wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2023 – 07:39 AM EDT

PDB ID	:	4HBJ
Title	:	Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with ILE M265 replaced with GLN
Authors	:	Mattis, A.J.; Wraight, C.A.
Deposited on	:	2012-09-28
Resolution	:	2.74 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:

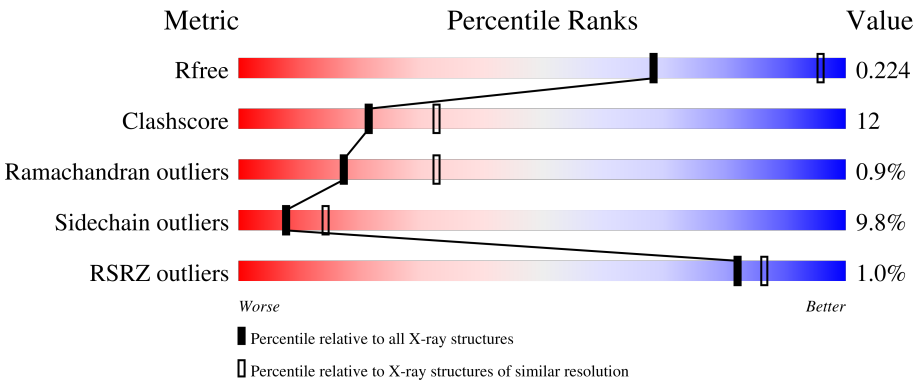
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.74 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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	L	281	% 78% 19% • •
2	M	313	% 74% 19% • • •
3	H	260	% 72% 16% • • 8%

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	BPH	L	303	X	-	-	-
5	BPH	M	404	X	-	-	-
6	U10	M	405	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6988 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 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2224	1502	352	362	8	0	0	0

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2406	1606	395	395	10	0	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	265	GLN	ILE	engineered mutation	UNP P0C0Y9
M	303	MET	-	expression tag	UNP P0C0Y9
M	304	ALA	-	expression tag	UNP P0C0Y9
M	305	PRO	-	expression tag	UNP P0C0Y9
M	306	LEU	-	expression tag	UNP P0C0Y9
M	307	ASN	-	expression tag	UNP P0C0Y9
M	308	HIS	-	expression tag	UNP P0C0Y9
M	309	HIS	-	expression tag	UNP P0C0Y9
M	310	HIS	-	expression tag	UNP P0C0Y9
M	311	HIS	-	expression tag	UNP P0C0Y9
M	312	HIS	-	expression tag	UNP P0C0Y9
M	313	HIS	-	expression tag	UNP P0C0Y9

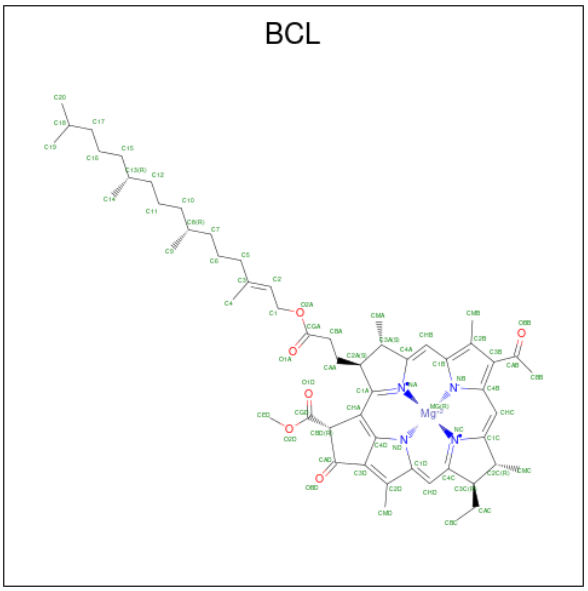
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	239	1795	1148	303	335	9	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	expression tag	UNP P0C0Y7
H	2	VAL	-	expression tag	UNP P0C0Y7
H	3	GLY	-	expression tag	UNP P0C0Y7
H	4	VAL	-	expression tag	UNP P0C0Y7
H	5	THR	-	expression tag	UNP P0C0Y7
H	6	ALA	-	expression tag	UNP P0C0Y7
H	7	PHE	-	expression tag	UNP P0C0Y7
H	8	GLY	-	expression tag	UNP P0C0Y7
H	9	ASN	-	expression tag	UNP P0C0Y7
H	10	PHE	-	expression tag	UNP P0C0Y7
H	251	VAL	-	expression tag	UNP P0C0Y7
H	252	VAL	-	expression tag	UNP P0C0Y7
H	253	ALA	-	expression tag	UNP P0C0Y7
H	254	ALA	-	expression tag	UNP P0C0Y7
H	255	MET	-	expression tag	UNP P0C0Y7
H	256	LEU	-	expression tag	UNP P0C0Y7
H	257	ALA	-	expression tag	UNP P0C0Y7
H	258	GLU	-	expression tag	UNP P0C0Y7
H	259	TYR	-	expression tag	UNP P0C0Y7
H	260	ALA	-	expression tag	UNP P0C0Y7

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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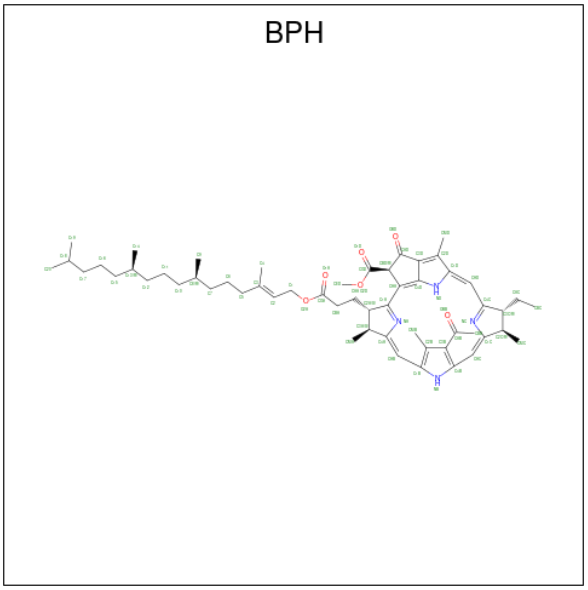
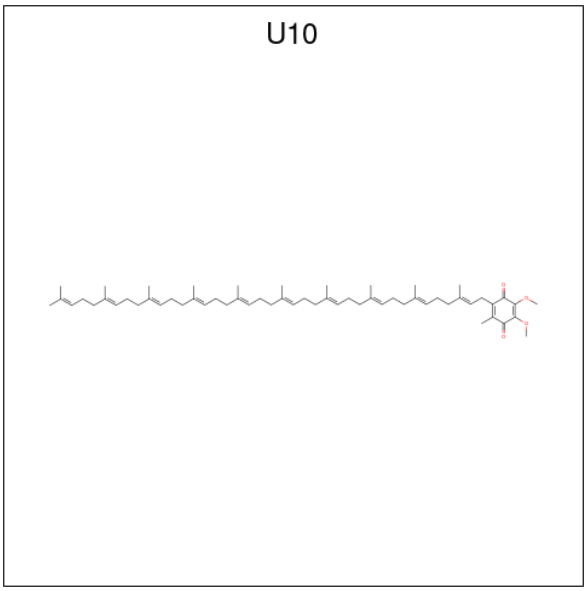
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
4	M	1	61	50	1	4	6	0	0
			Total	C	Mg	N	O		
4	M	1	66	55	1	4	6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

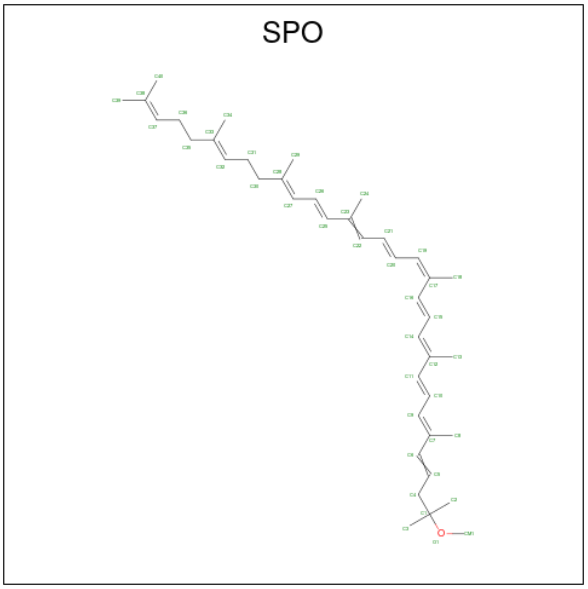


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	L	1	18	14	4	0	0
			Total	C	O		
6	M	1	48	44	4	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 9 is water.

