



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 06:49 AM EDT

PDB ID : 7MHA / pdb_00007mha
Title : Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant;
W252V mutant
Authors : Boxer, S.G.; Mathews, I.I.; Weaver, J.B.
Deposited on : 2021-04-14
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

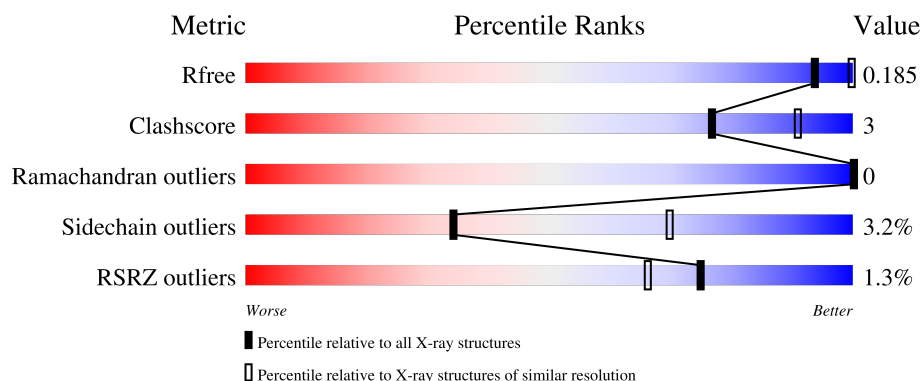
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	H	266	83% 6% 10%
2	L	282	94% 6%
3	M	308	90% 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
5	BPH	L	305	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	239	Total	C	N	O	S	0	0	0
			1823	1166	313	335	9			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	260	VAL	-	expression tag	UNP P0C0Y7
H	261	HIS	-	expression tag	UNP P0C0Y7
H	262	HIS	-	expression tag	UNP P0C0Y7
H	263	HIS	-	expression tag	UNP P0C0Y7
H	264	HIS	-	expression tag	UNP P0C0Y7
H	265	HIS	-	expression tag	UNP P0C0Y7
H	266	HIS	-	expression tag	UNP P0C0Y7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	1	0
			2240	1513	356	363	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	0	0
			2396	1598	392	396	10			

There is a discrepancy between the modelled and reference sequences:

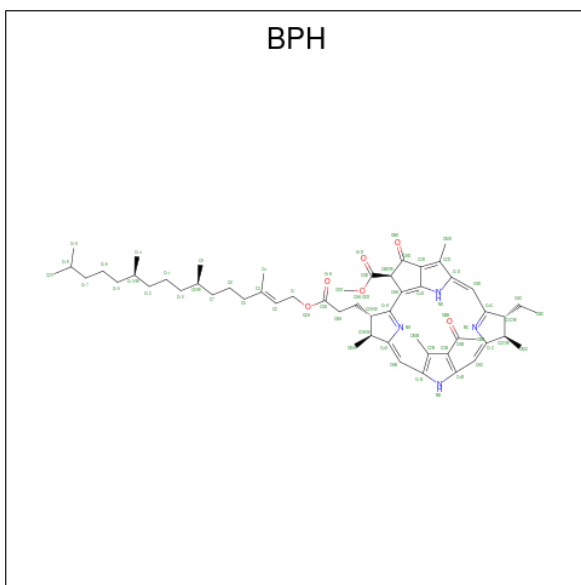
Chain	Residue	Modelled	Actual	Comment	Reference
M	252	VAL	TRP	engineered mutation	UNP P0C0Y9

- Molecule 4 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆)

BCL

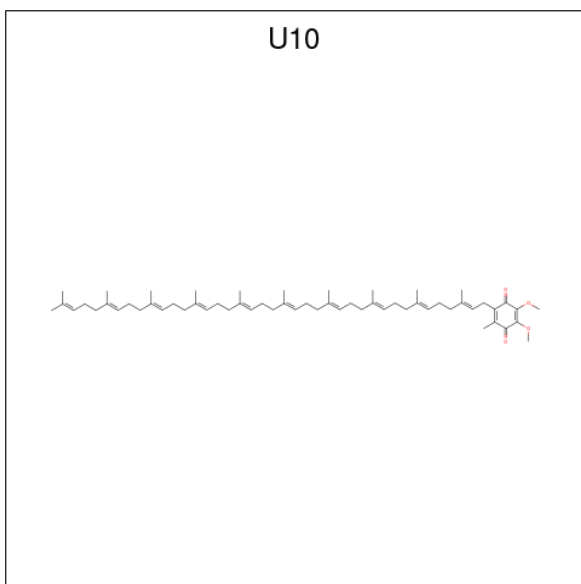
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	L	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 6 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

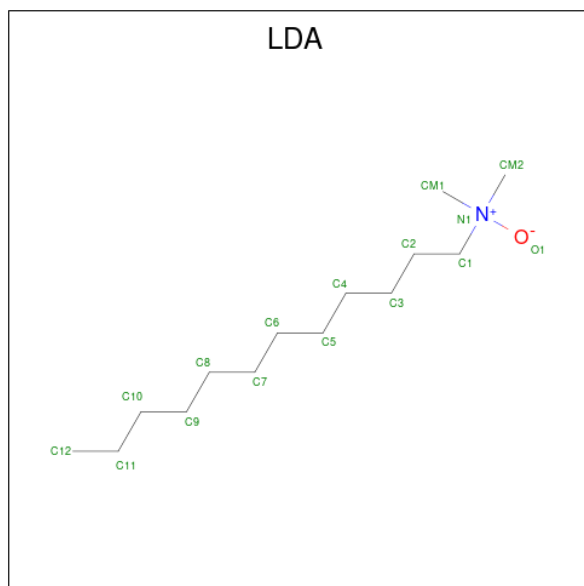


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total Cl 1 1	0	0

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

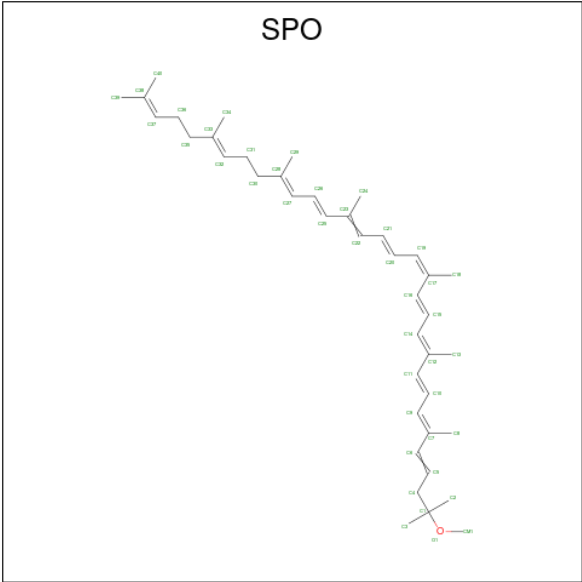


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total C N O 16 14 1 1	0	0
8	M	1	Total C N O 16 14 1 1	0	0
8	M	1	Total C N O 16 14 1 1	0	0

- Molecule 9 is FE (III) ION (CCD ID: FE) (formula: Fe).

