



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2024 – 02:57 AM EST

PDB ID : 4IN7
Title : (M)L214N mutant of the Rhodobacter sphaeroides Reaction Center
Authors : Saer, R.G.; Hardjasa, A.; Murphy, M.E.P.; Beatty, J.T.
Deposited on : 2013-01-04
Resolution : 2.85 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

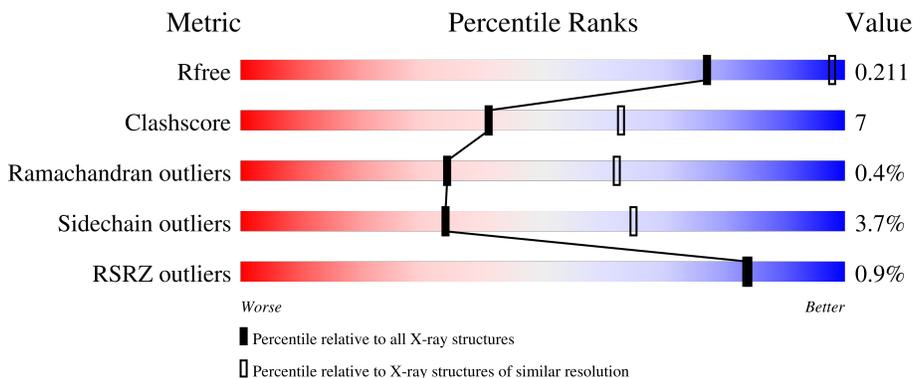
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	266	 2% 77% 11% 10%
2	L	282	 % 89% 10%
3	M	307	 84% 14%

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
11	HTO	L	309	-	X	-	X
16	PC1	M	410	-	-	-	X
4	GOL	H	303	-	-	-	X
6	GGD	H	307	-	-	-	X
8	LDA	L	302	-	-	-	X
8	LDA	L	303	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7359 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	1849	1183	320	337	9	0	5	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP P0C0Y7
H	-4	HIS	-	expression tag	UNP P0C0Y7
H	-3	HIS	-	expression tag	UNP P0C0Y7
H	-2	HIS	-	expression tag	UNP P0C0Y7
H	-1	HIS	-	expression tag	UNP P0C0Y7
H	0	HIS	-	expression tag	UNP P0C0Y7
H	251	VAL	-	expression tag	UNP P0C0Y7
H	252	VAL	-	expression tag	UNP P0C0Y7
H	253	ALA	-	expression tag	UNP P0C0Y7
H	254	ALA	-	expression tag	UNP P0C0Y7
H	255	MET	-	expression tag	UNP P0C0Y7
H	256	LEU	-	expression tag	UNP P0C0Y7
H	257	ALA	-	expression tag	UNP P0C0Y7
H	258	GLU	-	expression tag	UNP P0C0Y7
H	259	TYR	-	expression tag	UNP P0C0Y7
H	260	ALA	-	expression tag	UNP P0C0Y7

- Molecule 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	2239	1513	355	363	8	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	expression tag	UNP P0C0Y8

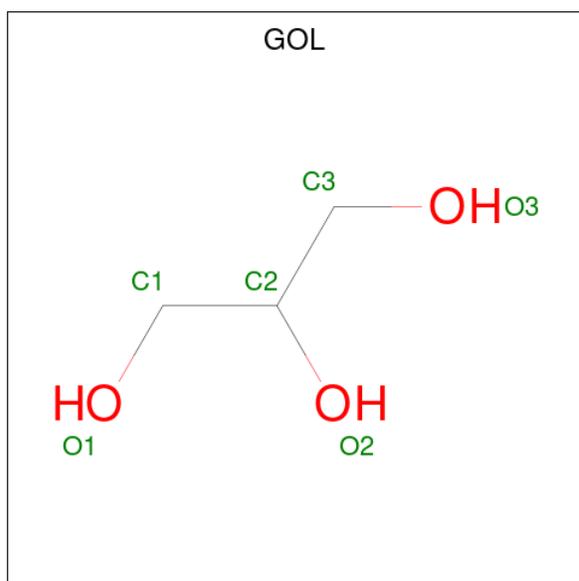
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2410	1605	396	399	10	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	expression tag	UNP P0C0Y9
M	214	ASN	LEU	engineered mutation	UNP P0C0Y9
M	303	MET	-	expression tag	UNP P0C0Y9
M	304	ALA	-	expression tag	UNP P0C0Y9
M	305	PRO	-	expression tag	UNP P0C0Y9
M	306	LEU	-	expression tag	UNP P0C0Y9

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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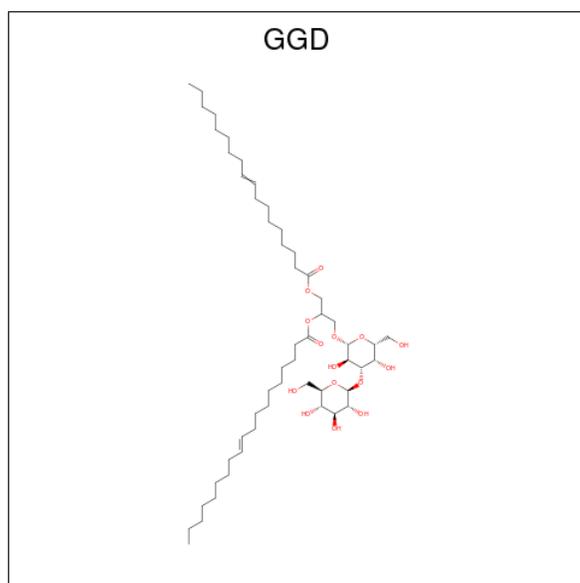
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

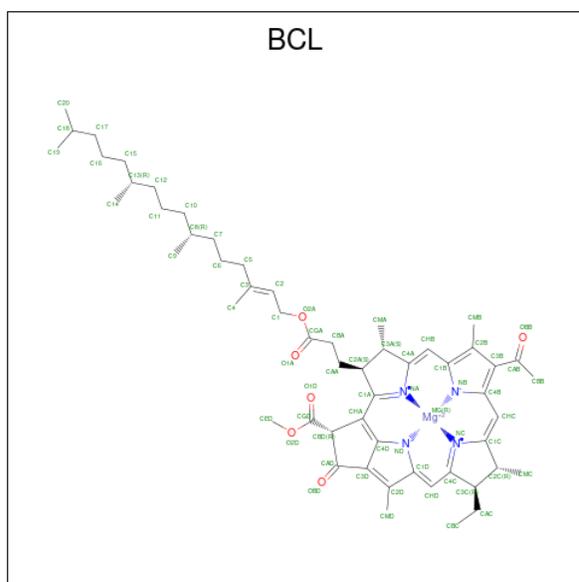
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

- Molecule 6 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY] -1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula: C₅₂H₉₄O₁₅).



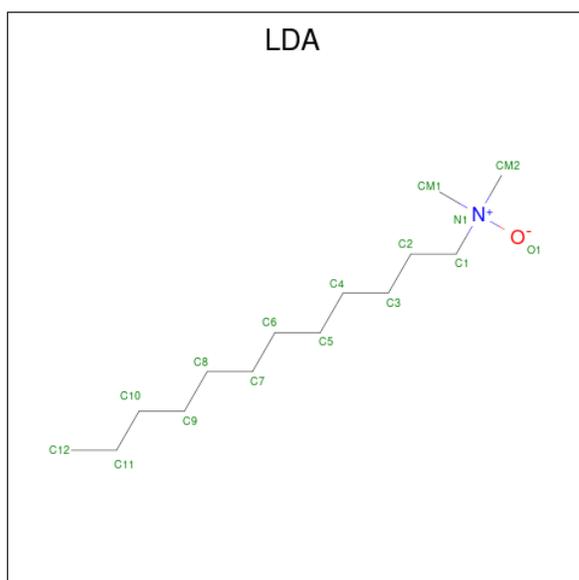
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			57	42	15		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



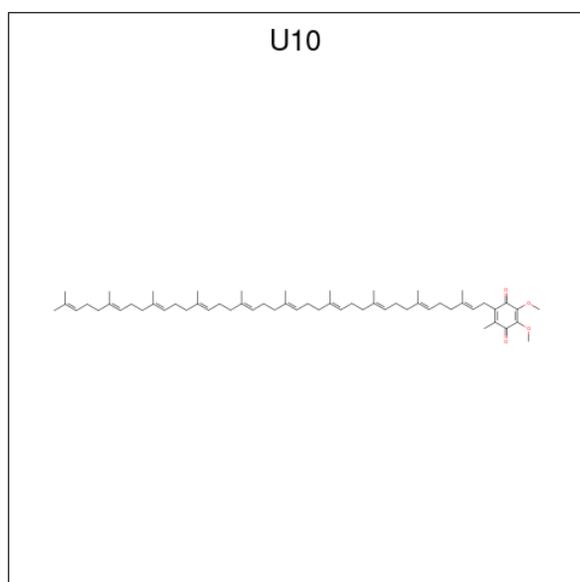
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mg	N			O
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



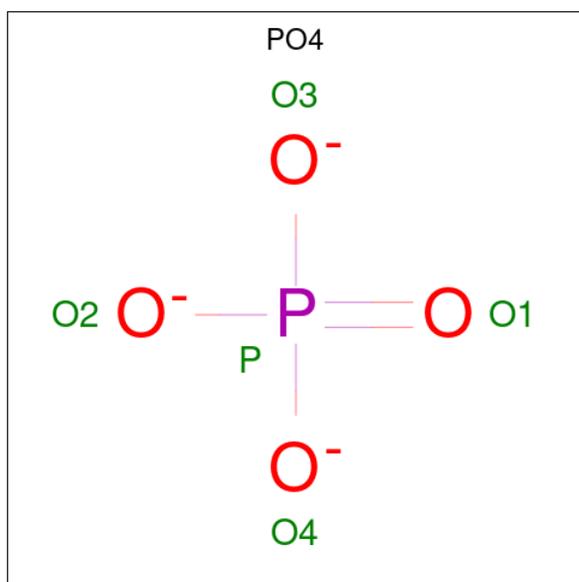
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	L	1	16	14	1	1	0	0
8	L	1	16	14	1	1	0	0
8	L	1	16	14	1	1	0	0
8	M	1	16	14	1	1	0	0
8	M	1	16	14	1	1	0	0

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



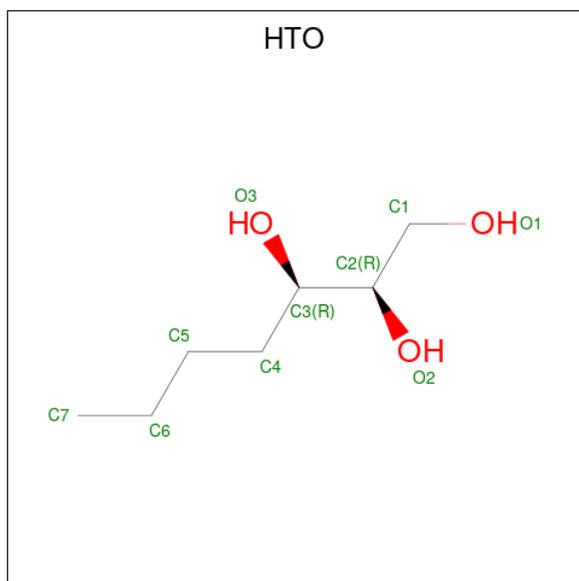
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	L	1	46	38	8	0	1
9	M	1	48	44	4	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 11 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

