



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 11:36 AM UTC

PDB ID : 8C3F / pdb_00008c3f
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

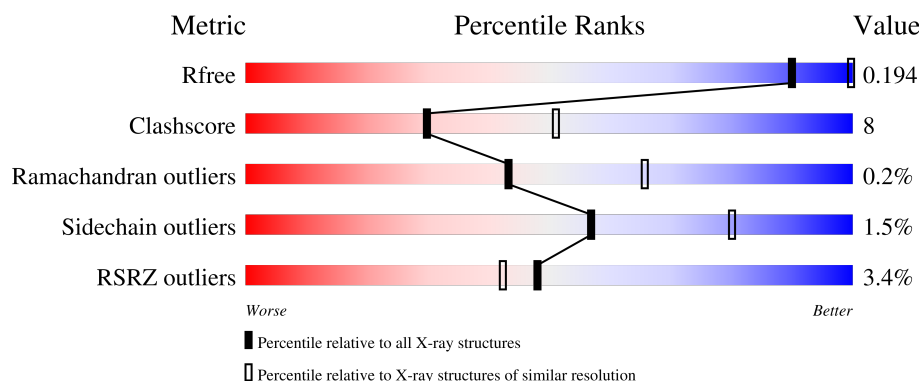
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

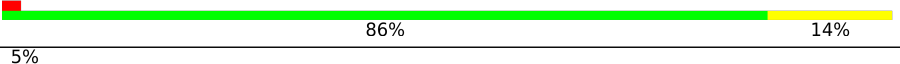
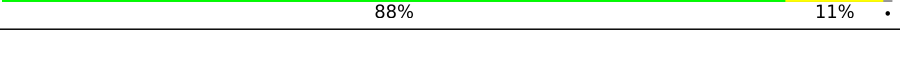
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	
2	M	303	
3	H	241	

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
6	HTO	M	402	-	-	X	-

2 Entry composition

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.

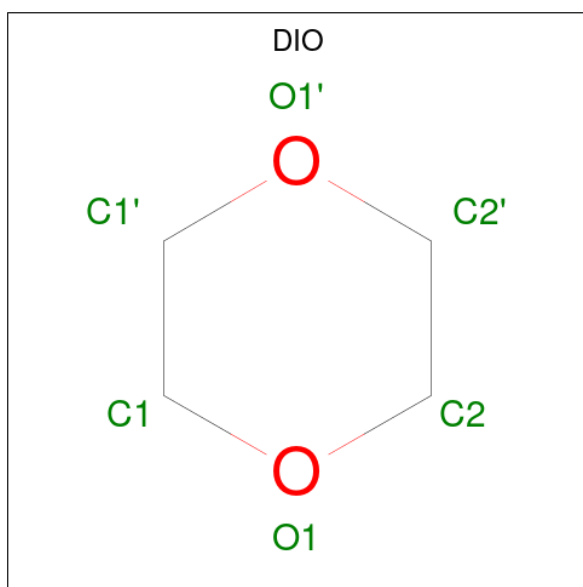
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	239	Total	C	N	O	S	0	0	0
			1823	1166	313	335	9			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



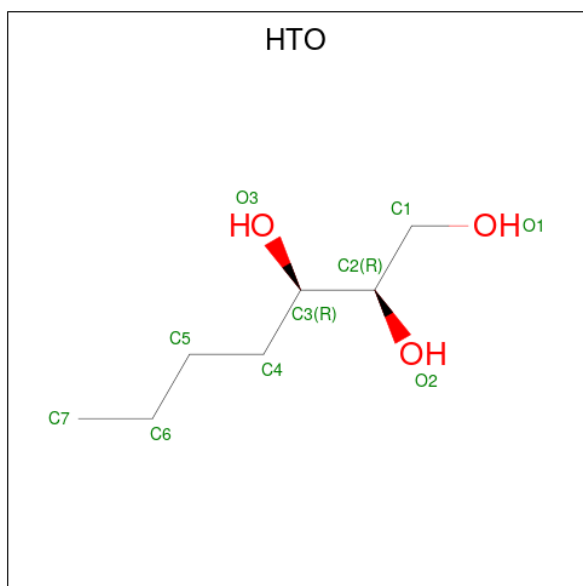
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: C₄H₈O₂).



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

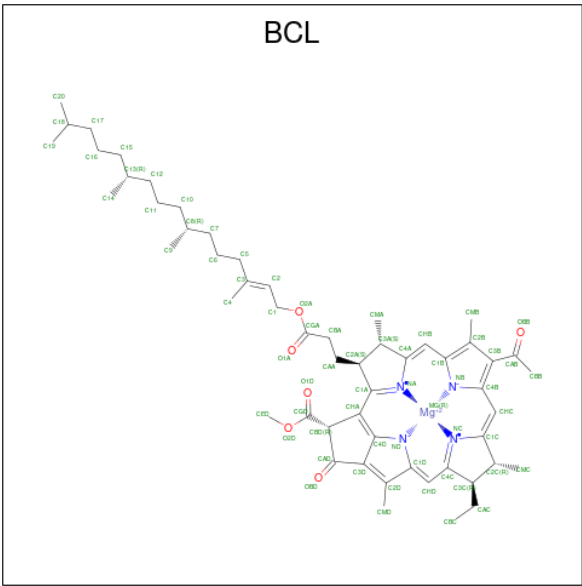
- Molecule 6 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



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

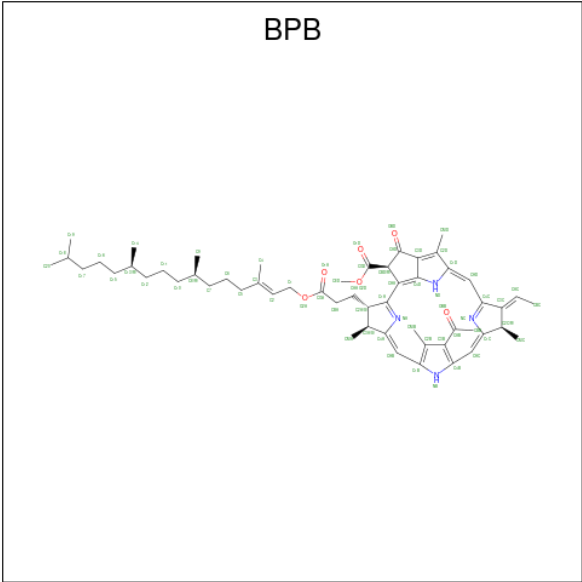
- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$)

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



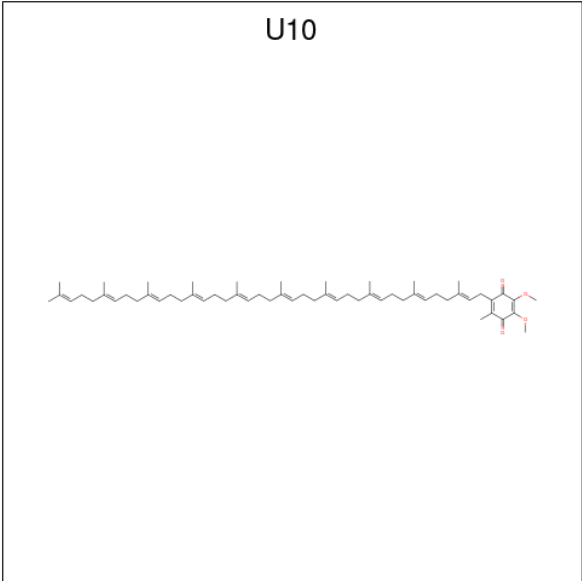
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: C₅₅H₇₄N₄O₆) (la-
beled 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 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



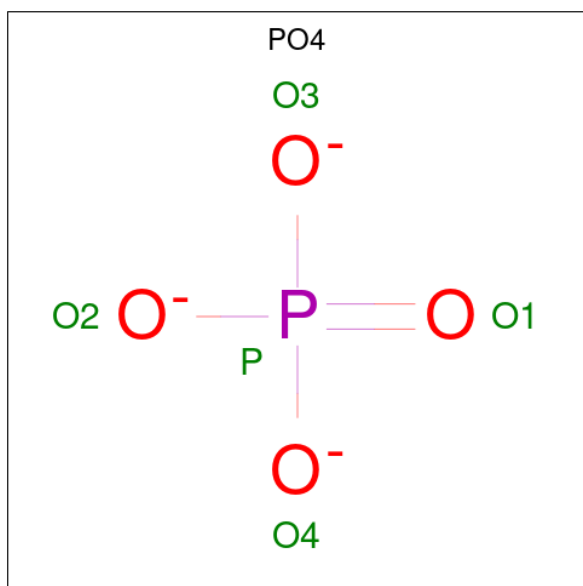
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			48	44	4		