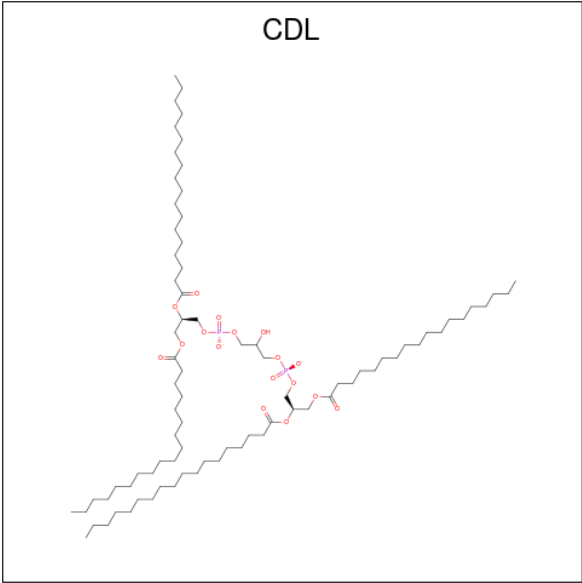
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O).



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

- Molecule 11 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			69	50	17	2		

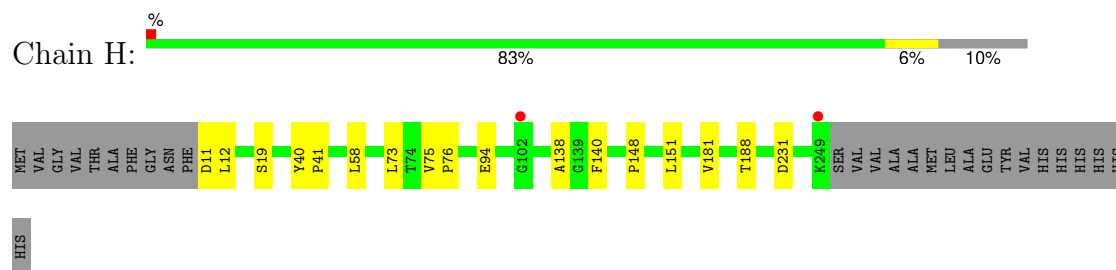
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	70	Total 70	O 70	0	0
12	L	39	Total 39	O 39	0	0
12	M	61	Total 62	O 62	0	1

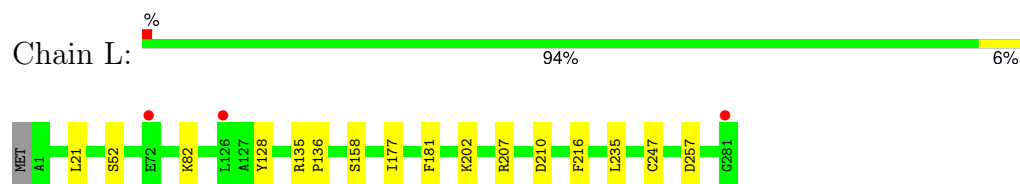
3 Residue-property plots [i](#)

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

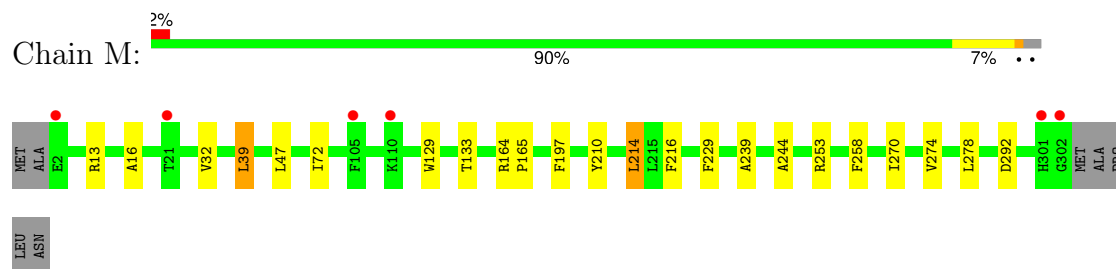
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.19Å 142.19Å 187.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.19 – 2.79 39.19 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.19-2.79) 99.9 (39.19-2.79)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.156 , 0.178 0.164 , 0.185	Depositor DCC
R_{free} test set	2643 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7178	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: CL, LDA, SPO, BCL, CDL, FE, BPH, 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	H	0.99	0/1871	1.34	0/2545
2	L	0.98	0/2328	1.39	1/3186 (0.0%)
3	M	0.97	0/2486	1.44	1/3393 (0.0%)
All	All	0.98	0/6685	1.40	2/9124 (0.0%)

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
1	H	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	292	ASP	CB-CA-C	-6.99	98.97	110.85
2	L	216	PHE	CA-CB-CG	-5.33	108.47	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	138	ALA	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	H	1823	0	1831	7	0
2	L	2240	0	2197	7	0
3	M	2396	0	2312	16	0
4	L	132	0	148	5	0
4	M	117	0	115	8	0
5	L	120	0	129	8	0
6	L	18	0	15	0	0
7	L	1	0	0	0	0
8	M	48	0	93	0	0
9	M	1	0	0	0	0
10	M	42	0	60	0	0
11	M	69	0	82	0	0
12	H	70	0	0	0	0
12	L	39	0	0	1	0
12	M	62	0	0	2	0
All	All	7178	0	6982	40	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 3.

All (40) 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)
4:L:301:BCL:HBB2	4:L:301:BCL:HHC	1.66	0.77
5:L:302:BPH:HBB3	5:L:302:BPH:HHC	1.65	0.76
5:L:302:BPH:HBB2	3:M:210:TYR:HB3	1.67	0.75
4:M:401:BCL:HBB2	4:M:401:BCL:HHC	1.79	0.64
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.86	0.58
3:M:197:PHE:CZ	4:M:402:BCL:HBB2	2.41	0.56
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.88	0.55
3:M:214:LEU:C	3:M:214:LEU:HD12	2.34	0.53
2:L:181:PHE:HB3	5:L:305:BPH:CBB	2.39	0.52
2:L:181:PHE:CD2	5:L:305:BPH:HBB1	2.45	0.52
1:H:140:PHE:HA	3:M:13:ARG:O	2.10	0.52
3:M:197:PHE:HZ	4:M:402:BCL:HBB2	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:181:PHE:HB3	5:L:305:BPH:HBB2	1.91	0.51
3:M:270:ILE:O	3:M:274:VAL:HG13	2.10	0.51
5:L:302:BPH:HBB1	3:M:210:TYR:CD2	2.46	0.51
4:M:401:BCL:HHC	4:M:401:BCL:CBB	2.41	0.50
4:M:401:BCL:HBB3	4:M:402:BCL:H41	1.95	0.49
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.96	0.48
2:L:128:TYR:HD1	4:L:301:BCL:HBB1	1.78	0.48
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.95	0.47
1:H:181:VAL:O	1:H:188:THR:HA	2.15	0.47
4:L:301:BCL:HHC	4:L:301:BCL:CBB	2.41	0.47
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.97	0.47
2:L:177:ILE:HD13	4:M:401:BCL:HMD2	1.97	0.46
5:L:305:BPH:HHC	5:L:305:BPH:HBB3	1.96	0.46
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.46
4:L:304:BCL:HMB3	4:L:304:BCL:CBB	2.45	0.46
3:M:253:ARG:NE	12:M:501:HOH:O	2.28	0.45
3:M:214:LEU:HD12	3:M:214:LEU:O	2.16	0.45
4:M:402:BCL:CBB	4:M:402:BCL:HHC	2.48	0.44
5:L:302:BPH:HHC	5:L:302:BPH:CBB	2.41	0.44
4:M:402:BCL:HAA2	4:M:402:BCL:HBD	1.99	0.43
3:M:253:ARG:NH1	12:M:501:HOH:O	2.48	0.42
1:H:58:LEU:HD23	1:H:58:LEU:HA	1.93	0.41
4:L:304:BCL:HHC	4:L:304:BCL:OBB	2.20	0.41
3:M:129:TRP:O	3:M:133:THR:HG23	2.20	0.41
1:H:73:LEU:HD22	3:M:239:ALA:O	2.21	0.41
3:M:39:LEU:HD12	3:M:39:LEU:HA	1.90	0.41
1:H:40:TYR:HA	1:H:41:PRO:C	2.45	0.41
2:L:257:ASP:HB3	12:L:422:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	237/266 (89%)	234 (99%)	3 (1%)	0	100	100
2	L	280/282 (99%)	272 (97%)	8 (3%)	0	100	100
3	M	299/308 (97%)	285 (95%)	14 (5%)	0	100	100
All	All	816/856 (95%)	791 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	H	194/215 (90%)	189 (97%)	5 (3%)	40	75
2	L	221/221 (100%)	212 (96%)	9 (4%)	27	62
3	M	236/241 (98%)	229 (97%)	7 (3%)	36	72
All	All	651/677 (96%)	630 (97%)	21 (3%)	34	70