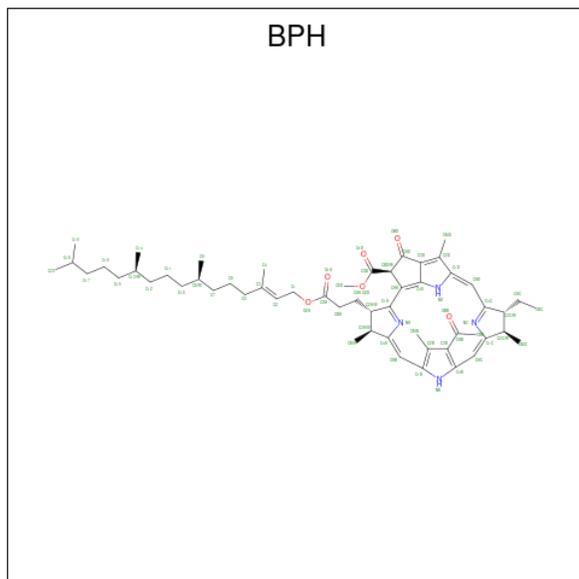


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			10	7	3		
11	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

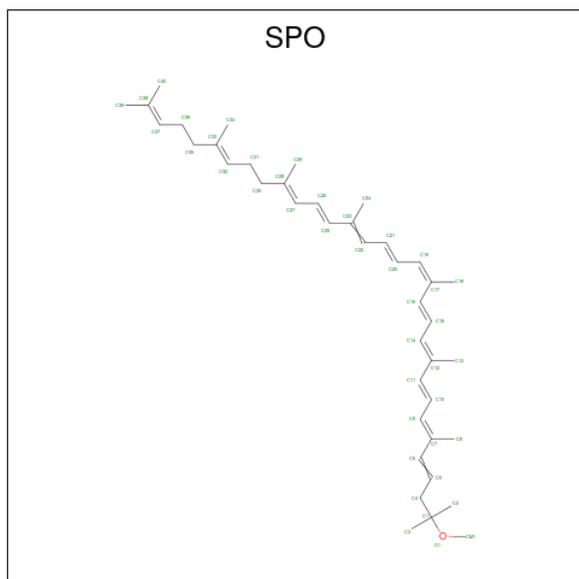
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total Fe 1 1	0	0

- Molecule 13 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



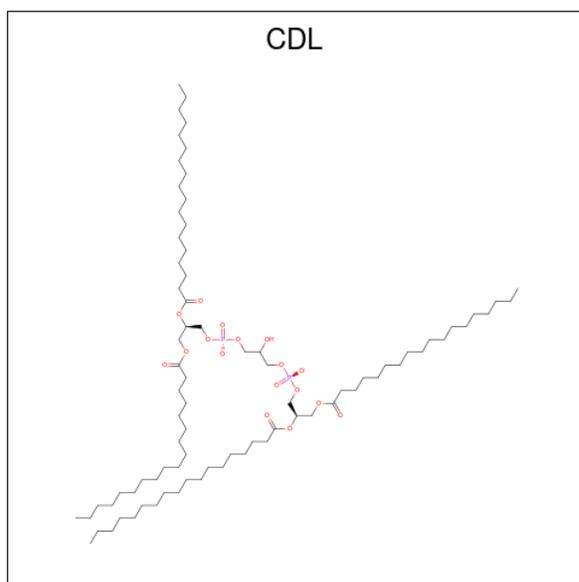
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	M	1	Total C N O 65 55 4 6	0	0
13	M	1	Total C N O 65 55 4 6	0	0

- Molecule 14 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



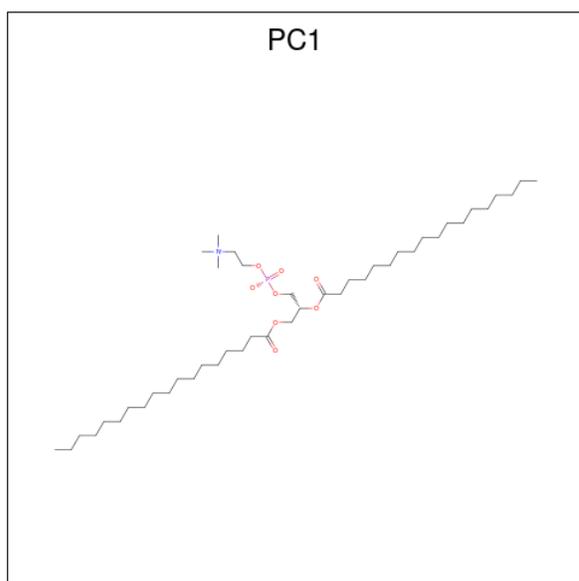
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	M	1	43	33	1	8	1	0	0

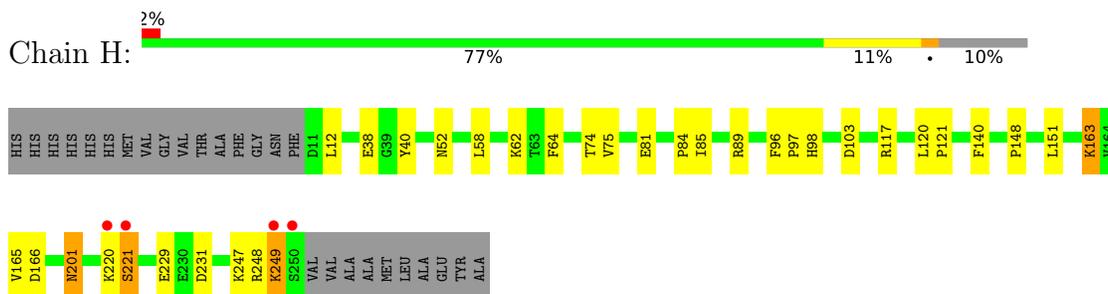
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
17	M	1	1	1	0	0

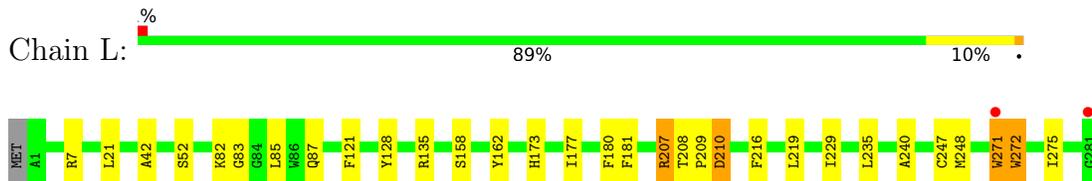
3 Residue-property plots [i](#)

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.

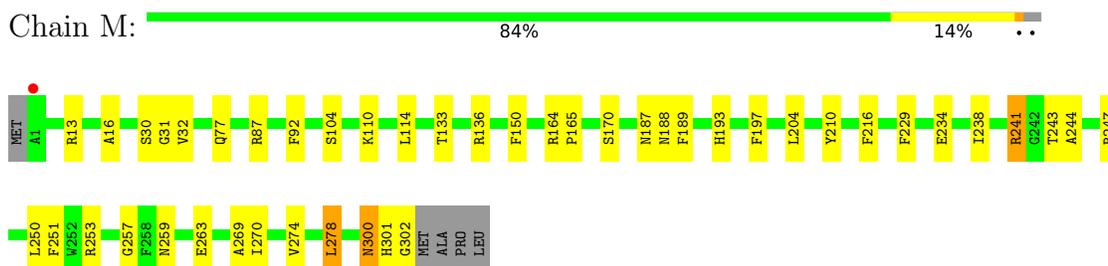
- Molecule 1: Reaction center protein H chain



- 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	139.14Å 139.14Å 185.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.57 – 2.85 38.54 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.57-2.85) 99.9 (38.54-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.86Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.174 , 0.213 0.179 , 0.211	Depositor DCC
R_{free} test set	2474 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtrriage
Anisotropy	0.042	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: PC1, HTO, K, SPO, GOL, U10, PO4, MG, BCL, CDL, BPH, FE, GGD, 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	H	0.89	0/1929	1.05	5/2619 (0.2%)
2	L	0.85	0/2339	0.90	5/3203 (0.2%)
3	M	0.86	1/2507 (0.0%)	0.90	3/3422 (0.1%)
All	All	0.86	1/6775 (0.0%)	0.95	13/9244 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	263	GLU	CD-OE1	5.51	1.31	1.25

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	210	ASP	CB-CG-OD1	7.19	124.77	118.30
2	L	207	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	H	89	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	M	241	ARG	NE-CZ-NH2	6.70	123.65	120.30
3	M	253	ARG	NE-CZ-NH1	-6.66	116.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

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	1849	0	1873	25	0
2	L	2239	0	2185	24	0
3	M	2410	0	2314	27	0
4	H	30	0	40	0	0
4	L	12	0	16	1	0
5	H	1	0	0	0	0
6	H	57	0	68	3	0
7	L	132	0	148	13	0
7	M	132	0	148	14	0
8	L	48	0	93	2	0
8	M	32	0	62	4	0
9	L	46	0	46	6	0
9	M	48	0	63	1	0
10	L	5	0	0	1	0
11	L	20	0	32	0	0
12	M	1	0	0	0	0
13	M	130	0	150	18	0
14	M	42	0	60	3	0
15	M	81	0	102	1	0
16	M	43	0	60	1	0
17	M	1	0	0	0	0
All	All	7359	0	7460	105	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 7.

