



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:05 AM UTC

PDB ID : 2HH1 / pdb_00002hh1
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylcholine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-27
Resolution : 2.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

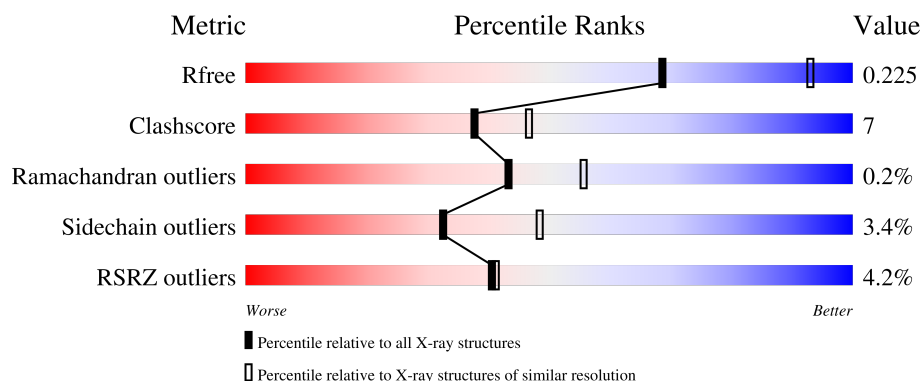
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	4% 89% 10% .
2	M	307	4% 82% 15% ..
3	H	260	4% 83% 9% . 6%

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
15	GOL	H	708	-	-	-	X
8	PC9	L	802	-	-	-	X

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 7923 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	2	0
			2234	1508	355	363	8			

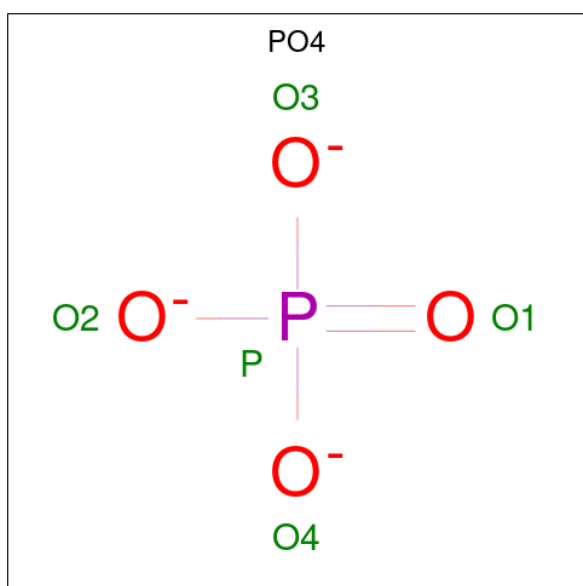
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	9	0
			2466	1643	403	409	11			

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

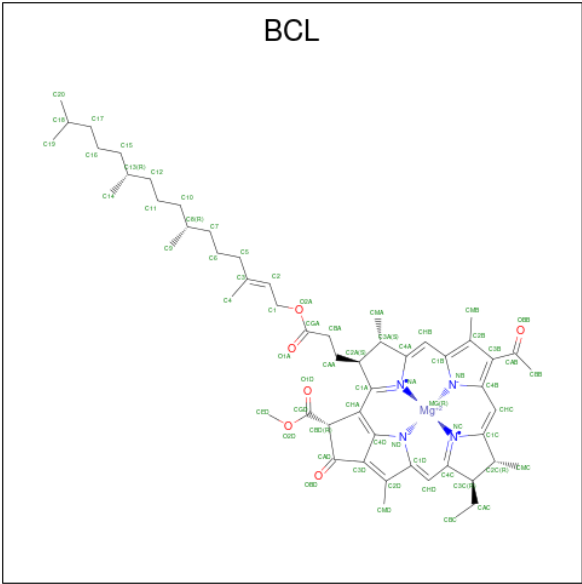
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	244	Total	C	N	O	S	0	9	0
			1891	1207	328	346	10			

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



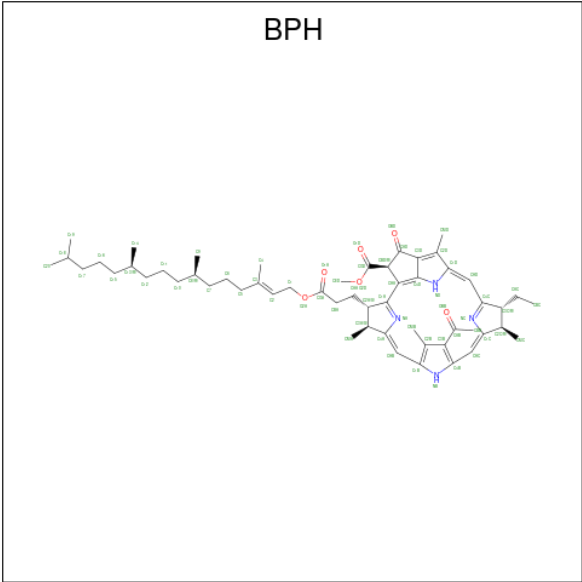
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	P	0	0
			5	4	1		
4	M	1	Total	O	P	0	0
			5	4	1		
4	M	1	Total	O	P	0	0
			5	4	1		
4	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



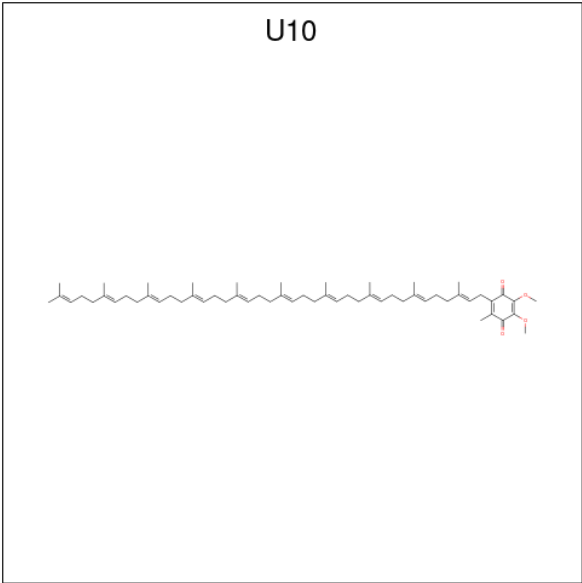
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: C₅₅H₇₆N₄O₆).



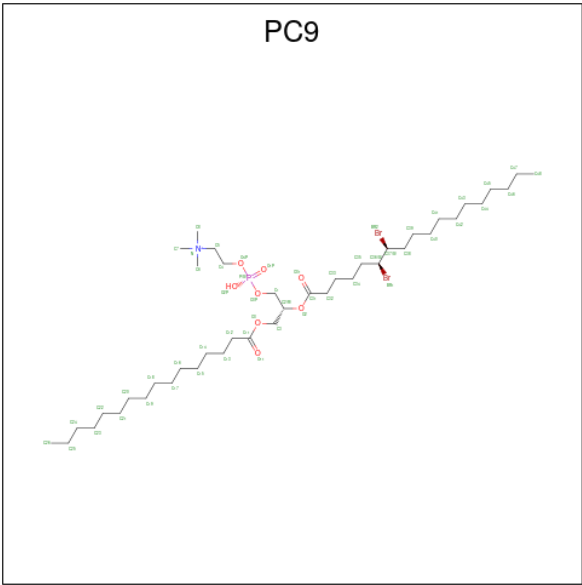
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄).



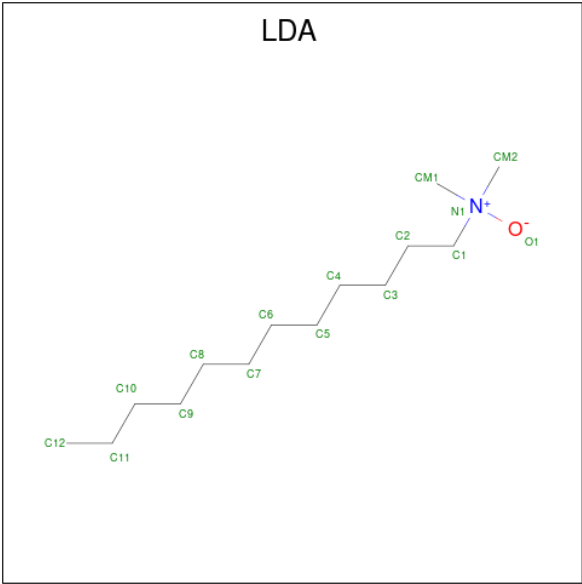
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is (7R,14S)-14,15-DIBROMO-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC9) (formula: C₄₂H₈₃Br₂NO₈P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	P		
8	L	1	54	2	42	1	8	1	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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