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	12	LEU
1	H	19	SER
1	H	94	GLU
1	H	231	ASP
2	L	21	LEU
2	L	52	SER
2	L	82	LYS
2	L	158	SER
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	235	LEU
2	L	247	CYS
3	M	39	LEU

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Mol	Chain	Res	Type
3	M	47	LEU
3	M	72	ILE
3	M	214	LEU
3	M	216	PHE
3	M	258	PHE
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	183	ASN
2	L	258	GLN
3	M	4	GLN
3	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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
8	LDA	M	405	-	13,15,15	0.20	0	14,17,17	0.16	0
4	BCL	M	402	3	69,74,74	1.71	12 (17%)	79,115,115	2.16	23 (29%)
4	BCL	L	304	2	69,74,74	1.67	14 (20%)	79,115,115	2.07	20 (25%)
5	BPH	L	305	-	49,60,70	0.93	2 (4%)	47,89,101	1.27	3 (6%)
4	BCL	M	401	3	54,59,74	1.94	15 (27%)	61,97,115	2.27	20 (32%)
5	BPH	L	302	-	59,70,70	0.84	2 (3%)	59,101,101	1.07	2 (3%)
8	LDA	M	403	-	13,15,15	0.19	0	14,17,17	0.29	0
4	BCL	L	301	2	69,74,74	1.67	16 (23%)	79,115,115	2.16	21 (26%)
11	CDL	M	408	-	68,68,99	0.43	0	74,80,111	0.47	0
8	LDA	M	404	-	13,15,15	0.16	0	14,17,17	0.30	0
10	SPO	M	407	-	41,41,41	1.24	5 (12%)	47,50,50	1.17	3 (6%)
6	U10	L	303	-	18,18,63	1.05	2 (11%)	24,25,79	1.08	2 (8%)

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
8	LDA	M	405	-	-	5/13/13/13	-
4	BCL	M	402	3	-	4/41/137/137	-
4	BCL	L	304	2	-	5/41/137/137	-
5	BPH	L	305	-	1/1/16/22	11/25/93/105	0/5/6/6
4	BCL	M	401	3	-	3/23/119/137	-
5	BPH	L	302	-	-	6/37/105/105	0/5/6/6
8	LDA	M	403	-	-	3/13/13/13	-
4	BCL	L	301	2	-	10/41/137/137	-
11	CDL	M	408	-	-	18/79/79/110	-
8	LDA	M	404	-	-	4/13/13/13	-
10	SPO	M	407	-	-	6/47/47/47	-
6	U10	L	303	-	-	6/9/33/87	0/1/1/1

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	402	BCL	O2D-CGD	5.06	1.45	1.33
4	L	304	BCL	O2D-CGD	5.04	1.45	1.33
4	M	401	BCL	O2A-CGA	4.73	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	301	BCL	O2D-CGD	4.68	1.44	1.33
4	L	304	BCL	C3D-C4D	-4.67	1.33	1.44
4	M	401	BCL	O2D-CGD	4.55	1.44	1.33
4	M	401	BCL	C3D-C4D	-4.43	1.34	1.44
4	M	402	BCL	C3D-C4D	-4.38	1.34	1.44
4	M	402	BCL	C3B-C4B	4.29	1.49	1.41
4	M	402	BCL	OBD-CAD	4.28	1.29	1.22
4	L	301	BCL	C3D-C4D	-4.23	1.34	1.44
4	L	301	BCL	O2A-CGA	4.18	1.45	1.33
4	M	401	BCL	CHB-C1B	4.05	1.48	1.39
4	L	304	BCL	OBD-CAD	4.00	1.29	1.22
4	L	304	BCL	O2A-CGA	3.90	1.44	1.33
4	L	301	BCL	CHB-C1B	3.88	1.48	1.39
4	M	401	BCL	C3B-C4B	3.82	1.48	1.41
5	L	305	BPH	C4D-CHA	3.62	1.45	1.39
4	M	401	BCL	CHC-C4B	3.57	1.47	1.39
4	M	402	BCL	O2A-CGA	3.53	1.43	1.33
4	L	304	BCL	C3B-C4B	3.36	1.47	1.41
4	L	301	BCL	C3B-C4B	3.36	1.47	1.41
4	M	401	BCL	CHD-C1D	3.33	1.44	1.38
5	L	302	BPH	C4D-CHA	3.32	1.44	1.39
4	L	304	BCL	CHC-C4B	3.31	1.46	1.39
4	L	301	BCL	OBD-CAD	3.30	1.28	1.22
5	L	302	BPH	C1B-C2B	3.29	1.43	1.39
4	L	304	BCL	CHB-C1B	3.25	1.46	1.39
4	M	401	BCL	OBD-CAD	3.23	1.28	1.22
4	L	304	BCL	C1D-ND	-3.19	1.33	1.37
4	M	402	BCL	CHB-C1B	3.13	1.46	1.39
5	L	305	BPH	C1B-C2B	3.12	1.43	1.39
4	M	401	BCL	C3D-C2D	3.08	1.47	1.39
4	L	301	BCL	CHC-C4B	3.08	1.46	1.39
4	M	402	BCL	CHC-C4B	3.05	1.46	1.39
4	M	402	BCL	CHD-C1D	3.00	1.44	1.38
4	M	402	BCL	C3D-C2D	2.89	1.46	1.39
4	L	301	BCL	C3D-C2D	2.88	1.46	1.39
6	L	303	U10	C6-C1	2.87	1.40	1.35
4	L	301	BCL	CHD-C1D	2.87	1.44	1.38
4	M	401	BCL	CHD-C4C	2.86	1.47	1.39
10	M	407	SPO	C16-C17	-2.79	1.40	1.46
10	M	407	SPO	C11-C12	-2.73	1.40	1.46
4	M	402	BCL	C1D-ND	-2.72	1.34	1.37
4	L	304	BCL	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	304	BCL	C3D-C2D	2.65	1.46	1.39
4	L	304	BCL	CHD-C1D	2.51	1.43	1.38
4	L	301	BCL	C1D-ND	-2.51	1.34	1.37
4	L	301	BCL	MG-NA	-2.48	2.00	2.06
4	L	301	BCL	C1B-C2B	2.47	1.48	1.43
4	L	304	BCL	C4B-NB	-2.45	1.34	1.37
4	M	401	BCL	C1D-ND	-2.44	1.34	1.37
4	L	304	BCL	CHD-C4C	2.43	1.46	1.39
4	M	402	BCL	CHD-C4C	2.41	1.46	1.39
10	M	407	SPO	C25-C23	-2.39	1.40	1.46
4	L	301	BCL	C4B-NB	-2.38	1.34	1.37
10	M	407	SPO	C6-C7	-2.32	1.41	1.46
4	M	401	BCL	C1B-C2B	2.29	1.48	1.43
10	M	407	SPO	C9-C7	2.24	1.41	1.35
4	L	301	BCL	C1B-NB	-2.21	1.35	1.37
4	L	304	BCL	C4D-CHA	2.20	1.46	1.38
4	L	301	BCL	CHD-C4C	2.19	1.45	1.39
4	L	301	BCL	MG-NC	-2.16	2.01	2.06
6	L	303	U10	C3-C2	-2.15	1.42	1.48
4	M	401	BCL	C1D-C2D	2.15	1.49	1.45
4	M	401	BCL	C4B-NB	-2.13	1.35	1.37
4	M	402	BCL	C1B-C2B	2.06	1.48	1.43
4	M	401	BCL	C4D-CHA	2.05	1.45	1.38

