



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 12:45 PM UTC

PDB ID : 2HJ6 / pdb_00002hj6
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylserine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-30
Resolution : 3.00 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

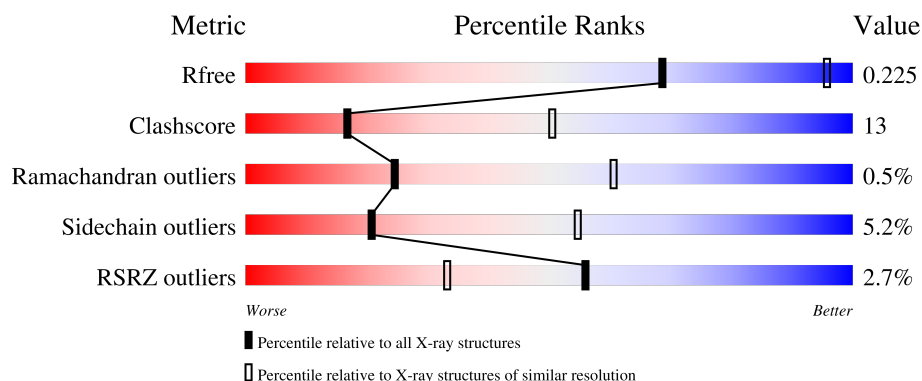
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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% 74% 23% .
2	M	307	2% 75% 21% ..
3	H	260	2% 68% 23% . 7%

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	LDA	M	920	-	-	X	-
13	GOL	M	704	-	-	-	X
9	HTO	M	703	-	-	-	X

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 7685 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	3	0
			2249	1520	357	364	8			

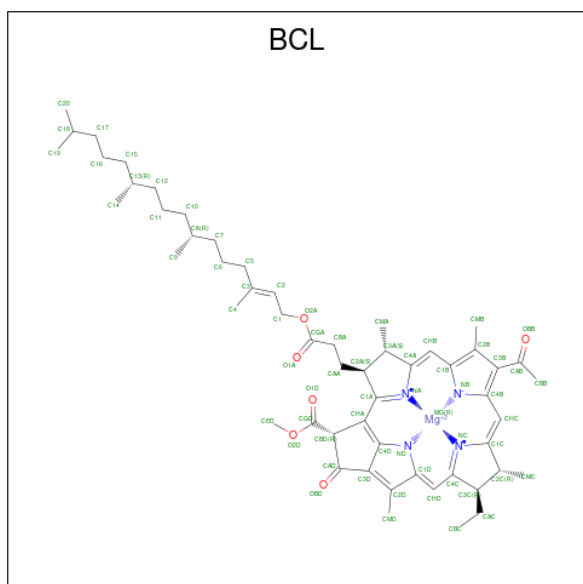
- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	5	0
			2452	1637	403	402	10			

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

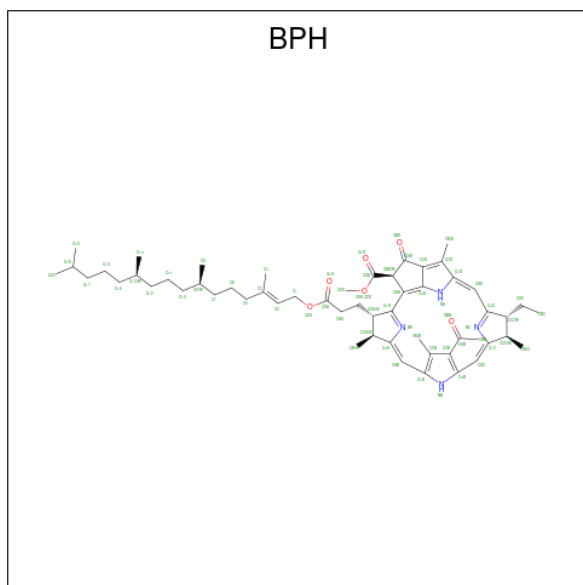
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	5	0
			1846	1180	316	339	11			

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



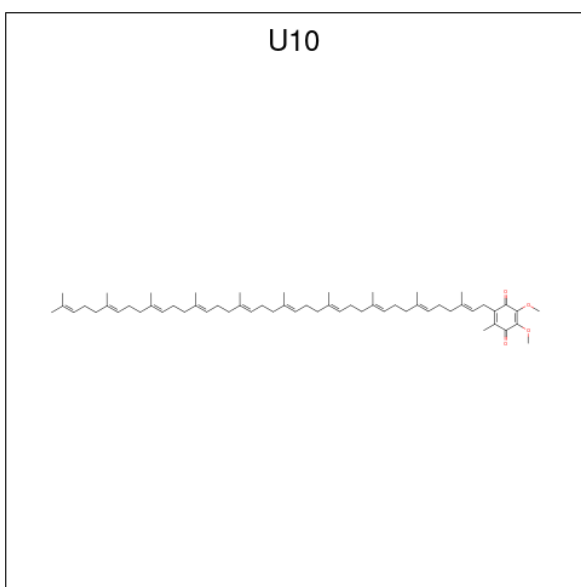
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).

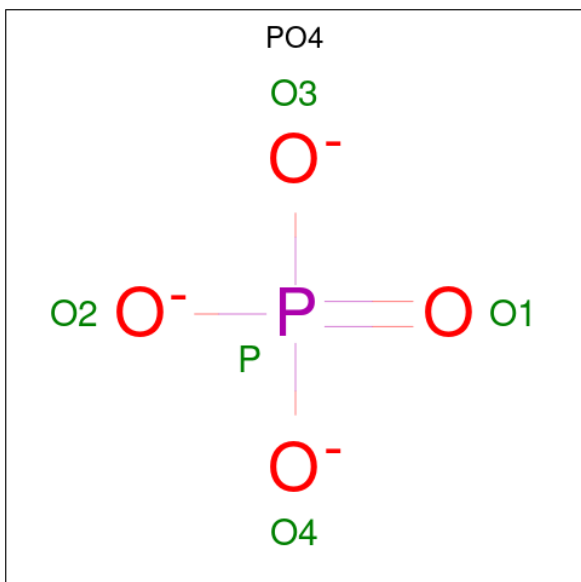


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			48	44	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

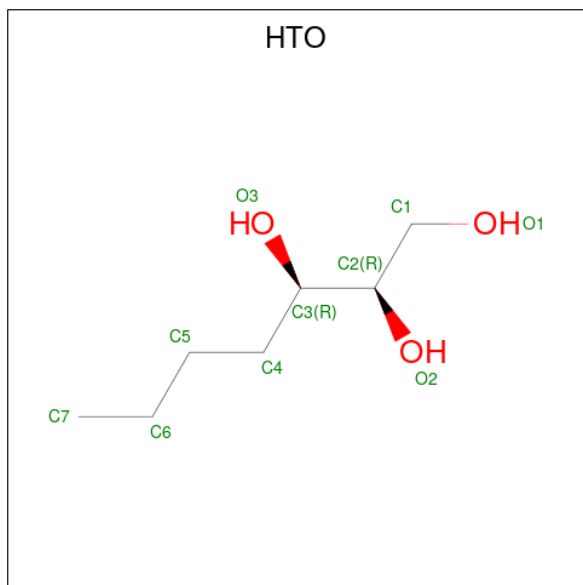
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



