



wwPDB X-ray Structure Validation Summary Report

Nov 14, 2023 – 12:46 pm GMT

PDB ID : 8C6K
Title : Double mutant A(L53)C/I(L64)C structure of Photosynthetic Reaction Center From Cereibacter sphaeroides strain RV
Authors : Gabdulkhakov, A.; Selikhanov, G.; Fufina, T.; Vasilieva, L.; Atamas, A.; Uhimchuk, D.
Deposited on : 2023-01-12
Resolution : 2.86 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (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

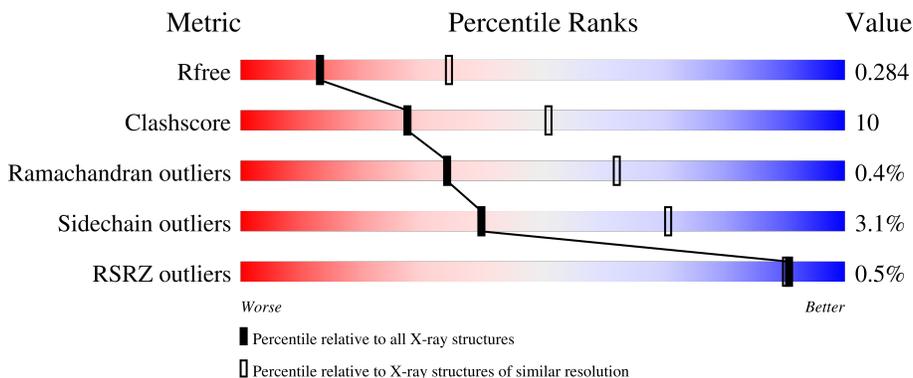
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

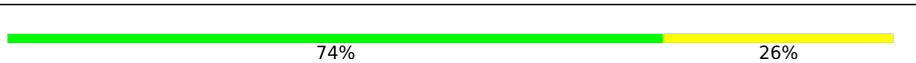
The reported resolution of this entry is 2.86 Å.

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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	H	242	 79% 19% ..
2	L	281	 76% 22% .
3	M	303	 74% 26%

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
13	HTO	L	311	-	-	-	X

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 7463 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	240	1848	1183	317	339	9	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	281	2240	1511	356	363	10	0	1	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	53	CYS	ALA	engineered mutation	UNP P0C0Y8
L	64	CYS	ILE	engineered mutation	UNP P0C0Y8
L	178	THR	SER	conflict	UNP P0C0Y8

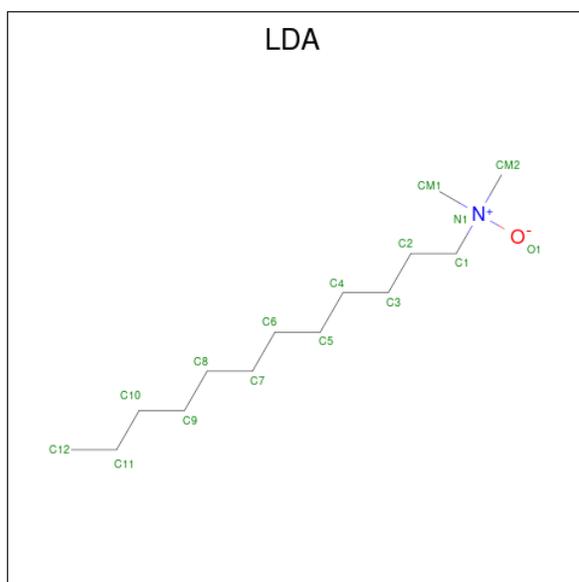
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2436	1630	397	399	10	0	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	conflict	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C₁₄H₃₁NO).

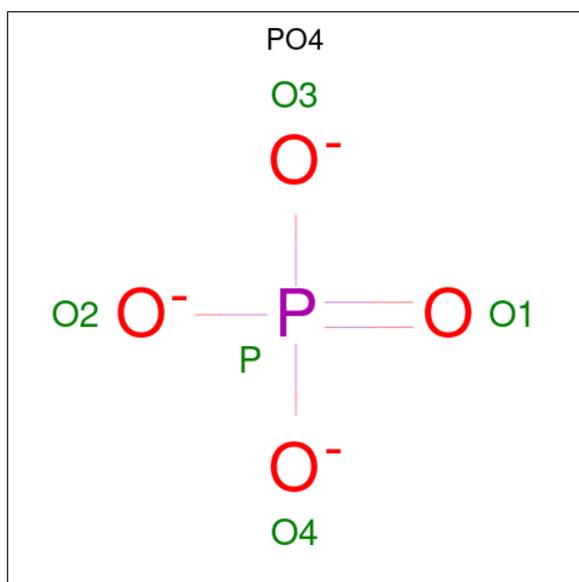


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	H	1	16	14	1	1	0	0
4	M	1	16	14	1	1	0	0
4	M	1	16	14	1	1	0	0
4	M	1	16	14	1	1	0	0
4	M	1	16	14	1	1	0	0
4	M	1	16	14	1	1	0	0

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

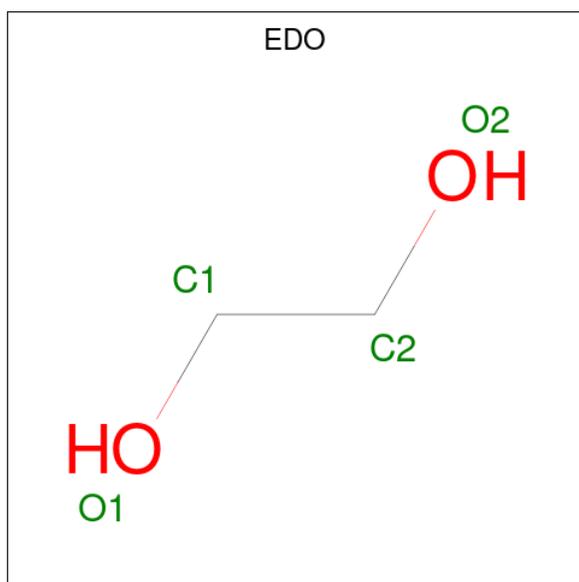
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
5	H	4	51	51	0	0
5	L	4	49	49	0	0
5	M	2	27	27	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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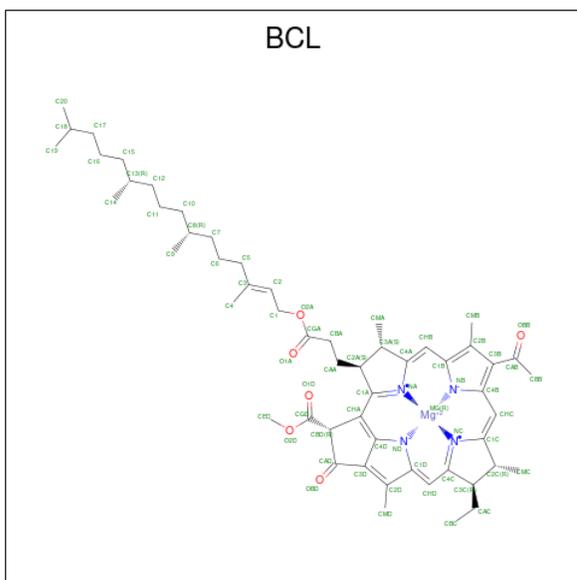
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	H	1	Total	C	O	0	0
			4	2	2		
7	L	1	Total	C	O	0	0
			4	2	2		
7	M	1	Total	C	O	0	0
			4	2	2		
7	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



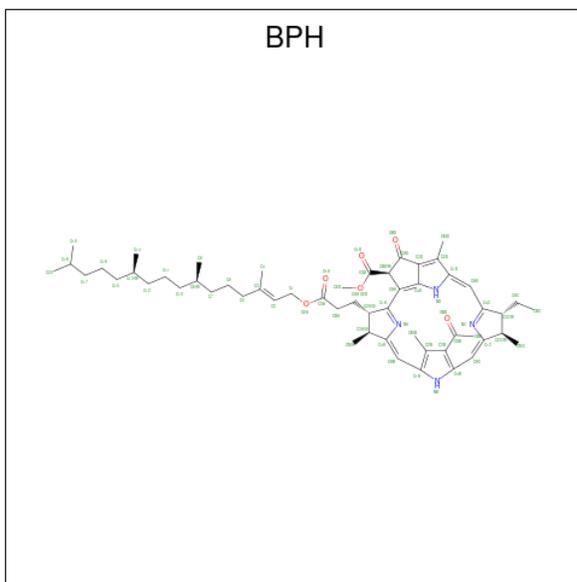
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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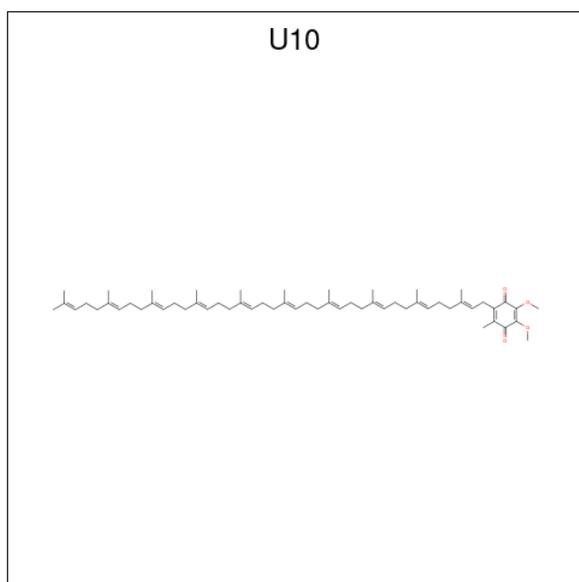
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



