



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 12:54 PM BST

PDB ID : 4H99
Title : Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with
ILE M265 replaced with THR
Authors : Mattis, A.J.; Wraight, C.A.
Deposited on : 2012-09-24
Resolution : 2.97 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

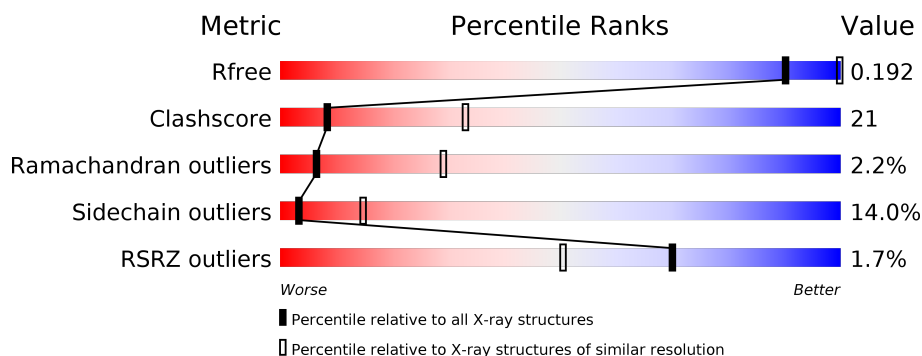
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.97 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 on 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 $\leq 5\%$. 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	<div> <div>0%</div> <div>60%</div> <div>26%</div> <div>11%</div> <div>•</div> </div>
2	M	313	<div> <div>2%</div> <div>52%</div> <div>34%</div> <div>8%</div> <div>• •</div> </div>
3	H	260	<div> <div>2%</div> <div>53%</div> <div>28%</div> <div>8%</div> <div>• 8%</div> </div>

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	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7005 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
1	L	281	Total	C	N	O	S	0	0	0
			2230	1505	355	362	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2406	1604	394	398	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	265	THR	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

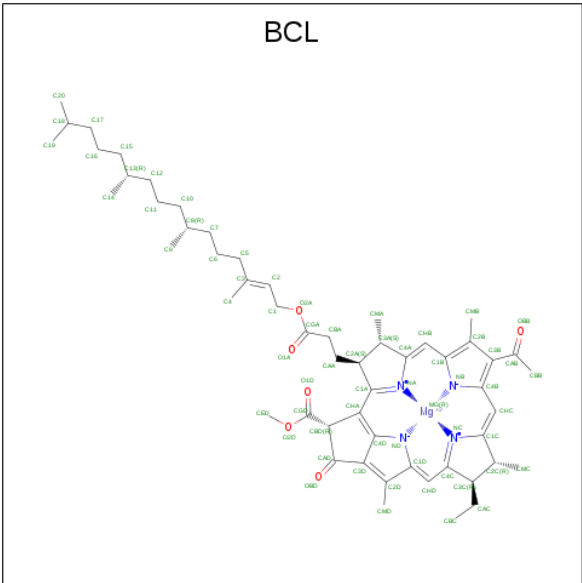
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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: C₅₅H₇₄MgN₄O₆).



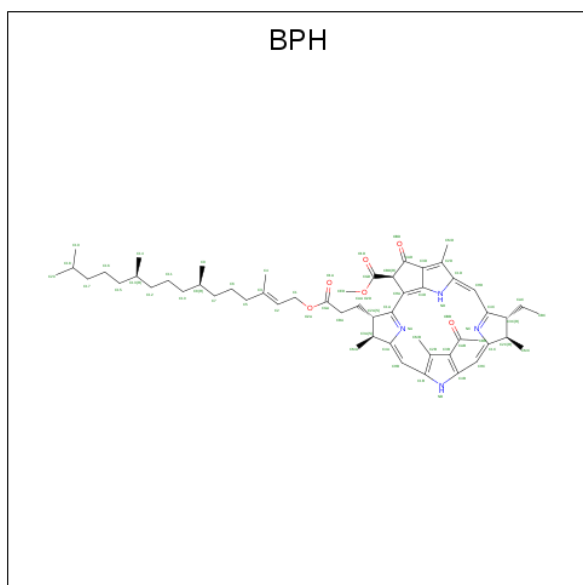
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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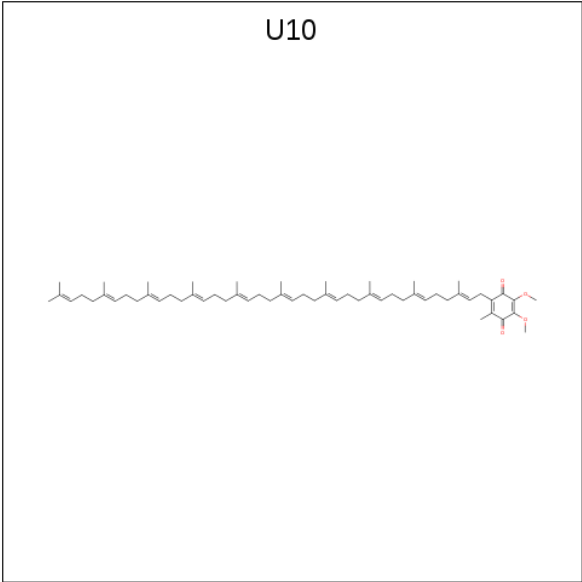
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	Mg	N	O	0	0
			50	39	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			51	41	4	6		

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

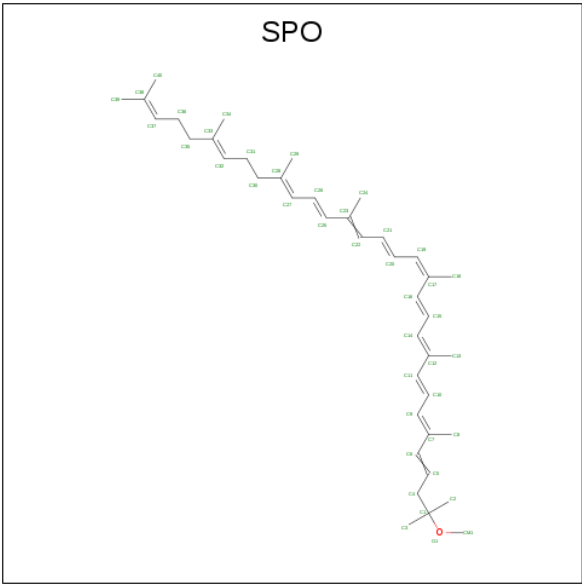


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			33	29	4		
6	M	1	Total	C	O	0	0
			48	44	4		

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

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

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



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

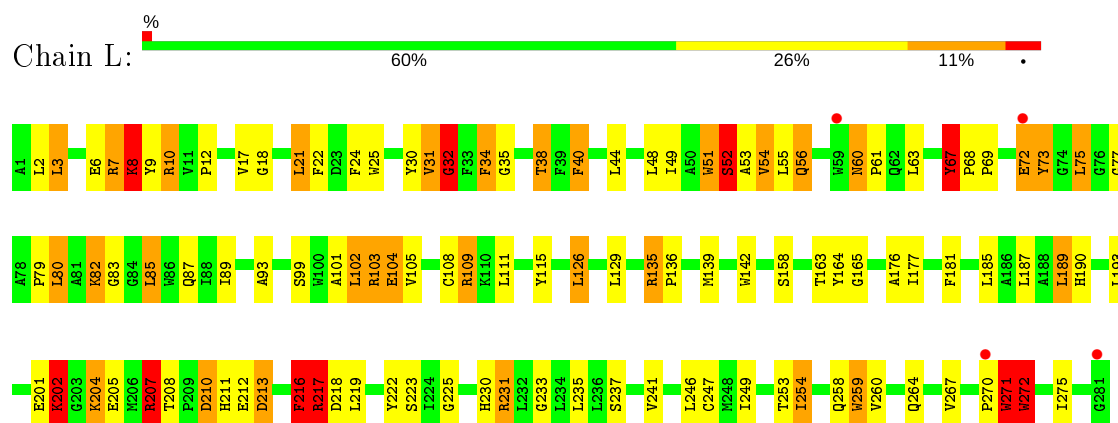
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	19	Total	O	0	0
			19	19		
9	M	18	Total	O	0	0
			18	18		
9	H	15	Total	O	0	0
			15	15		