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	304	BCL	CMD-C2D-C1D	7.38	137.72	124.73
4	M	402	BCL	CMD-C2D-C1D	7.27	137.53	124.73
4	M	401	BCL	CMD-C2D-C1D	7.20	137.40	124.73
4	L	301	BCL	CMD-C2D-C1D	6.40	136.00	124.73
4	L	301	BCL	O2D-CGD-CBD	5.97	121.66	111.23
4	M	402	BCL	C2B-C1B-NB	5.52	116.05	110.33
4	L	304	BCL	C2B-C1B-NB	5.32	115.85	110.33
5	L	302	BPH	C4D-CHA-CBD	-5.14	105.99	108.45
4	M	401	BCL	O2D-CGD-CBD	5.01	119.98	111.23
4	M	401	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
5	L	305	BPH	C4D-CHA-CBD	-4.84	106.13	108.45
4	L	304	BCL	C3D-C2D-C1D	-4.80	99.27	105.83
4	L	301	BCL	C3D-C2D-C1D	-4.75	99.34	105.83
4	M	401	BCL	CHD-C1D-ND	-4.75	118.12	124.80
4	L	301	BCL	C2B-C1B-NB	4.67	115.17	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	402	BCL	C3D-C2D-C1D	-4.66	99.48	105.83
4	M	402	BCL	CHD-C1D-ND	-4.64	118.27	124.80
4	M	402	BCL	C3C-C4C-CHD	-4.60	113.70	123.39
4	L	301	BCL	C3C-C4C-CHD	-4.51	113.88	123.39
4	L	304	BCL	CHD-C1D-ND	-4.46	118.53	124.80
4	L	301	BCL	C1C-NC-C4C	-4.45	104.65	106.68
4	L	304	BCL	C3C-C4C-CHD	-4.27	114.39	123.39
4	L	301	BCL	CHD-C1D-ND	-4.25	118.82	124.80
4	M	401	BCL	C3C-C4C-CHD	-4.24	114.46	123.39
4	L	304	BCL	C2D-C1D-ND	4.22	114.30	110.13
4	M	401	BCL	C2B-C1B-NB	4.21	114.69	110.33
4	M	401	BCL	C1C-NC-C4C	-4.13	104.79	106.68
4	L	301	BCL	C2D-C1D-ND	4.08	114.17	110.13
4	L	304	BCL	C1D-ND-C4D	-4.04	103.48	106.31
4	M	402	BCL	O2D-CGD-CBD	4.01	118.25	111.23
4	M	402	BCL	C2D-C1D-ND	4.01	114.10	110.13
4	M	402	BCL	C1D-ND-C4D	-3.98	103.52	106.31
5	L	305	BPH	C2B-C1B-NB	-3.98	106.56	109.43
4	L	301	BCL	C1D-ND-C4D	-3.94	103.55	106.31
4	M	401	BCL	C2D-C1D-ND	3.87	113.95	110.13
4	L	301	BCL	O2D-CGD-O1D	-3.78	116.50	123.85
4	L	301	BCL	C3B-C4B-NB	3.71	114.65	109.76
4	M	401	BCL	C1-O2A-CGA	3.65	125.48	116.65
5	L	302	BPH	C2B-C1B-NB	-3.65	106.79	109.43
4	L	304	BCL	C3B-C4B-NB	3.63	114.55	109.76
4	M	401	BCL	C1D-ND-C4D	-3.63	103.77	106.31
4	M	402	BCL	O2D-CGD-O1D	-3.53	116.98	123.85
4	M	402	BCL	CHC-C1C-NC	3.40	129.31	124.40
4	L	304	BCL	C1C-NC-C4C	-3.27	105.19	106.68
4	M	402	BCL	C3D-C4D-ND	3.23	115.24	109.99
4	L	304	BCL	O2A-CGA-O1A	-3.20	115.62	123.63
4	L	304	BCL	CHB-C4A-NA	3.16	128.96	124.40
5	L	305	BPH	C1A-C2A-C3A	-3.16	99.83	102.84
4	L	301	BCL	C3D-C4D-ND	3.15	115.11	109.99
4	L	304	BCL	CMB-C2B-C1B	3.11	130.16	125.42
4	L	301	BCL	C1D-CHD-C4C	-3.11	119.13	126.62
4	M	402	BCL	C4A-NA-C1A	3.10	108.09	106.68
4	M	401	BCL	C3D-C4D-ND	3.09	115.00	109.99
4	L	301	BCL	CHC-C1C-NC	3.04	128.79	124.40
4	M	402	BCL	CED-O2D-CGD	3.03	122.79	115.92
4	L	304	BCL	O2A-CGA-CBA	3.02	121.05	111.83
4	L	304	BCL	C4-C3-C5	3.00	120.43	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	402	BCL	CHB-C4A-NA	3.00	128.73	124.40
4	M	402	BCL	O2A-CGA-CBA	2.99	120.96	111.83
4	L	304	BCL	C3D-C4D-ND	2.97	114.82	109.99
10	M	407	SPO	C10-C9-C7	2.97	131.44	127.28
4	M	402	BCL	C1C-NC-C4C	-2.91	105.35	106.68
4	M	402	BCL	C1D-CHD-C4C	-2.91	119.61	126.62
4	L	304	BCL	C1D-CHD-C4C	-2.84	119.78	126.62
4	L	301	BCL	C4-C3-C5	2.84	120.15	115.23
4	M	402	BCL	C3B-C4B-NB	2.83	113.50	109.76
4	L	301	BCL	CHB-C4A-NA	2.79	128.42	124.40
4	M	402	BCL	C1-C2-C3	-2.66	121.83	126.20
4	M	402	BCL	O2A-CGA-O1A	-2.65	117.00	123.63
6	L	303	U10	C7-C6-C1	-2.60	120.44	124.89
4	L	304	BCL	CHC-C1C-NC	2.54	128.06	124.40
4	M	402	BCL	CHB-C1B-C2B	-2.51	120.13	127.43
4	M	401	BCL	C1D-CHD-C4C	-2.50	120.58	126.62
4	L	301	BCL	C4A-NA-C1A	2.49	107.81	106.68
4	M	401	BCL	CHB-C4A-NA	2.46	127.95	124.40
4	L	301	BCL	CMB-C2B-C1B	2.45	129.15	125.42
4	M	401	BCL	C3B-C4B-NB	2.40	112.93	109.76
4	M	402	BCL	CHC-C4B-NB	-2.40	120.45	124.05
4	L	301	BCL	C1-O2A-CGA	2.35	122.34	116.65
4	L	304	BCL	CHC-C4B-C3B	-2.20	123.00	131.72
4	M	401	BCL	CMB-C2B-C1B	2.18	128.73	125.42
4	M	401	BCL	C1-C2-C3	-2.17	123.26	126.76
4	L	304	BCL	C2A-C1A-CHA	-2.15	120.13	123.87
6	L	303	U10	C7-C6-C5	2.14	121.01	118.52
4	M	401	BCL	O1D-CGD-CBD	-2.14	120.30	124.52
4	M	401	BCL	CHC-C1C-NC	2.13	127.47	124.40
4	L	301	BCL	C6-C5-C3	-2.13	108.29	113.47
4	M	401	BCL	O2D-CGD-O1D	-2.12	119.71	123.85
4	L	301	BCL	CHC-C4B-NB	-2.12	120.87	124.05
4	M	401	BCL	O2A-CGA-CBA	2.08	118.18	111.83
4	L	304	BCL	CMD-C2D-C3D	-2.05	123.00	127.69
4	M	402	BCL	CMD-C2D-C3D	-2.05	123.00	127.69
10	M	407	SPO	C21-C20-C19	2.04	127.69	123.52
10	M	407	SPO	C13-C12-C14	-2.01	119.56	122.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	305	BPH	C8

