wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2023 – 06:02 pm GMT

PDB ID	:	8C3F
Title	:	Double mutant I(L177)H/F(M197)H structure of Photosynthetic Reaction Center From Cereibacter sphaeroides strain RV
Authors	:	Gabdulkhakov, A.G.; Selikhanov, G.K.; Fufina, T.Y.; Vasilieva, L.G.
Deposited on	:	2022-12-23
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

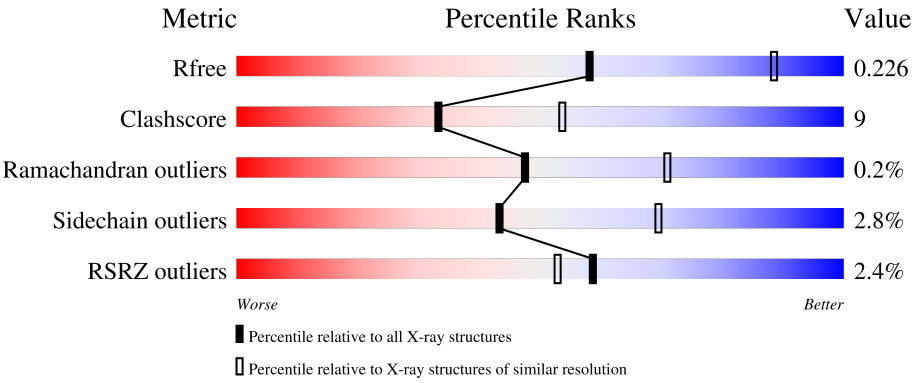
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	2% 80% 18%
2	M	303	2% 86% 12%
3	H	241	3% 88% 10%

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
12	LDA	M	417	-	-	-	X
12	LDA	M	418	-	-	-	X
6	HTO	M	402	-	-	X	-

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 7413 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
			2234	1508	357	361	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	177	HIS	ILE	engineered mutation	UNP P0C0Y8
L	178	THR	SER	engineered mutation	UNP P0C0Y8

- 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	1	0
			2416	1610	397	398	11			

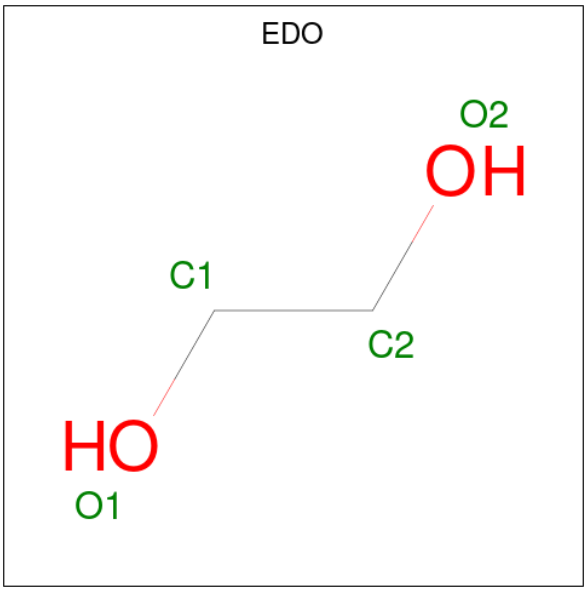
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	engineered mutation	UNP P0C0Y9
M	197	HIS	PHE	engineered mutation	UNP P0C0Y9

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

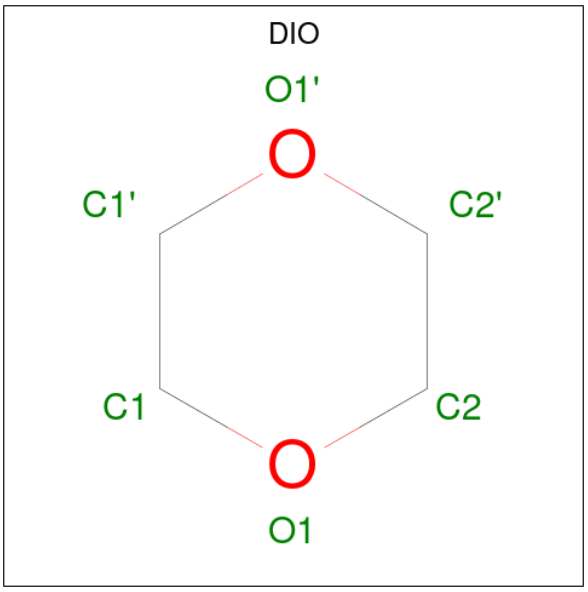
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	239	Total	C	N	O	S	0	0	0
			1823	1166	313	335	9			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



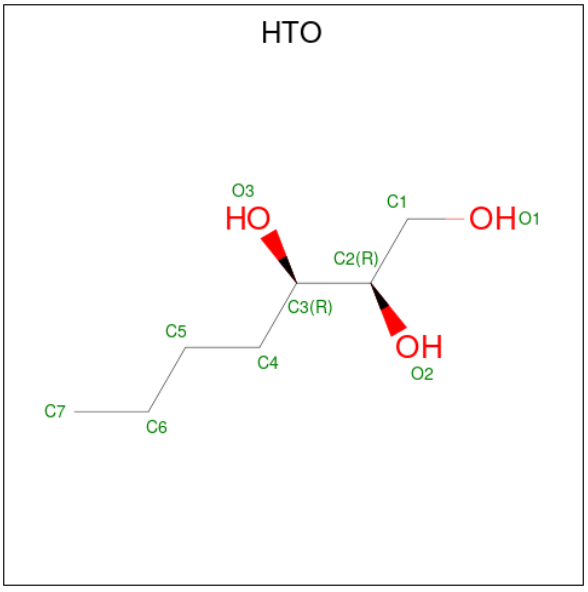
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	M	1	Total C O 4 2 2	0	0
4	M	1	Total C O 4 2 2	0	0
4	M	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total C O 6 4 2	0	0

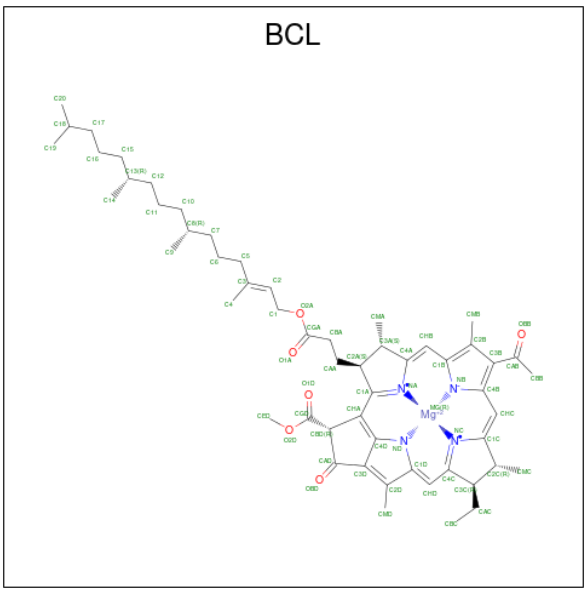
- Molecule 6 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 10 7 3	0	0
6	M	1	Total C O 10 7 3	0	0

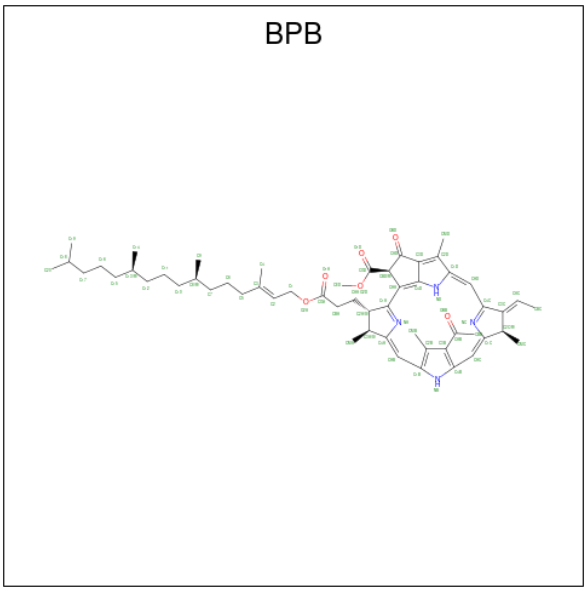
- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$)

(labeled as "Ligand of Interest" by depositor).



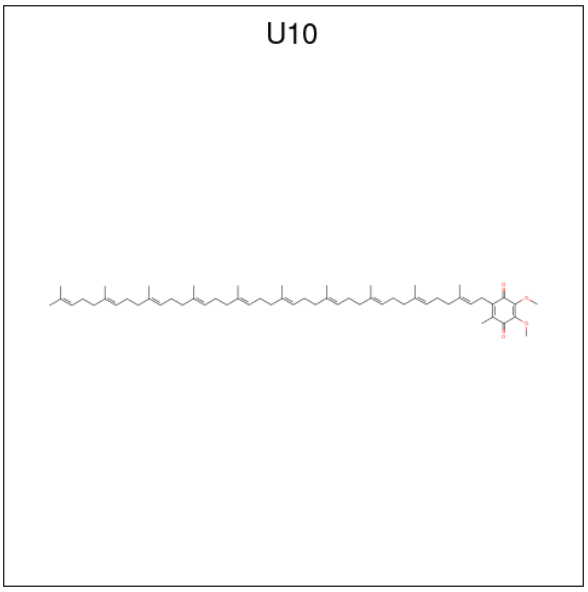
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



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

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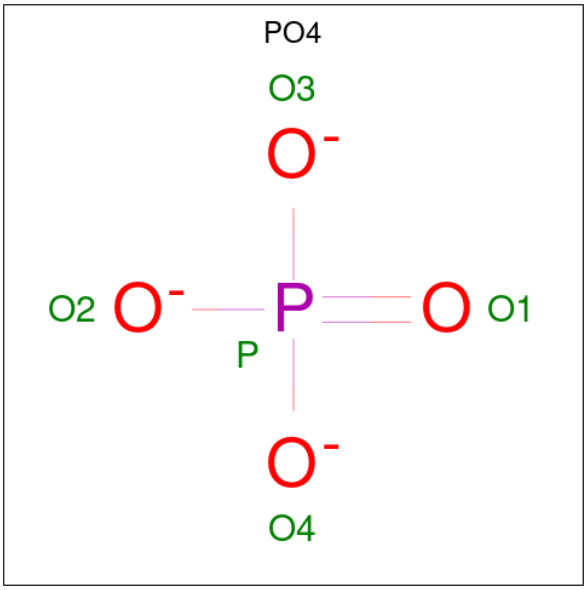
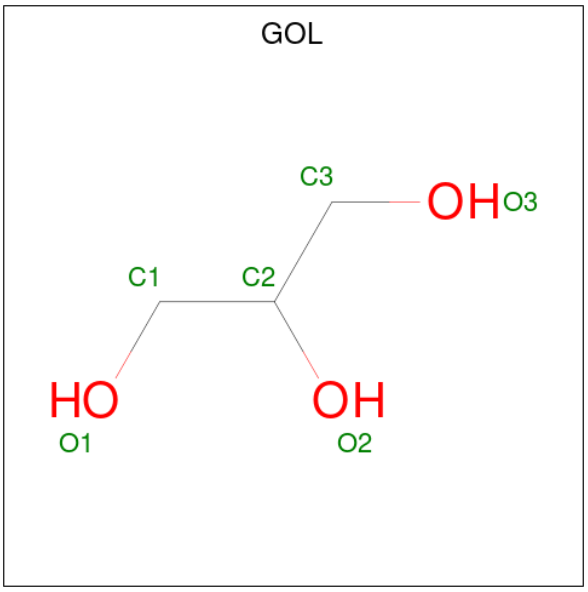
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total C O 48 44 4	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



