



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:41 pm BST

PDB ID : 4LWY
Title : L(M196)H,H(M202)L Double Mutant Structure of Photosynthetic Reaction Center From Rhodobacter Sphaeroides strain RV
Authors : Gabdulkhakov, A.G.
Deposited on : 2013-07-29
Resolution : 2.90 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 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	:	2.11
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)	:	2.11

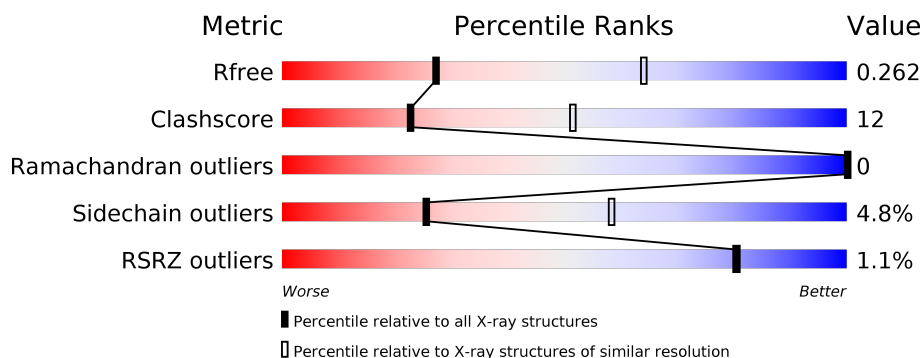
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	260	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>8%</div> </div> </div>
2	L	282	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>•</div> </div> </div>
3	M	303	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>•</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	BPH	L	303	X	-	-	-
12	BPH	M	402	X	-	-	-
12	BPH	M	404	X	-	-	-
14	CDL	M	401	-	-	-	X
4	LDA	M	411	-	-	-	X
5	UNL	L	305	-	-	-	X
5	UNL	L	307	-	-	-	X
7	DIO	H	307	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7434 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
1	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2233	1508	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

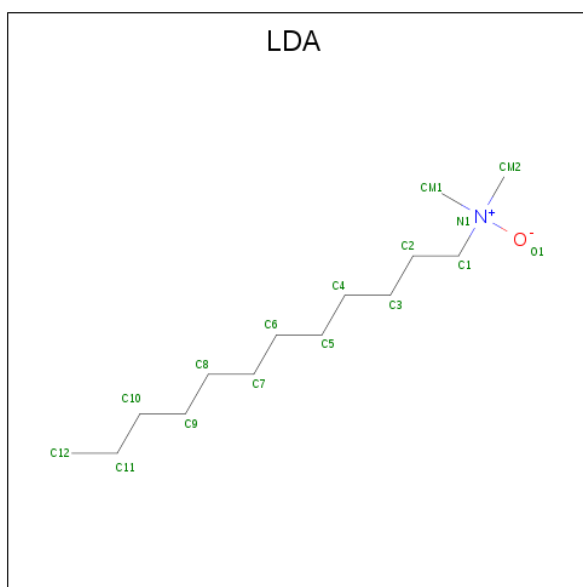
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9
M	196	HIS	LEU	ENGINEERED MUTATION	UNP P0C0Y9
M	202	LEU	HIS	ENGINEERED MUTATION	UNP P0C0Y9

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



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

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

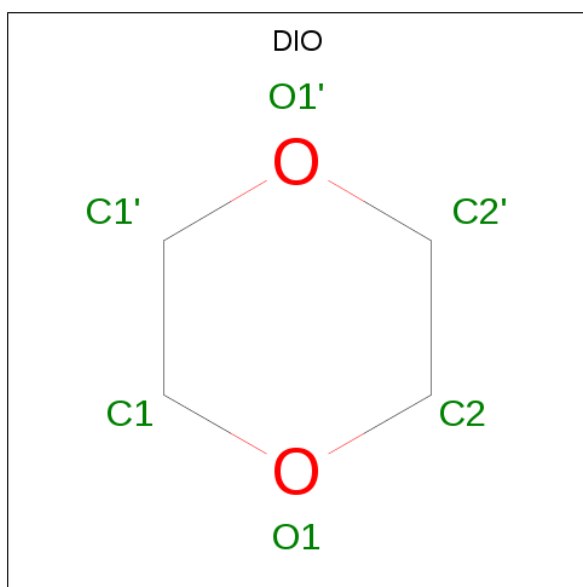
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	4	Total	C	0	0
			48	48		
5	L	4	Total	C	0	0
			46	46		
5	M	3	Total	C	0	0
			36	36		

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



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

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



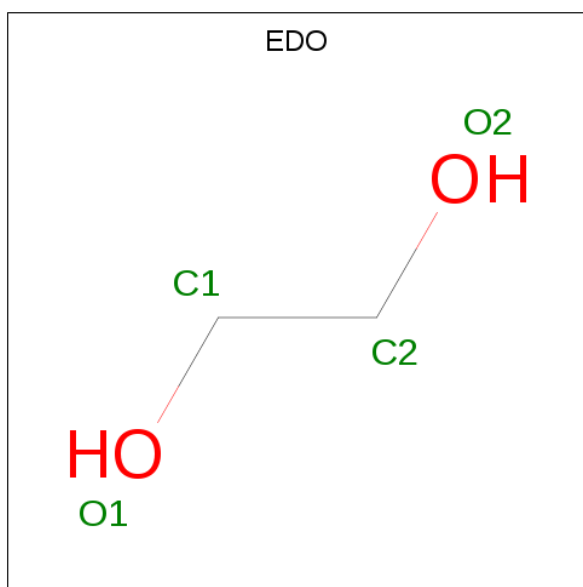
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			6	4	2		

Continued on next page...

Continued from previous page...

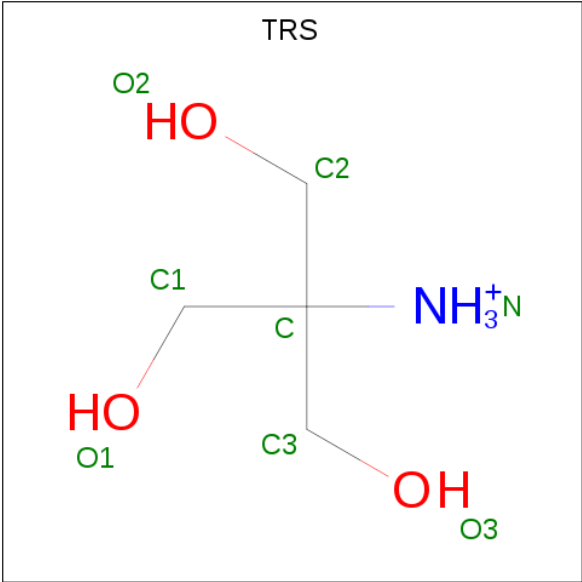
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			6	4	2		
7	L	1	Total	C	O	0	0
			6	4	2		
7	M	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

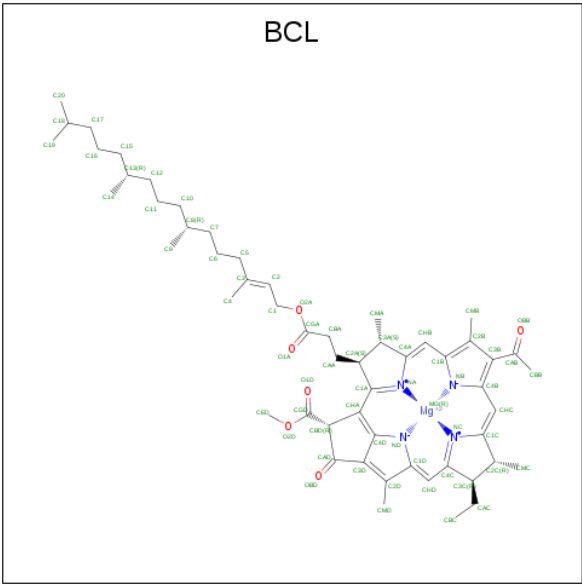


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			8	4	1	3		
9	L	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

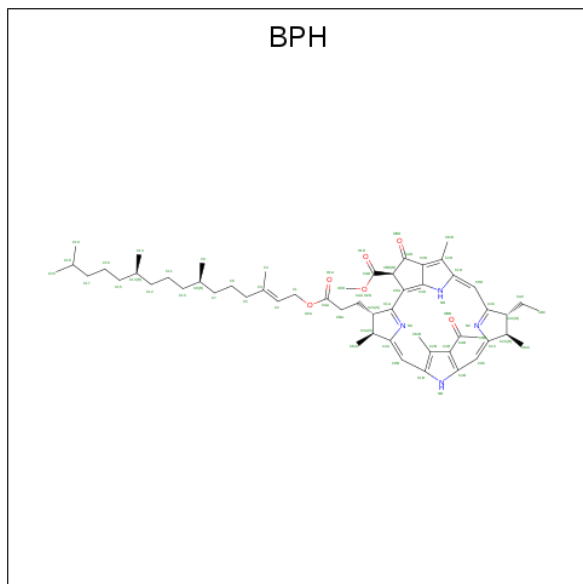
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	1	Total	K	0	0
			1	1		

- Molecule 11 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



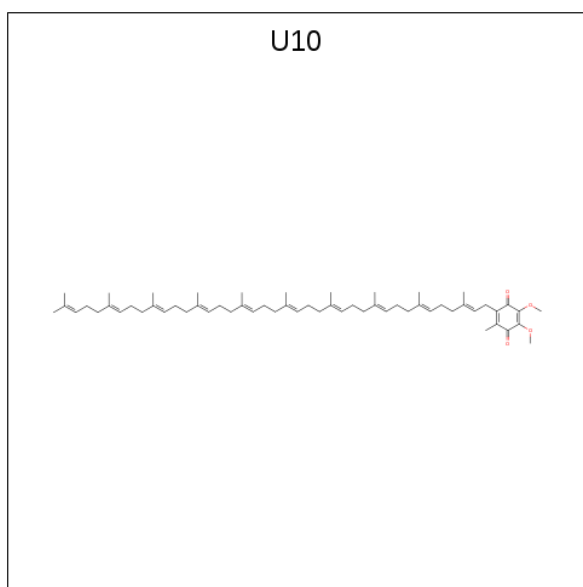
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	
			66	55	1	4	6	
11	L	1	Total	C	Mg	N	O	
			66	55	1	4	6	
11	M	1	Total	C	Mg	N	O	
			66	55	1	4	6	