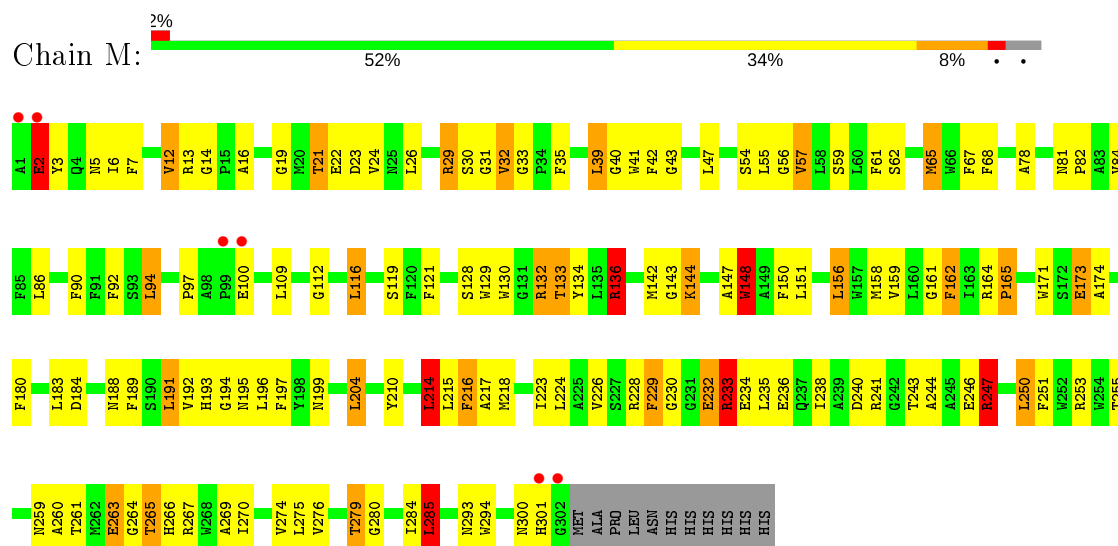
3 Residue-property plots

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

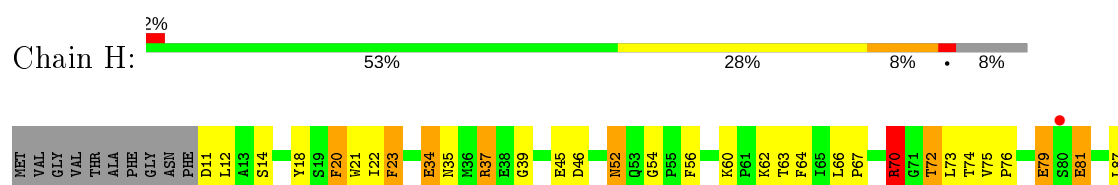
- Molecule 1: Reaction center protein L chain

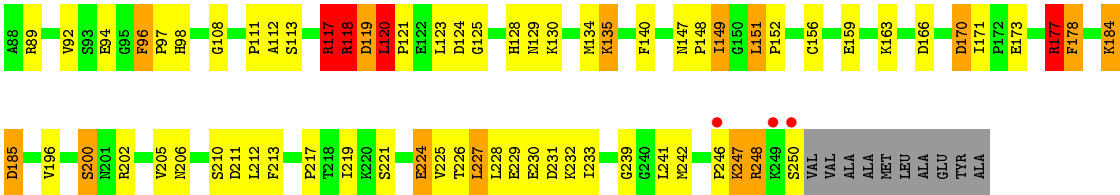


- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.87Å 138.87Å 185.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.77 – 2.97 19.77 – 2.97	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.77-2.97) 99.6 (19.77-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109, PHENIX	Depositor
R, R_{free}	0.174 , 0.194 0.184 , 0.192	Depositor DCC
R_{free} test set	2146 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7005	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: BCL, BPH, U10, FE, SPO

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	1.68	34/2318 (1.5%)	1.44	25/3172 (0.8%)
2	M	1.67	29/2498 (1.2%)	1.39	24/3410 (0.7%)
3	H	1.76	28/1877 (1.5%)	1.54	30/2553 (1.2%)
All	All	1.70	91/6693 (1.4%)	1.45	79/9135 (0.9%)

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
3	H	0	2
All	All	0	3

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	11.30	1.69	1.51
1	L	72	GLU	CG-CD	10.89	1.68	1.51
1	L	82	LYS	CB-CG	10.31	1.80	1.52
1	L	67	TYR	CD2-CE2	10.06	1.54	1.39
3	H	94	GLU	CD-OE1	9.99	1.36	1.25

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	231	ARG	NE-CZ-NH2	-13.09	113.76	120.30
1	L	231	ARG	NE-CZ-NH1	11.94	126.27	120.30
2	M	247	ARG	NE-CZ-NH1	11.91	126.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	217	ARG	NE-CZ-NH1	11.81	126.21	120.30
2	M	29	ARG	NE-CZ-NH2	-11.35	114.63	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	119	ASP	Peptide
3	H	79	GLU	Peptide
1	L	32	GLY	Peptide

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	L	2230	0	2178	100	0
2	M	2406	0	2313	107	0
3	H	1829	0	1836	68	0
4	L	132	0	148	9	0
4	M	116	0	115	20	0
5	L	65	0	76	14	0
5	M	51	0	43	9	0
6	L	33	0	39	10	0
6	M	48	0	63	1	0
7	M	1	0	0	0	0
8	M	42	0	60	13	0
9	H	15	0	0	5	0
9	L	19	0	0	3	0
9	M	18	0	0	0	0
All	All	7005	0	6871	289	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 21.

The worst 5 of 289 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:L:82:LYS:CB	1:L:82:LYS:CG	1.80	1.54
4:M:403:BCL:HHC	4:M:403:BCL:HBB3	1.27	1.14
6:L:304:U10:H1M1	6:L:304:U10:C8	1.79	1.12
1:L:38:THR:HG22	1:L:99:SER:HB2	1.20	1.11
1:L:7:ARG:HH11	3:H:98:HIS:CD2	1.69	1.10

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%)	246 (88%)	22 (8%)	11 (4%)	3	15
2	M	300/313 (96%)	260 (87%)	35 (12%)	5 (2%)	9	36
3	H	238/260 (92%)	212 (89%)	24 (10%)	2 (1%)	19	55
All	All	817/854 (96%)	718 (88%)	81 (10%)	18 (2%)	6	29

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	52	SER
1	L	55	LEU
1	L	202	LYS
2	M	301	HIS
3	H	185	ASP

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	219/220 (100%)	188 (86%)	31 (14%)	3	14
2	M	236/246 (96%)	204 (86%)	32 (14%)	3	15
3	H	195/208 (94%)	167 (86%)	28 (14%)	3	14
All	All	650/674 (96%)	559 (86%)	91 (14%)	3	15