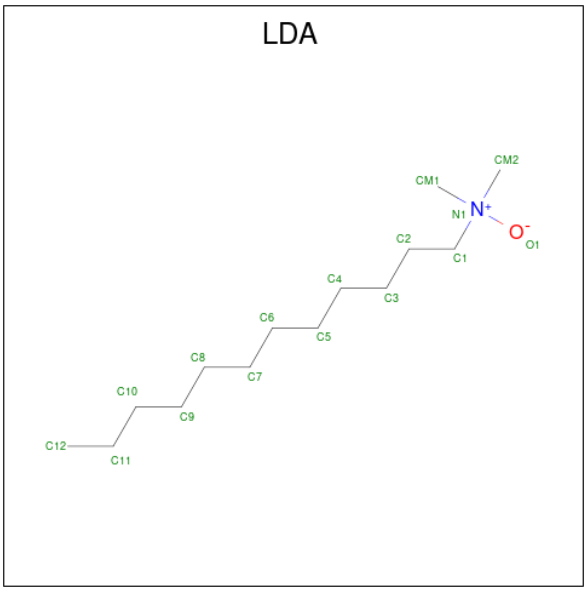
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total O P 5 4 1	0	0
10	L	1	Total O P 5 4 1	0	0
10	M	1	Total O P 5 4 1	0	0

- Molecule 11 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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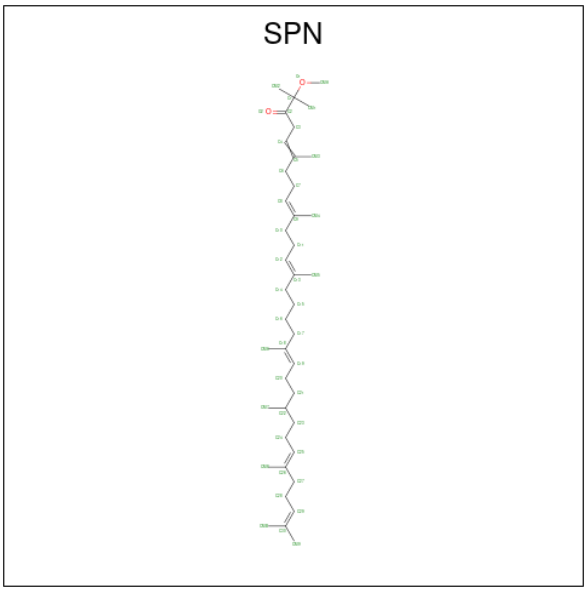
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 14 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



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

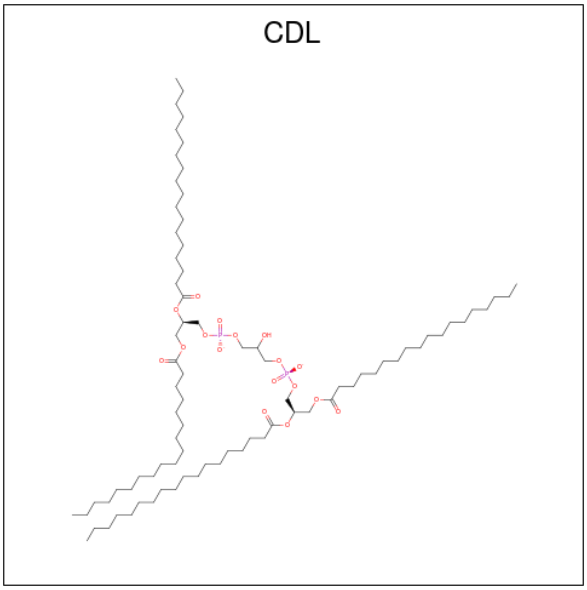
- Molecule 15 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	M	1	Total K 1 1	0	0
15	H	1	Total K 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

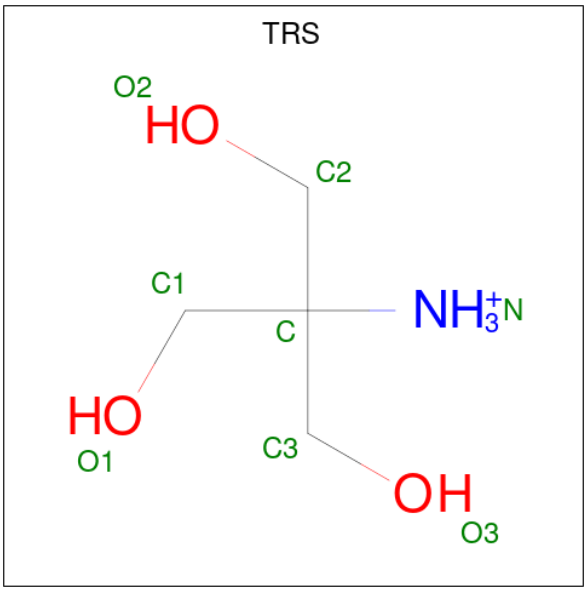
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total Cl 1 1	0	0

- Molecule 17 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 18 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	H	1	Total C N O 8 4 1 3	0	0

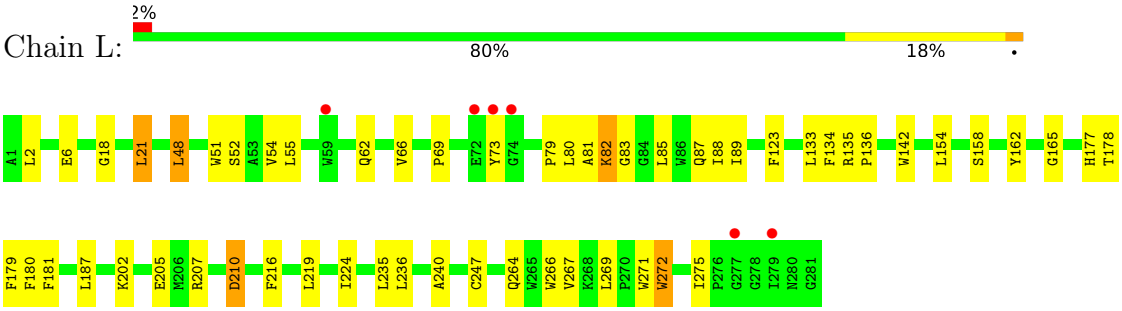
- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	L	32	Total O 32 32	0	0
19	M	39	Total O 39 39	0	0
19	H	40	Total O 40 40	0	0

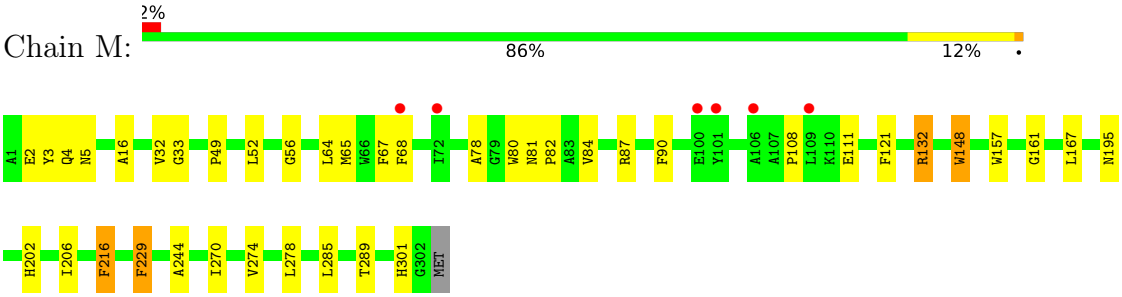
3 Residue-property plots (i)

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.

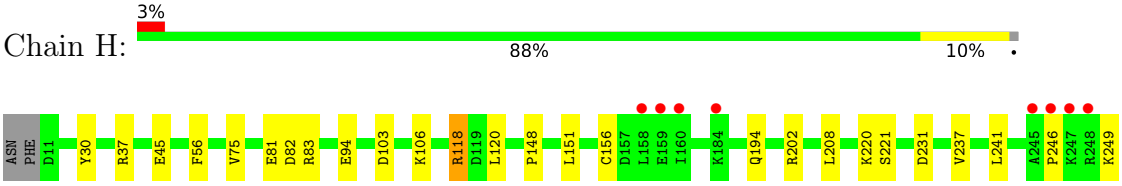
• Molecule 1: Reaction center protein L chain



• 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	139.35Å 139.35Å 184.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.12 – 2.60 46.12 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.12-2.60) 99.8 (46.12-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.220 0.197 , 0.226	Depositor DCC
R_{free} test set	3441 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.5	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	7413	wwPDB-VP
Average B, all atoms (Å^2)	64.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, PO4, HTO, FE, U10, EDO, CDL, CL, GOL, SPN, K, DIO, BPB, TRS, LDA

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	0.42	0/2323	0.59	2/3181 (0.1%)
2	M	0.40	0/2508	0.54	0/3424
3	H	0.43	0/1871	0.61	0/2545
All	All	0.42	0/6702	0.58	2/9150 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	48	LEU	CA-CB-CG	-7.74	97.49	115.30
1	L	235	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2234	0	2185	53	0
2	M	2416	0	2329	33	0
3	H	1823	0	1831	20	0
4	H	8	0	12	1	0
4	L	8	0	12	1	0
4	M	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	6	0	8	2	0
6	L	10	0	16	0	0
6	M	10	0	16	6	0
7	L	132	0	148	11	0
7	M	132	0	148	6	0
8	L	65	0	74	1	0
8	M	65	0	74	4	0
9	L	48	0	63	9	0
9	M	48	0	63	2	0
10	L	10	0	0	0	0
10	M	5	0	0	0	0
11	L	6	0	8	0	0
12	H	16	0	31	3	0
12	L	32	0	62	1	0
12	M	80	0	155	7	0
13	M	1	0	0	0	0
14	M	43	0	70	7	0
15	H	1	0	0	0	0
15	M	1	0	0	0	0
16	M	1	0	0	0	0
17	M	81	0	106	8	0
18	H	8	0	12	4	0
19	H	40	0	0	2	0
19	L	32	0	0	1	0
19	M	39	0	0	2	0
All	All	7413	0	7441	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 127 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:177:HIS:ND1	7:L:305:BCL:CMB	2.06	1.19
1:L:177:HIS:ND1	7:L:305:BCL:HMB3	1.54	1.18
1:L:177:HIS:ND1	7:L:305:BCL:HMB1	1.85	0.92
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.53	0.90
1:L:177:HIS:CE1	7:L:305:BCL:HMB1	2.09	0.88

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%)	267 (96%)	12 (4%)	0	100	100
2	M	301/303 (99%)	290 (96%)	10 (3%)	1 (0%)	41	64
3	H	237/241 (98%)	232 (98%)	4 (2%)	1 (0%)	34	57
All	All	817/825 (99%)	789 (97%)	26 (3%)	2 (0%)	47	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN
3	H	246	PRO

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	220/220 (100%)	211 (96%)	9 (4%)	30	56
2	M	237/237 (100%)	231 (98%)	6 (2%)	47	73
3	H	194/196 (99%)	191 (98%)	3 (2%)	65	83
All	All	651/653 (100%)	633 (97%)	18 (3%)	43	69

