



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 08:36 AM BST

PDB ID : 4IN6
Title : (M)L214A 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 : 2.70 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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

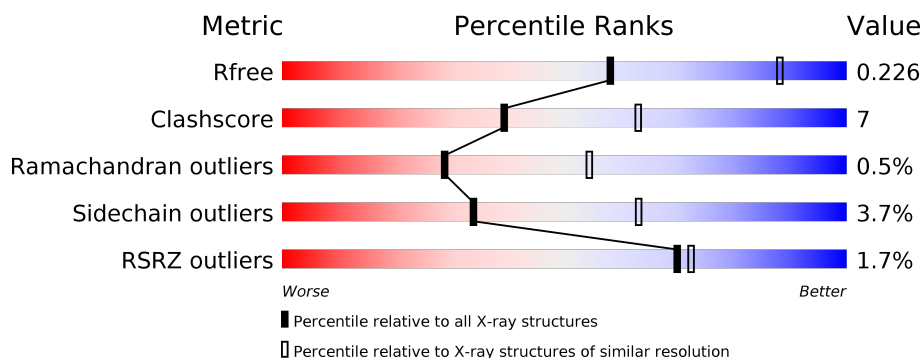
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	L	281	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 1%, green 89%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 89% 10% </div> </div>
2	M	302	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 18%, green 82%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 82% 18% </div> </div>
3	H	266	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 14%, green 74%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 2% 74% 14% 10% </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
7	PO4	H	304	-	-	X	-
7	PO4	L	310	-	-	-	X
8	HTO	L	305	-	X	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7418 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	1	0
			2230	1505	354	363	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	1	0
			2407	1604	395	398	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	214	ALA	LEU	ENGINEERED MUTATION	UNP P0C0Y9

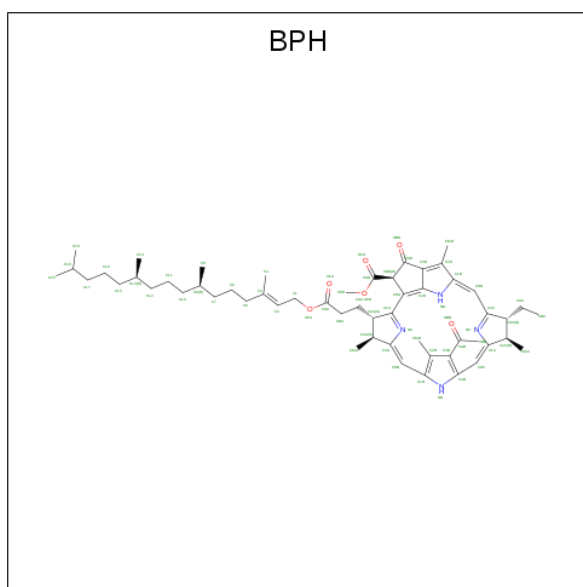
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	2	0
			1840	1178	316	337	9			

There are 6 discrepancies between the modelled and reference sequences:

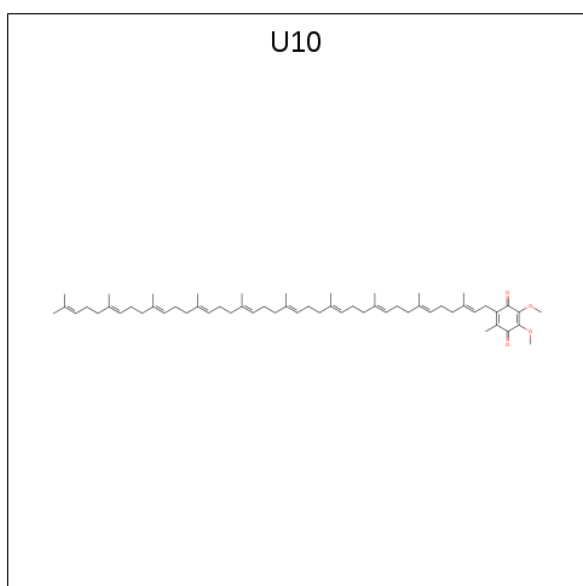
Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-4	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-3	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-2	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	-1	HIS	-	EXPRESSION TAG	UNP P0C0Y7
H	0	HIS	-	EXPRESSION TAG	UNP P0C0Y7

- Molecule 4 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



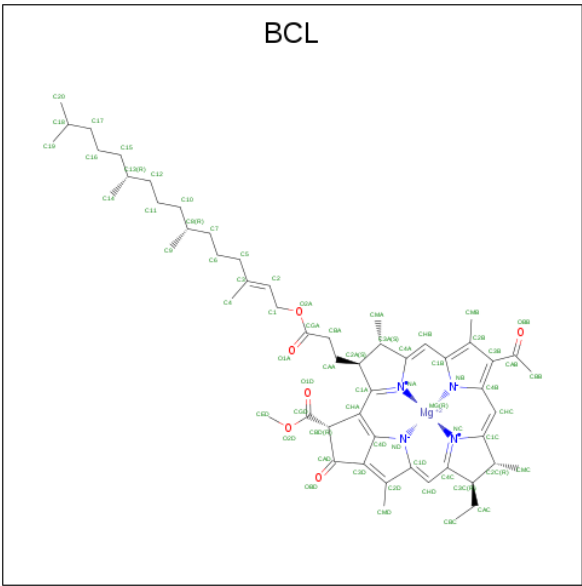
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	L	1	Total	C	N	O	0	0
			65	55	4	6		
4	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 5 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



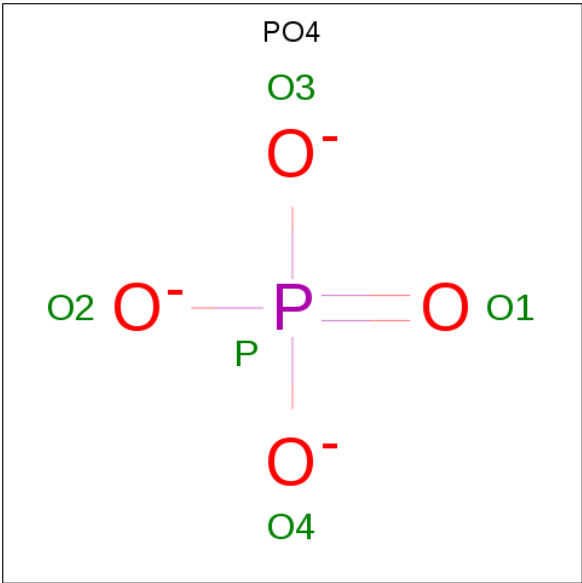
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	1
			46	38	8		
5	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



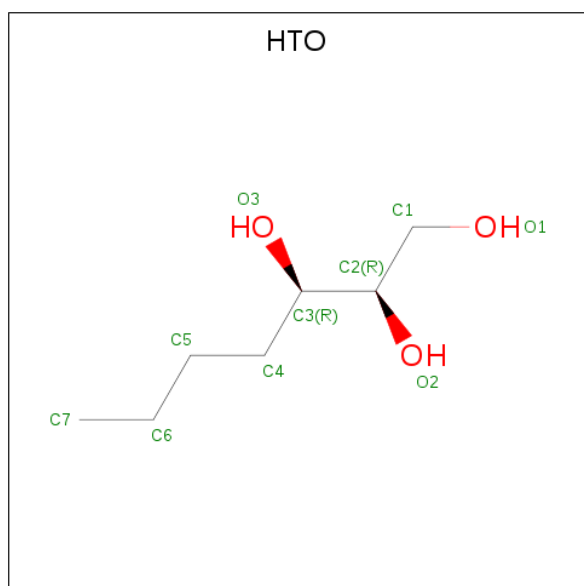
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



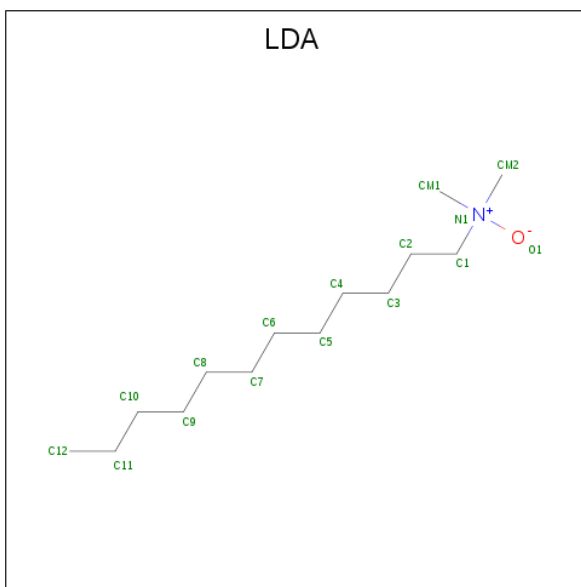
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

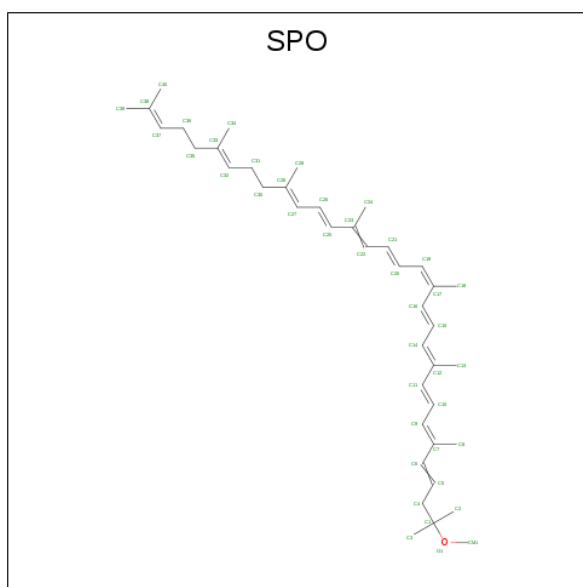


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

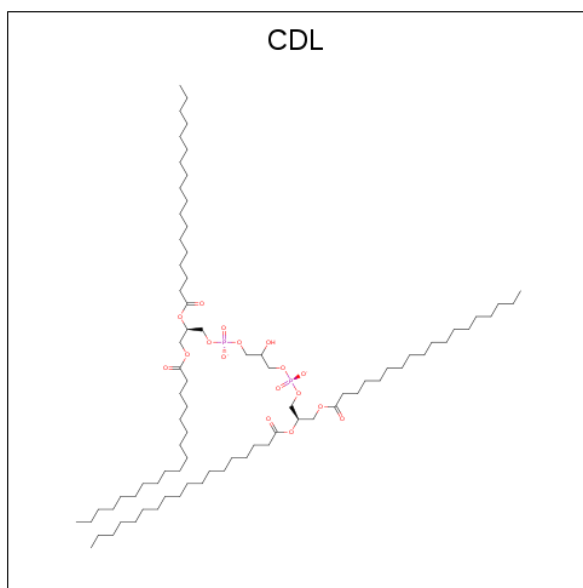
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C₄₁H₆₀O).



