wwPDB X-ray Structure Validation Summary Report (i)

Feb 8, 2024 – 11:17 AM EST

PDB ID	:	2HH1
Title	:	Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylcholine
Authors	:	Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2006-06-27
Resolution	:	2.55 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:

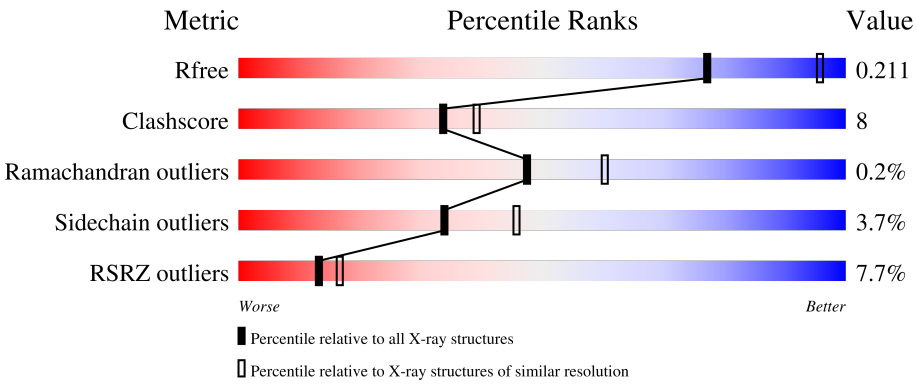
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	9% 89% 10% •
2	M	307	10% 83% 14% • •
3	H	260	3% 85% 7% • 6%

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
14	PC7	H	801	-	-	-	X
15	GOL	H	708	-	-	-	X
7	U10	L	502	-	-	-	X
8	PC9	L	802	-	-	X	X
9	LDA	H	903	-	-	-	X
9	LDA	H	904	-	-	-	X
9	LDA	H	905	-	-	-	X
9	LDA	L	902	-	-	-	X
9	LDA	M	907	-	-	-	X
9	LDA	M	920	-	-	-	X

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 7923 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	2234	1508	355	363	8	0	2	0

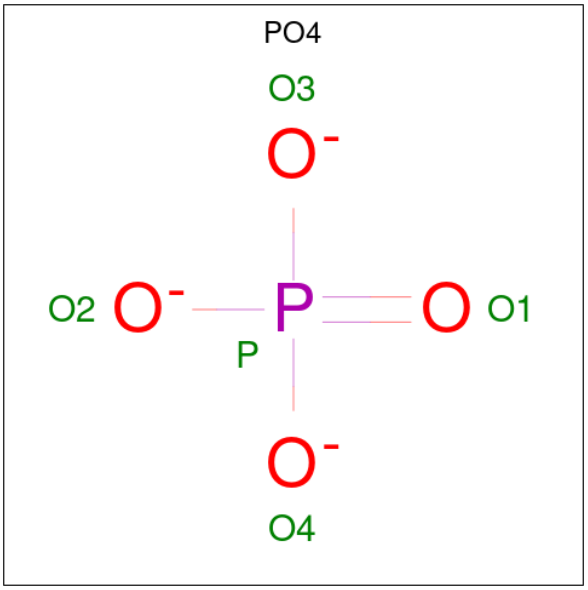
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2466	1643	403	409	11	0	9	0

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

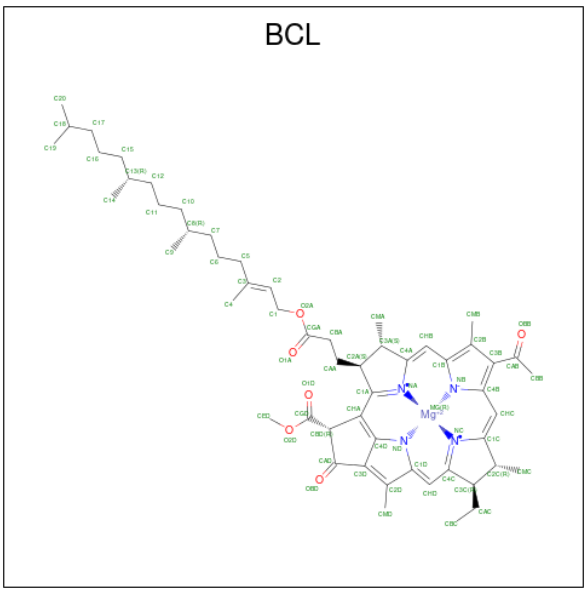
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	244	1891	1207	328	346	10	0	9	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



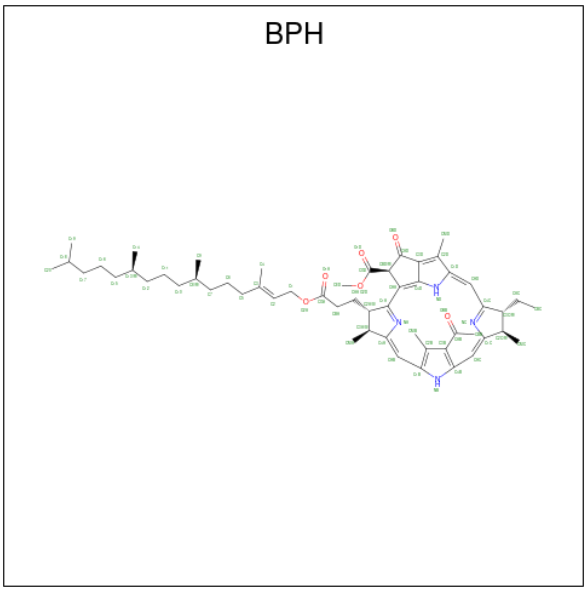
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
4	L	1	5	4	1		0	0
			Total	O	P			
4	M	1	5	4	1		0	0
			Total	O	P			
4	M	1	5	4	1		0	0
			Total	O	P			
4	M	1	5	4	1		0	0

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



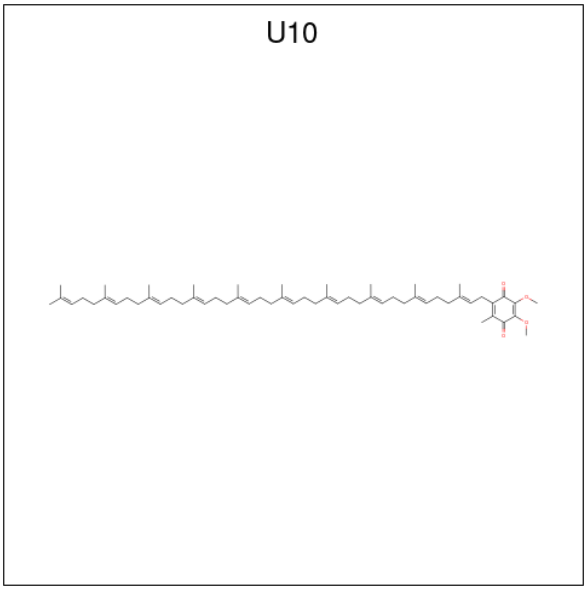
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
5	M	1	66	55	1	4	6	0	0

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



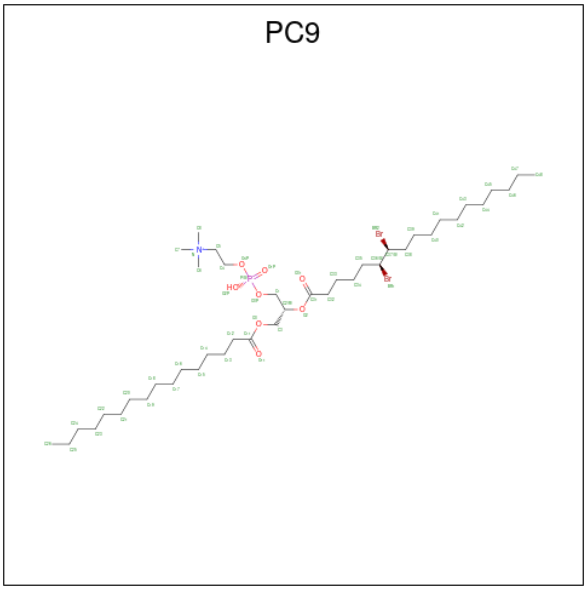
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	L	1	65	55	4	6	0	0
6	M	1	65	55	4	6	0	0

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



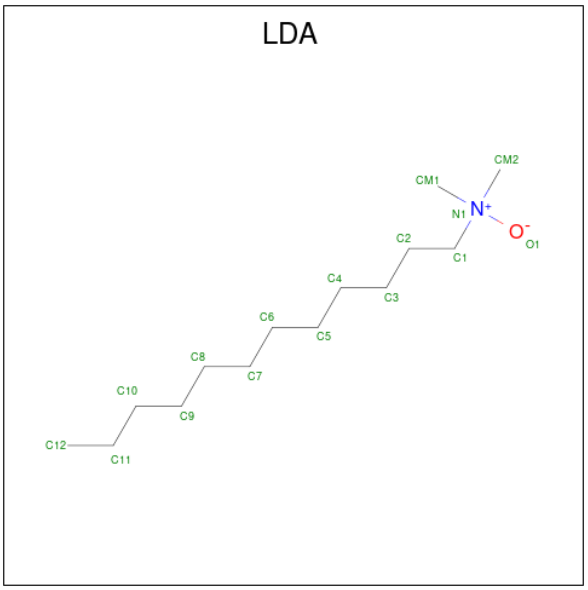
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	L	1	48	44	4	0	0
7	M	1	48	44	4	0	0

- Molecule 8 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC9) (formula: $C_{42}H_{83}Br_2NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	P		
8	L	1	54	2	42	1	8	1	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

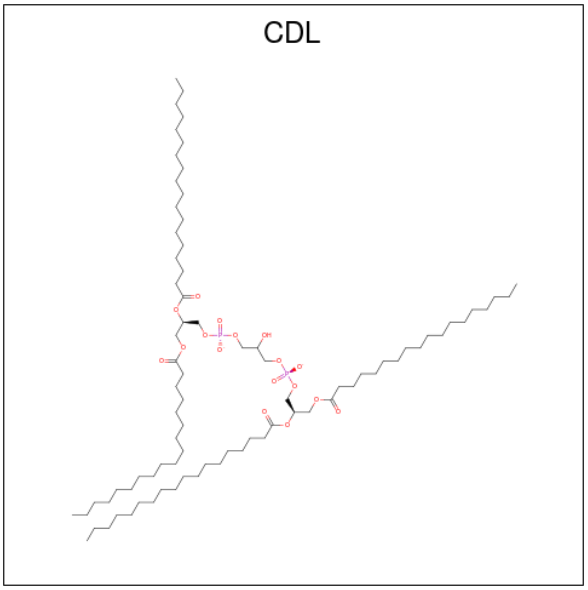


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	L	1	16	14	1	1	0	0
			Total	C	N	O		
9	L	1	16	14	1	1	0	0
			Total	C	N	O		
9	M	1	16	14	1	1	0	0
			Total	C	N	O		
9	M	1	16	14	1	1	0	0
			Total	C	N	O		
9	H	1	16	14	1	1	0	0
			Total	C	N	O		
9	H	1	16	14	1	1	0	0
			Total	C	N	O		
9	H	1	16	14	1	1	0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

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

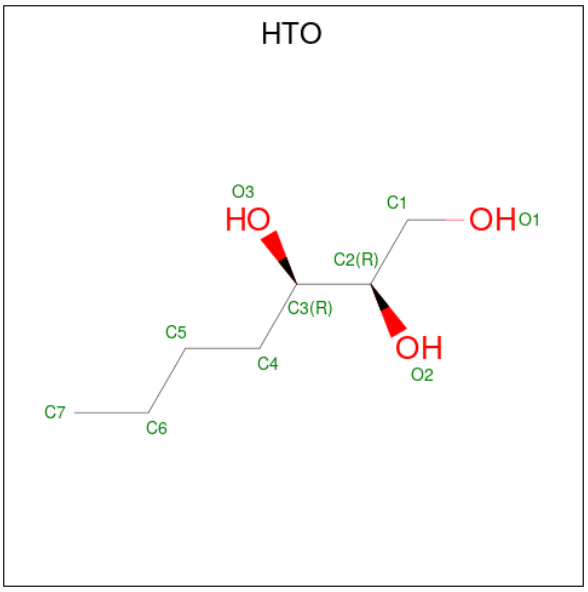


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
11	M	1	81	62	17	2	0	0

- Molecule 12 is POTASSIUM ION (three-letter code: K) (formula: K).