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	109	LEU
2	M	214	LEU
3	H	217	PRO
2	M	133	THR
2	M	156	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
2	M	193	HIS
3	H	52	ASN
3	H	98	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 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
4	BCL	L	302	-	58,74,74	1.54	5 (8%)	69,115,115	2.37	26 (37%)
8	SPO	M	406	-	40,41,41	2.18	8 (20%)	47,50,50	2.93	20 (42%)
4	BCL	M	403	-	58,74,74	1.47	4 (6%)	69,115,115	1.71	18 (26%)
6	U10	M	405	-	48,48,63	2.89	17 (35%)	58,61,79	2.44	19 (32%)
4	BCL	L	301	-	58,74,74	1.44	5 (8%)	69,115,115	1.64	12 (17%)
6	U10	L	304	-	33,33,63	3.55	11 (33%)	40,43,79	3.44	21 (52%)
5	BPH	M	404	-	49,55,70	1.77	11 (22%)	58,83,101	2.29	18 (31%)
4	BCL	M	401	-	42,58,74	2.99	7 (16%)	48,95,115	2.90	20 (41%)
5	BPH	L	303	-	64,70,70	1.67	9 (14%)	76,101,101	1.89	24 (31%)

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
4	BCL	L	302	-	-	6/37/137/137	-
8	SPO	M	406	-	-	9/47/47/47	-
4	BCL	M	403	-	-	7/37/137/137	-
6	U10	M	405	-	-	16/45/69/87	0/1/1/1
4	BCL	L	301	-	-	1/37/137/137	-
6	U10	L	304	-	-	13/27/51/87	0/1/1/1
5	BPH	M	404	-	-	8/36/87/105	0/5/6/6
4	BCL	M	401	-	-	4/18/118/137	-
5	BPH	L	303	-	2/2/18/22	15/54/105/105	0/5/6/6

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	401	BCL	C1B-NB	15.23	1.48	1.35
6	L	304	U10	C13-C14	9.42	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	406	SPO	C27-C28	9.22	1.43	1.34
6	L	304	U10	C8-C9	8.99	1.54	1.33
4	M	401	BCL	C4B-NB	8.52	1.42	1.35

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	BCL	O2A-C1-C2	9.77	131.82	108.97
8	M	406	SPO	C16-C17-C19	8.76	132.38	118.94
6	L	304	U10	O5-C5-C4	-7.94	104.08	120.93
4	M	401	BCL	O2D-CGD-CBD	7.52	124.64	111.27
4	L	302	BCL	O2D-CGD-CBD	7.15	123.97	111.27

All (2) chirality outliers are listed below:

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

5 of 79 torsion outliers are listed below:

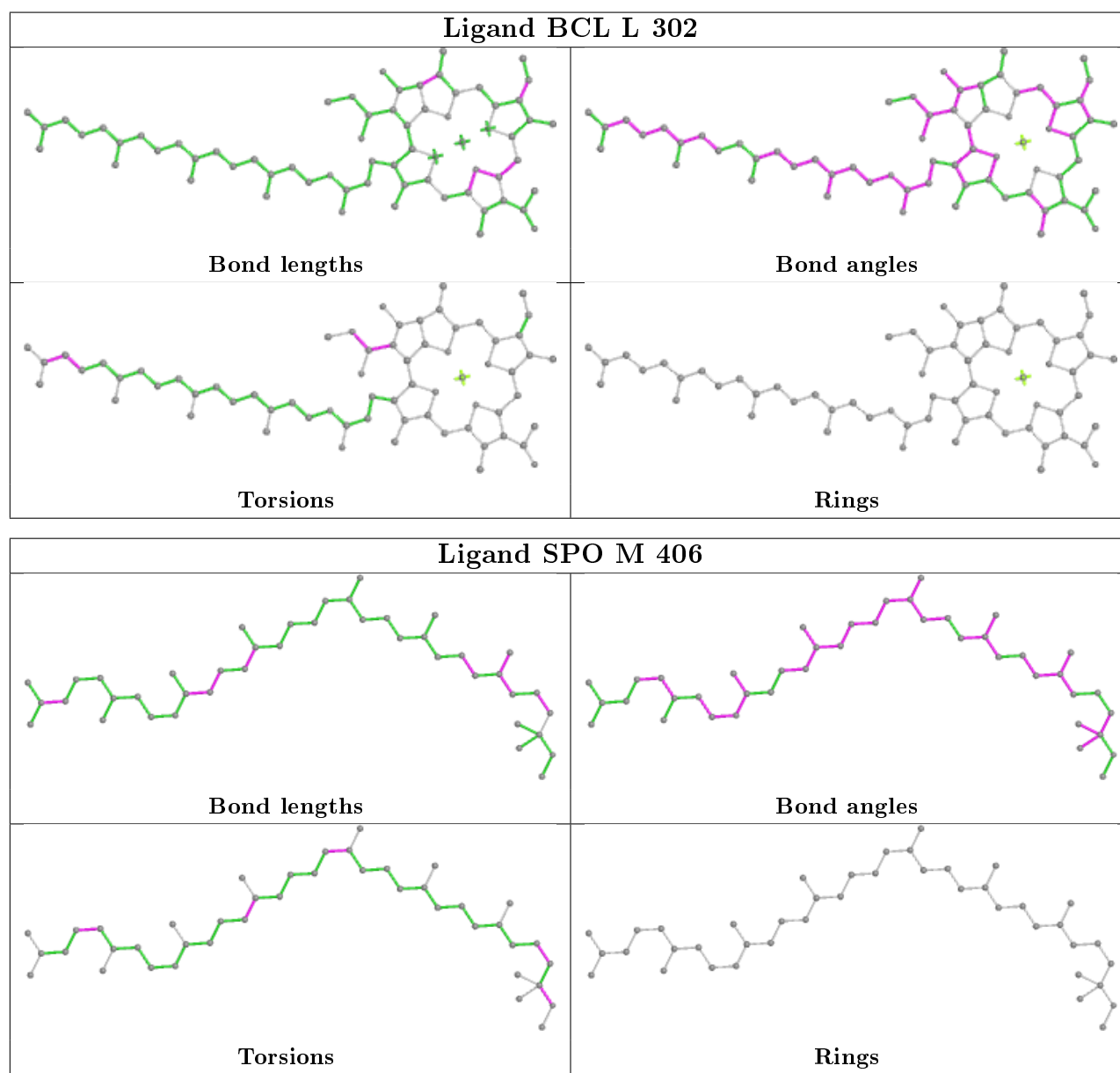
Mol	Chain	Res	Type	Atoms
8	M	406	SPO	C1-C4-C5-C6
8	M	406	SPO	C33-C35-C36-C37
6	M	405	U10	C12-C13-C14-C15
6	M	405	U10	C14-C16-C17-C18
6	M	405	U10	C27-C28-C29-C30