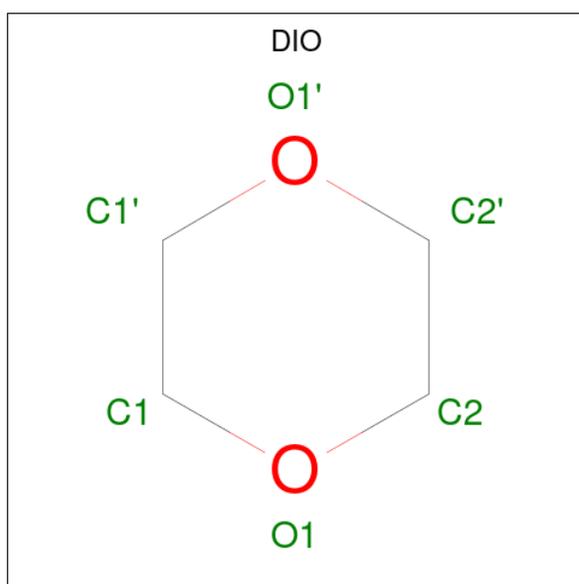
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



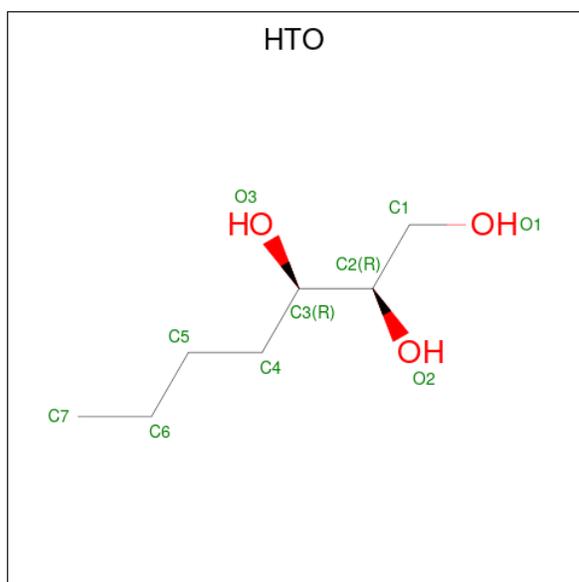
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			48	44	4		
11	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 12 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



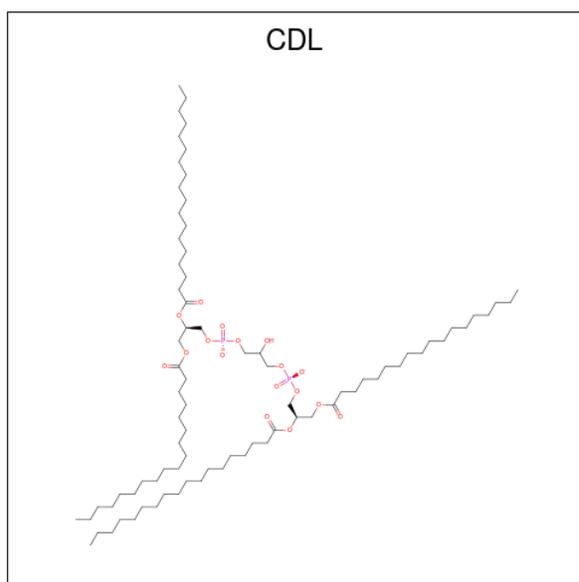
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			6	4	2		

- 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	L	1	Total	C	O	0	0
			10	7	3		
13	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

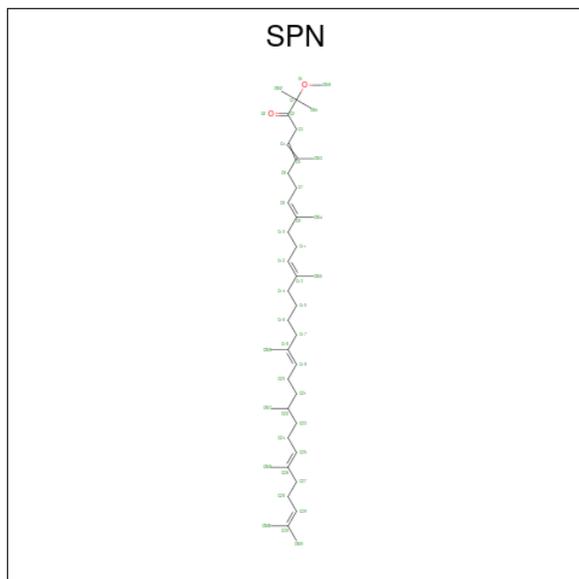


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 16 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂) (labeled as "Ligand of Interest" by depositor).



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

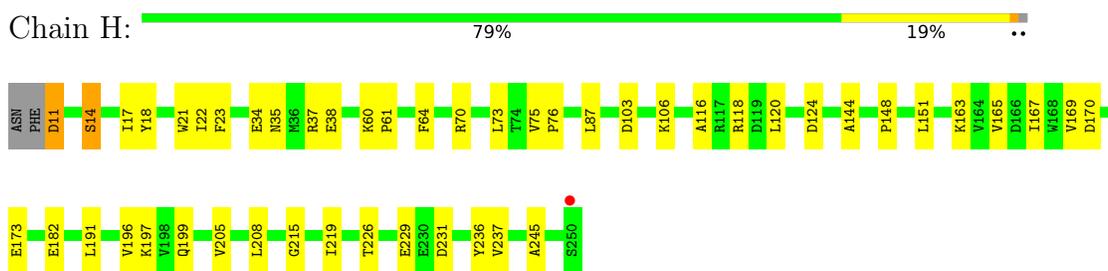
- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	H	11	Total O 11 11	0	0
17	L	12	Total O 12 12	0	0
17	M	8	Total O 8 8	0	0

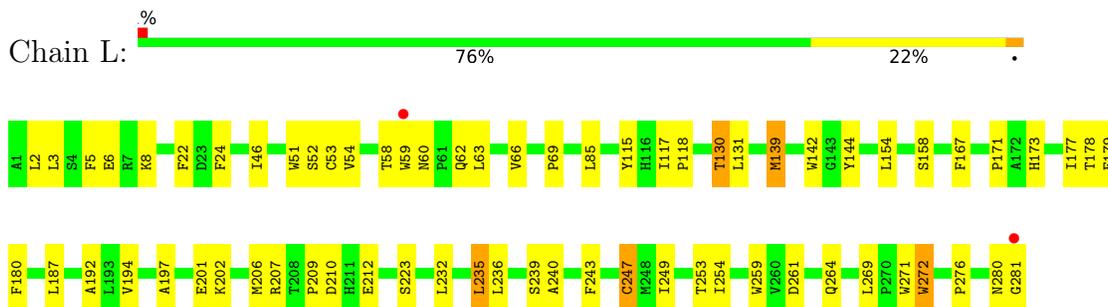
3 Residue-property plots [i](#)

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.

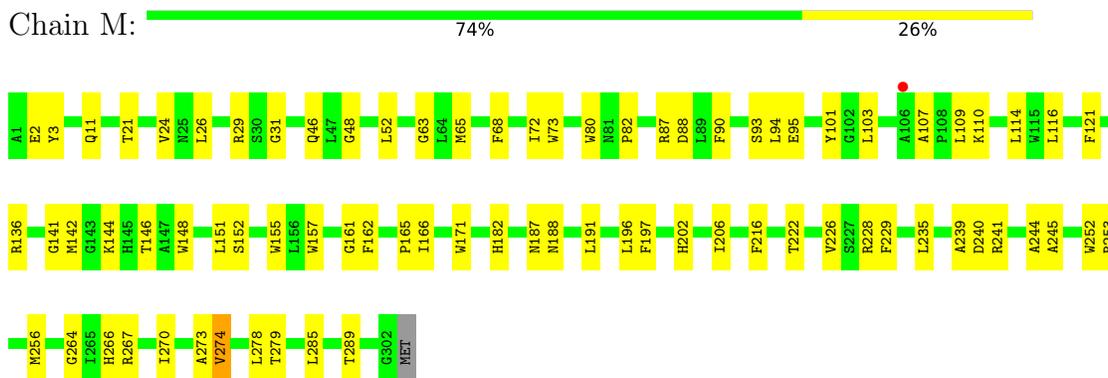
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M 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	139.64Å 139.64Å 185.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.89 – 2.86 57.48 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.89-2.86) 99.4 (57.48-2.85)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0352, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.229 , 0.279 0.240 , 0.284	Depositor DCC
R_{free} test set	2466 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	7.5	Xtrriage
Anisotropy	1.816	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	7463	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: PO4, HTO, FE, LDA, SPN, K, UNL, BCL, BPH, DIO, CDL, EDO, U10

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	H	0.47	0/1905	0.70	0/2590
2	L	0.49	0/2328	0.67	0/3186
3	M	0.46	0/2541	0.63	1/3468 (0.0%)
All	All	0.47	0/6774	0.66	1/9244 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	M	196	LEU	CA-CB-CG	5.19	127.23	115.30

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	H	1848	0	1866	32	0
2	L	2240	0	2191	52	0
3	M	2436	0	2362	62	0
4	H	16	0	31	3	0
4	M	80	0	155	4	0
5	H	51	0	0	0	0
5	L	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	27	0	0	0	0
6	H	5	0	0	0	0
6	M	10	0	0	0	0
7	H	16	0	24	2	0
7	L	4	0	6	0	0
7	M	8	0	12	2	0
8	H	1	0	0	0	0
9	L	132	0	148	7	0
9	M	132	0	148	11	0
10	L	65	0	76	1	0
10	M	65	0	76	5	0
11	L	48	0	63	3	0
11	M	48	0	63	2	0
12	L	6	0	8	1	0
13	L	20	0	32	0	0
14	M	81	0	106	10	0
15	M	1	0	0	0	0
16	M	43	0	70	5	0
17	H	11	0	0	0	0
17	L	12	0	0	0	0
17	M	8	0	0	0	0
All	All	7463	0	7437	148	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 10.

