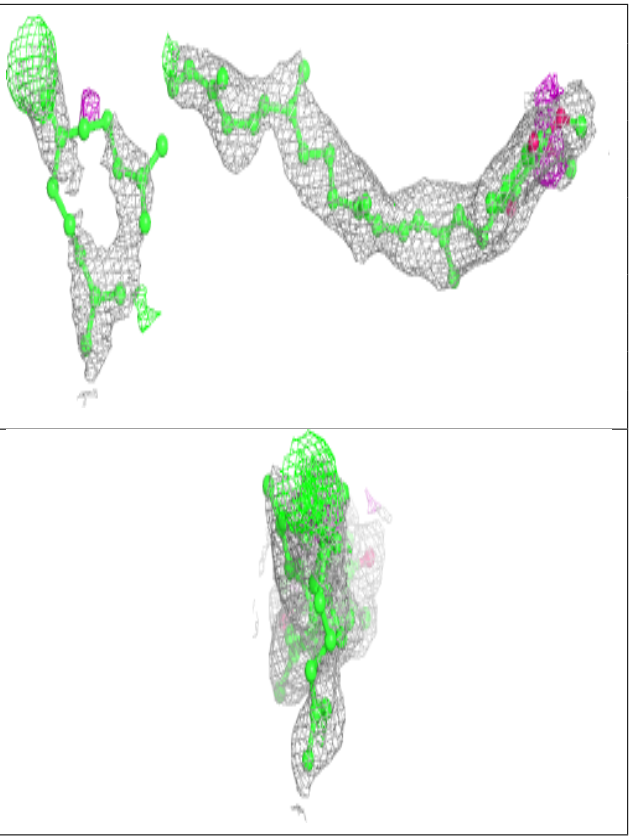
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	LDA	H	1256	16/16	0.49	0.30	70,79,106,107	0
4	LDA	M	1310	16/16	0.50	0.25	59,64,92,93	0
4	LDA	H	1254	16/16	0.51	0.29	68,81,117,117	0
4	LDA	L	1284	16/16	0.53	0.26	65,80,102,102	0
4	LDA	H	1252	16/16	0.54	0.27	61,72,107,107	0
4	LDA	H	1255	16/16	0.75	0.23	74,81,92,93	0
7	U10	L	1286	48/63	0.78	0.24	38,67,112,114	1
4	LDA	H	1253	12/16	0.85	0.15	64,67,73,74	0
4	LDA	M	1308	16/16	0.89	0.16	35,47,53,54	0
10	SPN	M	1312	43/43	0.93	0.12	26,42,72,80	0
7	U10	M	1313	48/63	0.94	0.12	16,38,66,68	0
4	LDA	M	1309	16/16	0.94	0.12	42,53,65,65	0
9	PO4	M	1306	5/5	0.95	0.22	66,68,71,72	0
5	BCL	M	1303	66/66	0.96	0.10	18,31,73,75	0
9	PO4	M	1307	5/5	0.96	0.20	36,50,55,58	0
6	BPH	M	1311	65/65	0.96	0.10	22,38,103,105	0
5	BCL	L	1283	66/66	0.97	0.08	13,25,44,55	0
5	BCL	L	1282	66/66	0.97	0.08	20,29,41,44	0
5	BCL	M	1304	66/66	0.97	0.08	19,29,50,64	0
6	BPH	L	1285	65/65	0.98	0.10	17,27,41,48	0
8	FE	M	1305	1/1	0.99	0.06	26,26,26,26	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.