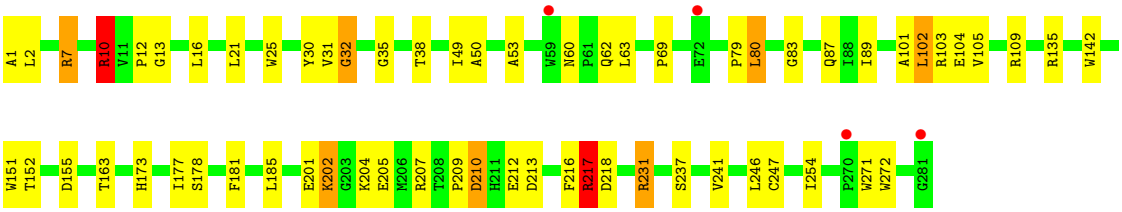
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	L	18	18	18	0	0
			Total	O		
9	M	19	19	19	0	0
			Total	O		
9	H	28	28	28	0	0

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.

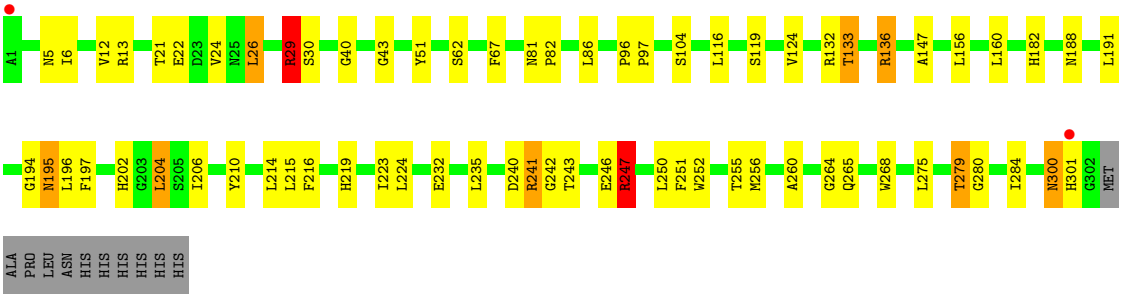
• Molecule 1: Reaction center protein L chain

Chain L:



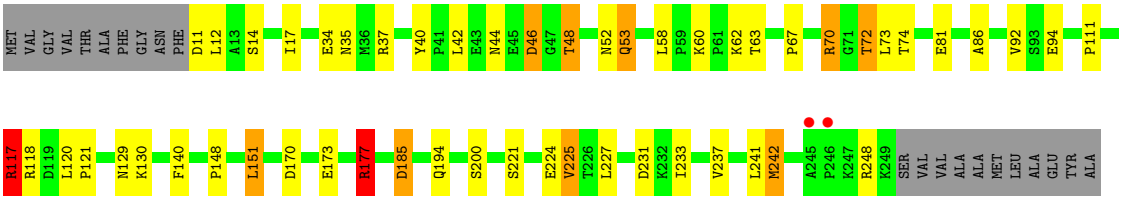
• Molecule 2: Reaction center protein M chain

Chain M:



• Molecule 3: Reaction center protein H chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.54Å 139.54Å 185.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.87 – 2.74 19.87 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.87-2.74) 99.7 (19.87-2.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.223 0.190 , 0.224	Depositor DCC
R_{free} test set	2748 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6988	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: BCL, FE, SPO, U10, 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	L	1.06	0/2312	1.01	12/3167 (0.4%)
2	M	0.97	0/2501	0.95	9/3415 (0.3%)
3	H	1.04	2/1843 (0.1%)	1.05	8/2517 (0.3%)
All	All	1.02	2/6656 (0.0%)	1.00	29/9099 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	5.86	1.60	1.51
3	H	72	THR	CB-CG2	5.21	1.69	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	7	ARG	NE-CZ-NH2	-11.13	114.74	120.30
3	H	177	ARG	NE-CZ-NH1	9.86	125.23	120.30
1	L	231	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	L	7	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	L	217	ARG	NE-CZ-NH1	8.56	124.58	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide

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	L	2224	0	2162	33	0
2	M	2406	0	2313	68	0
3	H	1795	0	1745	34	0
4	L	132	0	148	9	0
4	M	127	0	135	21	0
5	L	65	0	76	10	0
5	M	65	0	76	10	0
6	L	18	0	15	6	0
6	M	48	0	63	26	0
7	M	1	0	0	0	0
8	M	42	0	60	5	0
9	H	28	0	0	0	0
9	L	18	0	0	0	0
9	M	19	0	0	0	0
All	All	6988	0	6793	165	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 12.

The worst 5 of 165 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:304:U10:H3M2	6:L:304:U10:C4M	1.38	1.50
6:L:304:U10:H4M2	6:L:304:U10:C3M	1.63	1.28
6:L:304:U10:C4M	6:L:304:U10:C3M	2.18	1.17
5:L:303:BPH:HBB3	5:L:303:BPH:HHC	1.32	1.12
2:M:265[B]:GLN:HE22	6:M:405:U10:C3M	1.61	1.11

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	L	279/281 (99%)	261 (94%)	16 (6%)	2 (1%)	22	40
2	M	301/313 (96%)	283 (94%)	15 (5%)	3 (1%)	15	28
3	H	237/260 (91%)	226 (95%)	9 (4%)	2 (1%)	19	36
All	All	817/854 (96%)	770 (94%)	40 (5%)	7 (1%)	17	32

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
3	H	185	ASP
2	M	30	SER
2	M	301	HIS
1	L	80	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	L	217/220 (99%)	196 (90%)	21 (10%)	8	14
2	M	234/246 (95%)	210 (90%)	24 (10%)	7	13
3	H	184/208 (88%)	167 (91%)	17 (9%)	9	17
All	All	635/674 (94%)	573 (90%)	62 (10%)	8	14