- Molecule 12 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



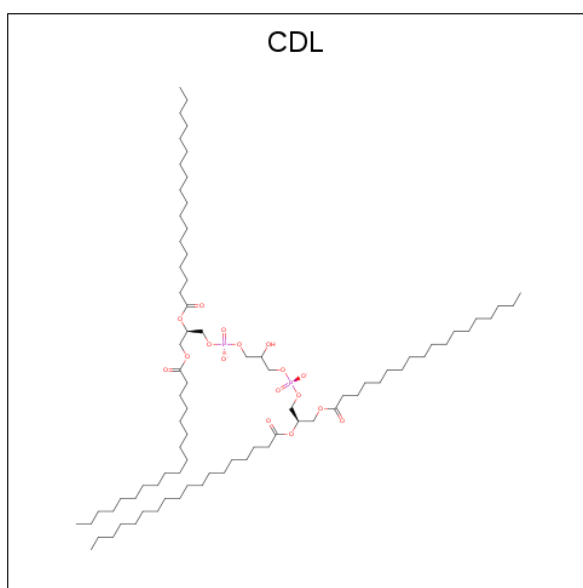
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O		
			65	55	4	6		
12	M	1	Total	C	N	O		
			65	55	4	6		
12	M	1	Total	C	N	O		
			65	55	4	6		

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



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

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

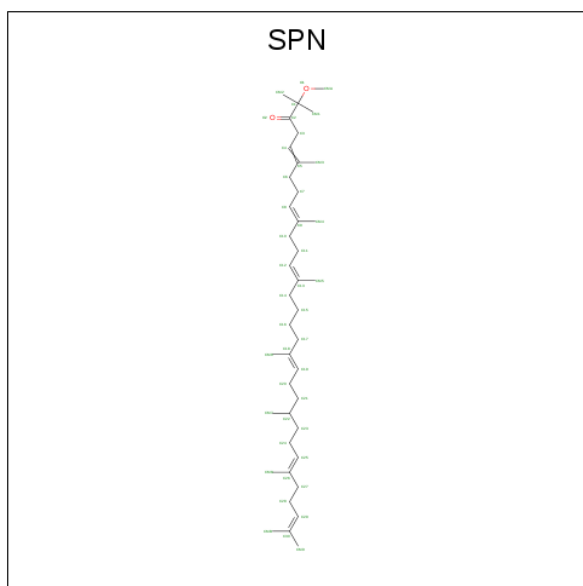


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 16 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



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

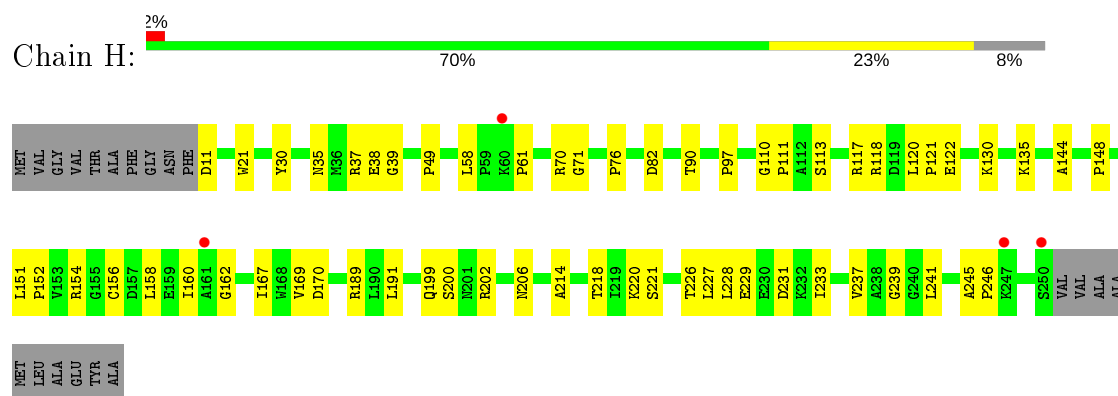
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	11	Total	O	0	0
			11	11		
17	L	10	Total	O	0	0
			10	10		
17	M	18	Total	O	0	0
			18	18		

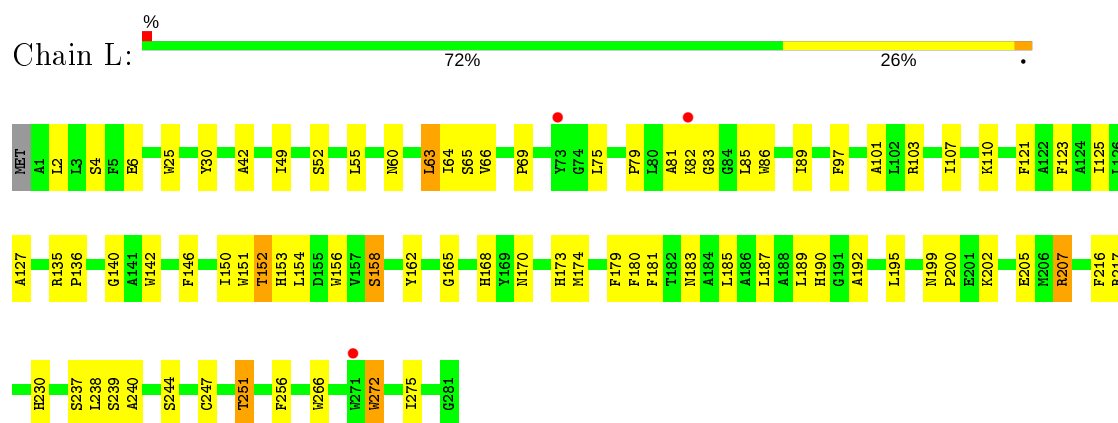
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

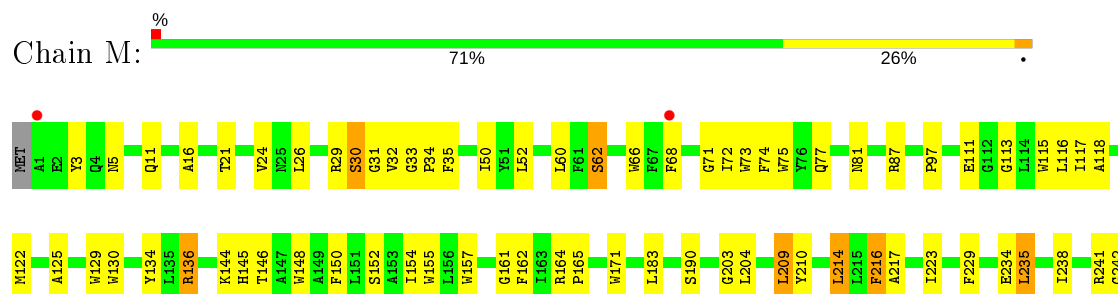
• Molecule 1: Reaction center protein H chain



• Molecule 2: Reaction center protein L chain



• Molecule 3: Reaction center protein M chain



T243	A244
R247	
W254	
T255	
W256	
G257	
F258	
G264	
R267	
W268	
A269	
I270	
V276	
T277	
L278	
I284	
W293	
V296	
W297	
G302	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.04Å 140.04Å 184.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.19 – 2.90 43.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.19-2.90) 99.8 (43.19-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, R_{free}	0.214 , 0.262 0.214 , 0.262	Depositor DCC
R_{free} test set	2335 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.066 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: BCL, LDA, DIO, CDL, BPH, K, EDO, FE, SPN, U10, TRS, UNL, PO4

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	0.43	0/1877	0.63	0/2553
2	L	0.46	0/2321	0.60	0/3177
3	M	0.44	0/2501	0.59	0/3415
All	All	0.44	0/6699	0.60	0/9145

There are no bond length outliers.

There are no bond angle outliers.

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	1829	0	1836	39	0
2	L	2233	0	2189	63	0
3	M	2409	0	2323	71	0
4	H	16	0	31	2	0
4	M	80	0	155	9	0
5	H	48	0	0	0	0
5	L	46	0	0	0	0
5	M	36	0	0	0	0
6	H	5	0	0	0	0
6	M	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	6	0	8	0	0
7	L	12	0	16	3	0
7	M	6	0	8	1	0
8	H	16	0	24	3	0
8	L	4	0	6	1	0
8	M	8	0	12	1	0
9	H	8	0	12	1	0
9	L	8	0	12	0	0
10	H	1	0	0	0	0
11	L	132	0	148	11	0
11	M	66	0	74	4	0
12	L	65	0	76	10	0
12	M	130	0	152	11	0
13	L	48	0	63	1	0
13	M	48	0	63	5	0
14	M	81	0	106	6	0
15	M	1	0	0	0	0
16	M	43	0	70	5	0
17	H	11	0	0	0	0
17	L	10	0	0	0	0
17	M	18	0	0	1	0
All	All	7434	0	7384	170	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 12.