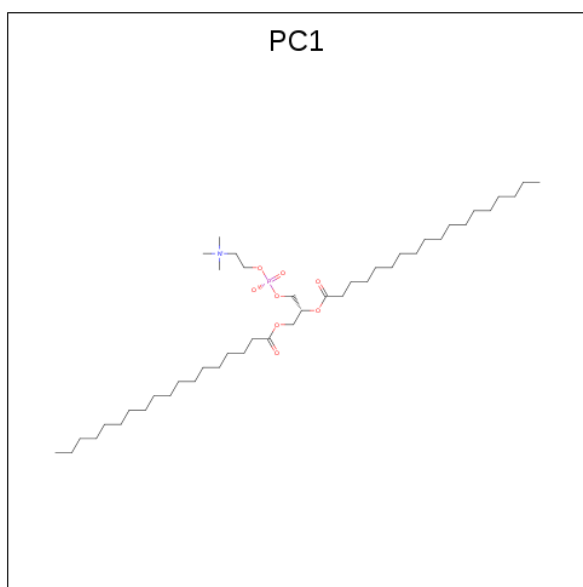
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



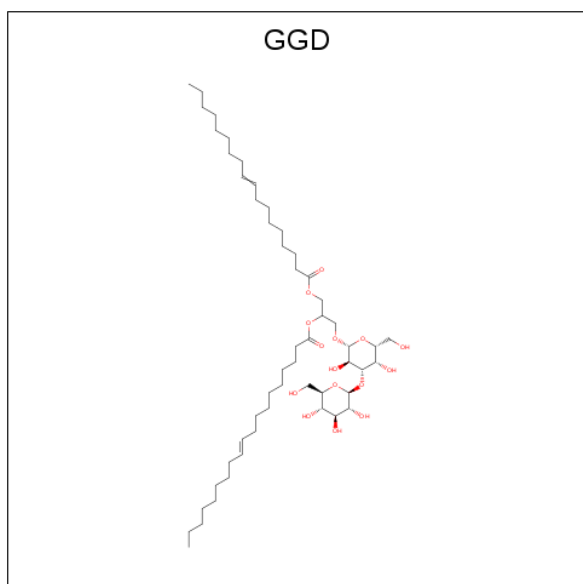
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 14 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
14	M	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 15 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-L-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: $C_{52}H_{94}O_{15}$).



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

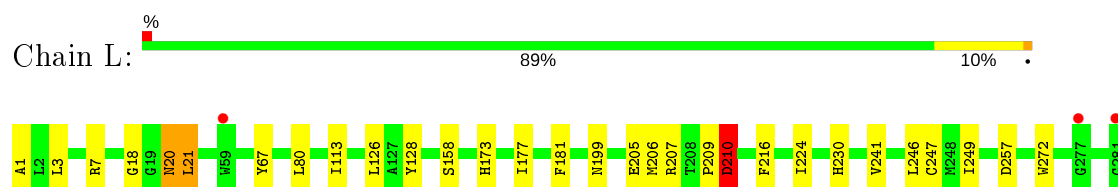
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	28	Total 28	O 28	0	0
16	M	22	Total 22	O 22	0	0
16	H	30	Total 30	O 30	0	0

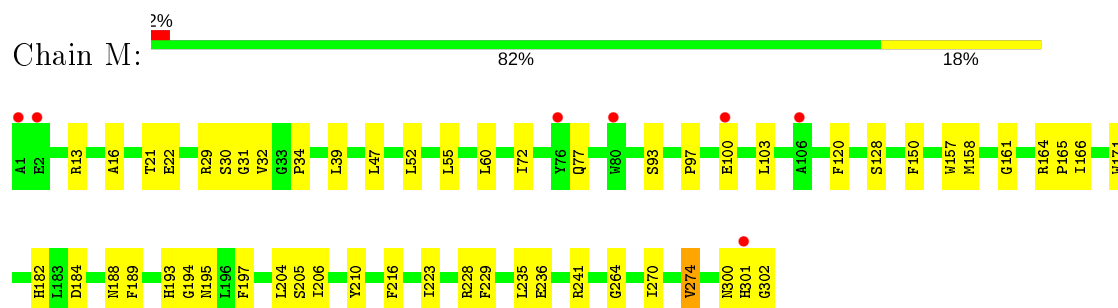
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

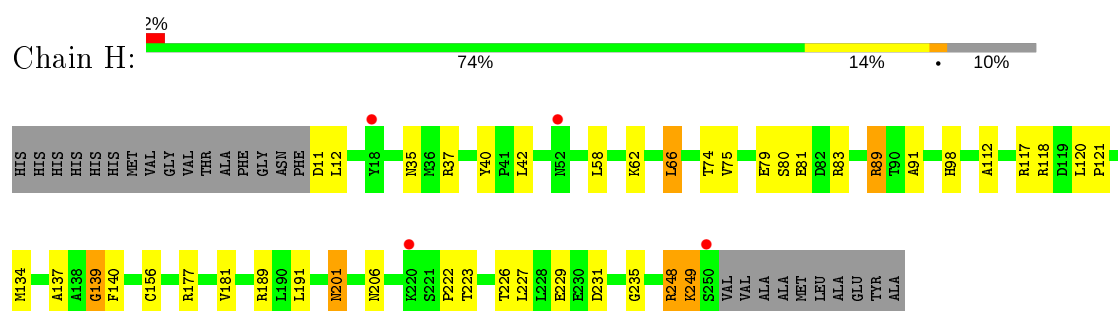
• Molecule 1: Reaction center protein L chain



• Molecule 2: Reaction center protein M chain



• Molecule 3: Reaction center protein H chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.03Å 139.03Å 184.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.62 – 2.70 33.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (33.62-2.70) 98.1 (33.60-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.223 0.188 , 0.226	Depositor DCC
R_{free} test set	2836 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7418	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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, GOL, LDA, GGD, CDL, BPH, PO4, PC1, HTO, FE, SPO, 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	L	0.87	0/2323	0.86	4/3180 (0.1%)
2	M	0.85	0/2504	0.90	4/3418 (0.1%)
3	H	0.87	0/1903	0.97	7/2586 (0.3%)
All	All	0.86	0/6730	0.91	15/9184 (0.2%)

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	H	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	228	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	M	228	ARG	NE-CZ-NH1	6.95	123.78	120.30
3	H	189	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	L	210	ASP	CB-CG-OD1	6.47	124.12	118.30
2	M	241	ARG	NE-CZ-NH2	6.21	123.41	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	248	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2230	0	2179	24	0
2	M	2407	0	2313	33	0
3	H	1840	0	1855	26	0
4	L	65	0	76	7	0
4	M	65	0	76	9	0
5	L	46	0	46	9	0
5	M	48	0	63	1	0
6	L	132	0	148	12	0
6	M	132	0	148	10	0
7	H	5	0	0	3	0
7	L	10	0	0	0	0
7	M	10	0	0	0	0
8	L	10	0	16	0	0
9	H	30	0	40	1	0
9	L	36	0	48	3	0
10	M	48	0	93	0	0
11	M	1	0	0	0	0
12	M	42	0	60	6	0
13	M	81	0	102	0	0
14	M	43	0	60	2	0
15	H	57	0	68	0	0
16	H	30	0	0	1	0
16	L	28	0	0	3	0
16	M	22	0	0	0	0
All	All	7418	0	7391	109	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 109 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)
5:L:302[B]:U10:C3M	5:L:302[B]:U10:H4M3	1.34	1.54
5:L:302[B]:U10:C4M	5:L:302[B]:U10:H3M3	1.38	1.54
4:M:406:BPH:HHC	4:M:406:BPH:HBB3	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:134:MET:O	7:H:304:PO4:O1	1.96	0.84
4:L:301:BPH:HBB3	4:L:301:BPH:HHC	1.59	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	301/302 (100%)	287 (95%)	11 (4%)	3 (1%)	15	37
3	H	241/266 (91%)	231 (96%)	9 (4%)	1 (0%)	34	60
All	All	822/849 (97%)	792 (96%)	26 (3%)	4 (0%)	29	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
3	H	249	LYS
2	M	30	SER
2	M	100	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	212 (96%)	8 (4%)	35	64
2	M	236/235 (100%)	227 (96%)	9 (4%)	33	62
3	H	198/214 (92%)	191 (96%)	7 (4%)	36	65
All	All	654/669 (98%)	630 (96%)	24 (4%)	34	63

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	52	LEU
2	M	182	HIS
3	H	201	ASN
2	M	60	LEU
2	M	72	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	77	GLN
2	M	187	ASN
2	M	300	ASN
1	L	264	GLN
2	M	193	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 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	GOL	L	312	-	5,5,5	0.65	0	5,5,5	0.81	0
5	U10	L	302[B]	-	23,23,63	2.29	4 (17%)	28,31,79	1.88	8 (28%)
12	SPO	M	408	-	40,41,41	0.94	2 (5%)	47,50,50	1.81	13 (27%)
15	GGD	H	301	-	58,58,68	1.13	3 (5%)	72,72,82	1.60	11 (15%)
7	PO4	M	412	-	4,4,4	1.16	0	6,6,6	0.72	0
9	GOL	L	307	-	5,5,5	0.54	0	5,5,5	0.91	0
9	GOL	L	309	-	5,5,5	0.60	0	5,5,5	0.66	0
6	BCL	L	308	-	58,74,74	1.53	10 (17%)	69,115,115	2.22	23 (33%)
6	BCL	L	303	-	58,74,74	1.63	8 (13%)	69,115,115	1.72	14 (20%)
7	PO4	M	411	-	4,4,4	0.53	0	6,6,6	0.81	0
7	PO4	L	310	-	4,4,4	0.86	0	6,6,6	0.62	0
7	PO4	H	304	-	4,4,4	1.47	1 (25%)	6,6,6	1.51	2 (33%)
7	PO4	L	304	-	4,4,4	0.41	0	6,6,6	0.98	0
6	BCL	M	401	-	58,74,74	1.68	10 (17%)	69,115,115	1.98	14 (20%)
9	GOL	H	302	-	5,5,5	0.45	0	5,5,5	0.23	0
4	BPH	M	406	-	64,70,70	1.99	13 (20%)	76,101,101	1.92	21 (27%)
6	BCL	M	402	-	58,74,74	1.57	10 (17%)	69,115,115	1.86	17 (24%)
9	GOL	H	306	-	5,5,5	0.56	0	5,5,5	0.72	0
14	PC1	M	410	-	42,42,53	1.48	4 (9%)	48,50,61	1.46	6 (12%)
8	HTO	L	305	-	9,9,9	1.19	1 (11%)	10,10,10	1.67	3 (30%)
9	GOL	L	313	-	5,5,5	0.49	0	5,5,5	0.67	0
10	LDA	M	403	-	12,15,15	2.25	1 (8%)	14,17,17	0.91	1 (7%)
10	LDA	M	404	-	12,15,15	2.06	1 (8%)	14,17,17	0.73	0
4	BPH	L	301	-	64,70,70	2.01	13 (20%)	76,101,101	1.80	14 (18%)
10	LDA	M	413	-	12,15,15	2.20	1 (8%)	14,17,17	0.60	0
9	GOL	L	311	-	5,5,5	0.56	0	5,5,5	0.59	0
9	GOL	H	305	-	5,5,5	0.47	0	5,5,5	0.32	0
9	GOL	L	306	-	5,5,5	0.68	0	5,5,5	1.30	0
9	GOL	H	303	-	5,5,5	0.16	0	5,5,5	0.82	0
5	U10	M	407	-	48,48,63	1.47	4 (8%)	58,61,79	1.68	14 (24%)
9	GOL	H	307	-	5,5,5	0.48	0	5,5,5	0.59	0
5	U10	L	302[A]	-	23,23,63	1.78	2 (8%)	28,31,79	1.92	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CDL	M	409	-	79,79,99	1.44	4 (5%)	84,90,111	1.42	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	L	312	-	-	2/4/4/4	-
5	U10	L	302[B]	-	-	4/15/39/87	0/1/1/1
12	SPO	M	408	-	-	6/47/47/47	-
15	GGD	H	301	-	-	27/47/87/97	0/2/2/2
9	GOL	L	307	-	-	3/4/4/4	-
9	GOL	L	309	-	-	3/4/4/4	-
6	BCL	L	308	-	-	5/37/137/137	-
6	BCL	L	303	-	-	5/37/137/137	-
9	GOL	H	302	-	-	0/4/4/4	-
6	BCL	M	401	-	-	11/37/137/137	-
4	BPH	M	406	-	-	17/54/105/105	0/5/6/6
6	BCL	M	402	-	-	4/37/137/137	-
9	GOL	H	306	-	-	0/4/4/4	-
14	PC1	M	410	-	-	19/46/46/57	-
8	HTO	L	305	-	-	8/10/10/10	-
9	GOL	L	313	-	-	2/4/4/4	-
10	LDA	M	403	-	-	4/13/13/13	-
10	LDA	M	404	-	-	9/13/13/13	-
4	BPH	L	301	-	-	7/54/105/105	0/5/6/6
10	LDA	M	413	-	-	3/13/13/13	-
9	GOL	L	311	-	-	2/4/4/4	-
9	GOL	H	305	-	-	0/4/4/4	-
9	GOL	L	306	-	-	2/4/4/4	-
9	GOL	H	303	-	-	2/4/4/4	-
5	U10	M	407	-	-	6/45/69/87	0/1/1/1
9	GOL	H	307	-	-	2/4/4/4	-
5	U10	L	302[A]	-	-	2/15/39/87	0/1/1/1
13	CDL	M	409	-	-	54/88/88/110	-