The worst 5 of 105 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)
13:M:412:BPH:HBB3	13:M:412:BPH:HHC	1.50	0.91
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:406:BPH:HHC	13:M:406:BPH:HBB3	1.66	0.78
1:H:248:ARG:HA	1:H:249[A]:LYS:HB2	1.68	0.75
1:H:220[B]:LYS:HE2	1:H:221:SER:OG	1.91	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	244/266 (92%)	231 (95%)	11 (4%)	2 (1%)	19	46
2	L	281/282 (100%)	265 (94%)	16 (6%)	0	100	100
3	M	301/307 (98%)	288 (96%)	11 (4%)	2 (1%)	22	50
All	All	826/855 (97%)	784 (95%)	38 (5%)	4 (0%)	34	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249[A]	LYS
1	H	249[B]	LYS
3	M	30	SER
3	M	301	HIS

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	200/214 (94%)	192 (96%)	8 (4%)	31	62
2	L	221/221 (100%)	211 (96%)	10 (4%)	27	57
3	M	237/240 (99%)	229 (97%)	8 (3%)	37	67
All	All	658/675 (98%)	632 (96%)	26 (4%)	34	62

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	247	CYS
2	L	272	TRP
3	M	259	ASN
2	L	271[B]	TRP
3	M	104	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	77	GLN
3	M	187	ASN
3	M	193	HIS
1	H	98	HIS
1	H	32	GLN

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 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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	M	407	-	48,48,63	1.35	5 (10%)	58,61,79	2.29	16 (27%)
4	GOL	H	303	-	5,5,5	0.57	0	5,5,5	0.64	0
10	PO4	L	307	-	4,4,4	1.18	1 (25%)	6,6,6	0.82	0
16	PC1	M	410	-	42,42,53	1.51	4 (9%)	48,50,61	1.49	6 (12%)
13	BPH	M	412	-	51,70,70	1.87	9 (17%)	52,101,101	2.42	18 (34%)
9	U10	L	305[A]	-	23,23,63	1.80	2 (8%)	28,31,79	1.58	6 (21%)
4	GOL	H	306	-	5,5,5	1.13	0	5,5,5	1.02	0
8	LDA	L	304	-	12,15,15	2.17	1 (8%)	14,17,17	0.80	0
11	HTO	L	309	-	9,9,9	1.52	3 (33%)	10,10,10	1.98	4 (40%)
4	GOL	L	310	-	5,5,5	0.46	0	5,5,5	0.51	0
4	GOL	H	304	-	5,5,5	0.80	0	5,5,5	0.75	0
11	HTO	L	308	-	9,9,9	1.32	2 (22%)	10,10,10	1.22	0
6	GGD	H	307	-	58,58,68	1.15	3 (5%)	72,72,82	1.68	14 (19%)
7	BCL	M	402	-	64,74,74	1.63	12 (18%)	78,115,115	2.10	19 (24%)
4	GOL	H	301	-	5,5,5	0.78	0	5,5,5	1.10	0
8	LDA	L	303	-	12,15,15	2.27	1 (8%)	14,17,17	0.79	1 (7%)
7	BCL	L	306	-	64,74,74	1.72	10 (15%)	78,115,115	1.91	21 (26%)
8	LDA	M	404	-	12,15,15	2.10	1 (8%)	14,17,17	0.56	0
9	U10	L	305[B]	-	23,23,63	2.07	2 (8%)	28,31,79	1.47	5 (17%)
14	SPO	M	408	-	40,41,41	0.81	1 (2%)	47,50,50	1.68	11 (23%)
15	CDL	M	409	-	79,79,99	1.52	5 (6%)	84,90,111	1.43	8 (9%)
13	BPH	M	406	-	51,70,70	1.80	9 (17%)	52,101,101	2.16	14 (26%)
4	GOL	H	302	-	5,5,5	0.49	0	5,5,5	0.65	0
8	LDA	M	403	-	12,15,15	2.25	1 (8%)	14,17,17	0.91	1 (7%)
7	BCL	L	301	-	64,74,74	1.60	14 (21%)	78,115,115	2.41	32 (41%)
4	GOL	L	311	-	5,5,5	0.36	0	5,5,5	0.34	0
8	LDA	L	302	-	12,15,15	2.14	1 (8%)	14,17,17	0.86	0
7	BCL	M	401	-	64,74,74	1.75	14 (21%)	78,115,115	2.17	25 (32%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	U10	M	407	-	-	9/45/69/87	0/1/1/1
4	GOL	H	303	-	-	2/4/4/4	-
16	PC1	M	410	-	-	24/46/46/57	-
13	BPH	M	412	-	-	9/37/105/105	0/5/6/6
9	U10	L	305[A]	-	-	1/15/39/87	0/1/1/1
4	GOL	H	306	-	-	2/4/4/4	-
8	LDA	L	304	-	-	8/13/13/13	-
11	HTO	L	309	-	-	5/10/10/10	-
4	GOL	L	310	-	-	4/4/4/4	-
4	GOL	H	304	-	-	2/4/4/4	-
11	HTO	L	308	-	-	5/10/10/10	-
6	GGD	H	307	-	-	20/47/87/97	0/2/2/2
7	BCL	M	402	-	-	6/37/137/137	-
4	GOL	H	301	-	-	2/4/4/4	-
8	LDA	L	303	-	-	7/13/13/13	-
7	BCL	L	306	-	-	4/37/137/137	-
8	LDA	M	404	-	-	7/13/13/13	-
9	U10	L	305[B]	-	-	3/15/39/87	0/1/1/1
14	SPO	M	408	-	-	4/47/47/47	-
15	CDL	M	409	-	-	49/88/88/110	-
13	BPH	M	406	-	-	17/37/105/105	0/5/6/6
4	GOL	H	302	-	-	2/4/4/4	-
8	LDA	M	403	-	-	7/13/13/13	-
7	BCL	L	301	-	-	5/37/137/137	-
4	GOL	L	311	-	-	4/4/4/4	-
8	LDA	L	302	-	-	6/13/13/13	-
7	BCL	M	401	-	-	13/37/137/137	-

The worst 5 of 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	305[B]	U10	C6-C1	8.47	1.50	1.35
9	L	305[A]	U10	C6-C1	7.66	1.49	1.35
8	L	303	LDA	O1-N1	-7.45	1.24	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	304	LDA	O1-N1	-7.32	1.25	1.42
8	M	403	LDA	O1-N1	-7.12	1.25	1.42

The worst 5 of 201 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	407	U10	C30-C29-C31	10.06	132.20	115.27
13	M	412	BPH	O1D-CGD-CBD	8.10	138.23	124.74
7	L	301	BCL	O2D-CGD-CBD	7.66	124.87	111.27
7	L	301	BCL	C2D-C1D-ND	6.59	114.96	110.10
7	M	402	BCL	C1C-NC-C4C	-6.51	103.78	106.71

There are no chirality outliers.

5 of 227 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	306	GOL	O1-C1-C2-O2
4	H	306	GOL	O1-C1-C2-C3
4	H	302	GOL	O1-C1-C2-O2
4	H	302	GOL	O1-C1-C2-C3
4	H	303	GOL	C1-C2-C3-O3

There are no ring outliers.

17 monomers are involved in 56 short contacts:

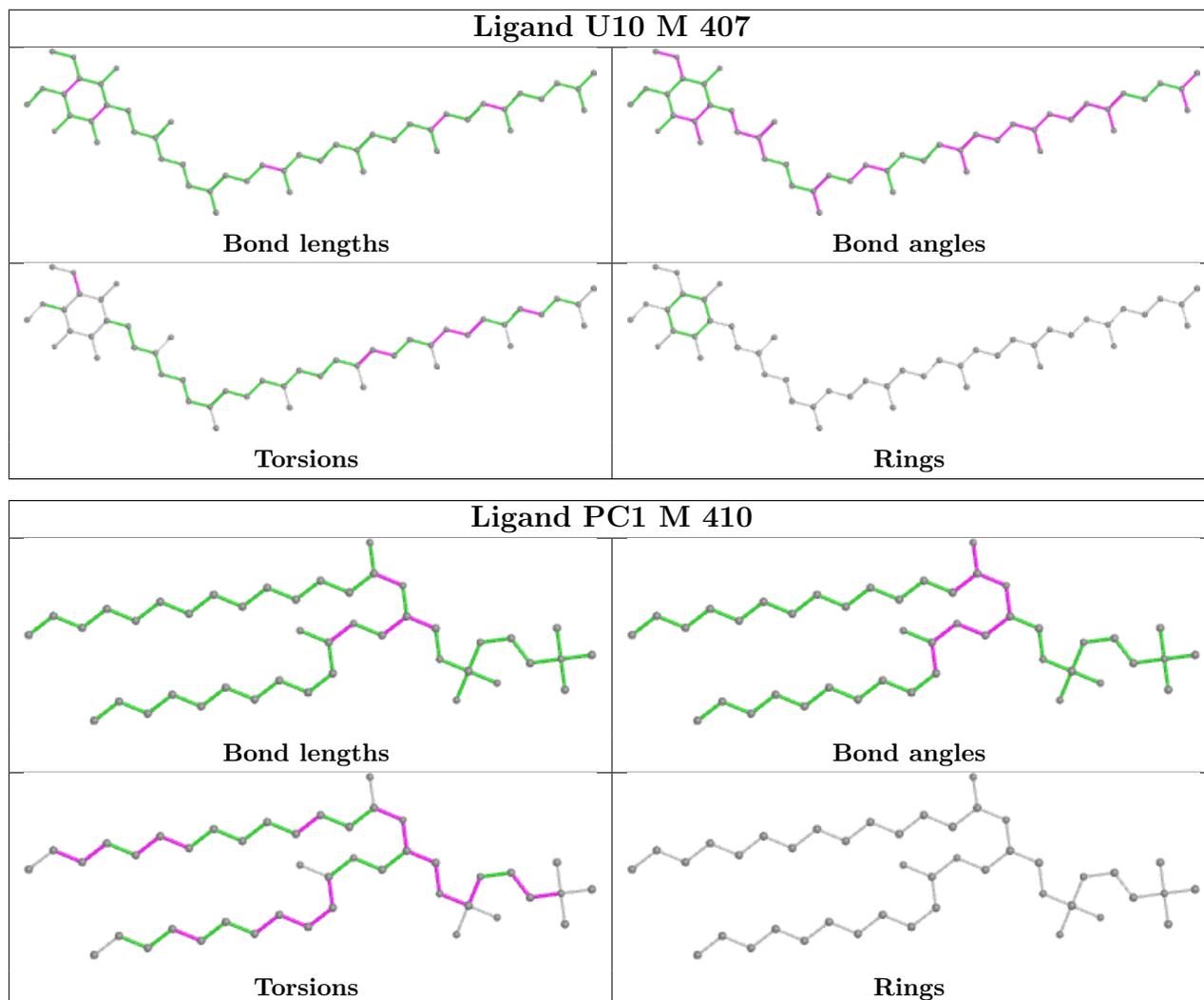
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	407	U10	1	0
10	L	307	PO4	1	0
16	M	410	PC1	1	0
13	M	412	BPH	12	0
8	L	304	LDA	2	0
6	H	307	GGD	3	0
7	M	402	BCL	9	0
7	L	306	BCL	7	0
8	M	404	LDA	2	0
9	L	305[B]	U10	6	0
14	M	408	SPO	3	0
15	M	409	CDL	1	0
13	M	406	BPH	6	0
8	M	403	LDA	2	0
7	L	301	BCL	7	0