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

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



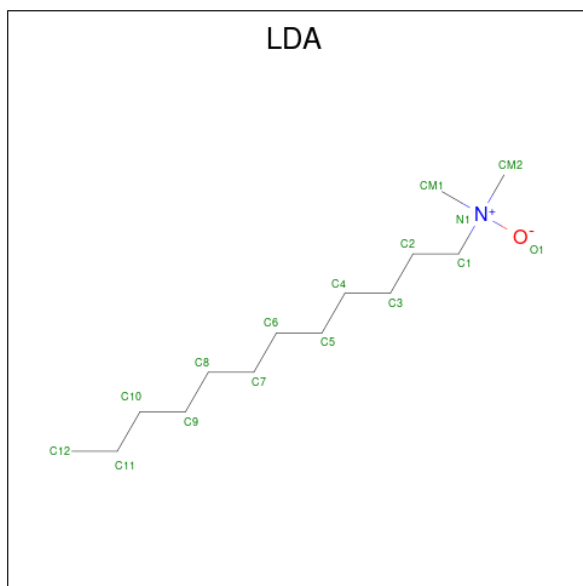
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	O	P	0	0
			5	4	1		
10	L	1	Total	O	P	0	0
			5	4	1		
10	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: 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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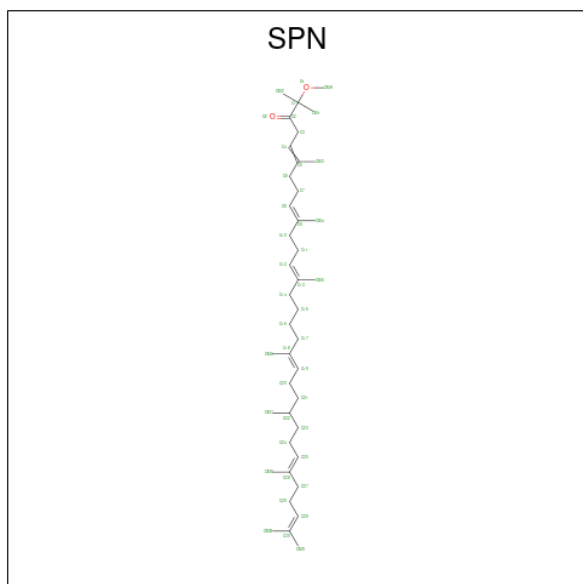
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	M	1	Total	C	N	O	0	0
			16	14	1	1		
12	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 13 is FE (III) ION (CCD ID: 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 (CCD ID: SPN) (formula: C₄₁H₇₀O₂) (labeled as "Ligand of Interest" by depositor).



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

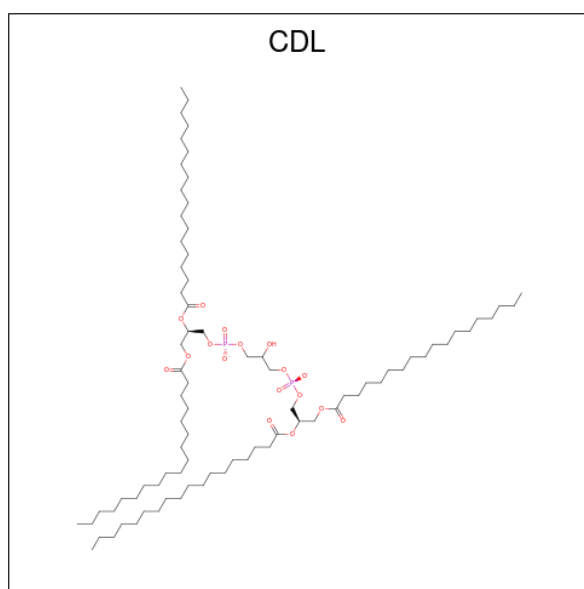
- Molecule 15 is POTASSIUM ION (CCD ID: K) (formula: K).

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 (CCD ID: CL) (formula: Cl).

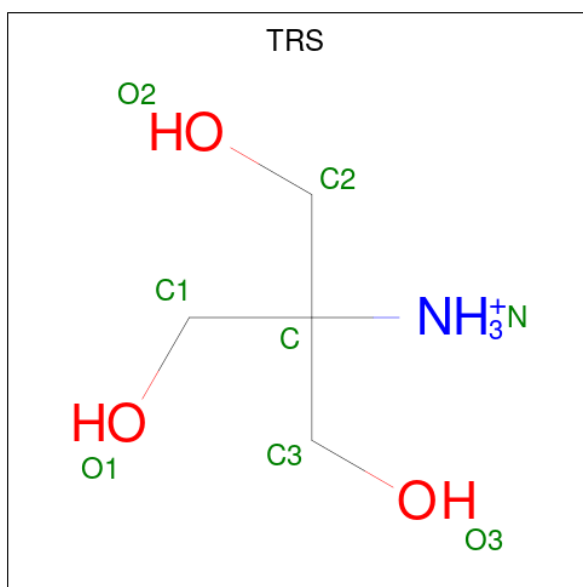
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	M	1	Total Cl 1 1	0	0

- Molecule 17 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (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 (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

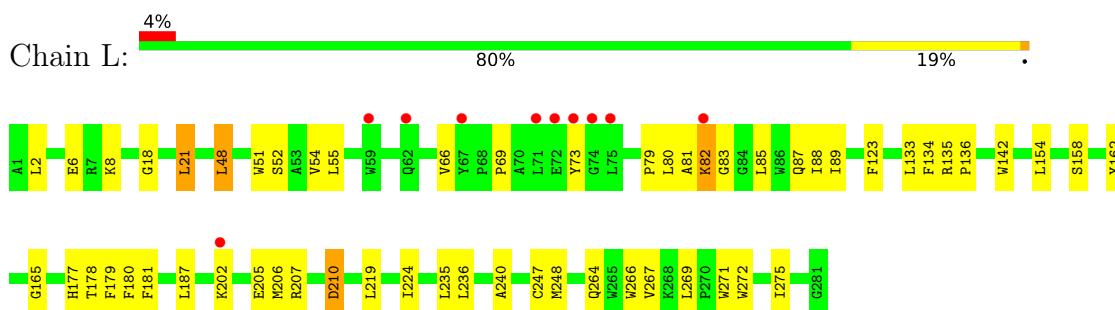
- Molecule 19 is water.

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

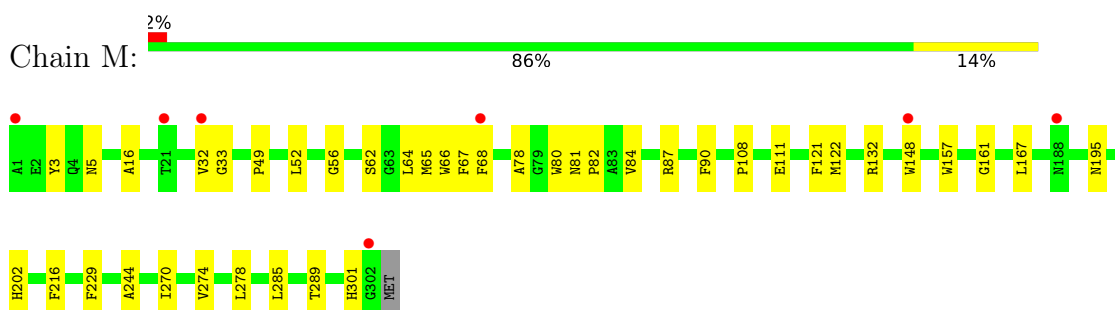
3 Residue-property plots [i](#)

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.