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	BCL	CHA-CBD-CGD-O1D
4	L	301	BCL	CHA-CBD-CGD-O2D
5	L	305	BPH	C4C-C3C-CAC-CBC
8	M	404	LDA	N1-C1-C2-C3
10	M	407	SPO	C4-C1-O1-CM1
10	M	407	SPO	C1-C4-C5-C6
11	M	408	CDL	CA3-OA5-PA1-OA2
11	M	408	CDL	CB2-OB2-PB2-OB3
4	L	301	BCL	CBD-CGD-O2D-CED
4	L	301	BCL	O1D-CGD-O2D-CED
6	L	303	U10	C7-C8-C9-C10
6	L	303	U10	C7-C8-C9-C11
11	M	408	CDL	CA7-C31-C32-C33
5	L	305	BPH	C5-C6-C7-C8
11	M	408	CDL	C33-C34-C35-C36
8	M	404	LDA	C1-C2-C3-C4
8	M	405	LDA	C3-C4-C5-C6
8	M	403	LDA	C11-C10-C9-C8
11	M	408	CDL	C39-C40-C41-C42
8	M	405	LDA	C1-C2-C3-C4
11	M	408	CDL	C11-CA5-OA6-CA4
4	M	402	BCL	C13-C15-C16-C17
8	M	403	LDA	C1-C2-C3-C4
8	M	403	LDA	C4-C5-C6-C7
5	L	305	BPH	C2C-C3C-CAC-CBC
11	M	408	CDL	OA7-CA5-OA6-CA4
5	L	305	BPH	CBA-CGA-O2A-C1
5	L	305	BPH	C6-C7-C8-C9
5	L	305	BPH	O1A-CGA-O2A-C1
10	M	407	SPO	C3-C1-O1-CM1
10	M	407	SPO	C34-C33-C35-C36
11	M	408	CDL	C11-C12-C13-C14
4	L	304	BCL	C15-C16-C17-C18
11	M	408	CDL	C72-C73-C74-C75
4	M	402	BCL	C16-C17-C18-C19
5	L	302	BPH	C13-C15-C16-C17
10	M	407	SPO	C32-C33-C35-C36
5	L	302	BPH	C6-C7-C8-C9
8	M	405	LDA	C7-C8-C9-C10
11	M	408	CDL	C36-C37-C38-C39
4	L	301	BCL	C12-C13-C15-C16
6	L	303	U10	C1-C6-C7-C8

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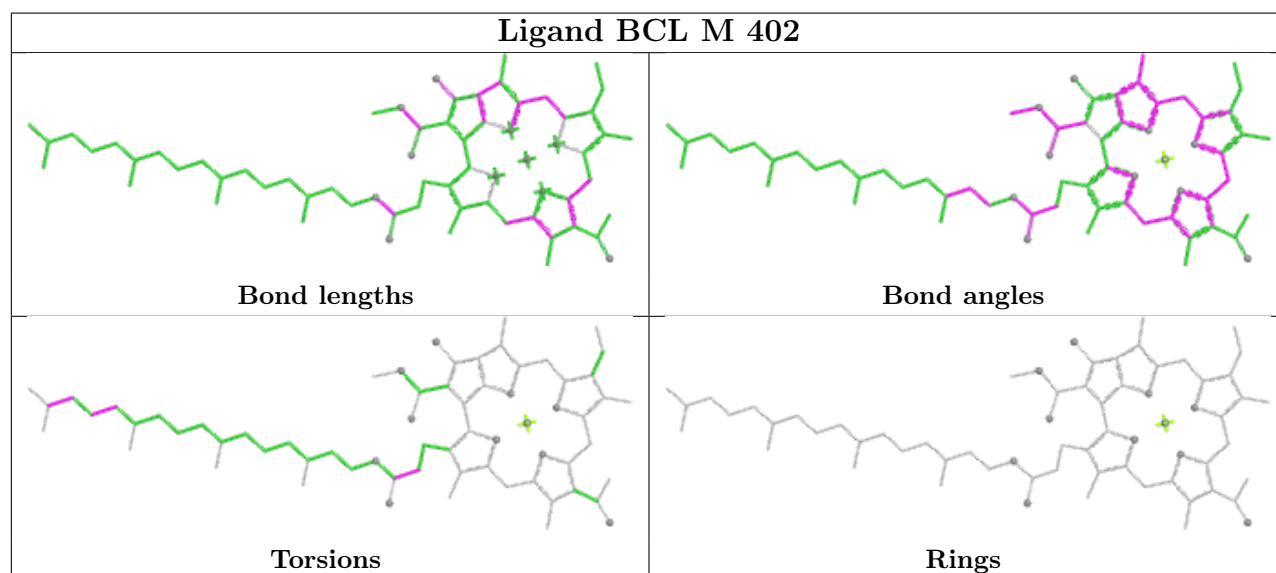
Mol	Chain	Res	Type	Atoms
5	L	302	BPH	C4-C3-C5-C6
5	L	305	BPH	C6-C7-C8-C10
6	L	303	U10	C5-C6-C7-C8
4	L	304	BCL	C16-C17-C18-C20
4	M	402	BCL	C16-C17-C18-C20
4	L	304	BCL	C2A-CAA-CBA-CGA
4	L	301	BCL	C14-C13-C15-C16
11	M	408	CDL	C17-C18-C19-C20
5	L	302	BPH	C2-C3-C5-C6
6	L	303	U10	C5-C4-O4-C4M
4	M	401	BCL	CHA-CBD-CGD-O1D
4	M	401	BCL	CHA-CBD-CGD-O2D
11	M	408	CDL	CA3-OA5-PA1-OA3
11	M	408	CDL	CB2-OB2-PB2-OB4
11	M	408	CDL	CB2-OB2-PB2-OB5
4	L	301	BCL	C2B-C3B-CAB-CBB
4	L	304	BCL	C16-C17-C18-C19
10	M	407	SPO	C2-C1-O1-CM1
5	L	305	BPH	C4-C3-C5-C6
4	L	304	BCL	C13-C15-C16-C17
5	L	302	BPH	C14-C13-C15-C16
4	L	301	BCL	C2B-C3B-CAB-OB
11	M	408	CDL	C13-C14-C15-C16
5	L	305	BPH	C2-C3-C5-C6
8	M	405	LDA	C2-C3-C4-C5
4	M	401	BCL	C4C-C3C-CAC-CBC
8	M	404	LDA	C7-C8-C9-C10
11	M	408	CDL	C74-C75-C76-C77
5	L	305	BPH	C2-C1-O2A-CGA
5	L	302	BPH	O2A-C1-C2-C3
4	L	301	BCL	C13-C15-C16-C17
4	L	301	BCL	C4B-C3B-CAB-CBB
11	M	408	CDL	OA5-CA3-CA4-CA6
6	L	303	U10	C3-C4-O4-C4M
8	M	404	LDA	C5-C6-C7-C8
4	M	402	BCL	CAA-CBA-CGA-O2A
11	M	408	CDL	OA5-CA3-CA4-OA6
8	M	405	LDA	C5-C6-C7-C8
5	L	305	BPH	CAD-CBD-CGD-O2D