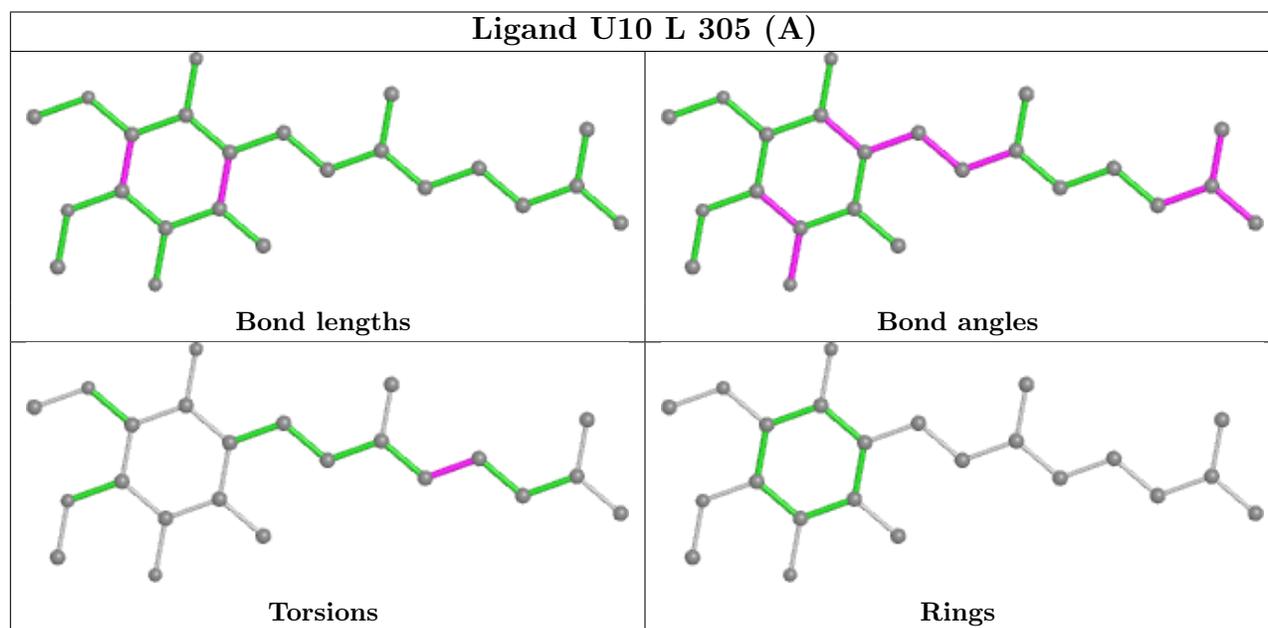
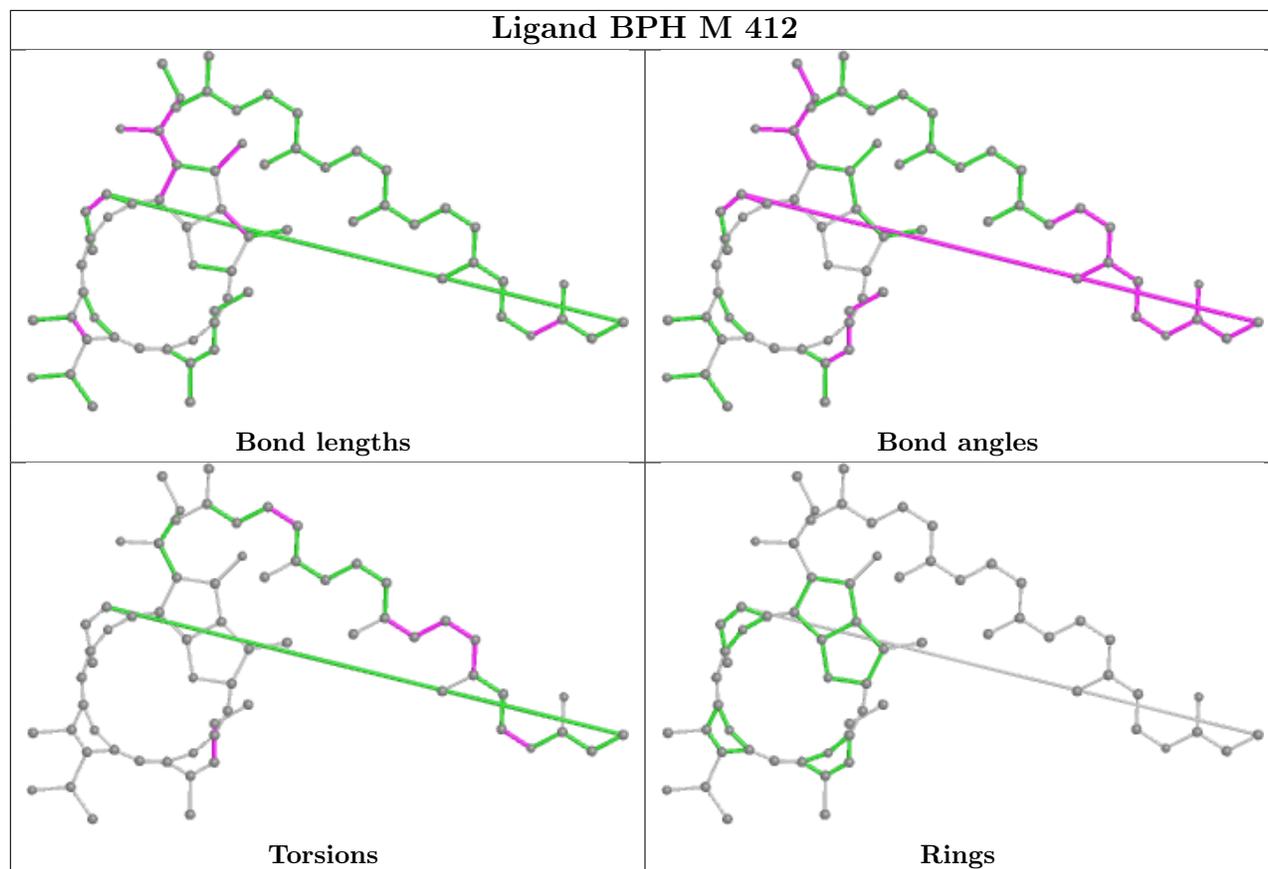
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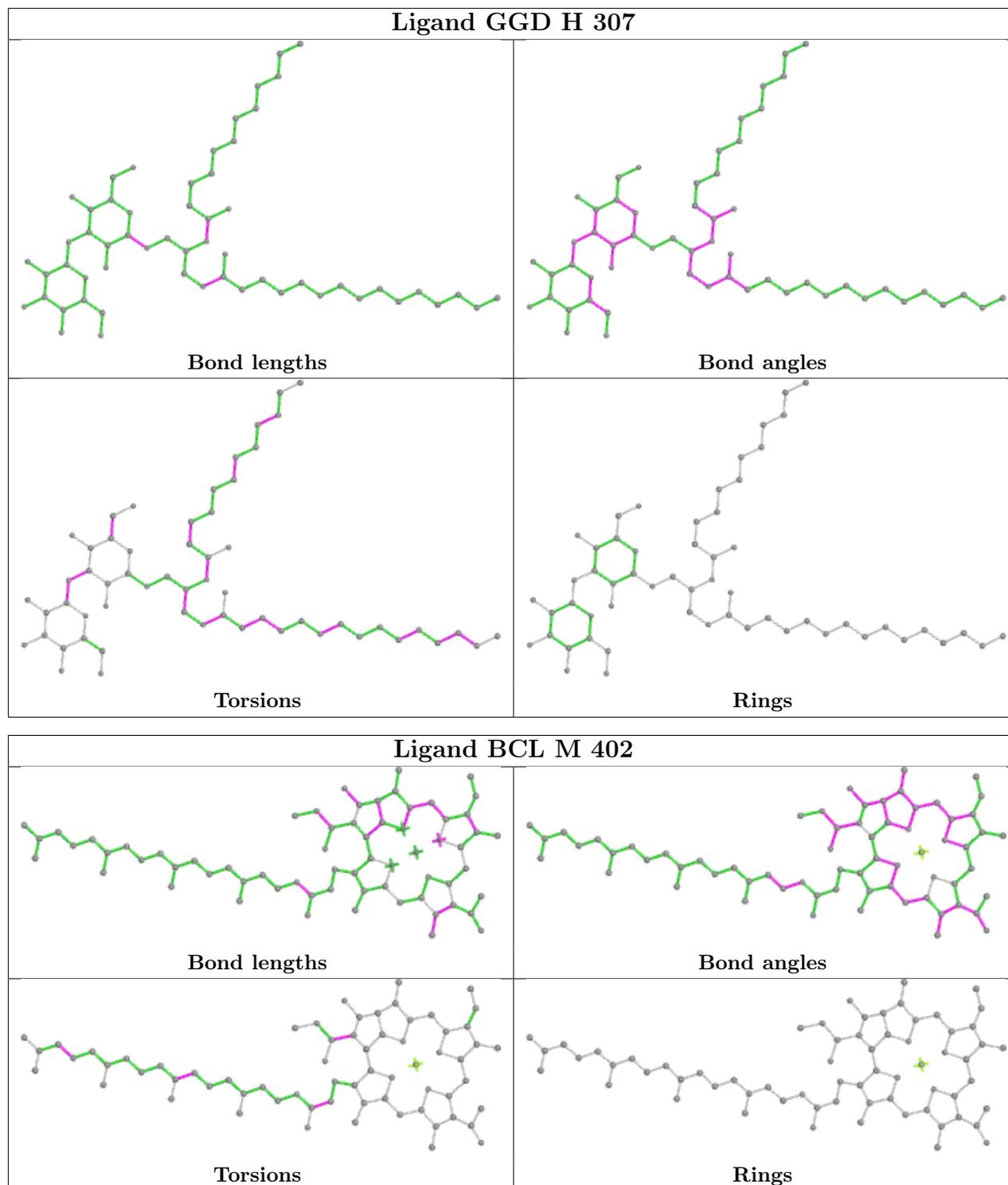
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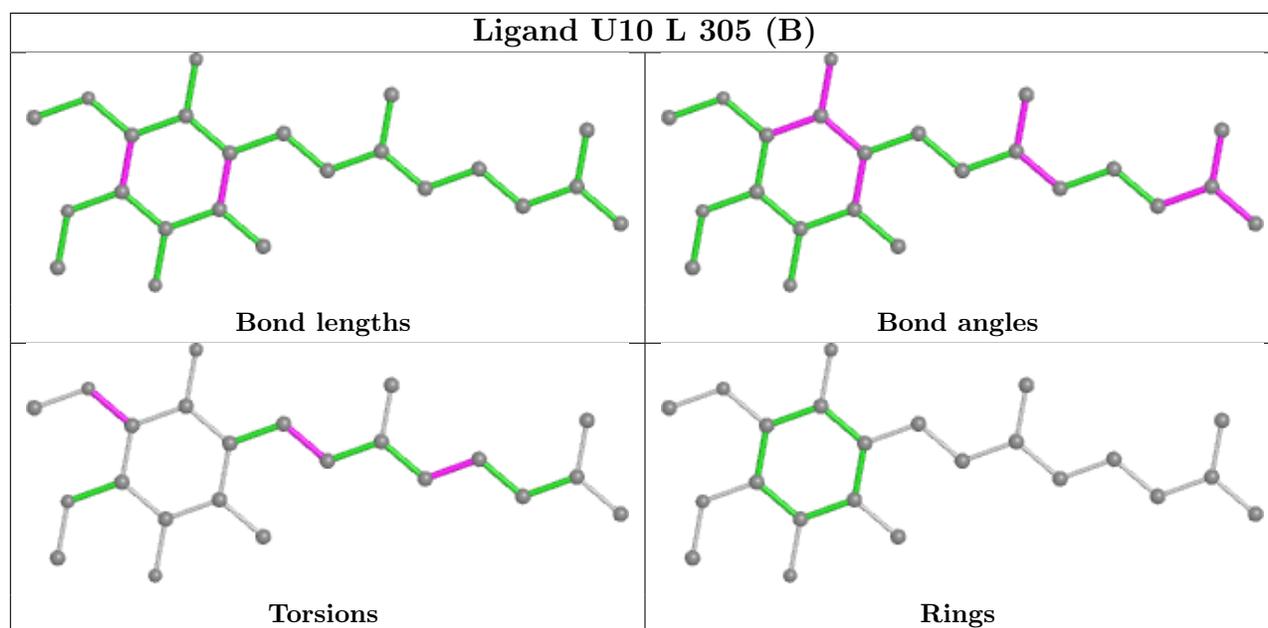
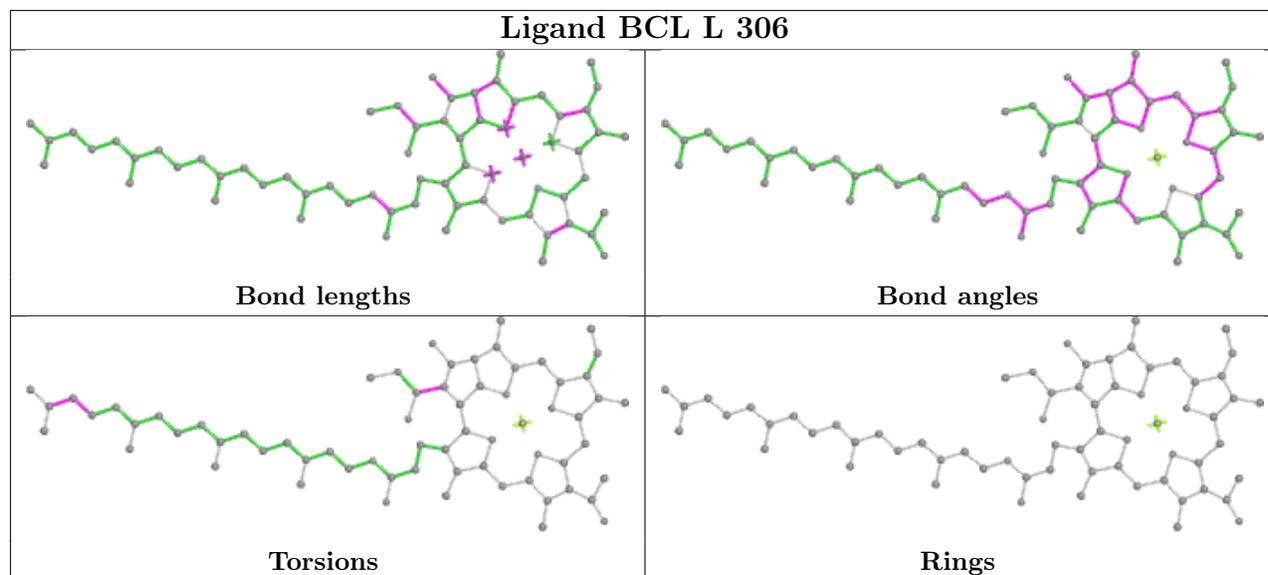
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	311	GOL	1	0
7	M	401	BCL	7	0