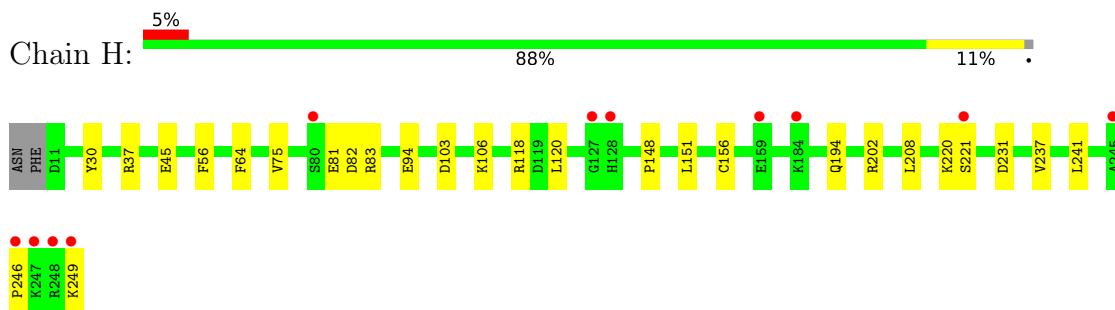
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

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 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.12-2.60) 100.0 (46.12-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (Not available) , 0.194	Depositor DCC
R_{free} test set	3442 reflections (4.80%)	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)	0.29 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/2323	0.53	1/3181 (0.0%)
2	M	0.31	0/2508	0.50	0/3424
3	H	0.35	0/1871	0.54	0/2545
All	All	0.33	0/6702	0.52	1/9150 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	48	LEU	CA-CB-CG	-5.37	97.49	116.30

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	2185	57	0
2	M	2416	0	2329	33	0
3	H	1823	0	1831	22	0
4	H	8	0	12	1	0
4	L	8	0	12	1	0
4	M	12	0	18	0	0
5	L	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	10	0	16	0	0
6	M	10	0	16	6	0
7	L	132	0	148	10	0
7	M	132	0	148	3	0
8	L	65	0	74	0	0
8	M	65	0	74	2	0
9	L	48	0	63	8	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	125	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 125 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:HMB2	1.23	1.43
1:L:177:HIS:ND1	7:L:305:BCL:CMB	2.06	1.18
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.53	0.90
1:L:266:TRP:CD1	6:M:402:HTO:H2	2.19	0.78
3:H:202:ARG:HH12	18:H:303:TRS:H12	1.49	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	36	58
3	H	237/241 (98%)	232 (98%)	4 (2%)	1 (0%)	30	51
All	All	817/825 (99%)	789 (97%)	26 (3%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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%)	213 (97%)	7 (3%)	34	62
2	M	237/237 (100%)	236 (100%)	1 (0%)	84	93
3	H	194/196 (99%)	192 (99%)	2 (1%)	68	86
All	All	651/653 (100%)	641 (98%)	10 (2%)	57	80

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	62	SER

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Mol	Chain	Res	Type
3	H	221	SER
3	H	231	ASP
1	L	207	ARG
1	L	210	ASP

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

Mol	Chain	Res	Type
1	L	258	GLN
2	M	300	ASN
3	H	129	ASN
3	H	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
9	U10	L	307	-	48,48,63	2.66	13 (27%)	60,61,79	1.92	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LDA	M	404	-	13,15,15	2.18	2 (15%)	14,17,17	0.55	0
4	EDO	L	301	-	3,3,3	0.56	0	2,2,2	0.34	0
4	EDO	L	302	-	3,3,3	0.60	0	2,2,2	0.14	0
17	CDL	M	414	-	80,80,99	1.14	4 (5%)	86,92,111	1.14	5 (5%)
7	BCL	M	403	-	69,74,74	1.21	8 (11%)	79,115,115	1.41	9 (11%)
6	HTO	L	304	-	9,9,9	0.27	0	10,10,10	1.11	1 (10%)
4	EDO	H	302	-	3,3,3	0.47	0	2,2,2	0.41	0
6	HTO	M	402	-	9,9,9	0.51	0	10,10,10	0.98	0
7	BCL	L	305	-	69,74,74	1.32	8 (11%)	79,115,115	1.30	7 (8%)
7	BCL	L	313	19	69,74,74	1.20	6 (8%)	79,115,115	1.83	12 (15%)
4	EDO	M	419	-	3,3,3	0.38	0	2,2,2	0.76	0
5	DIO	L	303	-	6,6,6	0.58	0	6,6,6	1.25	1 (16%)
8	BPB	L	306	-	57,70,70	1.16	6 (10%)	55,101,101	2.07	11 (20%)
12	LDA	M	417	-	13,15,15	2.25	2 (15%)	14,17,17	0.53	0
12	LDA	L	312	-	13,15,15	2.14	2 (15%)	14,17,17	0.80	0
8	BPB	M	407	-	57,70,70	1.12	7 (12%)	55,101,101	2.27	13 (23%)
12	LDA	L	311	-	13,15,15	2.27	2 (15%)	14,17,17	0.59	0
4	EDO	M	401	-	3,3,3	0.62	0	2,2,2	0.27	0
10	PO4	M	413	-	4,4,4	0.80	0	6,6,6	0.46	0
7	BCL	M	406	-	69,74,74	1.25	7 (10%)	79,115,115	1.50	9 (11%)
12	LDA	M	416	-	13,15,15	2.22	2 (15%)	14,17,17	0.40	0
14	SPN	M	410	-	42,42,42	0.73	1 (2%)	50,52,52	1.86	15 (30%)
9	U10	M	409	-	48,48,63	2.73	12 (25%)	60,61,79	1.71	14 (23%)
4	EDO	M	405	-	3,3,3	0.47	0	2,2,2	0.47	0
10	PO4	L	309	-	4,4,4	0.86	0	6,6,6	0.51	0
12	LDA	M	415	-	13,15,15	2.04	2 (15%)	14,17,17	0.56	0
10	PO4	L	308	-	4,4,4	0.81	0	6,6,6	0.45	0
11	GOL	L	310	-	5,5,5	0.79	0	5,5,5	1.11	0
12	LDA	H	304	-	13,15,15	2.14	2 (15%)	14,17,17	0.70	0
18	TRS	H	303	-	7,7,7	0.32	0	9,9,9	0.40	0
12	LDA	M	418	-	13,15,15	2.29	2 (15%)	14,17,17	0.51	0
4	EDO	H	301	-	3,3,3	0.37	0	2,2,2	0.50	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
9	U10	L	307	-	-	17/45/69/87	0/1/1/1
12	LDA	M	404	-	-	4/13/13/13	-
4	EDO	L	301	-	-	1/1/1/1	-
4	EDO	L	302	-	-	1/1/1/1	-
17	CDL	M	414	-	-	39/91/91/110	-
7	BCL	M	403	-	-	2/41/137/137	-
6	HTO	L	304	-	-	2/10/10/10	-
4	EDO	H	302	-	-	0/1/1/1	-
6	HTO	M	402	-	-	5/10/10/10	-
7	BCL	L	305	-	-	0/41/137/137	-
7	BCL	L	313	19	-	9/41/137/137	-
4	EDO	M	419	-	-	0/1/1/1	-
5	DIO	L	303	-	-	-	0/1/1/1
8	BPB	L	306	-	-	6/37/105/105	0/5/6/6
12	LDA	M	417	-	-	8/13/13/13	-
12	LDA	L	312	-	-	6/13/13/13	-
8	BPB	M	407	-	-	6/37/105/105	0/5/6/6
12	LDA	L	311	-	-	8/13/13/13	-
4	EDO	M	401	-	-	0/1/1/1	-
7	BCL	M	406	-	-	1/41/137/137	-
12	LDA	M	416	-	-	3/13/13/13	-
14	SPN	M	410	-	-	16/50/51/51	-
9	U10	M	409	-	-	12/45/69/87	0/1/1/1
4	EDO	M	405	-	-	1/1/1/1	-
12	LDA	M	415	-	-	10/13/13/13	-
11	GOL	L	310	-	-	0/4/4/4	-
12	LDA	H	304	-	-	8/13/13/13	-
18	TRS	H	303	-	-	5/9/9/9	-
12	LDA	M	418	-	-	5/13/13/13	-
4	EDO	H	301	-	-	1/1/1/1	-

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	409	U10	C13-C14	6.92	1.49	1.33
12	L	311	LDA	O1-N1	-6.67	1.25	1.42
12	M	418	LDA	O1-N1	-6.65	1.25	1.42
9	M	409	U10	C33-C34	6.59	1.48	1.33
9	L	307	U10	C33-C34	6.52	1.48	1.33

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	407	BPB	C4D-CHA-CBD	-10.62	103.36	108.45
8	L	306	BPB	C4D-CHA-CBD	-10.53	103.41	108.45
7	L	313	BCL	C1-O2A-CGA	8.87	138.12	116.65
7	M	406	BCL	C4D-CHA-C1A	5.60	127.93	121.24
7	L	313	BCL	C4D-CHA-C1A	5.36	127.64	121.24

There are no chirality outliers.