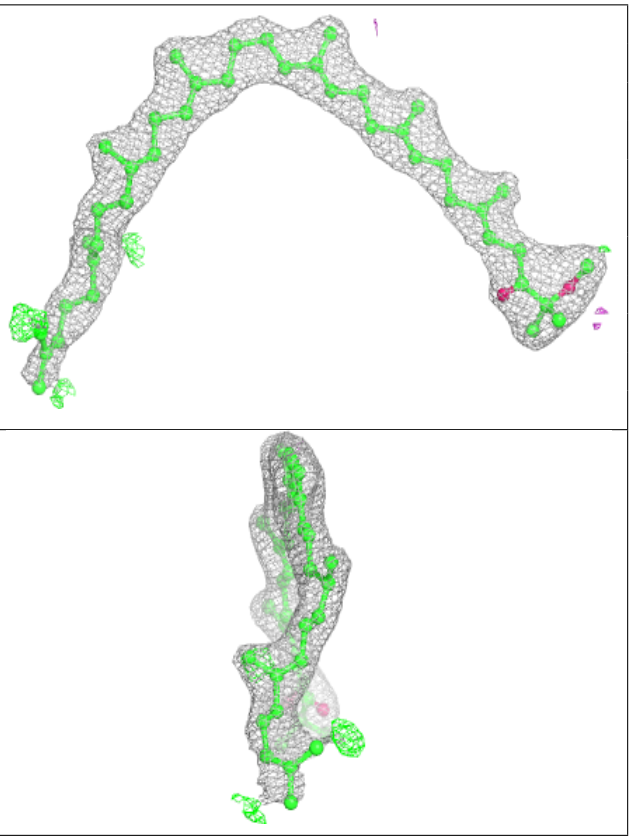
Electron density around U10 L 1286:

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



Electron density around SPN 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 U10 M 1313:

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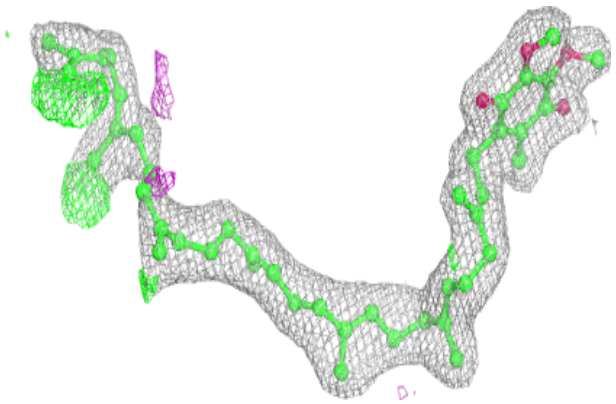
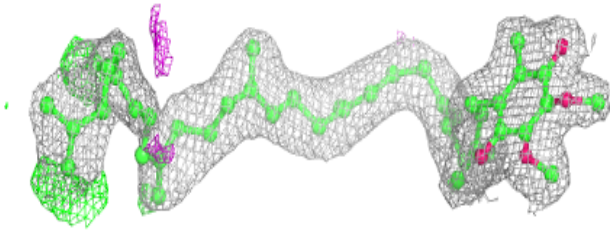
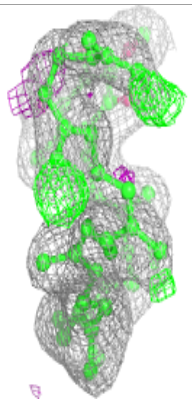
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around BCL M 1303:

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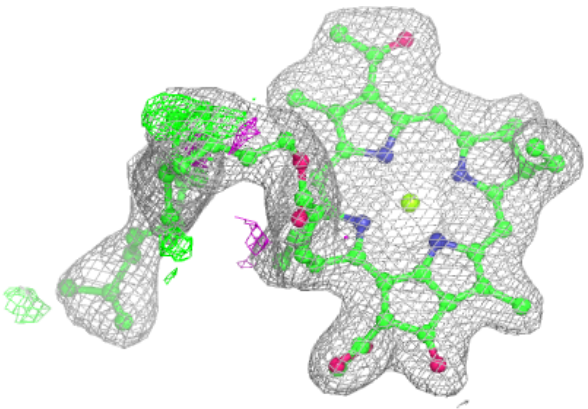
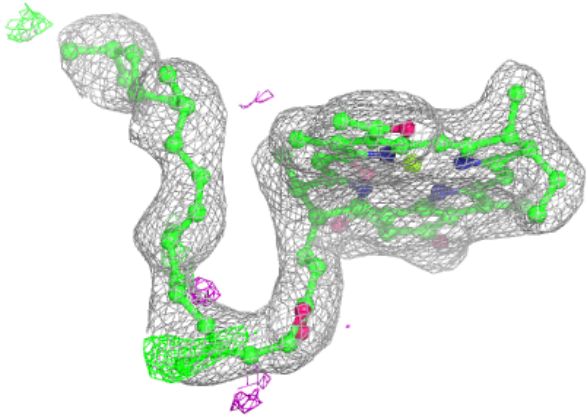
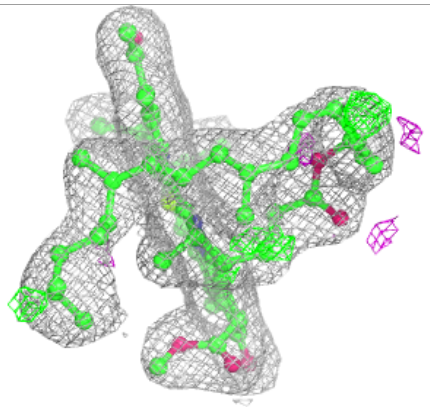
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