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	302[B]	U10	C6-C1	8.82	1.51	1.35
10	M	413	LDA	O1-N1	-7.48	1.24	1.42
5	L	302[A]	U10	C6-C1	7.40	1.48	1.35
10	M	403	LDA	O1-N1	-7.31	1.25	1.42
10	M	404	LDA	O1-N1	-6.81	1.26	1.42

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	402	BCL	C1C-NC-C4C	-7.45	103.36	106.71
4	L	301	BPH	C4A-NA-C1A	7.12	113.89	108.14
6	L	308	BCL	C1C-NC-C4C	-7.01	103.56	106.71
13	M	409	CDL	OB6-CB5-C51	6.39	125.27	111.50
6	M	401	BCL	O2D-CGD-CBD	6.11	122.13	111.27

There are no chirality outliers.

5 of 209 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	L	312	GOL	C1-C2-C3-O3
12	M	408	SPO	C2-C1-C4-C5
12	M	408	SPO	C3-C1-C4-C5
15	H	301	GGD	OA5-CA1-OA1-CC3
15	H	301	GGD	C14-CC5-OC6-CC4

There are no ring outliers.

16 monomers are involved in 59 short contacts:

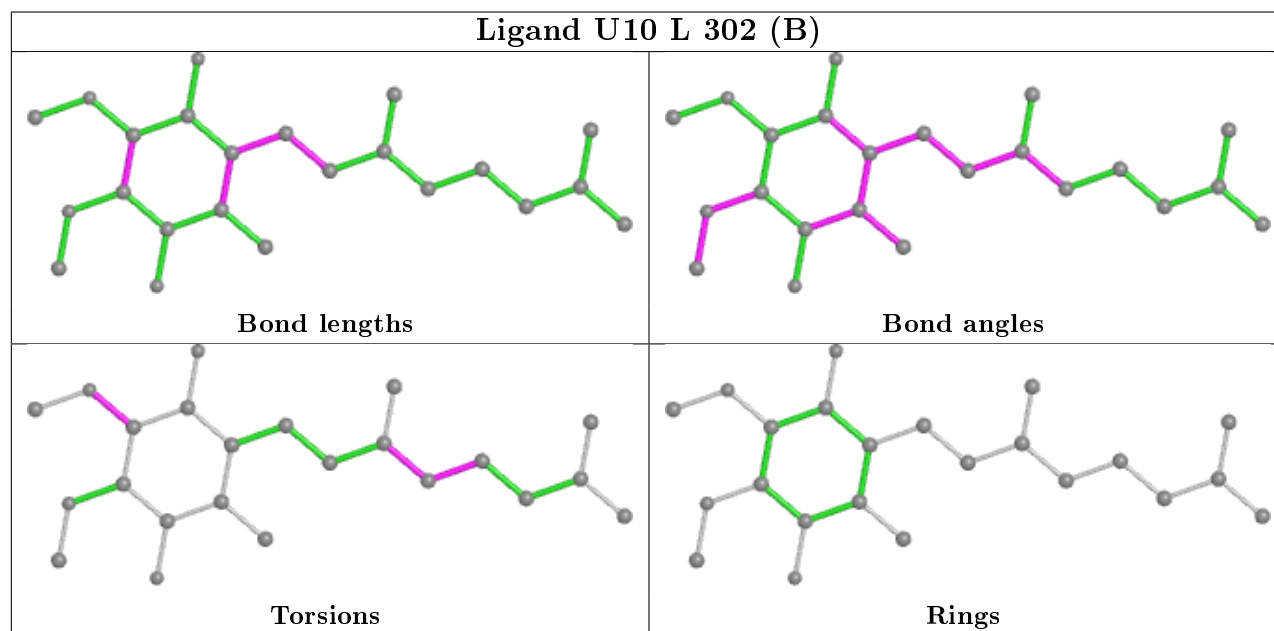
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302[B]	U10	8	0
12	M	408	SPO	6	0
9	L	307	GOL	1	0
6	L	308	BCL	10	0
6	L	303	BCL	4	0
7	H	304	PO4	3	0
6	M	401	BCL	5	0
4	M	406	BPH	9	0
6	M	402	BCL	6	0
14	M	410	PC1	2	0
9	L	313	GOL	1	0

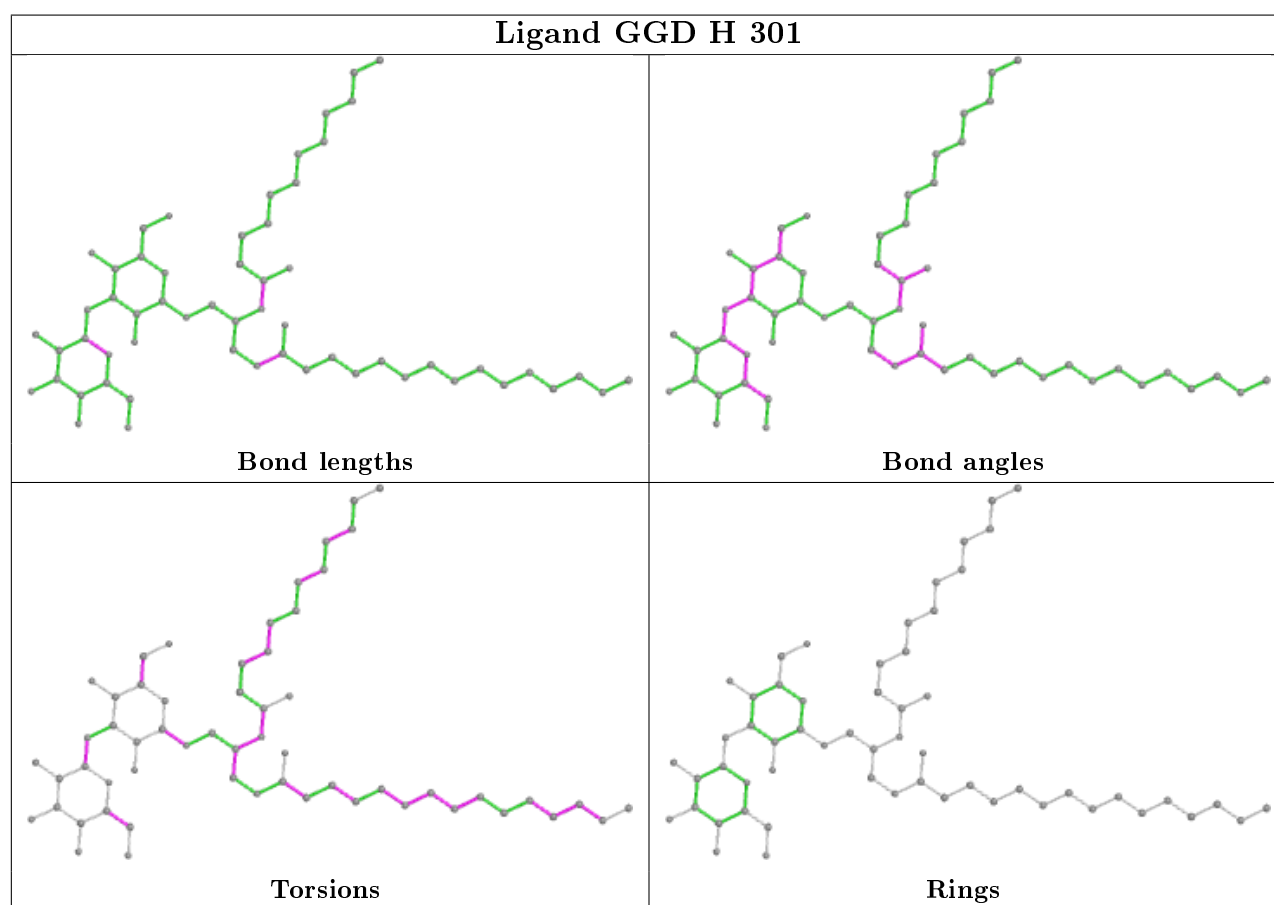
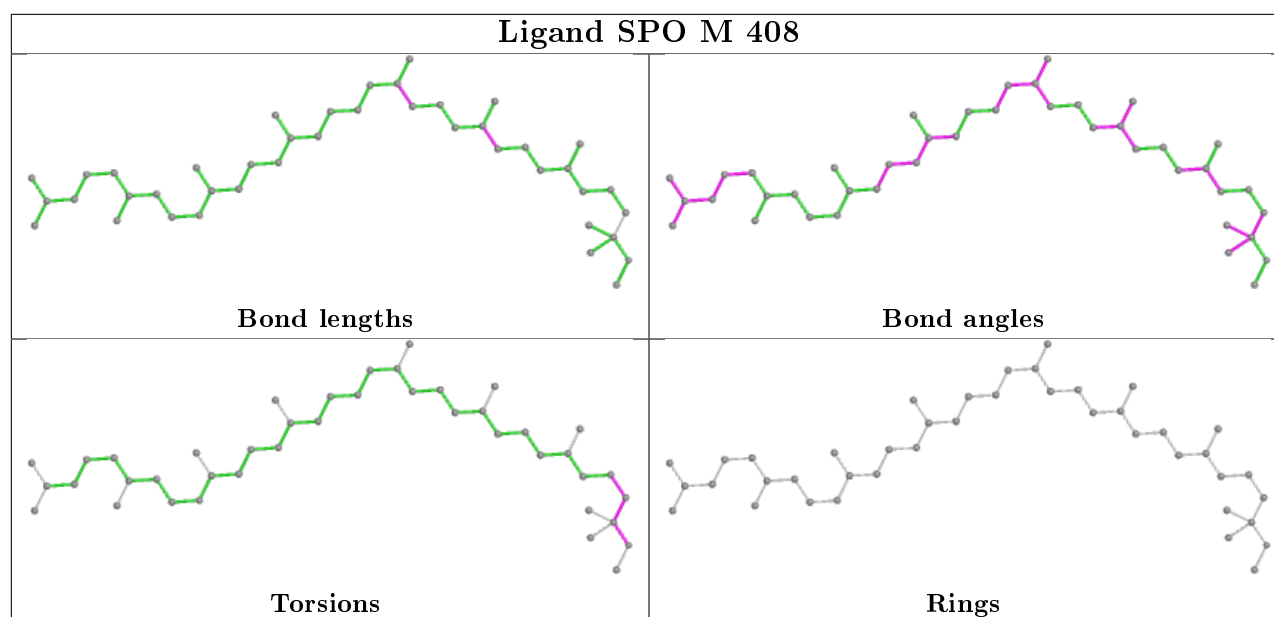
Continued on next page...