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	229	PHE

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Mol	Chain	Res	Type
3	H	231	ASP
3	H	221	SER
1	L	272	TRP
2	M	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 37 ligands modelled in this entry, 4 are monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	HTO	L	304	-	9,9,9	0.26	0	10,10,10	1.10	1 (10%)
12	LDA	M	416	-	12,15,15	1.98	1 (8%)	14,17,17	0.41	0
6	HTO	M	402	-	9,9,9	0.49	0	10,10,10	0.95	0
11	GOL	L	310	-	5,5,5	0.76	0	5,5,5	1.03	0
12	LDA	H	304	-	12,15,15	1.96	1 (8%)	14,17,17	0.70	0
7	BCL	L	313	19	58,74,74	1.37	4 (6%)	69,115,115	1.84	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	TRS	H	303	-	7,7,7	0.30	0	9,9,9	0.33	0
12	LDA	M	417	-	12,15,15	1.96	1 (8%)	14,17,17	0.54	0
12	LDA	L	312	-	12,15,15	1.99	1 (8%)	14,17,17	0.81	0
12	LDA	M	418	-	12,15,15	2.04	1 (8%)	14,17,17	0.51	0
4	EDO	H	302	-	3,3,3	0.51	0	2,2,2	0.36	0
4	EDO	M	401	-	3,3,3	0.65	0	2,2,2	0.27	0
5	DIO	L	303	-	6,6,6	0.57	0	6,6,6	1.21	1 (16%)
4	EDO	L	301	-	3,3,3	0.59	0	2,2,2	0.29	0
8	BPB	M	407	-	49,70,70	1.42	3 (6%)	47,101,101	1.82	10 (21%)
8	BPB	L	306	-	49,70,70	1.57	3 (6%)	47,101,101	1.43	7 (14%)
9	U10	M	409	-	48,48,63	2.67	13 (27%)	58,61,79	1.74	15 (25%)
14	SPN	M	410	-	40,42,42	0.74	1 (2%)	50,52,52	1.90	16 (32%)
4	EDO	M	405	-	3,3,3	0.50	0	2,2,2	0.43	0
12	LDA	M	415	-	12,15,15	2.03	1 (8%)	14,17,17	0.55	0
4	EDO	H	301	-	3,3,3	0.40	0	2,2,2	0.47	0
12	LDA	M	404	-	12,15,15	2.00	1 (8%)	14,17,17	0.55	0
10	PO4	M	413	-	4,4,4	0.76	0	6,6,6	0.43	0
7	BCL	M	403	-	58,74,74	1.32	7 (12%)	69,115,115	1.37	12 (17%)
17	CDL	M	414	-	80,80,99	1.14	4 (5%)	86,92,111	1.13	5 (5%)
4	EDO	L	302	-	3,3,3	0.63	0	2,2,2	0.09	0
10	PO4	L	308	-	4,4,4	0.77	0	6,6,6	0.42	0
10	PO4	L	309	-	4,4,4	0.81	0	6,6,6	0.48	0
12	LDA	L	311	-	12,15,15	2.05	1 (8%)	14,17,17	0.59	0
4	EDO	M	419	-	3,3,3	0.40	0	2,2,2	0.74	0
7	BCL	L	305	-	58,74,74	1.49	6 (10%)	69,115,115	1.34	9 (13%)
7	BCL	M	406	-	58,74,74	1.43	6 (10%)	69,115,115	1.54	11 (15%)
9	U10	L	307	-	48,48,63	2.60	13 (27%)	58,61,79	1.90	17 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HTO	L	304	-	-	2/10/10/10	-
12	LDA	M	416	-	-	3/13/13/13	-
6	HTO	M	402	-	-	5/10/10/10	-
11	GOL	L	310	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LDA	H	304	-	-	8/13/13/13	-
7	BCL	L	313	19	-	10/37/137/137	-
18	TRS	H	303	-	-	5/9/9/9	-
12	LDA	M	417	-	-	9/13/13/13	-
12	LDA	L	312	-	-	6/13/13/13	-
12	LDA	M	418	-	-	5/13/13/13	-
4	EDO	H	302	-	-	0/1/1/1	-
4	EDO	M	401	-	-	0/1/1/1	-
5	DIO	L	303	-	-	-	0/1/1/1
4	EDO	L	301	-	-	1/1/1/1	-
8	BPB	M	407	-	-	7/37/105/105	0/5/6/6
8	BPB	L	306	-	-	8/37/105/105	0/5/6/6
9	U10	M	409	-	-	15/45/69/87	0/1/1/1
14	SPN	M	410	-	-	16/50/51/51	-
4	EDO	M	405	-	-	1/1/1/1	-
12	LDA	M	415	-	-	10/13/13/13	-
4	EDO	H	301	-	-	1/1/1/1	-
12	LDA	M	404	-	-	4/13/13/13	-
7	BCL	M	403	-	-	1/37/137/137	-
17	CDL	M	414	-	-	39/91/91/110	-
4	EDO	L	302	-	-	1/1/1/1	-
12	LDA	L	311	-	-	8/13/13/13	-
4	EDO	M	419	-	-	0/1/1/1	-
7	BCL	L	305	-	-	2/37/137/137	-
7	BCL	M	406	-	-	1/37/137/137	-
9	U10	L	307	-	-	16/45/69/87	0/1/1/1

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	306	BPB	CAC-C3C	9.16	1.56	1.33
8	M	407	BPB	CAC-C3C	8.13	1.54	1.33
12	L	311	LDA	O1-N1	-6.99	1.25	1.42
12	M	418	LDA	O1-N1	-6.97	1.25	1.42
12	M	404	LDA	O1-N1	-6.83	1.26	1.42

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	313	BCL	C1-O2A-CGA	8.26	138.12	116.44
8	M	407	BPB	CBC-CAC-C3C	-6.25	110.11	126.70
9	L	307	U10	C17-C18-C19	-4.84	116.02	127.66
7	M	406	BCL	C1-C2-C3	-4.83	117.69	126.04
17	M	414	CDL	OB6-CB5-C51	4.66	121.53	111.50

There are no chirality outliers.

5 of 184 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	304	HTO	C2-C3-C4-C5
6	M	402	HTO	C1-C2-C3-O3
6	M	402	HTO	C1-C2-C3-C4
6	M	402	HTO	O2-C2-C3-O3
6	M	402	HTO	O2-C2-C3-C4

There are no ring outliers.

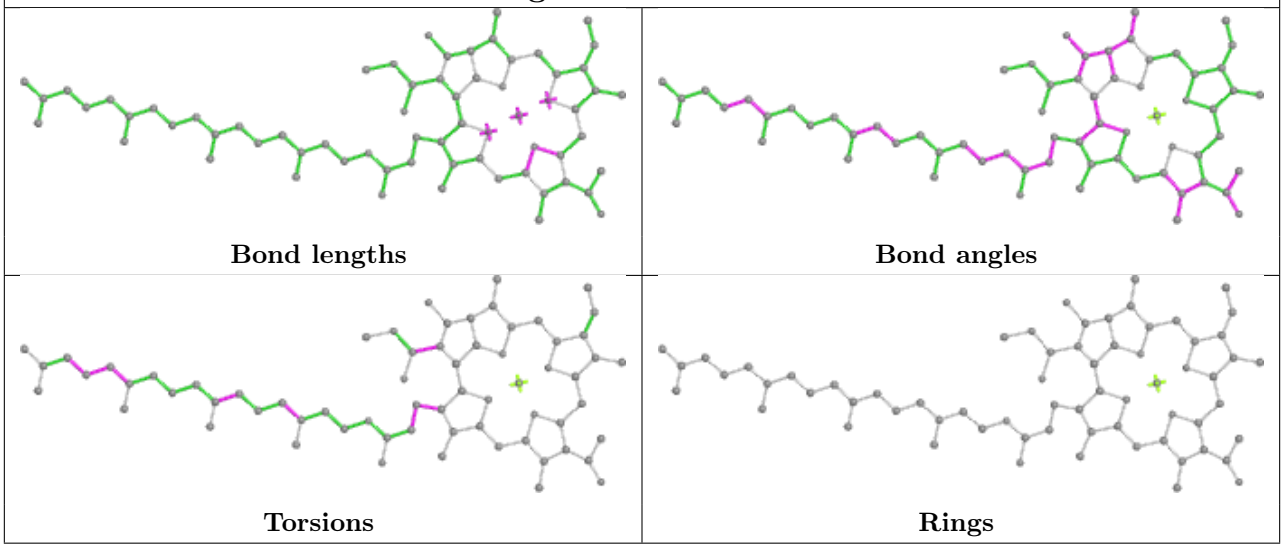
20 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	402	HTO	6	0
12	H	304	LDA	3	0
7	L	313	BCL	6	0
18	H	303	TRS	4	0
12	M	417	LDA	5	0
12	L	312	LDA	1	0
12	M	418	LDA	1	0
4	H	302	EDO	1	0
5	L	303	DIO	2	0
4	L	301	EDO	1	0
8	M	407	BPB	4	0
8	L	306	BPB	1	0
9	M	409	U10	2	0
14	M	410	SPN	7	0
12	M	404	LDA	1	0
7	M	403	BCL	2	0
17	M	414	CDL	8	0
7	L	305	BCL	5	0
7	M	406	BCL	4	0
9	L	307	U10	9	0

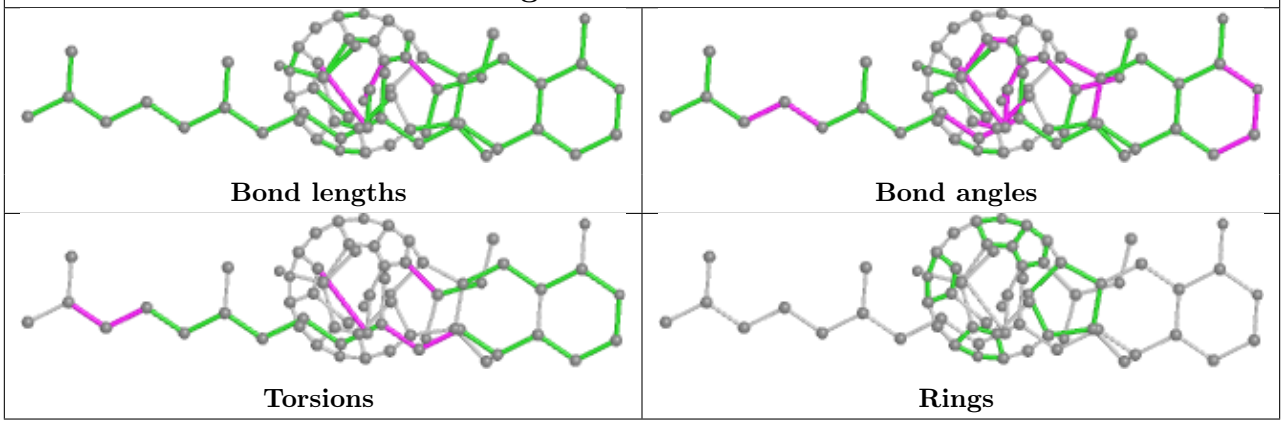
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