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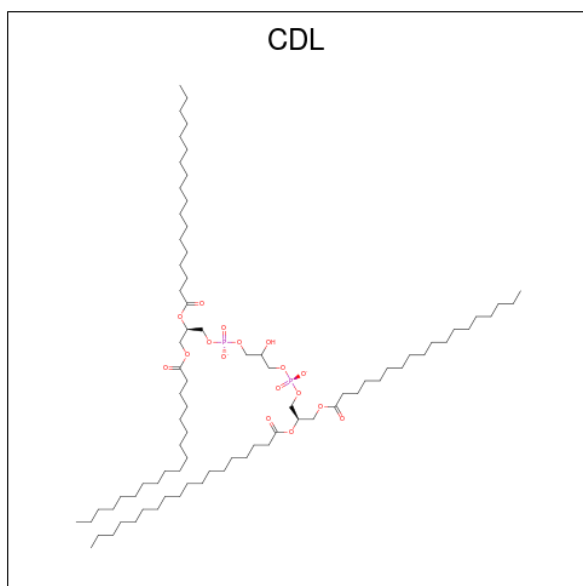
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	H	1	Total	C	N	O	0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

- Molecule 10 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

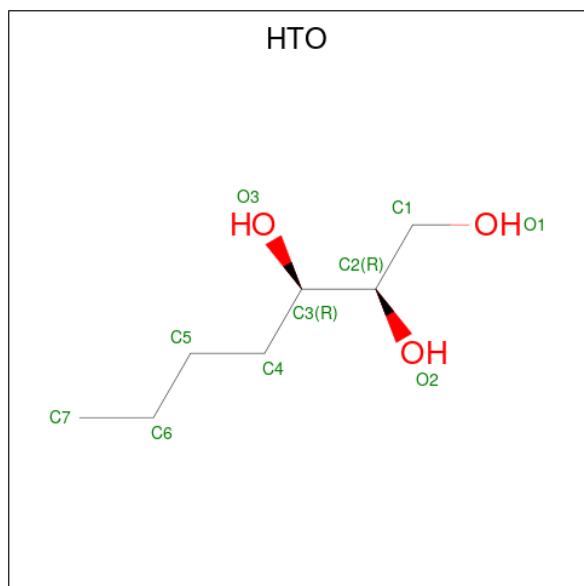


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 12 is POTASSIUM ION (CCD ID: K) (formula: K).

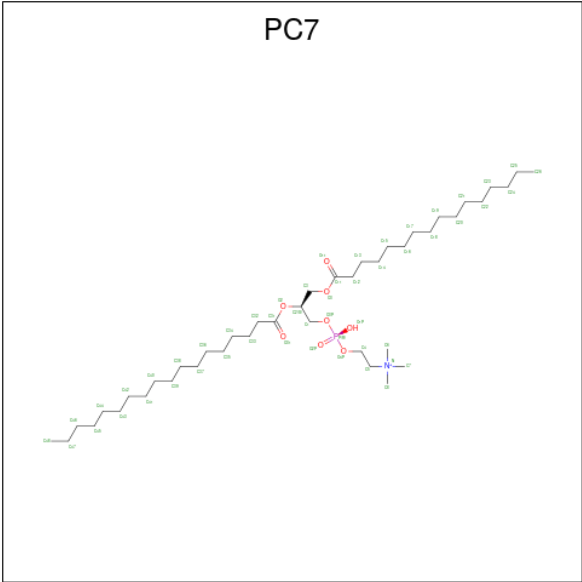
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	1	Total K 1 1	0	0

- Molecule 13 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: C₇H₁₆O₃).



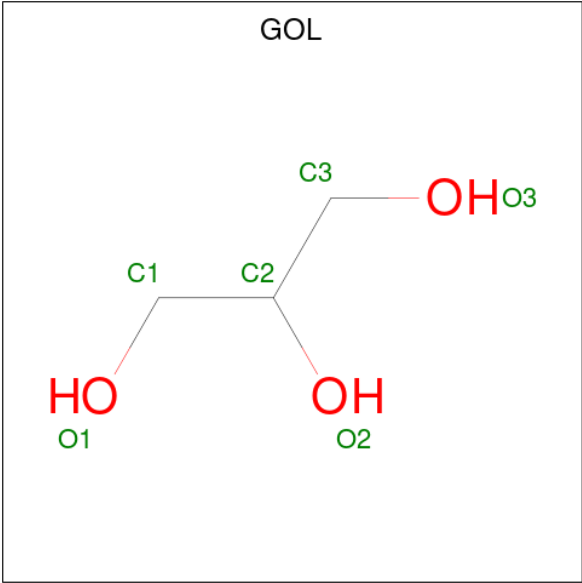
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	1	Total C O 10 7 3	0	0

- Molecule 14 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	H	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 15 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

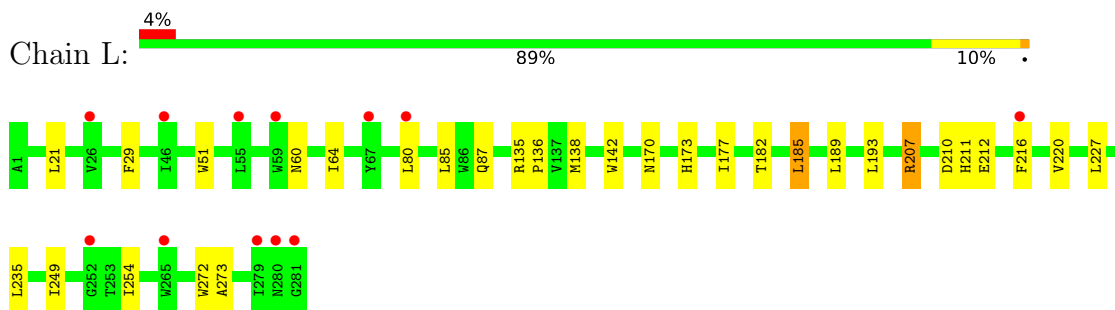
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	113	Total 113	O 113	0	0
16	M	139	Total 139	O 139	0	0
16	H	225	Total 225	O 225	0	0

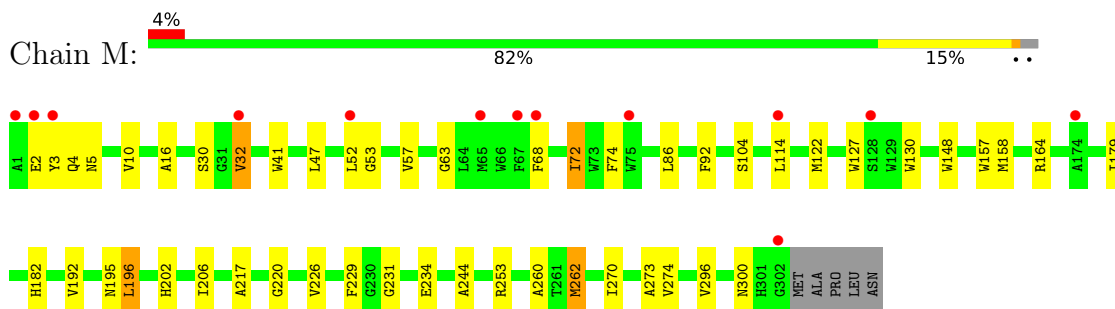
3 Residue-property plots [i](#)

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.

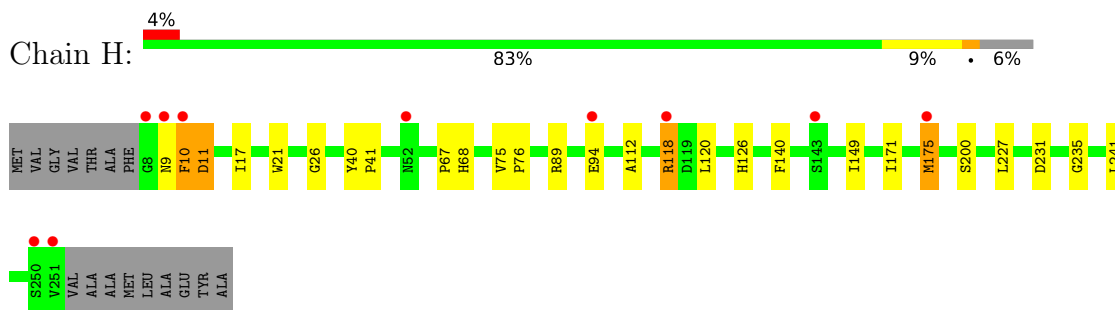
- Molecule 1: Reaction center protein L chain



- 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	139.54Å 139.54Å 183.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.03 – 2.55 46.03 – 2.55	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.03-2.55) 100.0 (46.03-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.69 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.210 (Not available) , 0.225	Depositor DCC
R_{free} test set	3362 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 87.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7923	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, BCL, FE, PO4, U10, K, HTO, PC9, GOL, PC7, LDA, BPH

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	1.09	0/2334	0.99	1/3194 (0.0%)
2	M	1.10	3/2590 (0.1%)	1.00	3/3532 (0.1%)
3	H	1.16	2/1986 (0.1%)	1.03	3/2697 (0.1%)
All	All	1.12	5/6910 (0.1%)	1.01	7/9423 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	260	ALA	CA-CB	6.41	1.63	1.53
3	H	126	HIS	C-O	-5.76	1.16	1.24
2	M	217	ALA	CA-C	5.58	1.59	1.52
3	H	17	ILE	CA-CB	5.18	1.61	1.54
2	M	273	ALA	CA-CB	5.11	1.61	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	149	ILE	N-CA-C	-5.64	102.25	109.30
1	L	227	LEU	N-CA-C	-5.59	105.11	111.14
3	H	120	LEU	CA-C-N	-5.35	115.07	120.31
3	H	120	LEU	C-N-CA	-5.35	115.07	120.31
2	M	220	GLY	N-CA-C	-5.34	106.32	112.73

There are no chirality outliers.