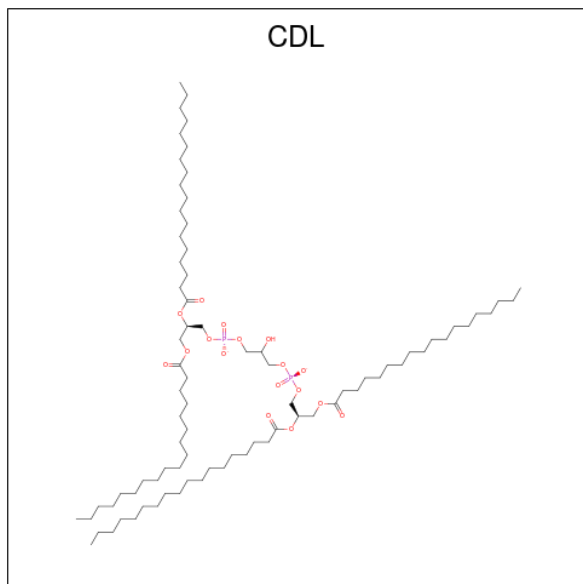
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	P	0	0
			5	4	1		
8	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



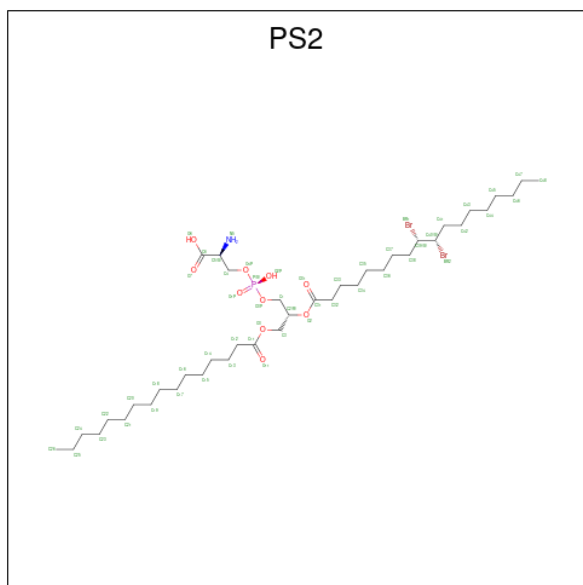
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



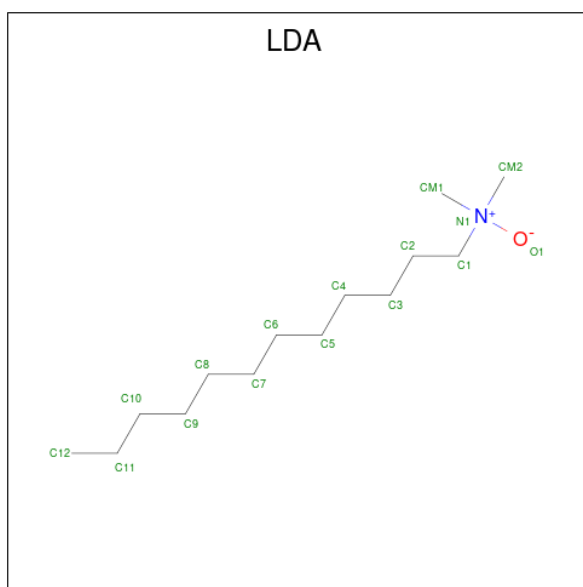
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is O-[[[(2R)-2-[[[(9S,10S)-9,10-DIBROMOOCTADECANOYL]OXY}-3-(PALMITOYLOXY)PROPYL]OXY}(HYDROXY)PHOSPHORYL]-L-SERINE (CCD ID: PS2) (formula: C₄₀H₇₆Br₂NO₁₀P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	M	1	Total	Br	C	N	O	P	0	0
			54	2	40	1	10	1		

- Molecule 12 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



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

- Molecule 13 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 14 is POTASSIUM ION (CCD ID: K) (formula: K).

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

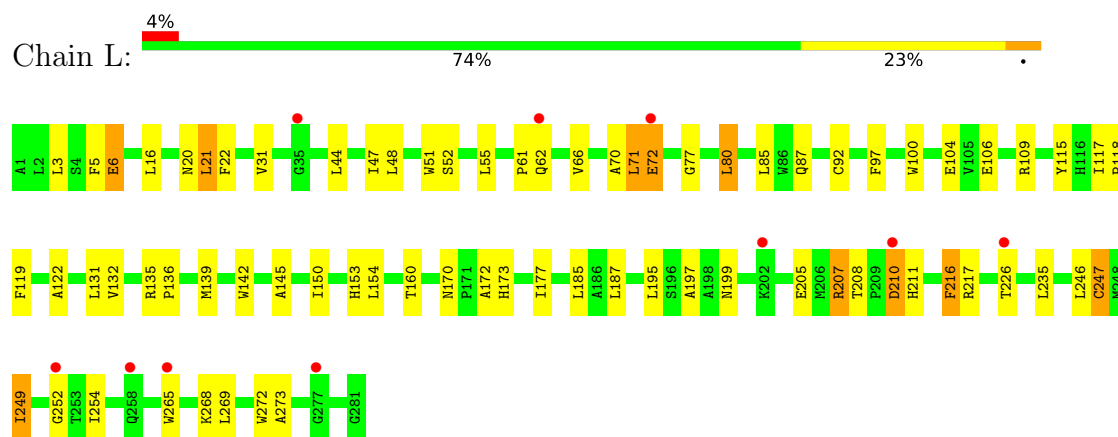
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	L	78	Total	O	0	0
			78	78		
15	M	108	Total	O	0	0
			108	108		
15	H	165	Total	O	0	0
			165	165		

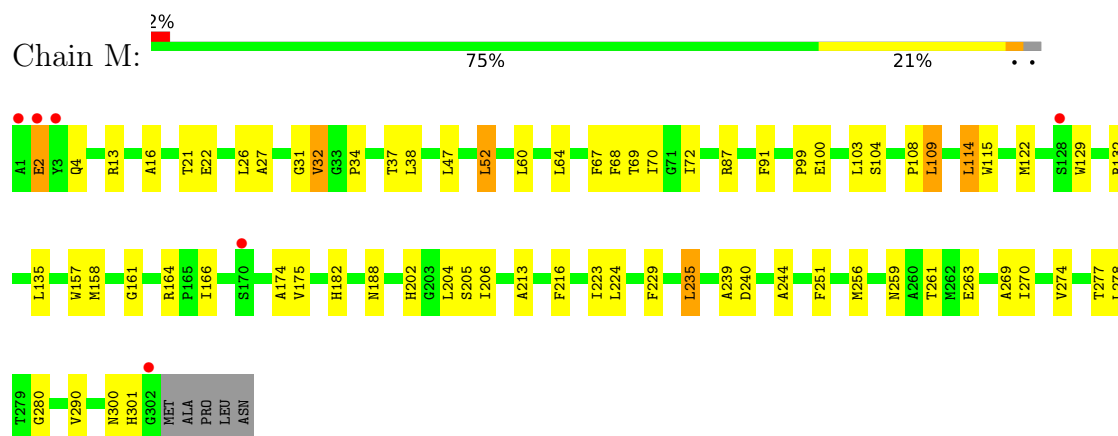
3 Residue-property plots [i](#)

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.