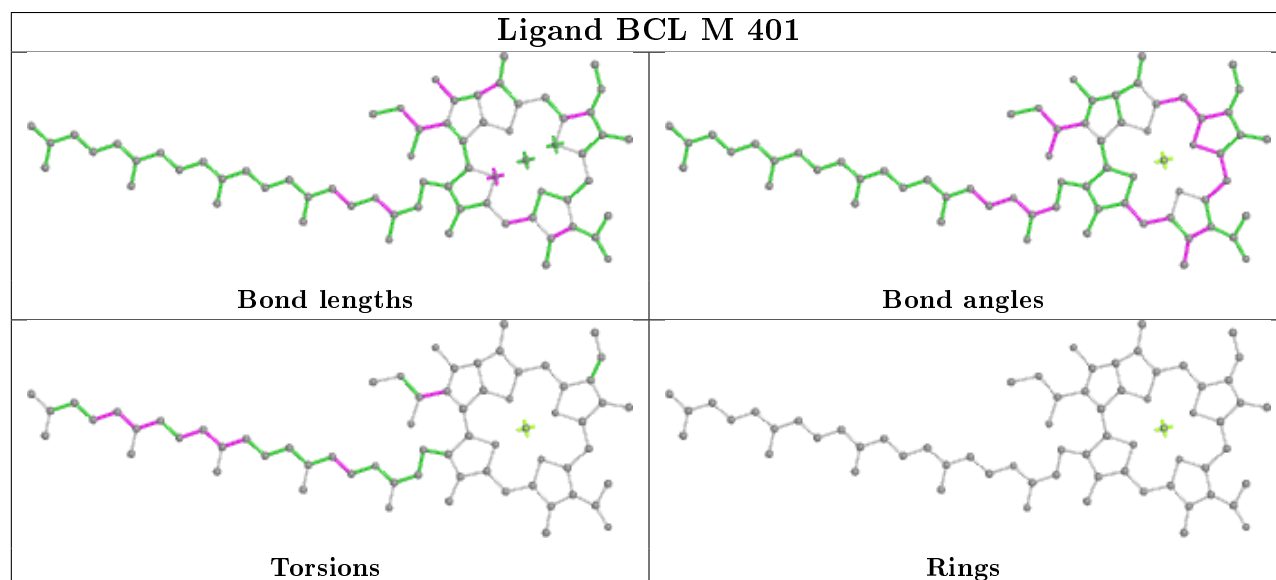
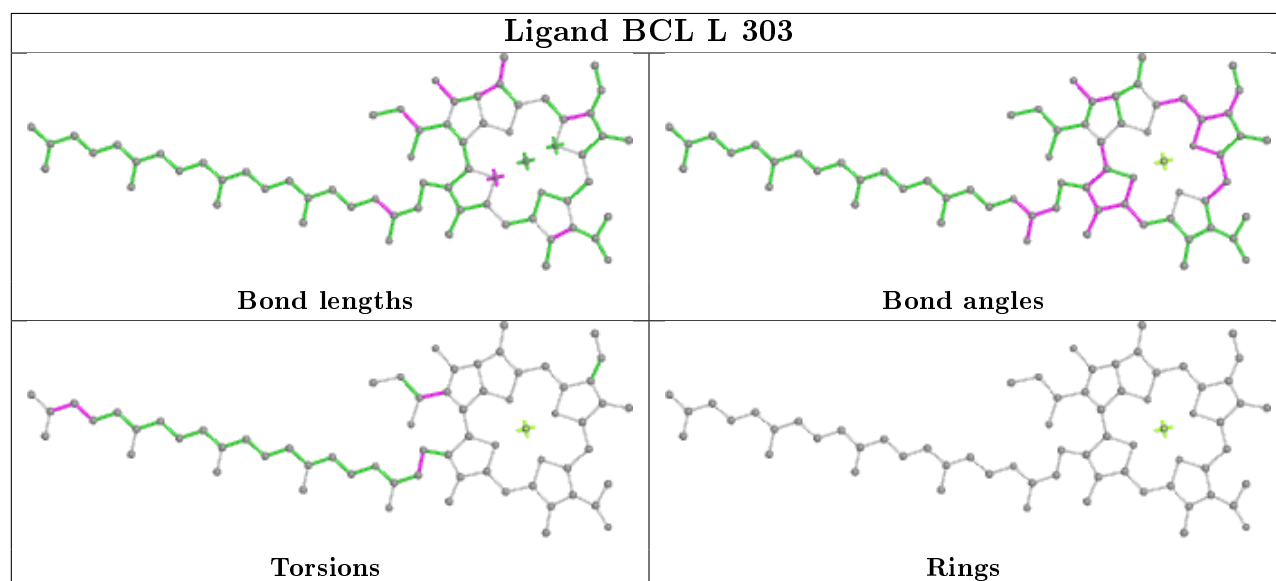
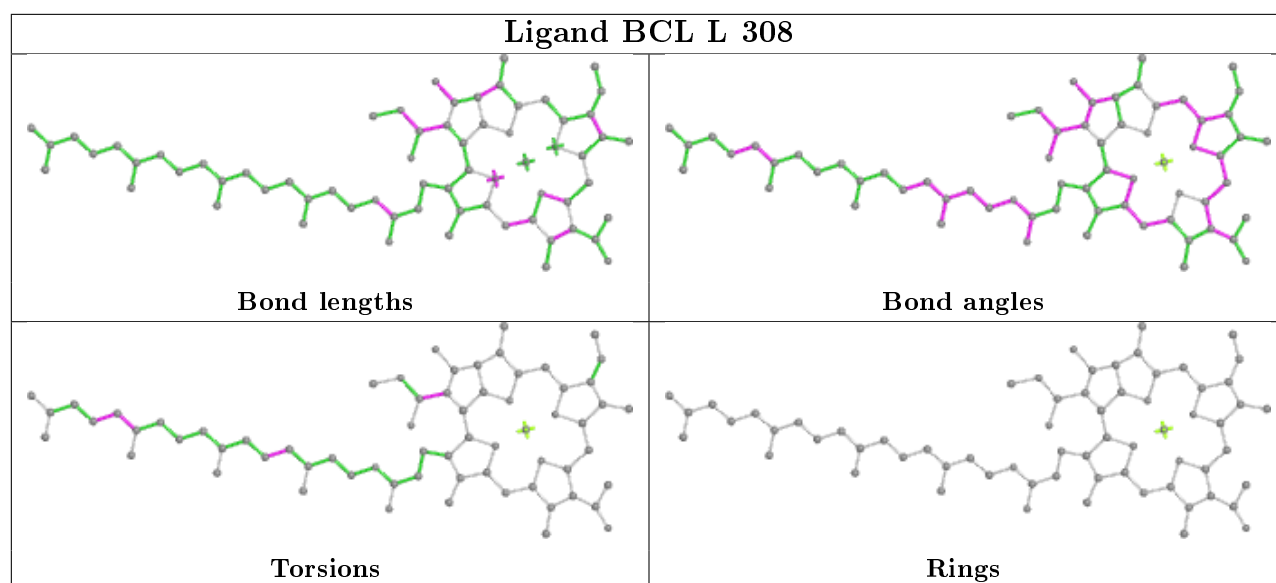
Continued from previous page...