There are no planarity outliers.

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	2234	0	2193	23	0
2	M	2466	0	2371	36	0
3	H	1891	0	1902	14	0
4	L	5	0	0	1	0
4	M	15	0	0	0	0
5	L	132	0	148	5	0
5	M	132	0	148	19	0
6	L	65	0	75	2	0
6	M	65	0	76	10	0
7	L	48	0	63	1	0
7	M	48	0	63	1	0
8	L	54	0	80	20	0
9	H	64	0	124	3	0
9	L	32	0	62	0	0
9	M	32	0	62	1	0
10	M	1	0	0	0	0
11	M	81	0	106	2	0
12	H	1	0	0	0	0
13	H	10	0	16	1	0
14	H	52	0	84	4	0
15	H	18	0	24	0	0
16	H	225	0	0	2	0
16	L	113	0	0	1	0
16	M	139	0	0	2	0
All	All	7923	0	7597	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)
8:L:802:PC9:H483	6:M:401:BPH:HED1	1.40	1.03
1:L:189:LEU:CD1	8:L:802:PC9:H472	1.96	0.95
14:H:801:PC7:H451	9:H:901:LDA:H122	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.59	0.84
5:M:311:BCL:H41	5:M:311:BCL:H71	1.61	0.81

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	281/281 (100%)	275 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	299 (96%)	10 (3%)	1 (0%)	36	45
3	H	251/260 (96%)	245 (98%)	5 (2%)	1 (0%)	30	39
All	All	842/848 (99%)	819 (97%)	21 (2%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	10	PHE
2	M	195	ASN

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	222/220 (101%)	216 (97%)	6 (3%)	39	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	246/240 (102%)	235 (96%)	11 (4%)	24	38
3	H	207/208 (100%)	201 (97%)	6 (3%)	37	55
All	All	675/668 (101%)	652 (97%)	23 (3%)	32	48

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	196	LEU
3	H	10	PHE
2	M	274	VAL
3	H	11	ASP
2	M	32	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	258	GLN
2	M	28	ASN
2	M	138	GLN
3	H	52	ASN
3	H	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 2 are monoatomic - leaving 27 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$
14	PC7	H	801	-	51,51,51	0.91	1 (1%)	57,59,59	1.02	4 (7%)
7	U10	M	501	-	48,48,63	1.21	6 (12%)	60,61,79	1.65	11 (18%)
9	LDA	H	905	-	13,15,15	2.07	2 (15%)	14,17,17	0.42	0
9	LDA	H	903	-	13,15,15	2.12	2 (15%)	14,17,17	0.59	0
15	GOL	H	708	-	5,5,5	0.38	0	5,5,5	0.64	0
7	U10	L	502	-	48,48,63	1.01	3 (6%)	60,61,79	1.71	12 (20%)
11	CDL	M	800	-	80,80,99	1.20	5 (6%)	86,92,111	1.31	8 (9%)
5	BCL	M	311	2	69,74,74	1.15	5 (7%)	79,115,115	1.57	18 (22%)
4	PO4	M	702	-	4,4,4	0.70	0	6,6,6	0.77	0
8	PC9	L	802	-	53,53,53	0.83	2 (3%)	59,63,63	1.26	6 (10%)
6	BPH	M	401	-	59,70,70	1.37	6 (10%)	59,101,101	1.94	16 (27%)
6	BPH	L	402	-	59,70,70	1.35	9 (15%)	59,101,101	1.59	10 (16%)
9	LDA	H	901	-	13,15,15	1.78	2 (15%)	14,17,17	0.66	0
4	PO4	M	704	-	4,4,4	0.88	0	6,6,6	0.78	0
15	GOL	H	706	-	5,5,5	0.55	0	5,5,5	0.98	0
4	PO4	L	703	-	4,4,4	0.80	0	6,6,6	0.88	0
4	PO4	M	701	-	4,4,4	0.85	0	6,6,6	0.82	0
9	LDA	M	907	-	13,15,15	2.04	2 (15%)	14,17,17	0.49	0
9	LDA	M	920	-	13,15,15	1.73	1 (7%)	14,17,17	0.83	1 (7%)
5	BCL	L	314	1	69,74,74	1.09	4 (5%)	79,115,115	1.57	14 (17%)
9	LDA	L	902	-	13,15,15	2.07	2 (15%)	14,17,17	0.85	1 (7%)
9	LDA	H	904	-	13,15,15	2.07	2 (15%)	14,17,17	0.54	0
15	GOL	H	705	-	5,5,5	0.50	0	5,5,5	0.49	0
5	BCL	L	312	1	69,74,74	1.18	6 (8%)	79,115,115	1.45	14 (17%)
13	HTO	H	709	-	9,9,9	0.47	0	10,10,10	0.48	0
5	BCL	M	313	2	69,74,74	1.23	4 (5%)	79,115,115	1.72	20 (25%)
9	LDA	L	906	-	13,15,15	2.17	2 (15%)	14,17,17	0.64	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
14	PC7	H	801	-	-	29/55/55/55	-
7	U10	M	501	-	-	4/45/69/87	0/1/1/1
9	LDA	H	905	-	-	9/13/13/13	-
9	LDA	H	903	-	-	4/13/13/13	-
15	GOL	H	708	-	-	2/4/4/4	-
11	CDL	M	800	-	-	31/91/91/110	-
7	U10	L	502	-	-	12/45/69/87	0/1/1/1
5	BCL	M	311	2	-	10/41/137/137	-
8	PC9	L	802	-	-	22/60/60/60	-
6	BPH	M	401	-	-	11/37/105/105	0/5/6/6
6	BPH	L	402	-	-	3/37/105/105	0/5/6/6
9	LDA	H	901	-	-	6/13/13/13	-
15	GOL	H	706	-	-	2/4/4/4	-
9	LDA	M	907	-	-	10/13/13/13	-
9	LDA	M	920	-	-	7/13/13/13	-
5	BCL	L	314	1	-	3/41/137/137	-
9	LDA	L	902	-	-	4/13/13/13	-
9	LDA	H	904	-	-	5/13/13/13	-
15	GOL	H	705	-	-	2/4/4/4	-
5	BCL	L	312	1	-	5/41/137/137	-
13	HTO	H	709	-	-	3/10/10/10	-
5	BCL	M	313	2	-	3/41/137/137	-
9	LDA	L	906	-	-	5/13/13/13	-

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	906	LDA	O1-N1	-6.54	1.26	1.42
9	H	905	LDA	O1-N1	-6.53	1.26	1.42
9	H	903	LDA	O1-N1	-6.51	1.26	1.42
9	H	904	LDA	O1-N1	-6.30	1.26	1.42
9	M	907	LDA	O1-N1	-6.16	1.27	1.42

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	402	BPH	O2D-CGD-CBD	6.60	118.19	110.95
6	M	401	BPH	O2D-CGD-CBD	6.43	118.02	110.95
11	M	800	CDL	OA6-CA5-C11	5.83	124.10	111.48
5	M	313	BCL	C1C-NC-C4C	5.55	109.21	106.68
6	M	401	BPH	OBD-CAD-CBD	-4.75	118.85	125.82

There are no chirality outliers.