The worst 5 of 148 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)
3:M:161:GLY:HA3	16:M:407:SPN:H201	1.60	0.82
9:L:301:BCL:H2C	9:M:403:BCL:HBC2	1.66	0.75
9:M:402:BCL:H202	16:M:407:SPN:H72	1.70	0.73
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.71	0.72
2:L:206:MET:HE3	3:M:239:ALA:HB2	1.73	0.71

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	H	241/242 (100%)	230 (95%)	9 (4%)	2 (1%)	19	46
2	L	280/281 (100%)	257 (92%)	23 (8%)	0	100	100
3	M	304/303 (100%)	285 (94%)	18 (6%)	1 (0%)	41	68
All	All	825/826 (100%)	772 (94%)	50 (6%)	3 (0%)	34	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
1	H	124	ASP
3	M	240	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	198/197 (100%)	192 (97%)	6 (3%)	41	72
2	L	222/221 (100%)	214 (96%)	8 (4%)	35	66
3	M	240/237 (101%)	232 (97%)	8 (3%)	38	68
All	All	660/655 (101%)	638 (97%)	22 (3%)	40	68

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	2[A]	GLU
3	M	52[B]	LEU
3	M	52[A]	LEU
3	M	182	HIS
2	L	130	THR

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

Mol	Chain	Res	Type
1	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 41 ligands modelled in this entry, 10 are unknown and 2 are monoatomic - leaving 29 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	$\# Z > 2$
11	U10	M	406	-	48,48,63	2.61	14 (29%)	58,61,79	1.93	16 (27%)
16	SPN	M	407	-	40,42,42	0.52	0	50,52,52	1.06	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	M	408	-	12,15,15	2.04	1 (8%)	14,17,17	0.96	1 (7%)
7	EDO	H	309	-	3,3,3	0.65	0	2,2,2	0.23	0
9	BCL	L	302	-	64,74,74	1.38	6 (9%)	78,115,115	1.77	17 (21%)
4	LDA	M	411	-	12,15,15	2.11	1 (8%)	14,17,17	0.51	0
13	HTO	L	311	-	9,9,9	0.56	0	10,10,10	1.44	2 (20%)
4	LDA	M	410	-	12,15,15	2.09	1 (8%)	14,17,17	0.75	1 (7%)
4	LDA	M	418	-	12,15,15	2.06	1 (8%)	14,17,17	0.53	0
6	PO4	H	306	-	4,4,4	0.77	0	6,6,6	0.61	0
10	BPH	M	404	-	51,70,70	0.84	1 (1%)	52,101,101	1.45	8 (15%)
9	BCL	L	301	-	64,74,74	1.43	7 (10%)	78,115,115	1.49	13 (16%)
13	HTO	L	312	-	9,9,9	0.49	0	10,10,10	0.88	1 (10%)
6	PO4	M	415	-	4,4,4	0.80	0	6,6,6	0.99	0
7	EDO	H	308	-	3,3,3	0.55	0	2,2,2	0.14	0
7	EDO	H	310	-	3,3,3	0.56	0	2,2,2	0.30	0
14	CDL	M	401	-	80,80,99	0.59	1 (1%)	86,92,111	0.41	0
7	EDO	M	417	-	3,3,3	0.52	0	2,2,2	0.48	0
9	BCL	M	403	-	64,74,74	1.45	8 (12%)	78,115,115	1.65	13 (16%)
12	DIO	L	309	-	6,6,6	1.17	1 (16%)	6,6,6	0.40	0
9	BCL	M	402	-	64,74,74	1.49	7 (10%)	78,115,115	1.75	16 (20%)
7	EDO	M	416	-	3,3,3	0.49	0	2,2,2	0.39	0
4	LDA	M	409	-	12,15,15	2.01	1 (8%)	14,17,17	0.55	0
4	LDA	H	301	-	12,15,15	1.88	1 (8%)	14,17,17	0.80	0
7	EDO	L	310	-	3,3,3	0.48	0	2,2,2	0.37	0
6	PO4	M	414	-	4,4,4	0.69	0	6,6,6	0.67	0
10	BPH	L	303	-	51,70,70	1.04	3 (5%)	52,101,101	1.43	8 (15%)
7	EDO	H	307	-	3,3,3	0.54	0	2,2,2	0.48	0
11	U10	L	304	-	48,48,63	2.60	13 (27%)	58,61,79	1.94	12 (20%)

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
11	U10	M	406	-	-	16/45/69/87	0/1/1/1
16	SPN	M	407	-	-	11/50/51/51	-
4	LDA	M	408	-	-	8/13/13/13	-
7	EDO	H	309	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	L	302	-	-	3/37/137/137	-
4	LDA	M	411	-	-	7/13/13/13	-
13	HTO	L	311	-	-	8/10/10/10	-
4	LDA	M	410	-	-	3/13/13/13	-
4	LDA	M	418	-	-	7/13/13/13	-
10	BPH	M	404	-	-	13/37/105/105	0/5/6/6
9	BCL	L	301	-	-	4/37/137/137	-
13	HTO	L	312	-	-	6/10/10/10	-
7	EDO	H	308	-	-	0/1/1/1	-
7	EDO	H	310	-	-	0/1/1/1	-
14	CDL	M	401	-	-	51/91/91/110	-
7	EDO	M	417	-	-	0/1/1/1	-
9	BCL	M	403	-	-	3/37/137/137	-
12	DIO	L	309	-	-	-	0/1/1/1
9	BCL	M	402	-	-	4/37/137/137	-
7	EDO	M	416	-	-	1/1/1/1	-
4	LDA	M	409	-	-	6/13/13/13	-
4	LDA	H	301	-	-	4/13/13/13	-
7	EDO	L	310	-	-	1/1/1/1	-
10	BPH	L	303	-	-	6/37/105/105	0/5/6/6
7	EDO	H	307	-	-	1/1/1/1	-
11	U10	L	304	-	-	19/45/69/87	0/1/1/1

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	411	LDA	O1-N1	-7.25	1.25	1.42
4	M	410	LDA	O1-N1	-7.12	1.25	1.42
4	M	418	LDA	O1-N1	-7.06	1.25	1.42
4	M	408	LDA	O1-N1	-6.94	1.25	1.42
4	M	409	LDA	O1-N1	-6.87	1.26	1.42

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	402	BCL	CHD-C1D-ND	-6.39	118.58	124.45
9	L	302	BCL	CHD-C1D-ND	-5.93	119.00	124.45
9	M	402	BCL	C1D-ND-C4D	-5.11	102.70	106.33
9	M	403	BCL	CHD-C1D-ND	-5.00	119.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	304	U10	C7-C8-C9	-4.89	118.65	126.79

There are no chirality outliers.

5 of 182 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	408	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-CM1
4	M	410	LDA	C2-C1-N1-CM2
4	M	418	LDA	C2-C1-N1-O1
4	M	418	LDA	C2-C1-N1-CM1

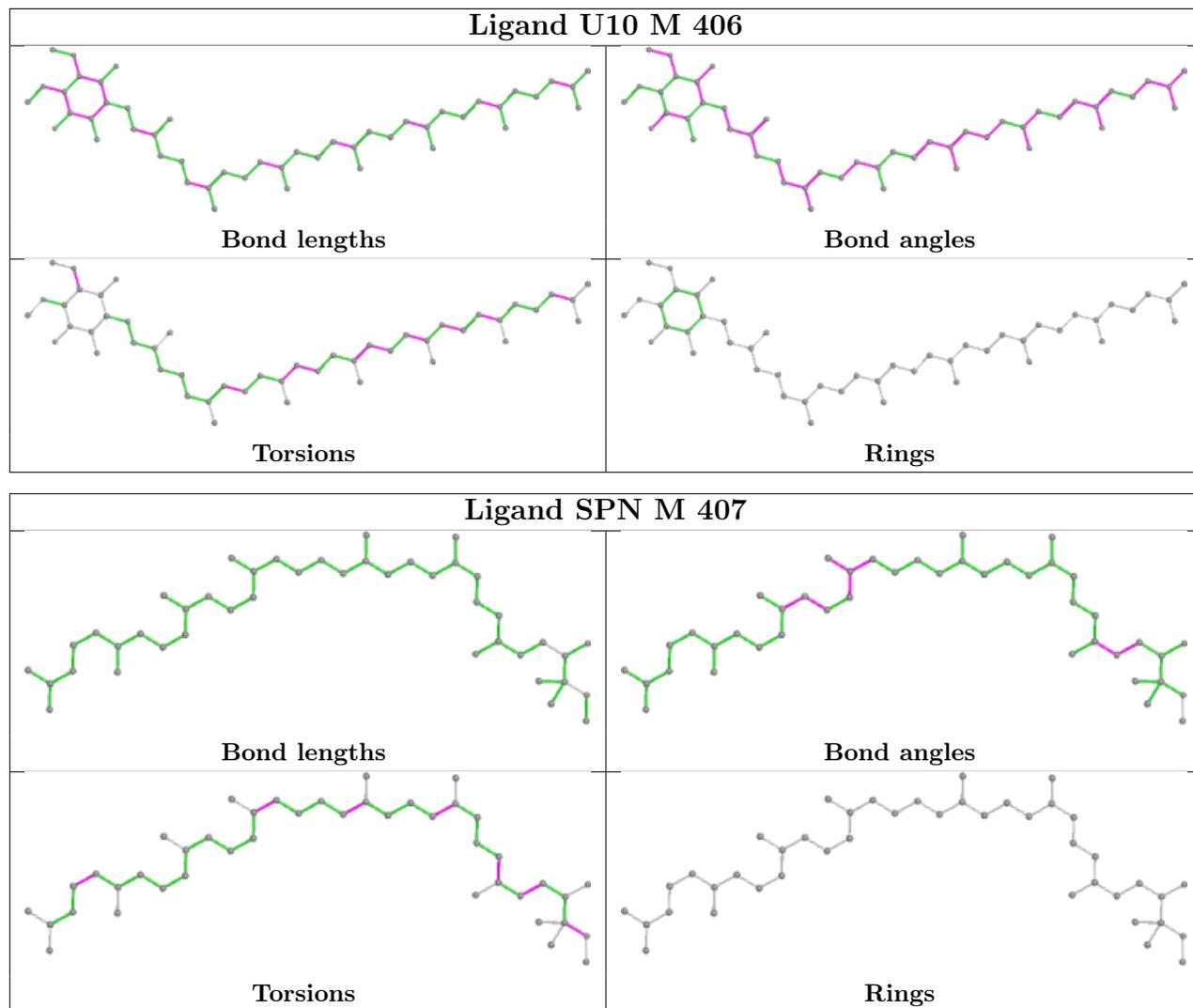
There are no ring outliers.