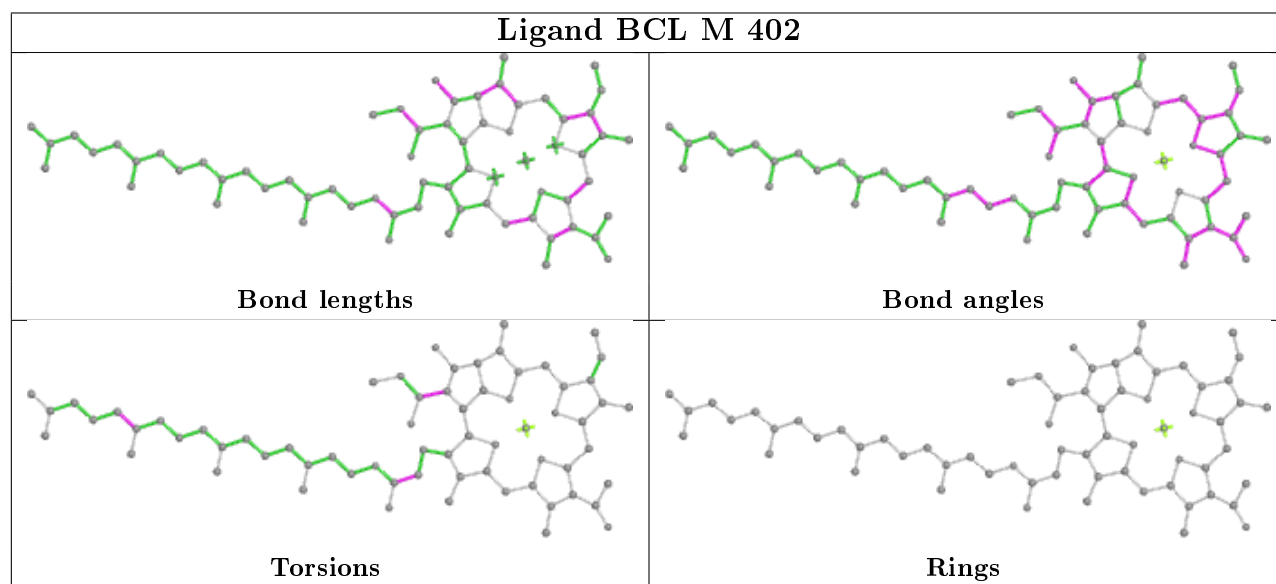
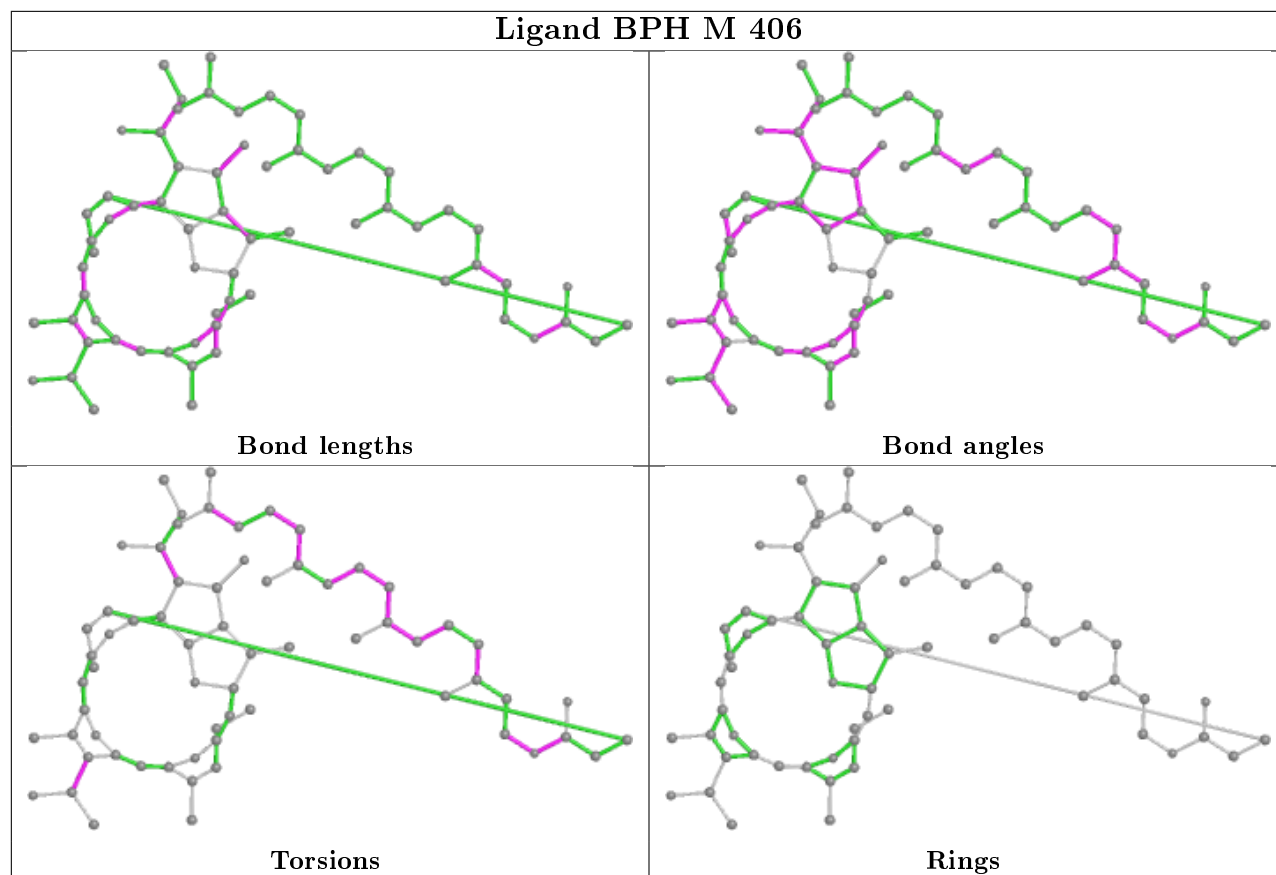
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	BPH	7	0
9	L	306	GOL	1	0
5	M	407	U10	1	0
9	H	307	GOL	1	0
5	L	302[A]	U10	1	0