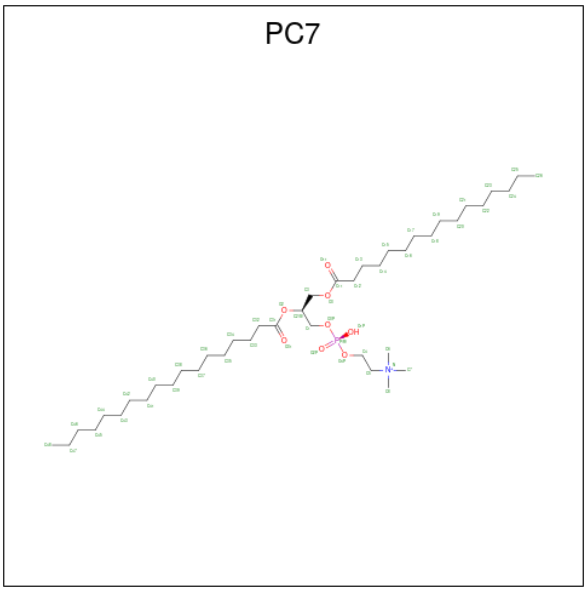
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	1	Total K 1 1	0	0

- Molecule 13 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



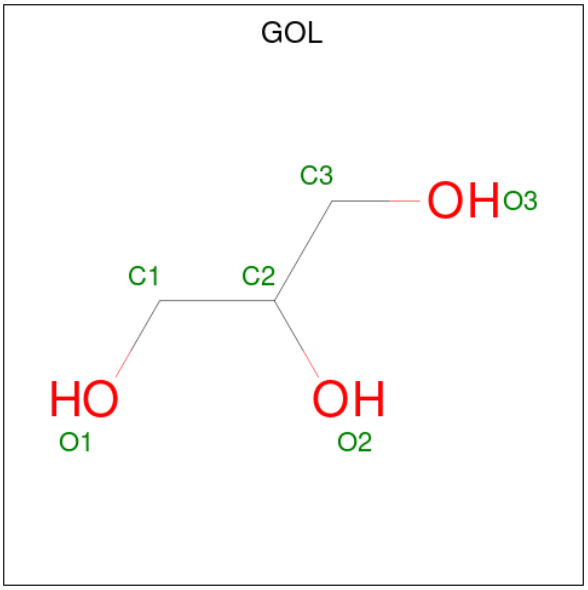
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	1	Total C O 10 7 3	0	0

- Molecule 14 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
14	H	1	52	42	1	8	1	0	0

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
15	H	1	6	3	3		0	0
			Total	C	O			
15	H	1	6	3	3		0	0
			Total	C	O			
15	H	1	6	3	3		0	0

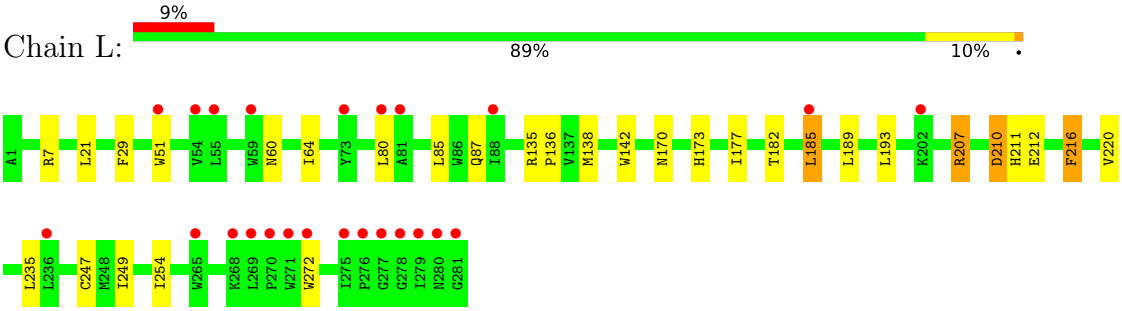
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	L	113	113	113	0	0
			Total	O		
16	M	139	139	139	0	0
			Total	O		
16	H	225	225	225	0	0

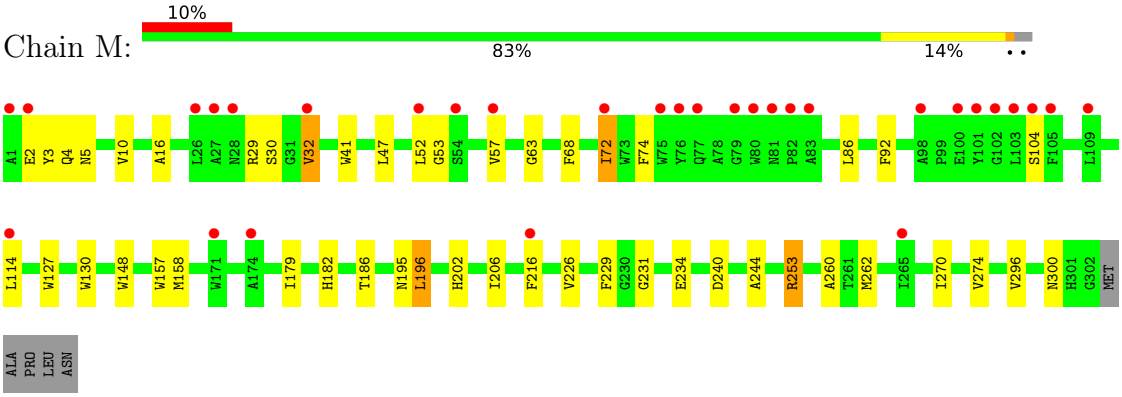
3 Residue-property plots (i)

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.

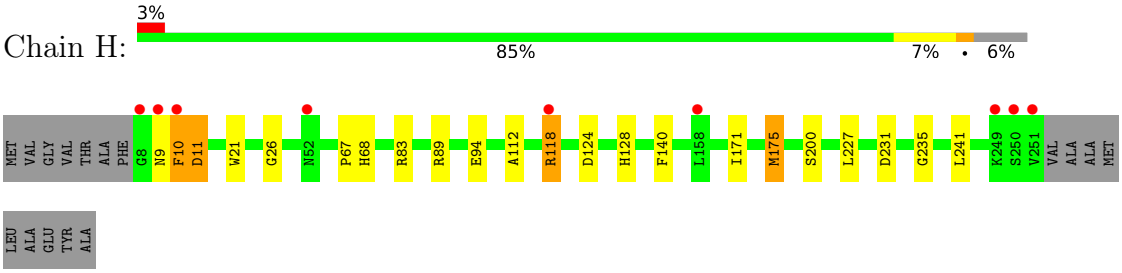
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



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 183.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.03 – 2.55 45.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.03-2.55) 100.0 (45.68-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.69 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.210 0.182 , 0.211	Depositor DCC
R_{free} test set	3362 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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: U10, LDA, HTO, K, PC9, BPH, FE, CDL, GOL, PO4, PC7, BCL

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	0.89	0/2334	0.75	2/3194 (0.1%)
2	M	0.88	1/2590 (0.0%)	0.80	5/3532 (0.1%)
3	H	0.93	0/1986	0.86	3/2697 (0.1%)
All	All	0.90	1/6910 (0.0%)	0.80	10/9423 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	260	ALA	CA-CB	5.14	1.63	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	253[A]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	M	253[B]	ARG	NE-CZ-NH2	-7.34	116.63	120.30
3	H	83	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	L	210	ASP	CB-CG-OD1	5.57	123.32	118.30
1	L	7	ARG	NE-CZ-NH2	5.51	123.05	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2234	0	2193	21	0
2	M	2466	0	2371	35	0
3	H	1891	0	1902	14	0
4	L	5	0	0	1	0
4	M	15	0	0	0	0
5	L	132	0	148	6	0
5	M	132	0	148	19	0
6	L	65	0	75	0	0
6	M	65	0	76	11	0
7	L	48	0	63	12	0
7	M	48	0	63	1	0
8	L	54	0	80	36	0
9	H	64	0	124	7	0
9	L	32	0	62	1	0
9	M	32	0	62	1	0
10	M	1	0	0	0	0
11	M	81	0	106	2	0
12	H	1	0	0	0	0
13	H	10	0	16	1	0
14	H	52	0	84	8	0
15	H	18	0	24	2	0
16	H	225	0	0	2	0
16	L	113	0	0	1	0
16	M	139	0	0	3	0
All	All	7923	0	7597	128	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 128 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)
8:L:802:PC9:H442	8:L:802:PC9:C48	1.58	1.26
8:L:802:PC9:H482	8:L:802:PC9:C44	1.67	1.19
7:L:502:U10:H351	7:L:502:U10:H38	1.28	1.15
8:L:802:PC9:H483	6:M:401:BPH:HED1	1.40	1.03
7:L:502:U10:H153	8:L:802:PC9:H471	1.38	1.02

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	281/281 (100%)	275 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	299 (96%)	10 (3%)	1 (0%)	41	51
3	H	251/260 (96%)	245 (98%)	5 (2%)	1 (0%)	34	46
All	All	842/848 (99%)	819 (97%)	21 (2%)	2 (0%)	47	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	10	PHE
2	M	195	ASN

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	222/220 (101%)	213 (96%)	9 (4%)	30	41
2	M	246/240 (102%)	236 (96%)	10 (4%)	30	41
3	H	207/208 (100%)	201 (97%)	6 (3%)	42	57
All	All	675/668 (101%)	650 (96%)	25 (4%)	34	46

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	216	PHE
3	H	231	ASP
2	M	196	LEU
2	M	274	VAL