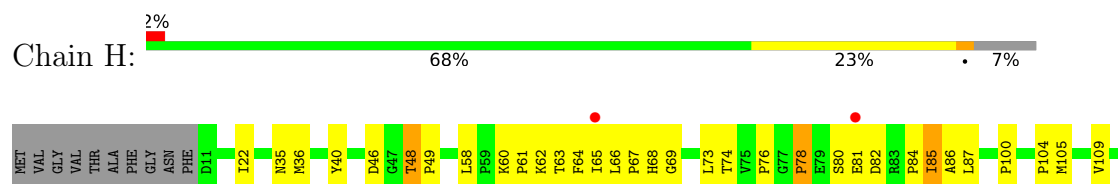
- Molecule 1: Reaction center protein L chain

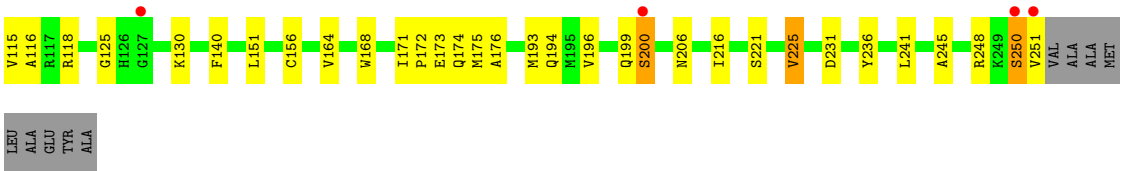


- Molecule 2: Reaction center protein M chain



- 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	139.35Å 139.35Å 183.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.29 – 3.00 39.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.29-3.00) 99.4 (39.29-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.174 , 0.227 0.178 , 0.225	Depositor DCC
R_{free} test set	2083 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	75.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 83.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7685	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: LDA, HTO, CDL, BPH, PO4, K, GOL, BCL, U10, PS2, FE

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	1.05	1/2350 (0.0%)	1.06	2/3216 (0.1%)
2	M	1.06	1/2552 (0.0%)	1.09	5/3482 (0.1%)
3	H	1.12	2/1921 (0.1%)	1.17	6/2612 (0.2%)
All	All	1.07	4/6823 (0.1%)	1.10	13/9310 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	132	VAL	C-N	7.42	1.43	1.33
3	H	64	PHE	C-O	-6.95	1.15	1.23
3	H	22	ILE	CA-CB	6.04	1.60	1.54
2	M	235	LEU	CA-C	5.45	1.59	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	259	ASN	N-CA-C	8.31	120.77	108.14
3	H	216	ILE	CA-C-N	6.76	126.80	119.90
3	H	216	ILE	C-N-CA	6.76	126.80	119.90
2	M	2	GLU	N-CA-C	-5.81	102.45	110.35
2	M	290	VAL	CB-CA-C	-5.73	104.96	111.55

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	L	2249	0	2210	55	0
2	M	2452	0	2357	68	0
3	H	1846	0	1866	48	0
4	L	132	0	148	12	0
4	M	132	0	148	15	0
5	L	65	0	76	4	0
5	M	65	0	76	3	0
6	L	48	0	63	3	0
6	M	48	0	63	4	0
7	M	1	0	0	0	0
8	M	10	0	0	0	0
9	M	10	0	16	0	0
10	M	81	0	106	3	0
11	M	54	0	72	4	0
12	H	48	0	93	0	0
12	M	80	0	155	22	0
13	H	6	0	8	0	0
13	M	6	0	8	2	0
14	H	1	0	0	0	0
15	H	165	0	0	9	0
15	L	78	0	0	1	0
15	M	108	0	0	3	0
All	All	7685	0	7465	189	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 13.

The worst 5 of 189 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:H:250:SER:O	3:H:251:VAL:CG2	2.11	0.99
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.46	0.97
3:H:250:SER:O	3:H:251:VAL:HG23	1.64	0.97
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.54	0.88
4:M:311:BCL:HMB3	4:M:311:BCL:HBB2	1.63	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	282/281 (100%)	263 (93%)	18 (6%)	1 (0%)	30	65
2	M	305/307 (99%)	283 (93%)	21 (7%)	1 (0%)	36	70
3	H	244/260 (94%)	237 (97%)	5 (2%)	2 (1%)	16	50
All	All	831/848 (98%)	783 (94%)	44 (5%)	4 (0%)	24	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	109	LEU
1	L	31	VAL
3	H	86	ALA
3	H	78	PRO

5.3.2 Protein sidechains

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	223/220 (101%)	209 (94%)	14 (6%)	16	48
2	M	241/240 (100%)	229 (95%)	12 (5%)	22	56
3	H	201/208 (97%)	192 (96%)	9 (4%)	24	59
All	All	665/668 (100%)	630 (95%)	35 (5%)	21	54

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	78	PRO
3	H	80	SER
3	H	221[B]	SER
1	L	249	ILE
1	L	247	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	129	ASN
3	H	141	HIS
1	L	274	ASN
2	M	202	HIS
2	M	300	ASN

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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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
12	LDA	M	920	-	13,15,15	1.72	2 (15%)	14,17,17	0.70	0
12	LDA	M	901	-	13,15,15	2.18	2 (15%)	14,17,17	0.54	0
4	BCL	L	312	1	69,74,74	1.35	5 (7%)	79,115,115	1.27	10 (12%)
4	BCL	M	311	2	69,74,74	1.34	6 (8%)	79,115,115	1.62	15 (18%)
12	LDA	M	903	-	13,15,15	1.95	1 (7%)	14,17,17	1.15	1 (7%)
12	LDA	H	905	-	13,15,15	2.20	2 (15%)	14,17,17	0.50	0
12	LDA	H	904	-	13,15,15	2.07	2 (15%)	14,17,17	0.56	0
12	LDA	H	902	-	13,15,15	1.95	2 (15%)	14,17,17	0.87	1 (7%)
12	LDA	M	907	-	13,15,15	1.78	2 (15%)	14,17,17	0.66	0
11	PS2	M	802	-	52,53,53	1.17	4 (7%)	54,62,62	2.39	11 (20%)
4	BCL	M	313	2	69,74,74	1.08	3 (4%)	79,115,115	1.43	15 (18%)
9	HTO	M	703	-	9,9,9	0.94	0	10,10,10	2.39	4 (40%)
12	LDA	M	906	-	13,15,15	1.61	2 (15%)	14,17,17	0.79	1 (7%)
13	GOL	M	704	-	5,5,5	0.54	0	5,5,5	0.43	0
5	BPH	M	401	-	59,70,70	1.20	3 (5%)	59,101,101	2.20	17 (28%)
6	U10	M	501	-	48,48,63	1.16	6 (12%)	60,61,79	1.32	6 (10%)
8	PO4	M	702	-	4,4,4	0.79	0	6,6,6	1.02	0
8	PO4	M	701	-	4,4,4	0.57	0	6,6,6	1.10	0
4	BCL	L	314	1	69,74,74	1.33	7 (10%)	79,115,115	1.69	19 (24%)
13	GOL	H	705	-	5,5,5	0.40	0	5,5,5	0.31	0
6	U10	L	502	-	48,48,63	1.17	2 (4%)	60,61,79	1.55	9 (15%)
10	CDL	M	800	-	80,80,99	1.28	5 (6%)	86,92,111	1.35	11 (12%)
5	BPH	L	402	-	59,70,70	1.41	7 (11%)	59,101,101	1.76	13 (22%)