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

Mol	Chain	Res	Type
2	M	124	VAL
3	H	151	LEU
2	M	196	LEU
3	H	120	LEU
3	H	221	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
3	H	44	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	BPH	M	404	-	51,70,70	1.01	2 (3%)	52,101,101	2.03	17 (32%)
8	SPO	M	406	-	40,41,41	1.31	4 (10%)	47,50,50	2.34	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	BCL	M	401	-	53,69,74	1.89	3 (5%)	63,109,115	2.09	19 (30%)
5	BPH	L	303	-	51,70,70	1.02	3 (5%)	52,101,101	1.81	12 (23%)
4	BCL	M	403	-	58,74,74	1.36	2 (3%)	69,115,115	1.74	12 (17%)
4	BCL	L	301	-	58,74,74	1.60	4 (6%)	69,115,115	1.55	15 (21%)
4	BCL	L	302	-	58,74,74	1.62	3 (5%)	69,115,115	2.05	16 (23%)
6	U10	L	304	-	18,18,63	2.74	7 (38%)	22,25,79	3.34	10 (45%)
6	U10	M	405	-	48,48,63	2.71	11 (22%)	58,61,79	2.02	13 (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
5	BPH	M	404	-	2/2/18/22	15/37/105/105	0/5/6/6
8	SPO	M	406	-	-	13/47/47/47	-
4	BCL	M	401	-	-	8/31/131/137	-
5	BPH	L	303	-	2/2/18/22	14/37/105/105	0/5/6/6
4	BCL	M	403	-	-	3/37/137/137	-
4	BCL	L	301	-	-	6/37/137/137	-
4	BCL	L	302	-	-	5/37/137/137	-
6	U10	L	304	-	-	3/9/33/87	0/1/1/1
6	U10	M	405	-	-	14/45/69/87	0/1/1/1

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	401	BCL	C1B-NB	9.09	1.43	1.35
4	L	302	BCL	C4B-NB	8.86	1.43	1.35
4	L	301	BCL	C1B-NB	8.21	1.42	1.35
4	M	401	BCL	C4B-NB	7.85	1.42	1.35
6	M	405	U10	C33-C34	6.91	1.49	1.33

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	304	U10	C7-C6-C5	-10.02	106.42	118.48
4	L	302	BCL	O2D-CGD-CBD	7.53	124.66	111.27

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Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	406	SPO	C16-C17-C19	7.27	130.09	118.94
6	L	304	U10	O5-C5-C6	-6.78	109.66	121.55
8	M	406	SPO	C18-C17-C19	-6.45	113.89	122.92

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	303	BPH	C8
5	L	303	BPH	C13
5	M	404	BPH	C8
5	M	404	BPH	C13

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	303	BPH	O2A-C1-C2-C3
5	M	404	BPH	C4-C3-C5-C6
6	L	304	U10	C7-C8-C9-C11
6	M	405	U10	C12-C13-C14-C15
6	M	405	U10	C12-C13-C14-C16

There are no ring outliers.

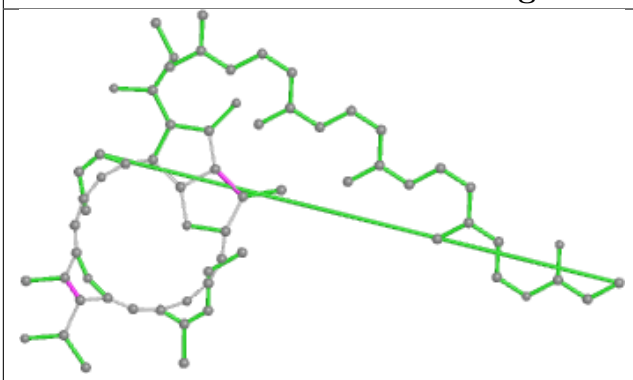
9 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	404	BPH	10	0
8	M	406	SPO	5	0
4	M	401	BCL	10	0
5	L	303	BPH	10	0
4	M	403	BCL	13	0
4	L	301	BCL	4	0
4	L	302	BCL	6	0
6	L	304	U10	6	0
6	M	405	U10	26	0

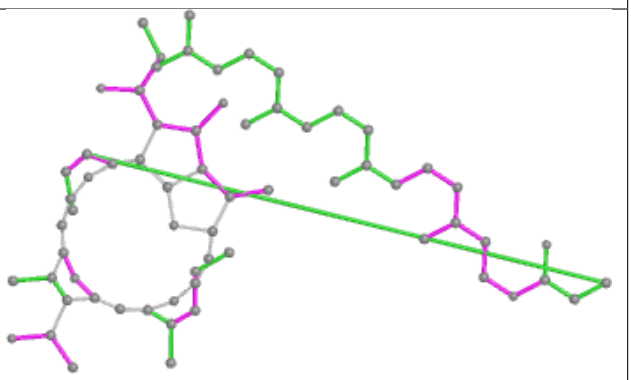
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