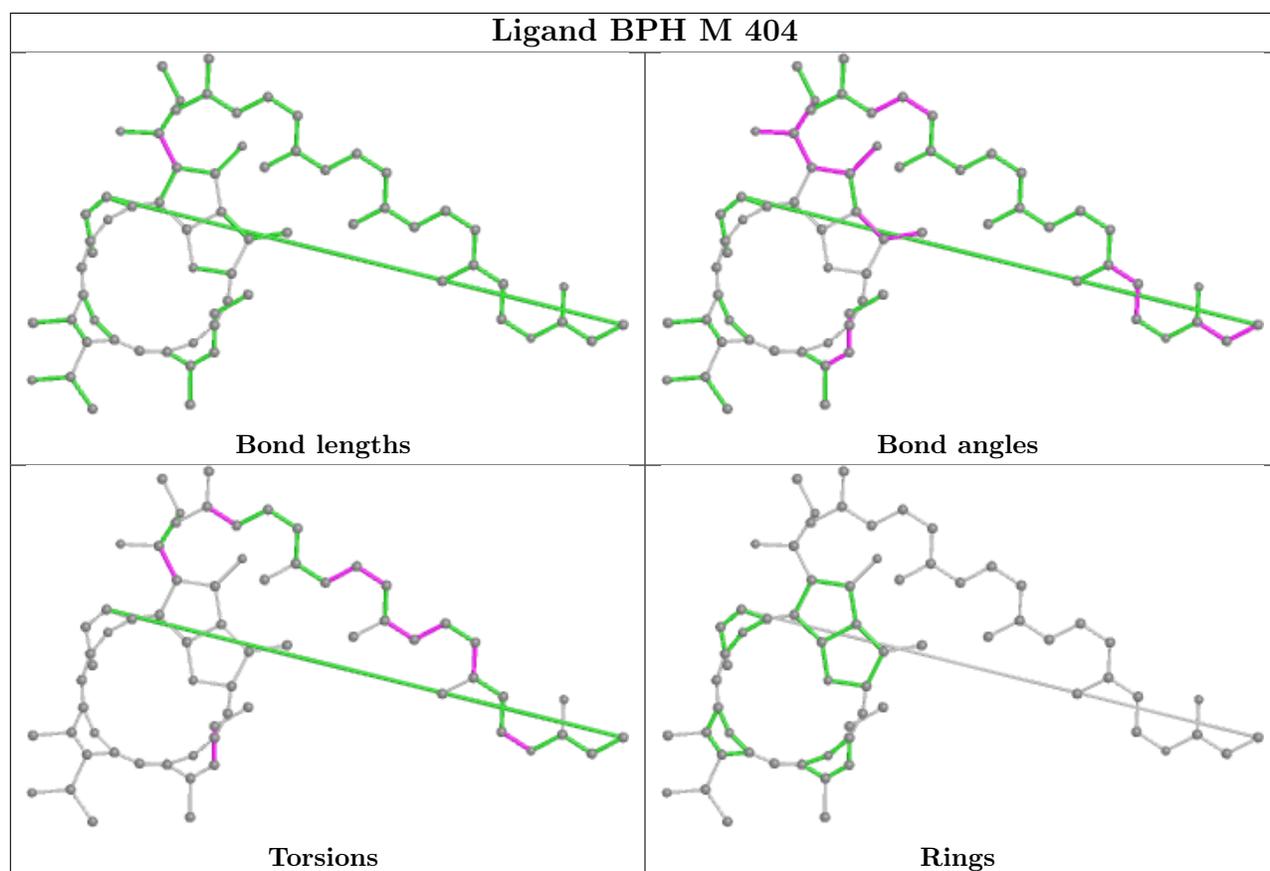
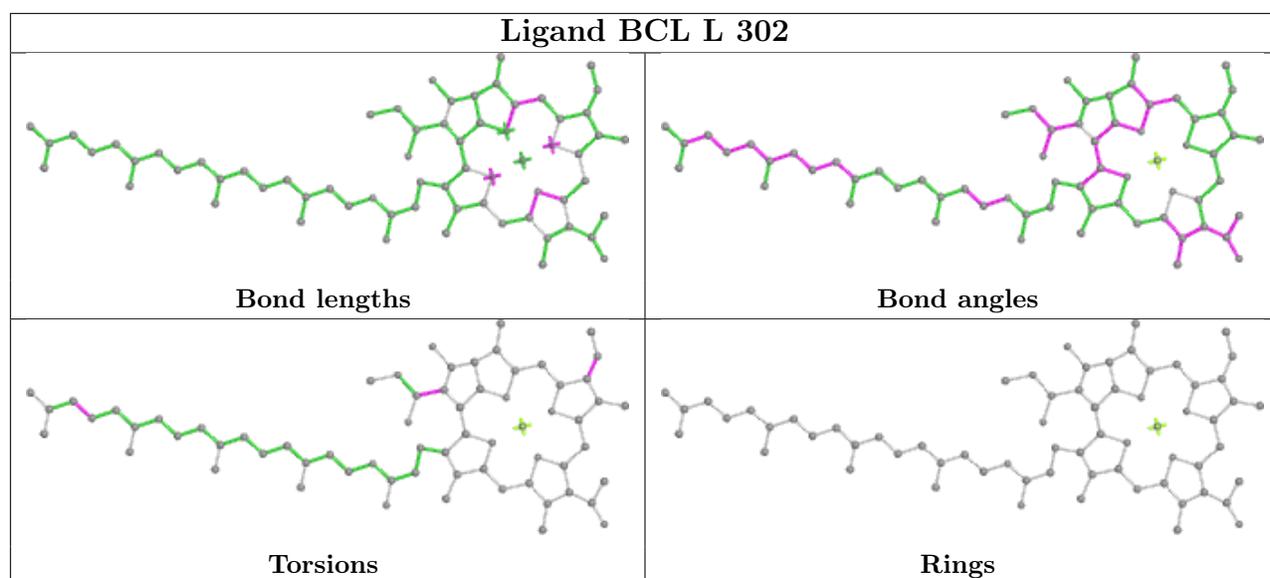
18 monomers are involved in 46 short contacts:

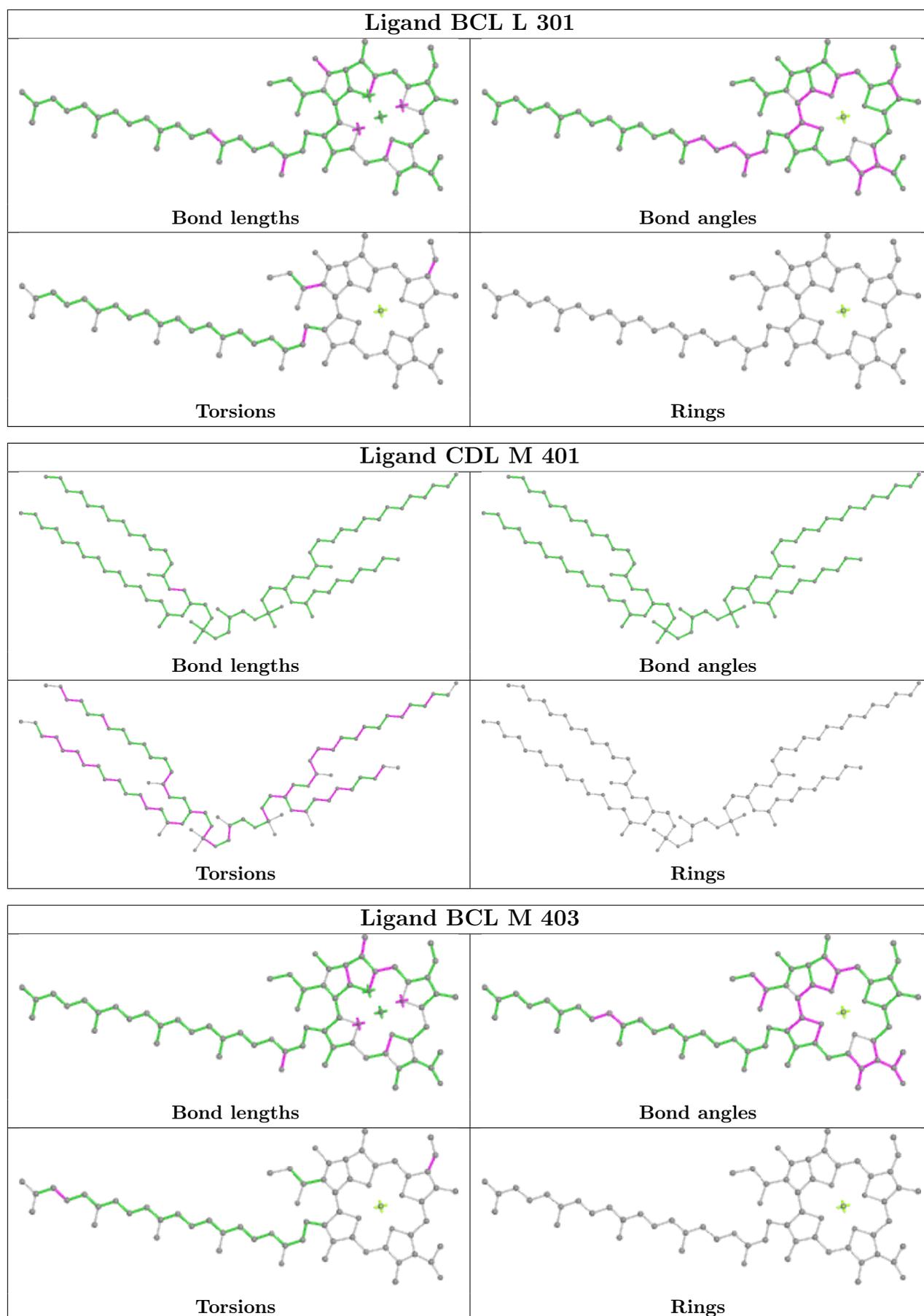
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	406	U10	2	0
16	M	407	SPN	5	0
4	M	408	LDA	1	0
9	L	302	BCL	3	0
4	M	410	LDA	1	0
4	M	418	LDA	2	0
10	M	404	BPH	5	0
9	L	301	BCL	5	0
7	H	308	EDO	1	0
7	H	310	EDO	1	0
14	M	401	CDL	10	0
9	M	403	BCL	6	0
12	L	309	DIO	1	0
9	M	402	BCL	5	0
7	M	416	EDO	2	0
4	H	301	LDA	3	0
10	L	303	BPH	1	0
11	L	304	U10	3	0

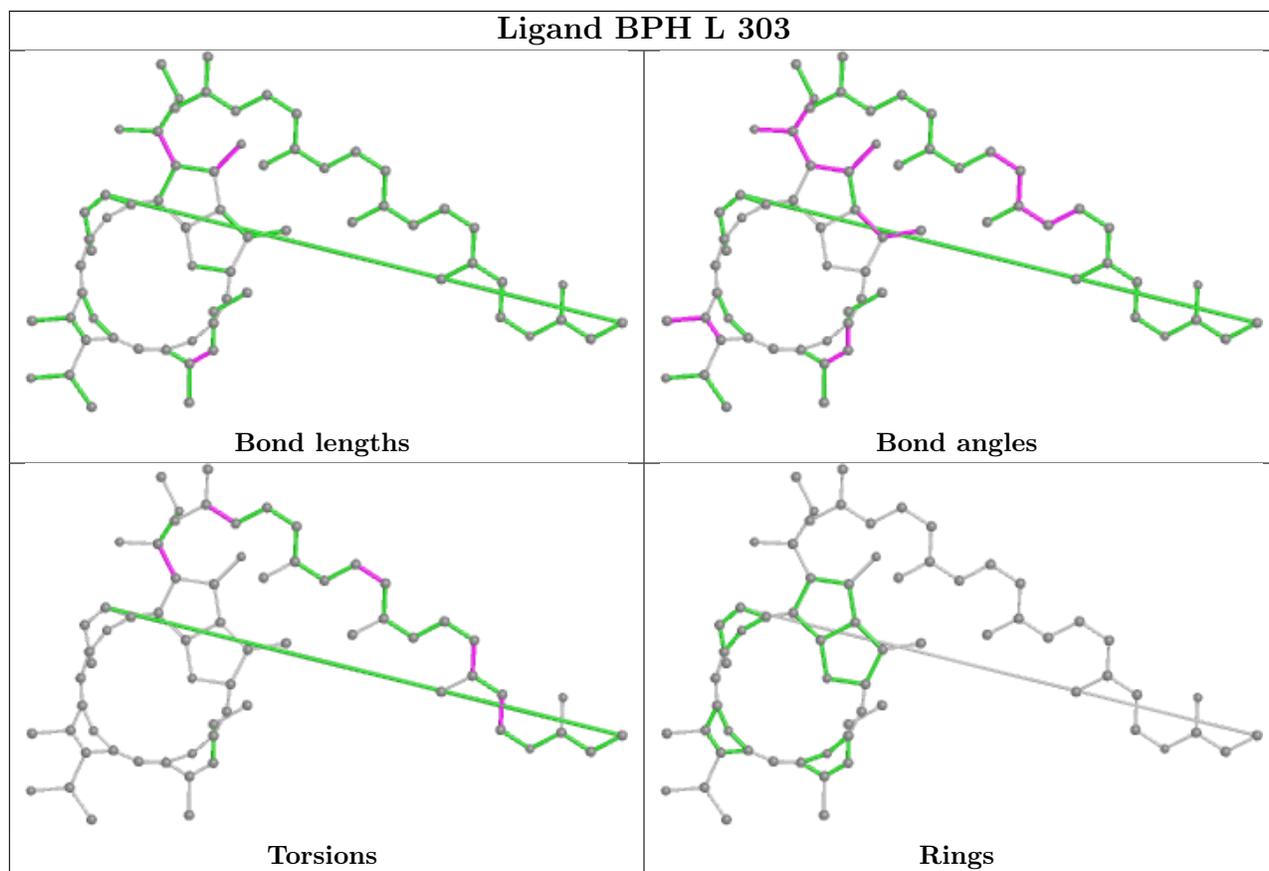
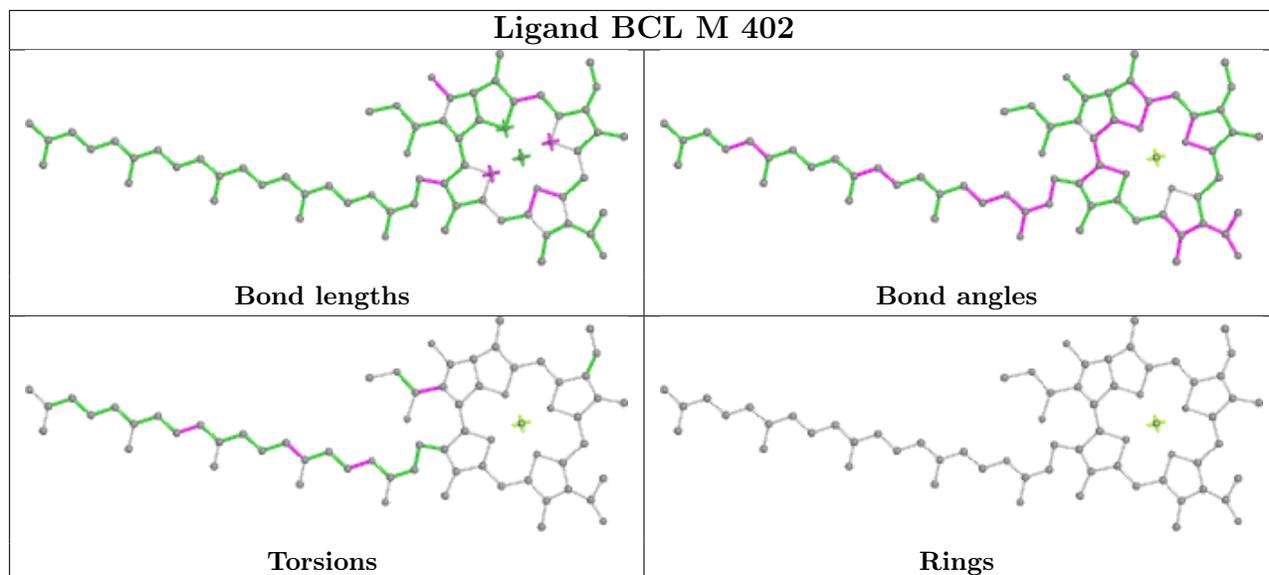
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