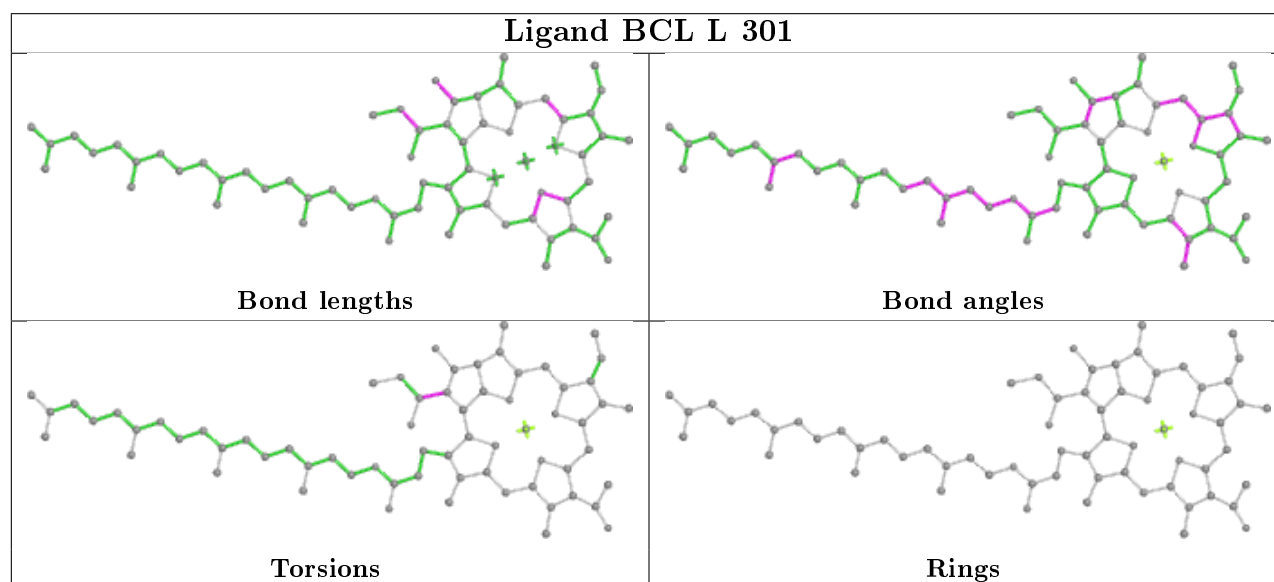
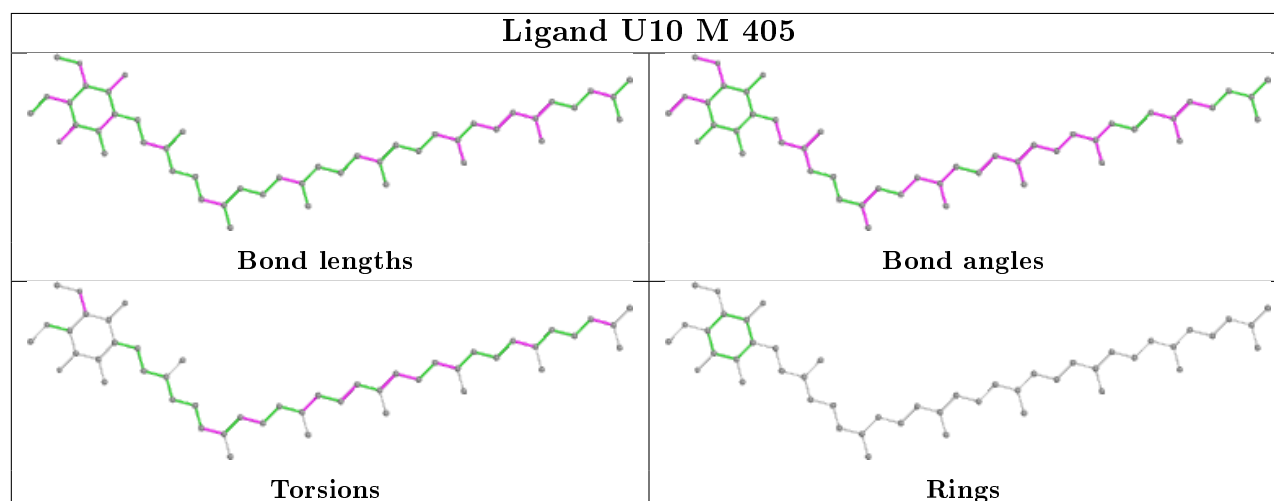
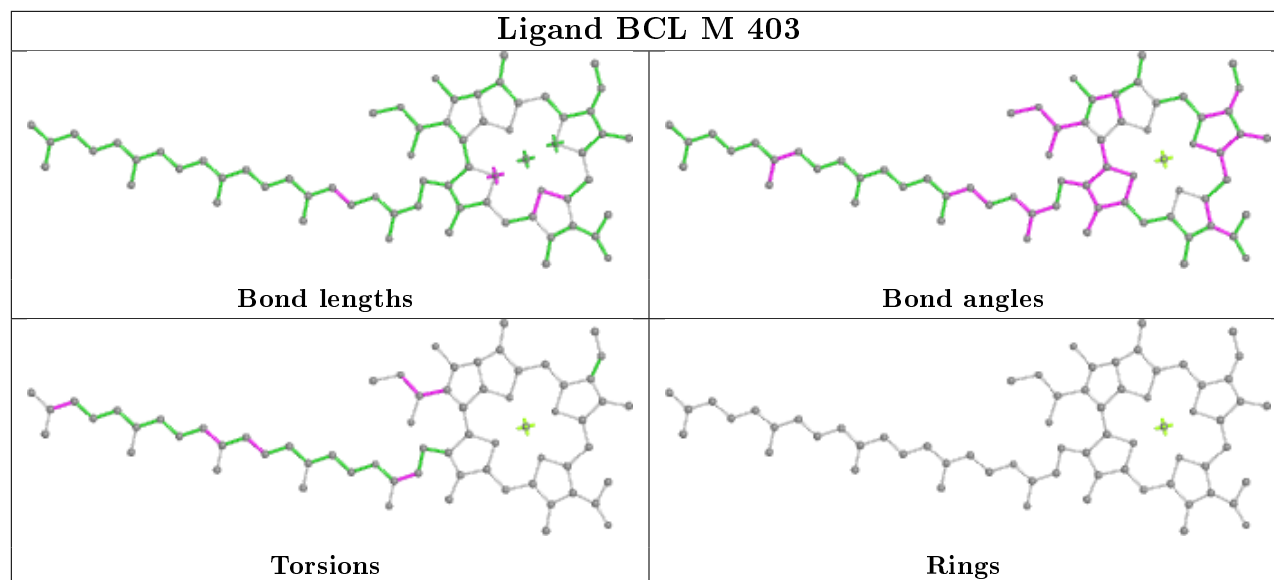
There are no ring outliers.

9 monomers are involved in 70 short contacts:

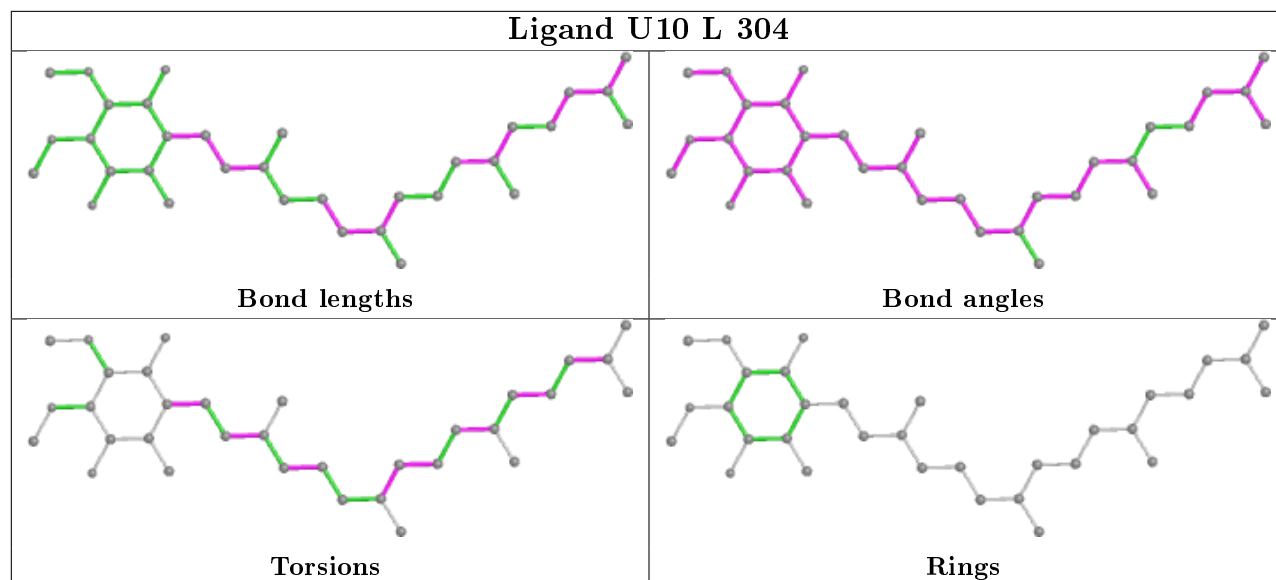
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	302	BCL	6	0
8	M	406	SPO	13	0
4	M	403	BCL	15	0
6	M	405	U10	1	0
4	L	301	BCL	3	0
6	L	304	U10	10	0
5	M	404	BPH	9	0
4	M	401	BCL	7	0
5	L	303	BPH	14	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