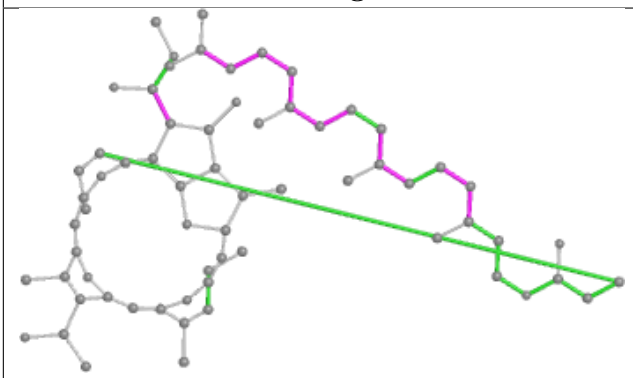
Ligand BPH M 404



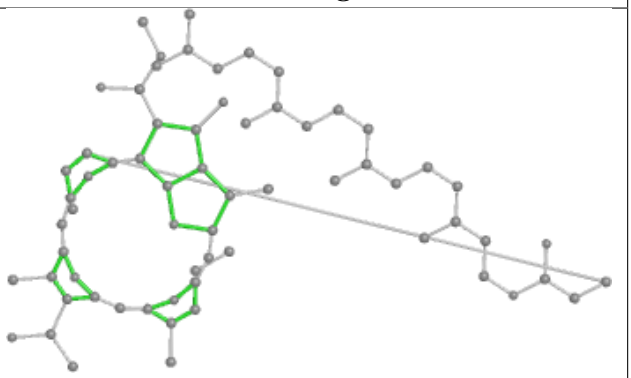
Bond lengths



Bond angles

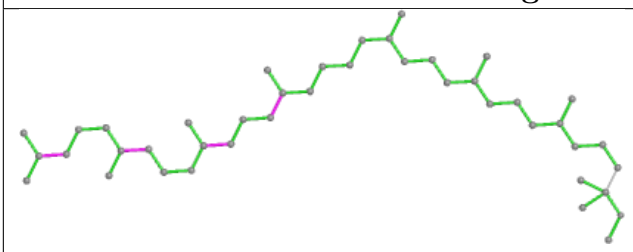


Torsions

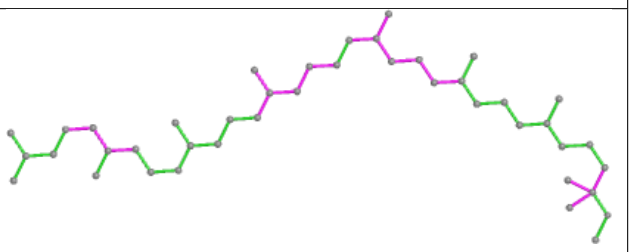


Rings

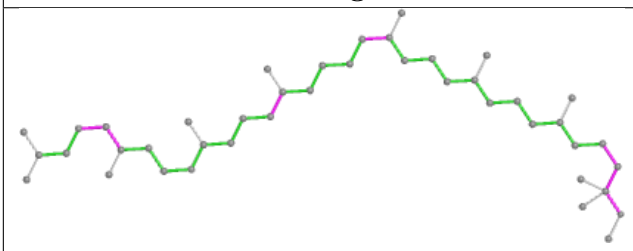
Ligand SPO M 406



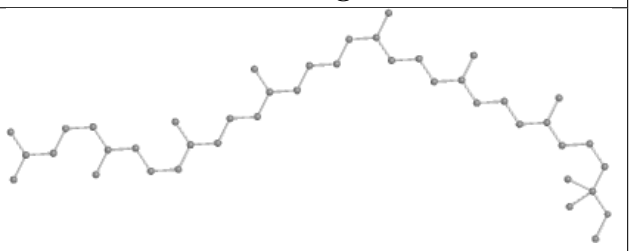
Bond lengths



Bond angles

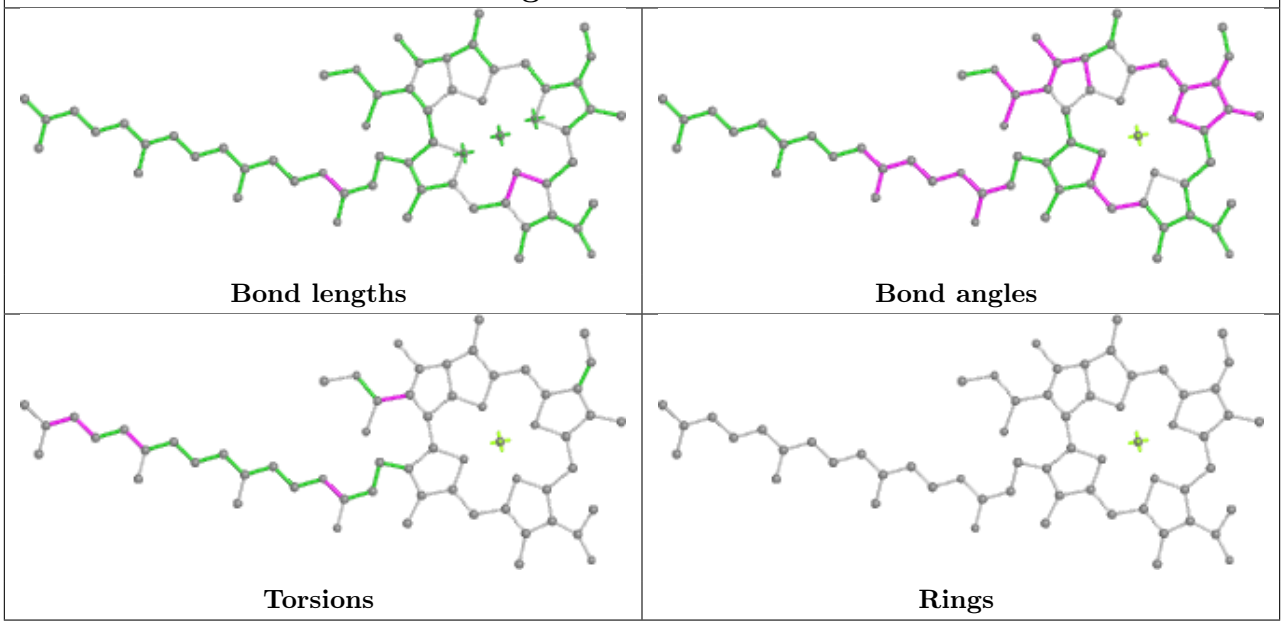


Torsions

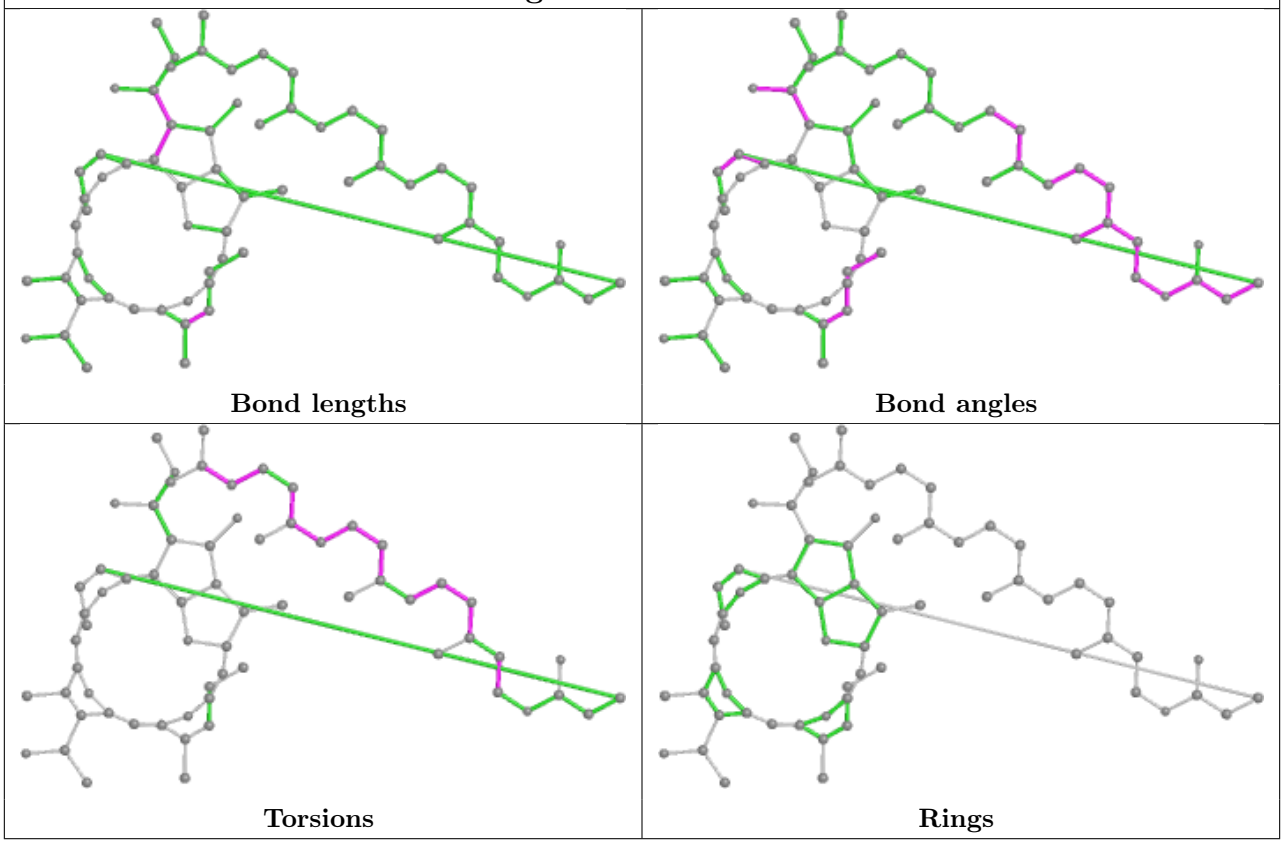


Rings

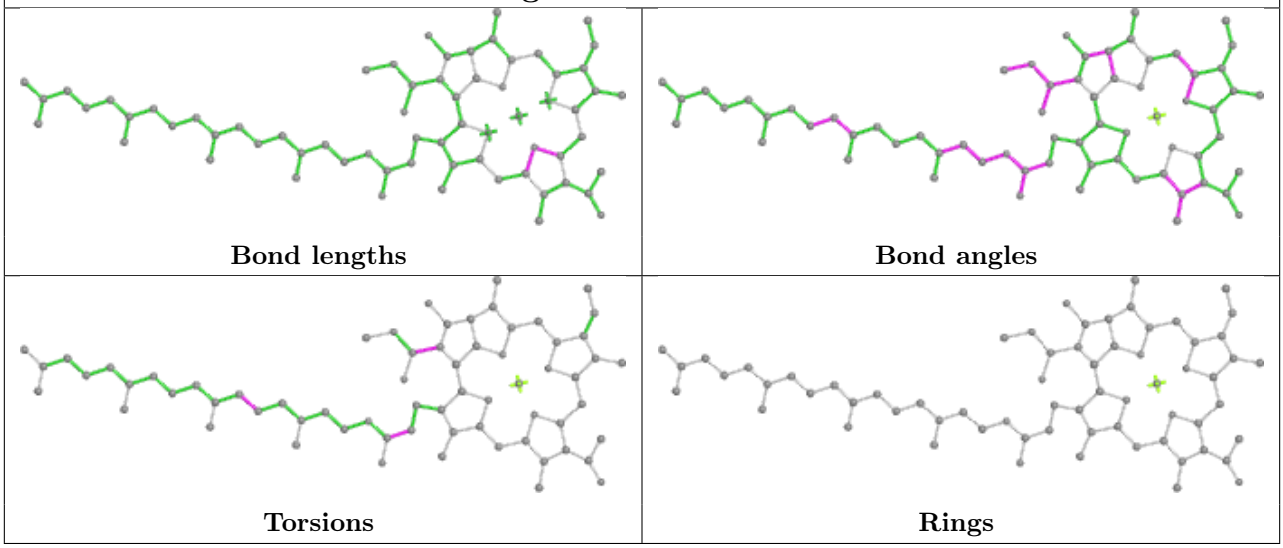
Ligand BCL M 401



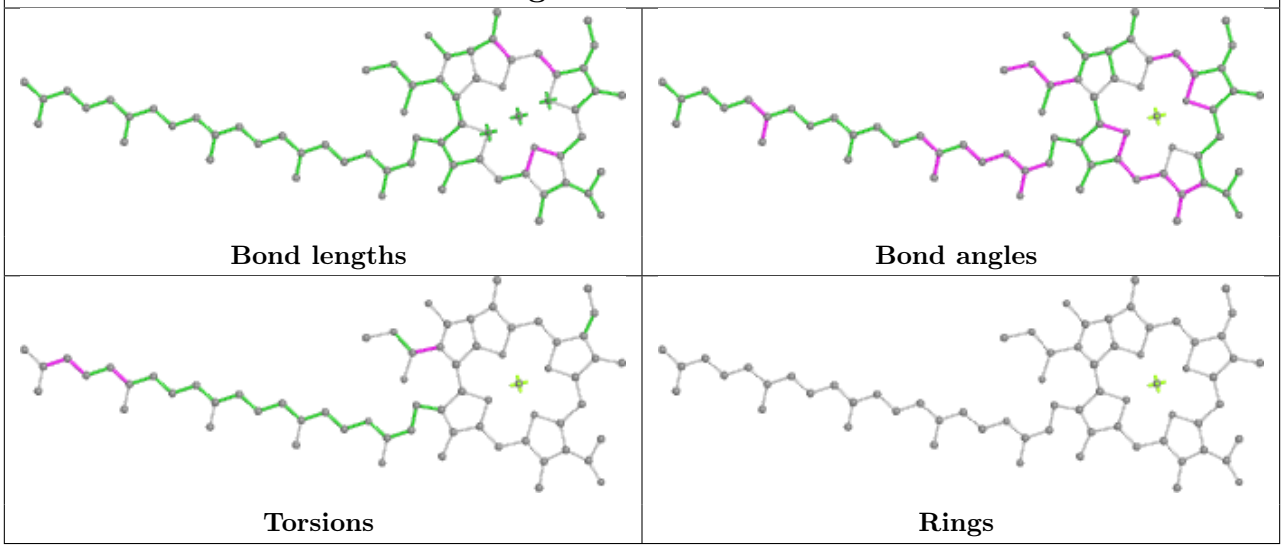
Ligand BPH L 303



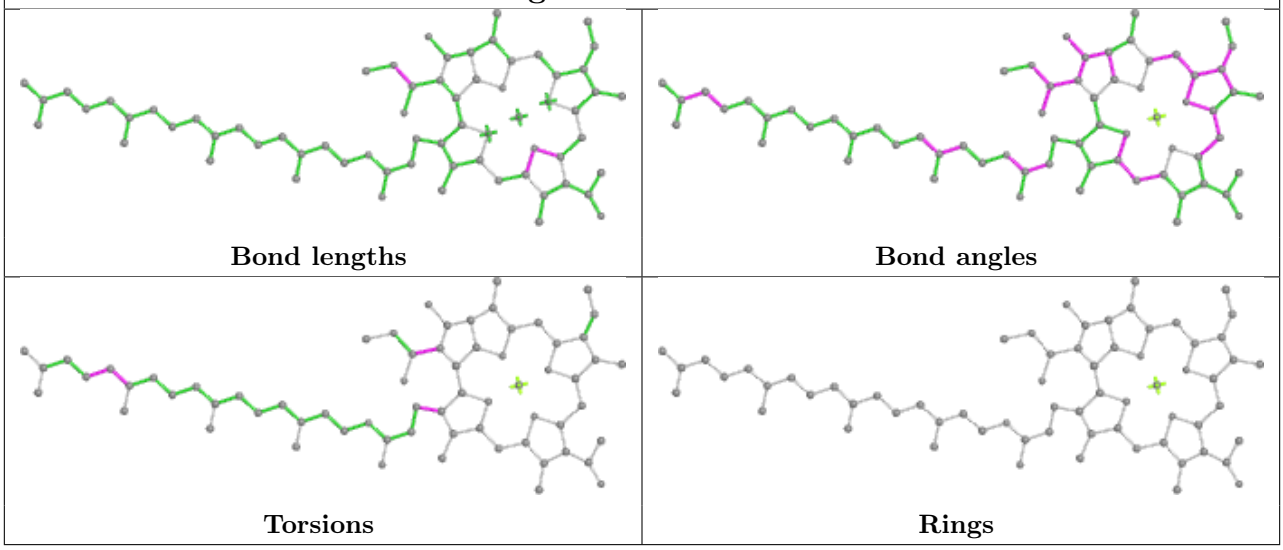