Electron density around BPH M 1311:

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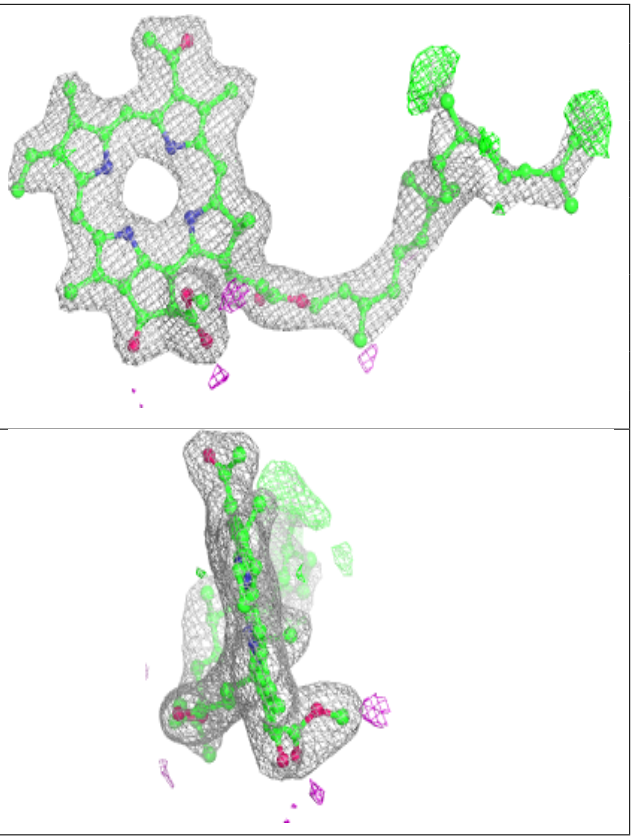
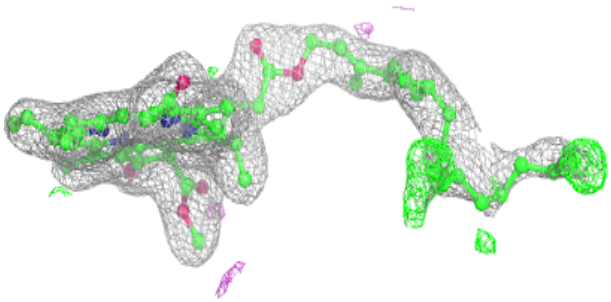
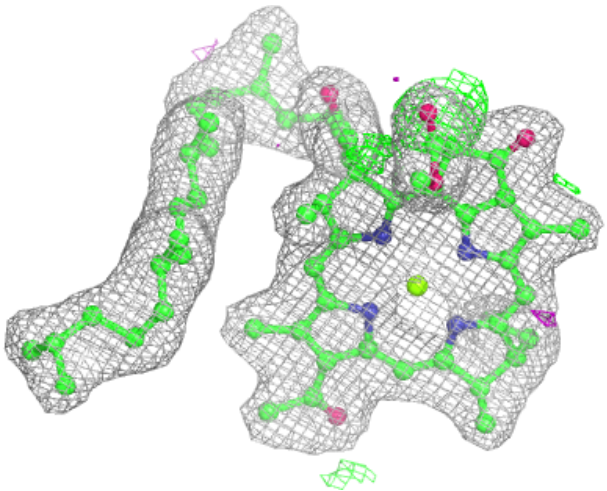
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