The worst 5 of 170 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:34:PRO:HA	4:M:412:LDA:H71	1.55	0.89
2:L:200:PRO:HD2	7:L:309:DIO:H22	1.64	0.80
1:H:202:ARG:HH12	9:H:312:TRS:H21	1.53	0.73
2:L:42:ALA:HA	12:L:303:BPH:H9C3	1.71	0.73
2:L:65:SER:HB2	2:L:152:THR:HG21	1.70	0.72

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	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/282 (99%)	261 (94%)	18 (6%)	0	100	100
3	M	300/303 (99%)	280 (93%)	20 (7%)	0	100	100
All	All	817/845 (97%)	774 (95%)	43 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	195/208 (94%)	188 (96%)	7 (4%)	35	69
2	L	220/221 (100%)	208 (94%)	12 (6%)	21	53
3	M	236/237 (100%)	224 (95%)	12 (5%)	24	56
All	All	651/666 (98%)	620 (95%)	31 (5%)	25	58

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	216	PHE
2	L	256	PHE
3	M	235	LEU
2	L	247	CYS
2	L	272	TRP

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

Mol	Chain	Res	Type
3	M	77	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 45 ligands modelled in this entry, 11 are unknown and 2 are monoatomic - leaving 32 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	BCL	L	302	-	58,74,74	1.29	5 (8%)	69,115,115	1.69	14 (20%)
8	EDO	M	420	-	3,3,3	0.52	0	2,2,2	0.20	0
8	EDO	H	308	-	3,3,3	0.47	0	2,2,2	0.28	0
6	PO4	M	417	-	4,4,4	0.87	0	6,6,6	0.35	0
4	LDA	M	412	-	12,15,15	2.04	1 (8%)	14,17,17	0.35	0
12	BPH	L	303	-	64,70,70	1.45	8 (12%)	76,101,101	1.31	8 (10%)
6	PO4	M	416	-	4,4,4	0.84	0	6,6,6	0.43	0
7	DIO	H	307	-	6,6,6	0.86	0	6,6,6	0.76	0
7	DIO	L	309	-	6,6,6	0.81	0	6,6,6	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	TRS	H	312	-	7,7,7	0.30	0	9,9,9	0.34	0
4	LDA	M	409	-	12,15,15	2.04	1 (8%)	14,17,17	0.43	0
16	SPN	M	407	-	40,42,42	1.22	6 (15%)	50,52,52	1.66	13 (26%)
13	U10	M	406	-	48,48,63	2.64	14 (29%)	58,61,79	1.84	14 (24%)
8	EDO	H	310	-	3,3,3	0.46	0	2,2,2	0.48	0
8	EDO	M	419	-	3,3,3	0.51	0	2,2,2	0.28	0
12	BPH	M	402	-	64,70,70	1.37	8 (12%)	76,101,101	1.26	9 (11%)
6	PO4	H	306	-	4,4,4	0.93	0	6,6,6	0.31	0
4	LDA	M	410	-	12,15,15	2.08	1 (8%)	14,17,17	0.60	0
4	LDA	M	408	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0
11	BCL	L	301	-	58,74,74	1.31	3 (5%)	69,115,115	1.71	13 (18%)
8	EDO	L	311	-	3,3,3	0.55	0	2,2,2	0.09	0
12	BPH	M	404	-	64,70,70	1.38	7 (10%)	76,101,101	1.44	9 (11%)
7	DIO	M	418	-	6,6,6	0.85	0	6,6,6	0.85	0
4	LDA	M	411	-	12,15,15	2.07	1 (8%)	14,17,17	0.38	0
9	TRS	L	312	-	7,7,7	0.32	0	9,9,9	0.30	0
11	BCL	M	403	-	58,74,74	1.42	6 (10%)	69,115,115	1.84	15 (21%)
13	U10	L	304	-	48,48,63	2.60	13 (27%)	58,61,79	1.84	15 (25%)
14	CDL	M	401	-	80,80,99	0.90	4 (5%)	86,92,111	1.30	7 (8%)
8	EDO	H	311	-	3,3,3	0.54	0	2,2,2	0.17	0
8	EDO	H	309	-	3,3,3	0.44	0	2,2,2	0.55	0
4	LDA	H	301	-	12,15,15	2.03	1 (8%)	14,17,17	0.55	0
7	DIO	L	310	-	6,6,6	0.70	0	6,6,6	1.07	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
11	BCL	L	302	-	-	7/37/137/137	-
8	EDO	M	420	-	-	1/1/1/1	-
8	EDO	H	308	-	-	0/1/1/1	-
4	LDA	M	412	-	-	6/13/13/13	-
12	BPH	L	303	-	2/2/18/22	13/54/105/105	0/5/6/6
7	DIO	H	307	-	-	-	0/1/1/1
7	DIO	L	309	-	-	-	0/1/1/1
9	TRS	H	312	-	-	6/9/9/9	-
4	LDA	M	409	-	-	5/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	SPN	M	407	-	-	17/50/51/51	-
13	U10	M	406	-	-	12/45/69/87	0/1/1/1
8	EDO	H	310	-	-	0/1/1/1	-
8	EDO	M	419	-	-	1/1/1/1	-
12	BPH	M	402	-	2/2/18/22	8/54/105/105	0/5/6/6
4	LDA	M	410	-	-	1/13/13/13	-
4	LDA	M	408	-	-	2/13/13/13	-
11	BCL	L	301	-	-	10/37/137/137	-
8	EDO	L	311	-	-	0/1/1/1	-
12	BPH	M	404	-	2/2/18/22	7/54/105/105	0/5/6/6
7	DIO	M	418	-	-	-	0/1/1/1
4	LDA	M	411	-	-	7/13/13/13	-
9	TRS	L	312	-	-	7/9/9/9	-
11	BCL	M	403	-	-	7/37/137/137	-
13	U10	L	304	-	-	11/45/69/87	0/1/1/1
14	CDL	M	401	-	-	44/91/91/110	-
8	EDO	H	311	-	-	0/1/1/1	-
8	EDO	H	309	-	-	0/1/1/1	-
4	LDA	H	301	-	-	8/13/13/13	-
7	DIO	L	310	-	-	-	0/1/1/1

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	408	LDA	O1-N1	-7.13	1.25	1.42
4	M	410	LDA	O1-N1	-7.11	1.25	1.42
4	M	411	LDA	O1-N1	-7.07	1.25	1.42
4	H	301	LDA	O1-N1	-6.97	1.25	1.42
4	M	412	LDA	O1-N1	-6.96	1.25	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	403	BCL	C1C-NC-C4C	6.48	109.62	106.71
11	L	301	BCL	C1C-NC-C4C	5.95	109.38	106.71
13	L	304	U10	C7-C8-C9	-5.69	117.32	126.79
11	L	302	BCL	CMB-C2B-C1B	-4.99	120.80	128.46
11	L	301	BCL	O2D-CGD-CBD	4.89	119.96	111.27

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	303	BPH	C8
12	L	303	BPH	C13
12	M	402	BPH	C8
12	M	402	BPH	C13
12	M	404	BPH	C8

5 of 180 torsion outliers are listed below:

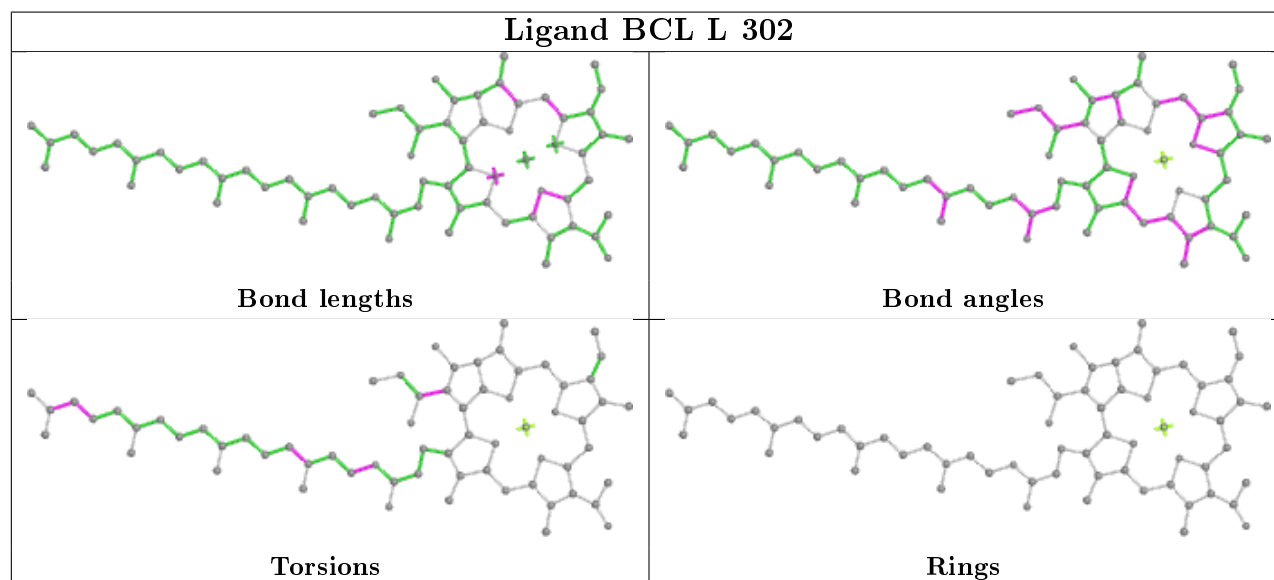
Mol	Chain	Res	Type	Atoms
11	L	302	BCL	C4-C3-C5-C6
12	L	303	BPH	C4B-C3B-CAB-CBB
12	L	303	BPH	C4B-C3B-CAB-OB
4	M	409	LDA	N1-C1-C2-C3
16	M	407	SPN	C7-C8-C9-C10