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
12	LDA	M	920	-	-	7/13/13/13	-
12	LDA	M	901	-	-	4/13/13/13	-
4	BCL	L	312	1	-	0/41/137/137	-
4	BCL	M	311	2	-	7/41/137/137	-
12	LDA	M	903	-	-	10/13/13/13	-
12	LDA	H	905	-	-	7/13/13/13	-
12	LDA	H	904	-	-	5/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LDA	H	902	-	-	6/13/13/13	-
12	LDA	M	907	-	-	6/13/13/13	-
11	PS2	M	802	-	-	40/62/62/62	-
4	BCL	M	313	2	-	5/41/137/137	-
9	HTO	M	703	-	-	6/10/10/10	-
12	LDA	M	906	-	-	9/13/13/13	-
13	GOL	M	704	-	-	4/4/4/4	-
5	BPH	M	401	-	-	7/37/105/105	0/5/6/6
6	U10	M	501	-	-	2/45/69/87	0/1/1/1
4	BCL	L	314	1	-	5/41/137/137	-
13	GOL	H	705	-	-	3/4/4/4	-
6	U10	L	502	-	-	12/45/69/87	0/1/1/1
10	CDL	M	800	-	-	43/91/91/110	-
5	BPH	L	402	-	-	8/37/105/105	0/5/6/6

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	901	LDA	O1-N1	-7.12	1.24	1.42
12	H	905	LDA	O1-N1	-6.68	1.25	1.42
12	H	904	LDA	O1-N1	-6.42	1.26	1.42
12	M	903	LDA	O1-N1	-6.19	1.27	1.42
4	L	312	BCL	MG-NB	6.16	2.18	2.05

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	802	PS2	O4P-C4-C5	9.03	115.94	108.06
5	M	401	BPH	O2D-CGD-CBD	7.77	119.48	110.95
5	M	401	BPH	C4D-CHA-CBD	-6.55	105.31	108.45
11	M	802	PS2	C3-C2-C1	-6.42	96.81	111.78
11	M	802	PS2	BR1-C39-C40	-6.13	98.40	110.27

There are no chirality outliers.

5 of 196 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	401	BPH	C4C-C3C-CAC-CBC

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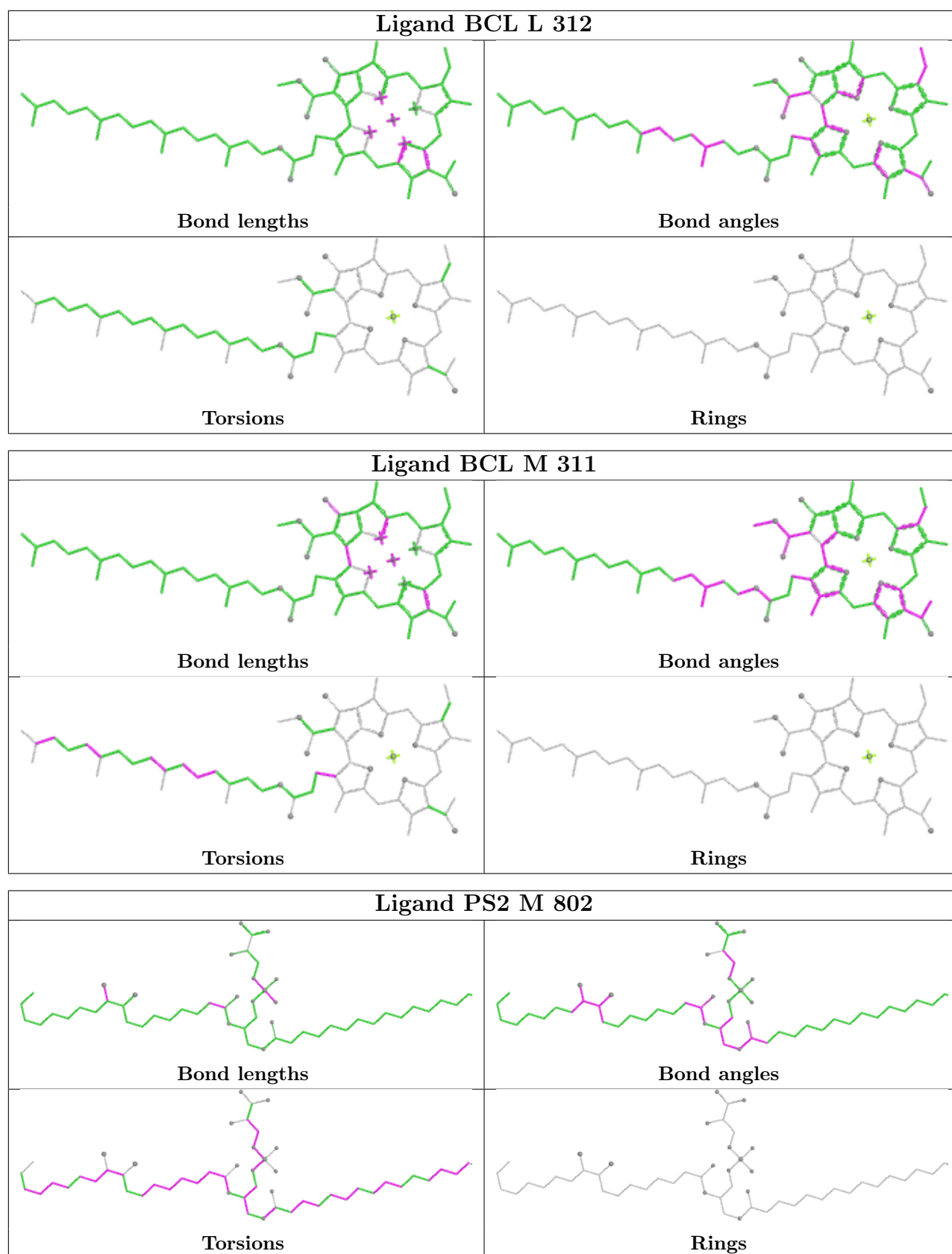
Mol	Chain	Res	Type	Atoms
9	M	703	HTO	C1-C2-C3-C4
10	M	800	CDL	CB2-C1-CA2-OA2
10	M	800	CDL	CA2-OA2-PA1-OA3
10	M	800	CDL	CA2-OA2-PA1-OA5