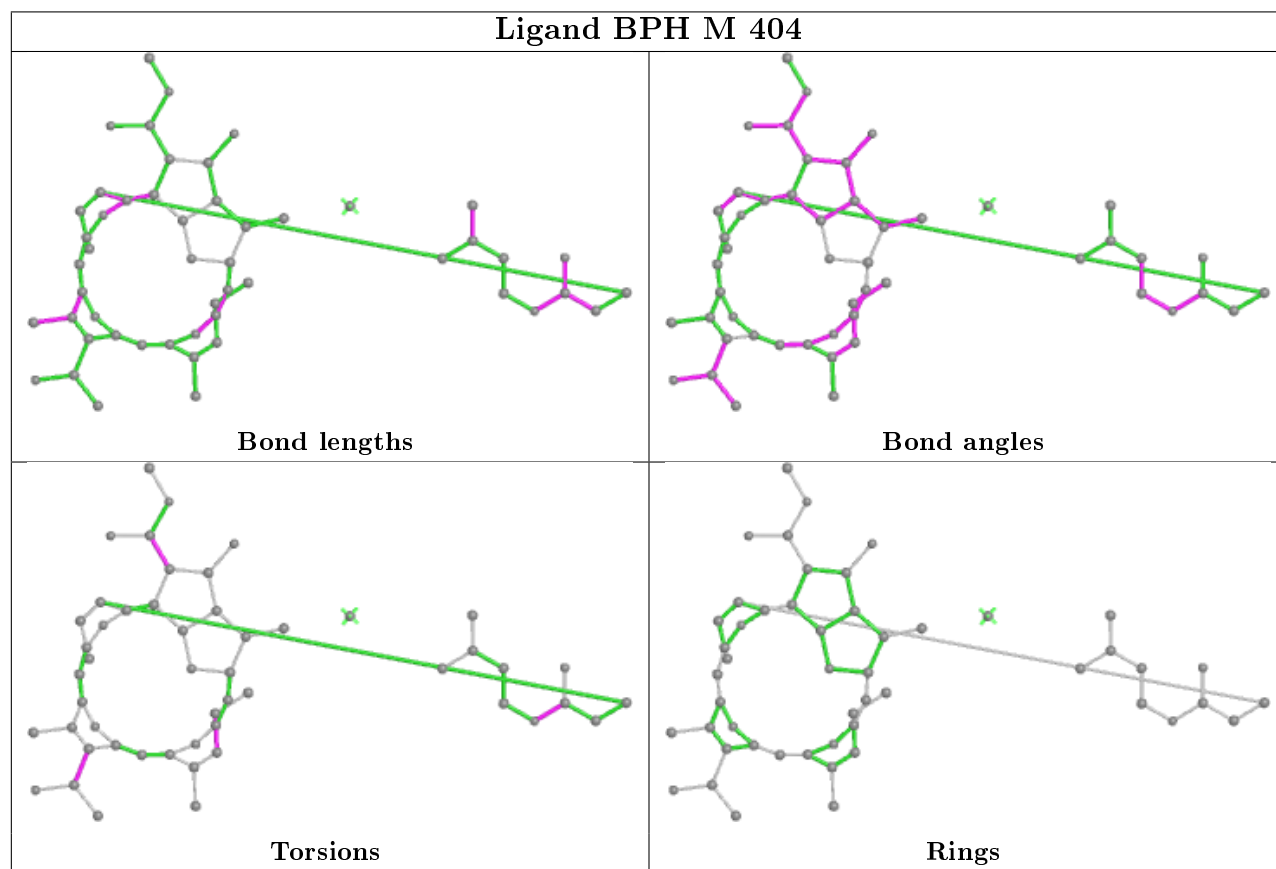


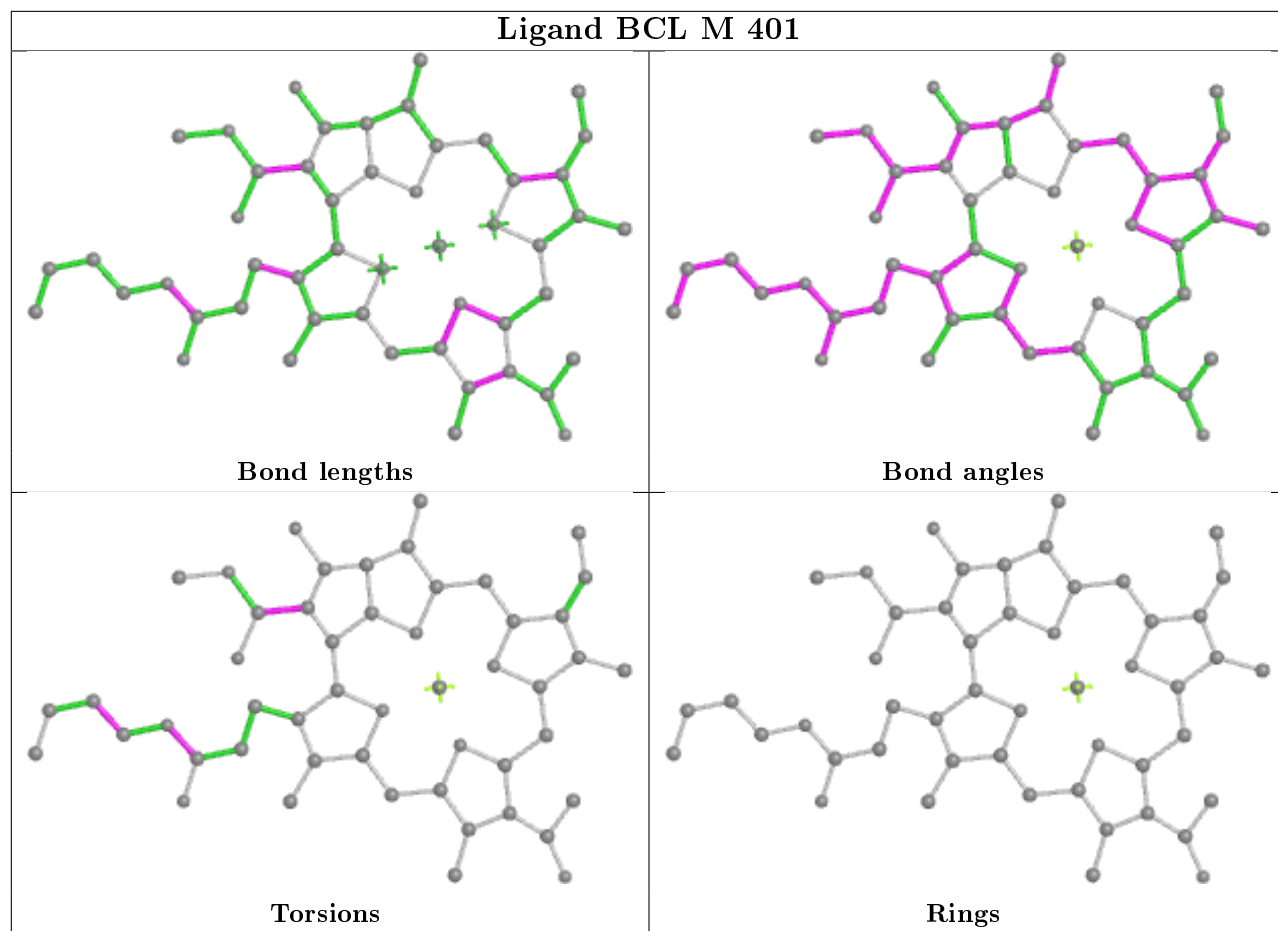


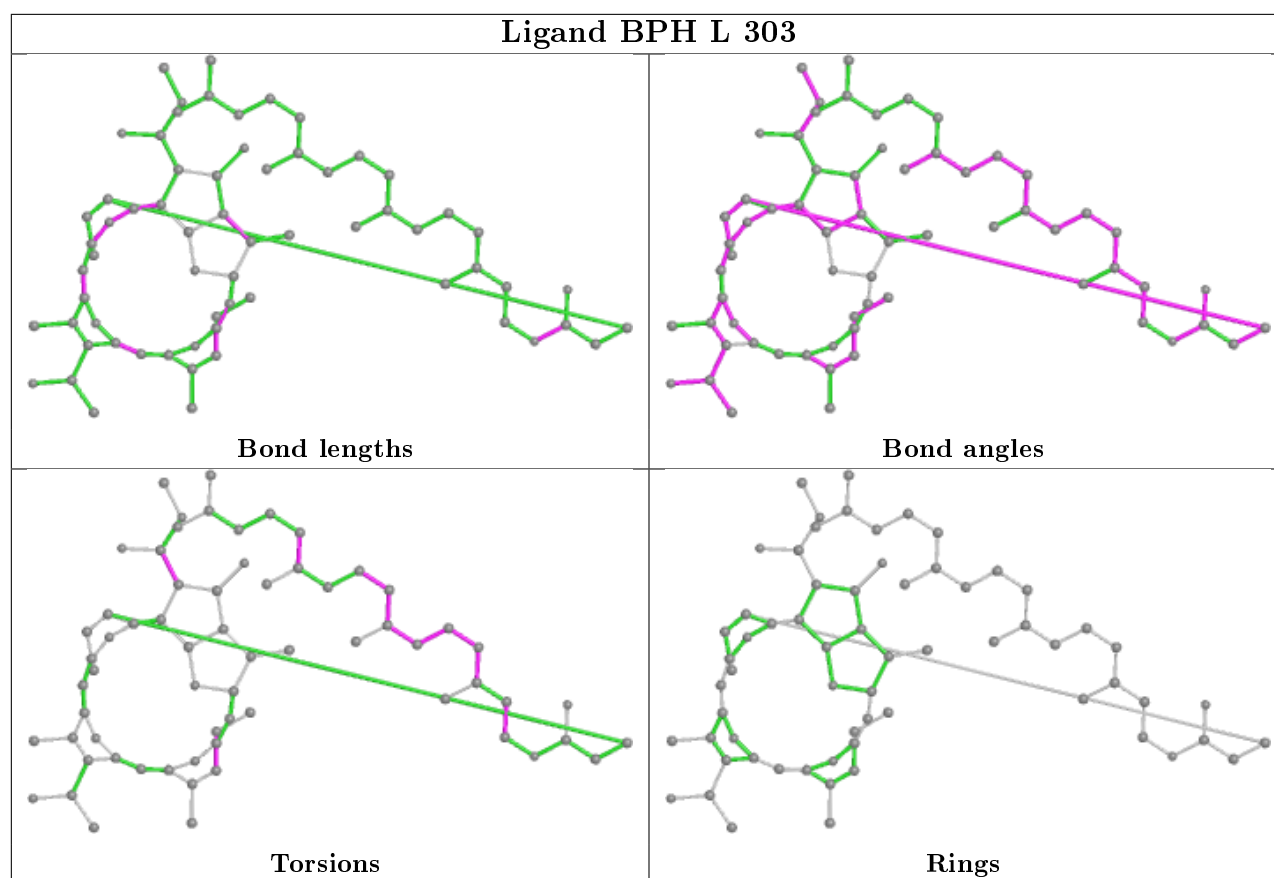
Ligand U10 L 304



Ligand BPH M 404







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%)	-0.66	4 (1%) 75 57	35, 48, 83, 98	0
2	M	302/313 (96%)	-0.67	6 (1%) 65 45	34, 52, 82, 108	0
3	H	240/260 (92%)	-0.48	4 (1%) 70 50	38, 52, 69, 96	0
All	All	823/854 (96%)	-0.61	14 (1%) 70 50	34, 50, 81, 108	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	6.3
3	H	250	SER	4.5
3	H	80	SER	3.2
2	M	301	HIS	2.9
2	M	302	GLY	2.9

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](#)

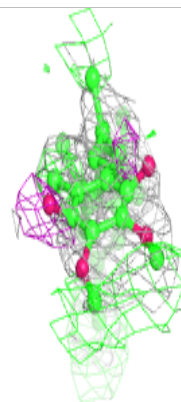
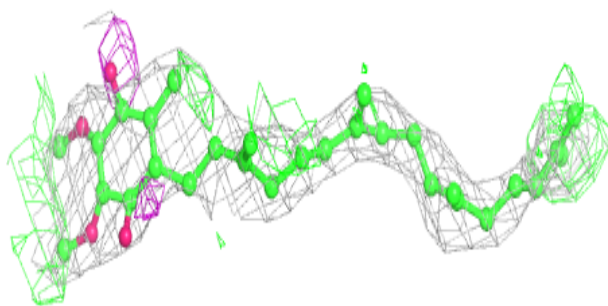