5 of 176 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

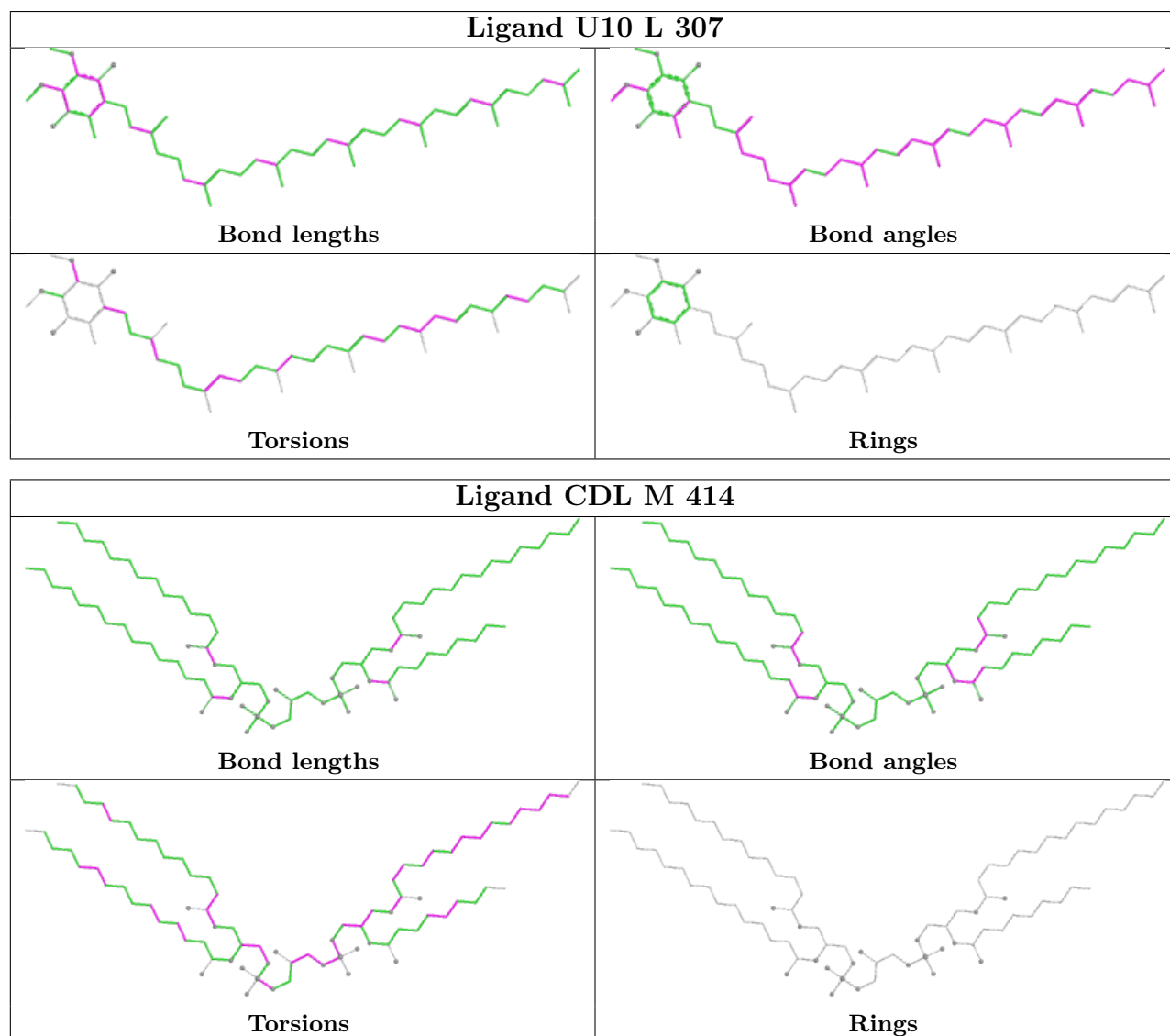
There are no ring outliers.

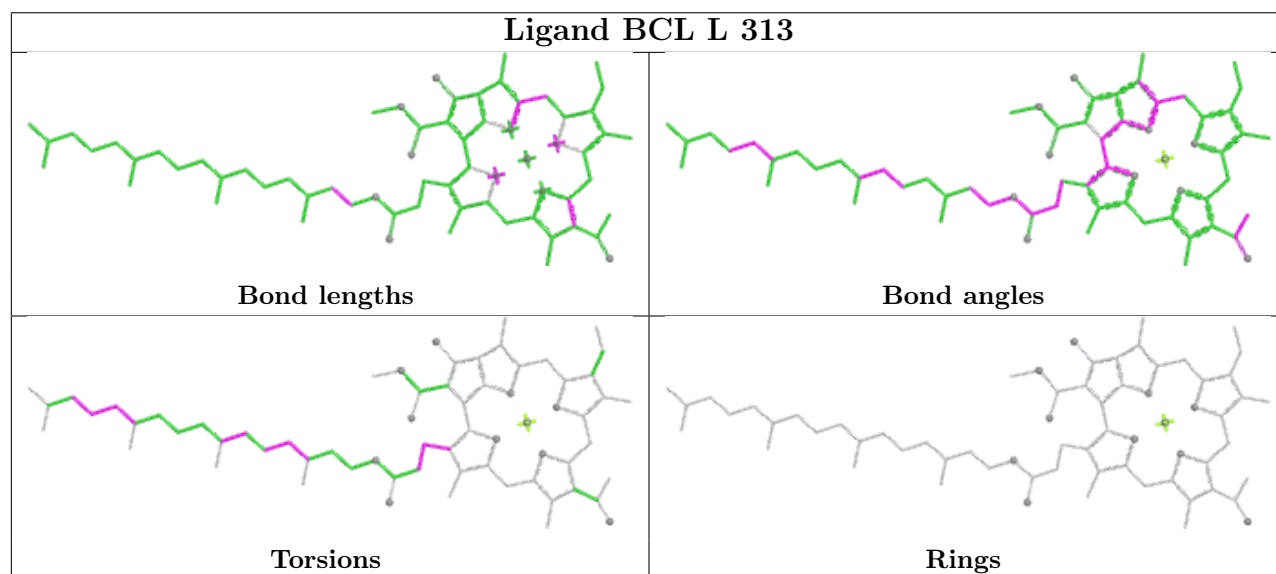
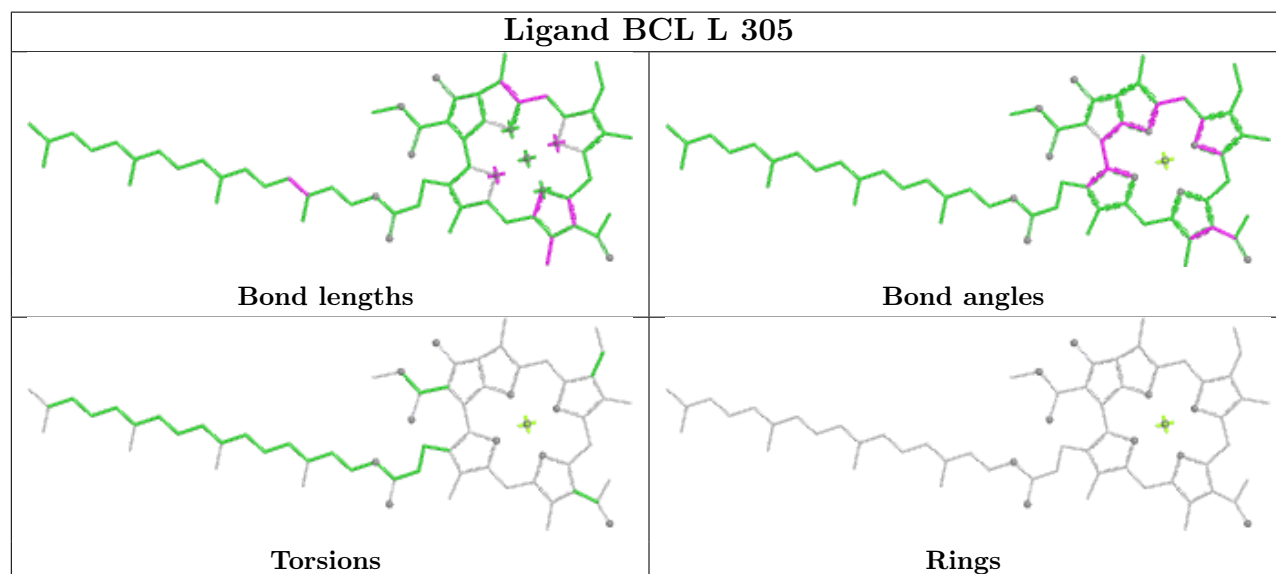
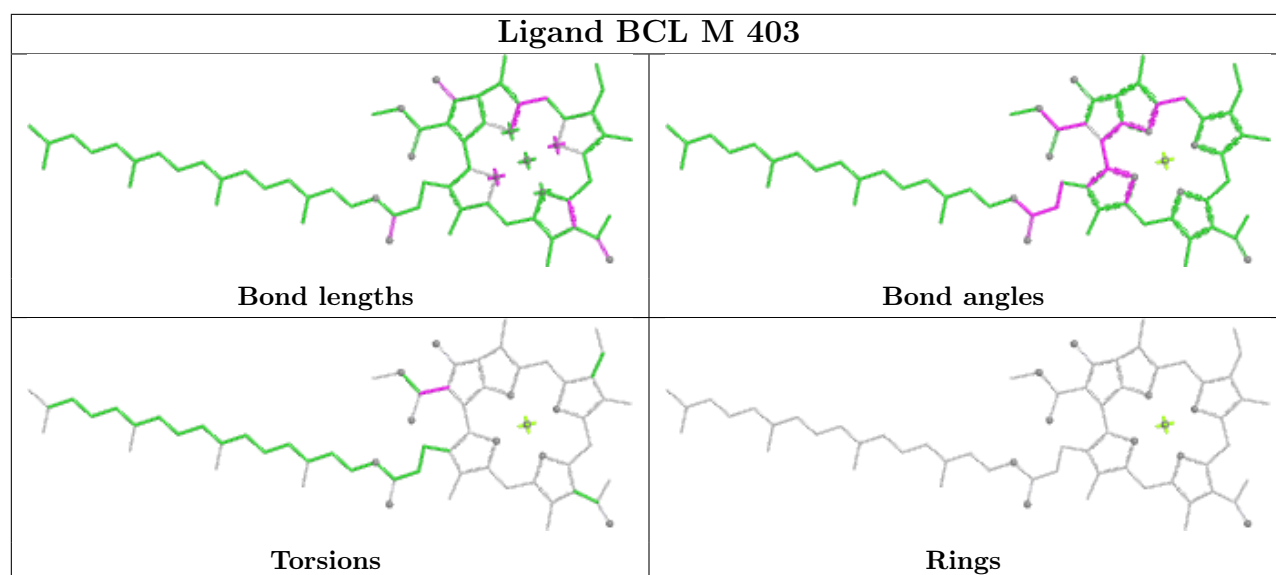
19 monomers are involved in 58 short contacts:

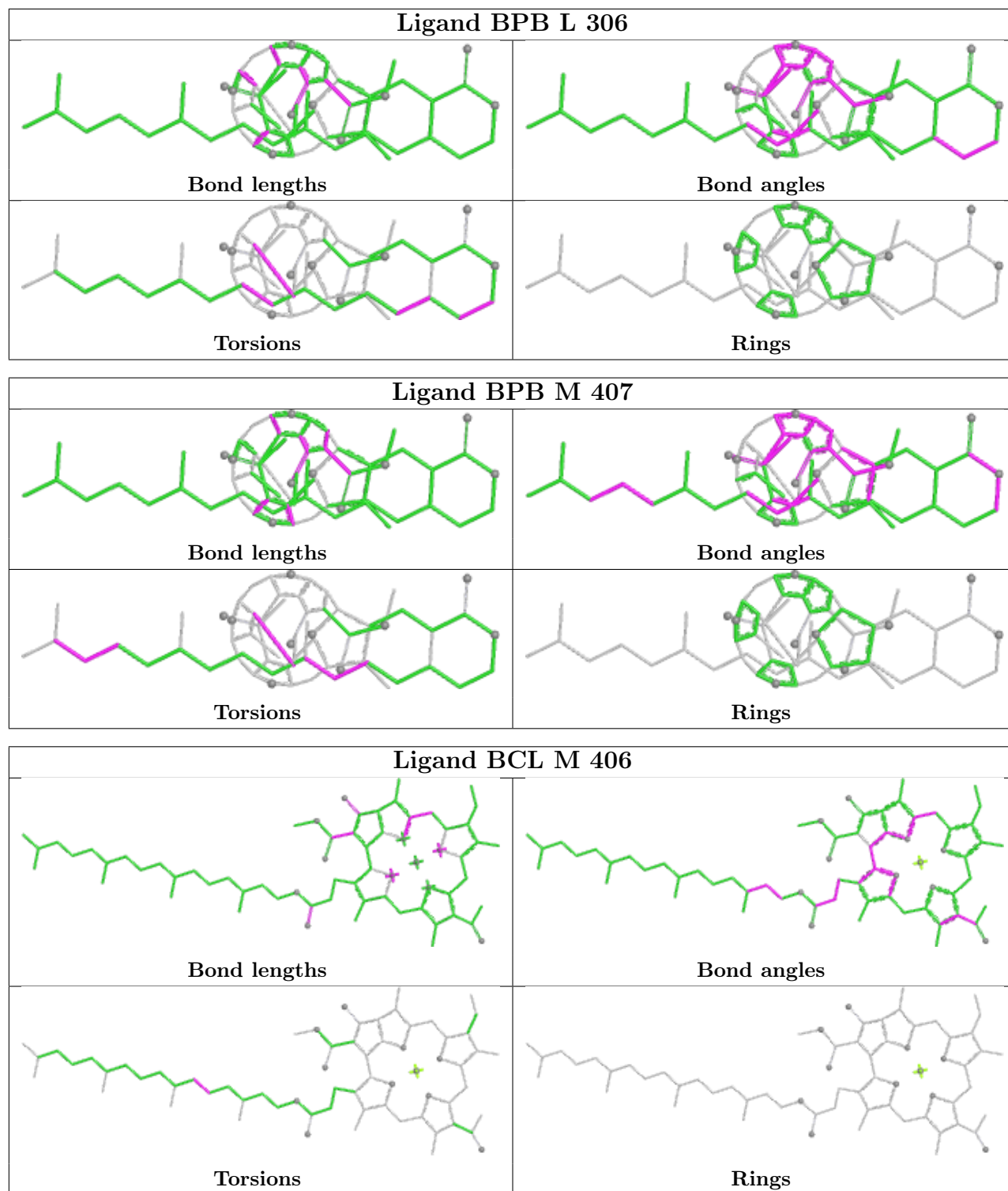
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	307	U10	8	0
12	M	404	LDA	1	0
4	L	301	EDO	1	0
17	M	414	CDL	8	0
7	M	403	BCL	1	0
4	H	302	EDO	1	0
6	M	402	HTO	6	0
7	L	305	BCL	5	0
7	L	313	BCL	5	0
5	L	303	DIO	2	0
12	M	417	LDA	5	0
12	L	312	LDA	1	0
8	M	407	BPB	2	0
7	M	406	BCL	2	0
14	M	410	SPN	7	0
9	M	409	U10	2	0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