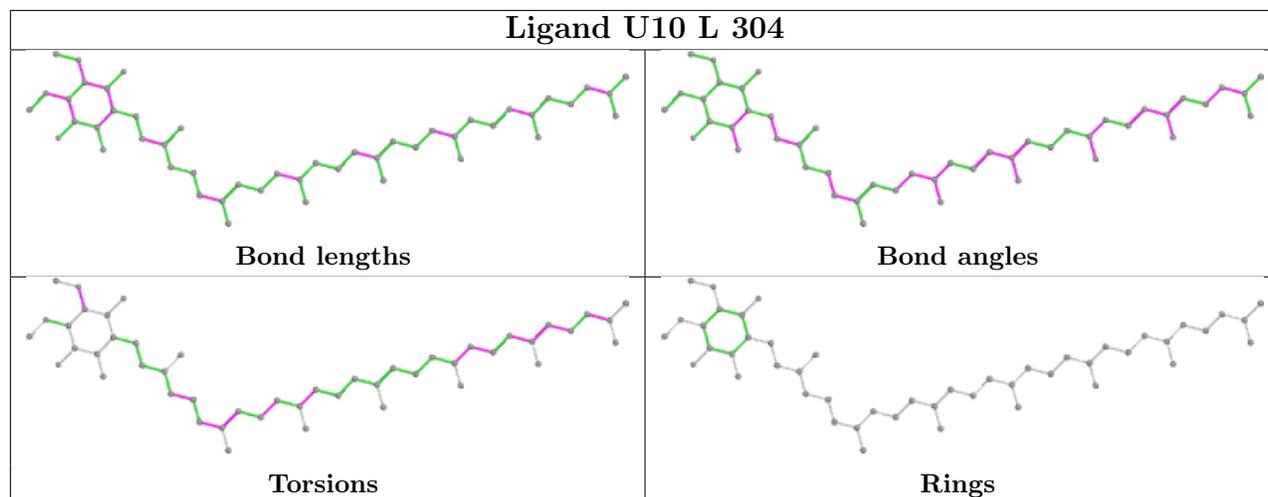
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers 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	H	240/242 (99%)	-0.60	1 (0%) 92 92	3, 12, 31, 88	0
2	L	281/281 (100%)	-0.56	2 (0%) 87 87	2, 11, 45, 99	0
3	M	302/303 (99%)	-0.57	1 (0%) 94 94	2, 12, 33, 64	0
All	All	823/826 (99%)	-0.58	4 (0%) 91 90	2, 12, 36, 99	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.9
2	L	59	TRP	4.1
2	L	281	GLY	3.3
3	M	106	ALA	2.3

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

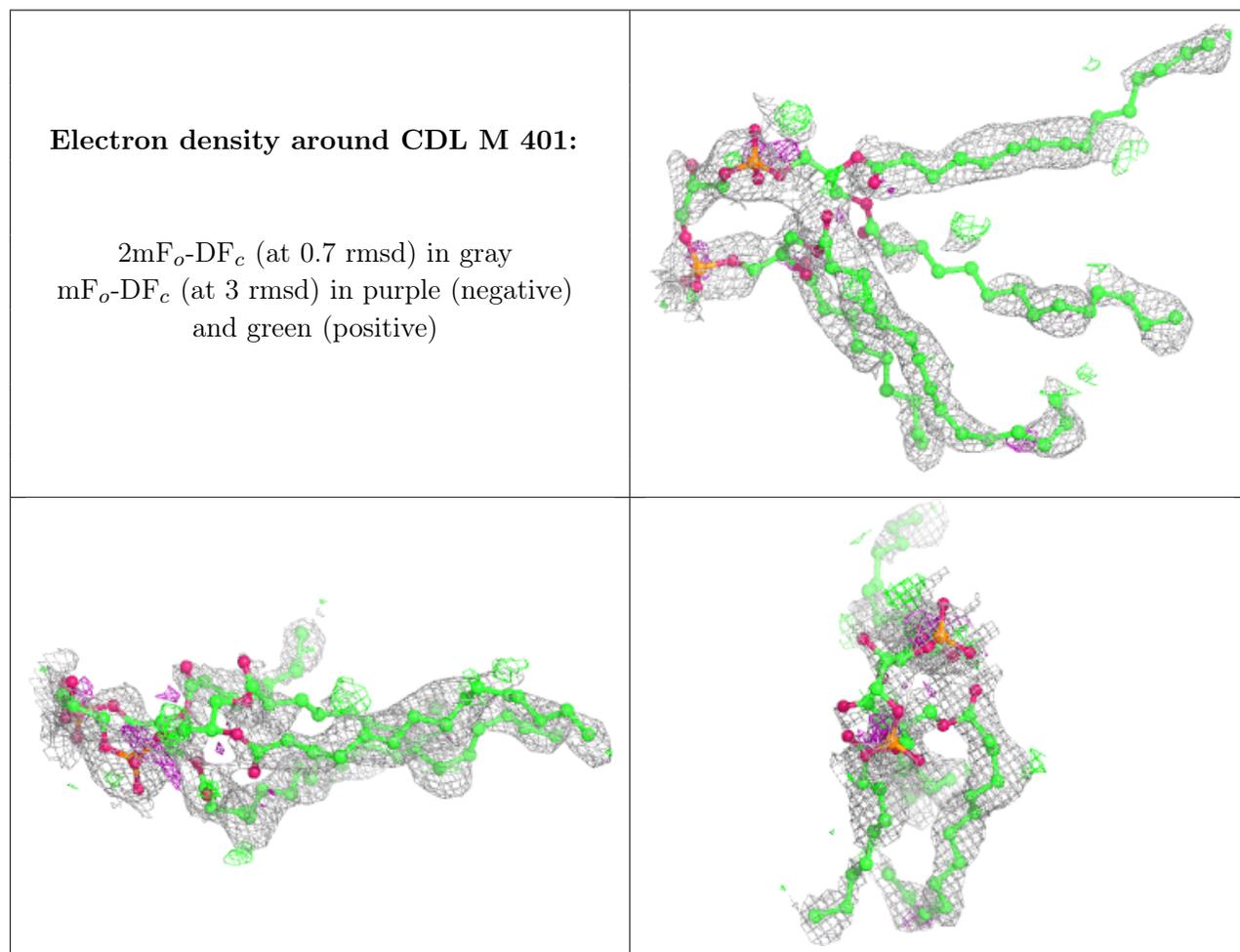
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	HTO	L	311	10/10	0.79	0.46	13,40,50,61	10
7	EDO	H	310	4/4	0.81	0.25	17,21,30,33	0
14	CDL	M	401	81/100	0.81	0.37	5,45,99,121	0
4	LDA	M	410	16/16	0.83	0.28	12,22,71,79	0
5	UNL	L	307	10/-	0.84	0.57	19,42,59,70	0
4	LDA	M	411	16/16	0.84	0.57	22,46,70,71	0
4	LDA	M	418	16/16	0.85	0.48	31,42,60,62	0
11	U10	L	304	48/63	0.85	0.26	7,25,39,51	0
5	UNL	L	308	12/-	0.86	0.28	6,30,58,62	0
5	UNL	M	413	12/-	0.86	0.30	12,25,37,40	0
4	LDA	M	409	16/16	0.86	0.28	6,25,61,69	0
6	PO4	M	415	5/5	0.88	0.27	16,32,55,61	5
5	UNL	H	303	12/-	0.89	0.38	18,25,44,56	0
5	UNL	M	412	15/-	0.89	0.18	15,20,35,39	0
5	UNL	H	305	15/-	0.90	0.33	1,31,51,60	0
12	DIO	L	309	6/6	0.90	0.24	25,31,37,37	0
7	EDO	H	309	4/4	0.90	0.26	12,16,34,35	0
5	UNL	L	305	12/-	0.90	0.35	15,30,40,48	0
5	UNL	L	306	15/-	0.91	0.32	5,18,41,48	0
13	HTO	L	312	10/10	0.91	0.67	22,64,78,78	0
4	LDA	H	301	16/16	0.91	0.24	14,27,43,44	0
7	EDO	H	308	4/4	0.92	0.41	20,43,44,55	0
5	UNL	H	304	12/-	0.93	0.27	14,34,46,52	0
16	SPN	M	407	43/43	0.93	0.21	2,14,30,56	0
8	K	H	311	1/1	0.94	0.08	19,19,19,19	0
10	BPH	M	404	65/65	0.94	0.16	2,12,48,64	0
4	LDA	M	408	16/16	0.94	0.17	1,9,25,26	0
11	U10	M	406	48/63	0.94	0.17	1,8,26,43	0
5	UNL	H	302	12/-	0.94	0.20	6,17,24,39	0
7	EDO	H	307	4/4	0.94	0.15	9,14,15,19	0
7	EDO	L	310	4/4	0.94	0.33	19,31,40,44	0
7	EDO	M	416	4/4	0.94	0.27	19,23,27,36	0
7	EDO	M	417	4/4	0.94	0.21	6,8,9,10	0
6	PO4	M	414	5/5	0.95	0.09	22,24,52,58	0
6	PO4	H	306	5/5	0.95	0.15	29,55,63,72	0
9	BCL	M	402	66/66	0.95	0.15	1,7,30,41	0
9	BCL	M	403	66/66	0.95	0.15	1,4,19,28	0
9	BCL	L	301	66/66	0.96	0.14	1,3,11,24	0
9	BCL	L	302	66/66	0.96	0.15	1,7,18,30	0
10	BPH	L	303	65/65	0.97	0.12	1,5,13,22	0
15	FE	M	405	1/1	0.99	0.06	6,6,6,6	0

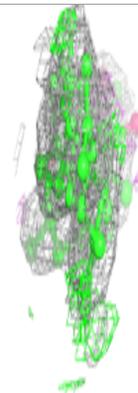
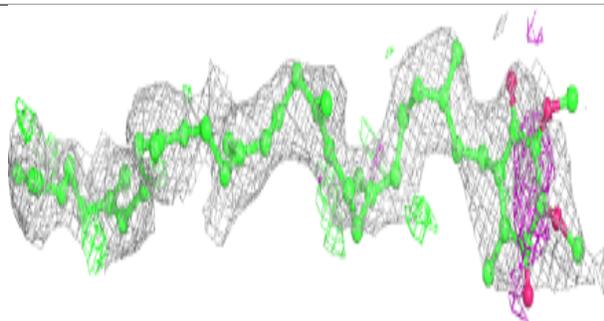
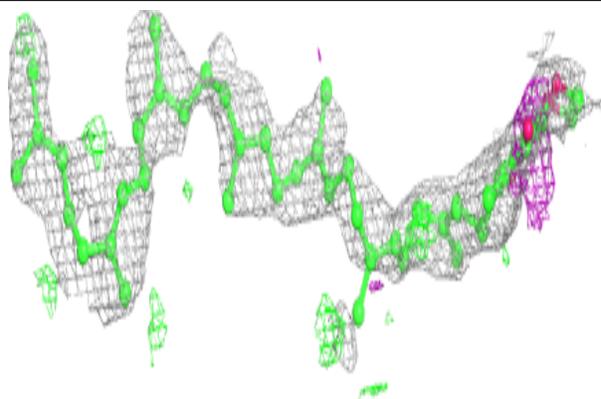
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