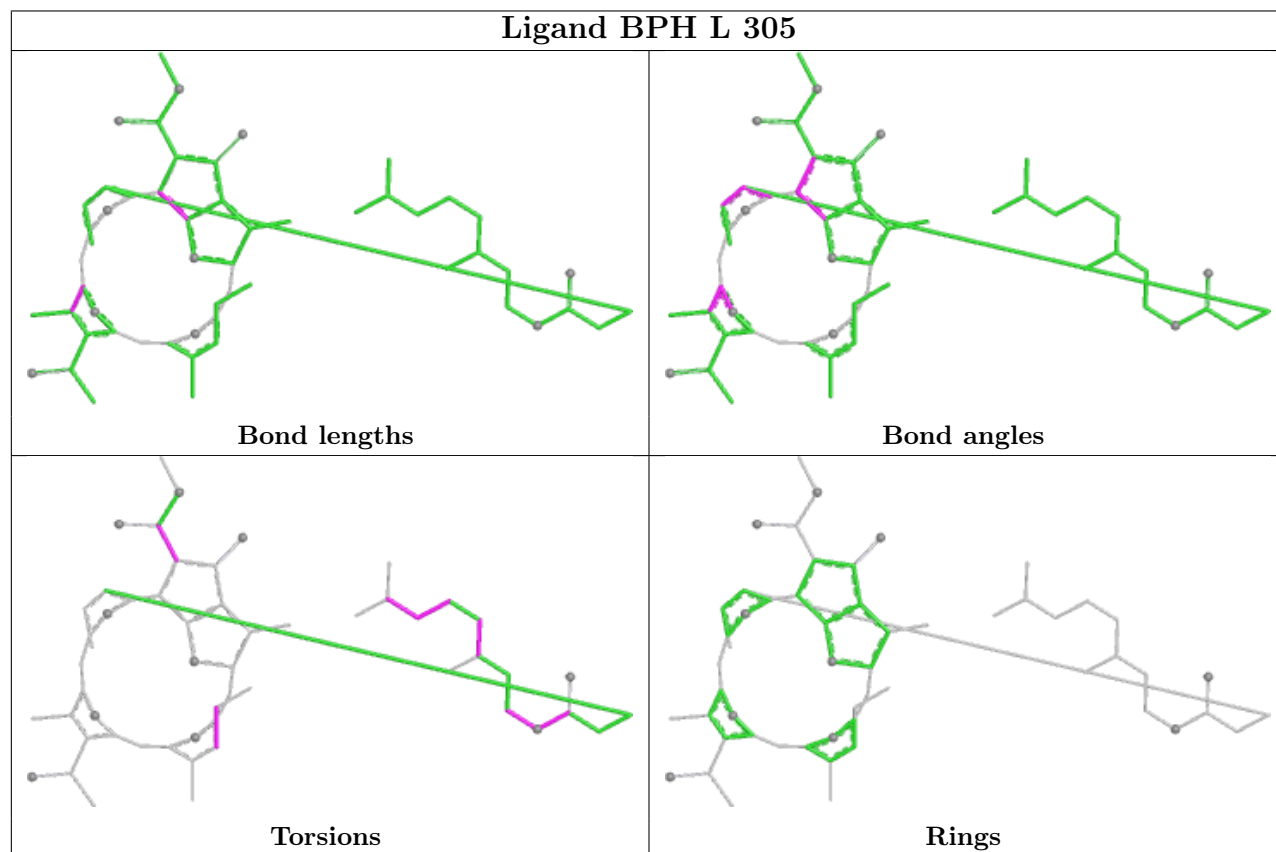
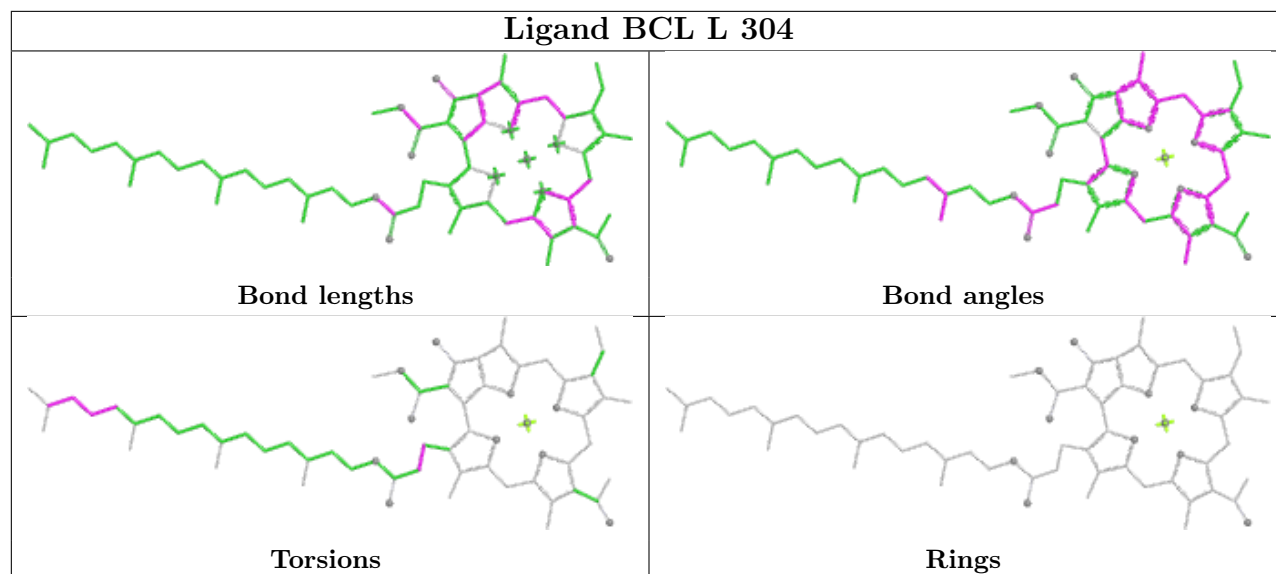
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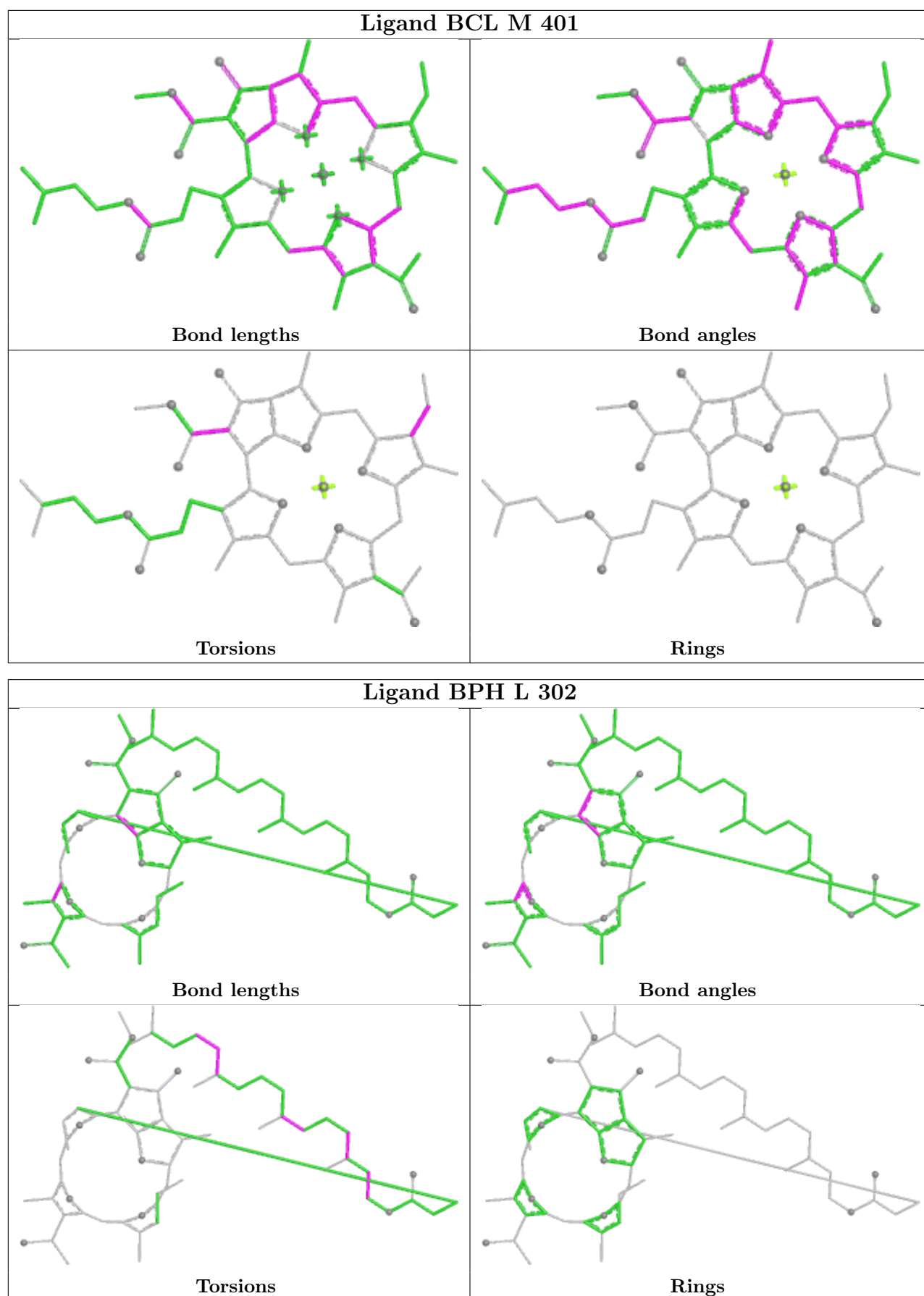
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