5 of 192 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	401	BPH	C2C-C3C-CAC-CBC
6	M	401	BPH	C11-C12-C13-C14
8	L	802	PC9	C1-O3P-P-O2P
8	L	802	PC9	C1-O3P-P-O4P
9	L	906	LDA	N1-C1-C2-C3

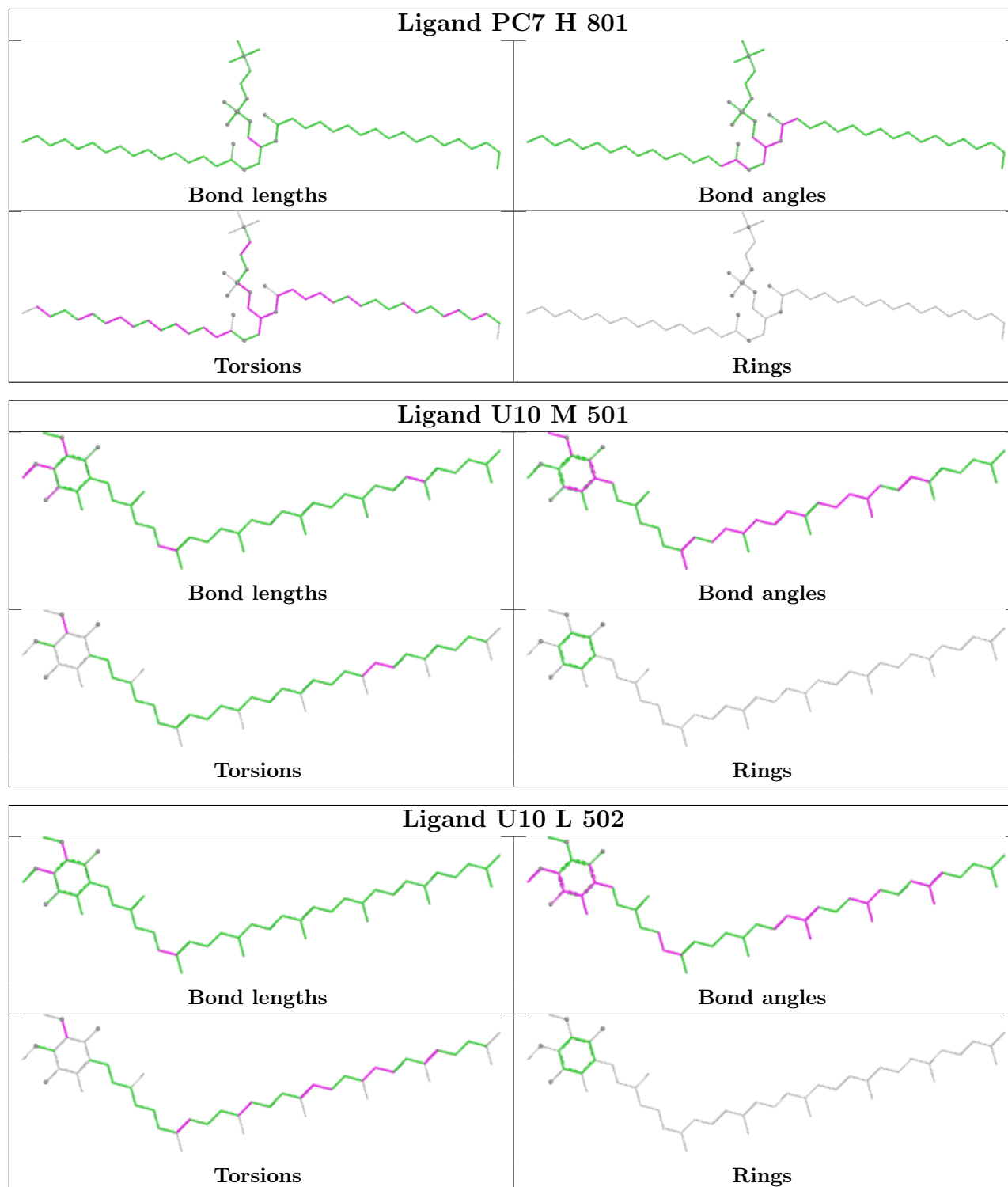
There are no ring outliers.

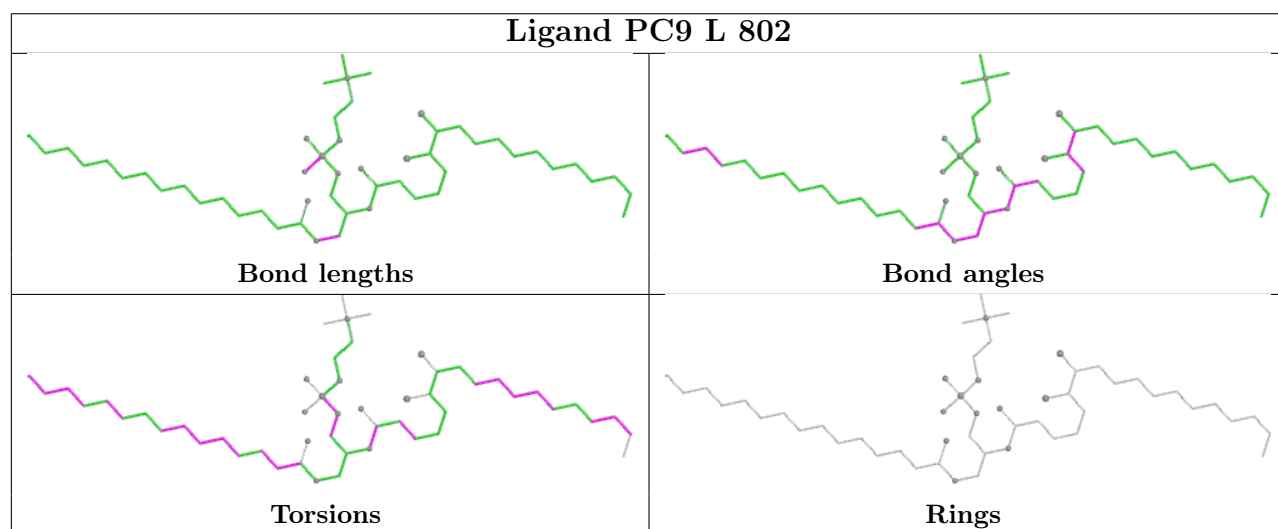
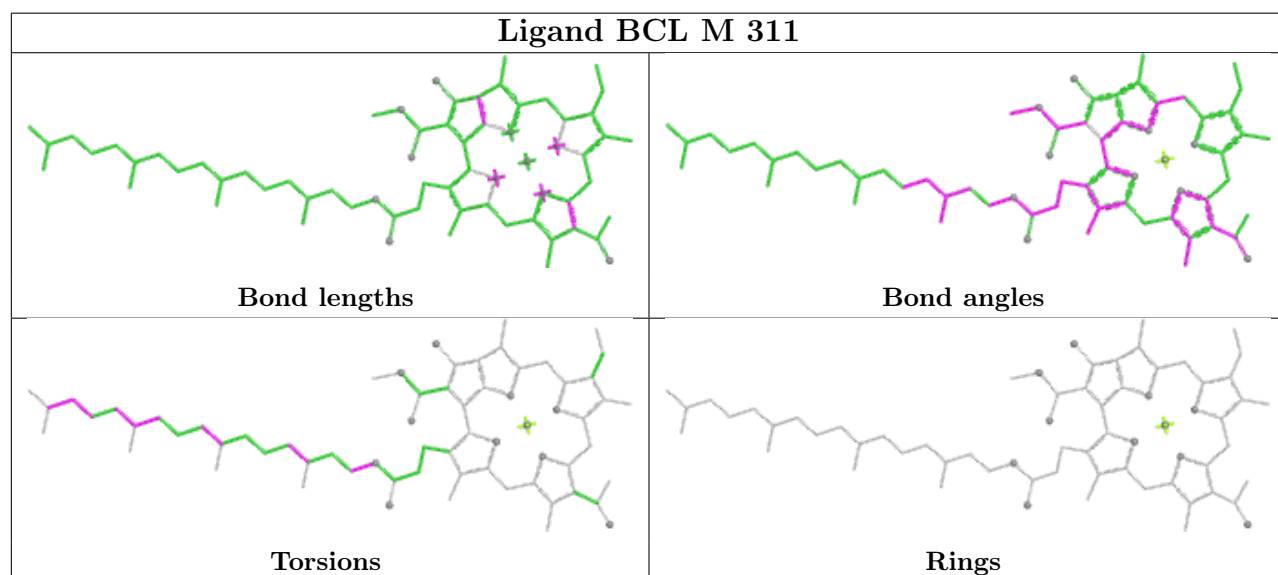
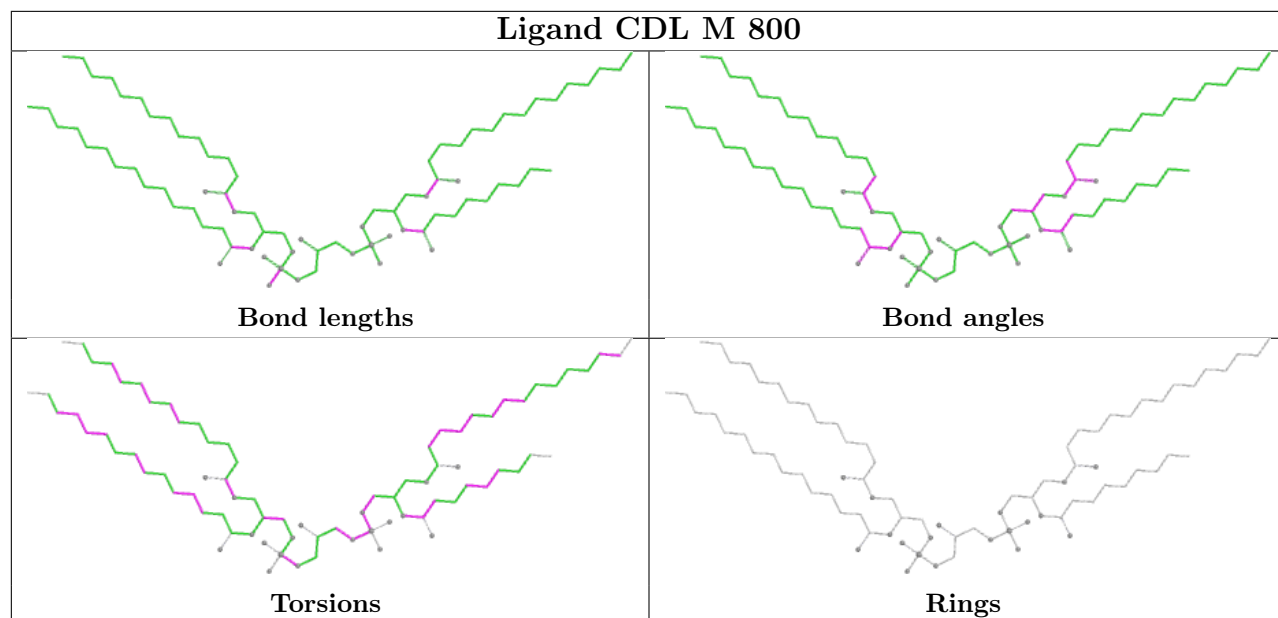
15 monomers are involved in 53 short contacts:

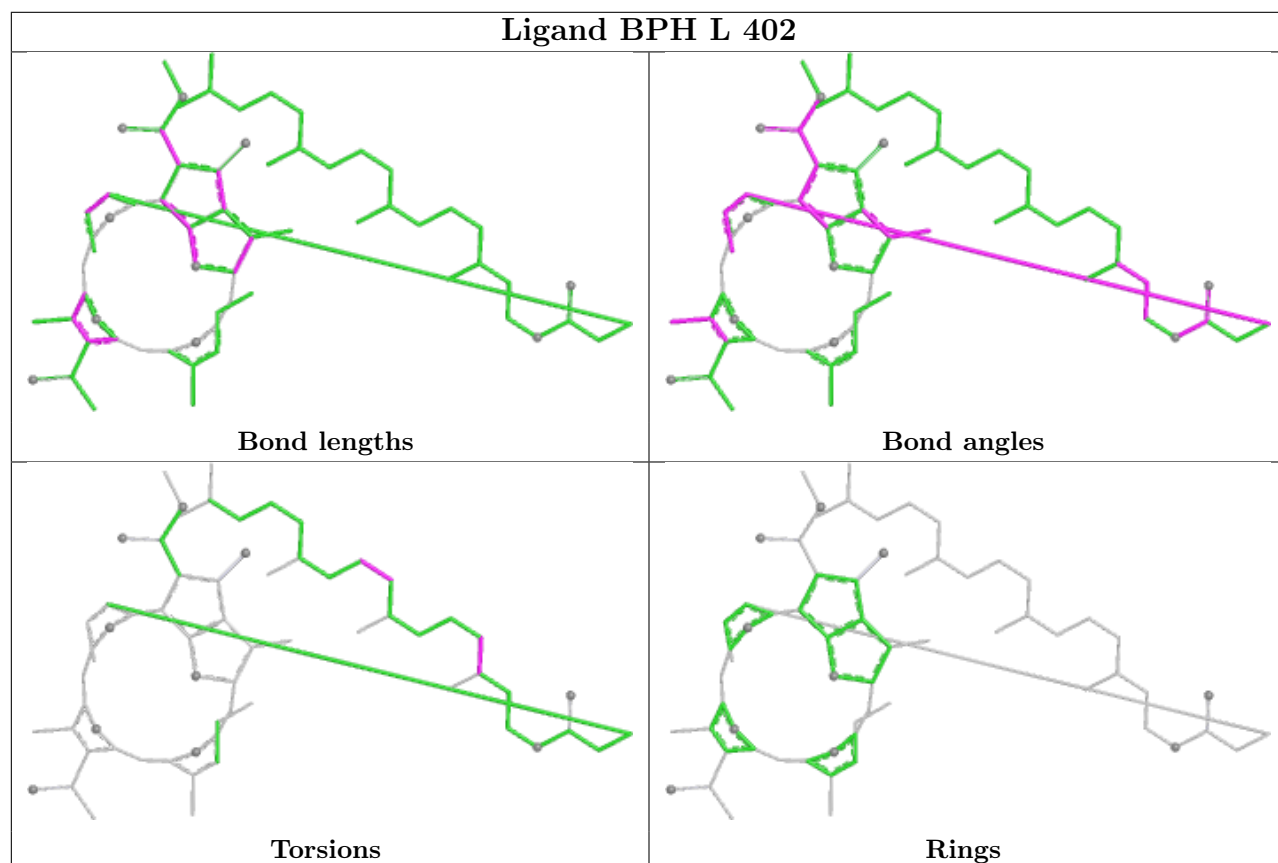
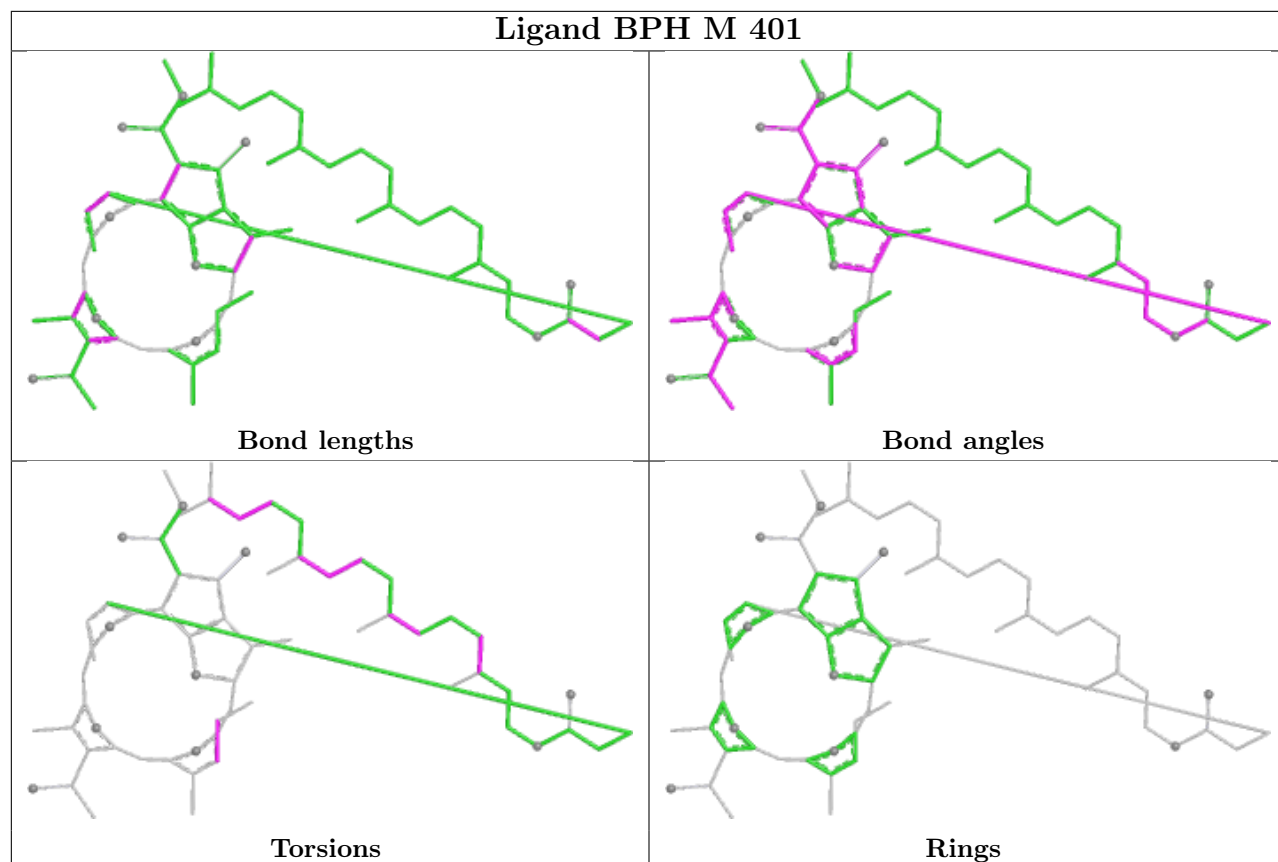
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	801	PC7	4	0
7	M	501	U10	1	0
7	L	502	U10	1	0
11	M	800	CDL	2	0
5	M	311	BCL	12	0
8	L	802	PC9	20	0
6	M	401	BPH	10	0
6	L	402	BPH	2	0
9	H	901	LDA	3	0
4	L	703	PO4	1	0
9	M	907	LDA	1	0
5	L	314	BCL	3	0
5	L	312	BCL	2	0
13	H	709	HTO	1	0
5	M	313	BCL	9	0