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

Mol	Chain	Res	Type
3	H	68	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 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
13	HTO	H	709	-	9,9,9	0.45	0	10,10,10	0.46	0
9	LDA	H	904	-	12,15,15	1.94	1 (8%)	14,17,17	0.55	0
9	LDA	M	907	-	12,15,15	1.90	1 (8%)	14,17,17	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	LDA	M	920	-	12,15,15	1.80	1 (8%)	14,17,17	0.84	1 (7%)
9	LDA	L	902	-	12,15,15	1.87	1 (8%)	14,17,17	0.86	1 (7%)
6	BPH	M	401	-	51,70,70	0.79	2 (3%)	52,101,101	1.82	12 (23%)
5	BCL	L	314	1	64,74,74	1.13	4 (6%)	78,115,115	1.69	16 (20%)
8	PC9	L	802	-	53,53,53	0.82	2 (3%)	59,63,63	1.25	6 (10%)
5	BCL	M	311	2	64,74,74	1.16	4 (6%)	78,115,115	1.61	15 (19%)
7	U10	M	501	-	48,48,63	1.19	6 (12%)	58,61,79	1.71	12 (20%)
9	LDA	H	903	-	12,15,15	1.99	1 (8%)	14,17,17	0.59	0
9	LDA	L	906	-	12,15,15	2.02	1 (8%)	14,17,17	0.65	0
15	GOL	H	706	-	5,5,5	0.52	0	5,5,5	0.92	0
14	PC7	H	801	-	51,51,51	0.89	1 (1%)	57,59,59	1.01	3 (5%)
4	PO4	M	701	-	4,4,4	0.80	0	6,6,6	0.79	0
5	BCL	L	312	1	64,74,74	1.16	5 (7%)	78,115,115	1.60	15 (19%)
9	LDA	H	905	-	12,15,15	2.01	1 (8%)	14,17,17	0.42	0
7	U10	L	502	-	48,48,63	1.00	3 (6%)	58,61,79	1.78	13 (22%)
15	GOL	H	708	-	5,5,5	0.37	0	5,5,5	0.58	0
5	BCL	M	313	2	64,74,74	1.35	5 (7%)	78,115,115	1.92	21 (26%)
15	GOL	H	705	-	5,5,5	0.48	0	5,5,5	0.48	0
11	CDL	M	800	-	80,80,99	1.19	5 (6%)	86,92,111	1.30	8 (9%)
9	LDA	H	901	-	12,15,15	1.75	1 (8%)	14,17,17	0.67	0
6	BPH	L	402	-	51,70,70	0.91	2 (3%)	52,101,101	1.58	9 (17%)
4	PO4	M	704	-	4,4,4	0.84	0	6,6,6	0.74	0
4	PO4	M	702	-	4,4,4	0.67	0	6,6,6	0.73	0
4	PO4	L	703	-	4,4,4	0.75	0	6,6,6	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HTO	H	709	-	-	2/10/10/10	-
9	LDA	H	904	-	-	5/13/13/13	-
9	LDA	M	907	-	-	10/13/13/13	-
9	LDA	M	920	-	-	7/13/13/13	-
9	LDA	L	902	-	-	4/13/13/13	-
6	BPH	M	401	-	-	12/37/105/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	L	314	1	-	3/37/137/137	-
8	PC9	L	802	-	-	24/60/60/60	-
5	BCL	M	311	2	-	11/37/137/137	-
7	U10	M	501	-	-	4/45/69/87	0/1/1/1
9	LDA	H	903	-	-	4/13/13/13	-
9	LDA	L	906	-	-	5/13/13/13	-
15	GOL	H	706	-	-	2/4/4/4	-
14	PC7	H	801	-	-	30/55/55/55	-
9	LDA	H	905	-	-	9/13/13/13	-
7	U10	L	502	-	-	12/45/69/87	0/1/1/1
15	GOL	H	708	-	-	2/4/4/4	-
5	BCL	M	313	2	-	3/37/137/137	-
15	GOL	H	705	-	-	3/4/4/4	-
11	CDL	M	800	-	-	33/91/91/110	-
9	LDA	H	901	-	-	6/13/13/13	-
6	BPH	L	402	-	-	5/37/105/105	0/5/6/6
5	BCL	L	312	1	-	6/37/137/137	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	906	LDA	O1-N1	-6.86	1.26	1.42
9	H	905	LDA	O1-N1	-6.85	1.26	1.42
9	H	903	LDA	O1-N1	-6.83	1.26	1.42
9	H	904	LDA	O1-N1	-6.60	1.26	1.42
9	M	907	LDA	O1-N1	-6.46	1.27	1.42

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	313	BCL	CMB-C2B-C1B	-6.45	118.55	128.46
11	M	800	CDL	OA6-CA5-C11	5.84	124.10	111.50
6	L	402	BPH	O2D-CGD-CBD	5.68	118.19	111.00
5	M	313	BCL	C1C-NC-C4C	5.57	109.21	106.71
6	M	401	BPH	O2D-CGD-CBD	5.54	118.02	111.00

There are no chirality outliers.

5 of 202 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	311	BCL	C4-C3-C5-C6
6	M	401	BPH	C2C-C3C-CAC-CBC
6	M	401	BPH	C11-C12-C13-C14
8	L	802	PC9	C1-O3P-P-O4P
9	L	906	LDA	N1-C1-C2-C3

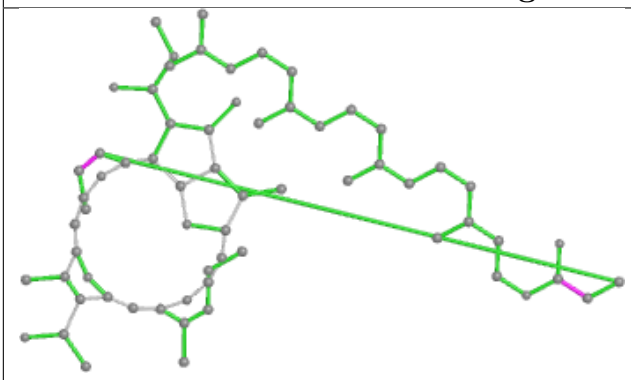
There are no ring outliers.

18 monomers are involved in 80 short contacts:

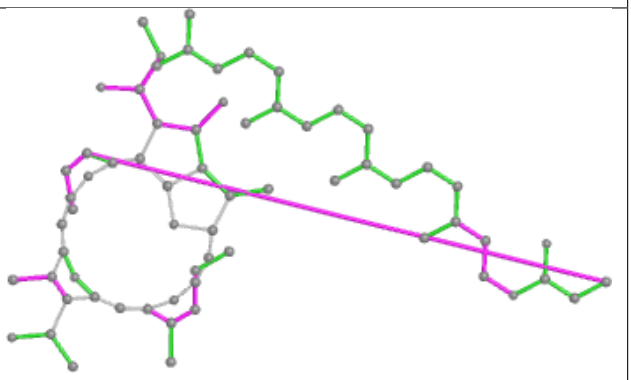
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	H	709	HTO	1	0
9	H	904	LDA	2	0
9	M	907	LDA	1	0
6	M	401	BPH	11	0
5	L	314	BCL	3	0
8	L	802	PC9	36	0
5	M	311	BCL	11	0
7	M	501	U10	1	0
9	L	906	LDA	1	0
14	H	801	PC7	8	0
5	L	312	BCL	3	0
9	H	905	LDA	2	0
7	L	502	U10	12	0
15	H	708	GOL	2	0
5	M	313	BCL	10	0
11	M	800	CDL	2	0
9	H	901	LDA	3	0
4	L	703	PO4	1	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.

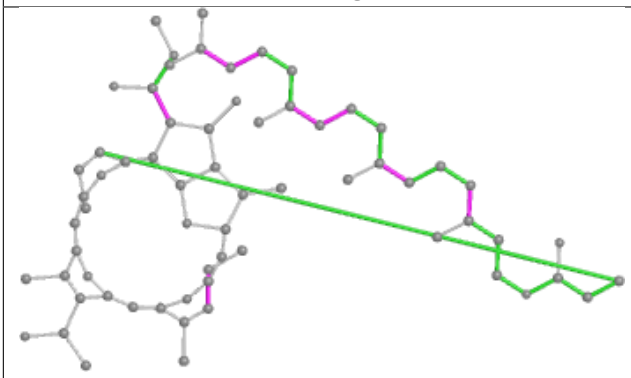
Ligand BPH M 401



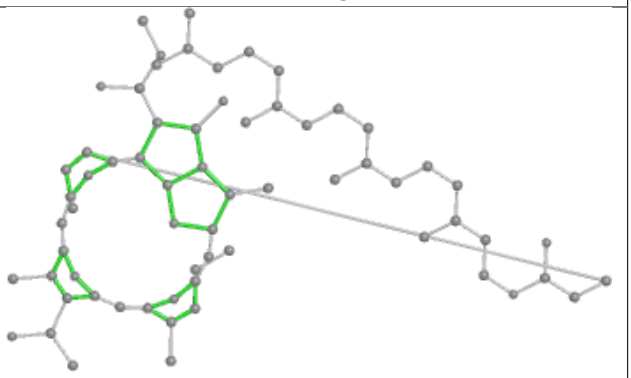
Bond lengths



Bond angles

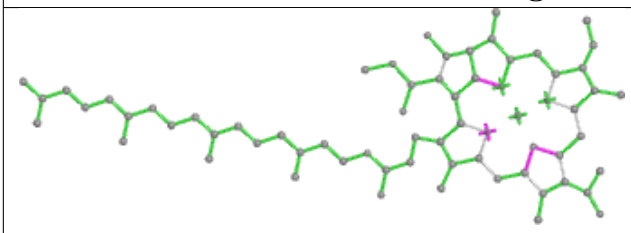


Torsions



Rings

Ligand BCL L 314



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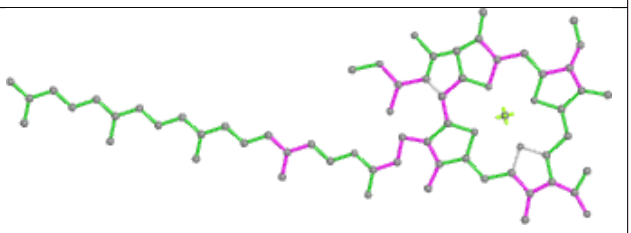
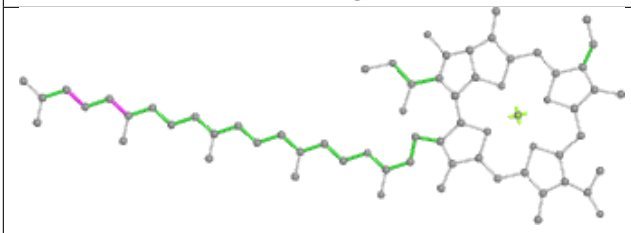
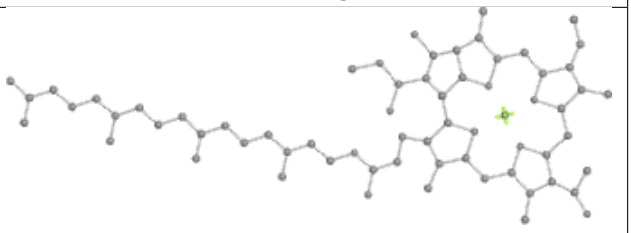