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

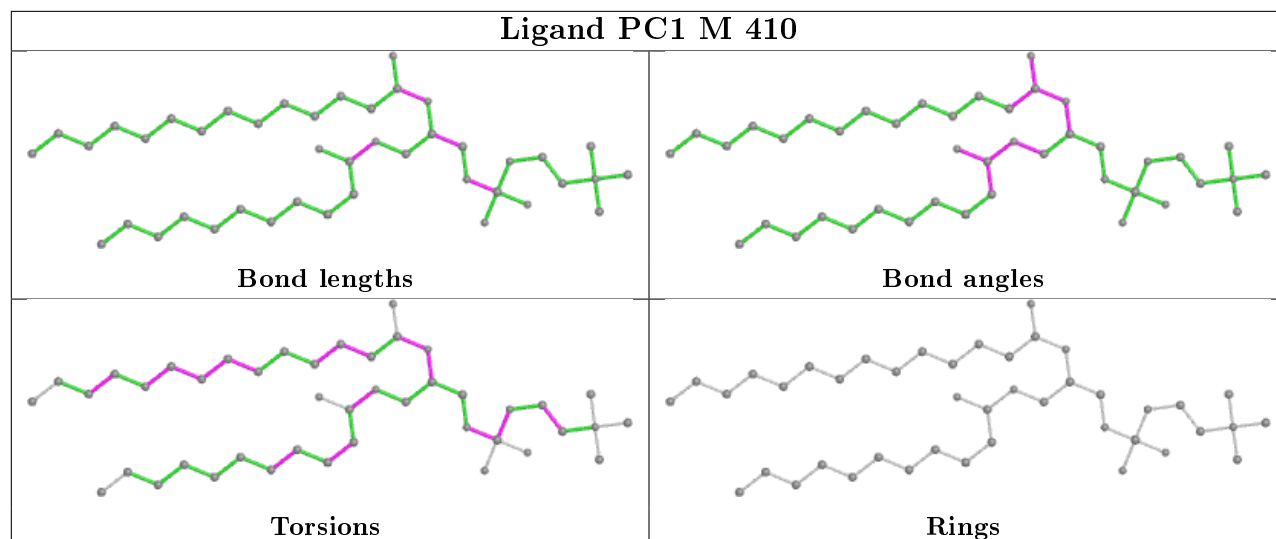




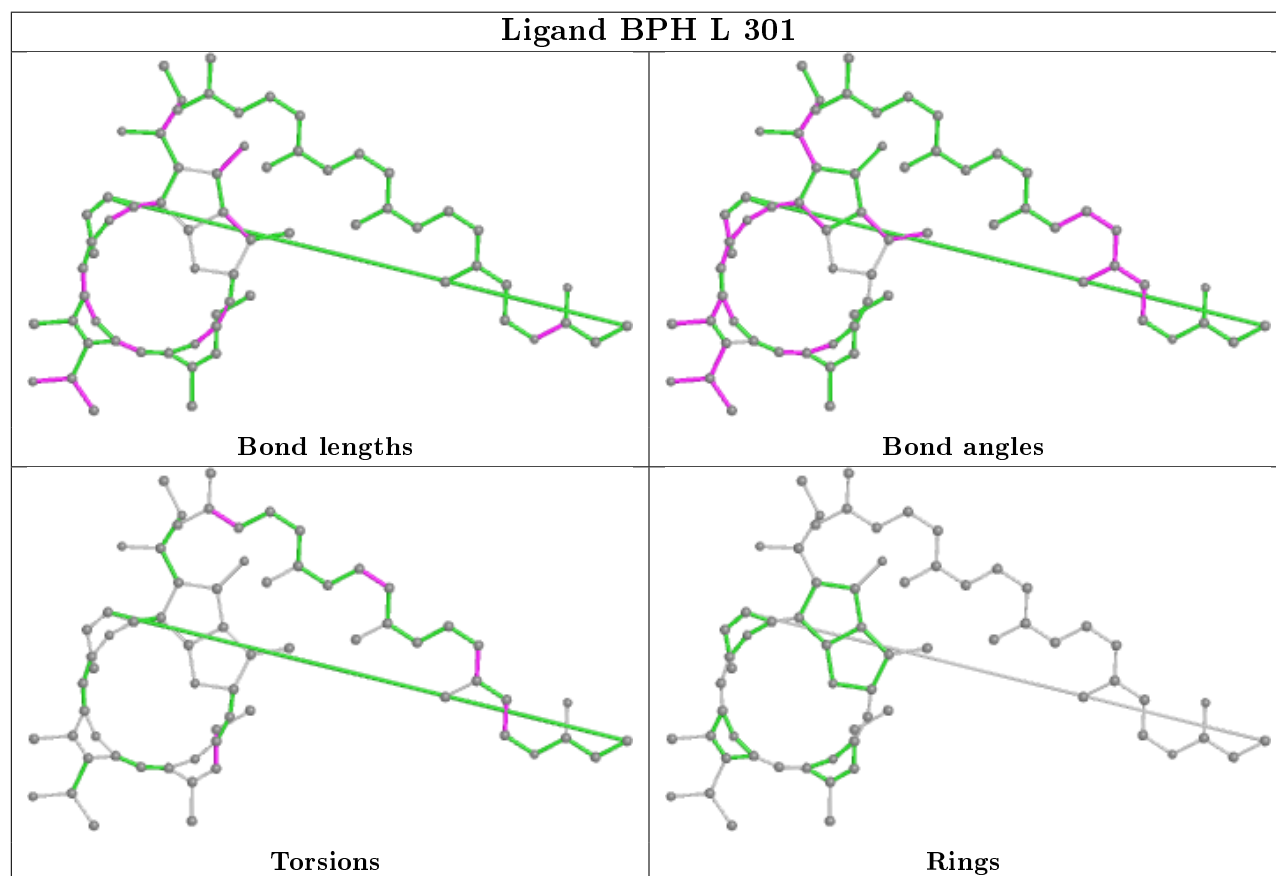




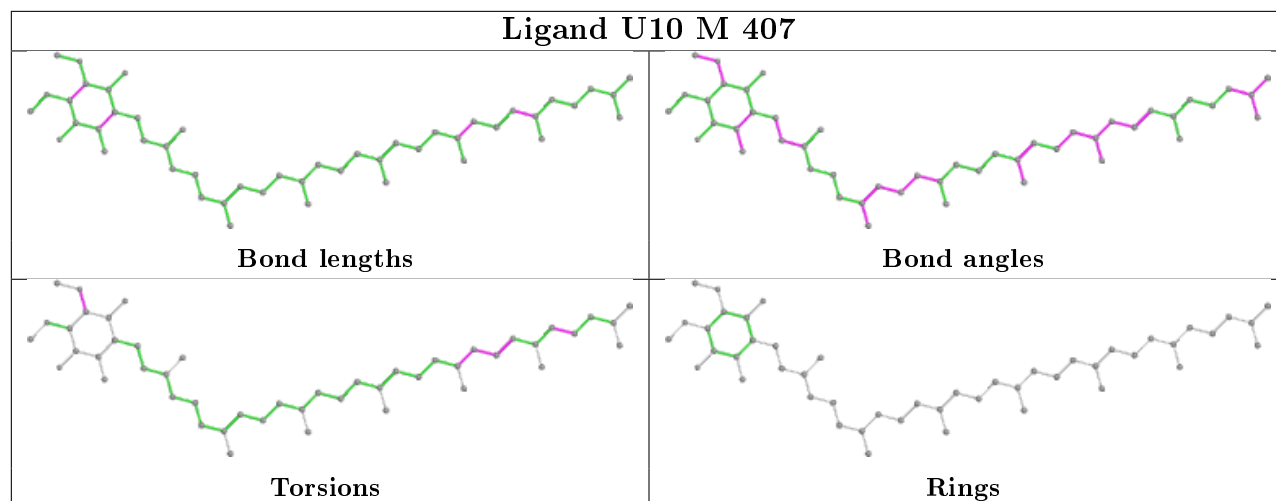
Ligand PC1 M 410



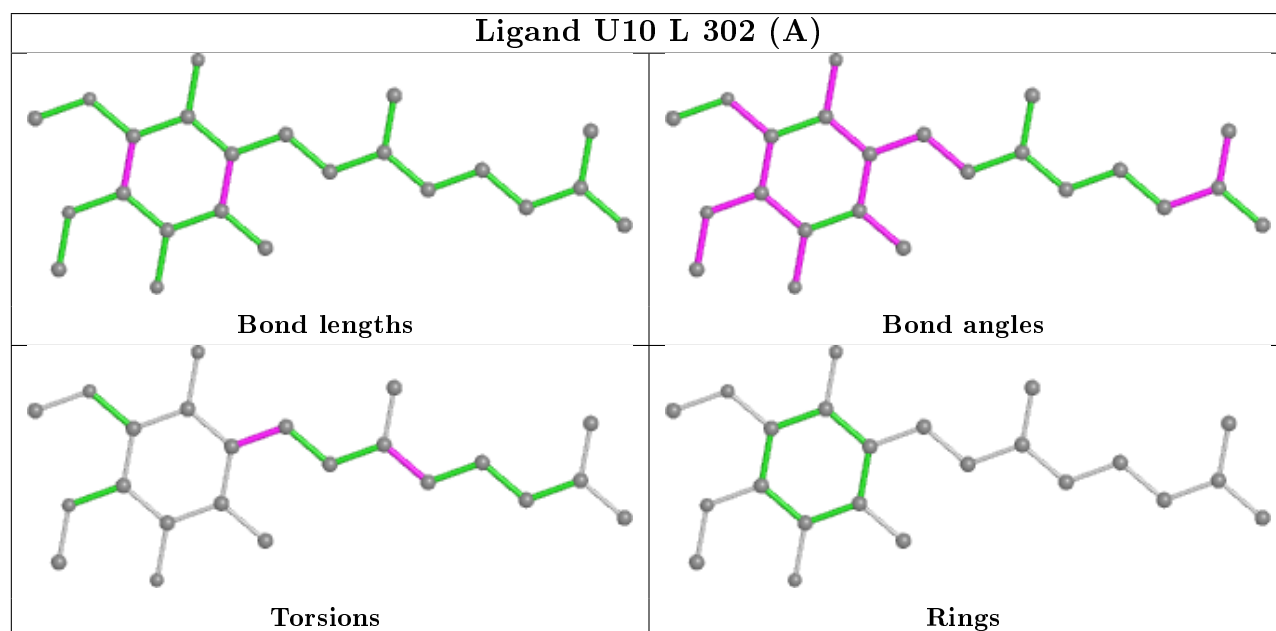
Ligand BPH L 301



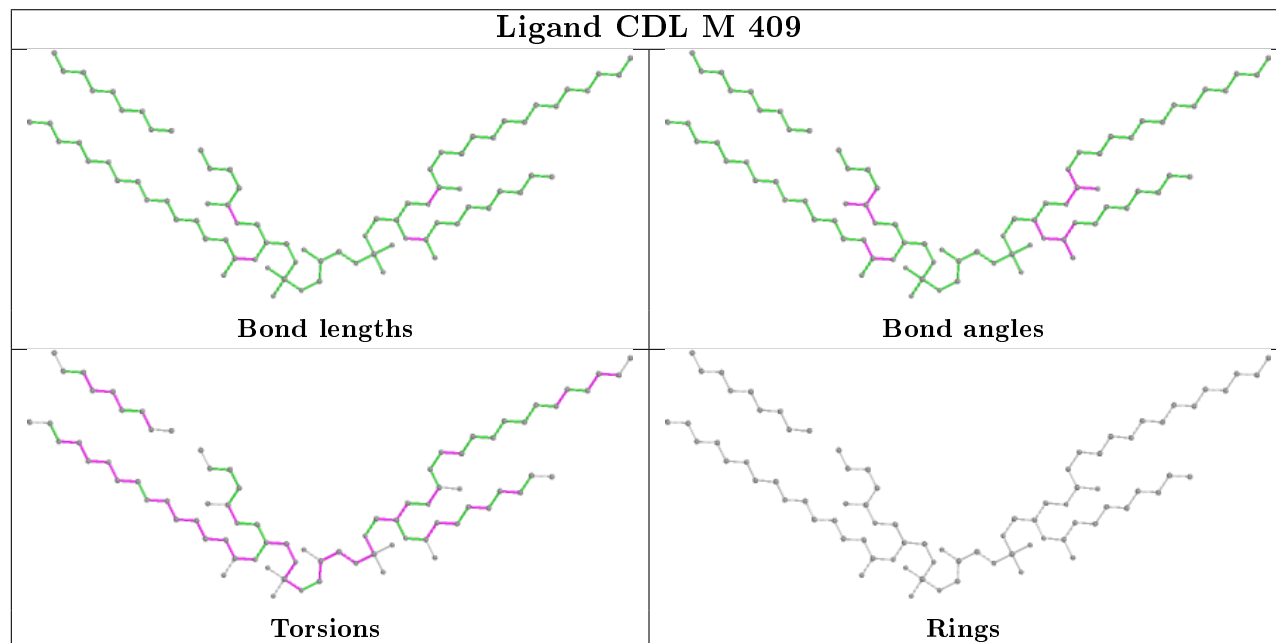
Ligand U10 M 407



Ligand U10 L 302 (A)



Ligand CDL M 409



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	281/281 (100%)	-0.72	3 (1%) 80 82	30, 39, 60, 78	0
2	M	302/302 (100%)	-0.35	7 (2%) 60 62	29, 43, 64, 104	6 (1%)
3	H	240/266 (90%)	-0.47	4 (1%) 70 72	33, 43, 58, 95	3 (1%)
All	All	823/849 (96%)	-0.51	14 (1%) 70 72	29, 42, 62, 104	9 (1%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	7.7
3	H	250	SER	4.5
2	M	301	HIS	3.2
3	H	220[A]	LYS	2.8
1	L	281	GLY	2.7

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](#)

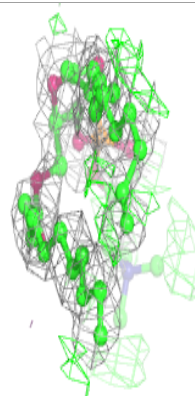
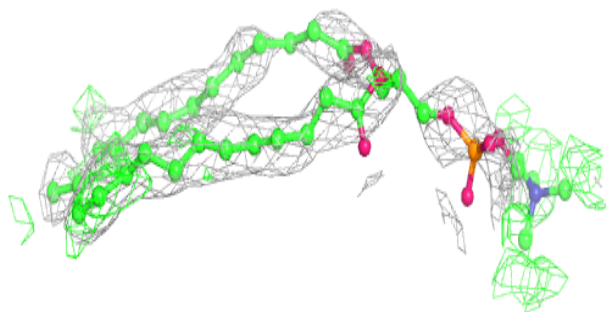
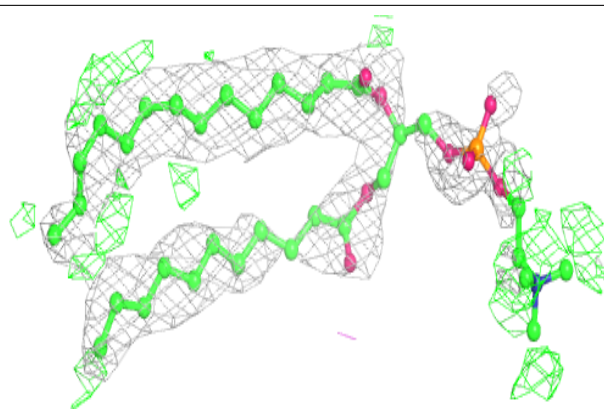
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	PC1	M	410	43/54	0.52	0.37	64,94,167,184	0
15	GGD	H	301	57/67	0.62	0.39	56,100,200,209	0
7	PO4	L	310	5/5	0.77	1.05	129,132,166,171	0
9	GOL	H	305	6/6	0.79	0.24	62,73,83,87	0
9	GOL	L	309	6/6	0.80	0.28	74,81,83,83	0
7	PO4	M	412	5/5	0.81	0.32	73,121,129,134	0
9	GOL	H	303	6/6	0.83	0.23	71,77,78,80	0
10	LDA	M	413	16/16	0.86	0.34	61,77,118,135	0
9	GOL	H	302	6/6	0.86	0.42	71,92,101,107	0
8	HTO	L	305	10/10	0.86	0.40	64,79,90,97	0
5	U10	L	302[B]	23/63	0.87	0.31	20,34,40,41	23
5	U10	L	302[A]	23/63	0.87	0.31	33,42,71,75	23
13	CDL	M	409	81/100	0.87	0.28	48,79,111,124	0
10	LDA	M	404	16/16	0.90	0.36	61,66,89,91	0
9	GOL	L	307	6/6	0.91	0.19	58,60,69,74	0
9	GOL	L	312	6/6	0.91	0.19	53,61,64,80	0
9	GOL	L	313	6/6	0.91	0.25	58,79,88,90	0
4	BPH	M	406	65/65	0.92	0.24	33,39,116,120	0
9	GOL	H	307	6/6	0.92	0.15	57,65,67,67	0
7	PO4	M	411	5/5	0.92	0.24	65,71,79,87	0
10	LDA	M	403	16/16	0.92	0.24	50,69,92,94	0
7	PO4	H	304	5/5	0.93	0.16	52,72,89,90	0
5	U10	M	407	48/63	0.93	0.22	32,51,92,101	0
9	GOL	L	311	6/6	0.93	0.15	49,59,63,63	0
12	SPO	M	408	42/42	0.93	0.17	36,49,77,91	0
9	GOL	L	306	6/6	0.93	0.27	44,59,64,68	0
9	GOL	H	306	6/6	0.96	0.24	49,56,60,65	0
6	BCL	M	401	66/66	0.97	0.17	29,36,82,94	0
6	BCL	M	402	66/66	0.97	0.17	30,38,54,79	0
4	BPH	L	301	65/65	0.97	0.14	28,34,46,49	0
6	BCL	L	308	66/66	0.97	0.17	23,32,58,62	0
6	BCL	L	303	66/66	0.98	0.13	33,37,52,66	0
7	PO4	L	304	5/5	0.98	0.16	53,60,60,61	0
11	FE	M	405	1/1	1.00	0.14	34,34,34,34	0