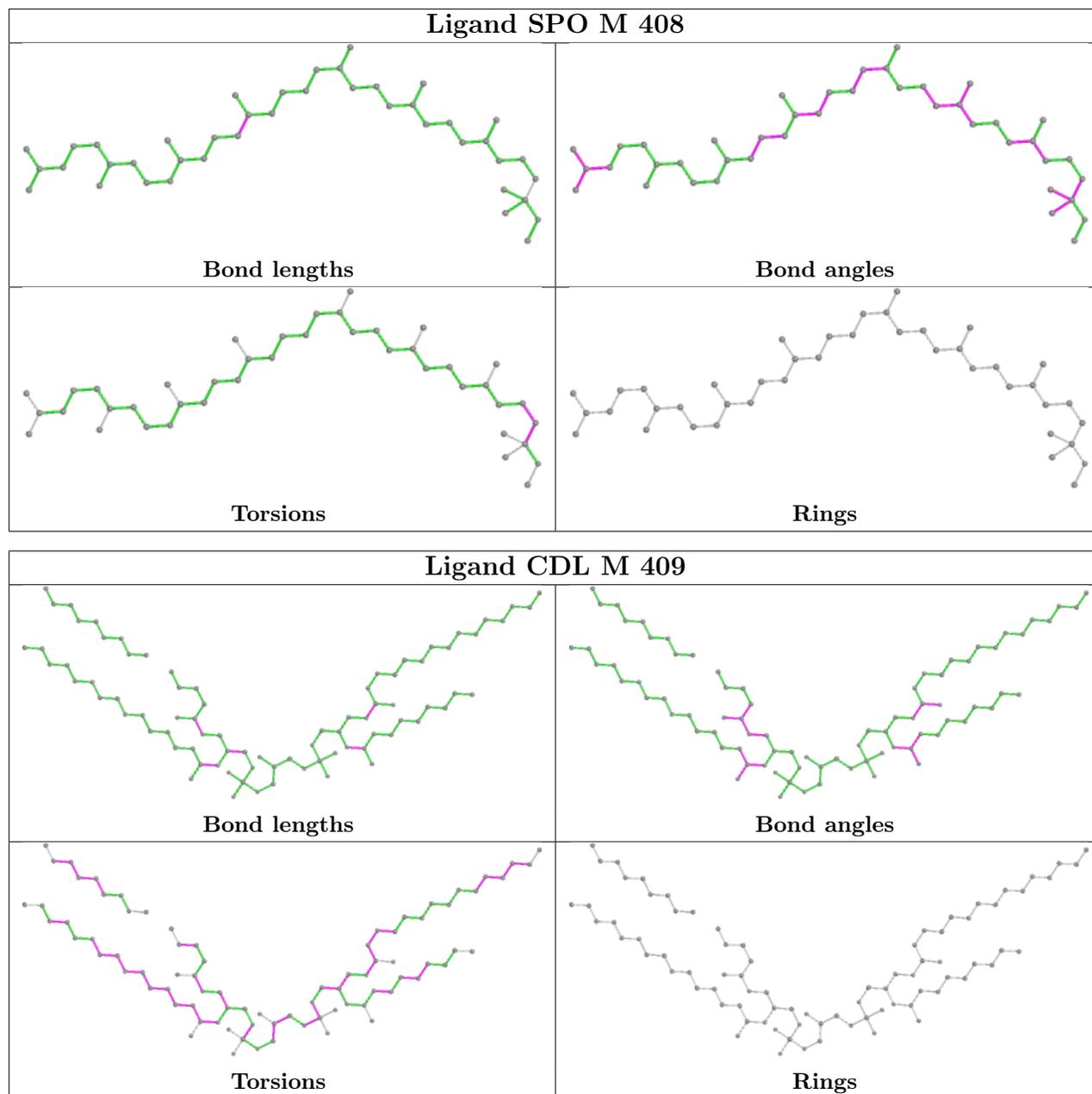
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

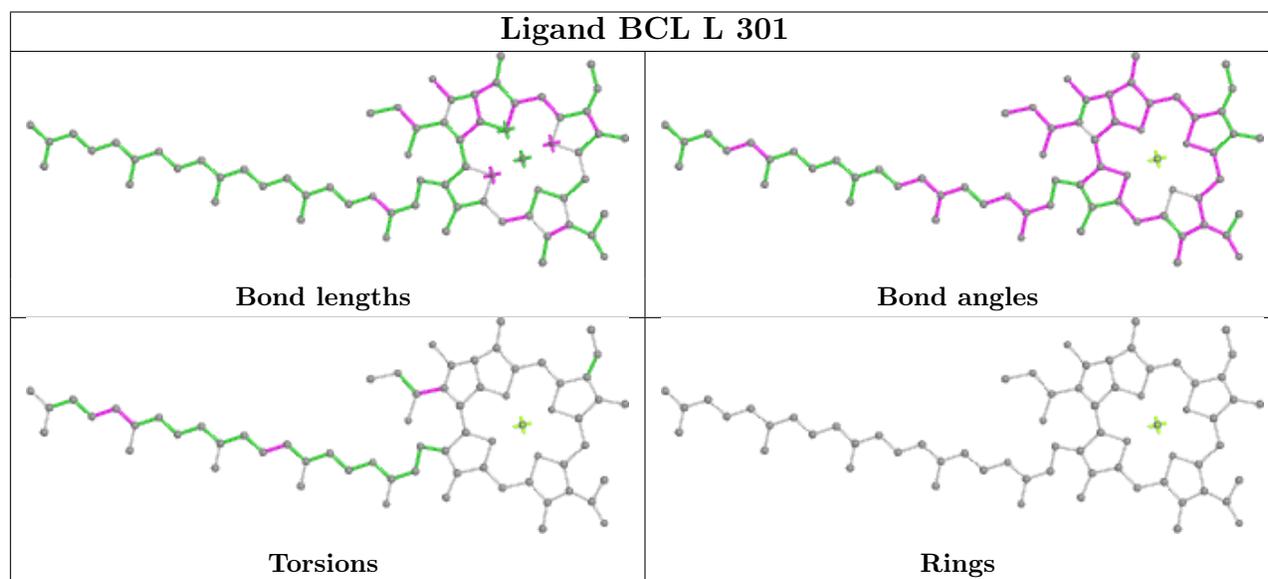
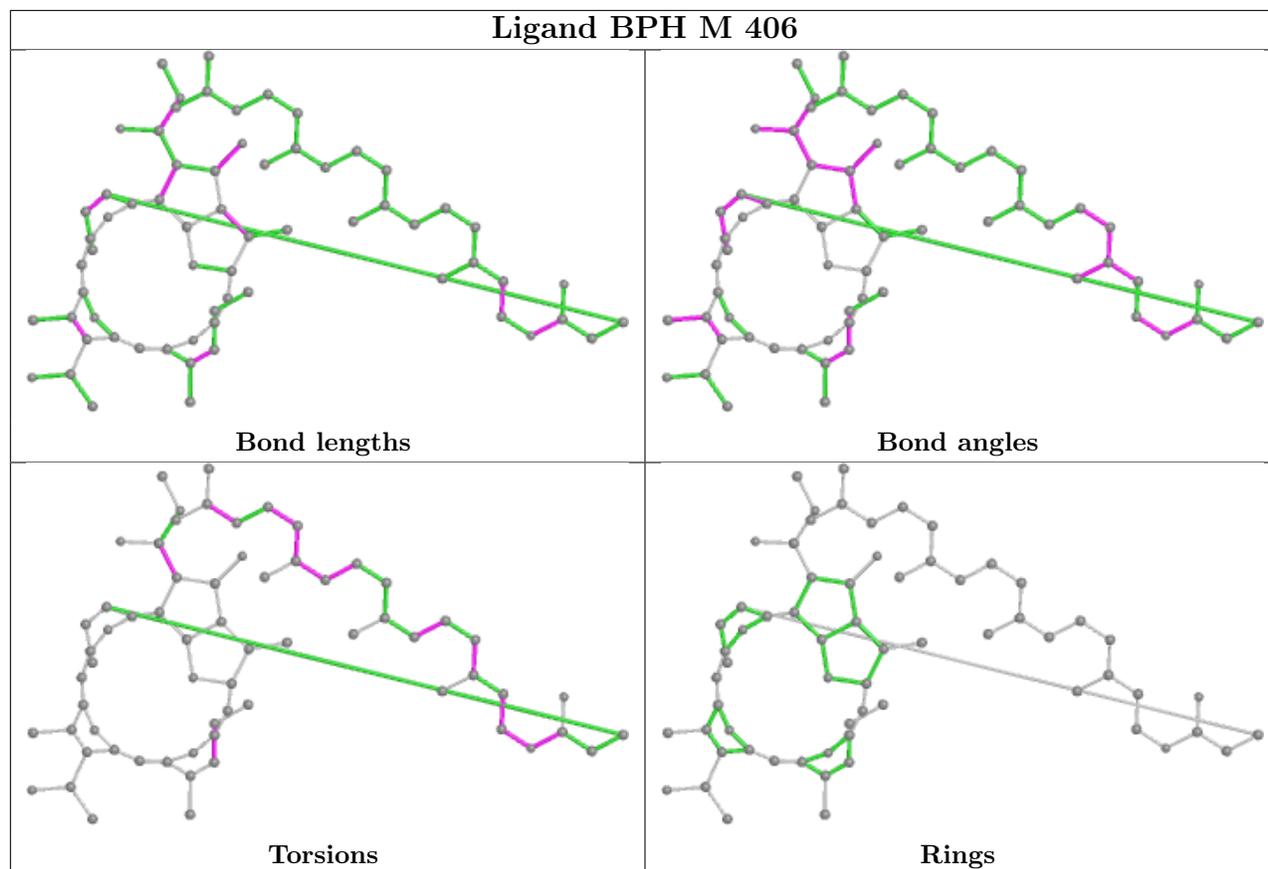