Bond angles

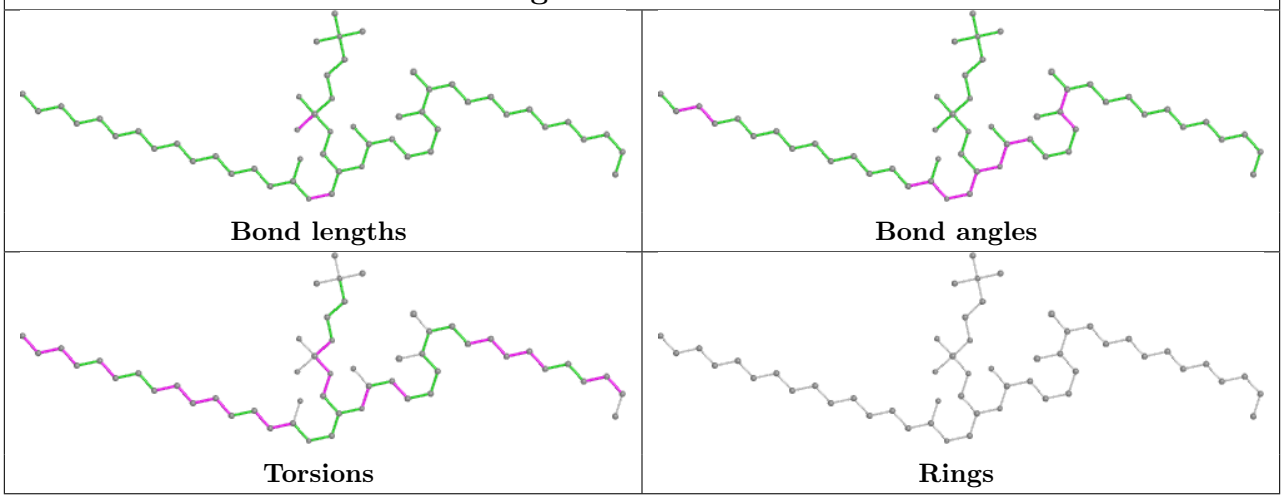


Torsions

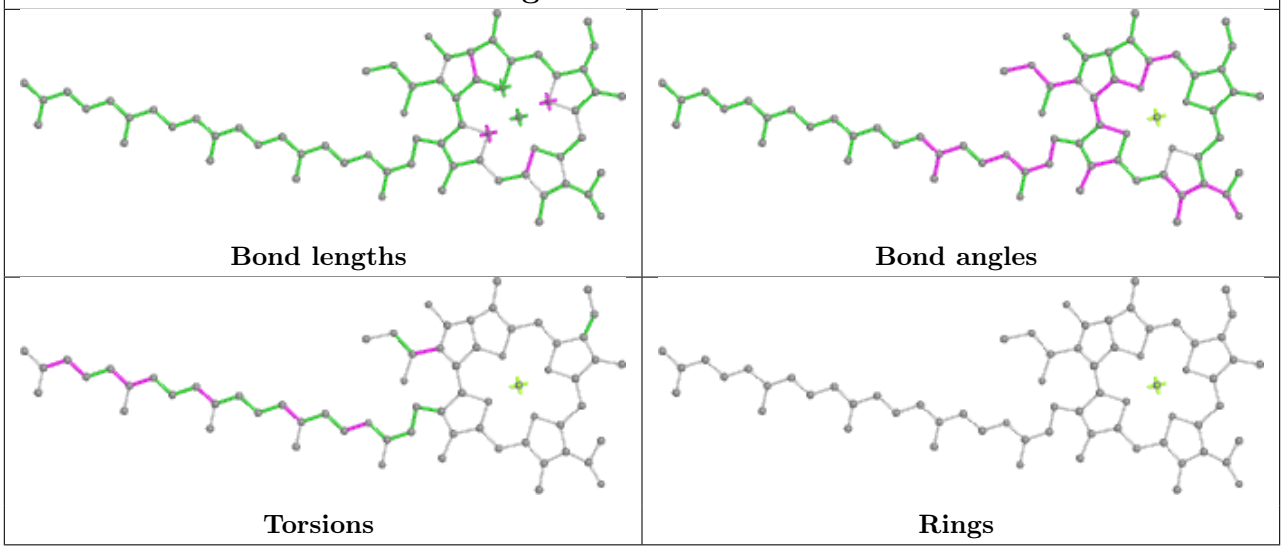


Rings

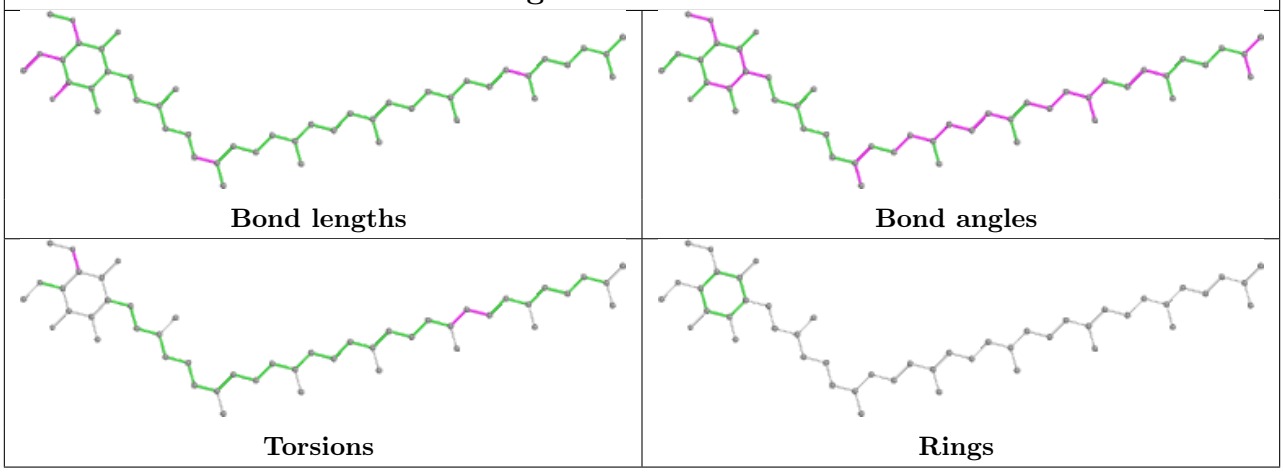
Ligand PC9 L 802



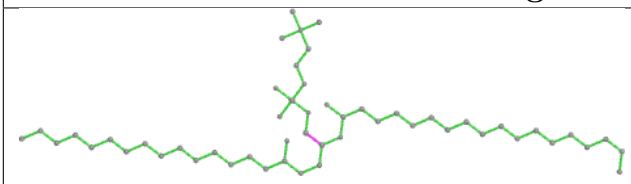
Ligand BCL M 311



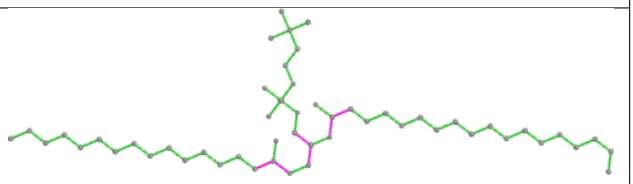
Ligand U10 M 501



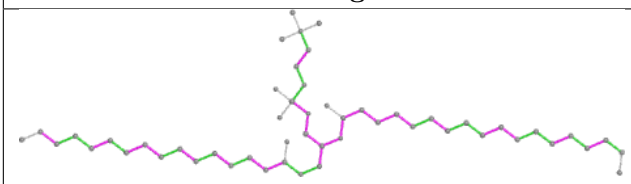
Ligand PC7 H 801



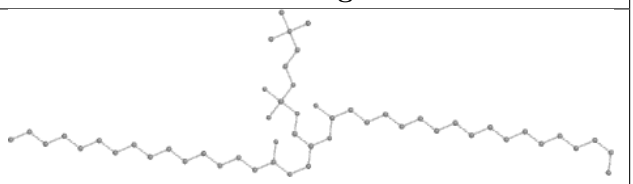
Bond lengths



Bond angles

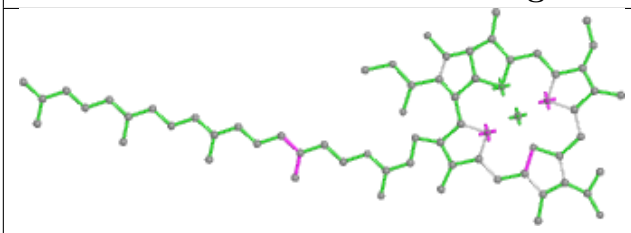


Torsions

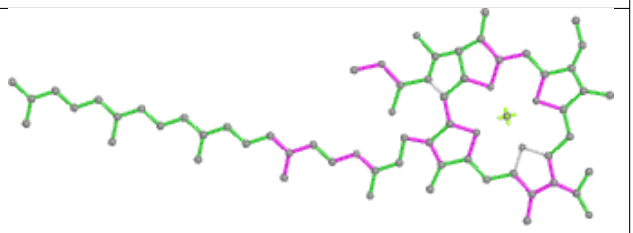


Rings

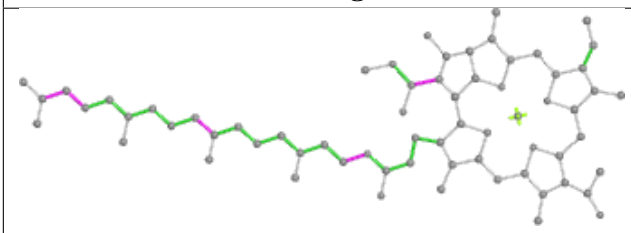
Ligand BCL L 312



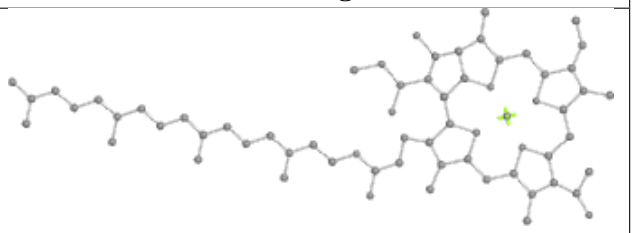
Bond lengths



Bond angles

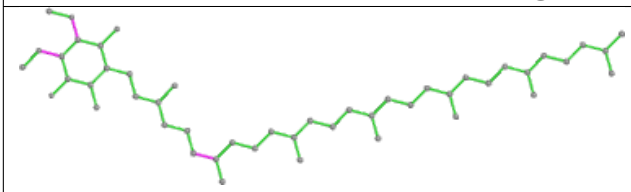


Torsions

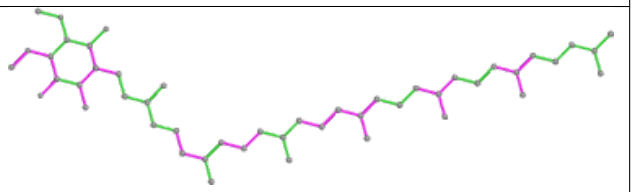


Rings