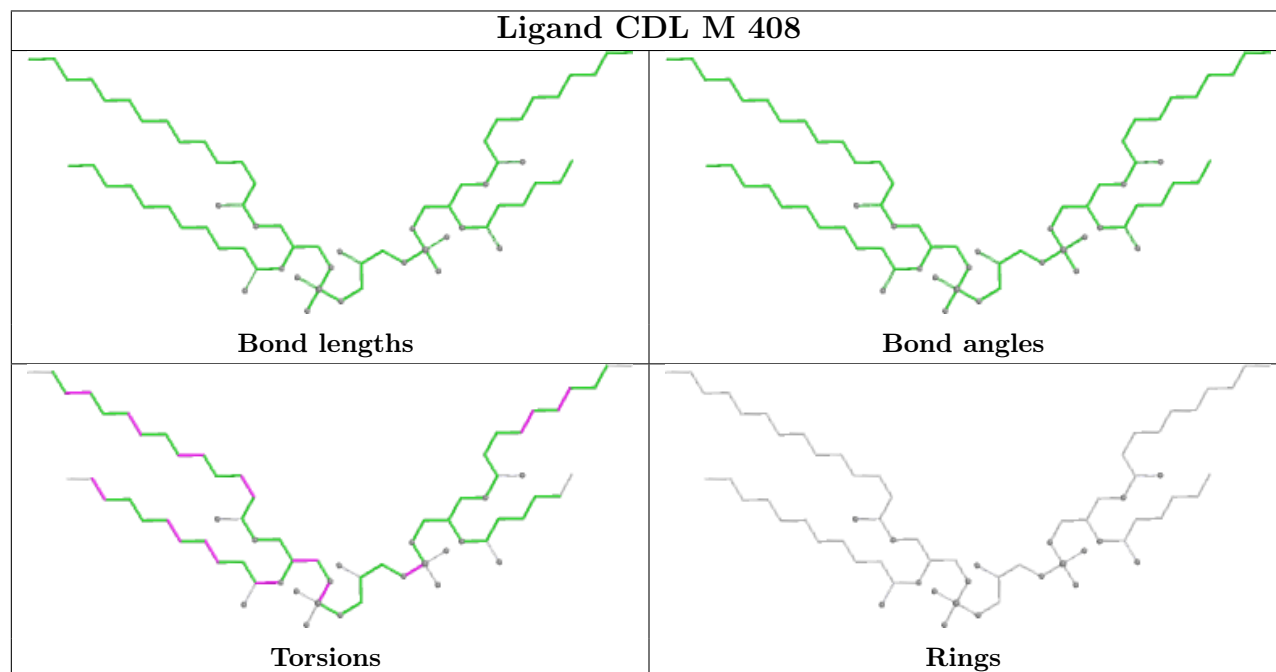
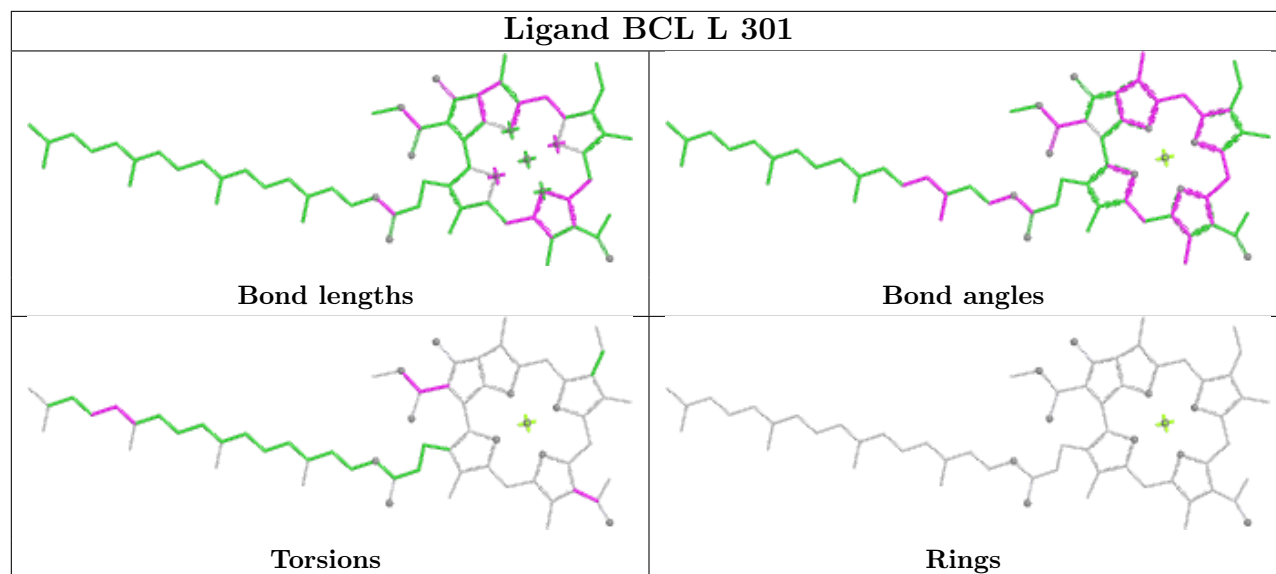
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	402	BCL	5	0
4	L	304	BCL	2	0
5	L	305	BPH	4	0
4	M	401	BCL	4	0
5	L	302	BPH	4	0
4	L	301	BCL	3	0