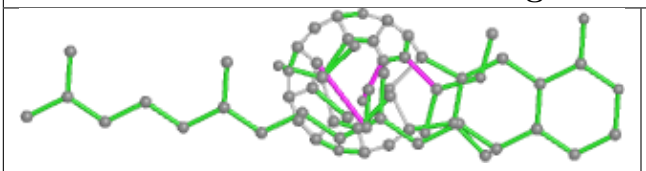
Ligand BCL L 313



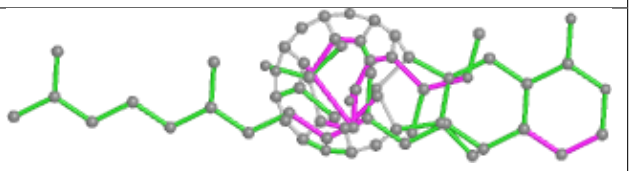
Ligand BPB M 407



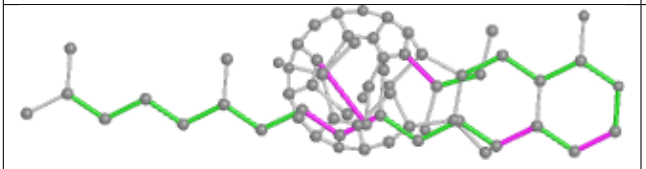
Ligand BPB L 306



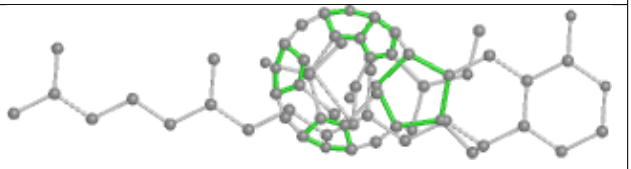
Bond lengths



Bond angles

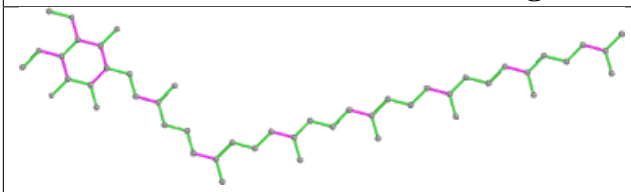


Torsions

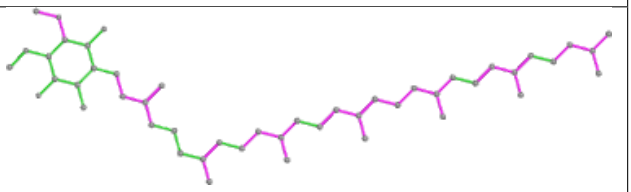


Rings

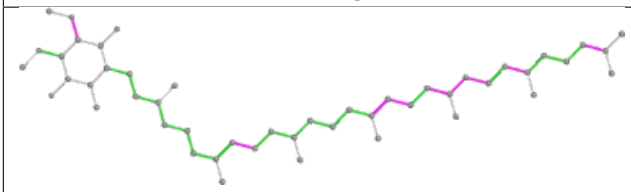
Ligand U10 M 409



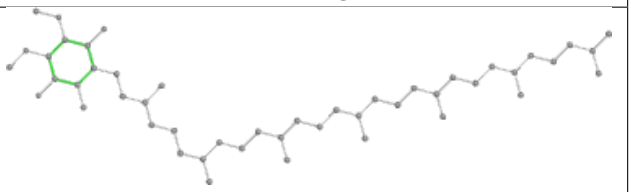
Bond lengths



Bond angles

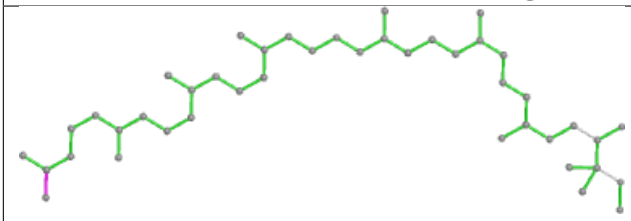


Torsions

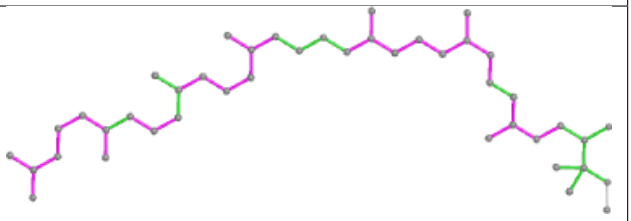


Rings

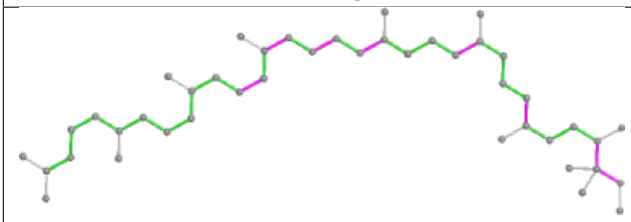
Ligand SPN M 410



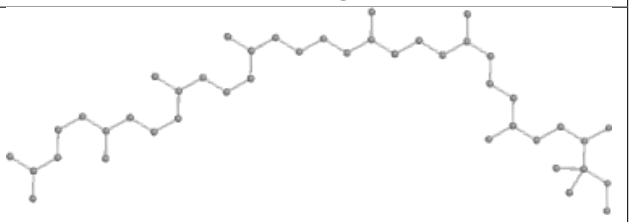
Bond lengths



Bond angles

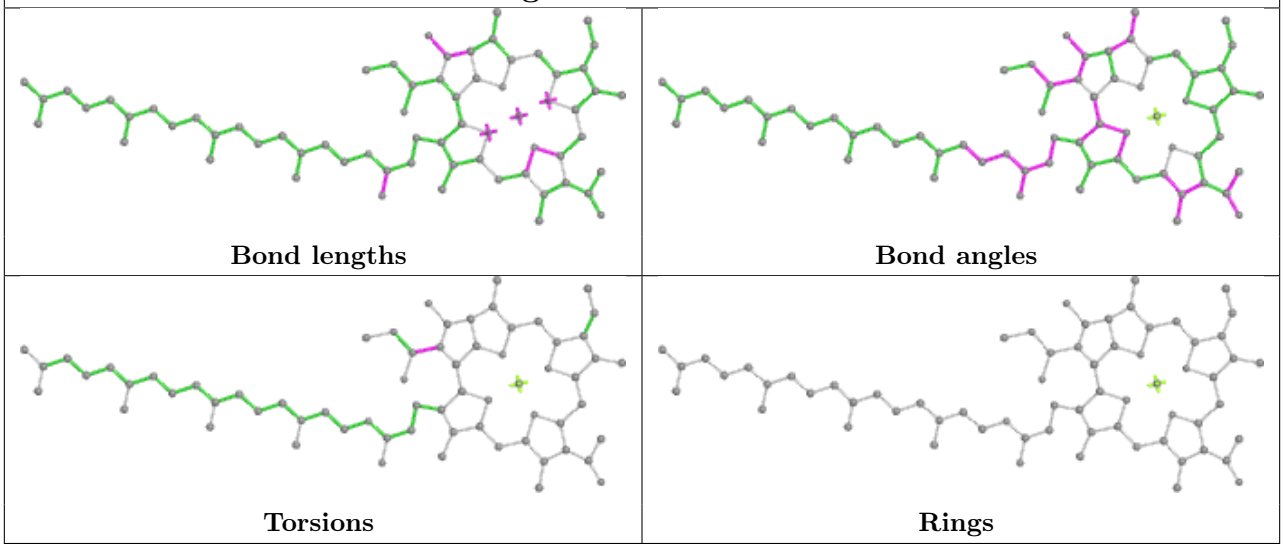


Torsions

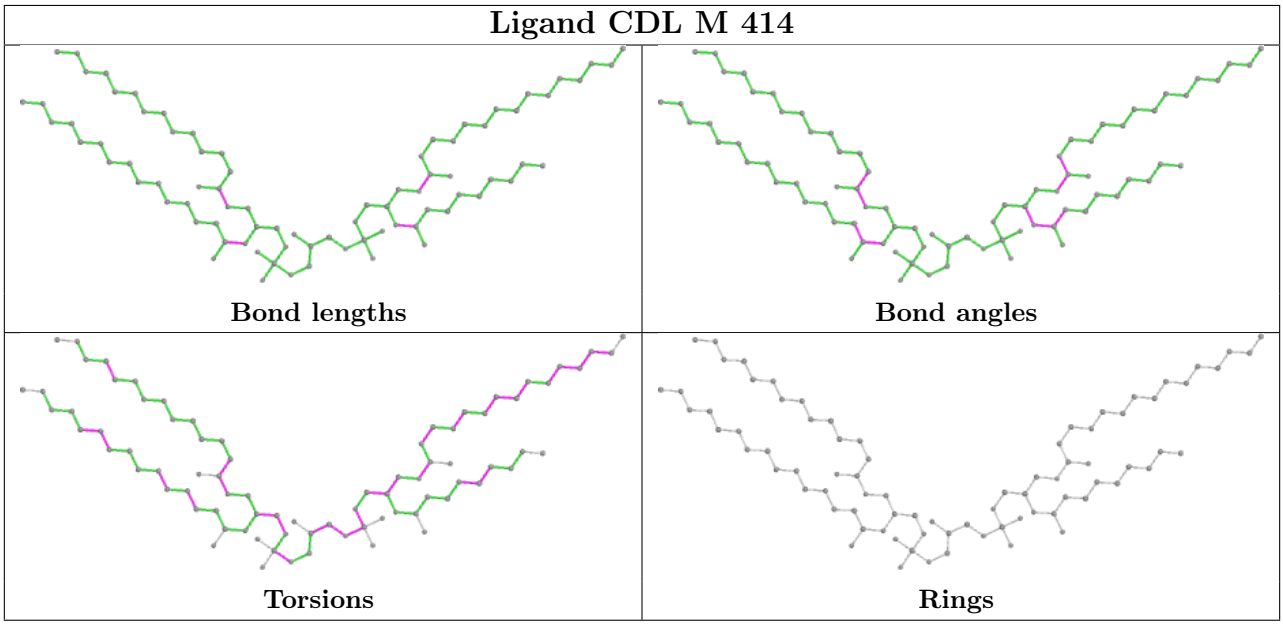


Rings

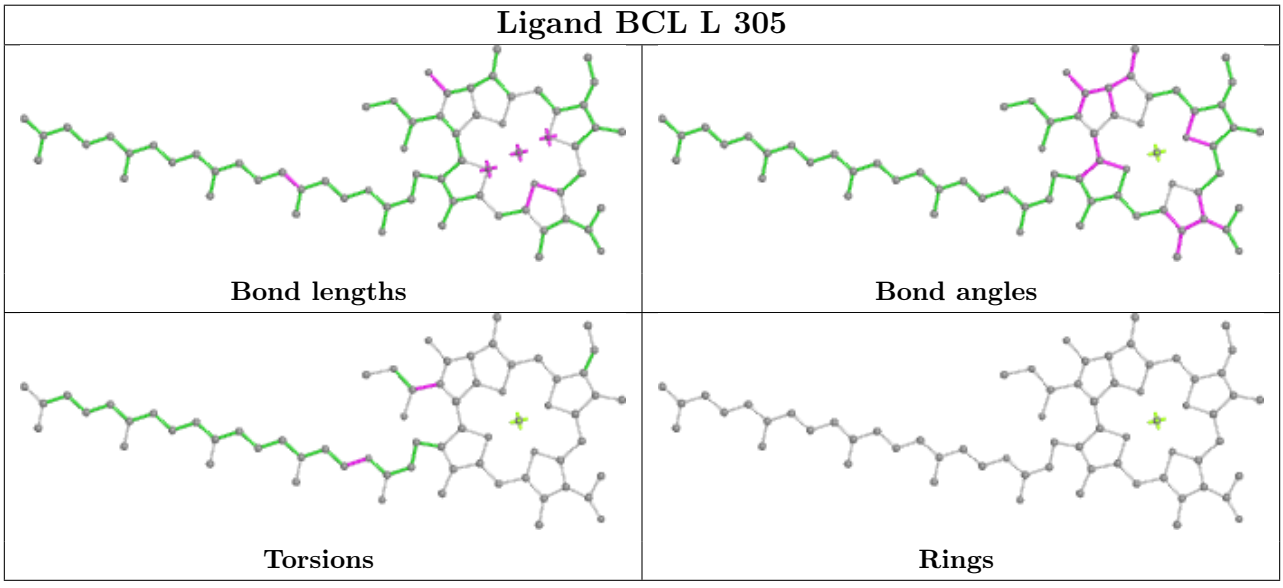
Ligand BCL M 403



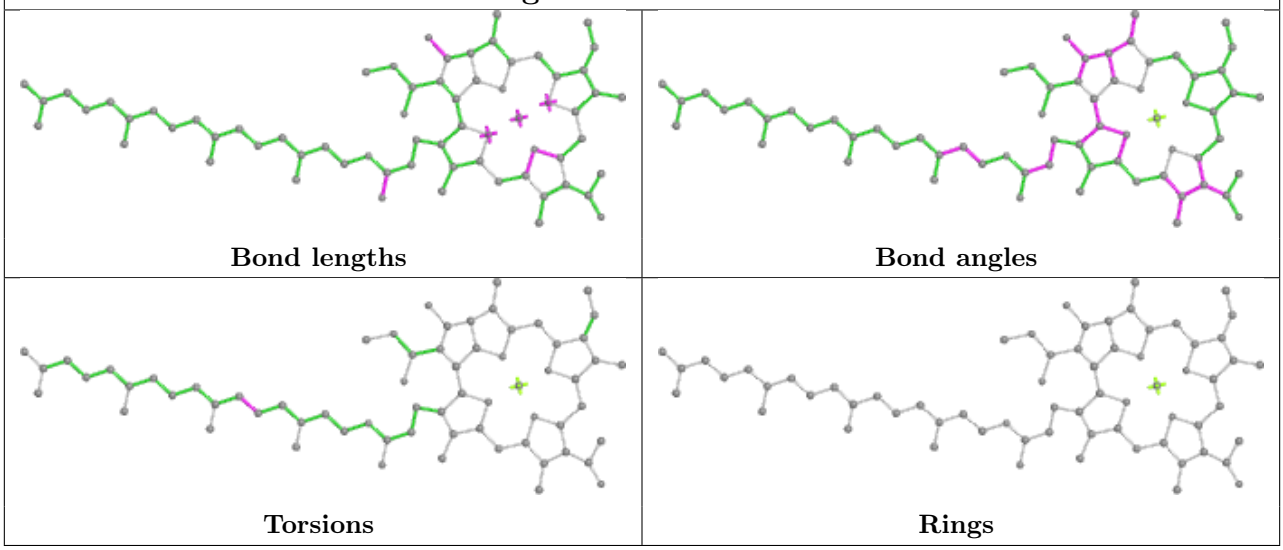
Ligand CDL M 414



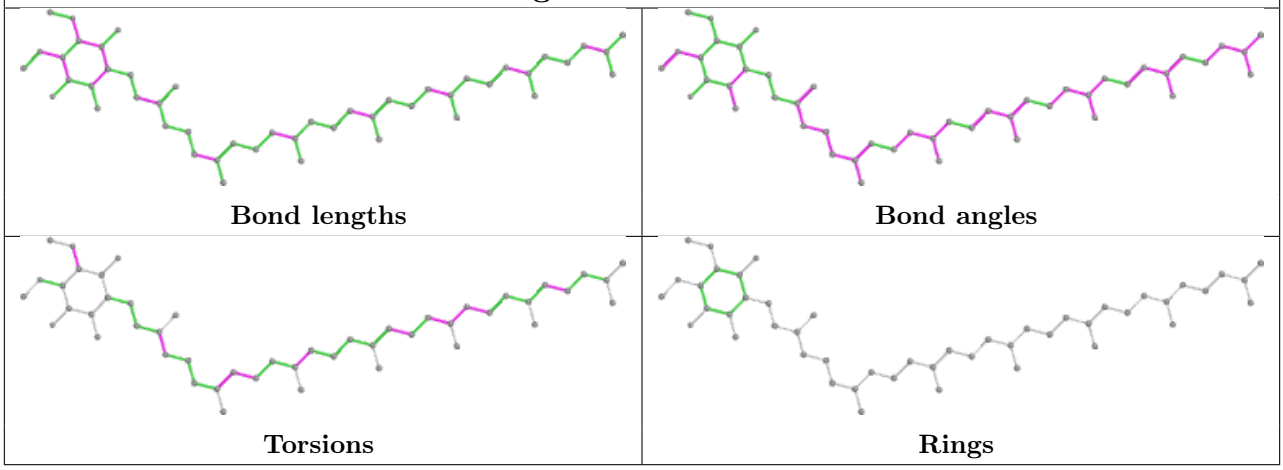
Ligand BCL L 305



Ligand BCL M 406



Ligand U10 L 307



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	L	281/281 (100%)	-0.25	6 (2%)	63	58	47, 60, 89, 104	0
2	M	302/303 (99%)	-0.27	6 (1%)	65	60	46, 64, 88, 104	0
3	H	239/241 (99%)	-0.39	8 (3%)	46	39	50, 60, 75, 129	0
All	All	822/825 (99%)	-0.30	20 (2%)	59	53	46, 61, 88, 129	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	248	ARG	8.6
3	H	246	PRO	5.3
3	H	247	LYS	4.9
1	L	72	GLU	4.6
3	H	245	ALA	3.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

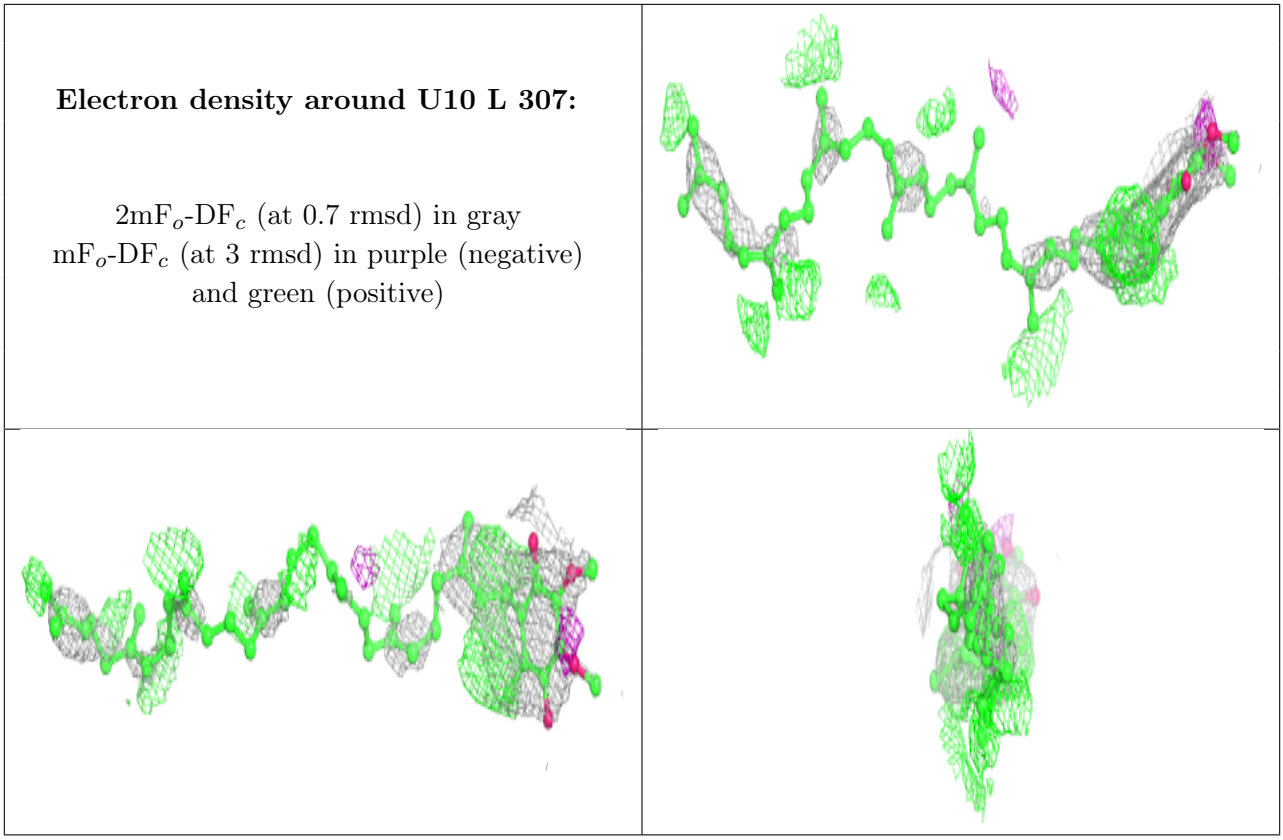
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	LDA	M	418	16/16	0.44	0.48	74,96,122,123	0