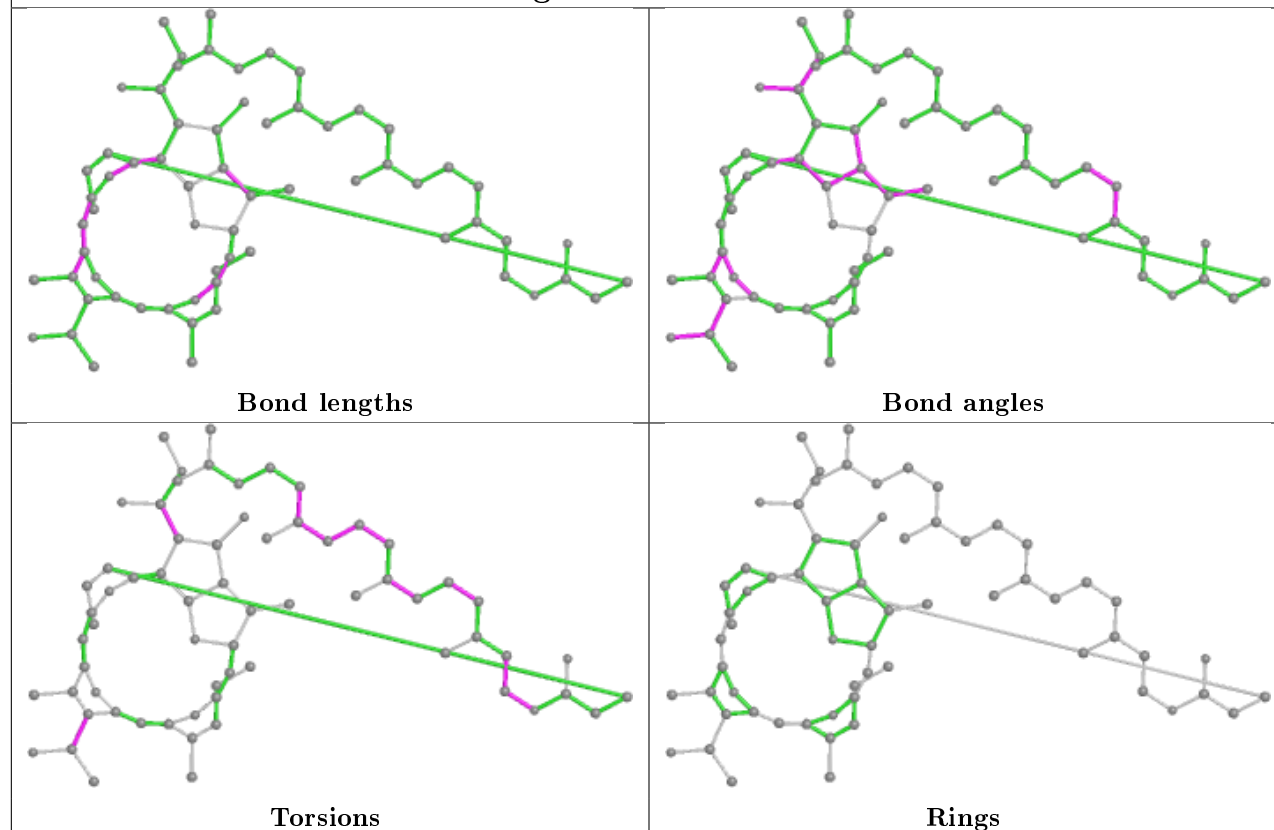
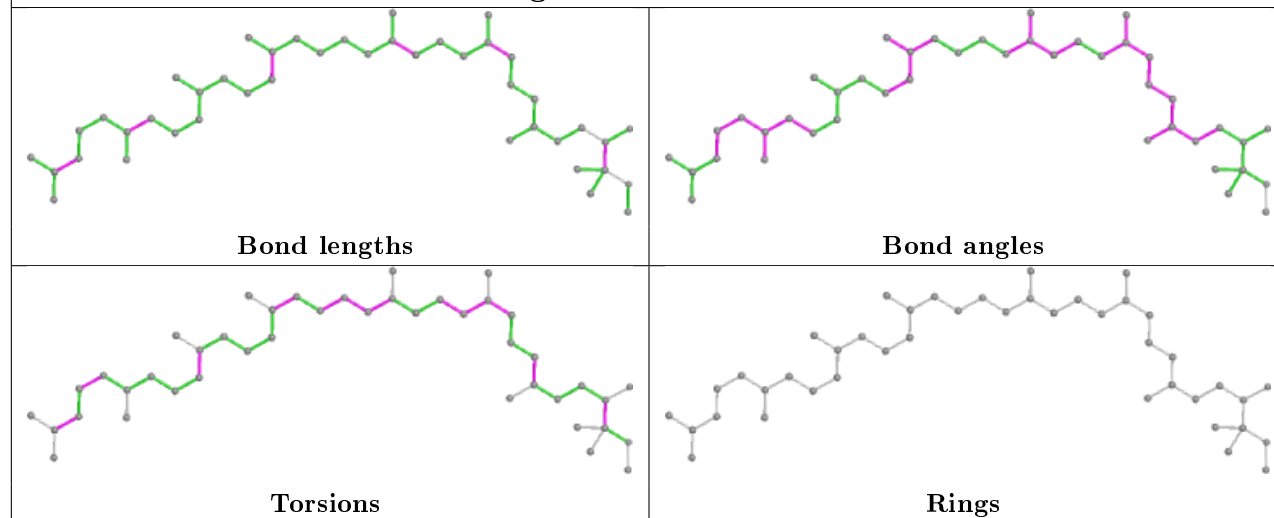
There are no ring outliers.

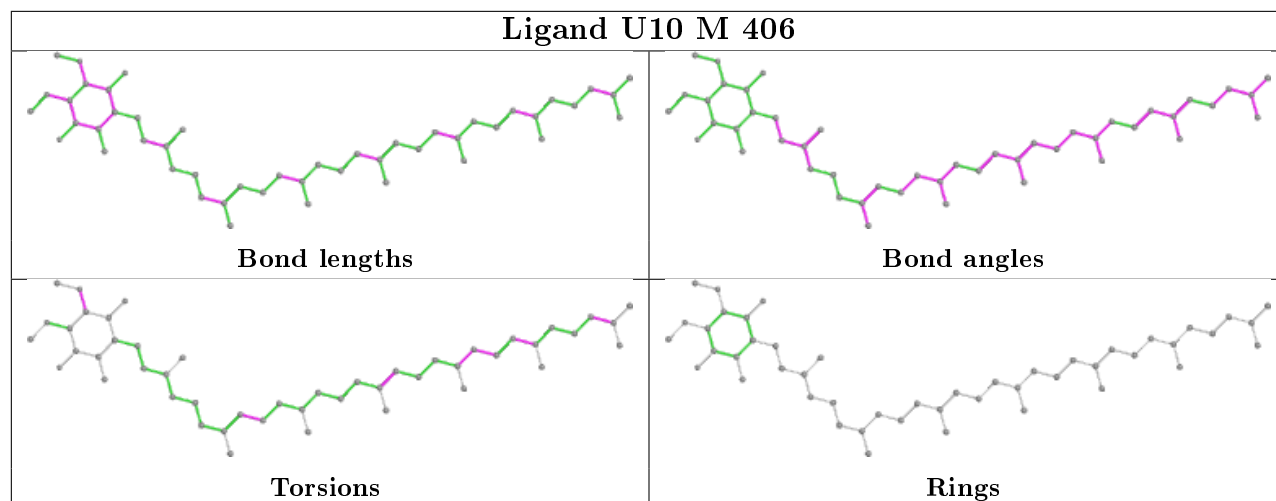
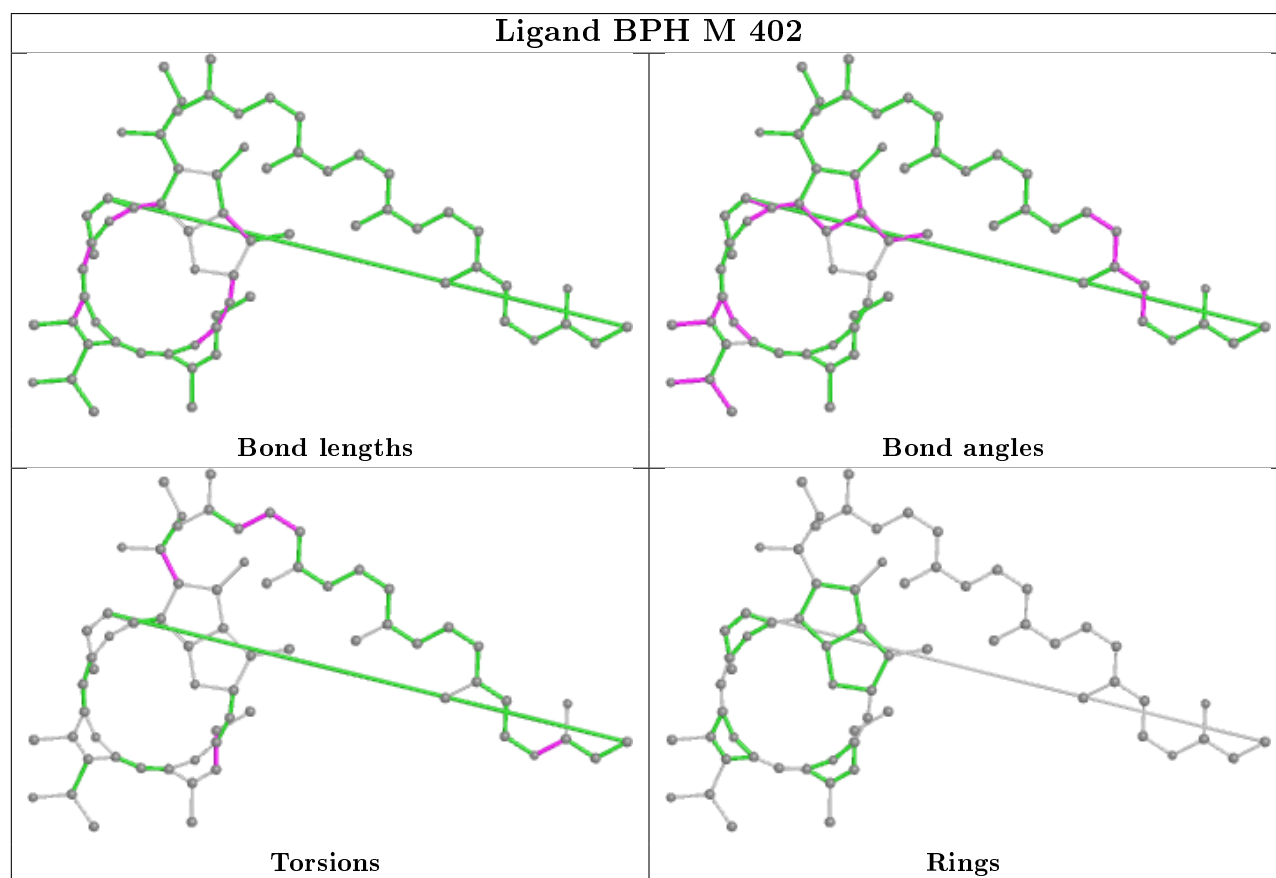
21 monomers are involved in 65 short contacts:

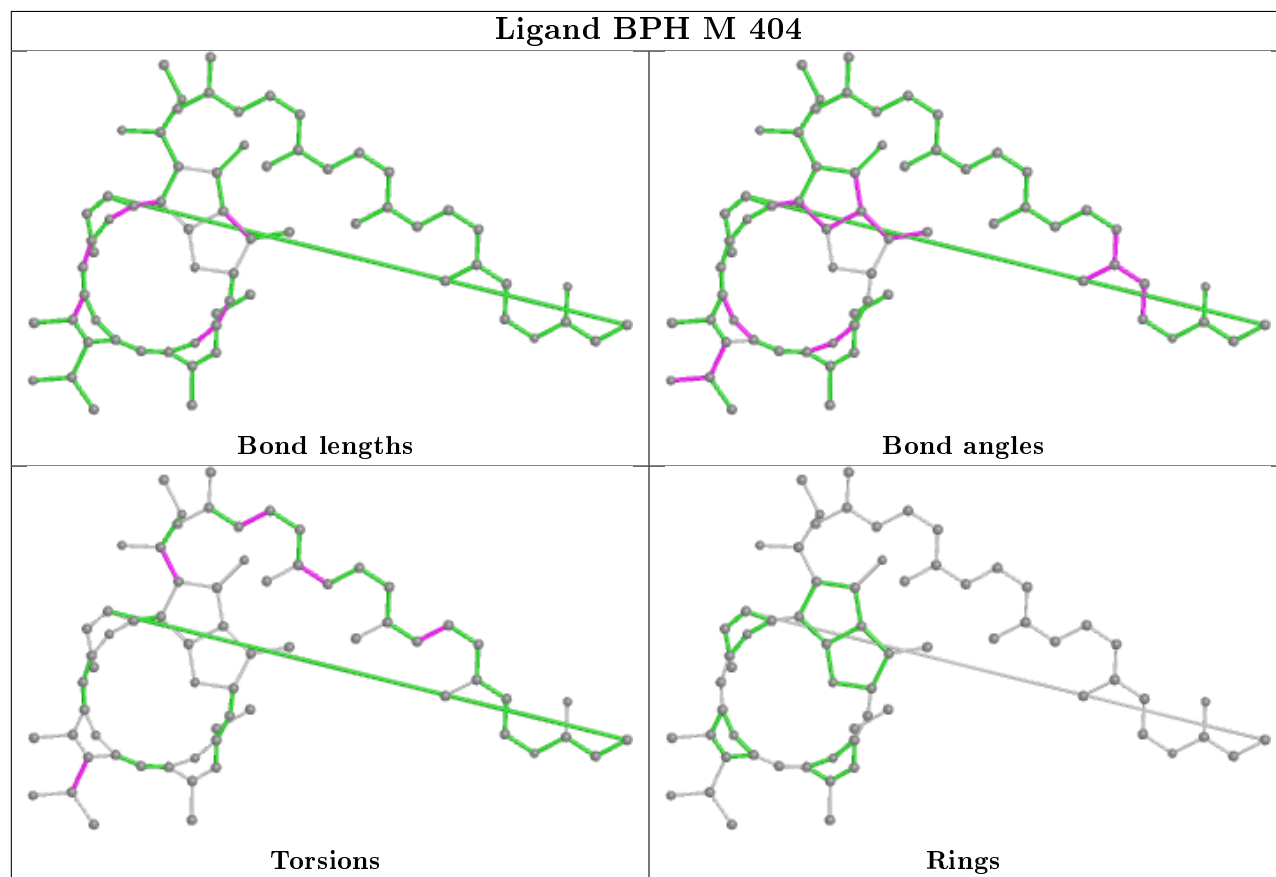
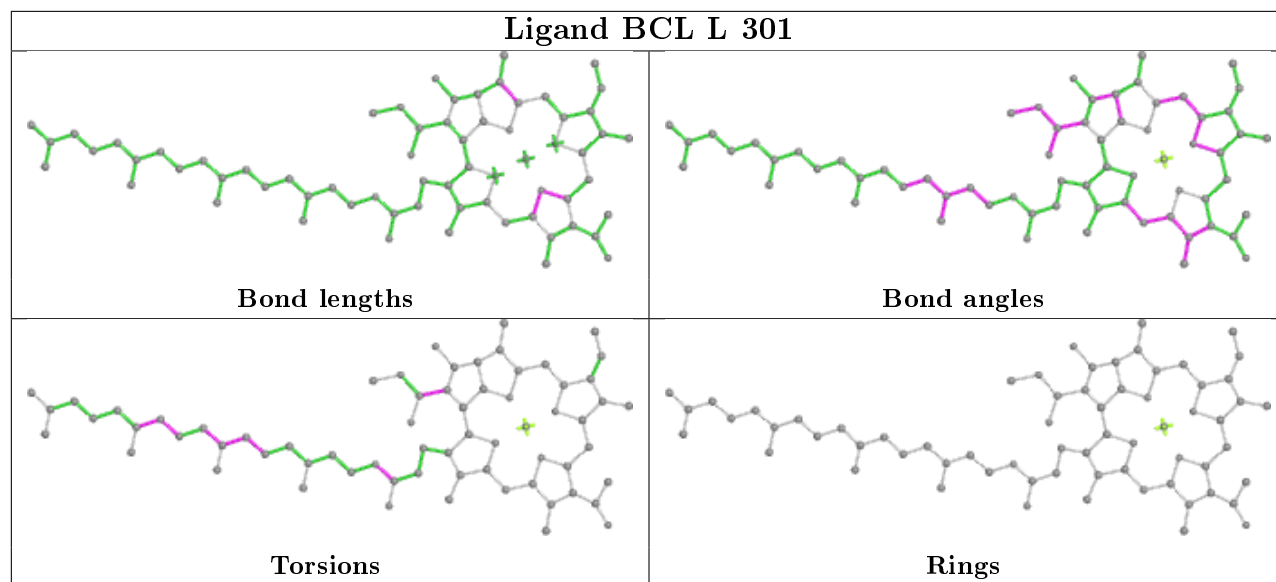
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	302	BCL	6	0
4	M	412	LDA	4	0
12	L	303	BPH	10	0
7	L	309	DIO	3	0
9	H	312	TRS	1	0
16	M	407	SPN	5	0
13	M	406	U10	5	0
8	H	310	EDO	2	0
8	M	419	EDO	1	0
12	M	402	BPH	5	0
4	M	410	LDA	1	0
4	M	408	LDA	4	0
11	L	301	BCL	5	0
8	L	311	EDO	1	0
12	M	404	BPH	7	0
7	M	418	DIO	1	0
11	M	403	BCL	4	0
13	L	304	U10	1	0
14	M	401	CDL	6	0
8	H	311	EDO	1	0
4	H	301	LDA	2	0