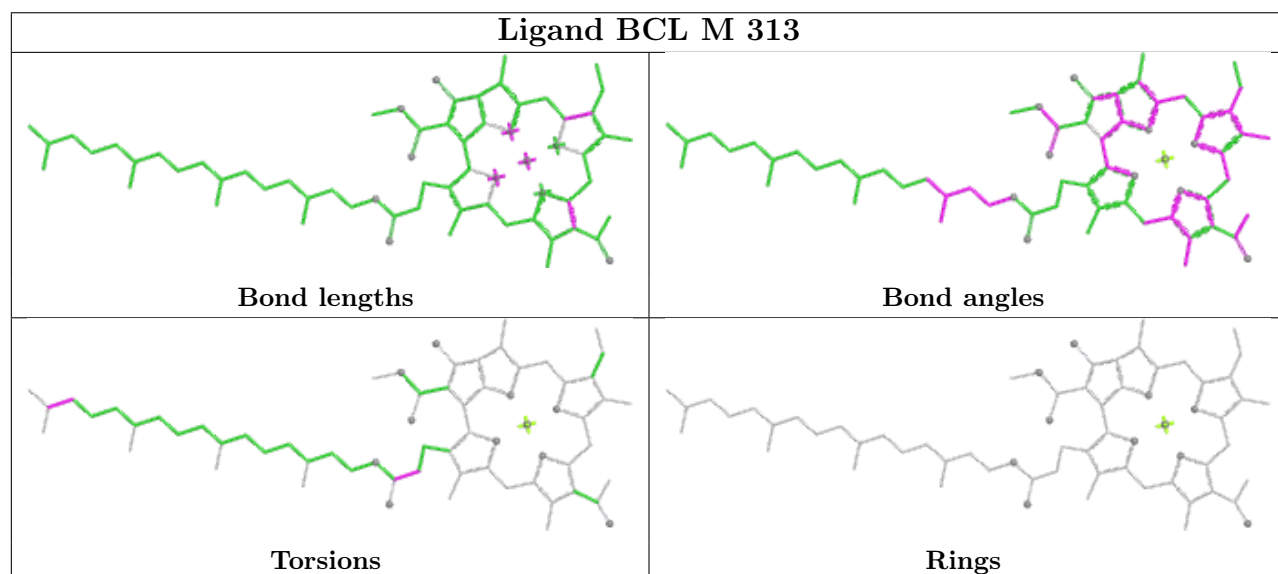
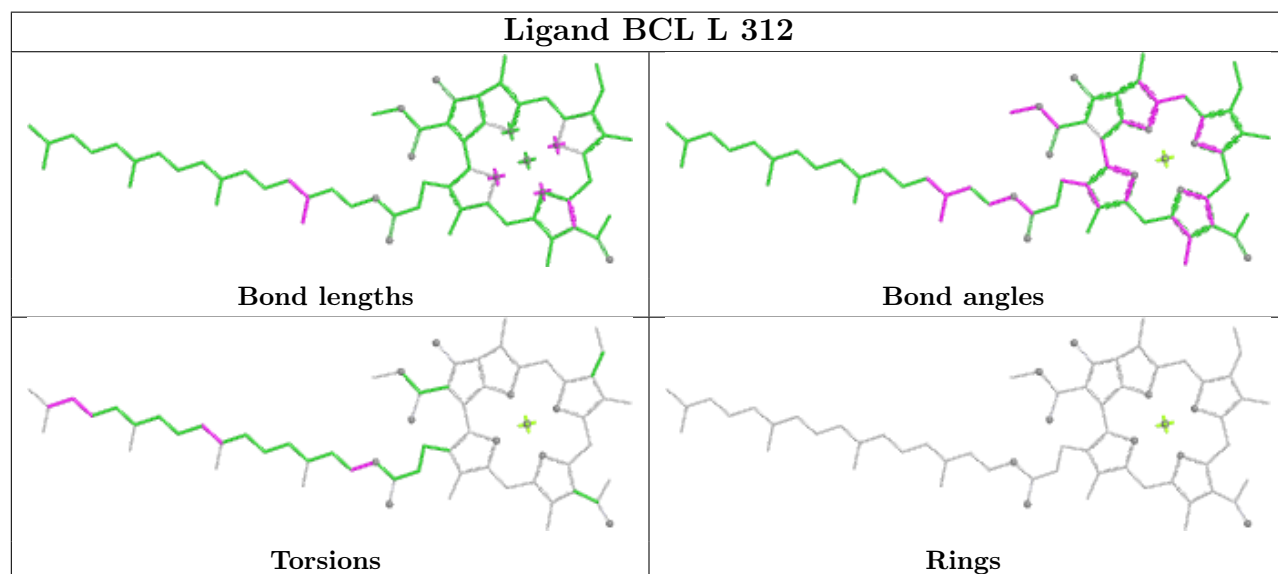
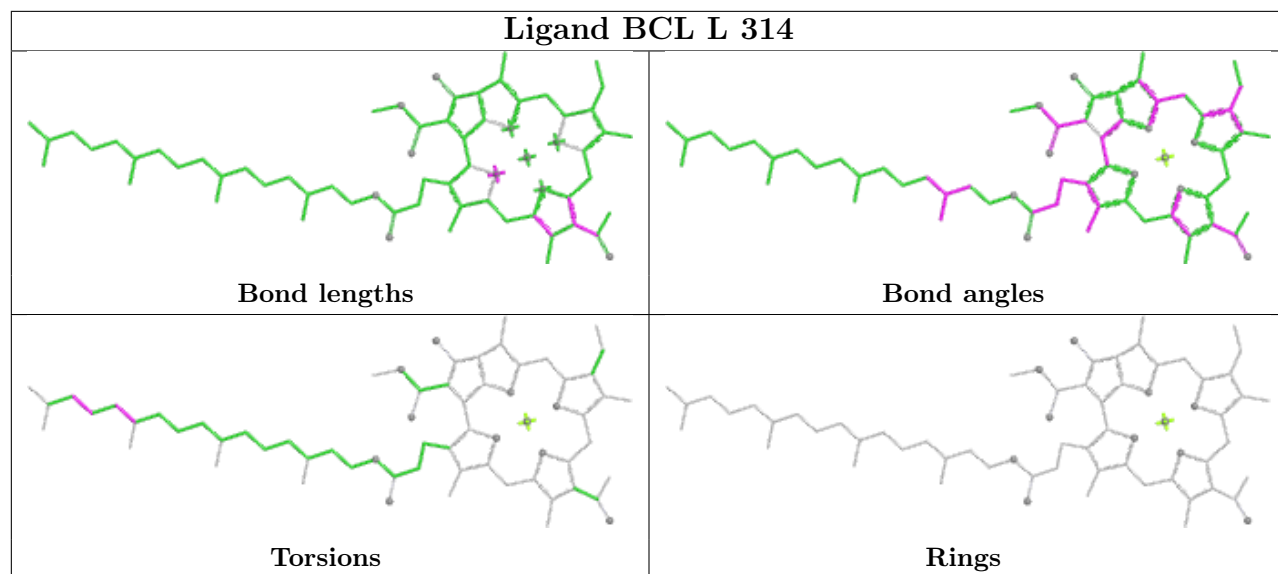
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	L	281/281 (100%)	0.46	12 (4%)	40	40	38, 51, 60, 72	2 (0%)
2	M	302/307 (98%)	0.48	13 (4%)	40	40	24, 50, 60, 76	9 (2%)
3	H	244/260 (93%)	0.35	10 (4%)	41	42	24, 49, 60, 87	8 (3%)
All	All	827/848 (97%)	0.43	35 (4%)	40	41	24, 50, 61, 87	19 (2%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	251	VAL	8.6
3	H	9	ASN	7.4
3	H	118[A]	ARG	6.1
3	H	10	PHE	5.2
3	H	8	GLY	4.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