Ligand BCL M 403



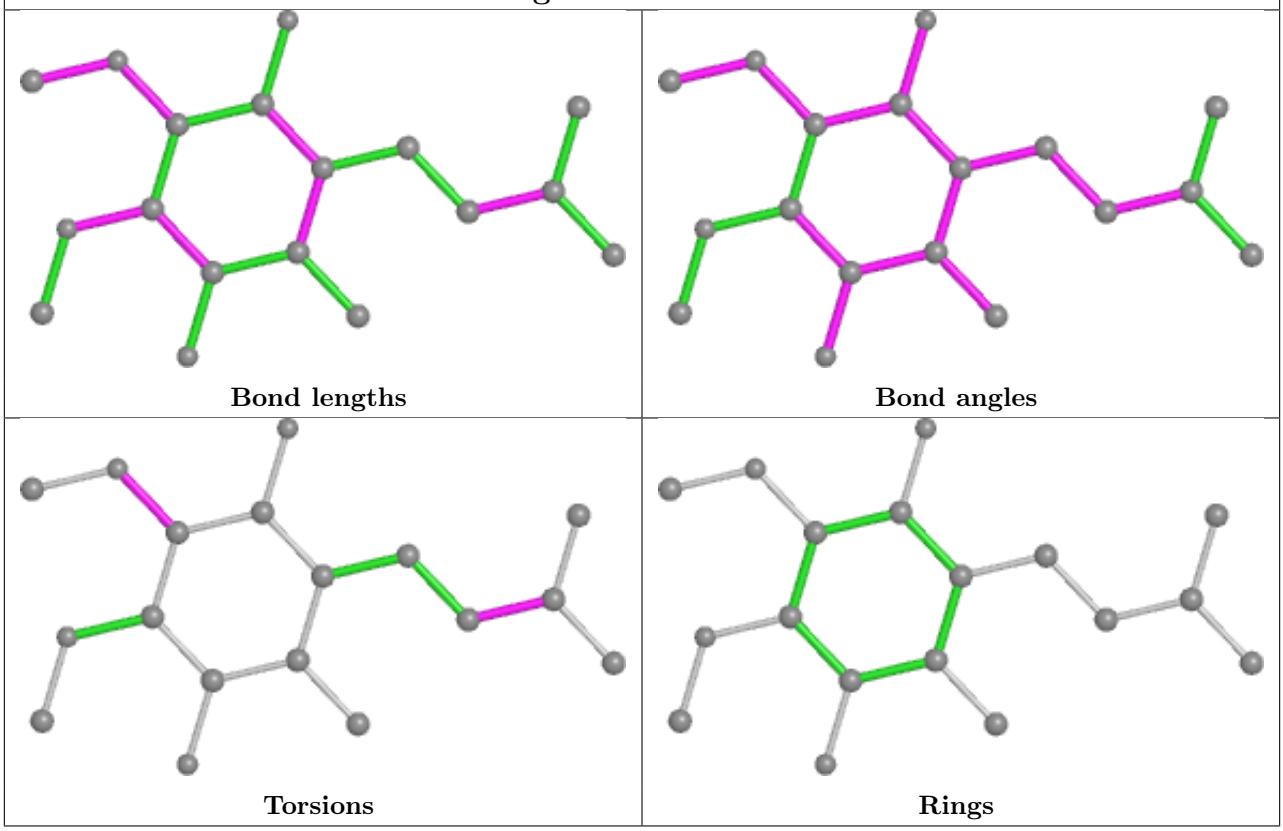
Ligand BCL L 301



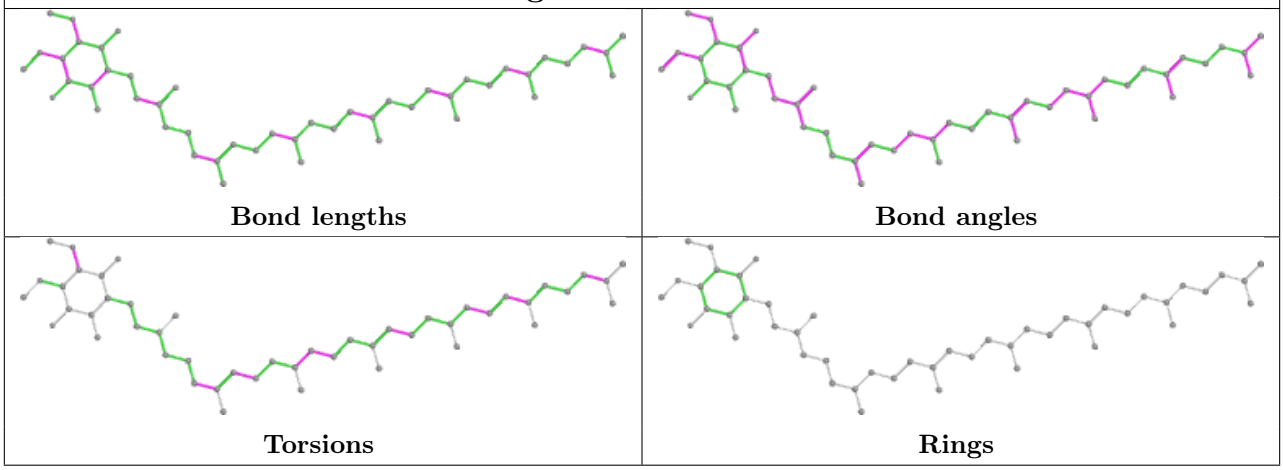
Ligand BCL L 302



Ligand U10 L 304



Ligand U10 M 405



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	L	281/281 (100%)	-0.62	4 (1%)	75	80	28, 40, 77, 93	0
2	M	302/313 (96%)	-0.69	2 (0%)	87	90	28, 44, 71, 90	0
3	H	239/260 (91%)	-0.61	2 (0%)	86	89	27, 42, 57, 74	0
All	All	822/854 (96%)	-0.64	8 (0%)	82	86	27, 42, 71, 93	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.0
1	L	281	GLY	4.7
2	M	301	HIS	4.4
3	H	246	PRO	3.8
1	L	270	PRO	3.3