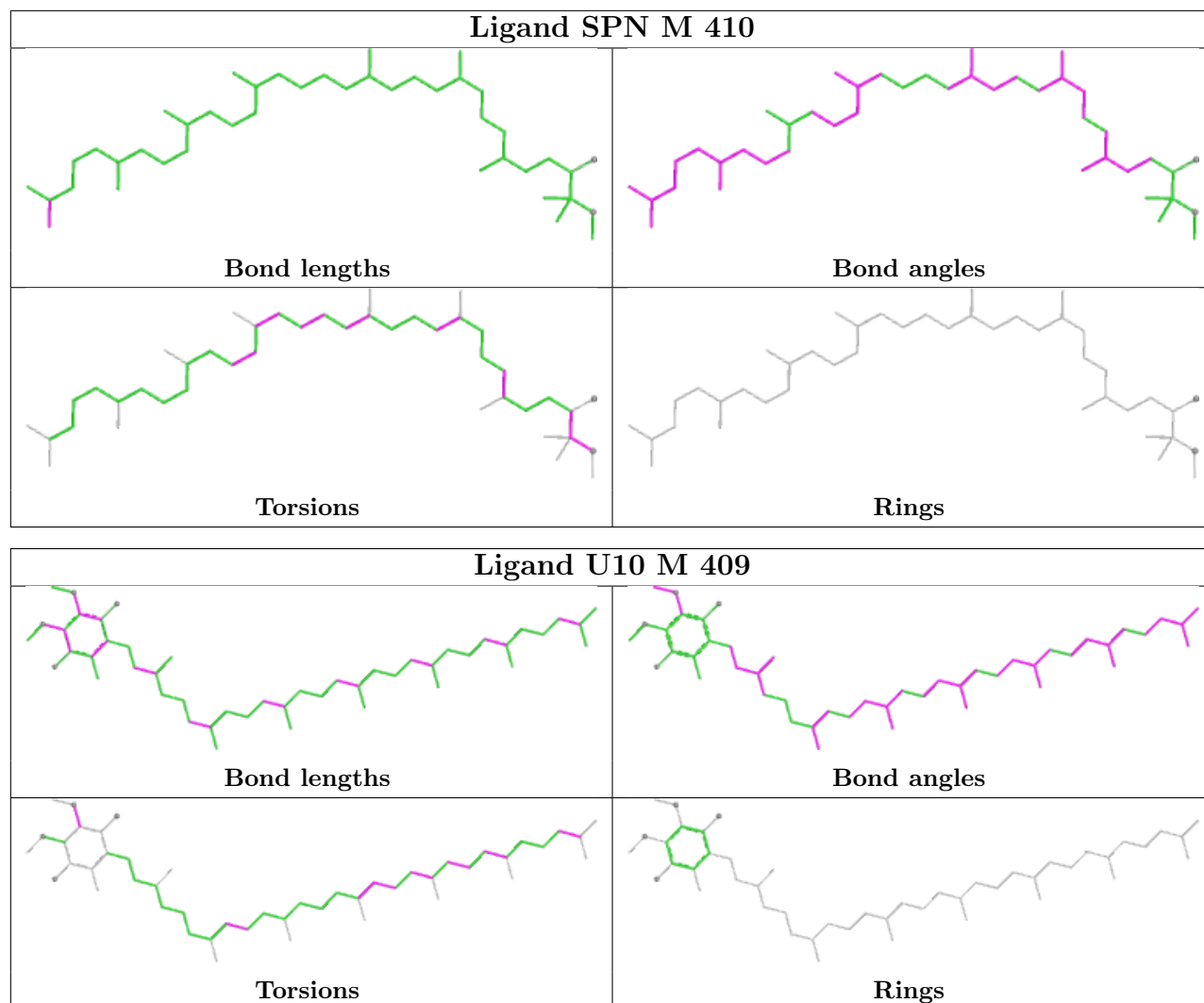
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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.









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%)	0.10	10 (3%) 46 40	47, 60, 89, 104	0
2	M	302/303 (99%)	-0.12	7 (2%) 61 55	33, 63, 88, 104	1 (0%)
3	H	239/241 (99%)	-0.01	11 (4%) 37 32	50, 60, 75, 129	0
All	All	822/825 (99%)	-0.01	28 (3%) 48 42	33, 61, 88, 129	1 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	72	GLU	6.3
1	L	73	TYR	4.9
3	H	249	LYS	4.8
3	H	247	LYS	4.1
3	H	246	PRO	4.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

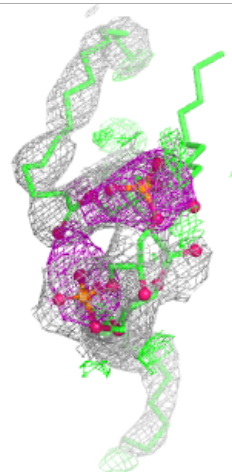
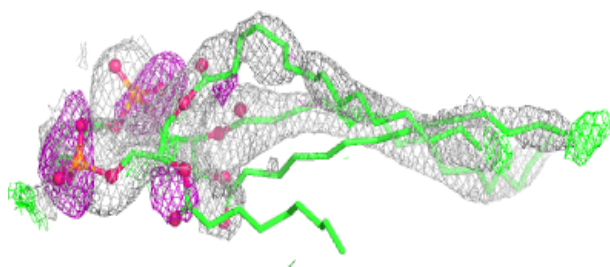
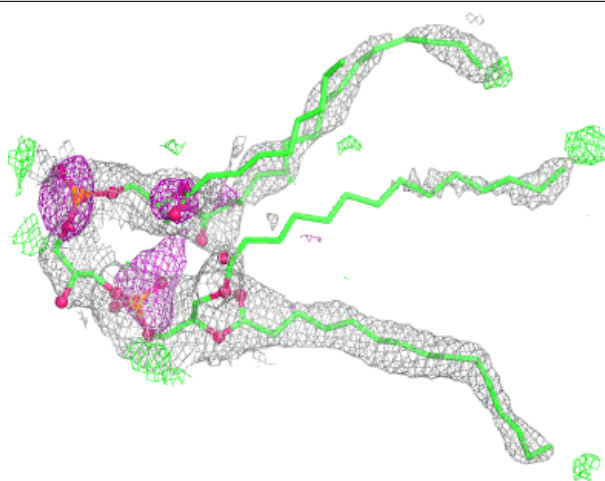
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	H	302	4/4	0.56	0.38	68,82,86,96	0
10	PO4	L	308	5/5	0.64	0.14	111,111,117,127	0
18	TRS	H	303	8/8	0.65	0.14	83,88,93,93	0
12	LDA	M	417	16/16	0.75	0.35	82,92,136,138	0
12	LDA	L	311	16/16	0.77	0.31	58,85,101,107	0
12	LDA	M	418	16/16	0.78	0.39	74,96,122,123	0
6	HTO	M	402	10/10	0.80	0.28	78,86,96,97	0
6	HTO	L	304	10/10	0.80	0.22	79,91,99,104	0
4	EDO	L	302	4/4	0.82	0.38	73,79,83,87	0
12	LDA	L	312	16/16	0.83	0.27	67,79,107,107	0
4	EDO	L	301	4/4	0.84	0.23	60,70,71,74	0
5	DIO	L	303	6/6	0.85	0.28	73,76,85,89	0
12	LDA	M	404	16/16	0.85	0.30	69,79,110,111	0
17	CDL	M	414	81/100	0.85	0.23	60,91,123,138	0
12	LDA	M	416	16/16	0.85	0.24	59,74,97,101	0
4	EDO	M	419	4/4	0.87	0.17	53,57,60,62	0
4	EDO	H	301	4/4	0.87	0.19	71,80,84,92	0
9	U10	L	307	48/63	0.87	0.33	47,71,80,84	48
4	EDO	M	405	4/4	0.88	0.16	59,68,71,78	0
10	PO4	L	309	5/5	0.88	0.42	82,88,105,111	0
11	GOL	L	310	6/6	0.89	0.16	80,84,89,90	0
14	SPN	M	410	43/43	0.91	0.17	57,74,85,93	0
12	LDA	M	415	16/16	0.92	0.19	49,69,78,79	0
10	PO4	M	413	5/5	0.93	0.06	80,83,95,95	0
9	U10	M	409	48/63	0.93	0.15	45,58,77,84	0
7	BCL	L	313	66/66	0.94	0.17	54,66,112,119	0
4	EDO	M	401	4/4	0.94	0.15	56,58,63,64	0
12	LDA	H	304	16/16	0.94	0.18	65,73,83,88	0
15	K	M	411	1/1	0.95	0.12	87,87,87,87	0
16	CL	M	412	1/1	0.95	0.15	70,70,70,70	0
8	BPB	M	407	65/65	0.96	0.12	47,66,116,124	0
8	BPB	L	306	65/65	0.96	0.09	44,51,63,70	0
7	BCL	M	406	66/66	0.97	0.10	52,59,76,96	0
7	BCL	L	305	66/66	0.97	0.08	48,56,61,65	0
15	K	H	305	1/1	0.98	0.04	69,69,69,69	0
7	BCL	M	403	66/66	0.98	0.08	40,51,64,76	0
13	FE	M	408	1/1	1.00	0.01	50,50,50,50	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.