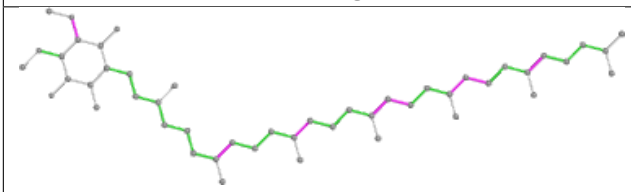
Ligand U10 L 502



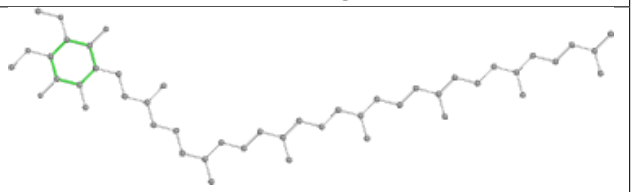
Bond lengths



Bond angles

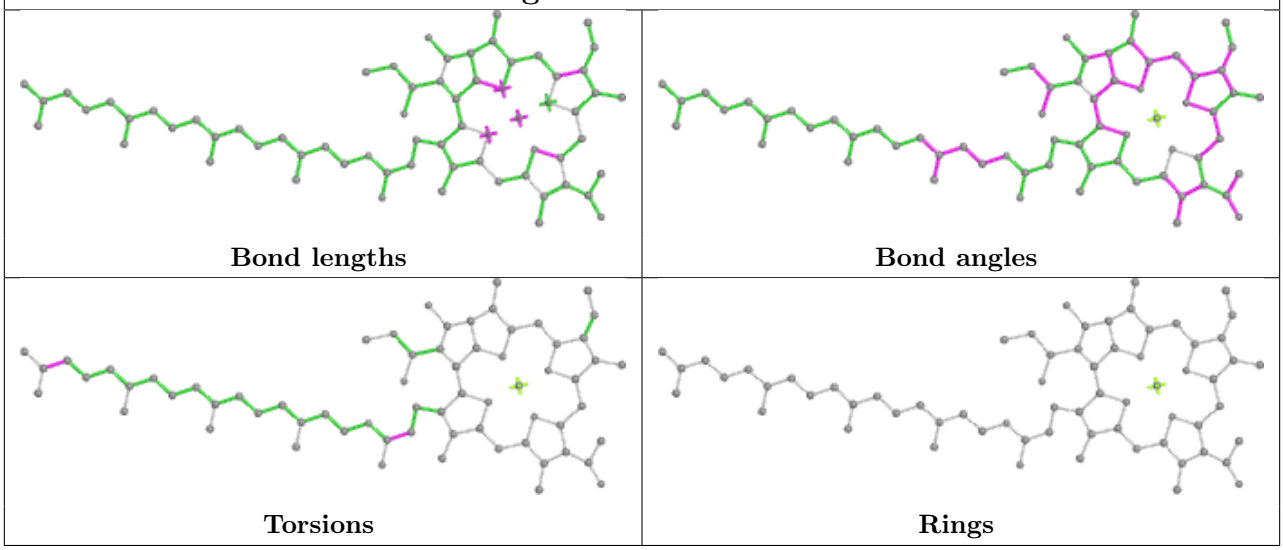


Torsions

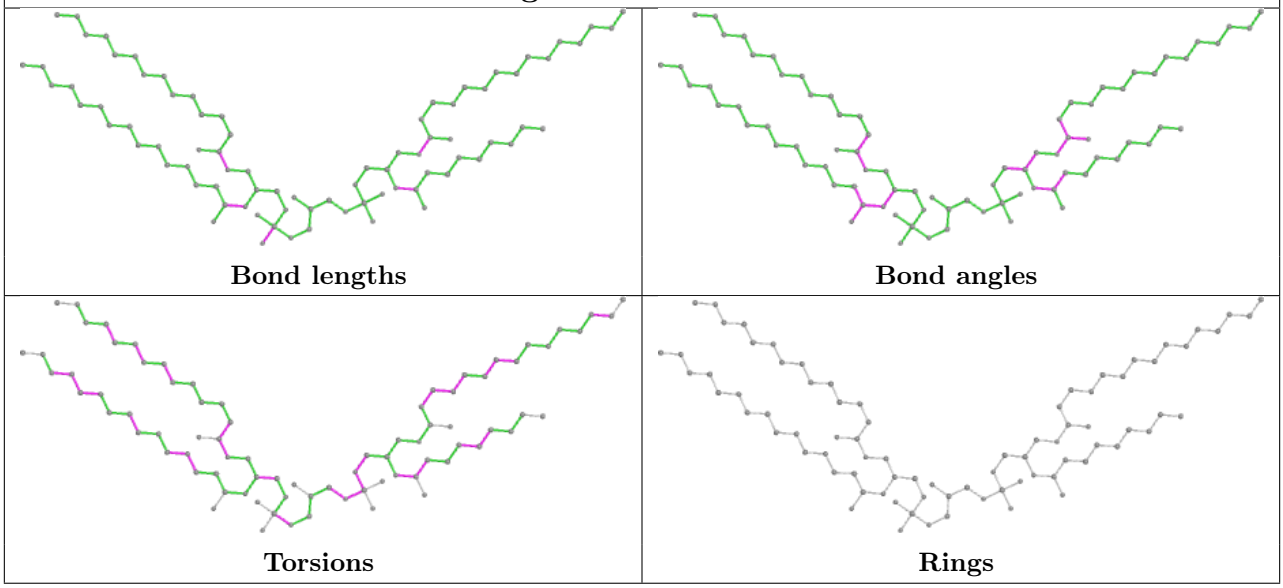


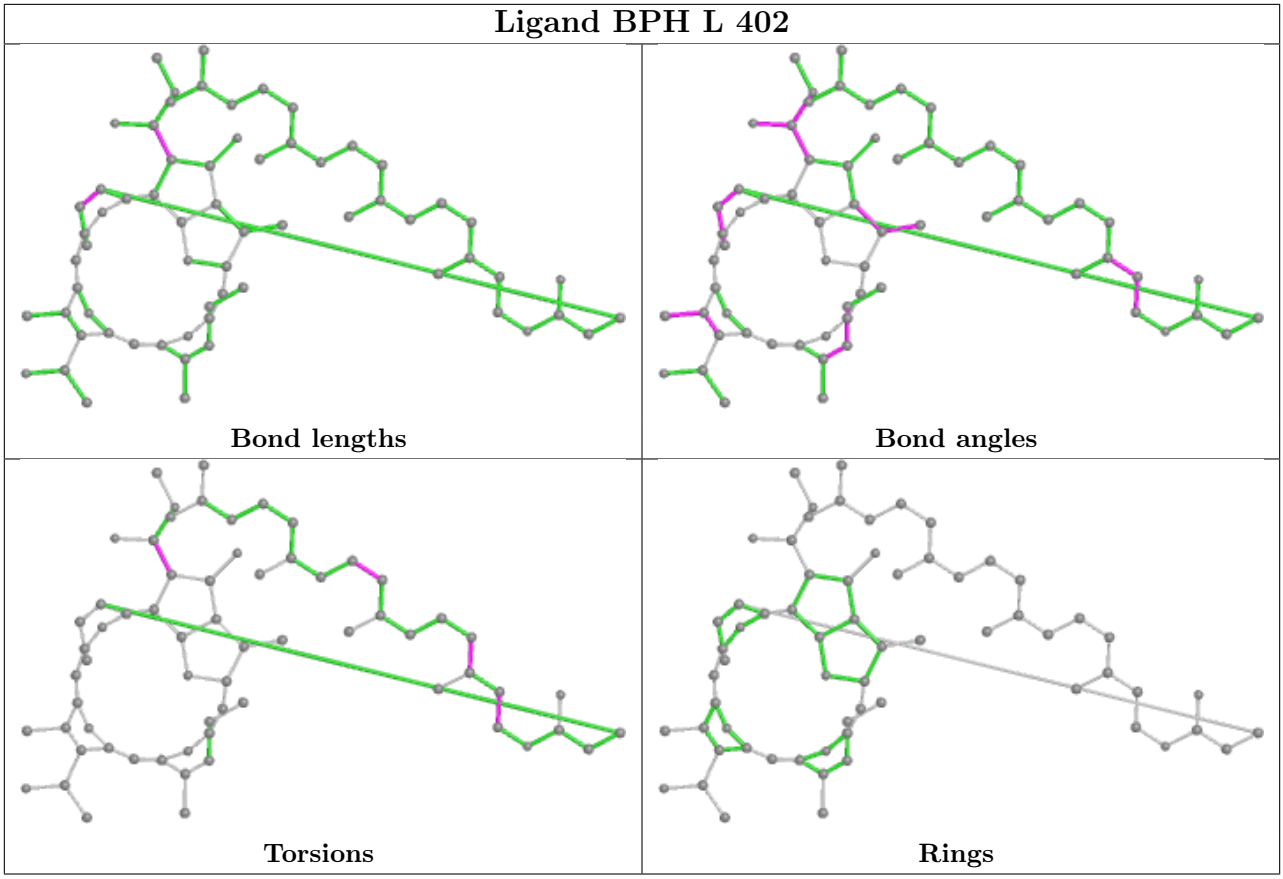
Rings

Ligand BCL M 313



Ligand CDL M 800





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%)	0.16	24 (8%) 10 12	38, 51, 61, 72	0
2	M	302/307 (98%)	0.36	31 (10%) 6 8	40, 50, 60, 76	0
3	H	244/260 (93%)	0.03	9 (3%) 41 48	42, 49, 60, 87	1 (0%)
All	All	827/848 (97%)	0.19	64 (7%) 13 17	38, 50, 61, 87	1 (0%)

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	9	ASN	8.8
3	H	8	GLY	8.5
3	H	251	VAL	7.7
3	H	10	PHE	7.2
3	H	250	SER	6.4

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)