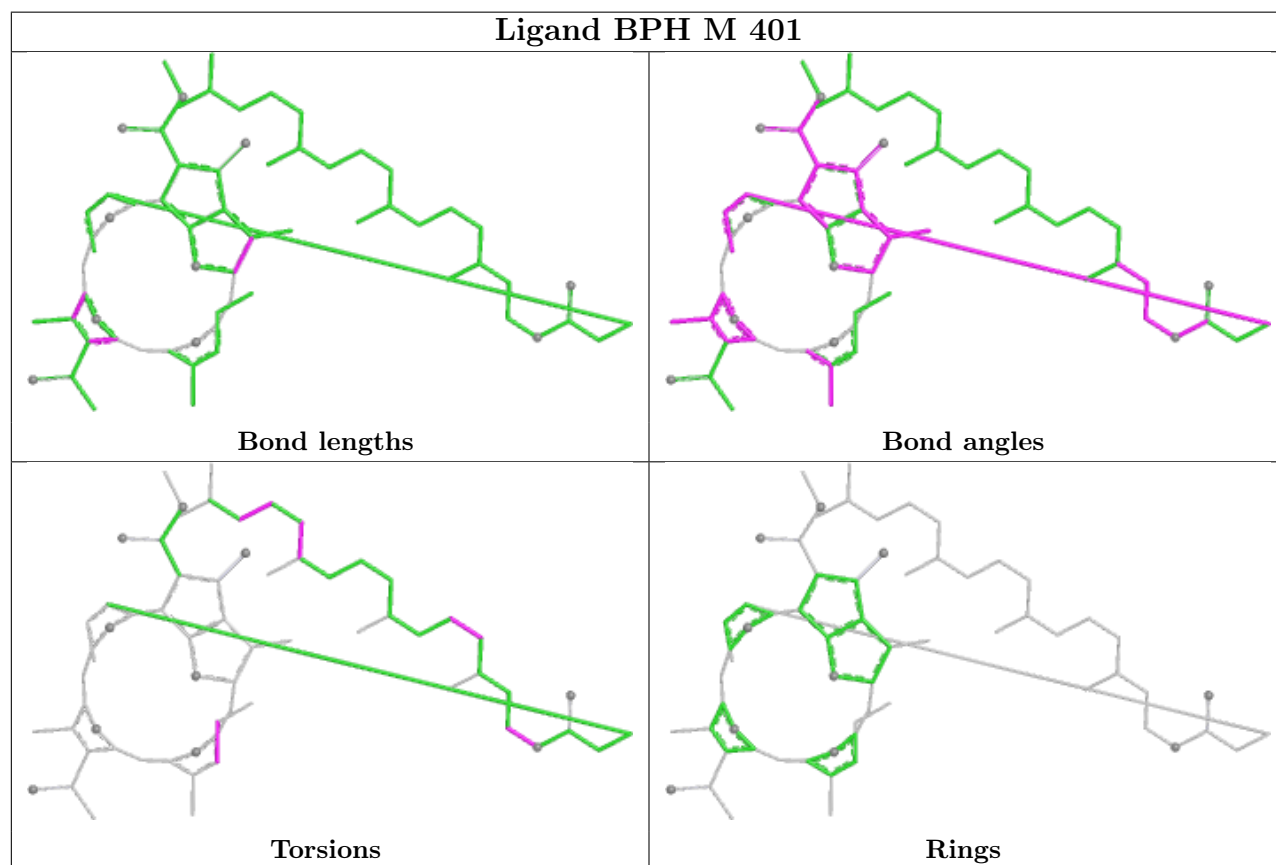
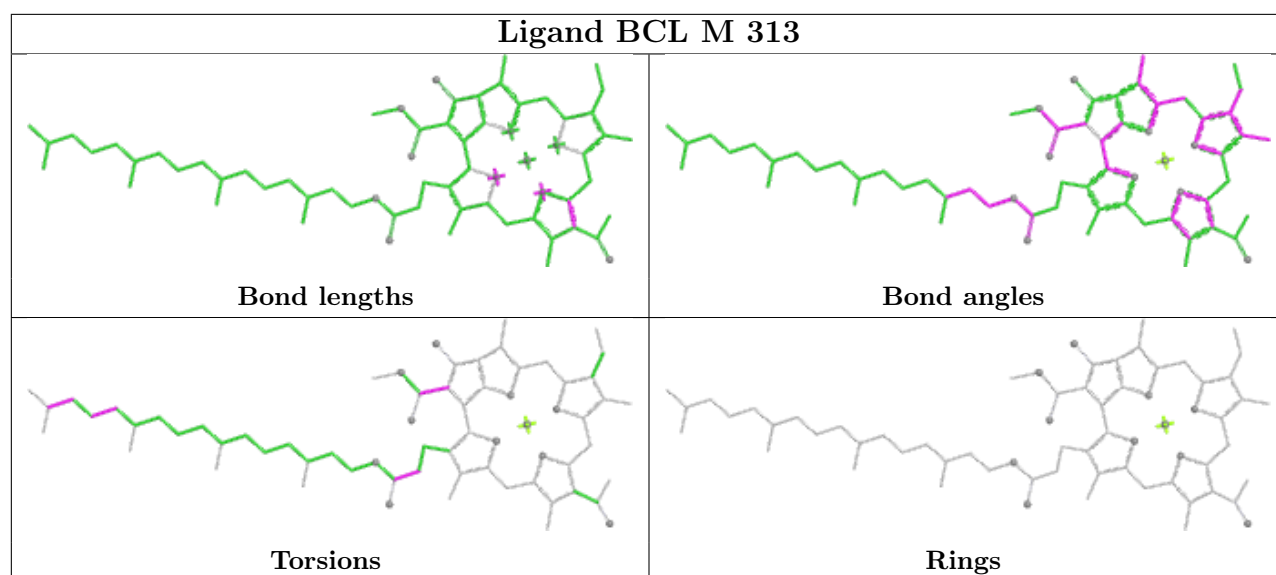
There are no ring outliers.

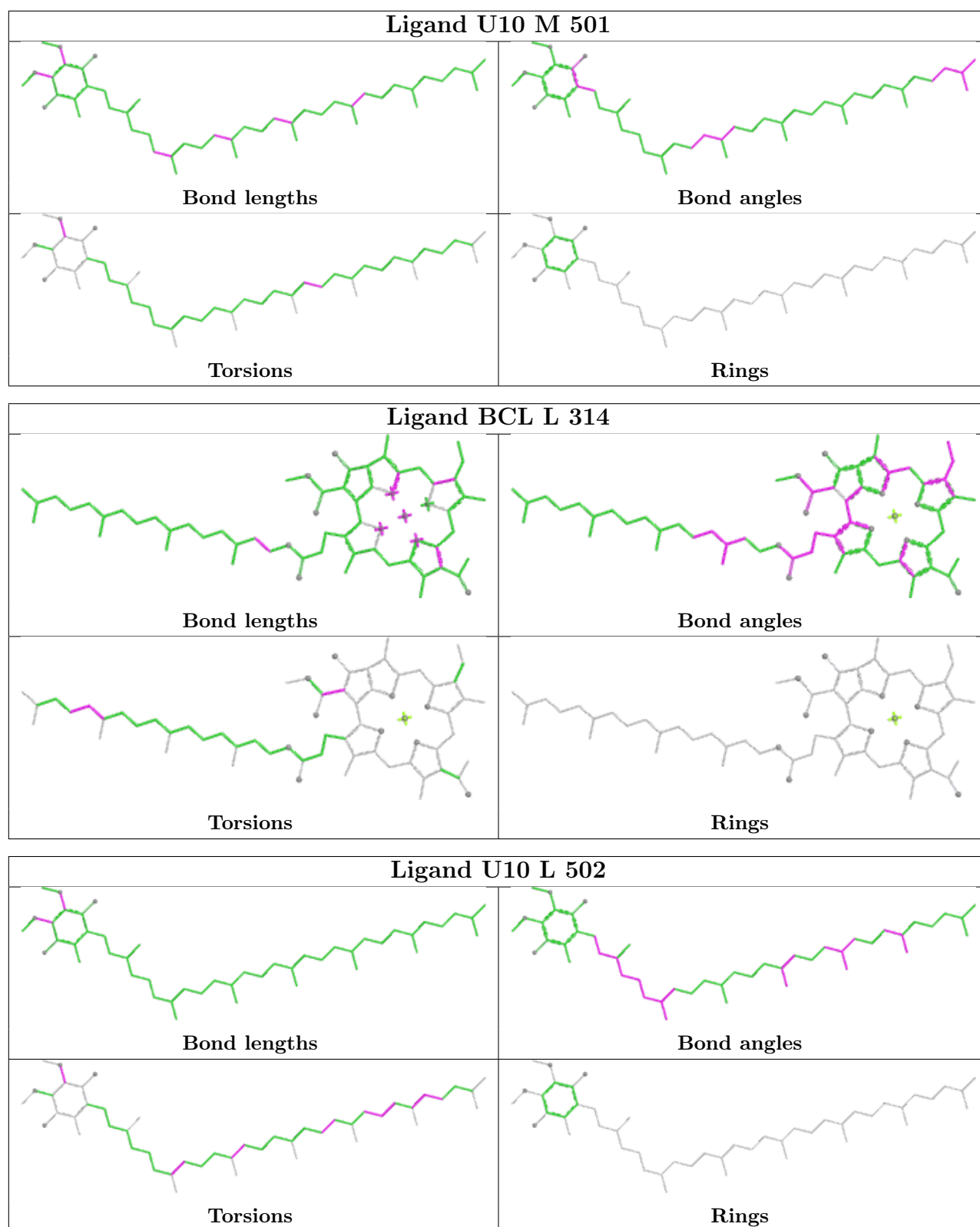
16 monomers are involved in 67 short contacts:

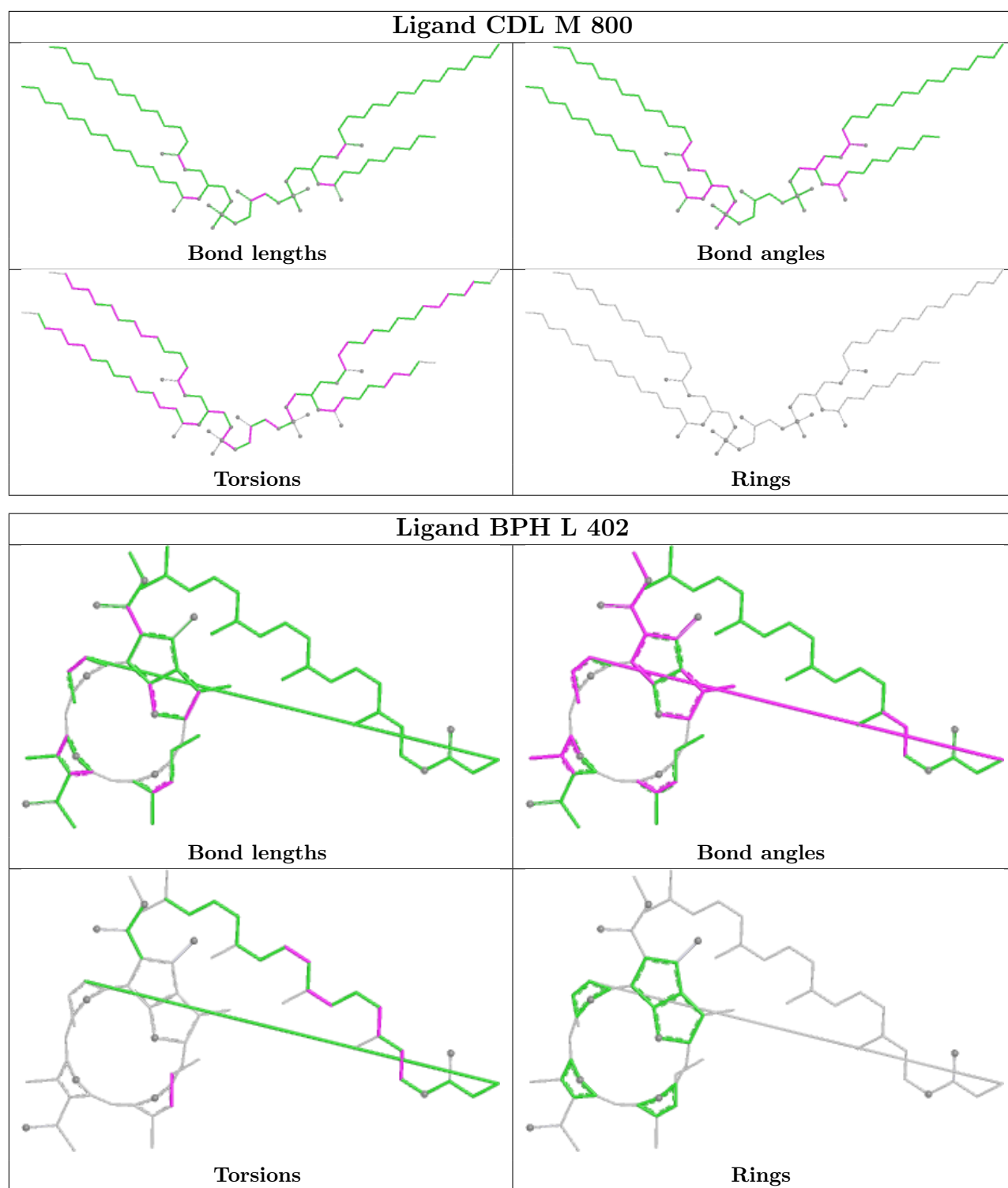
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	920	LDA	12	0
12	M	901	LDA	7	0
4	L	312	BCL	10	0
4	M	311	BCL	12	0
12	M	903	LDA	5	0
12	M	907	LDA	1	0
11	M	802	PS2	4	0
4	M	313	BCL	4	0
12	M	906	LDA	2	0
13	M	704	GOL	2	0
5	M	401	BPH	3	0
6	M	501	U10	4	0
4	L	314	BCL	3	0
6	L	502	U10	3	0
10	M	800	CDL	3	0
5	L	402	BPH	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.15	10 (3%) 46 26	32, 70, 78, 86	3 (1%)
2	M	302/307 (98%)	0.01	6 (1%) 65 41	34, 69, 78, 113	5 (1%)
3	H	241/260 (92%)	0.03	6 (2%) 58 35	49, 69, 80, 100	5 (2%)
All	All	824/848 (97%)	0.06	22 (2%) 56 33	32, 69, 78, 113	13 (1%)

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.0
1	L	202	LYS	4.0
2	M	2	GLU	3.3
2	M	3	TYR	3.3
2	M	302	GLY	2.9

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](#)