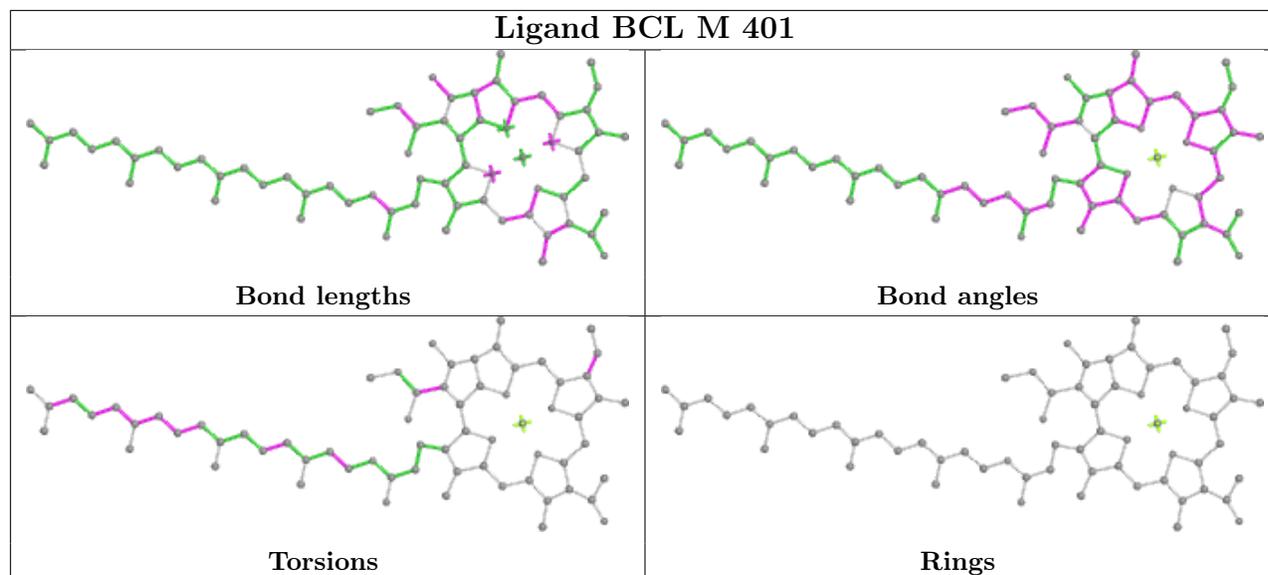












5.7 Other polymers [i](#)

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	240/266 (90%)	-0.48	4 (1%) 70 68	33, 43, 61, 133	3 (1%)
2	L	281/282 (99%)	-0.63	2 (0%) 87 87	30, 41, 64, 89	0
3	M	302/307 (98%)	-0.46	1 (0%) 94 94	31, 45, 66, 99	6 (1%)
All	All	823/855 (96%)	-0.52	7 (0%) 84 84	30, 43, 64, 133	9 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	7.1
1	H	249[A]	LYS	3.2
3	M	1	ALA	3.1
2	L	281	GLY	2.5
1	H	220[A]	LYS	2.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

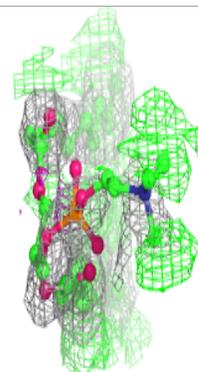
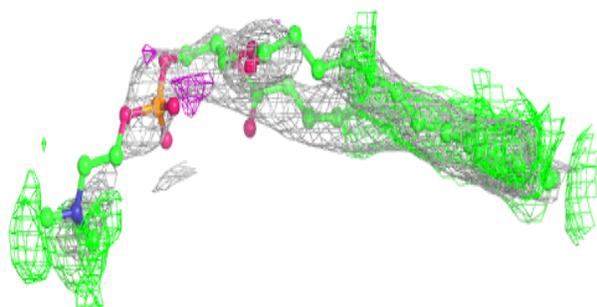
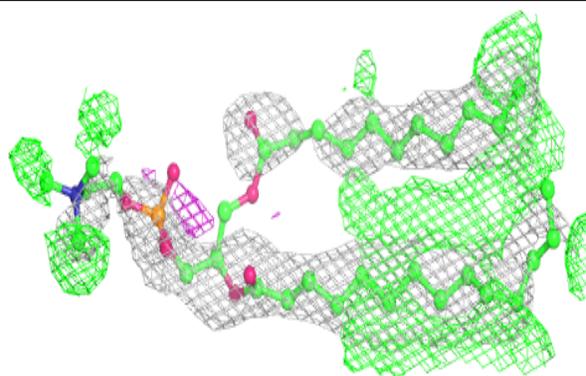
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
16	PC1	M	410	43/54	0.47	0.45	61,99,145,170	0
8	LDA	L	303	16/16	0.57	0.54	80,90,108,114	0
8	LDA	L	304	16/16	0.58	0.40	71,98,123,128	0
8	LDA	L	302	16/16	0.67	0.57	47,125,153,155	0
11	HTO	L	309	10/10	0.70	0.87	72,96,120,121	0
6	GGD	H	307	57/67	0.75	0.41	51,108,185,203	0
4	GOL	H	303	6/6	0.76	0.42	85,89,92,95	0
4	GOL	H	306	6/6	0.78	0.37	69,76,89,90	0
4	GOL	L	311	6/6	0.83	0.33	83,88,91,94	0
11	HTO	L	308	10/10	0.84	0.50	66,87,102,105	0
15	CDL	M	409	81/100	0.85	0.40	53,96,139,153	0
4	GOL	H	302	6/6	0.85	0.34	81,82,85,90	0
4	GOL	L	310	6/6	0.87	0.47	73,81,85,86	0
4	GOL	H	301	6/6	0.90	0.39	59,65,69,80	0
8	LDA	M	404	16/16	0.91	0.33	59,69,92,96	0
8	LDA	M	403	16/16	0.92	0.20	52,68,77,78	0
4	GOL	H	304	6/6	0.92	0.32	40,52,63,71	0
9	U10	L	305[A]	23/63	0.92	0.26	33,37,65,71	23
9	U10	L	305[B]	23/63	0.92	0.26	35,50,60,62	23
13	BPH	M	406	65/65	0.93	0.23	35,47,119,134	0
9	U10	M	407	48/63	0.94	0.24	33,46,91,110	0
14	SPO	M	408	42/42	0.94	0.21	33,47,80,92	0
5	K	H	305	1/1	0.95	0.12	50,50,50,50	0
10	PO4	L	307	5/5	0.96	0.11	60,62,66,67	0
17	MG	M	411	1/1	0.96	0.15	39,39,39,39	0
7	BCL	L	306	66/66	0.97	0.15	28,39,49,65	0
7	BCL	M	401	66/66	0.97	0.21	28,38,95,105	0
7	BCL	L	301	66/66	0.97	0.13	26,34,56,61	0
7	BCL	M	402	66/66	0.98	0.20	33,40,51,75	0
13	BPH	M	412	65/65	0.98	0.15	30,39,48,57	0
12	FE	M	405	1/1	0.99	0.16	36,36,36,36	0

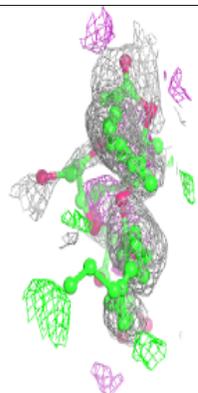
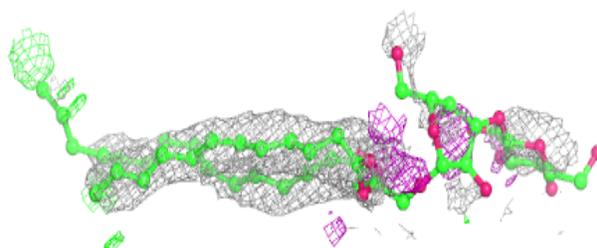
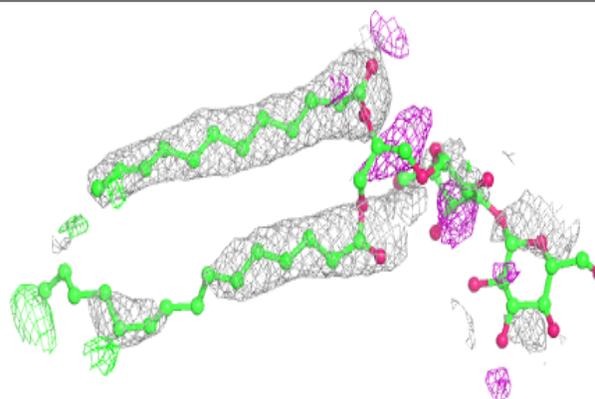
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC1 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)