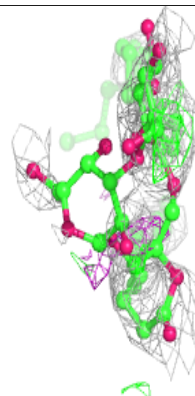
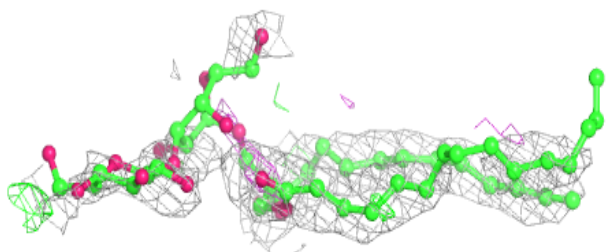
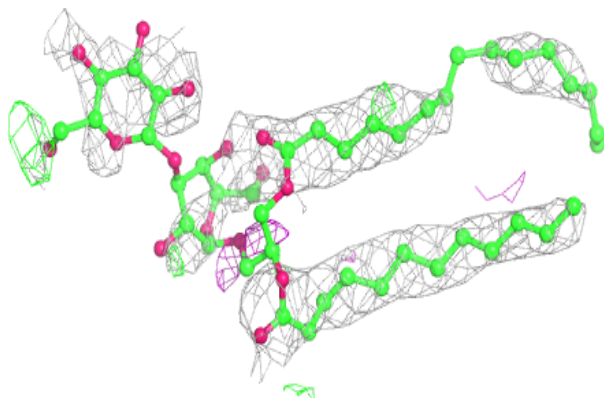
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

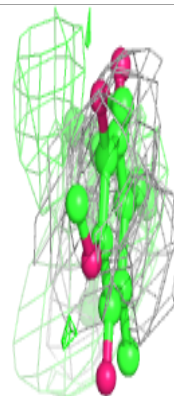
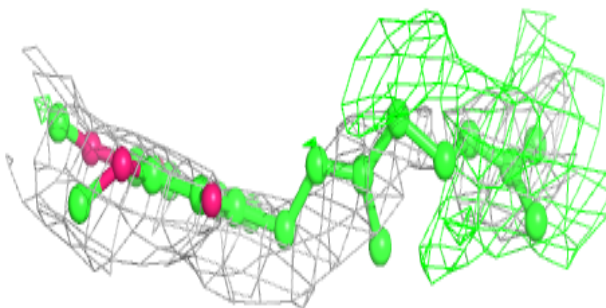
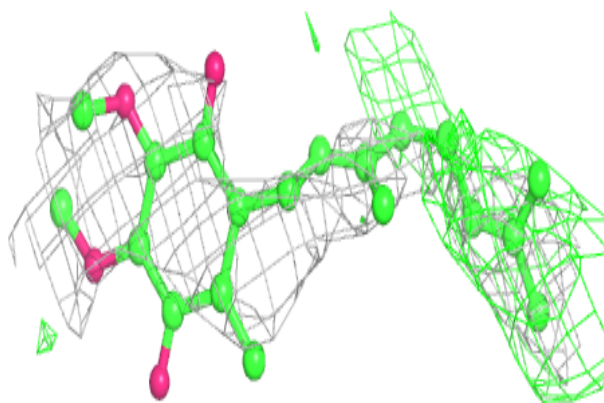
**Electron density around GGD H 301:**

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

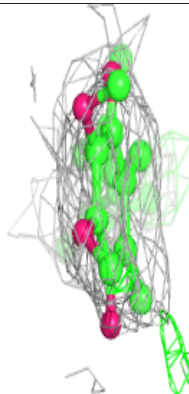
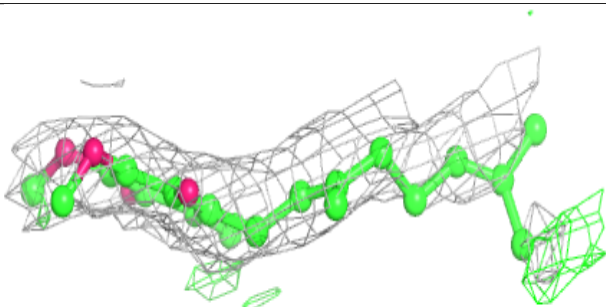
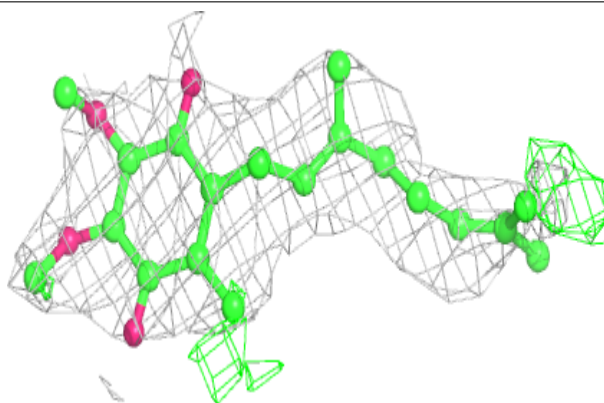


Electron density around U10 L 302 (B):

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

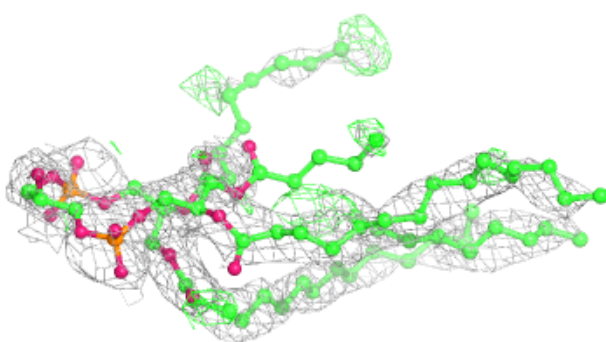
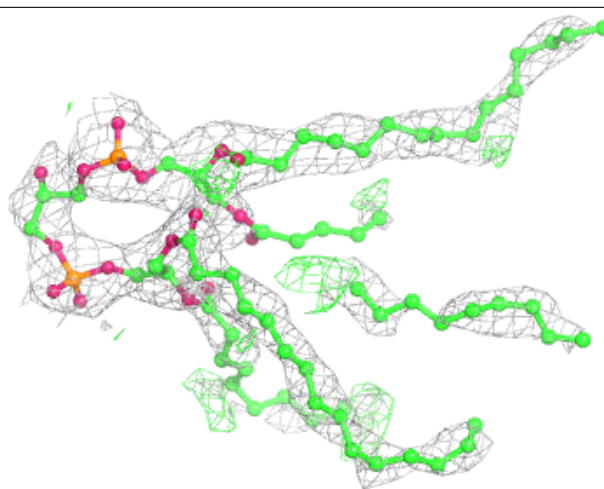
**Electron density around U10 L 302 (A):**

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



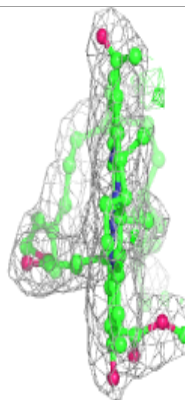
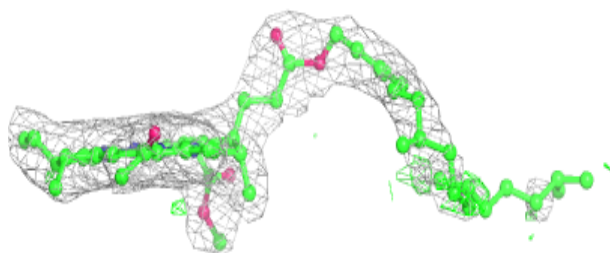
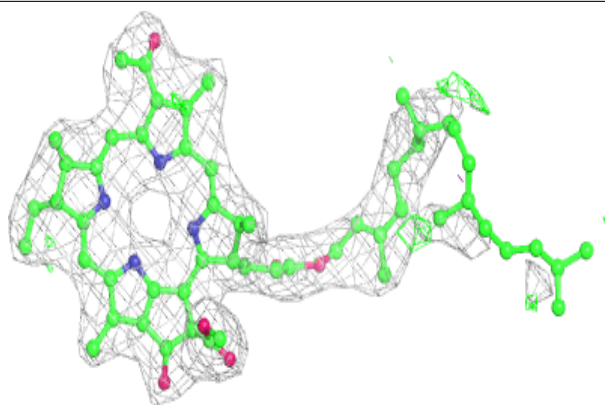
Electron density around CDL M 409:

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

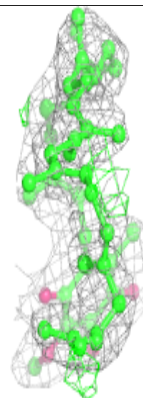
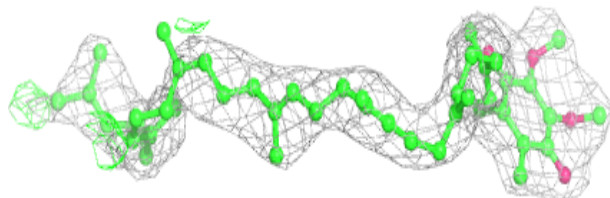
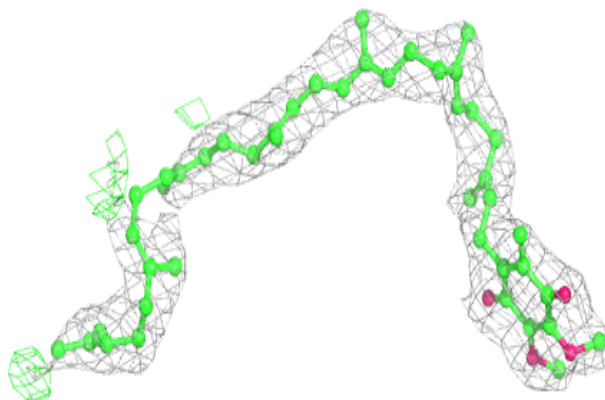


Electron density around BPH M 406:

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

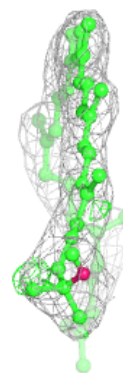
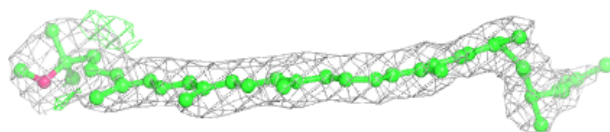
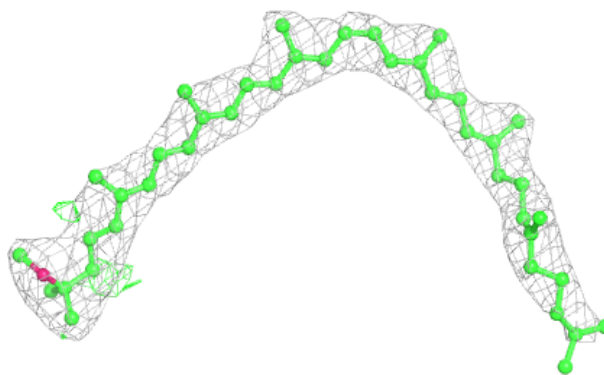
**Electron density around U10 M 407:**