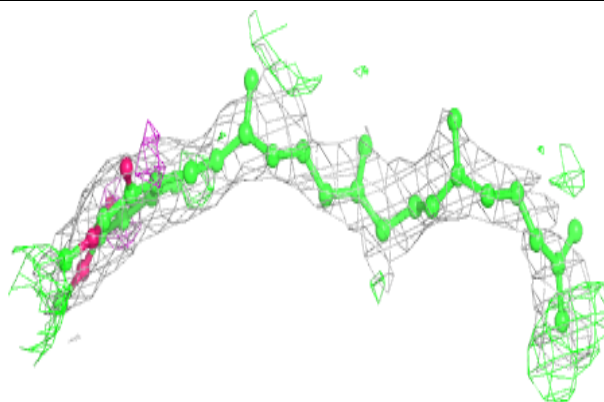
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	U10	L	304	33/63	0.75	0.35	64,85,99,101	0
8	SPO	M	406	42/42	0.87	0.28	64,87,114,116	0
6	U10	M	405	48/63	0.94	0.15	31,50,76,82	0
4	BCL	M	403	66/66	0.96	0.15	30,51,61,77	0
4	BCL	L	301	66/66	0.97	0.16	34,48,55,58	0
4	BCL	L	302	66/66	0.98	0.09	24,34,54,64	0
5	BPH	M	404	51/65	0.98	0.11	36,54,66,101	0
4	BCL	M	401	50/66	0.98	0.10	35,43,80,100	0
5	BPH	L	303	65/65	0.98	0.12	27,38,50,54	0
7	FE	M	402	1/1	1.00	0.07	41,41,41,41	0

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

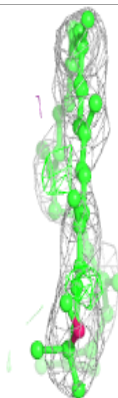
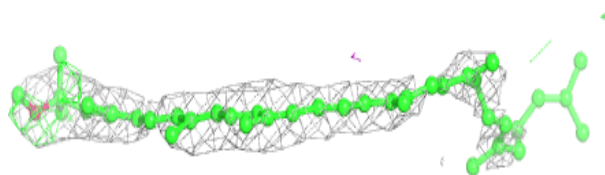
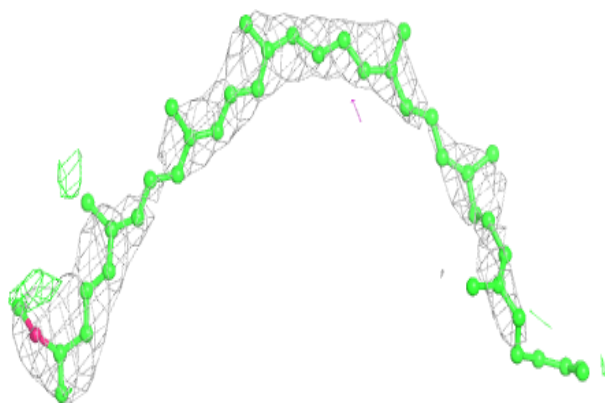
Electron density around U10 L 304:

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

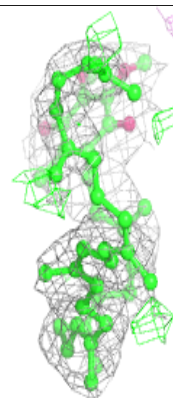
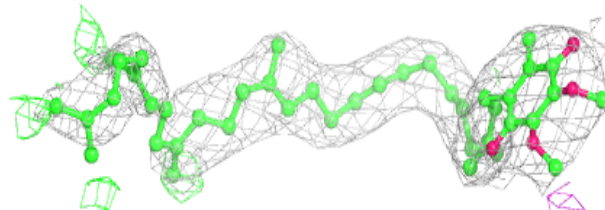
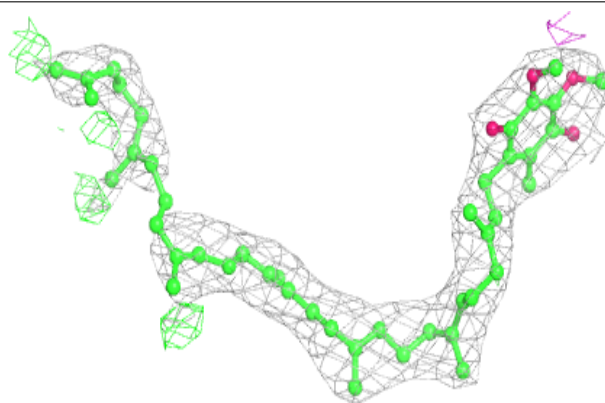


Electron density around SPO M 406:

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

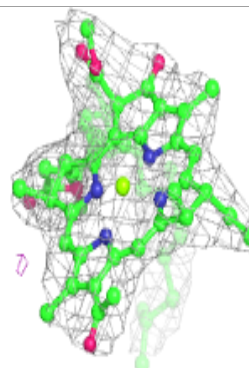
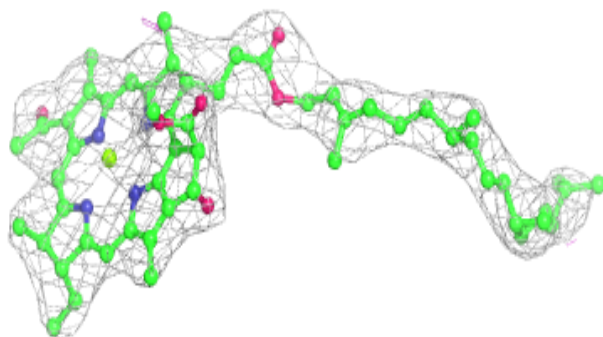
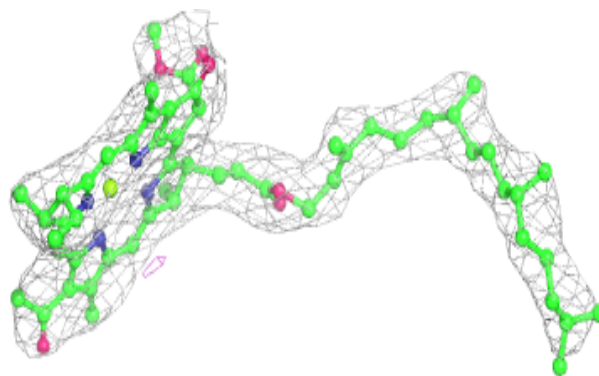
**Electron density around U10 M 405:**

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

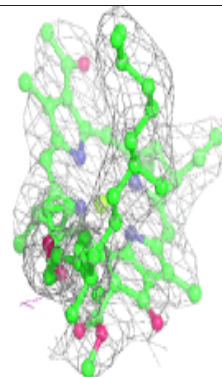
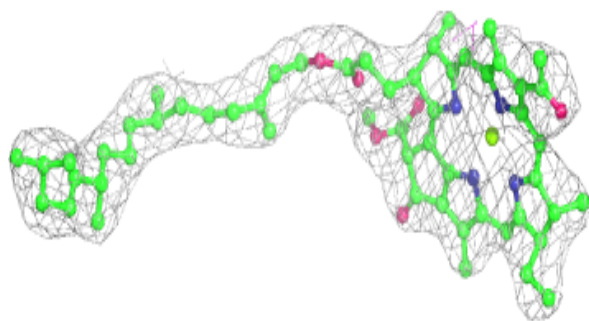
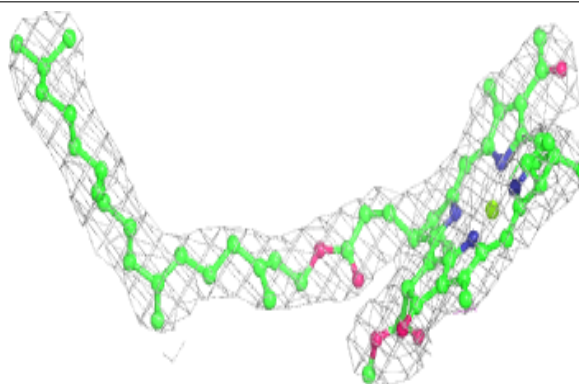


Electron density around BCL M 403:

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

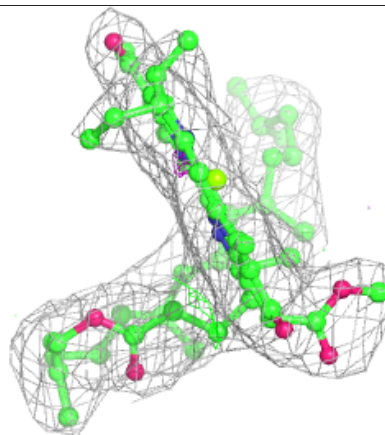
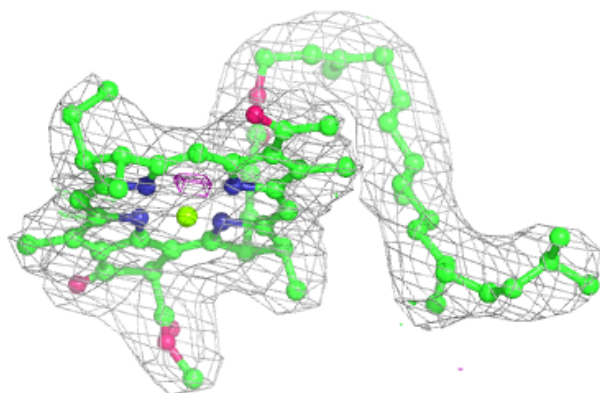
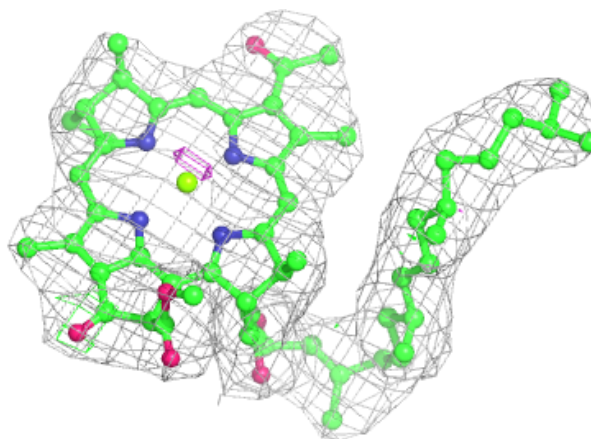
**Electron density around BCL L 301:**