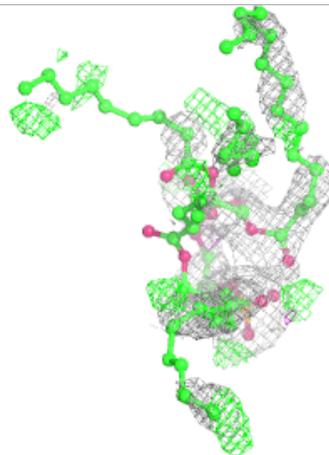
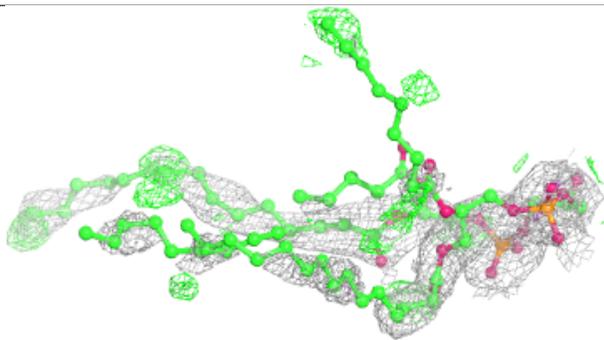
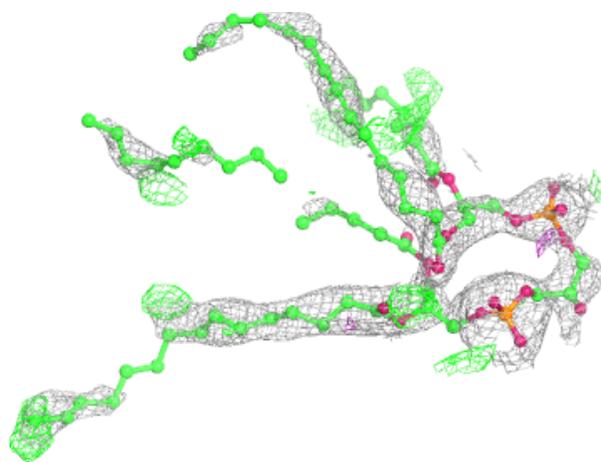
**Electron density around GGD H 307:**

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



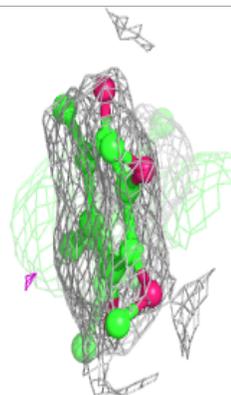
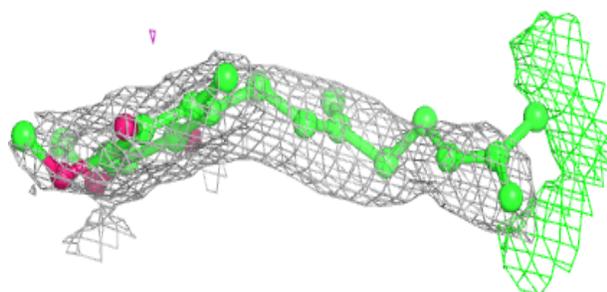
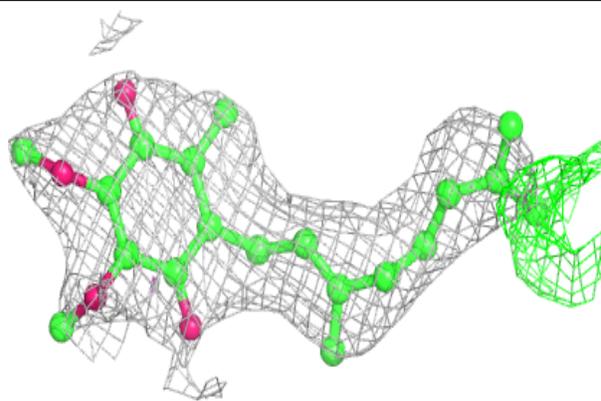
Electron density around CDL M 409:

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and green (positive)

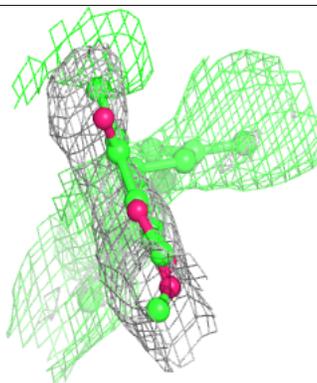
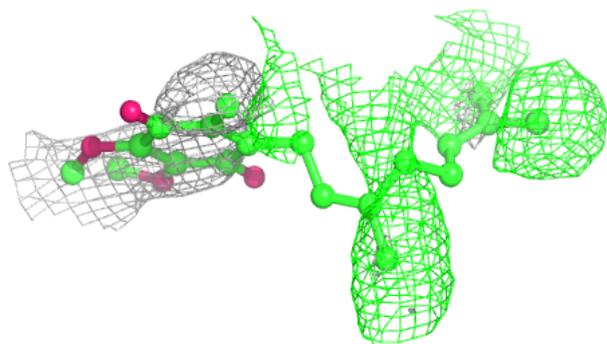
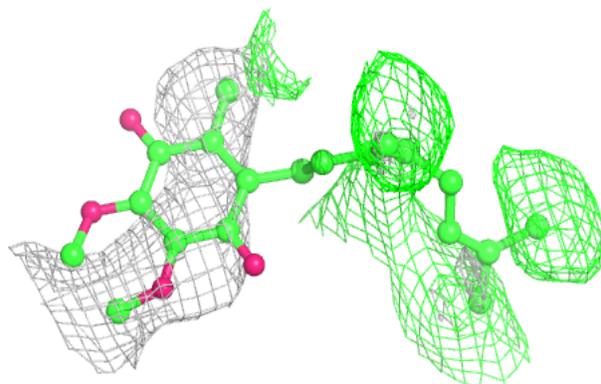


Electron density around U10 L 305 (A):

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and green (positive)

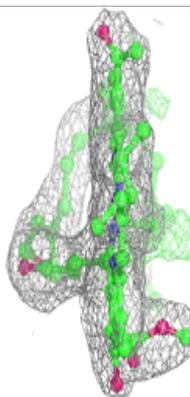
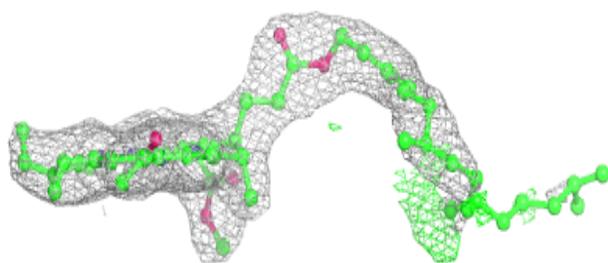
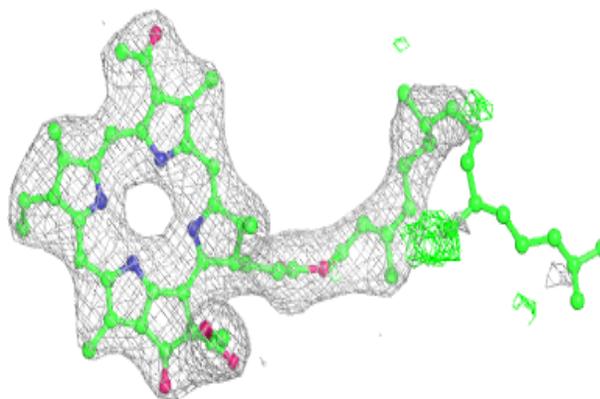
**Electron density around U10 L 305 (B):**

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and green (positive)

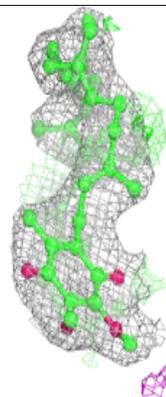
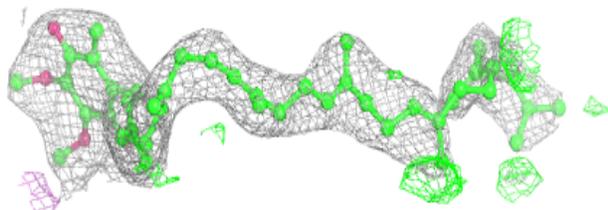
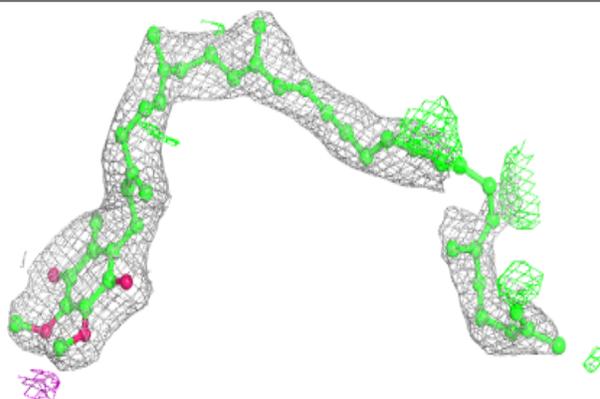


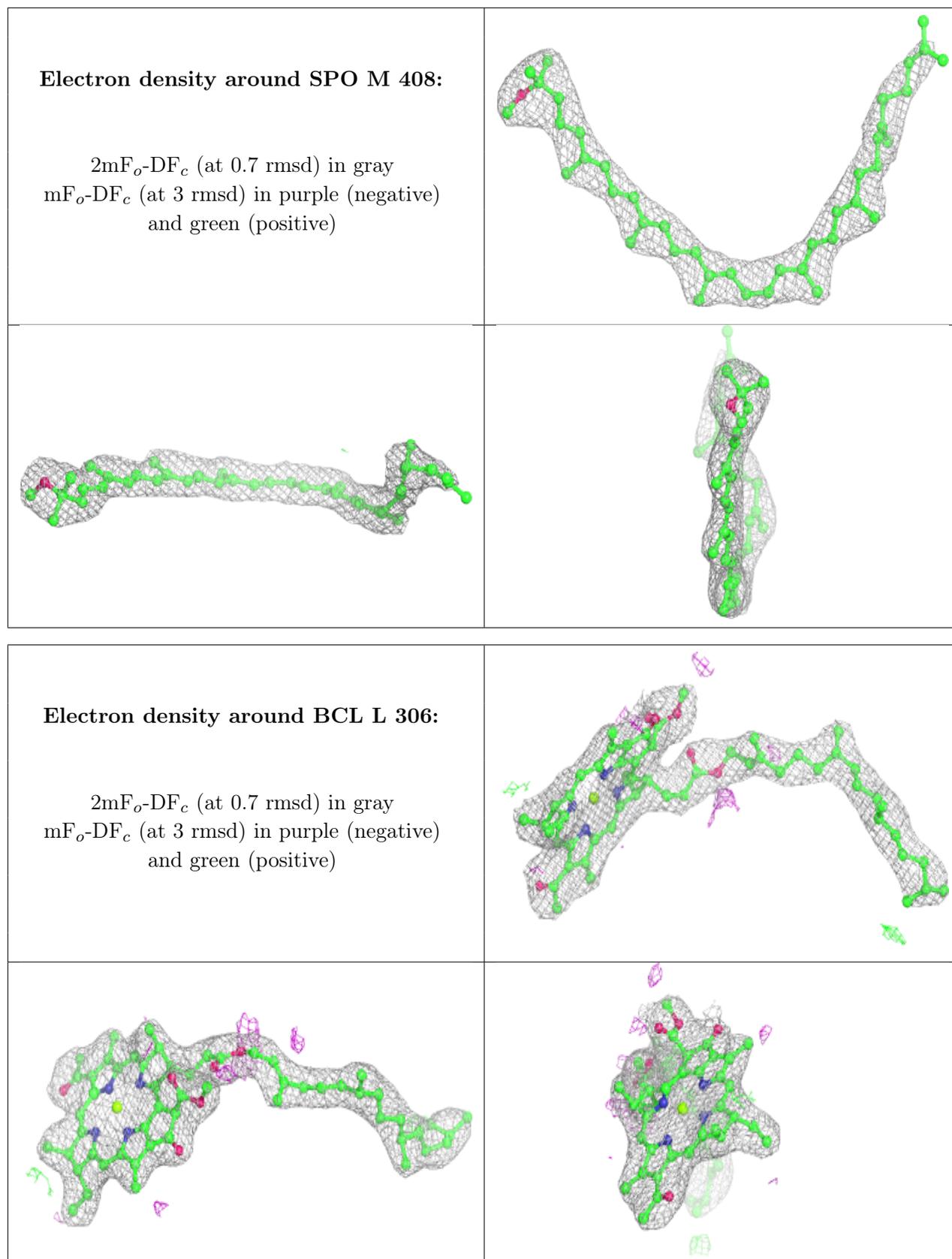
Electron density around BPH M 406:

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and green (positive)

**Electron density around U10 M 407:**

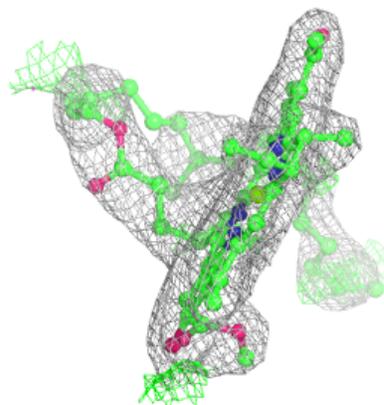
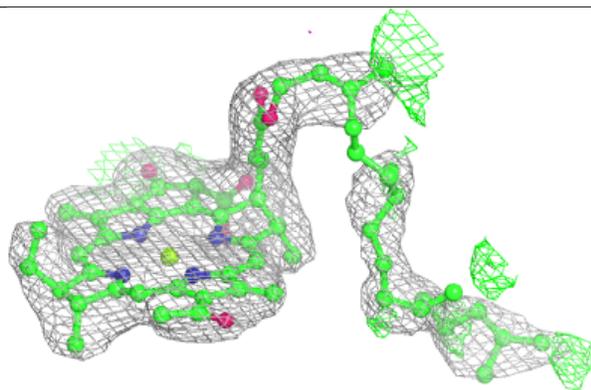
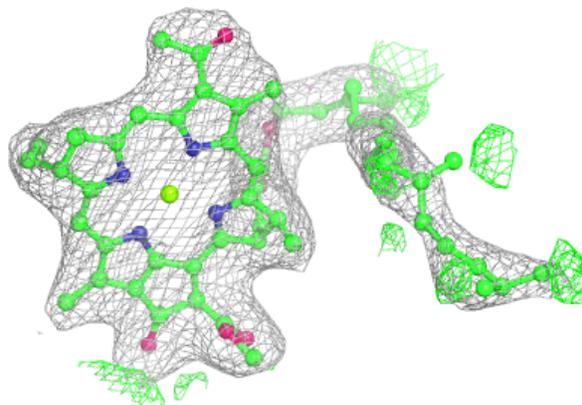
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





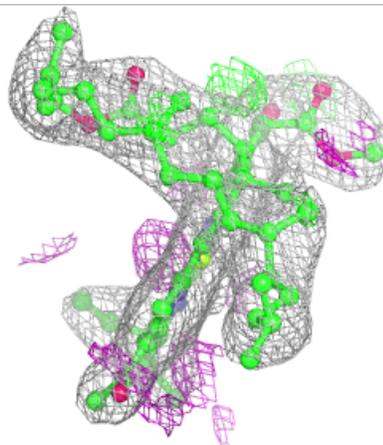
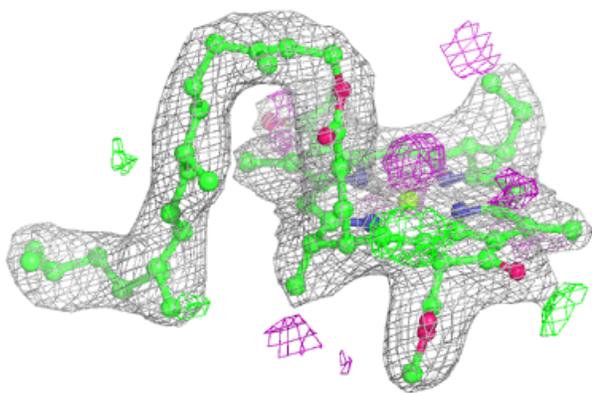
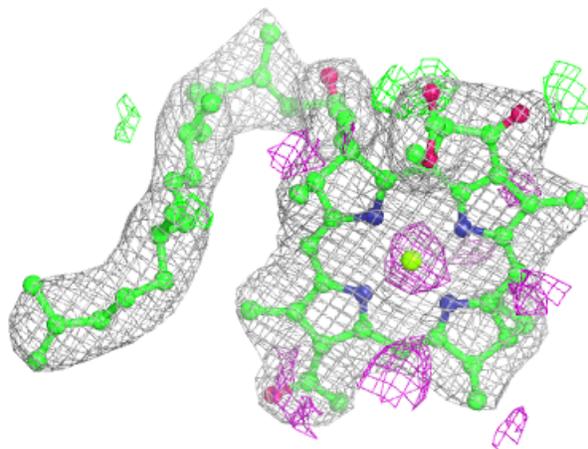
Electron density around BCL M 401:

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



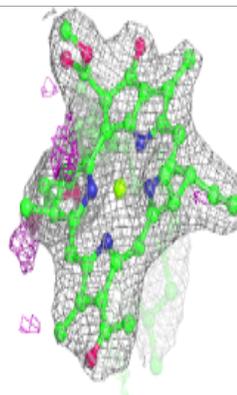
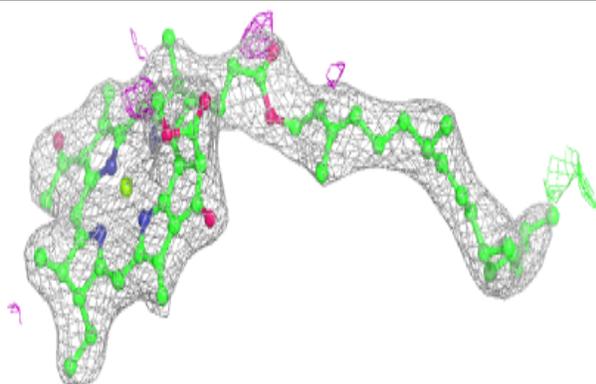
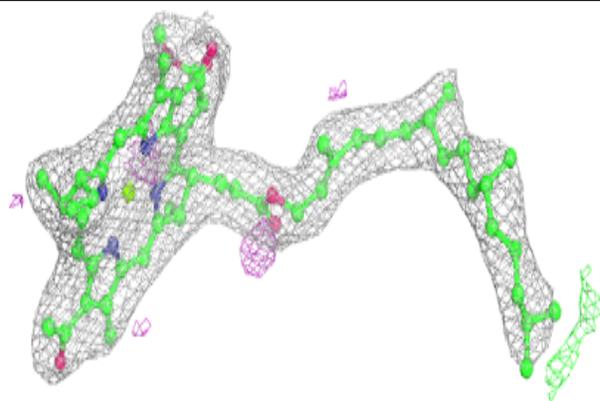
Electron density around BCL L 301:

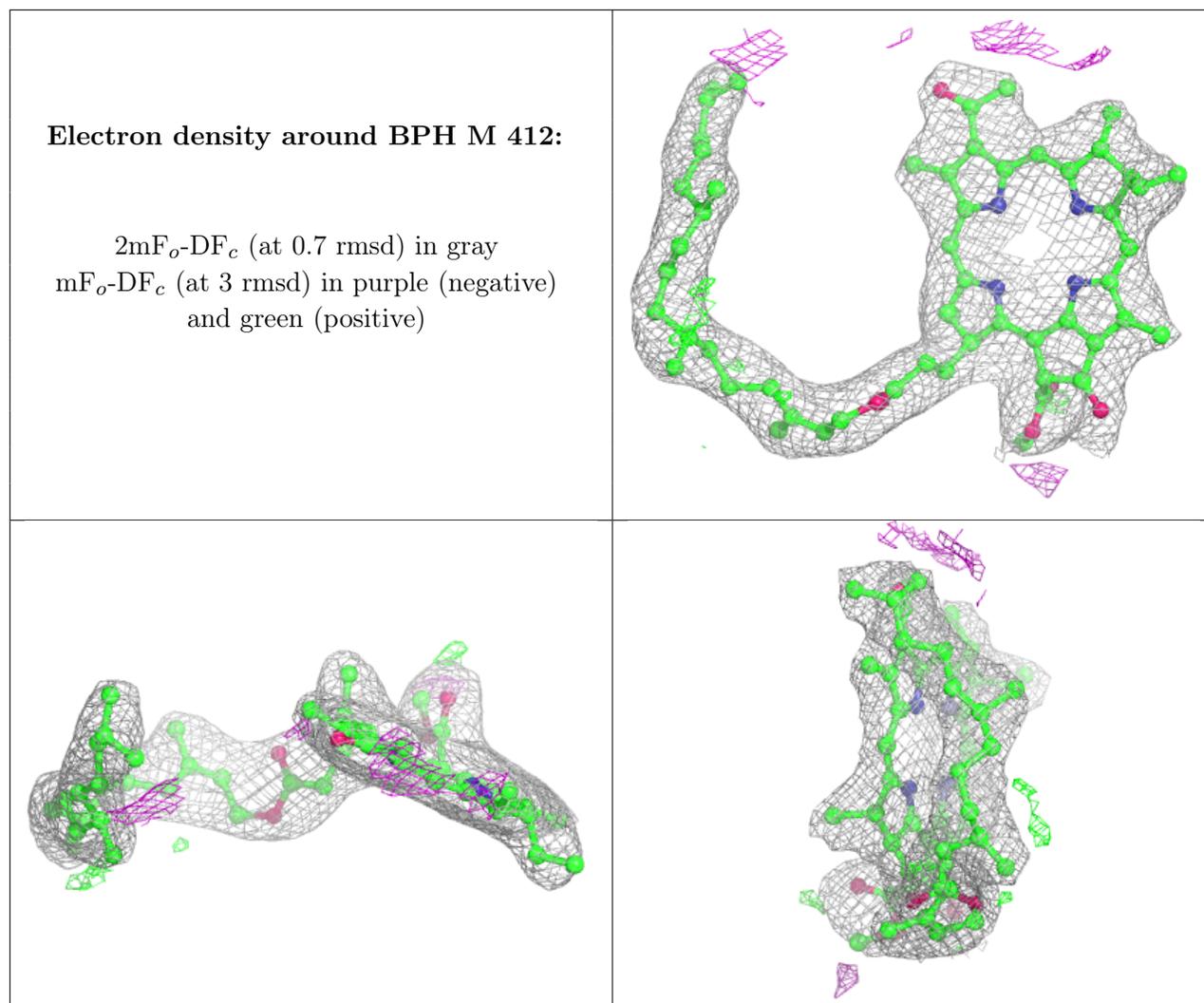
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.