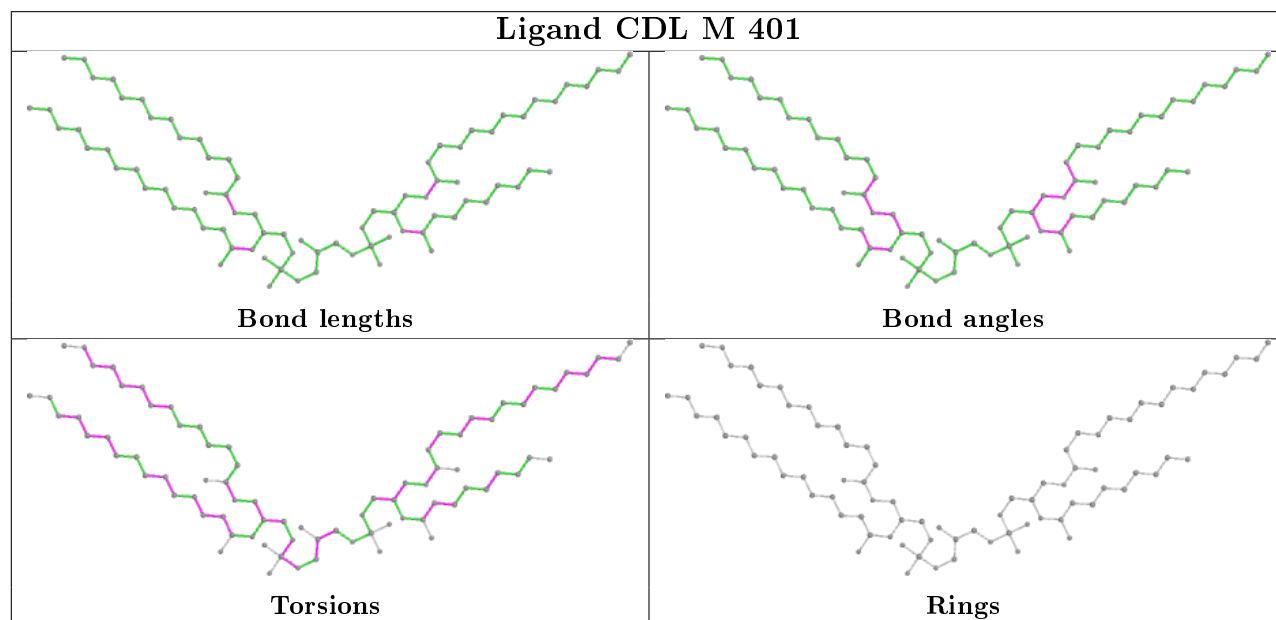
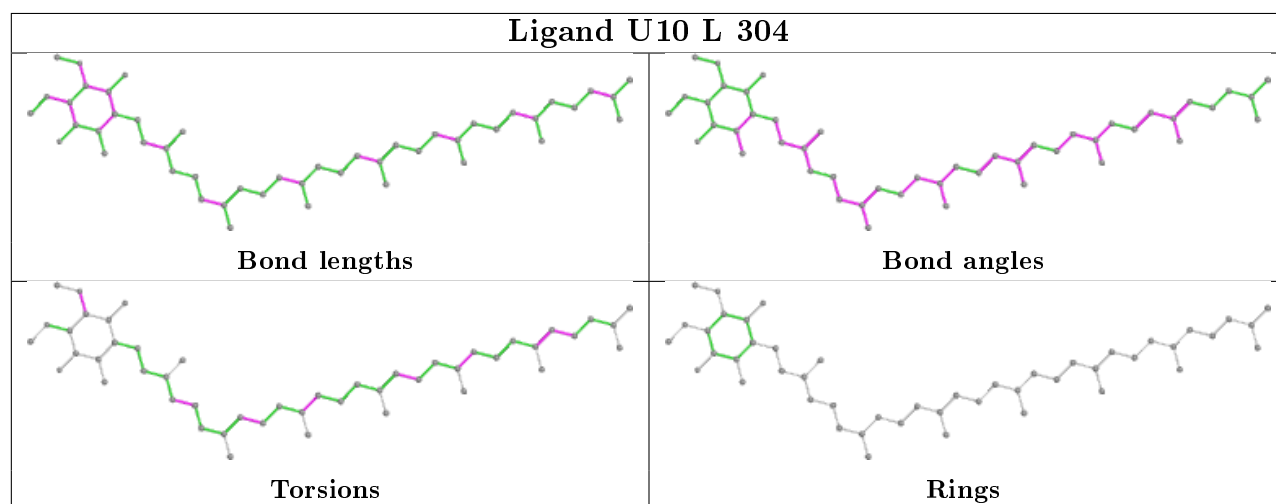
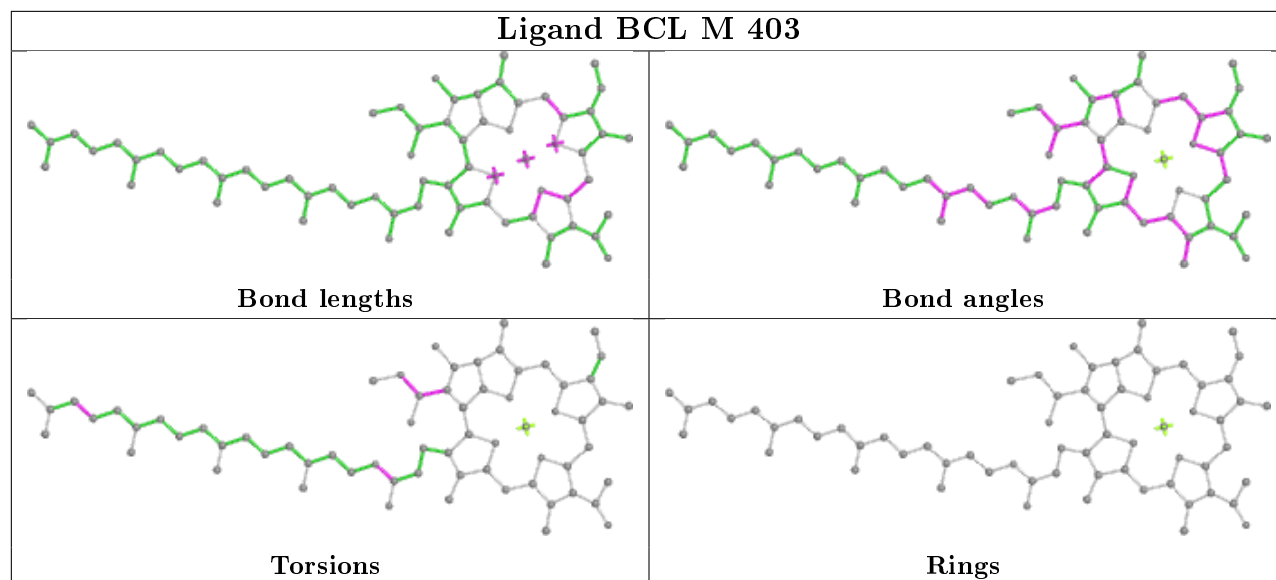
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand BPH L 303**Ligand SPN M 407**

Ligand U10 M 406**Ligand BPH M 402**





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	240/260 (92%)	-0.41	4 (1%) 70 69	19, 45, 74, 127	0
2	L	281/282 (99%)	-0.32	3 (1%) 80 80	13, 42, 83, 130	0
3	M	302/303 (99%)	-0.30	2 (0%) 87 87	18, 45, 84, 118	0
All	All	823/845 (97%)	-0.34	9 (1%) 80 80	13, 44, 82, 130	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	4.5
1	H	247	LYS	3.1
3	M	1	ALA	2.7
2	L	82	LYS	2.2
3	M	68	PHE	2.2

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 carbohydrates 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.

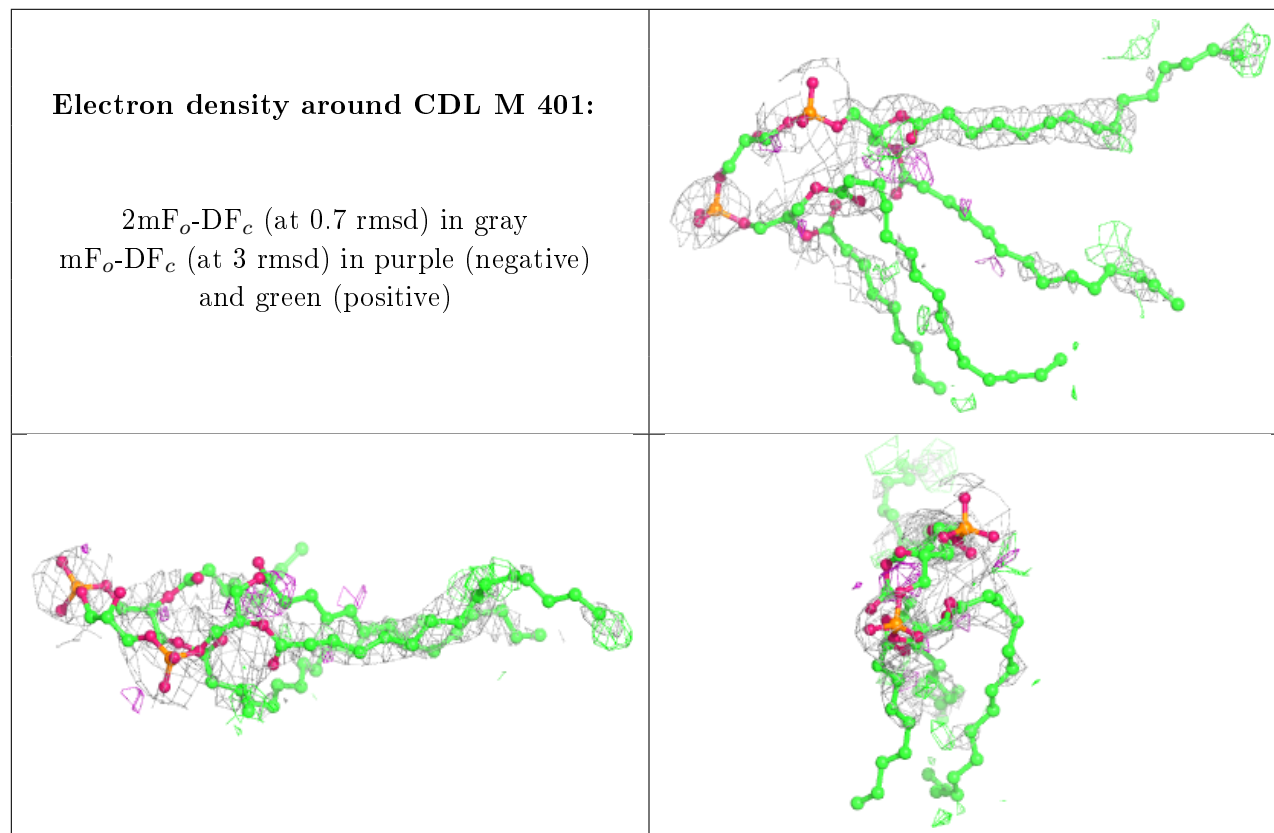
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LDA	M	411	16/16	0.63	0.93	63,106,135,139	0
8	EDO	H	311	4/4	0.71	0.37	58,60,62,63	0
5	UNL	L	308	12/-	0.73	0.36	39,70,76,79	0
7	DIO	H	307	6/6	0.75	0.60	100,102,102,102	0
5	UNL	L	305	12/-	0.76	0.83	67,78,91,94	0
5	UNL	L	307	10/-	0.76	0.91	53,79,104,107	0
5	UNL	M	414	12/-	0.79	0.32	45,66,80,85	0
4	LDA	M	412	16/16	0.80	0.34	63,87,99,105	0
14	CDL	M	401	81/100	0.80	0.48	58,97,140,158	0
5	UNL	H	304	12/-	0.81	0.51	39,53,80,83	0
5	UNL	M	415	12/-	0.82	0.69	70,82,90,92	0
9	TRS	H	312	8/8	0.83	0.26	76,84,92,102	0
8	EDO	M	419	4/4	0.84	0.29	60,73,77,78	0
9	TRS	L	312	8/8	0.85	0.39	73,77,88,89	0
5	UNL	L	306	12/-	0.85	0.38	35,54,67,68	0
6	PO4	M	416	5/5	0.85	0.13	95,108,121,134	0
5	UNL	M	413	12/-	0.85	0.25	32,47,55,58	0
5	UNL	H	303	12/-	0.85	0.55	43,54,70,73	0
4	LDA	M	410	16/16	0.85	0.29	48,66,88,98	0
6	PO4	M	417	5/5	0.86	0.22	94,102,115,118	0
5	UNL	H	305	12/-	0.86	0.38	54,66,81,82	0
4	LDA	M	409	16/16	0.86	0.46	34,45,80,83	0
7	DIO	L	310	6/6	0.87	0.23	64,68,73,82	0
5	UNL	H	302	12/-	0.87	0.41	53,59,78,82	0
13	U10	L	304	48/63	0.88	0.24	53,70,84,90	0
8	EDO	H	310	4/4	0.88	0.34	61,65,68,70	0
10	K	H	313	1/1	0.88	0.15	64,64,64,64	0
8	EDO	H	308	4/4	0.89	0.18	79,79,82,86	0
6	PO4	H	306	5/5	0.89	0.16	94,105,115,120	0
8	EDO	L	311	4/4	0.90	0.20	68,73,73,81	0
7	DIO	M	418	6/6	0.91	0.36	99,104,105,112	0
13	U10	M	406	48/63	0.91	0.24	28,39,57,64	0
12	BPH	M	404	65/65	0.92	0.26	39,54,101,113	0
16	SPN	M	407	43/43	0.92	0.40	30,52,74,78	0
7	DIO	L	309	6/6	0.93	0.32	34,36,40,46	6
4	LDA	H	301	16/16	0.94	0.18	48,58,63,69	0
12	BPH	L	303	65/65	0.95	0.18	25,31,44,51	0
8	EDO	H	309	4/4	0.95	0.17	55,56,59,61	0
4	LDA	M	408	16/16	0.95	0.18	45,55,64,66	0
8	EDO	M	420	4/4	0.96	0.19	37,40,46,47	0
11	BCL	L	302	66/66	0.97	0.16	24,32,42,46	0
11	BCL	M	403	66/66	0.97	0.16	19,24,37,41	0
12	BPH	M	402	65/65	0.97	0.16	27,33,55,67	0