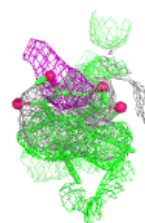
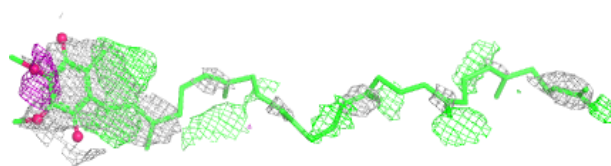
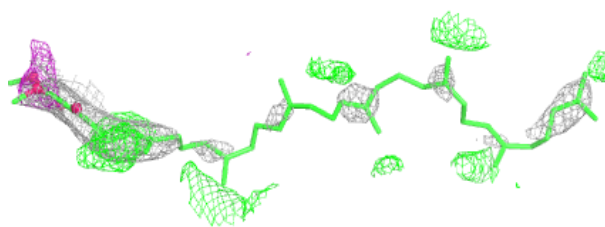
Electron density around CDL M 414:

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

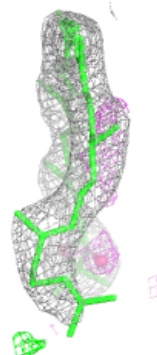
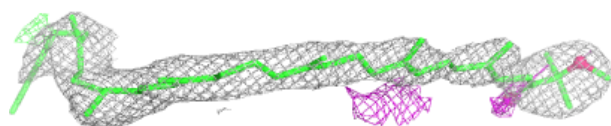
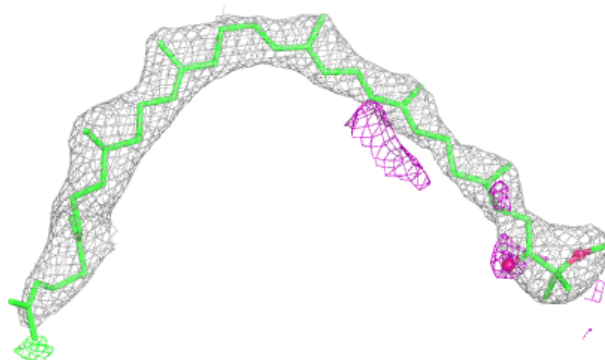


Electron density around U10 L 307:

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

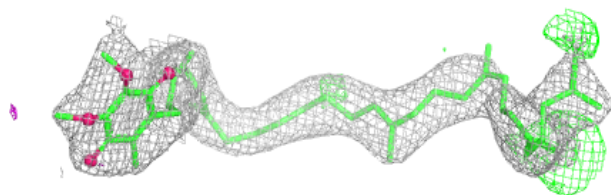
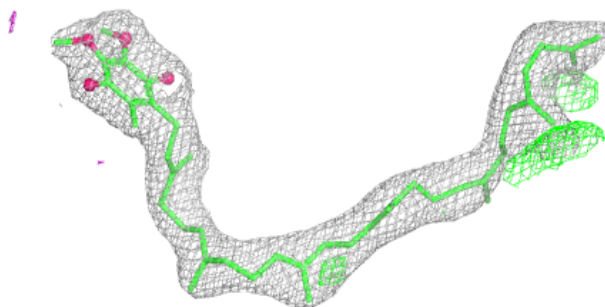
**Electron density around SPN M 410:**

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

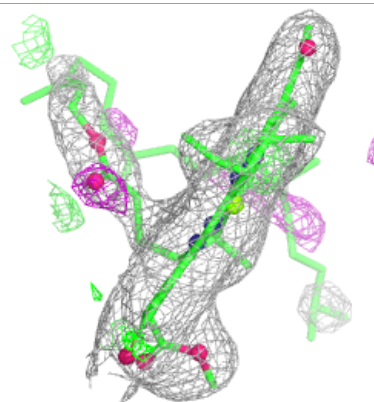
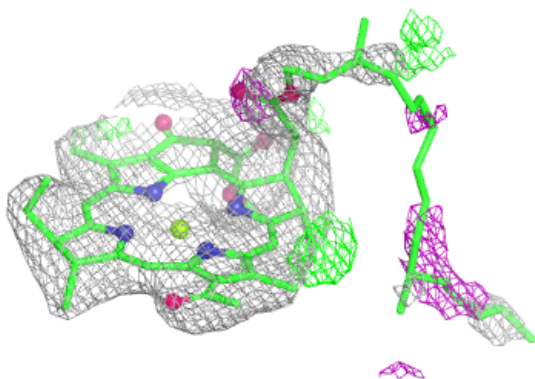
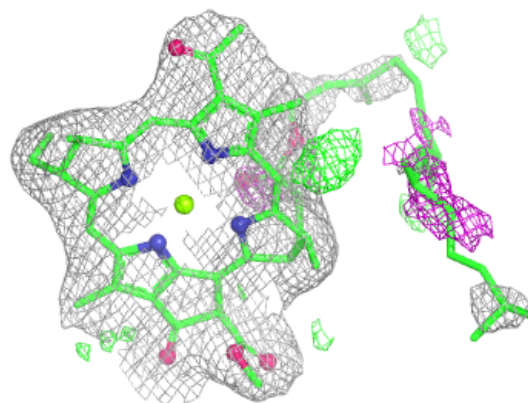


Electron density around U10 M 409:

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

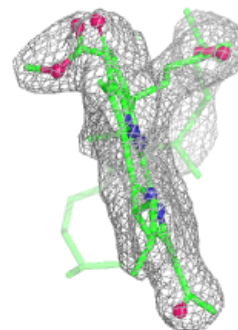
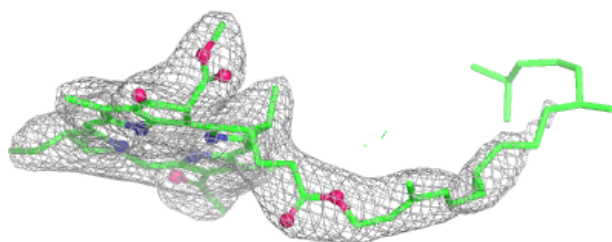
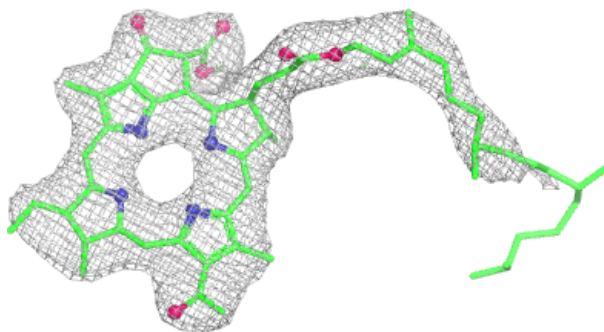
**Electron density around BCL L 313:**

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and green (positive)



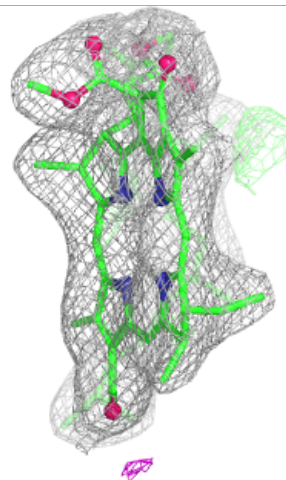
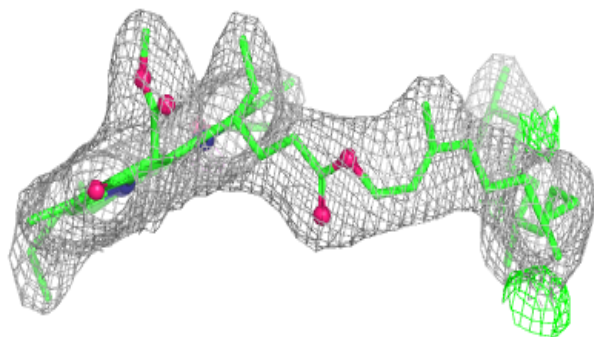
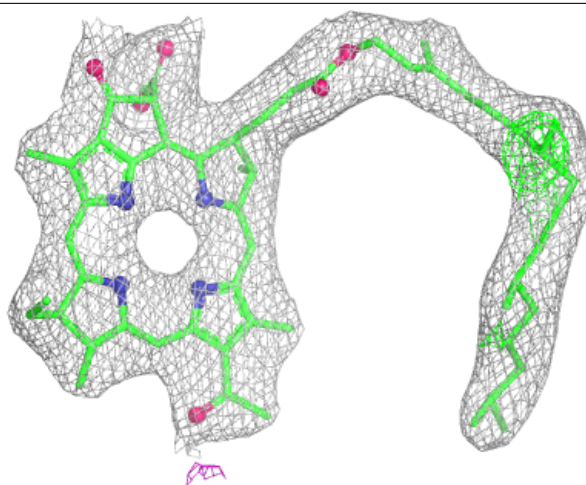
Electron density around BPB M 407:

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and green (positive)



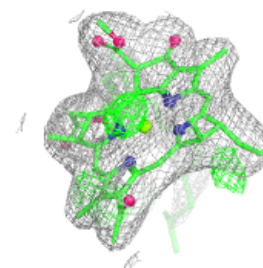
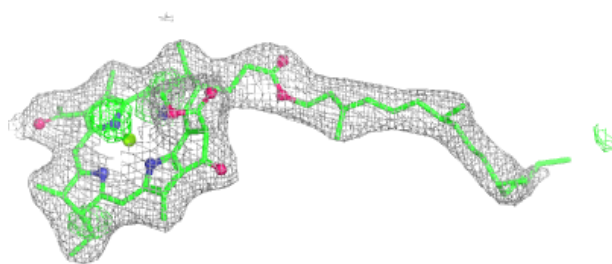
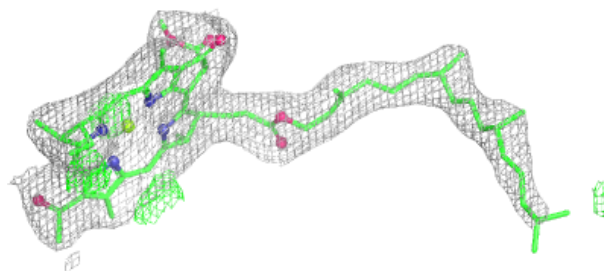
Electron density around BPB L 306:

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

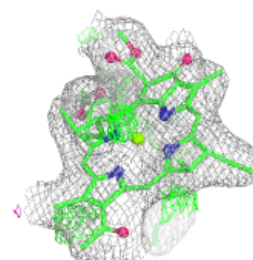
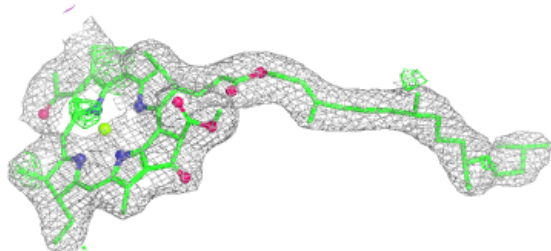
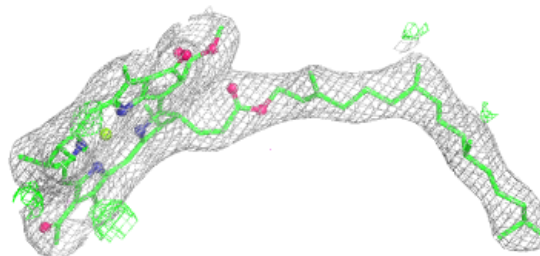


Electron density around BCL M 406:

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

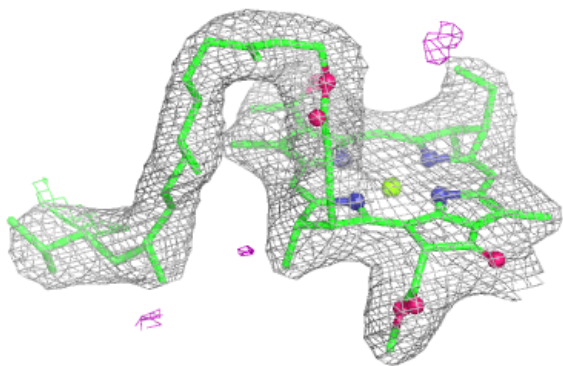
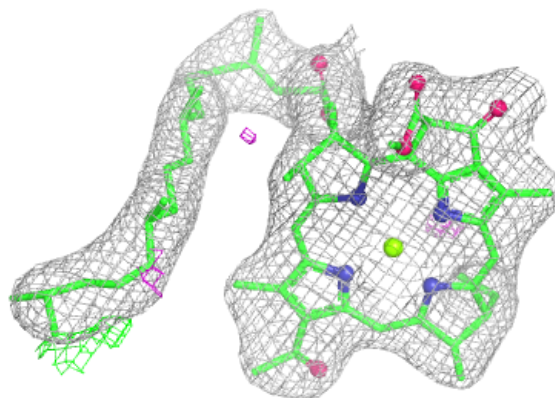
**Electron density around BCL L 305:**

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



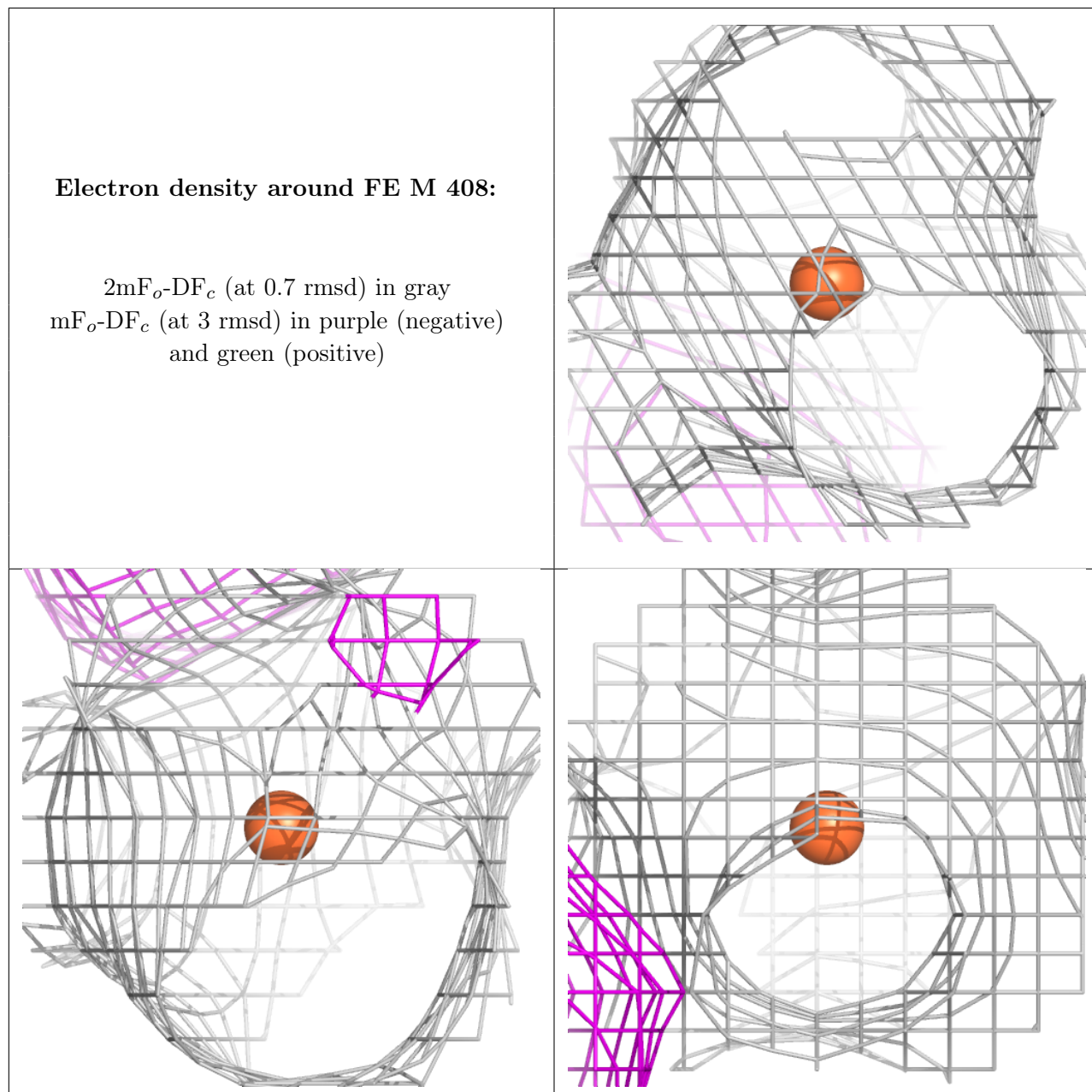
Electron density around BCL M 403:

$2mF_o-DF_c$ (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.