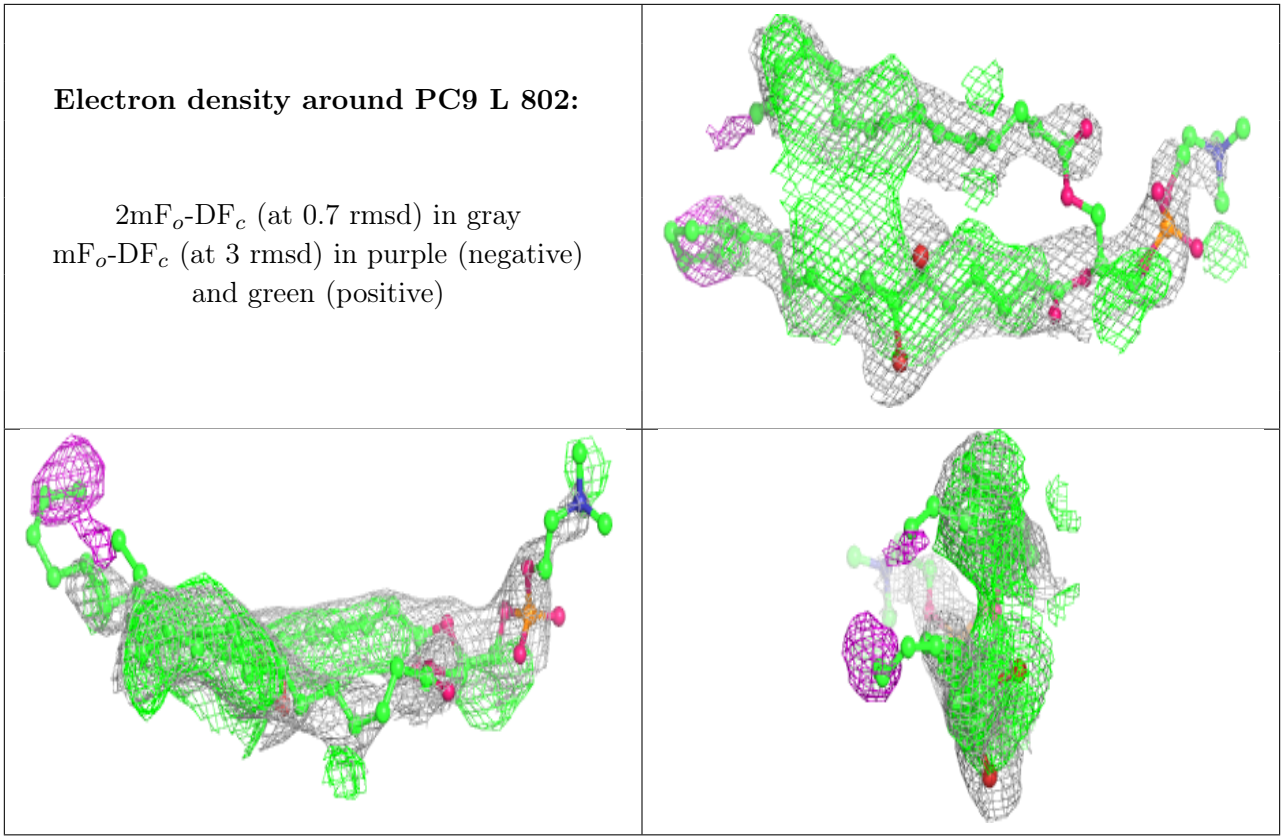
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	LDA	H	905	16/16	0.20	0.75	61,69,78,78	16
9	LDA	H	904	16/16	0.30	0.61	65,68,72,72	16
9	LDA	H	903	16/16	0.44	0.48	63,65,74,75	16
8	PC9	L	802	54/54	0.55	0.62	57,66,75,79	54
9	LDA	M	920	16/16	0.56	0.48	59,74,88,88	16
14	PC7	H	801	52/52	0.60	0.81	26,68,76,78	52
9	LDA	L	902	16/16	0.66	0.50	68,73,77,80	16
13	HTO	H	709	10/10	0.67	0.26	50,56,56,58	10
9	LDA	L	906	16/16	0.68	0.35	54,56,59,60	16
11	CDL	M	800	81/100	0.68	0.40	43,71,83,85	81
9	LDA	M	907	16/16	0.71	0.42	56,61,66,67	16
15	GOL	H	708	6/6	0.77	0.89	46,46,47,49	6
7	U10	L	502	48/63	0.78	0.65	34,48,60,62	48
15	GOL	H	705	6/6	0.84	0.30	58,69,70,72	0
4	PO4	M	702	5/5	0.84	0.22	66,67,68,68	5
4	PO4	M	704	5/5	0.85	0.34	76,76,77,78	5
15	GOL	H	706	6/6	0.87	0.29	74,76,77,77	0
9	LDA	H	901	16/16	0.89	0.28	60,65,69,71	0
7	U10	M	501	48/63	0.89	0.22	43,54,77,80	0
4	PO4	L	703	5/5	0.90	0.39	70,72,73,75	5
6	BPH	M	401	65/65	0.91	0.18	45,51,92,93	0
5	BCL	L	314	66/66	0.94	0.17	38,47,62,66	0
5	BCL	L	312	66/66	0.95	0.15	41,46,58,61	0
5	BCL	M	311	66/66	0.95	0.17	42,51,96,97	0
6	BPH	L	402	65/65	0.95	0.15	35,47,52,53	0
5	BCL	M	313	66/66	0.97	0.15	38,46,70,79	0
4	PO4	M	701	5/5	0.97	0.31	57,59,62,63	0
12	K	H	700	1/1	0.98	0.07	54,54,54,54	0
10	FE	M	500	1/1	1.00	0.16	49,49,49,49	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.

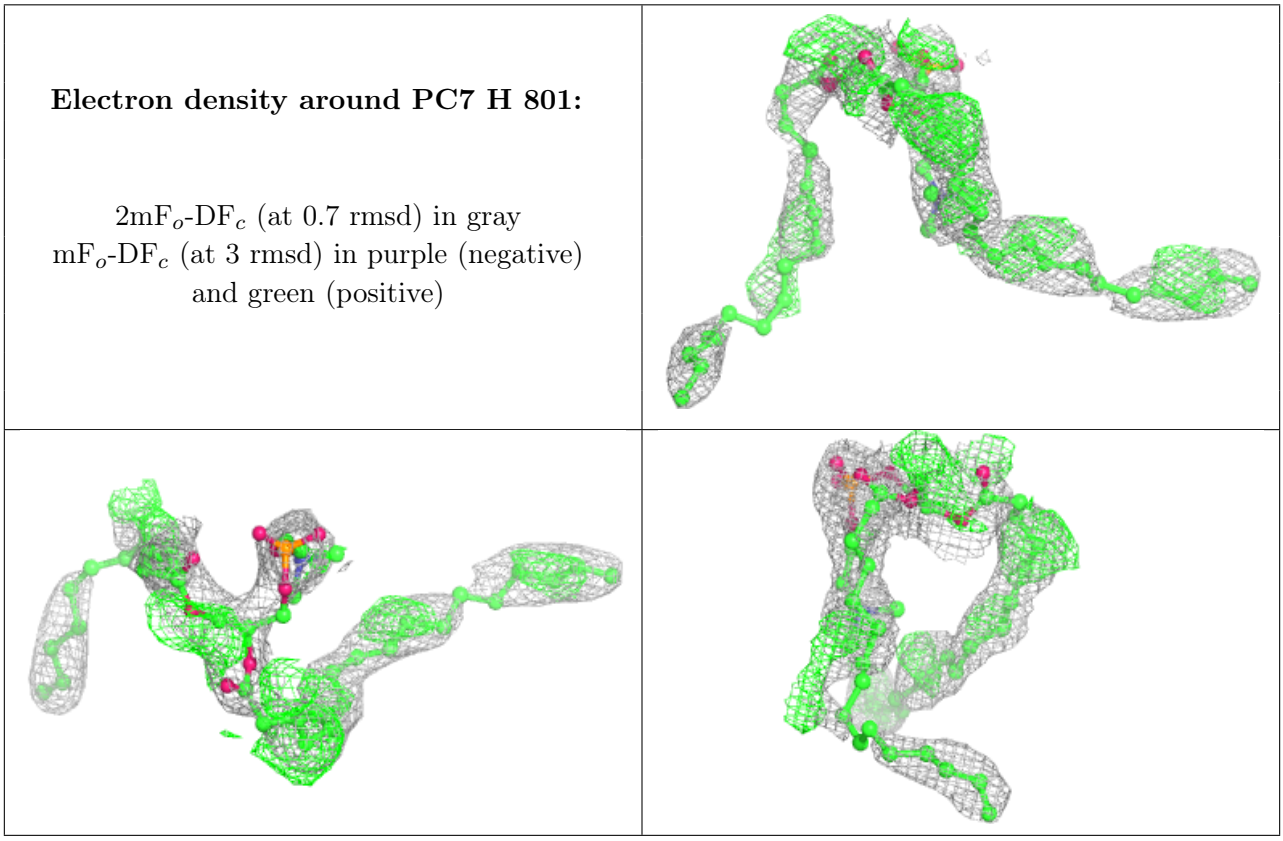
Electron density around PC9 L 802:

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



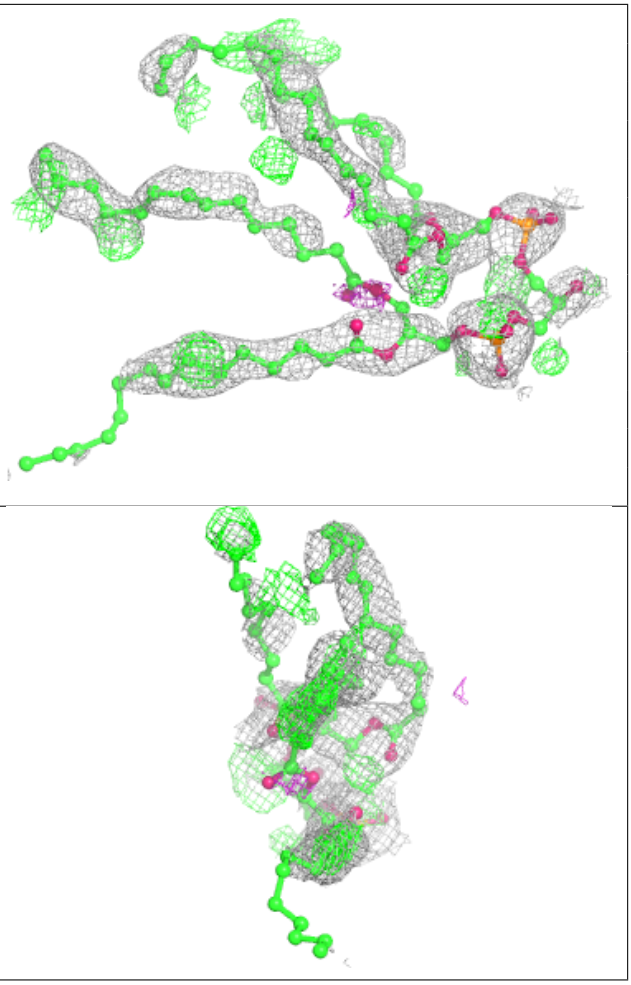
Electron density around PC7 H 801:

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



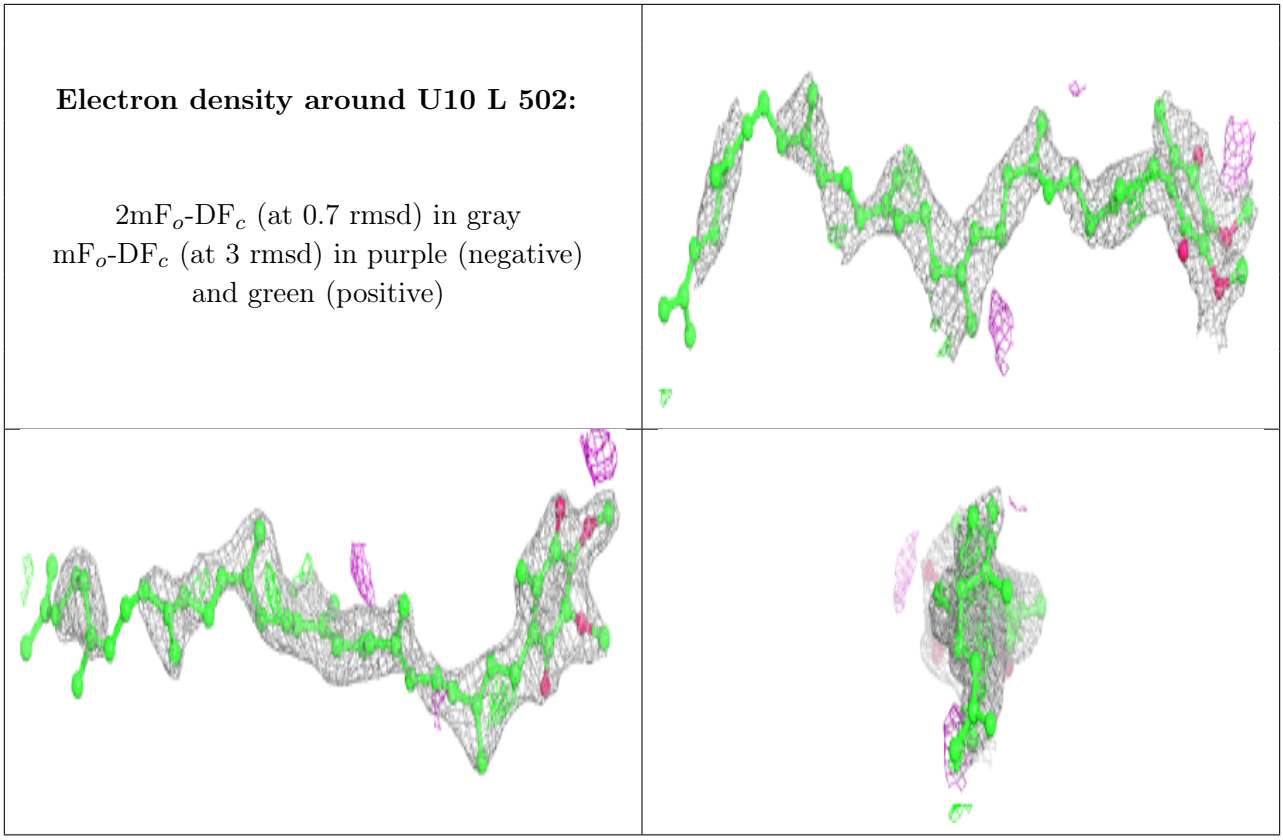
Electron density around CDL M 800:

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



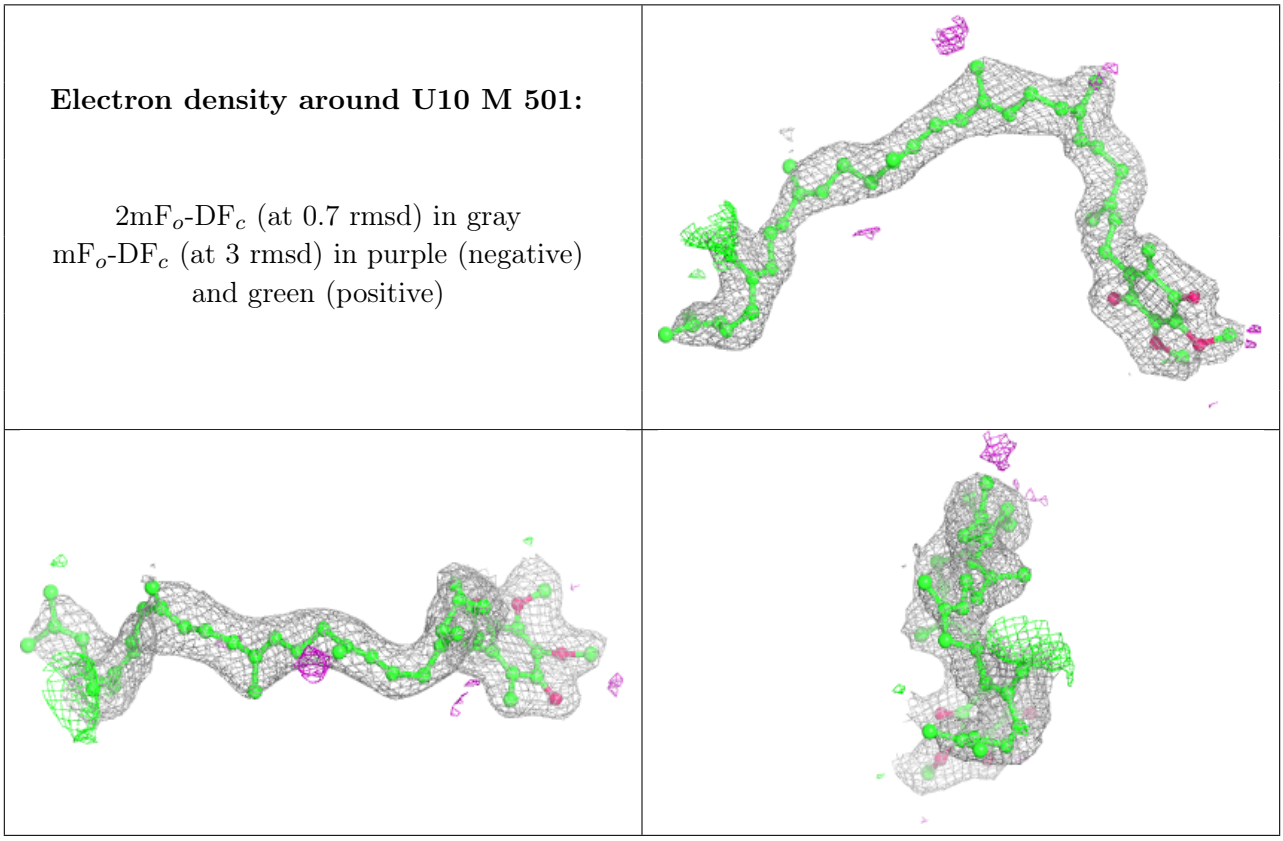
Electron density around U10 L 502:

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



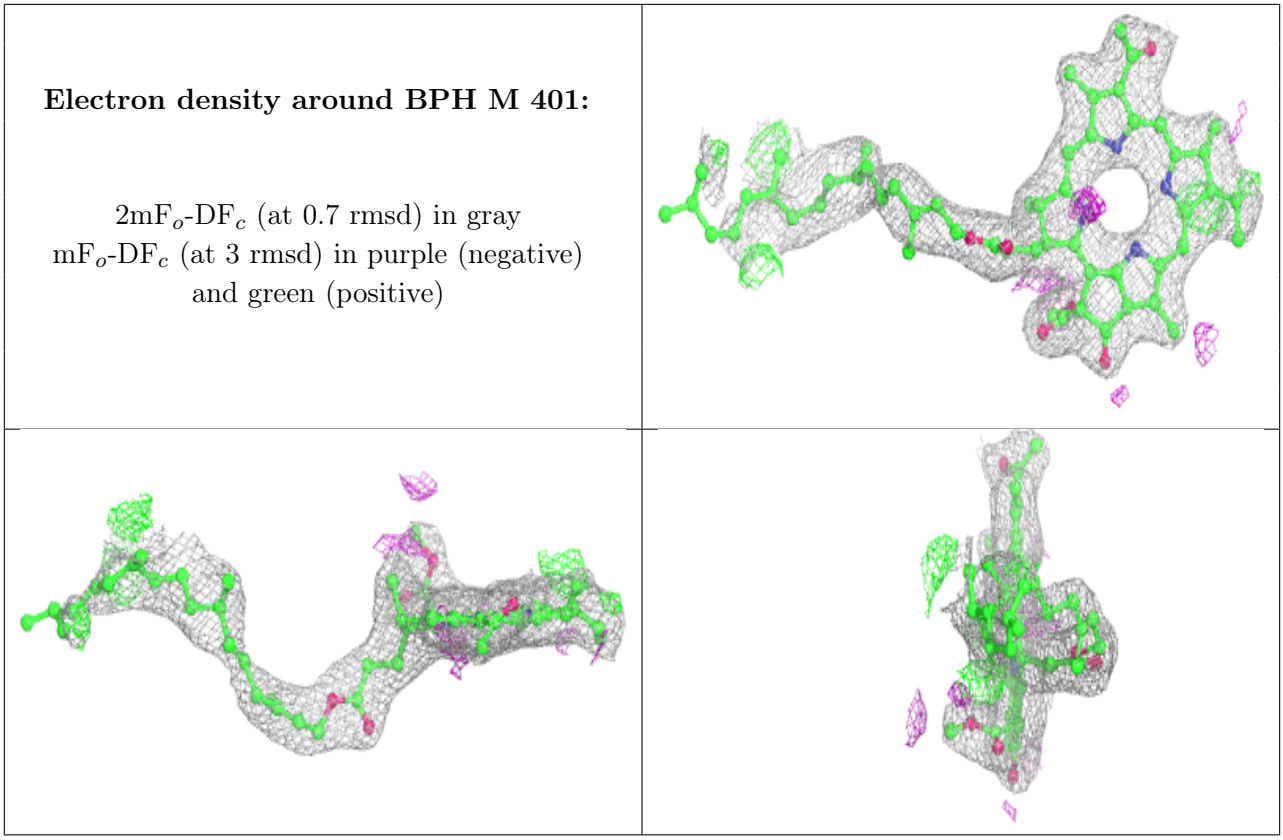
Electron density around U10 M 501:

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



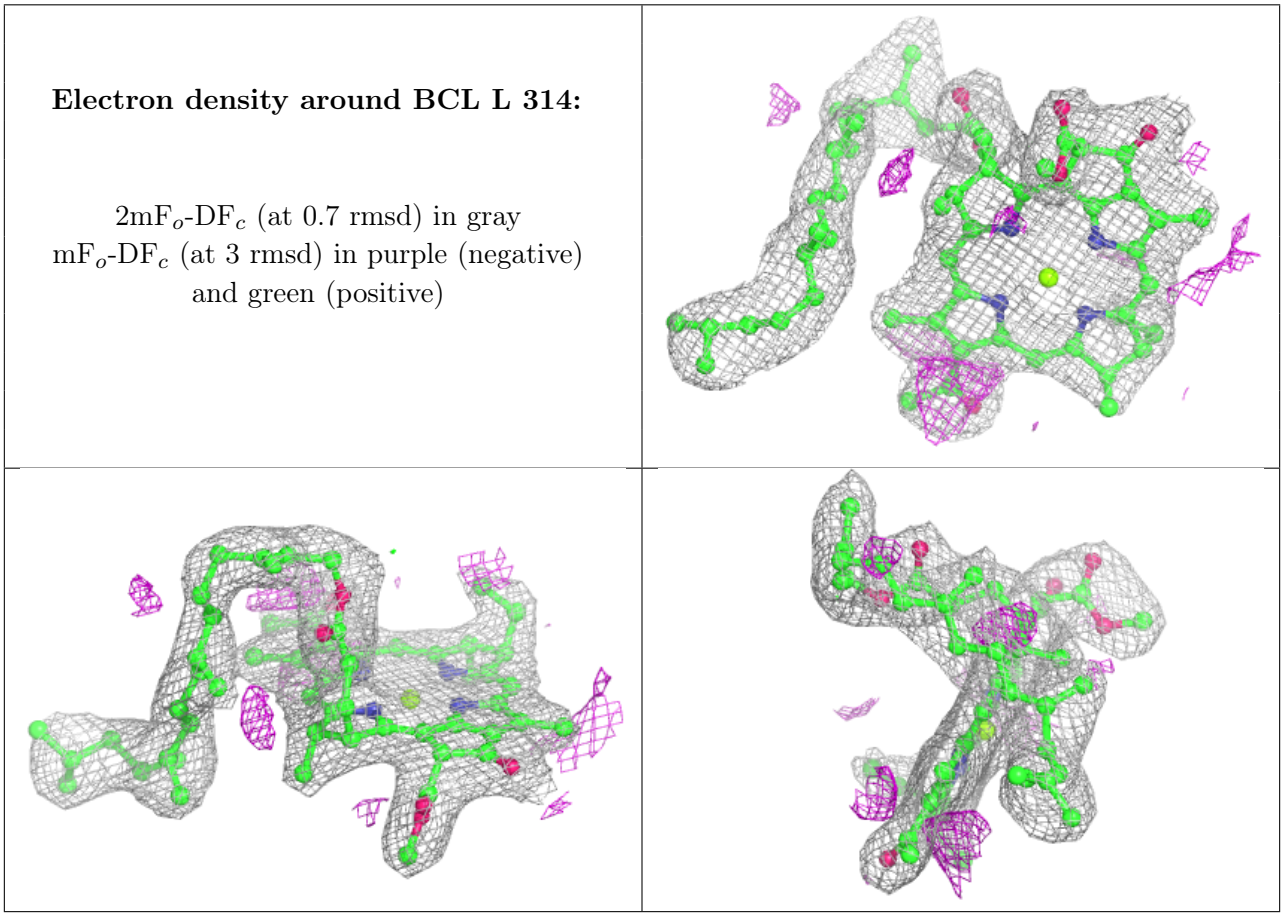
Electron density around BPH M 401:

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



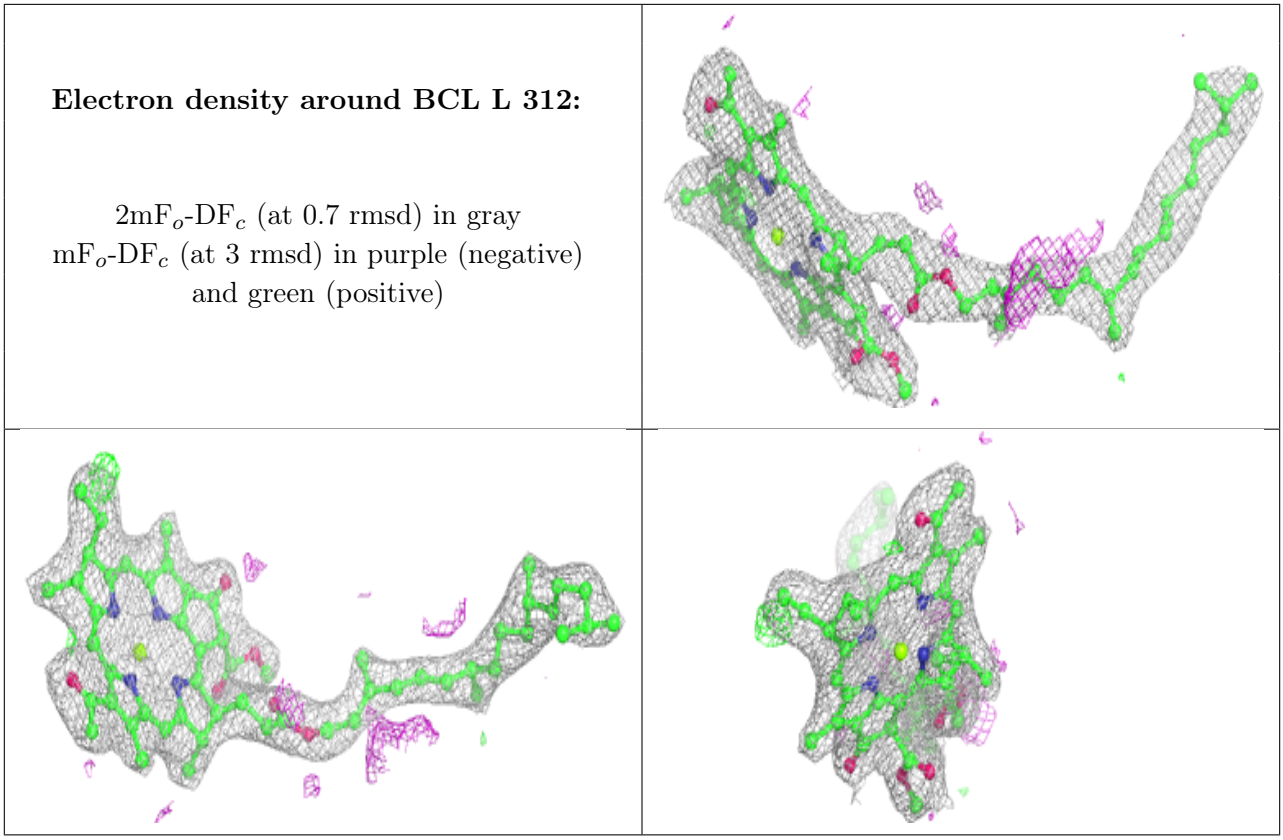
Electron density around BCL L 314:

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



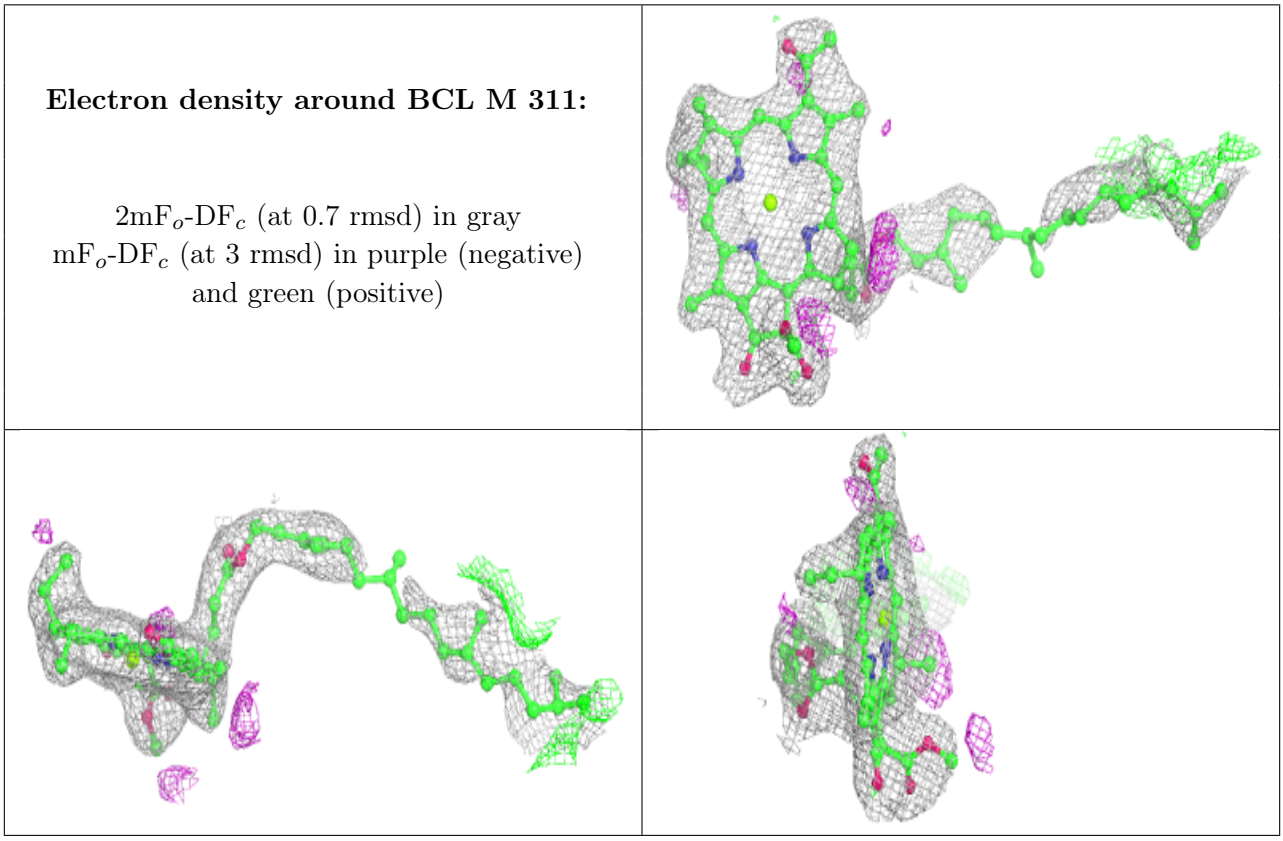
Electron density around BCL L 312:

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



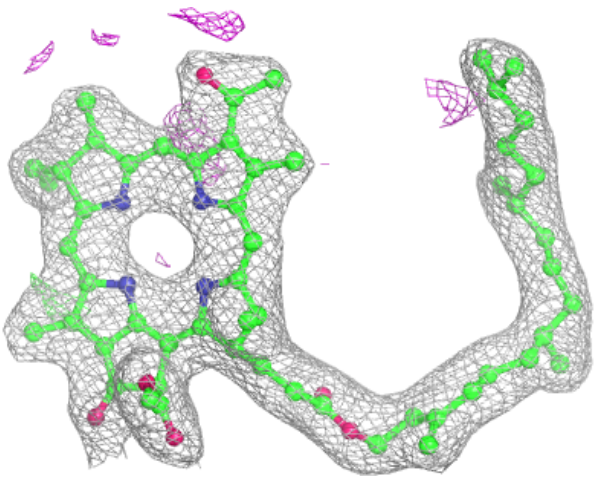
Electron density around BCL M 311:

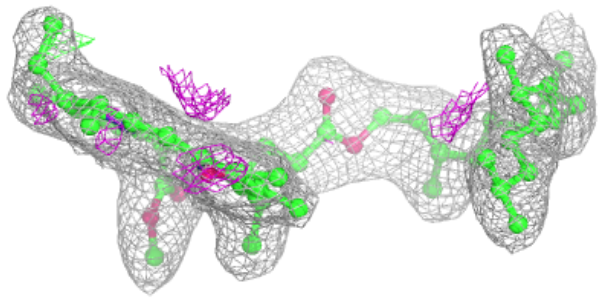
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

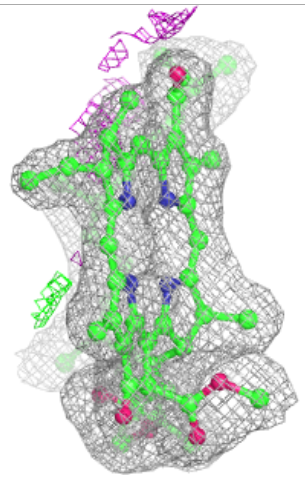


Electron density around BPH L 402:

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

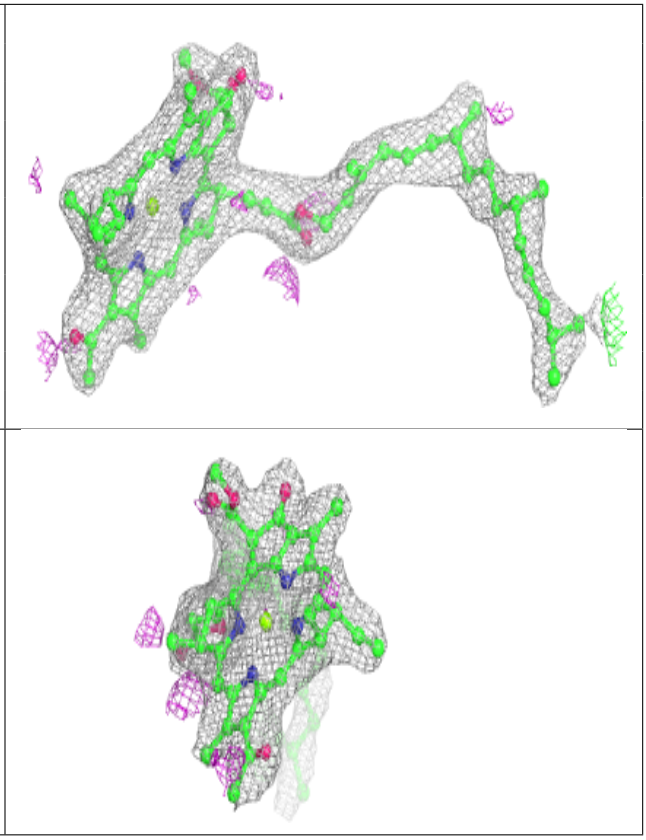






Electron density around BCL M 313:

$2mF_o$-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.