Continued on next page...

Continued from previous page...

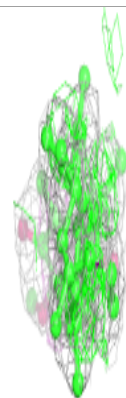
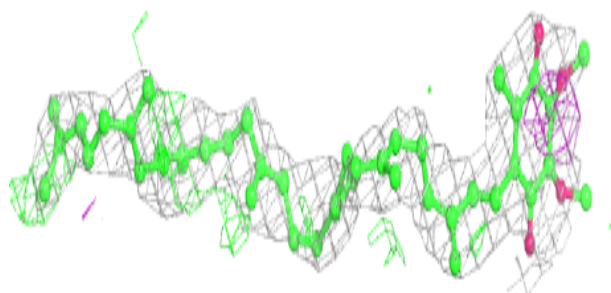
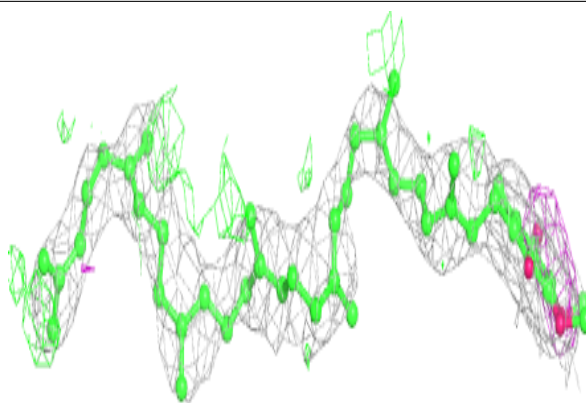
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	BCL	L	301	66/66	0.97	0.17	21,34,65,72	0
15	FE	M	405	1/1	1.00	0.15	25,25,25,25	0

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.

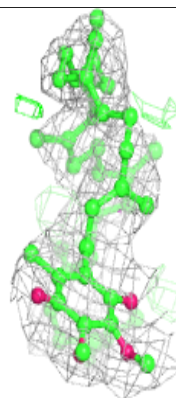
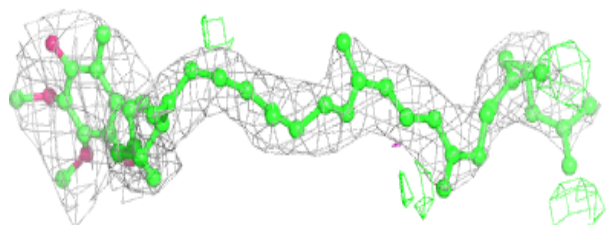
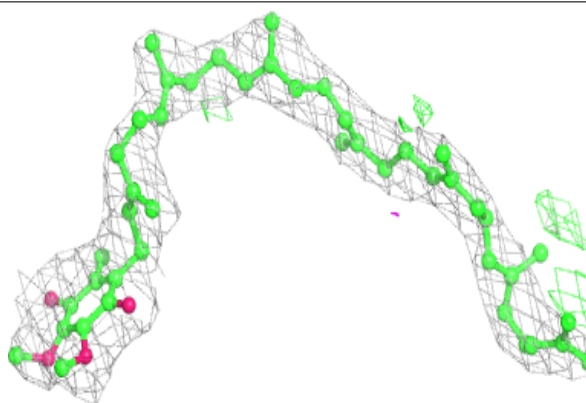


Electron density around U10 L 304:

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

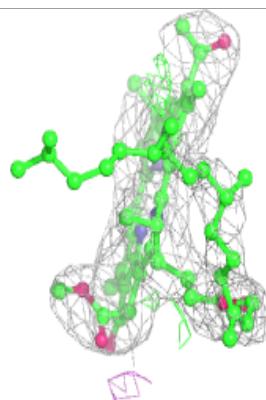
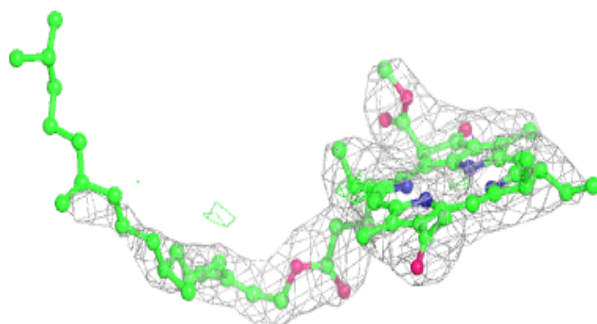
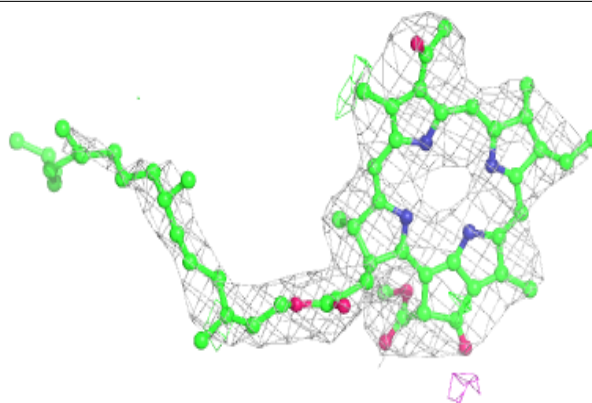
**Electron density around U10 M 406:**

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

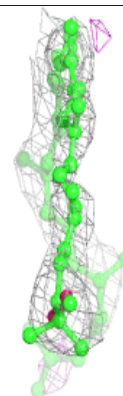
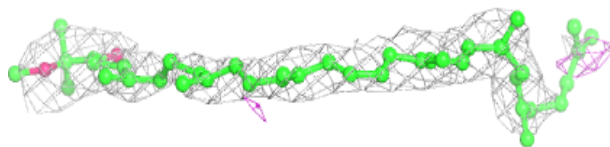
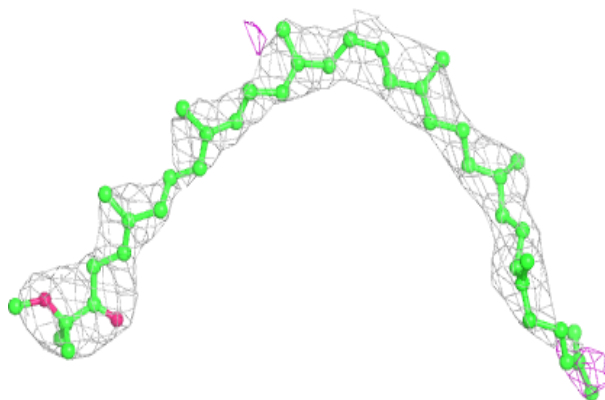


Electron density around BPH M 404:

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

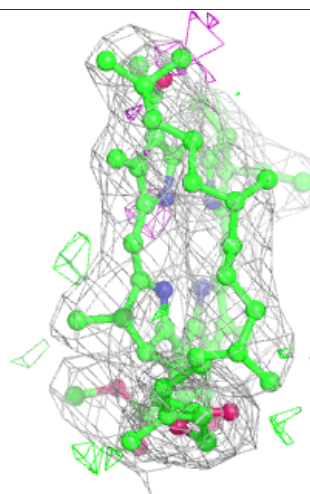
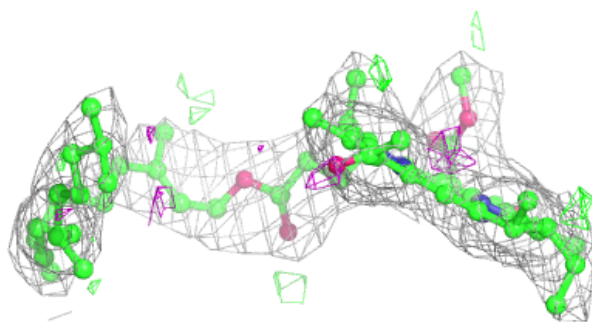
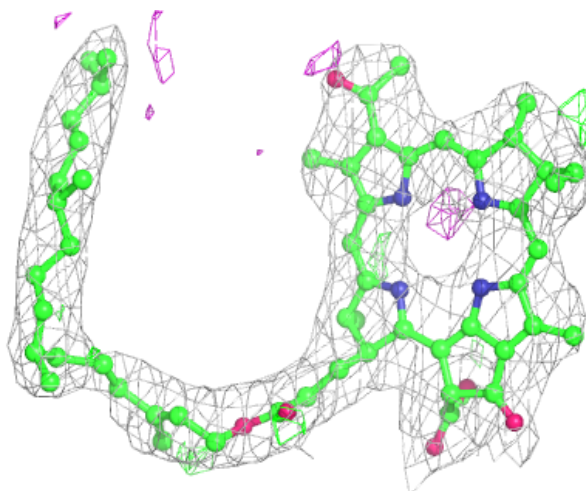
**Electron density around SPN M 407:**

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



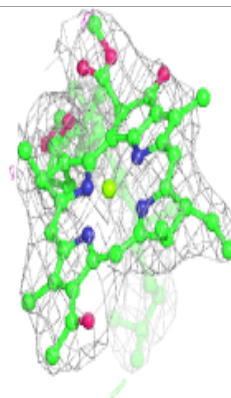
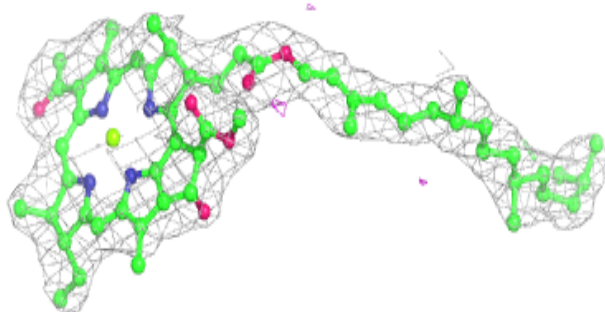
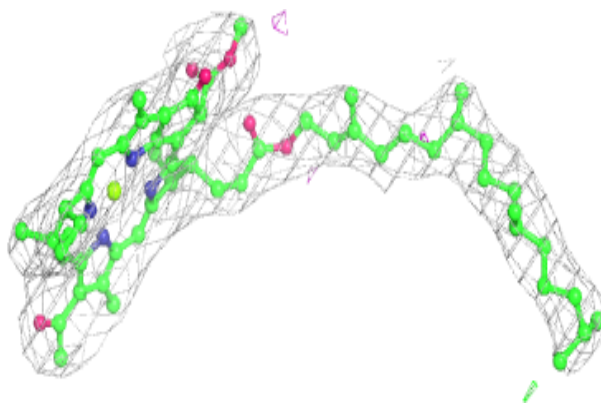
Electron density around BPH L 303:

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



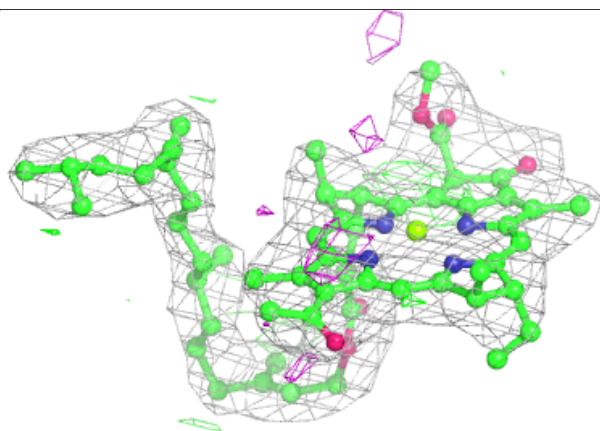
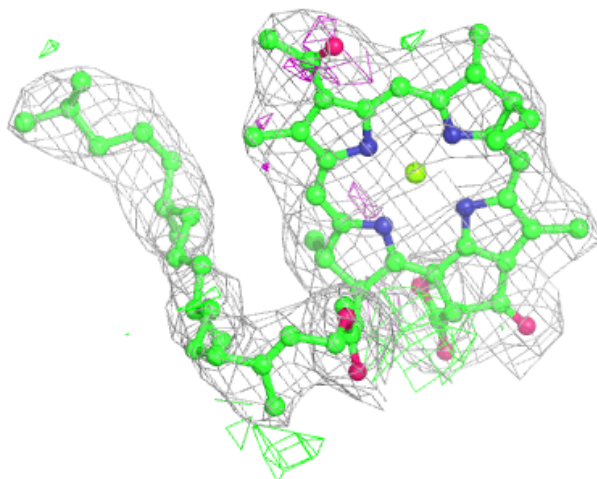
Electron density around BCL L 302:

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



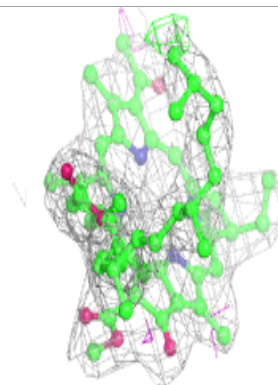
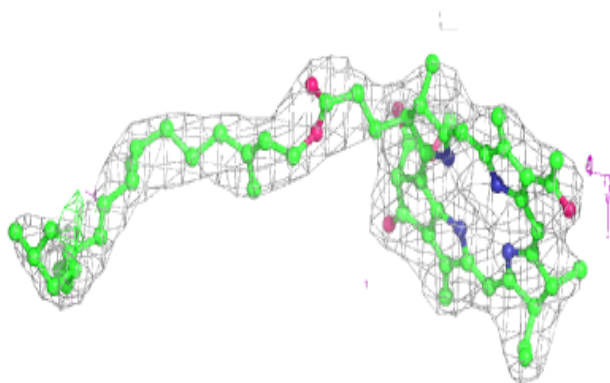
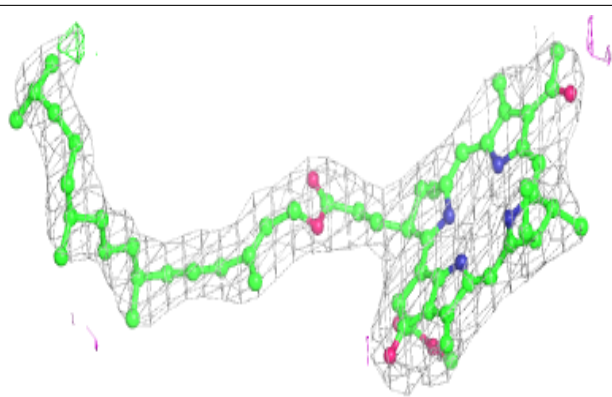
Electron density around BCL M 403:

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



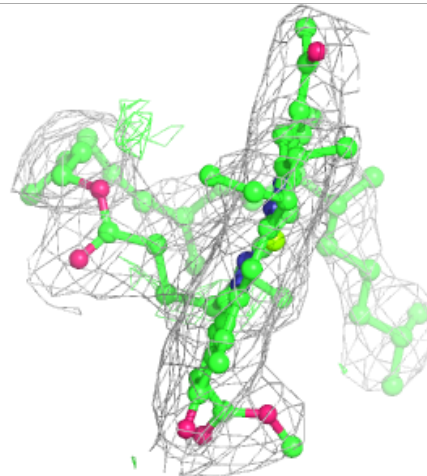
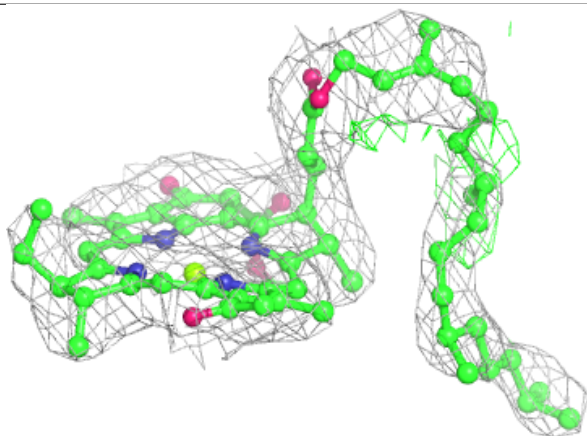
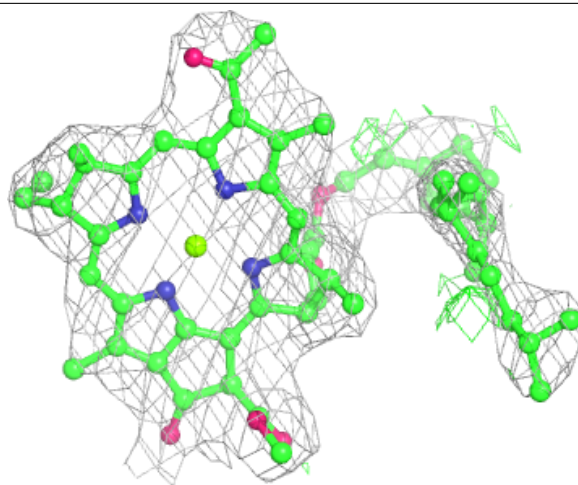
Electron density around BPH M 402:

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



Electron density around BCL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.