12	LDA	M	404	16/16	0.74	0.27	69,79,110,111	0
6	HTO	L	304	10/10	0.74	0.35	79,91,99,104	0
12	LDA	M	417	16/16	0.75	0.55	82,92,136,138	0
9	U10	L	307	48/63	0.77	0.35	47,71,80,84	48
12	LDA	L	312	16/16	0.78	0.20	67,79,107,107	0
12	LDA	L	311	16/16	0.78	0.34	58,85,101,107	0
4	EDO	H	302	4/4	0.79	0.24	68,82,86,96	0
18	TRS	H	303	8/8	0.81	0.40	83,88,93,93	0
17	CDL	M	414	81/100	0.85	0.38	60,91,123,138	0
12	LDA	H	304	16/16	0.85	0.28	65,73,83,88	0
15	K	M	411	1/1	0.86	0.17	87,87,87,87	0
6	HTO	M	402	10/10	0.86	0.40	78,86,96,97	0
4	EDO	L	301	4/4	0.86	0.25	60,70,71,74	0
10	PO4	L	308	5/5	0.87	0.49	111,111,117,127	0
12	LDA	M	415	16/16	0.87	0.24	49,69,78,79	0
4	EDO	L	302	4/4	0.87	0.17	73,79,83,87	0
4	EDO	H	301	4/4	0.87	0.31	71,80,84,92	0
14	SPN	M	410	43/43	0.88	0.32	57,74,85,93	0
11	GOL	L	310	6/6	0.89	0.54	80,84,89,90	0
12	LDA	M	416	16/16	0.89	0.37	59,74,97,101	0
4	EDO	M	405	4/4	0.89	0.12	59,68,71,78	0
4	EDO	M	419	4/4	0.90	0.23	53,57,60,62	0
10	PO4	L	309	5/5	0.91	0.59	82,88,105,111	0
5	DIO	L	303	6/6	0.91	0.29	73,76,85,89	0
9	U10	M	409	48/63	0.92	0.21	45,58,77,84	0
8	BPB	M	407	65/65	0.93	0.21	47,66,116,124	0
15	K	H	305	1/1	0.93	0.11	69,69,69,69	0
4	EDO	M	401	4/4	0.94	0.18	56,58,63,64	0
7	BCL	L	313	66/66	0.95	0.24	54,66,112,119	0
10	PO4	M	413	5/5	0.95	0.08	80,83,95,95	0
8	BPB	L	306	65/65	0.97	0.20	44,51,63,70	0
7	BCL	L	305	66/66	0.97	0.19	48,56,61,65	0
7	BCL	M	406	66/66	0.97	0.21	52,59,76,96	0
7	BCL	M	403	66/66	0.98	0.17	40,51,64,76	0
13	FE	M	408	1/1	0.99	0.15	50,50,50,50	0
16	CL	M	412	1/1	0.99	0.07	70,70,70,70	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.