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

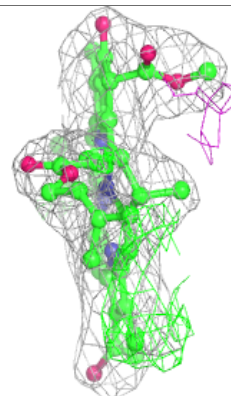
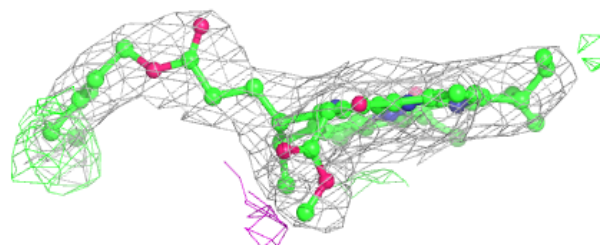
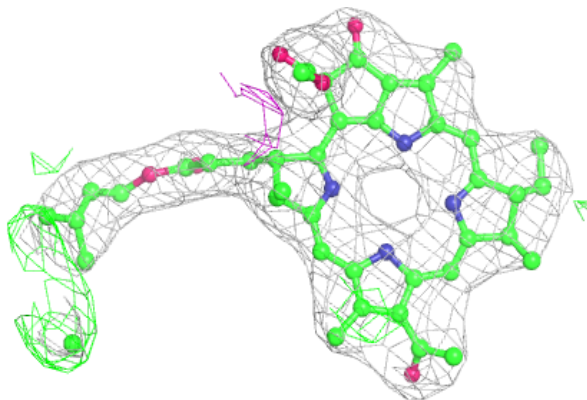


Electron density around BCL L 302:

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

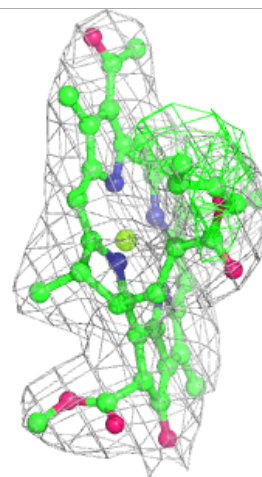
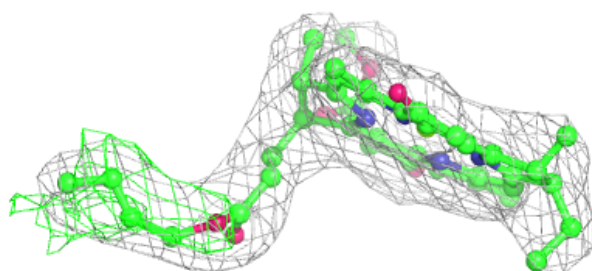
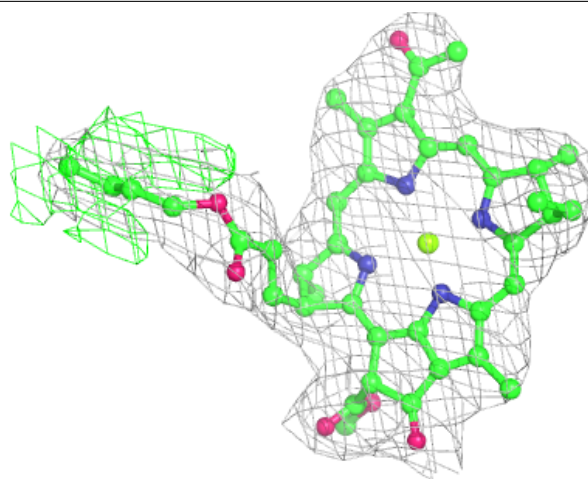
**Electron density around BPH M 404:**

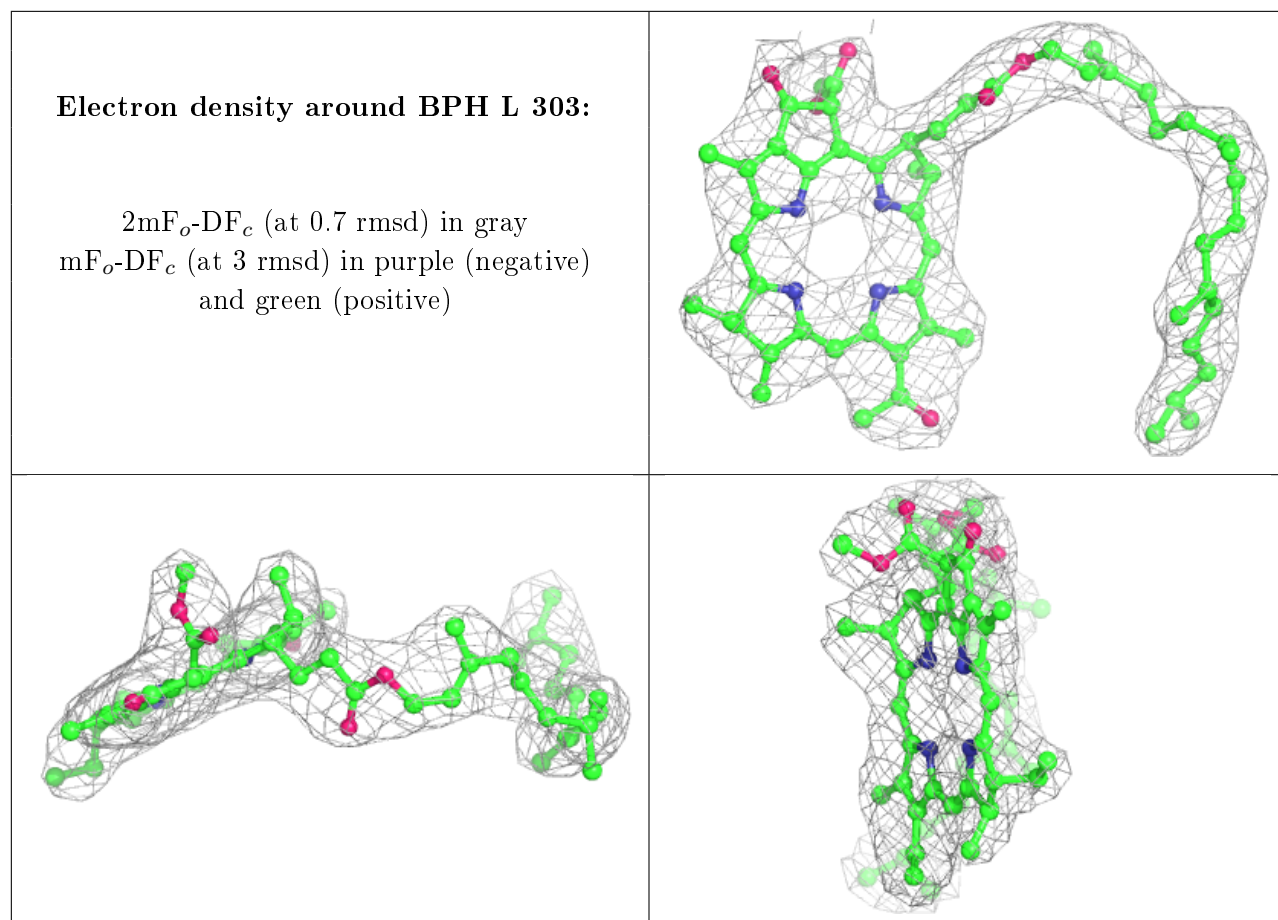
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL M 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.