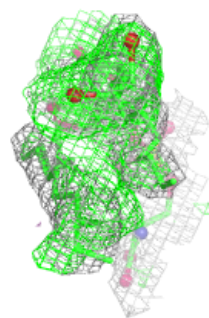
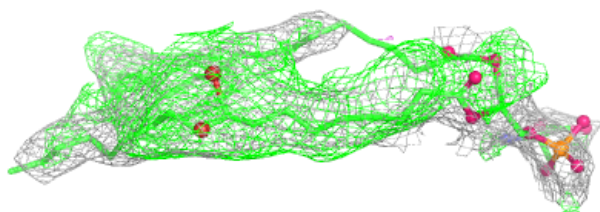
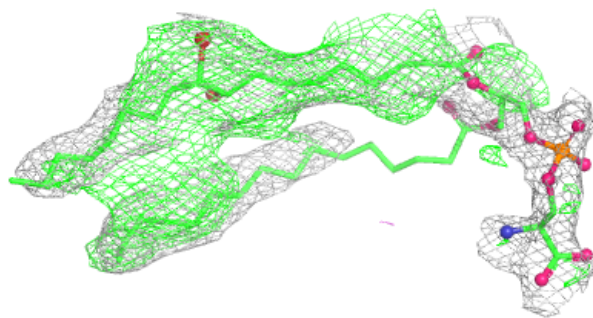
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists 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
9	HTO	M	703	10/10	0.54	0.55	58,61,63,63	10
13	GOL	H	705	6/6	0.77	0.23	56,58,60,61	6
13	GOL	M	704	6/6	0.78	0.62	68,71,72,74	6
11	PS2	M	802	54/54	0.83	0.36	48,62,75,77	54
12	LDA	H	904	16/16	0.84	0.39	53,57,61,62	16
10	CDL	M	800	81/100	0.86	0.26	57,70,81,82	81
12	LDA	H	902	16/16	0.87	0.35	55,59,73,73	16
12	LDA	M	907	16/16	0.89	0.30	63,67,78,78	16
12	LDA	H	905	16/16	0.89	0.40	65,69,74,75	16
8	PO4	M	702	5/5	0.90	0.17	64,66,68,68	5
6	U10	L	502	48/63	0.91	0.31	52,57,69,71	48
6	U10	M	501	48/63	0.91	0.17	64,72,91,92	0
12	LDA	M	906	16/16	0.92	0.29	57,61,68,70	16
12	LDA	M	901	16/16	0.92	0.18	67,70,73,74	16
12	LDA	M	920	16/16	0.92	0.29	65,70,85,87	16
12	LDA	M	903	16/16	0.92	0.22	41,60,71,72	16
4	BCL	M	311	66/66	0.93	0.14	52,66,113,114	0
8	PO4	M	701	5/5	0.93	0.08	61,62,63,64	5
5	BPH	M	401	65/65	0.94	0.12	61,71,110,111	0
4	BCL	L	312	66/66	0.96	0.11	60,66,77,82	0
4	BCL	M	313	66/66	0.96	0.11	55,65,80,84	0
5	BPH	L	402	65/65	0.96	0.11	61,71,74,75	0
4	BCL	L	314	66/66	0.97	0.08	62,69,74,78	0
14	K	H	700	1/1	0.97	0.05	63,63,63,63	0
7	FE	M	500	1/1	1.00	0.03	70,70,70,70	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.

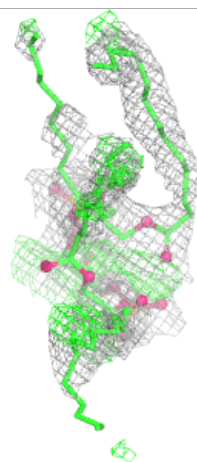
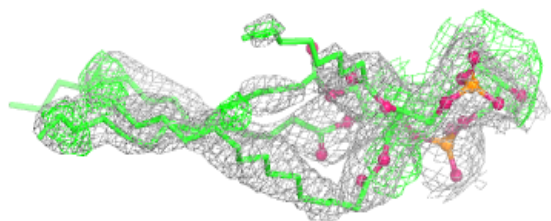
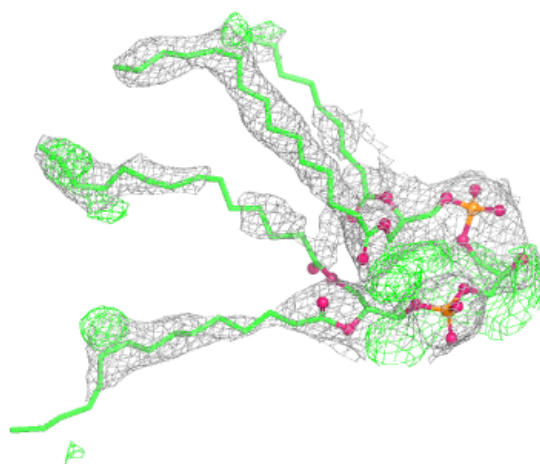
Electron density around PS2 M 802:

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



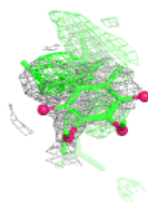
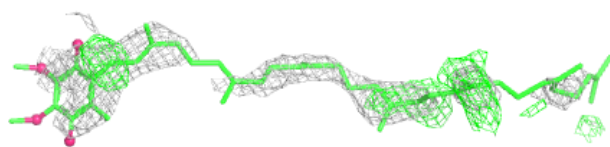
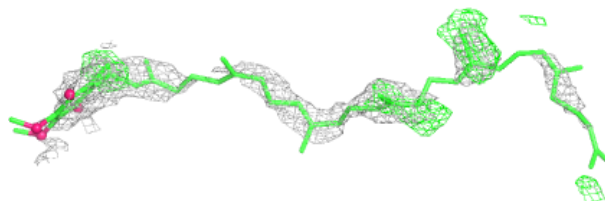
Electron density around CDL M 800:

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

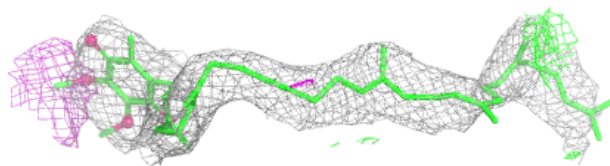
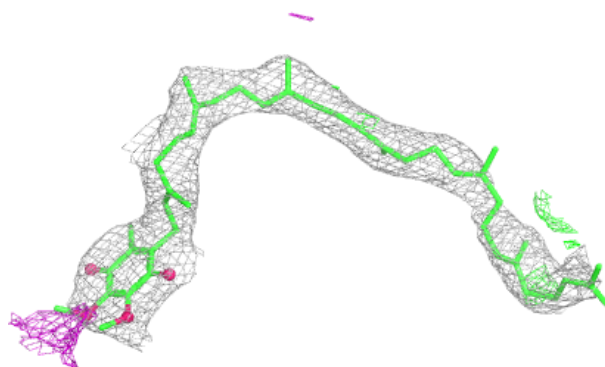


Electron density around U10 L 502:

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

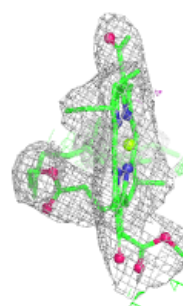
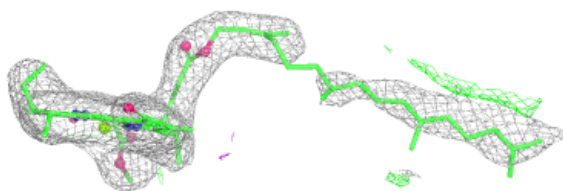
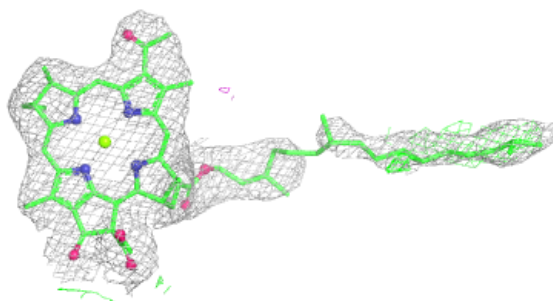
**Electron density around U10 M 501:**