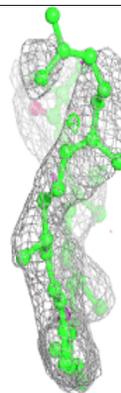
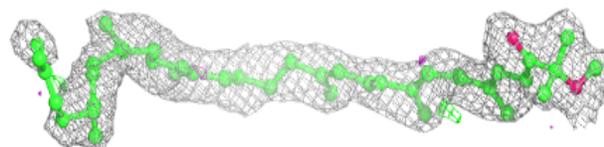
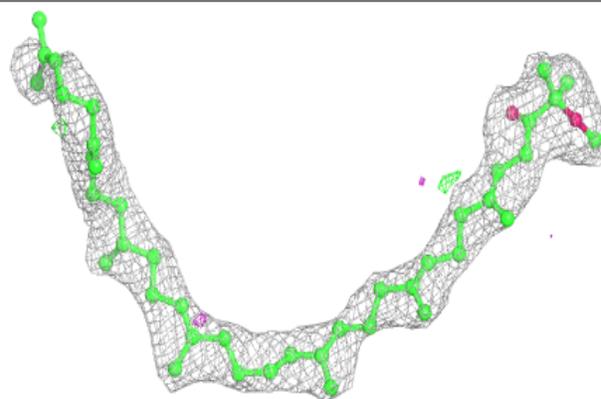


Electron density around U10 L 304:

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

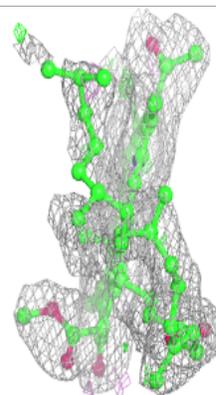
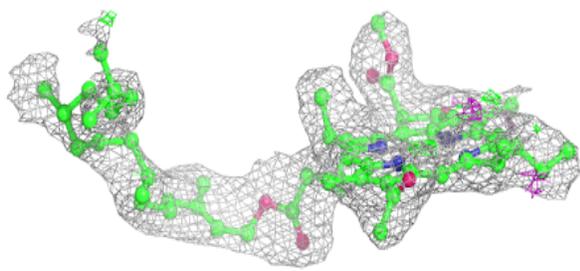
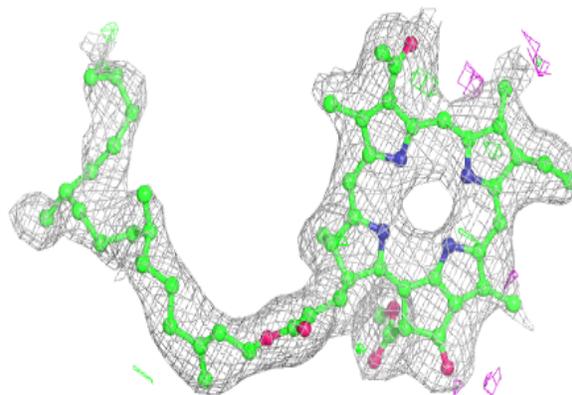
**Electron density around SPN M 407:**

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

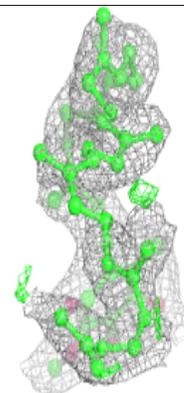
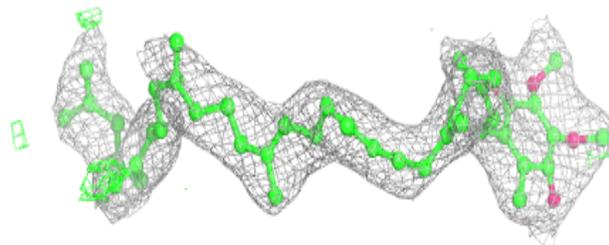
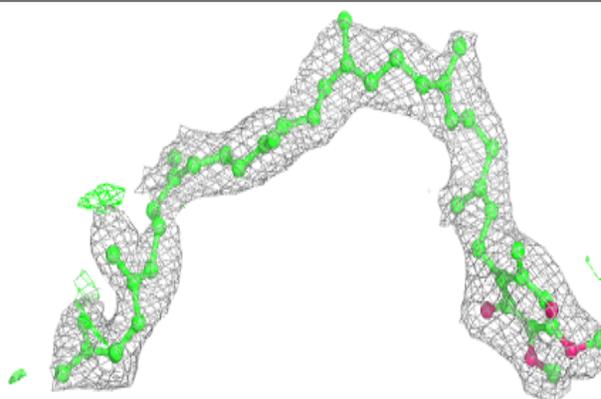


Electron density around BPH M 404:

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

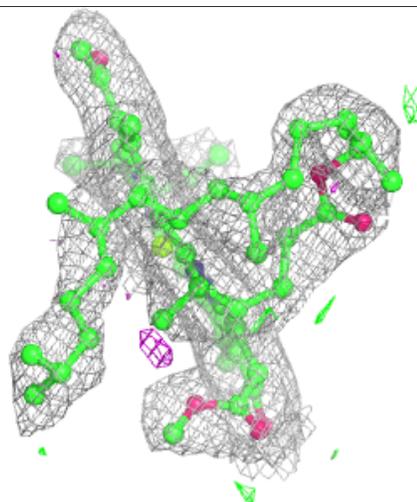
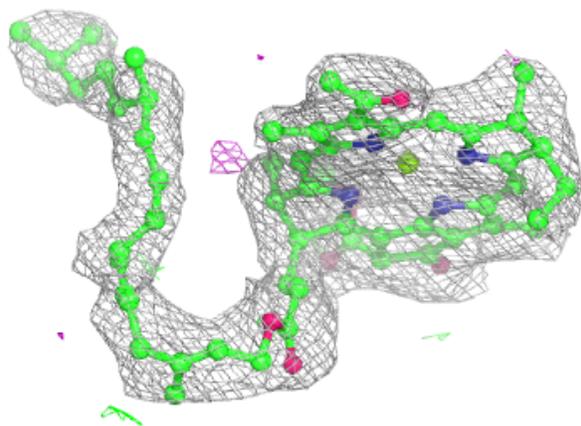
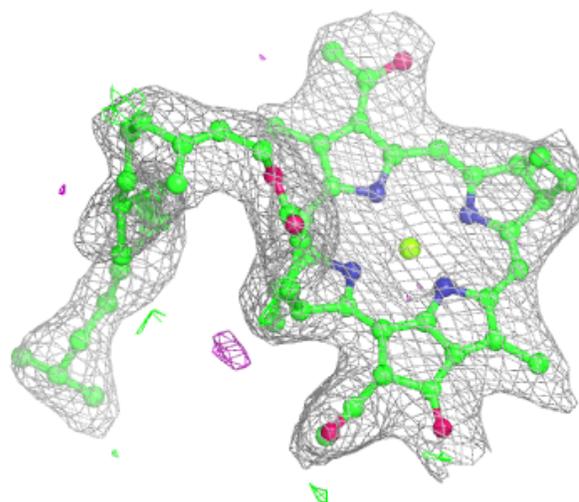
**Electron density around U10 M 406:**

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



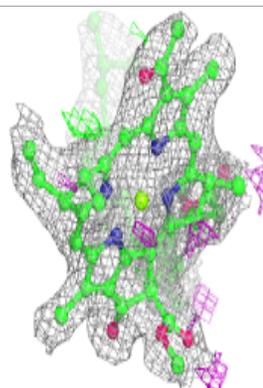
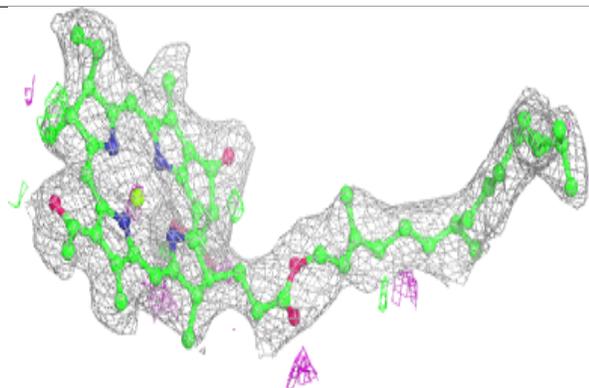
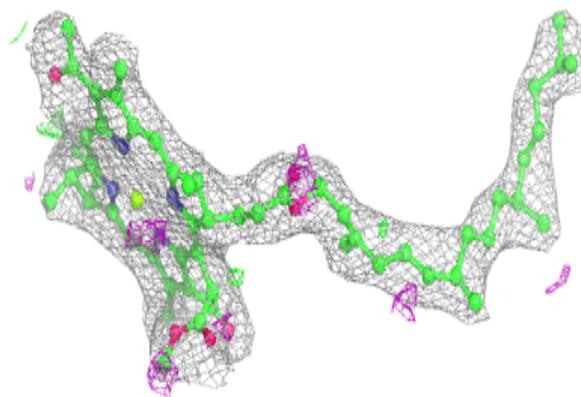
Electron density around BCL M 402:

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

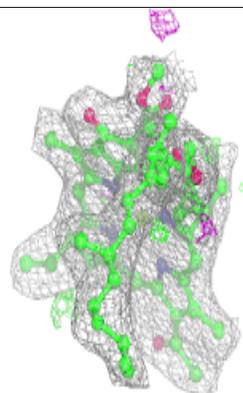
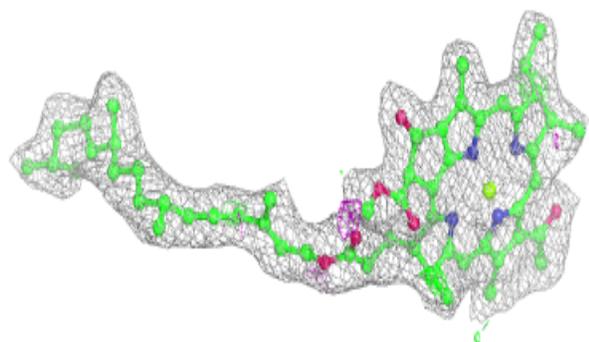
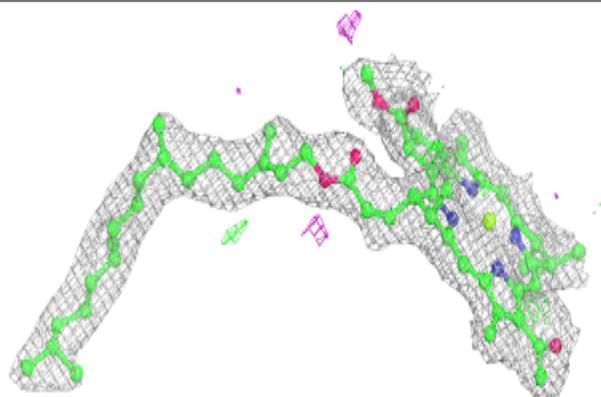


Electron density around BCL M 403:

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

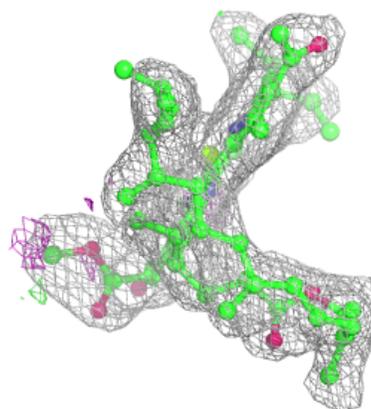
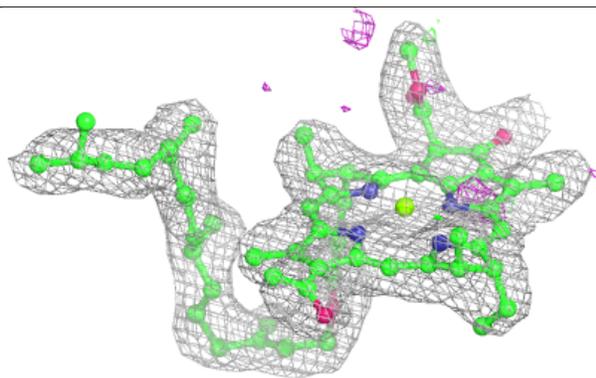
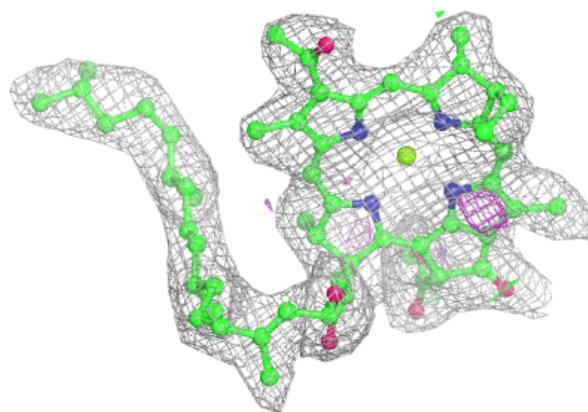
**Electron density around BCL L 301:**

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



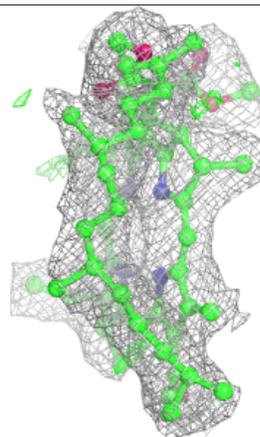
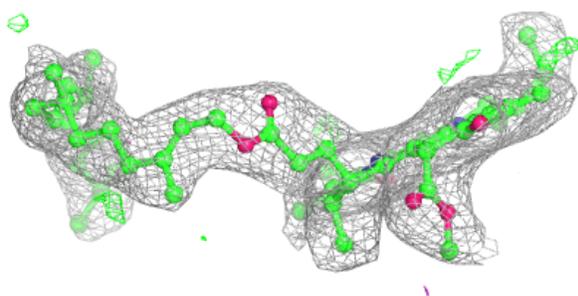
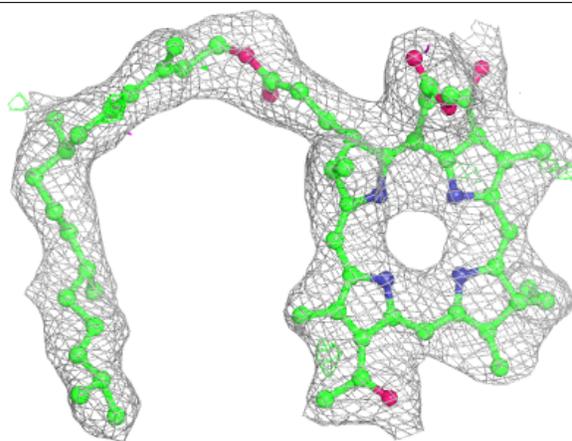
Electron density around BCL L 302:

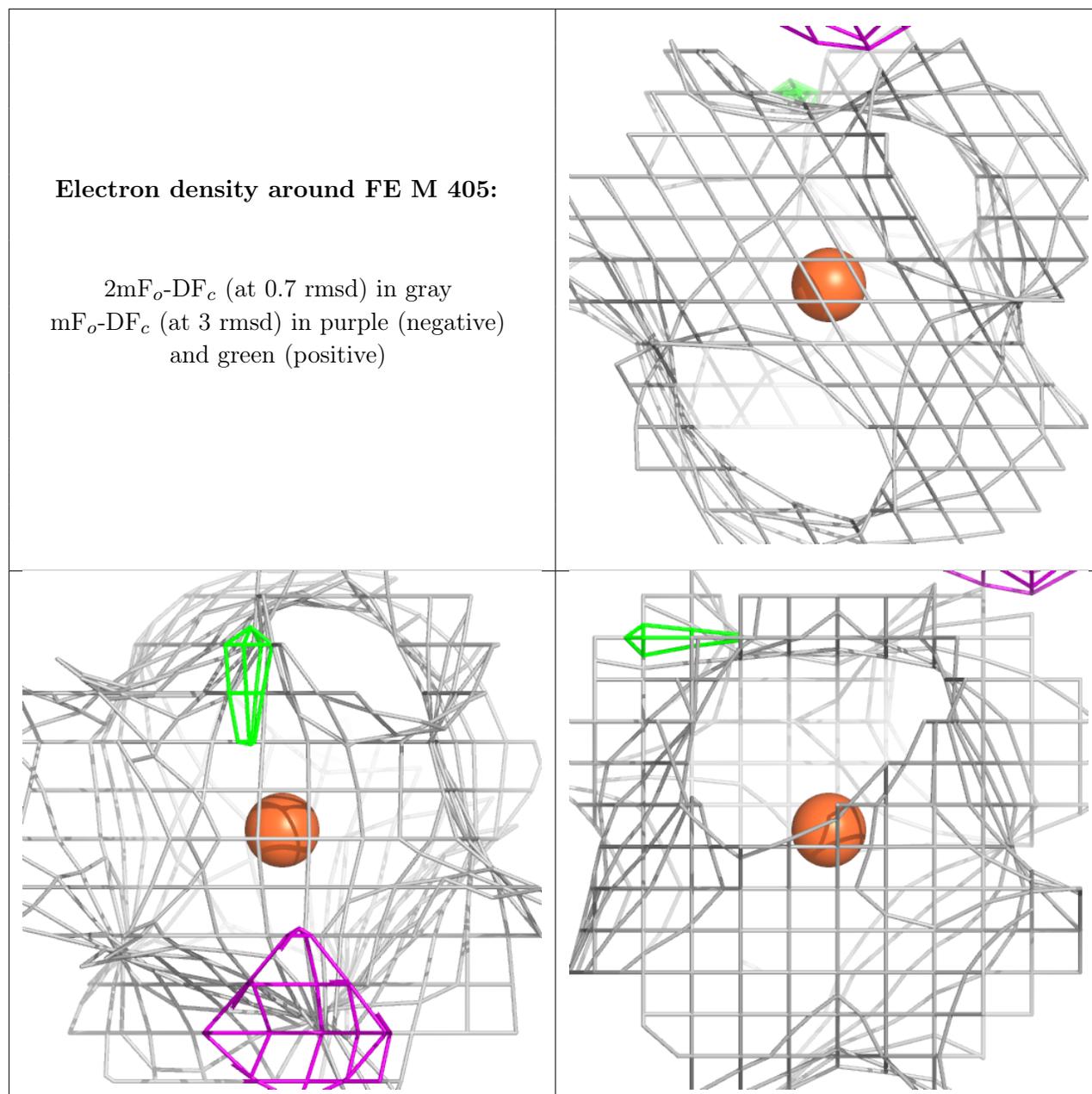
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BPH L 303:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.