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

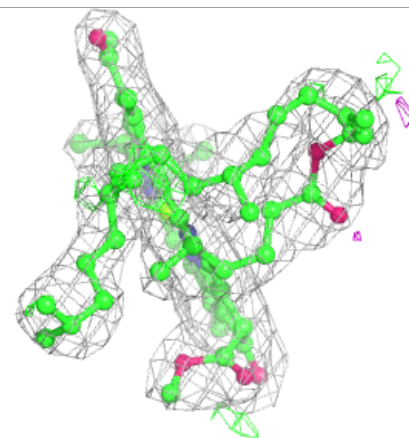
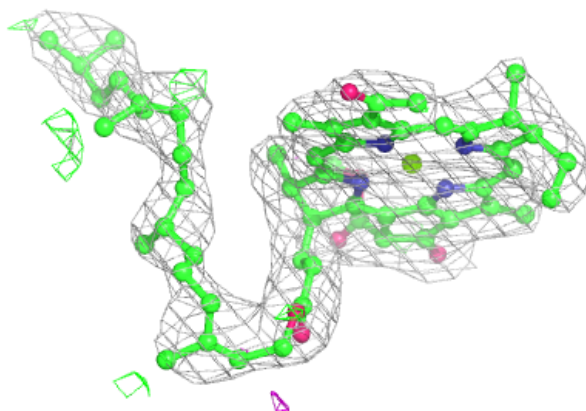
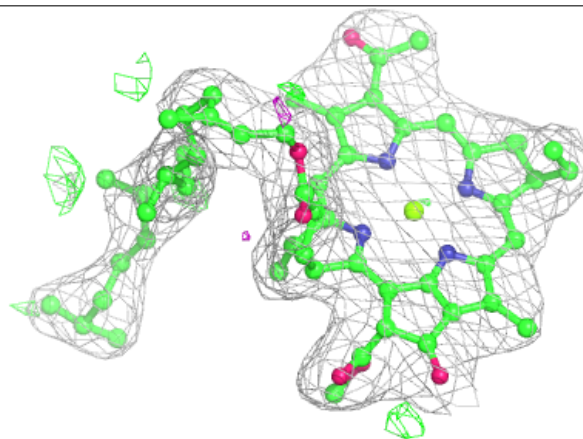


Electron density around SPO M 408:

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

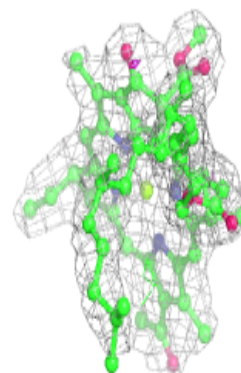
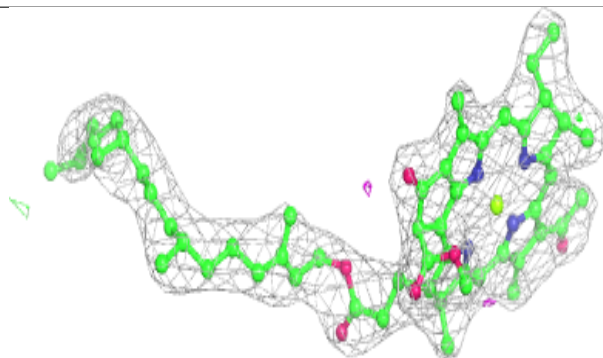
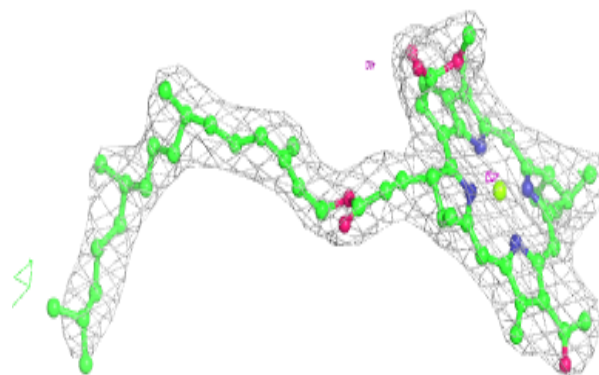
**Electron density around BCL M 401:**

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

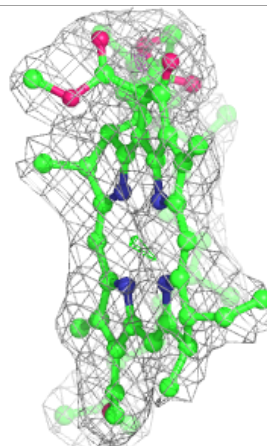
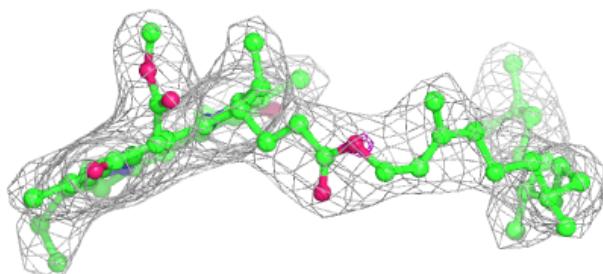
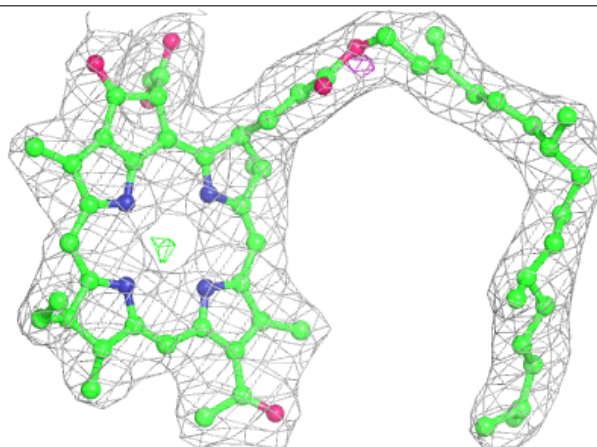


Electron density around BCL M 402:

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

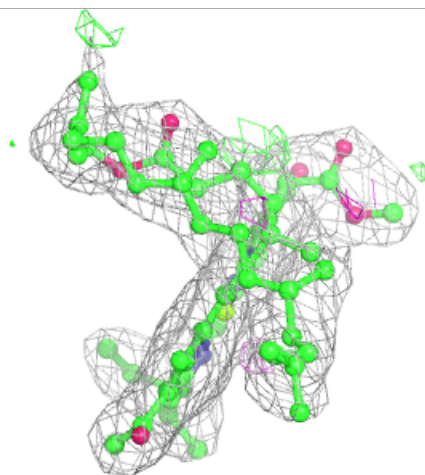
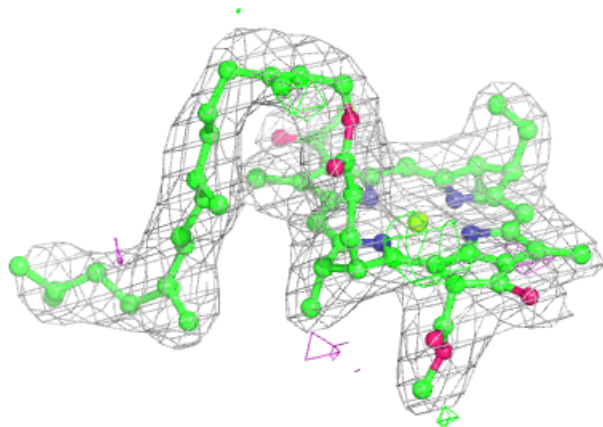
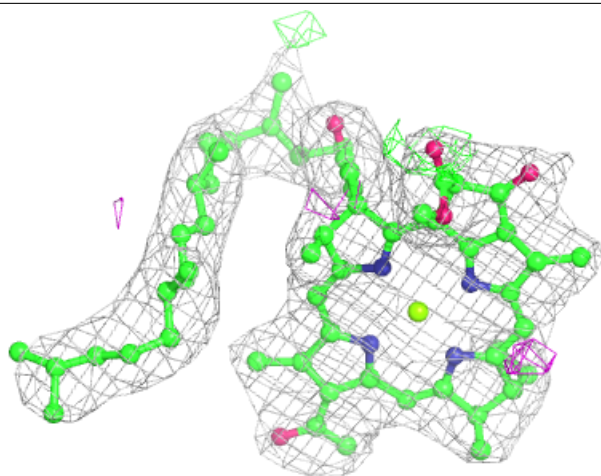
**Electron density around BPH L 301:**

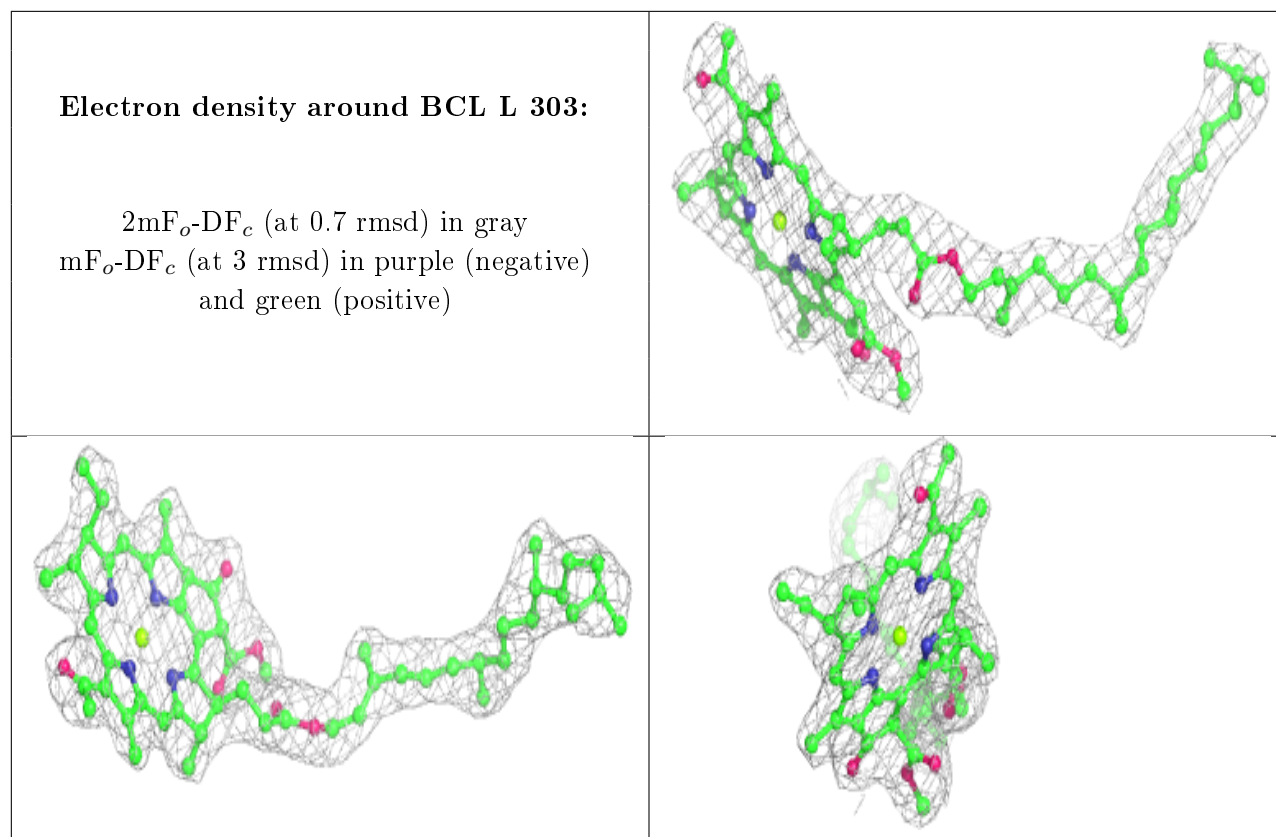
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL L 308:

$2mF_o-DF_c$ (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.