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

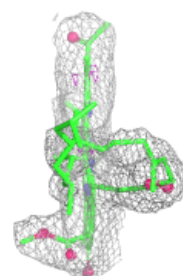
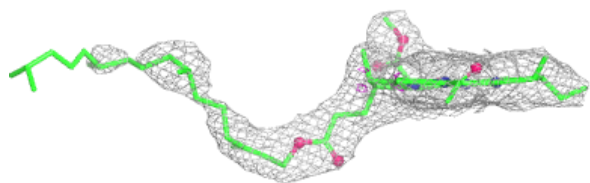
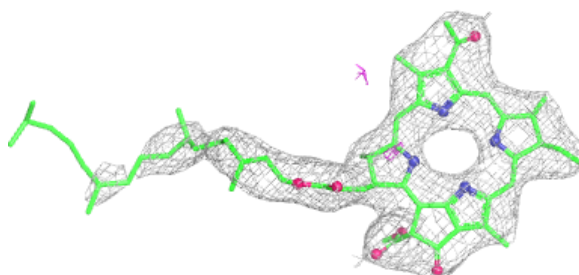


Electron density around BCL M 311:

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

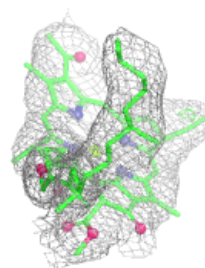
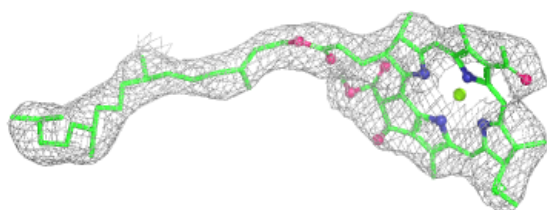
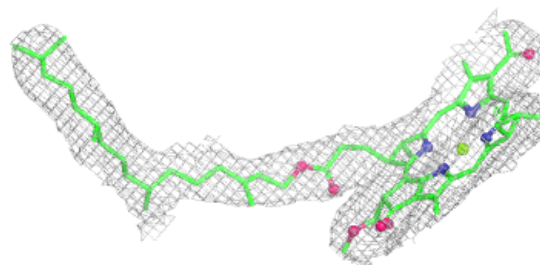
**Electron density around BPH M 401:**

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

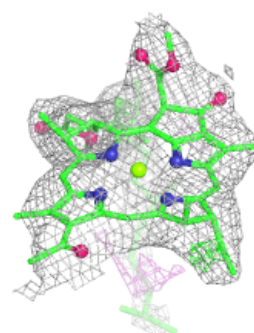
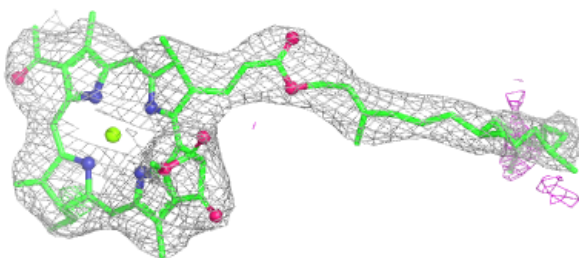
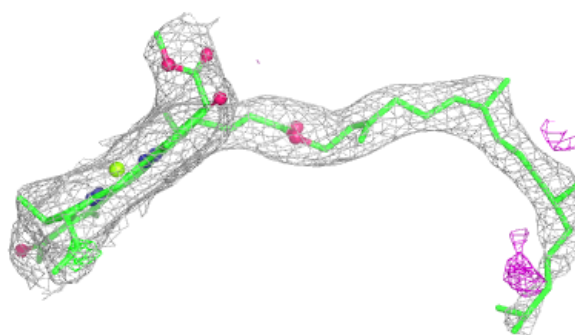


Electron density around BCL L 312:

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

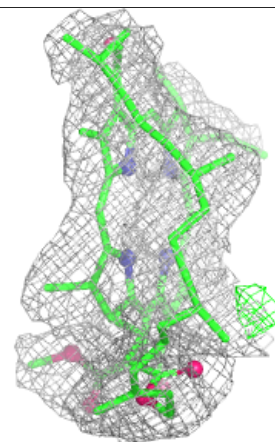
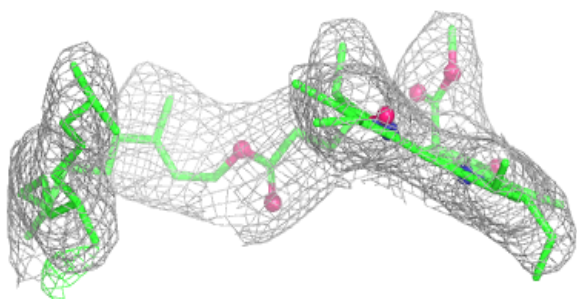
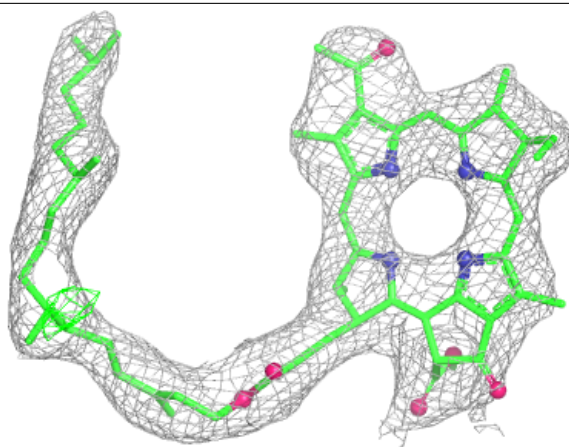
**Electron density around BCL M 313:**

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



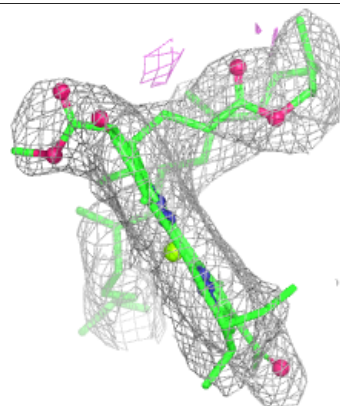
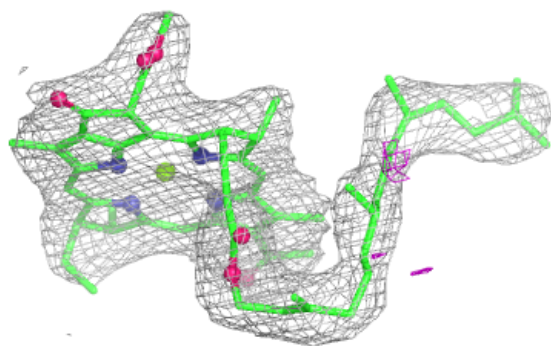
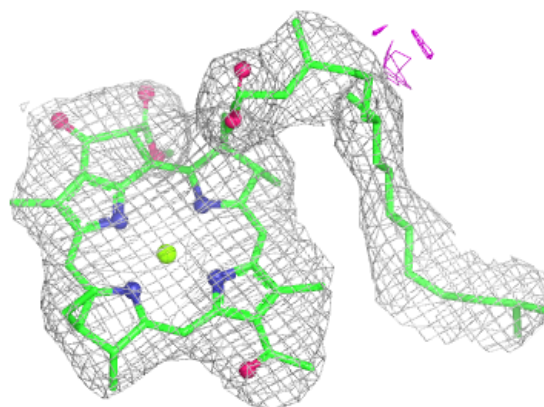
Electron density around BPH L 402:

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



Electron density around BCL L 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.