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 monosaccharides in this entry.

6.4 Ligands (i)

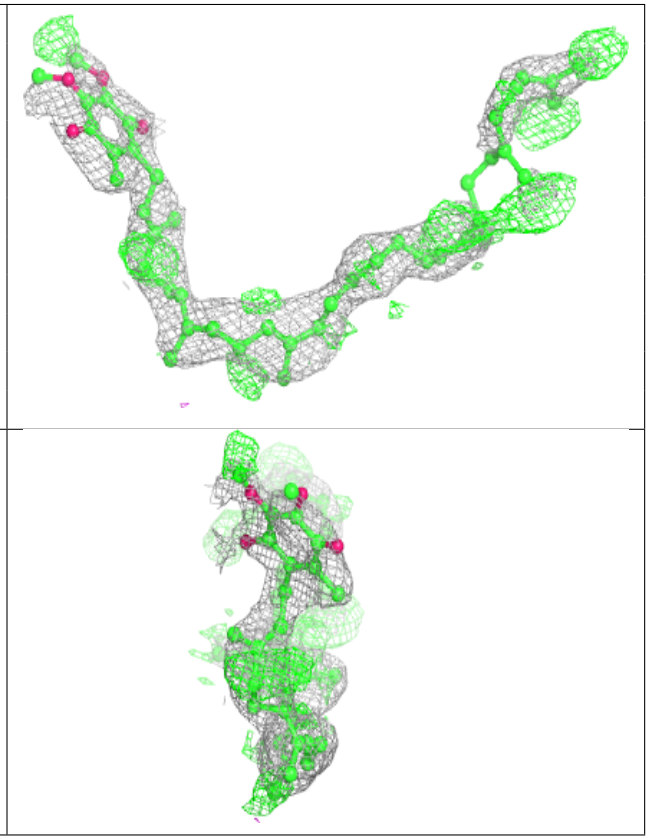
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	U10	M	405	48/63	0.80	0.31	31,42,52,55	48
6	U10	L	304	18/63	0.82	0.50	9,13,18,20	18
8	SPO	M	406	42/42	0.90	0.22	45,68,98,100	0
5	BPH	M	404	65/65	0.93	0.15	28,39,114,116	0
4	BCL	M	401	61/66	0.94	0.14	23,33,87,89	0
4	BCL	L	301	66/66	0.96	0.14	25,36,43,56	0
4	BCL	M	403	66/66	0.97	0.13	30,38,56,68	0
5	BPH	L	303	65/65	0.97	0.12	18,31,43,46	0
4	BCL	L	302	66/66	0.97	0.08	16,27,51,53	0
7	FE	M	402	1/1	1.00	0.08	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.