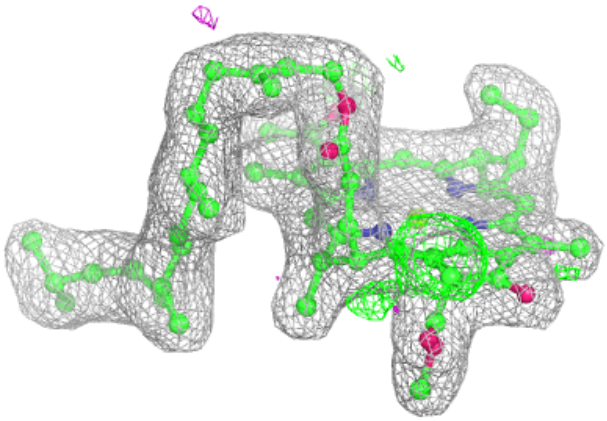


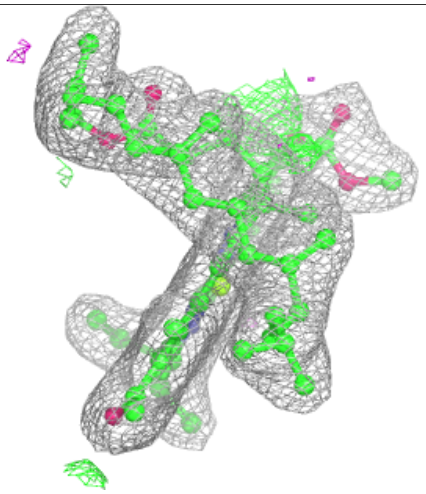


Electron density around BCL L 1283:

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

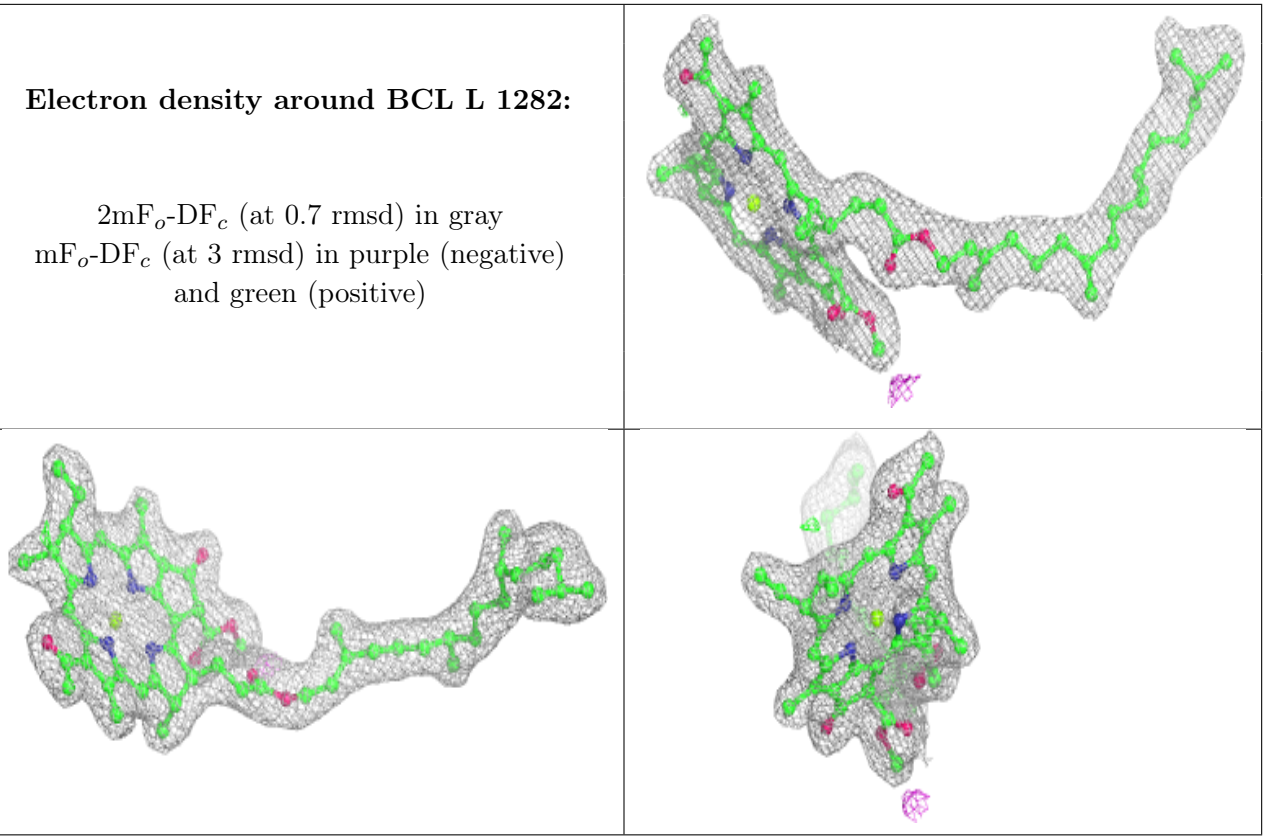






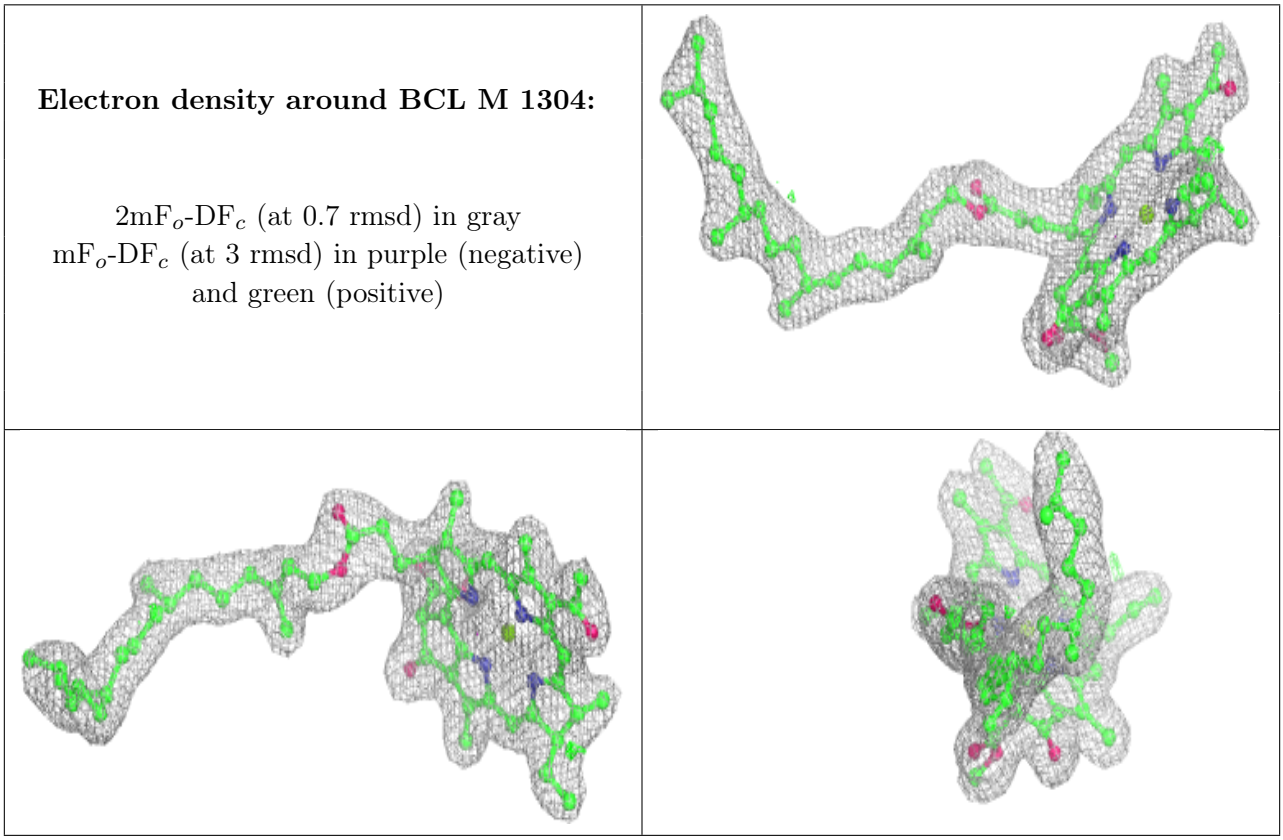
Electron density around BCL L 1282:

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



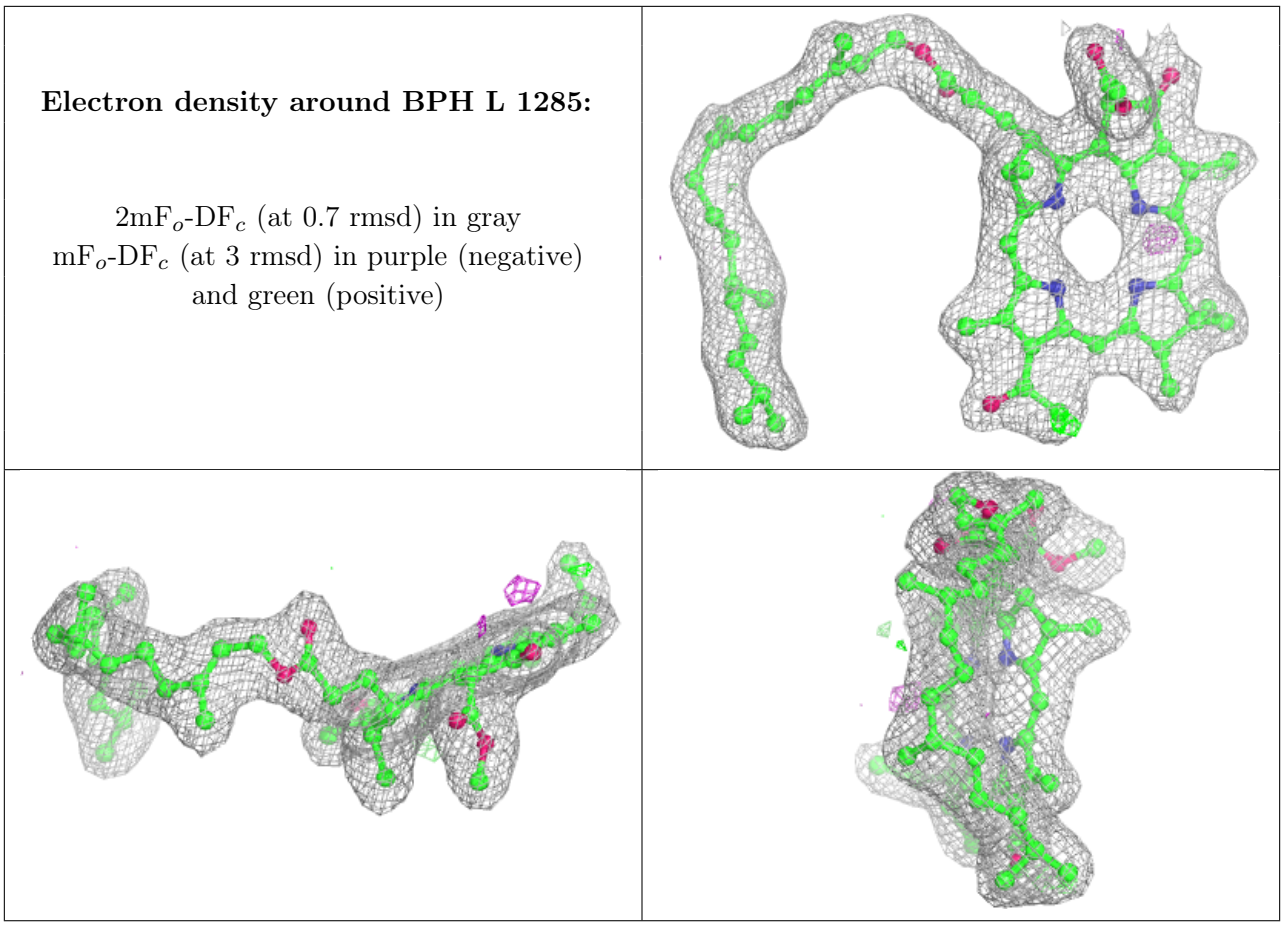
Electron density around BCL M 1304:

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



Electron density around BPH L 1285:

$2mF_o$-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.