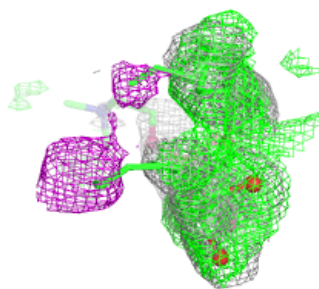
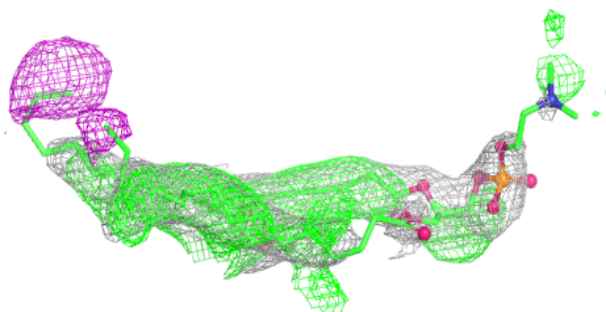
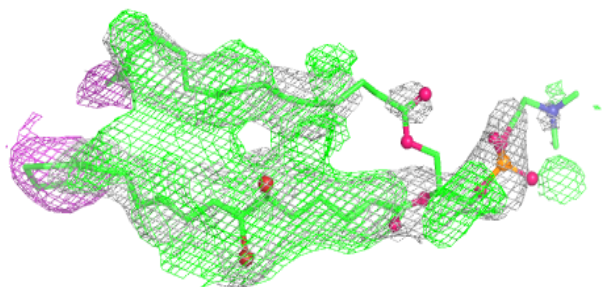
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	GOL	H	708	6/6	0.65	0.57	46,46,47,49	6
8	PC9	L	802	54/54	0.76	0.52	57,66,75,79	54
9	LDA	H	903	16/16	0.79	0.36	63,65,74,75	16
14	PC7	H	801	52/52	0.81	0.37	26,68,76,78	52
11	CDL	M	800	81/100	0.81	0.33	43,71,83,85	81
13	HTO	H	709	10/10	0.82	0.40	50,56,56,58	10
9	LDA	H	904	16/16	0.83	0.39	65,68,72,72	16
9	LDA	L	902	16/16	0.86	0.29	68,73,77,80	16
9	LDA	H	905	16/16	0.86	0.41	61,69,78,78	16
4	PO4	M	704	5/5	0.86	0.12	76,76,77,78	5
9	LDA	M	907	16/16	0.87	0.35	56,61,66,67	16
9	LDA	M	920	16/16	0.87	0.29	59,74,88,88	16
4	PO4	M	702	5/5	0.87	0.12	66,67,68,68	5
9	LDA	L	906	16/16	0.88	0.36	54,56,59,60	16
7	U10	L	502	48/63	0.89	0.30	34,48,60,62	48
15	GOL	H	706	6/6	0.91	0.21	74,76,77,77	0
6	BPH	M	401	65/65	0.91	0.14	45,51,92,93	0
7	U10	M	501	48/63	0.92	0.14	43,54,77,80	0
5	BCL	M	311	66/66	0.92	0.14	42,51,96,97	0
4	PO4	L	703	5/5	0.93	0.17	70,72,73,75	5
9	LDA	H	901	16/16	0.95	0.14	60,65,69,71	0
15	GOL	H	705	6/6	0.95	0.15	58,69,70,72	0
4	PO4	M	701	5/5	0.95	0.13	57,59,62,63	0
6	BPH	L	402	65/65	0.95	0.10	35,47,52,53	0
5	BCL	L	312	66/66	0.96	0.10	41,46,58,61	0
5	BCL	M	313	66/66	0.96	0.10	38,46,70,79	0
5	BCL	L	314	66/66	0.96	0.09	38,47,62,66	0
12	K	H	700	1/1	0.99	0.03	54,54,54,54	0
10	FE	M	500	1/1	1.00	0.03	49,49,49,49	0

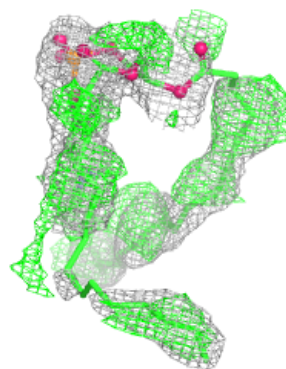
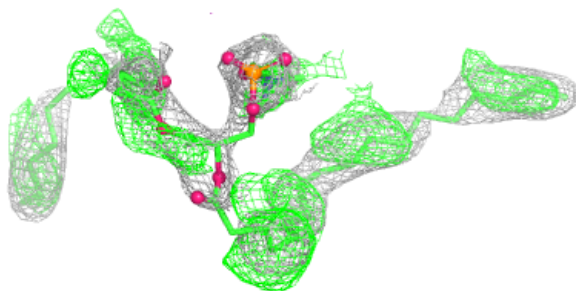
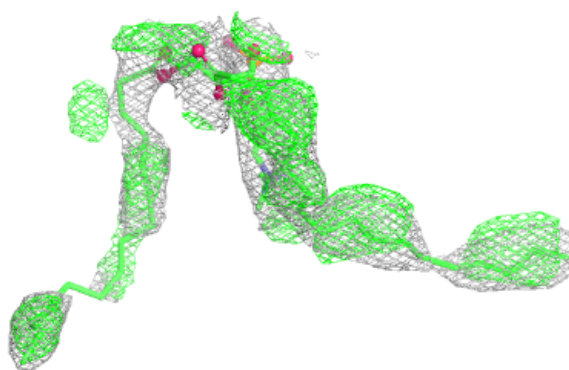
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PC9 L 802:

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

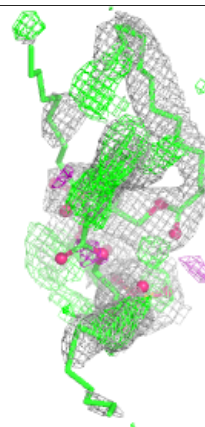
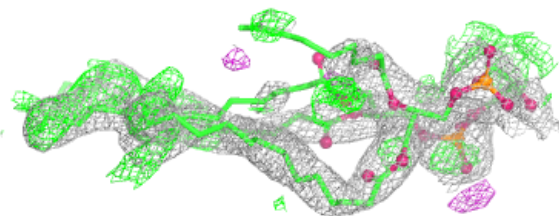
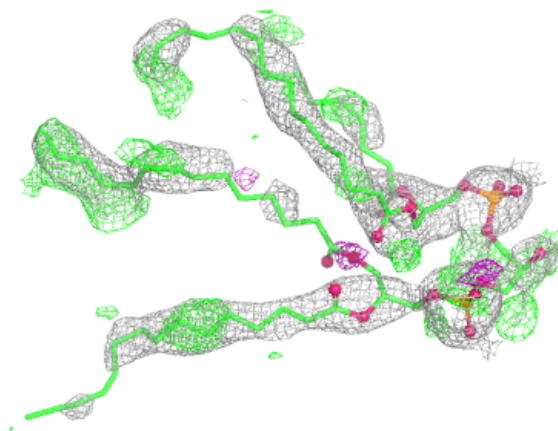
**Electron density around PC7 H 801:**

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

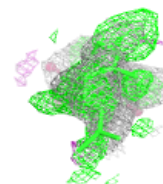
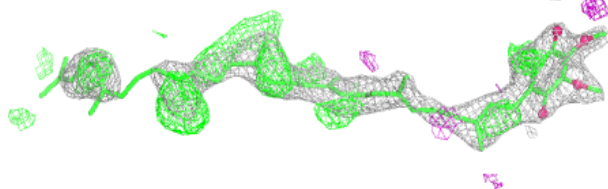
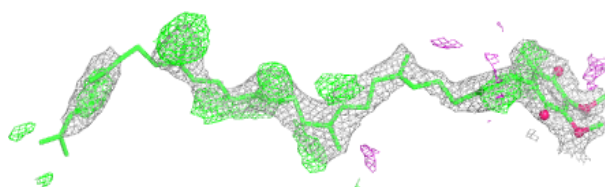


Electron density around CDL M 800:

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

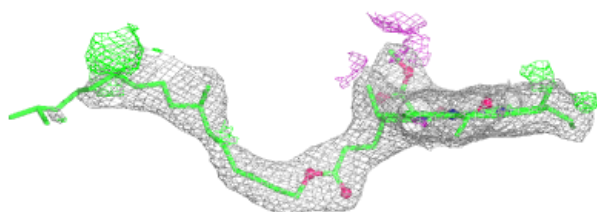
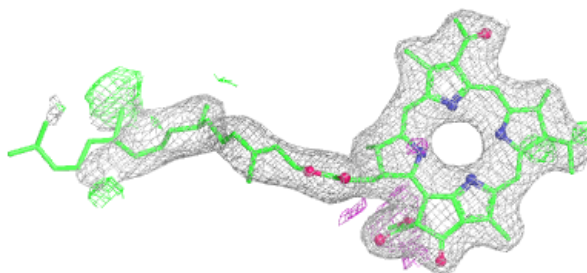
**Electron density around U10 L 502:**