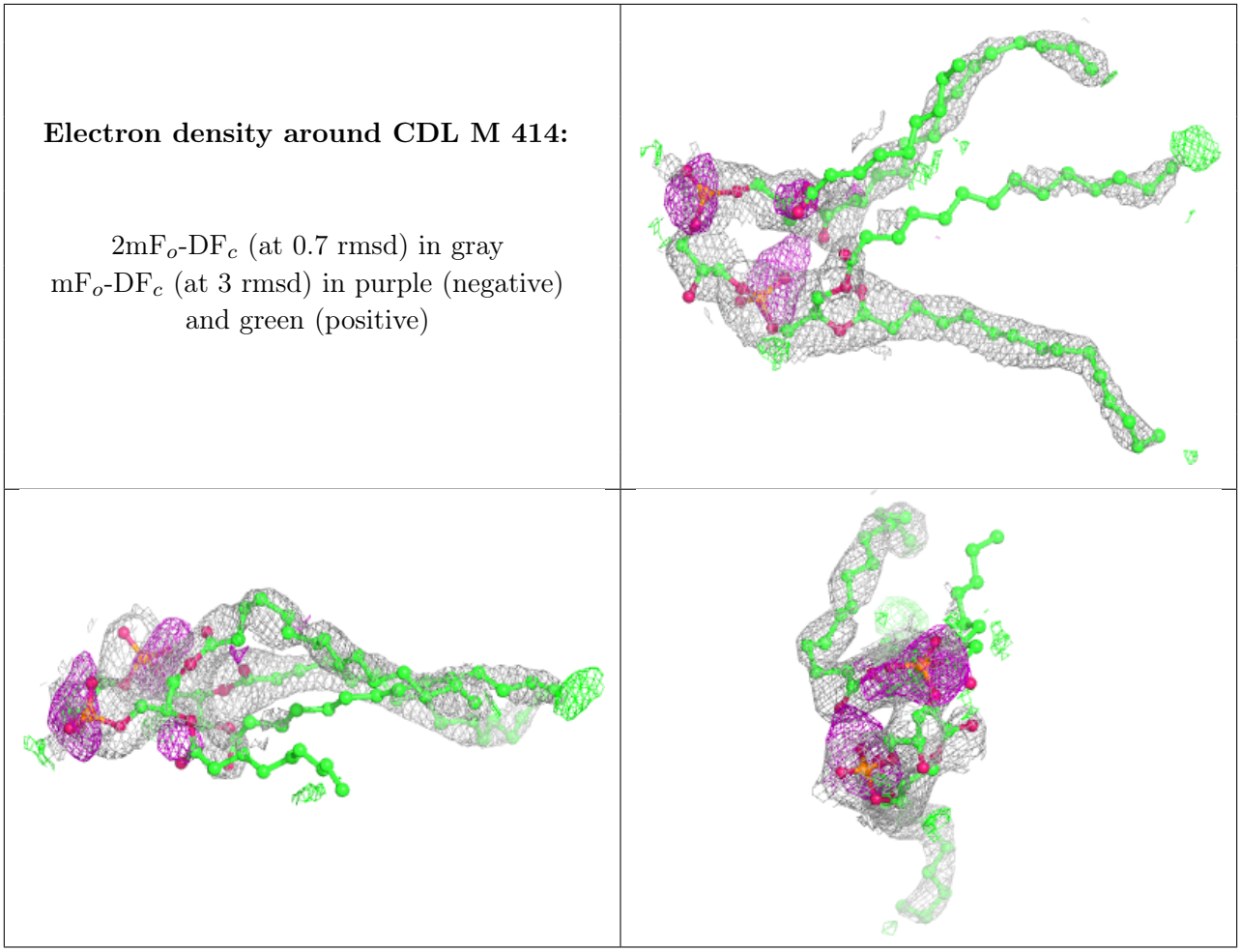
Electron density around U10 L 307:

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



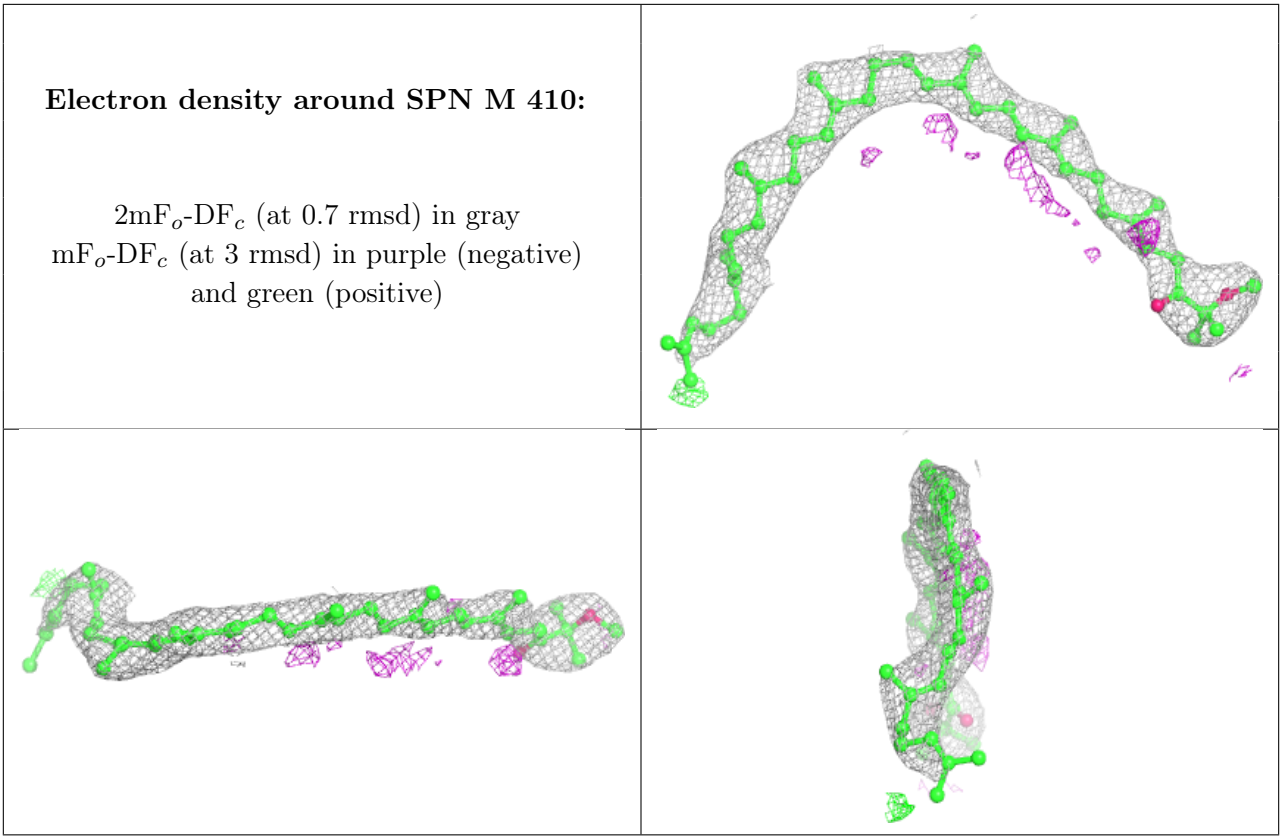
Electron density around CDL M 414:

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



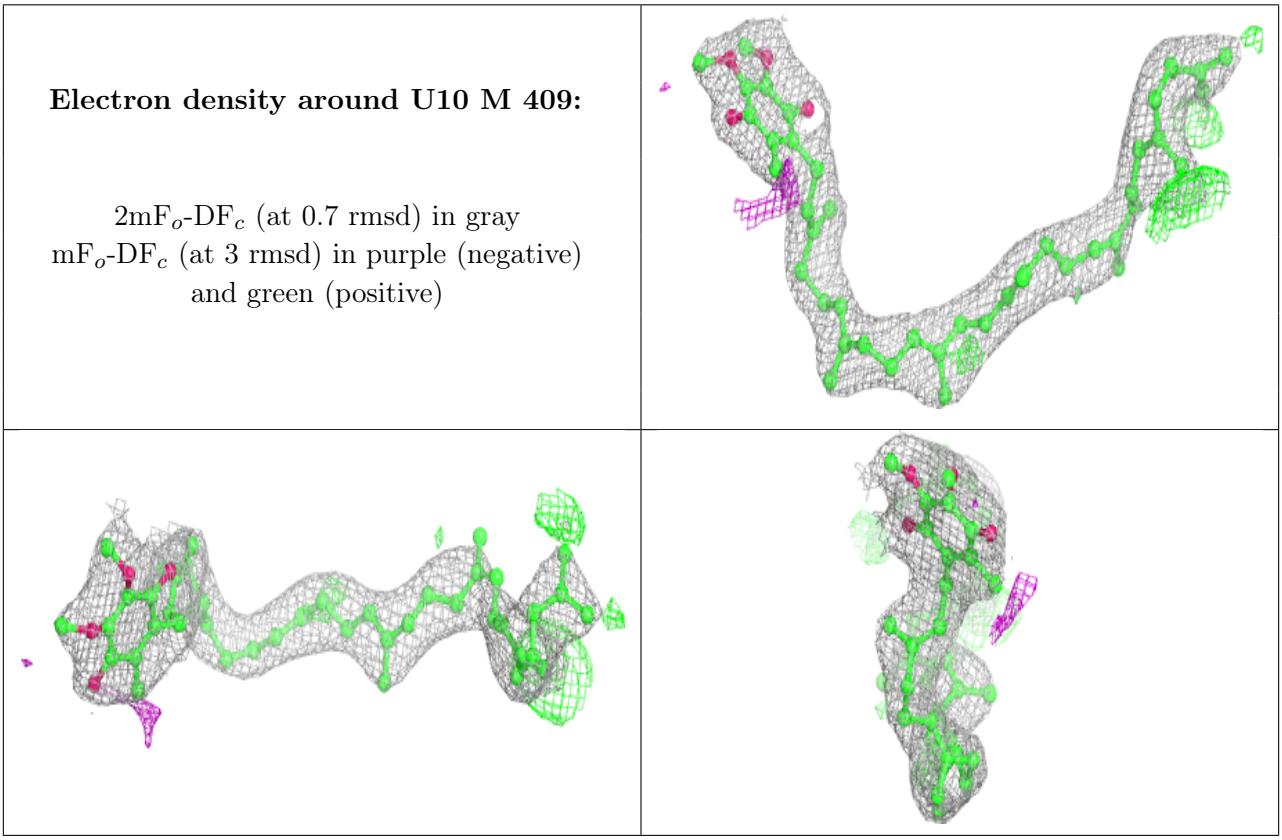
Electron density around SPN M 410:

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



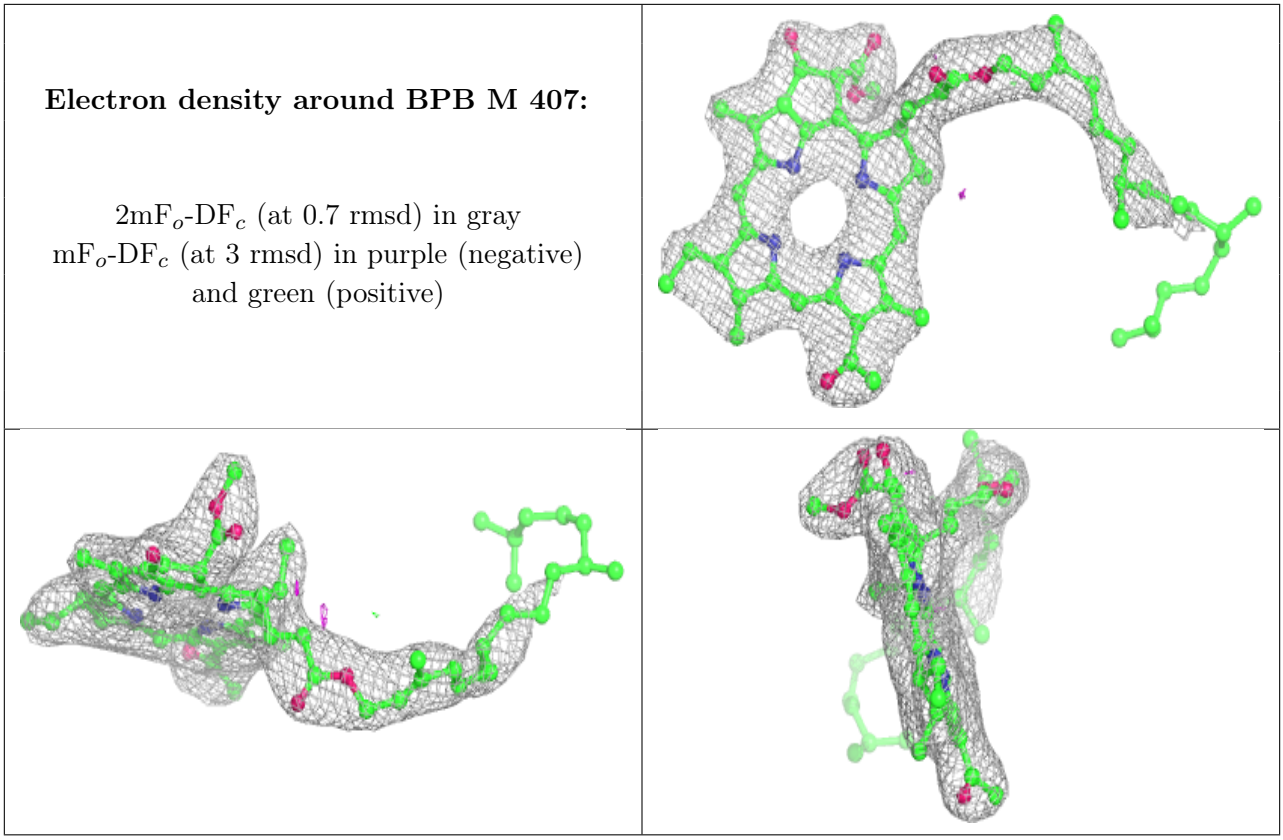
Electron density around U10 M 409:

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



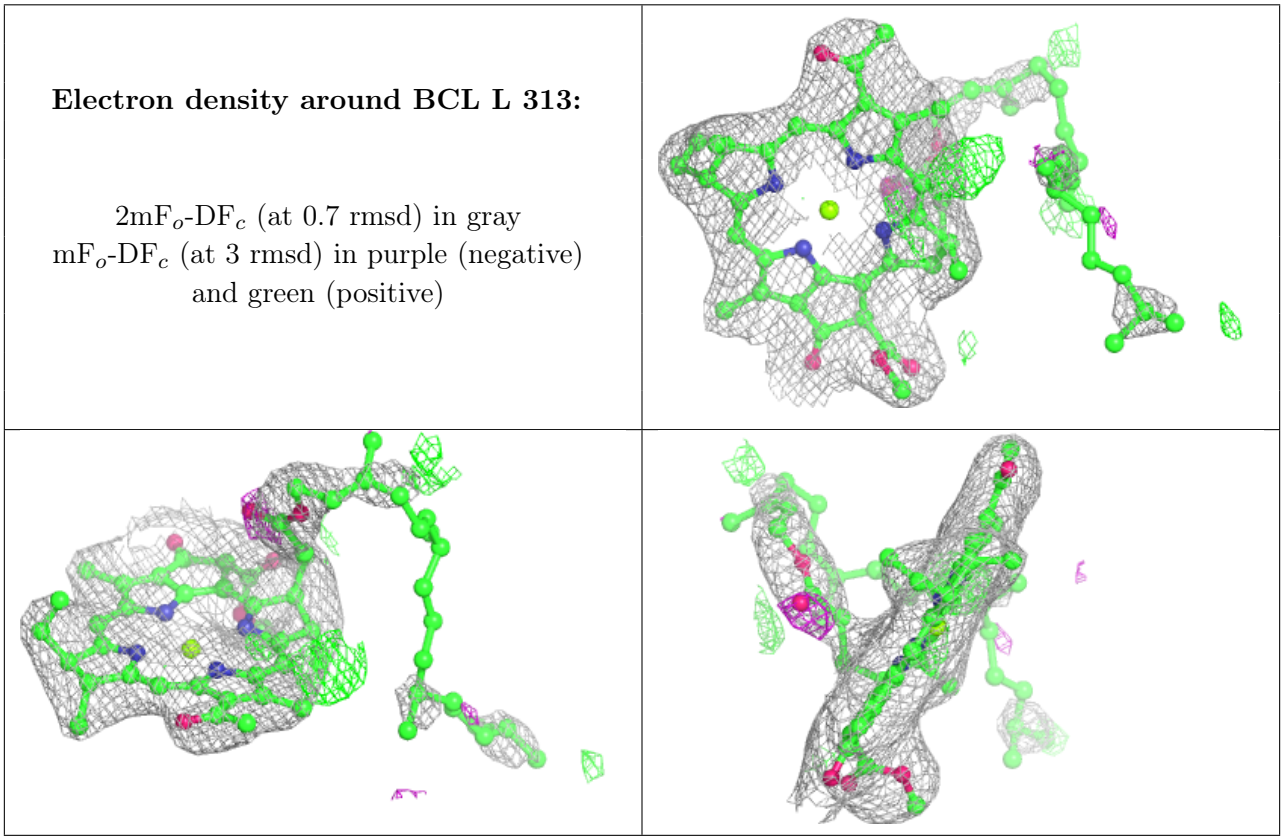
Electron density around BPB M 407:

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



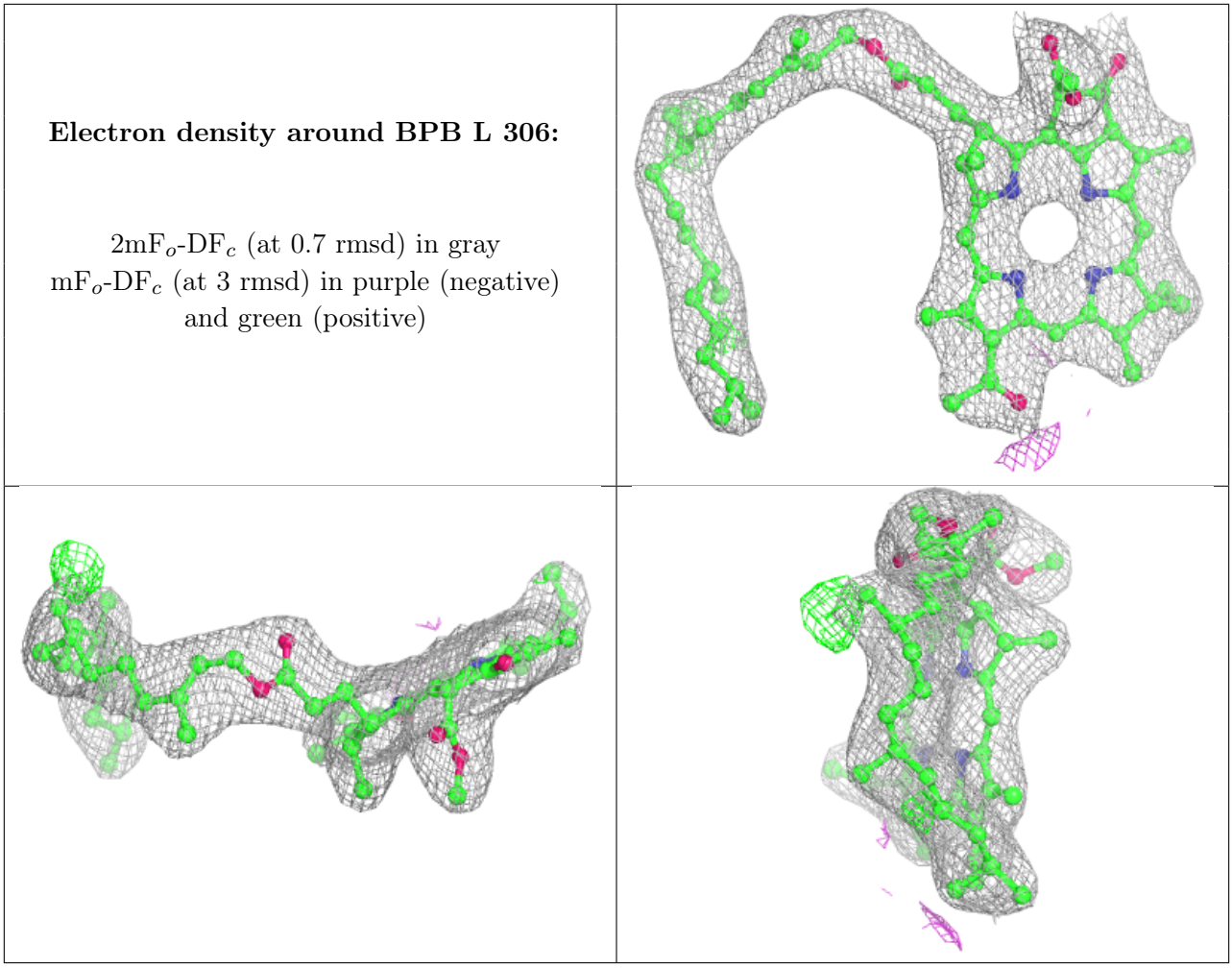
Electron density around BCL L 313:

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



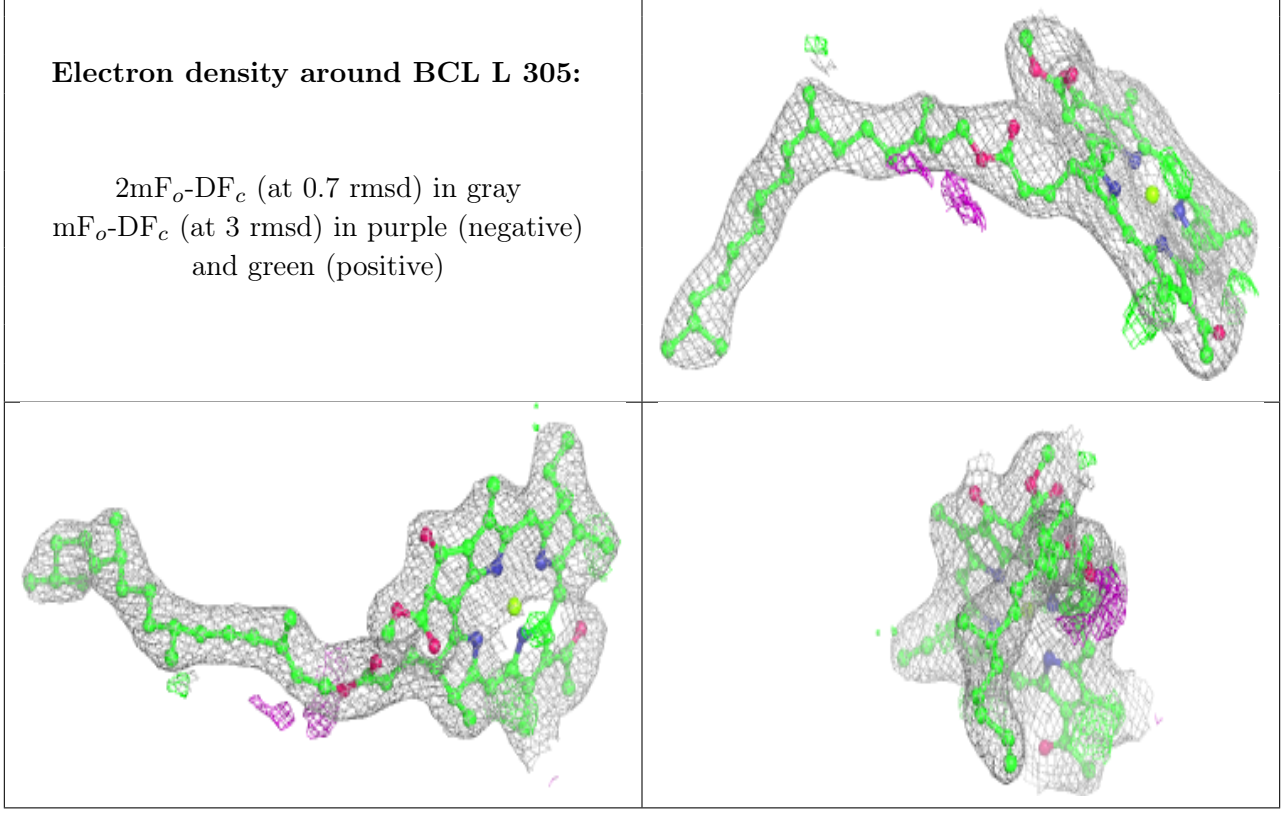
Electron density around BPB L 306:

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



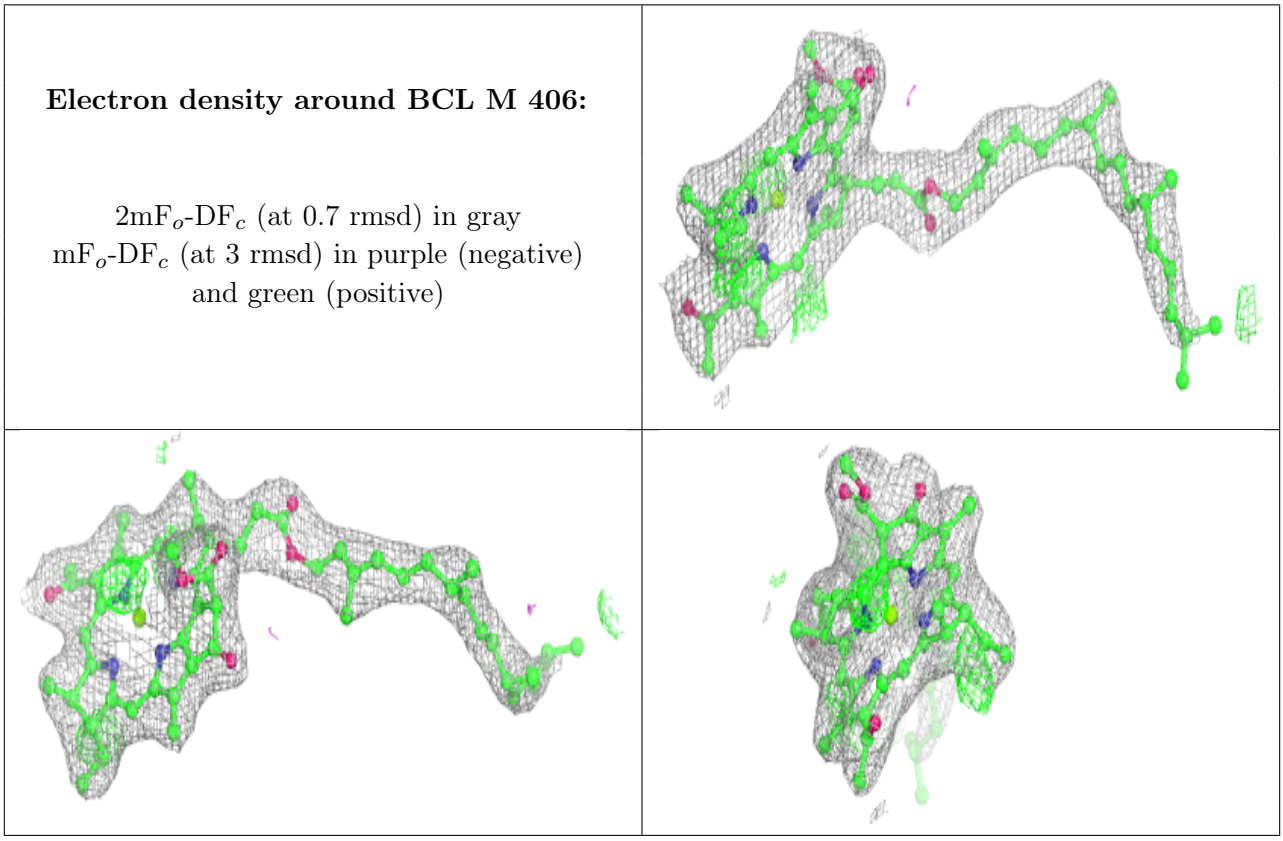
Electron density around BCL L 305:

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



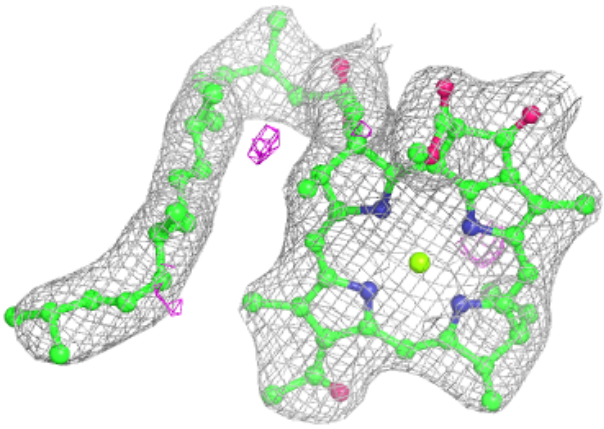
Electron density around BCL M 406:

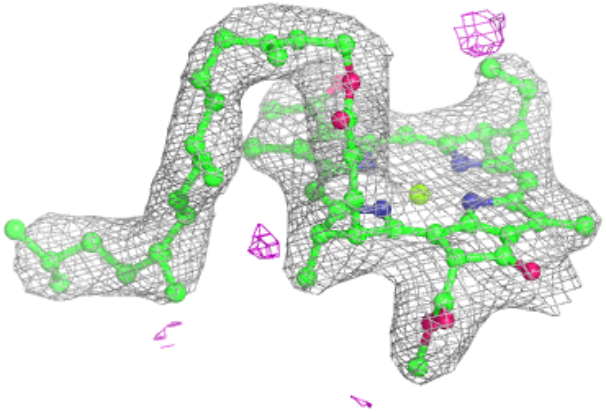
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

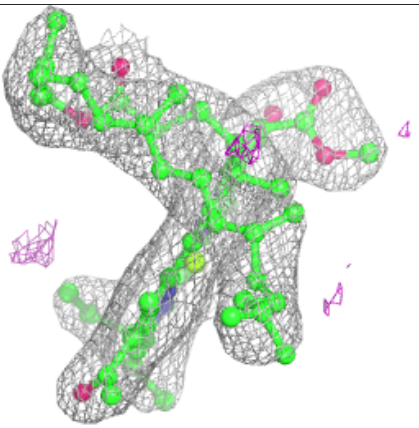


Electron density around BCL M 403:

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

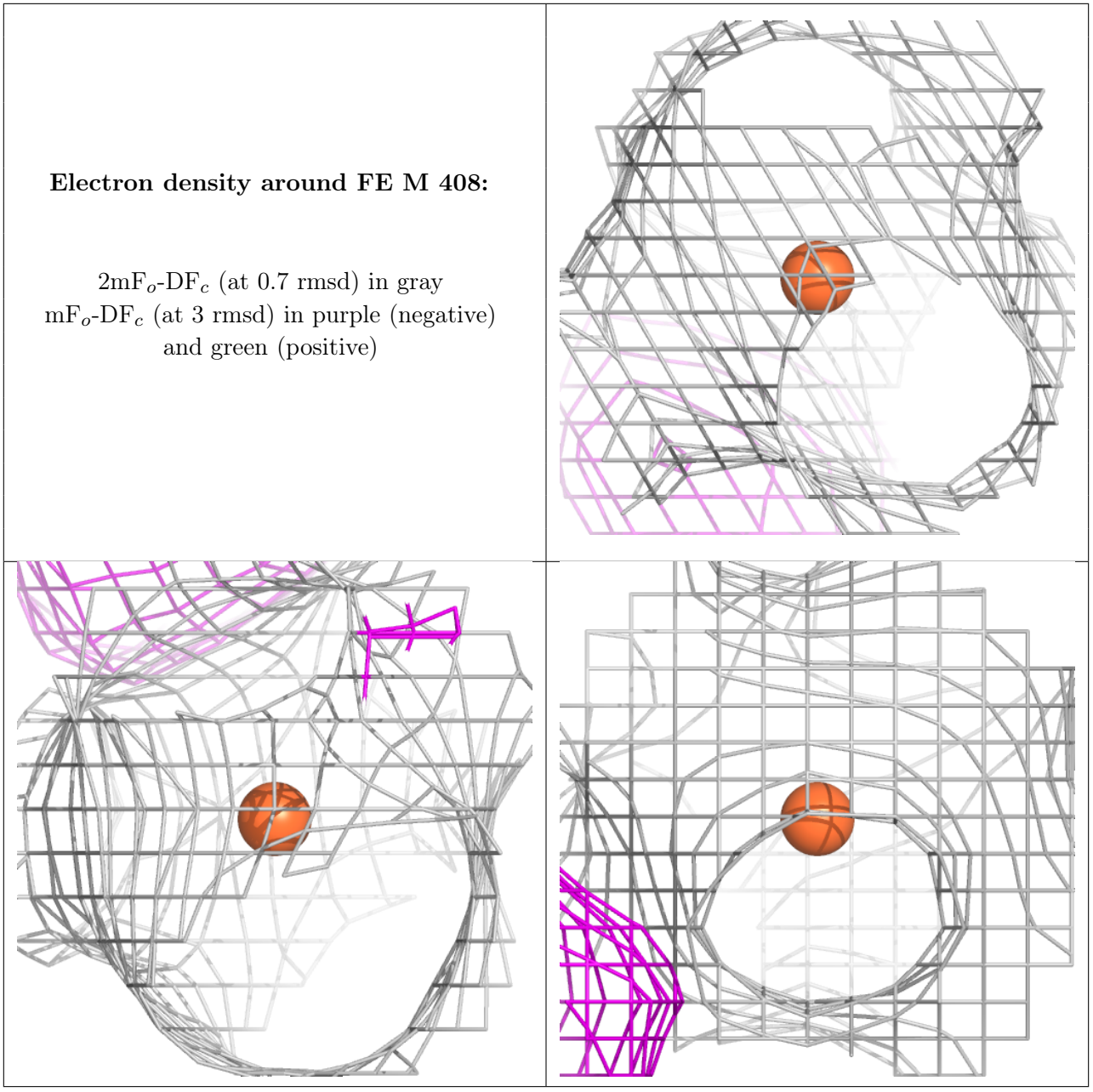






Electron density around FE M 408:

$2mF_o$-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.