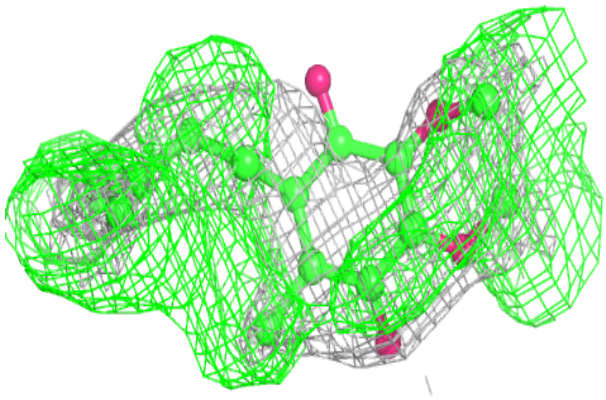
Electron density around U10 M 405:

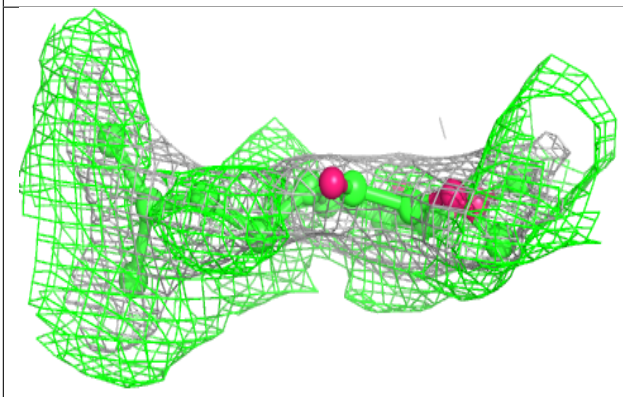
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

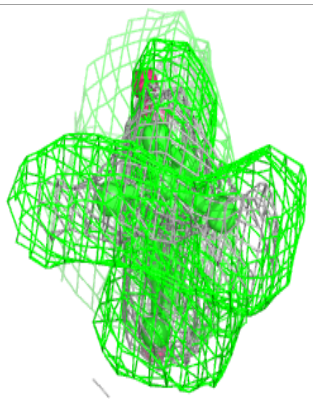


Electron density around U10 L 304:

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

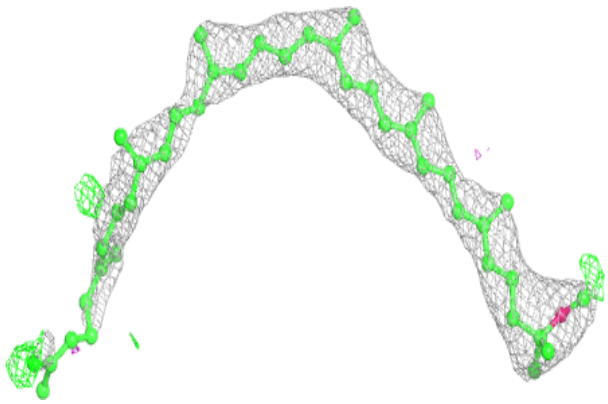


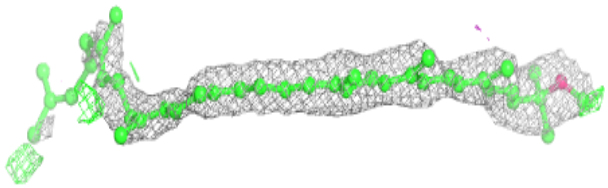


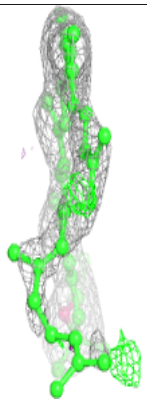


Electron density around SPO M 406:

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

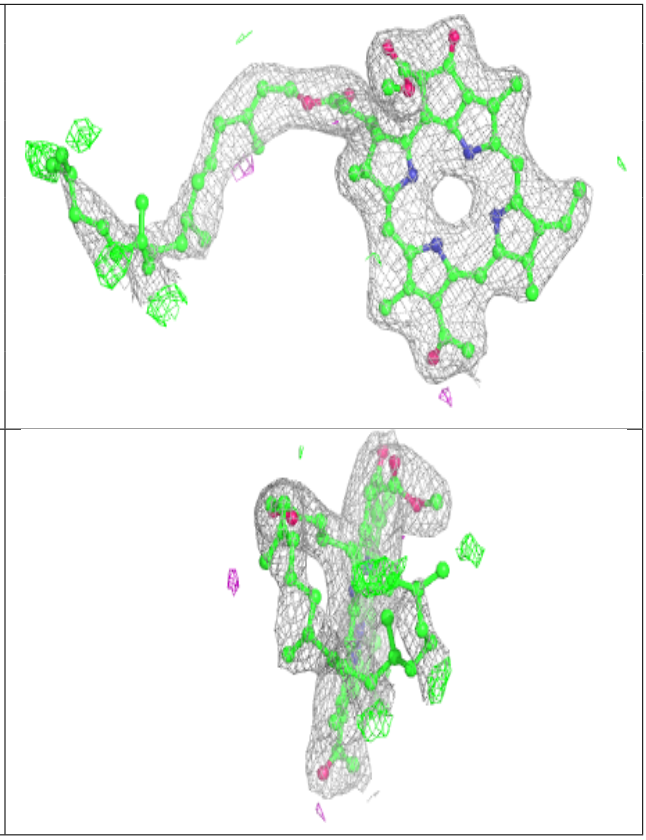






Electron density around BPH M 404:

$2mF_o$-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 401:

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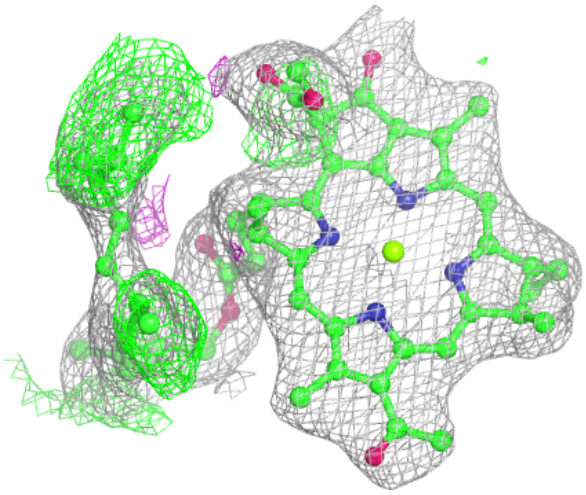
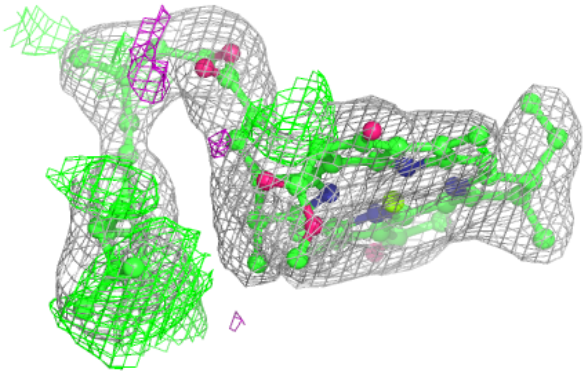
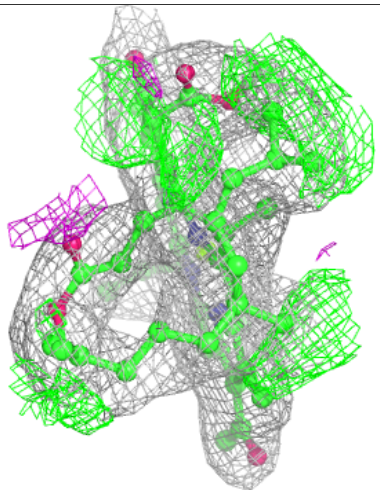
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCL L 301:

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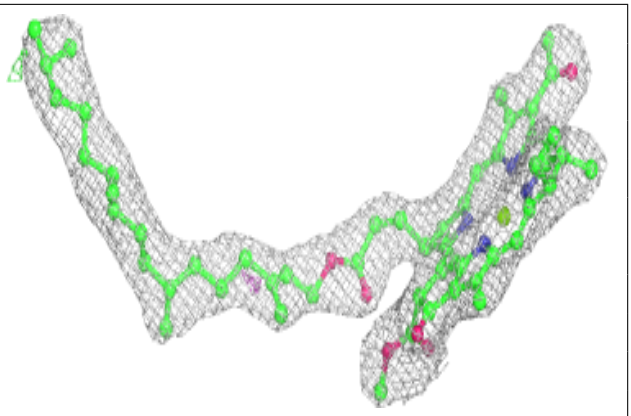
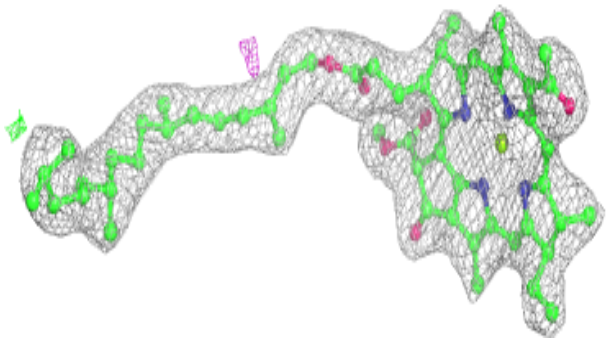
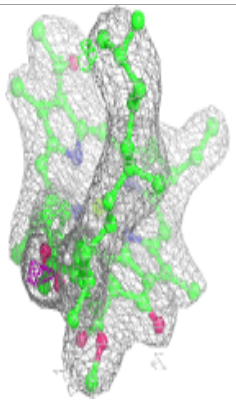
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCL M 403:

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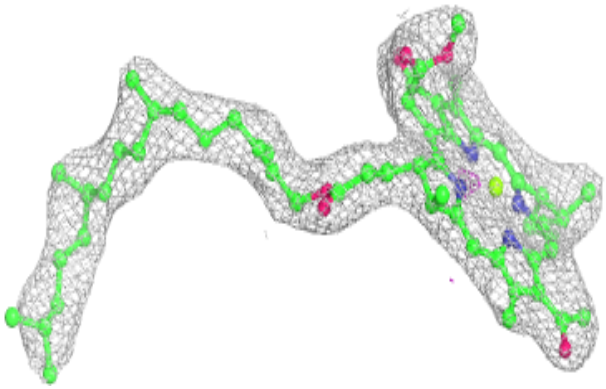
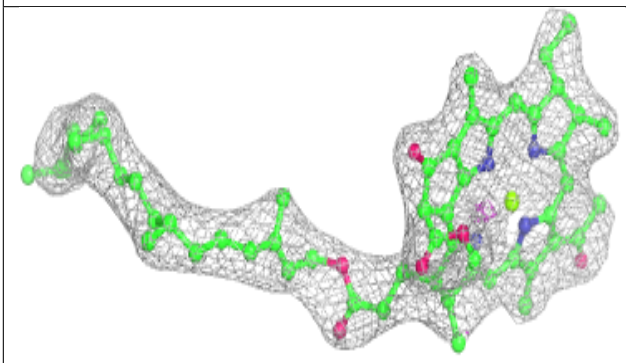
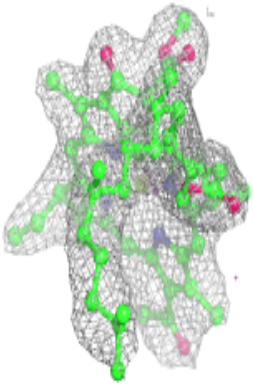
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BPH L 303:

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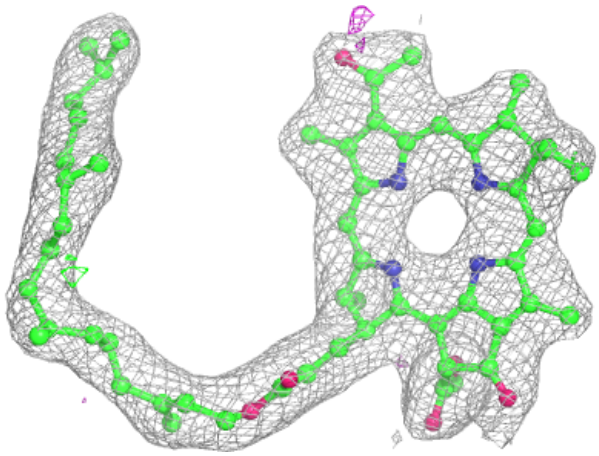
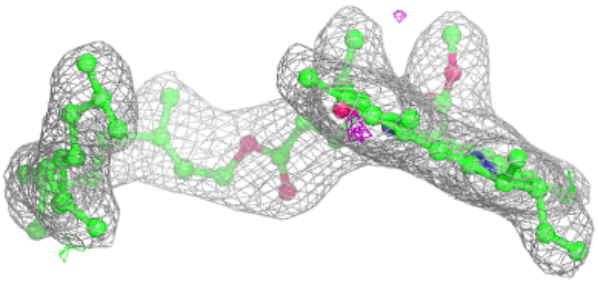
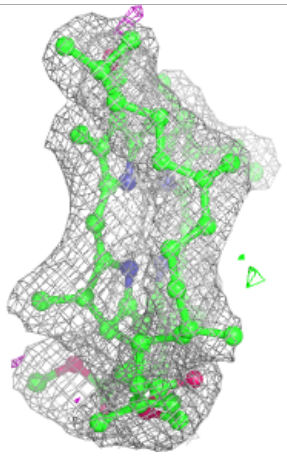
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BCL L 302:

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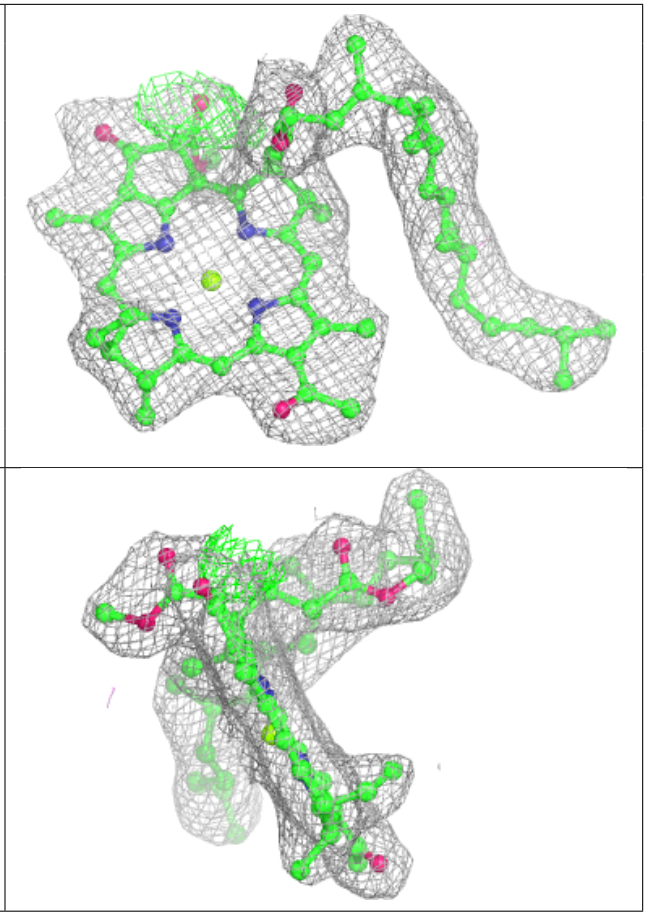
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.