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

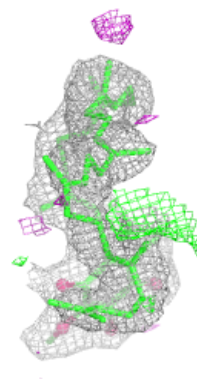
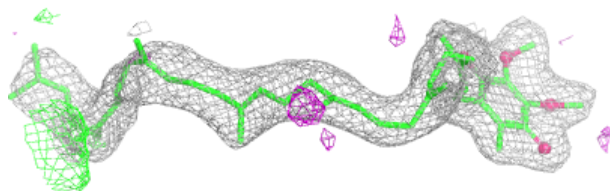


Electron density around BPH M 401:

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

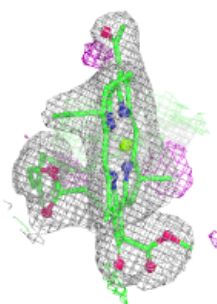
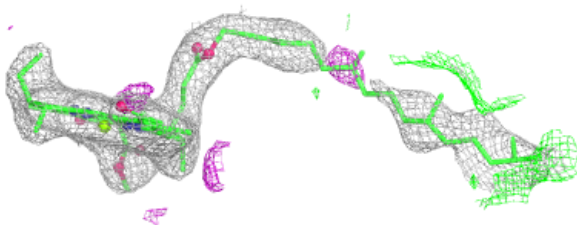
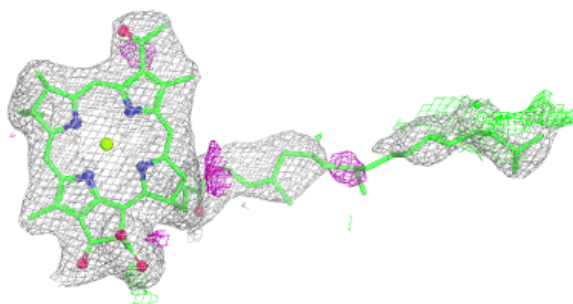
**Electron density around U10 M 501:**

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and green (positive)



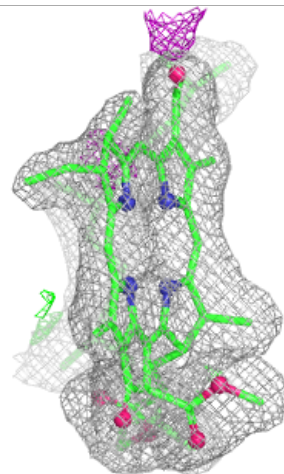
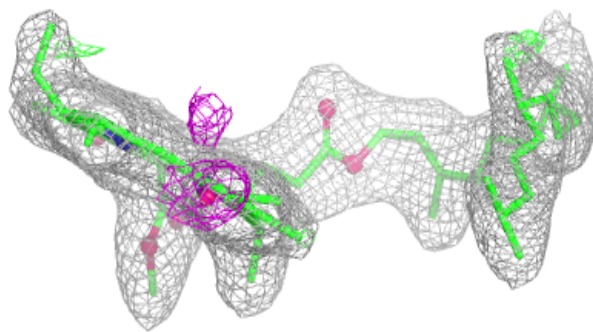
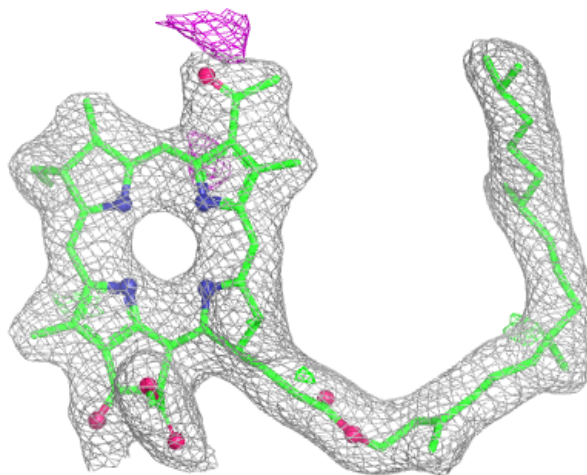
Electron density around BCL M 311:

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and green (positive)



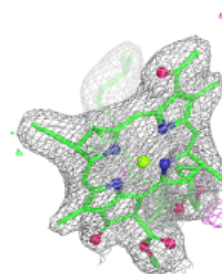
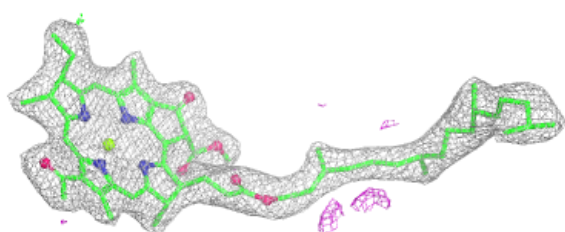
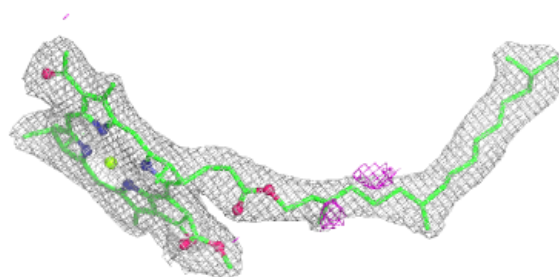
Electron density around BPH L 402:

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

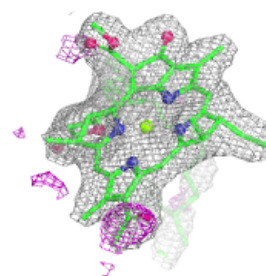
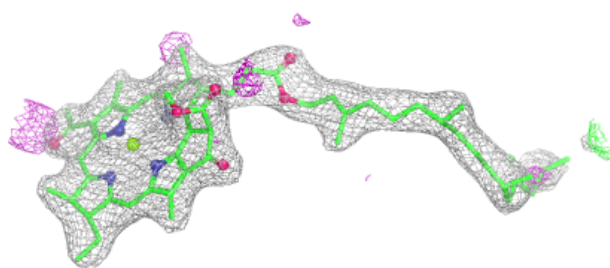
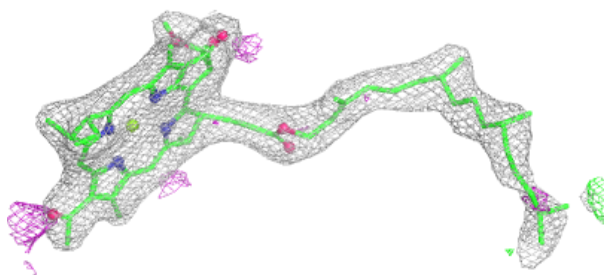


Electron density around BCL L 312:

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

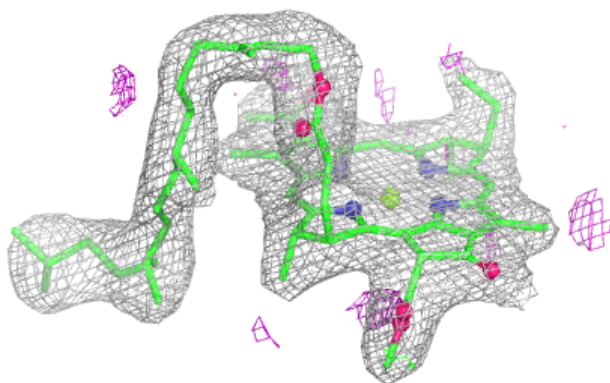
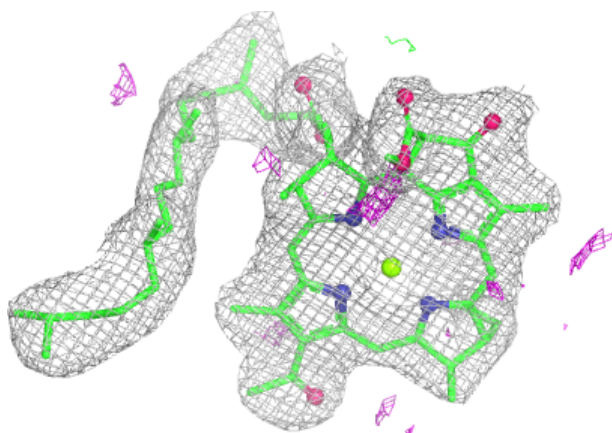
**Electron density around BCL M 313:**

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



Electron density around BCL L 314:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.