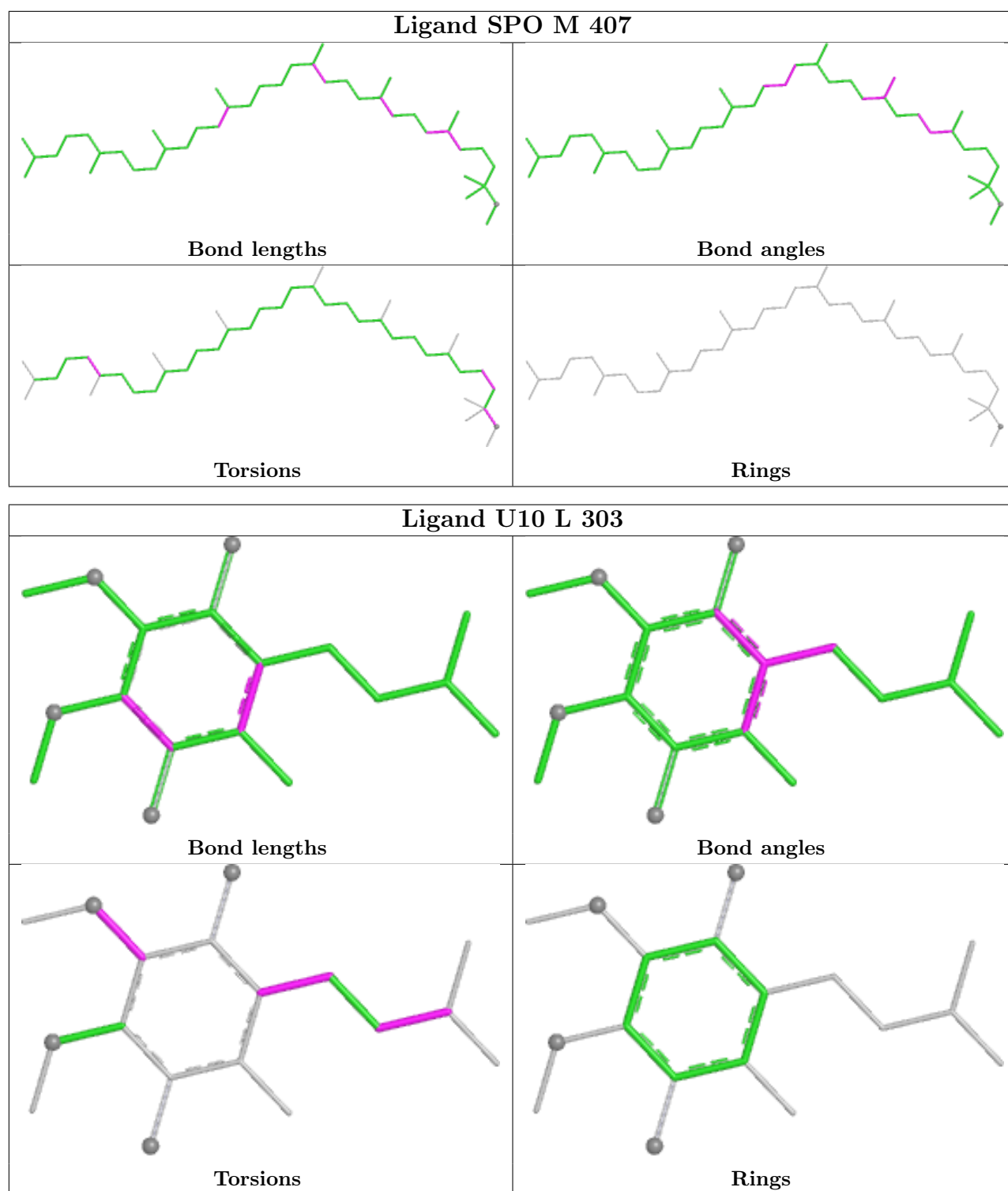
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	H	239/266 (89%)	-0.31	2 (0%) 82 75	41, 56, 81, 100	0
2	L	281/282 (99%)	-0.26	3 (1%) 78 70	24, 52, 90, 104	1 (0%)
3	M	301/308 (97%)	-0.19	6 (1%) 65 56	38, 58, 93, 104	0
All	All	821/856 (95%)	-0.25	11 (1%) 75 66	24, 56, 89, 104	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	2	GLU	3.3
1	H	102	GLY	3.1
3	M	302	GLY	3.1
2	L	72	GLU	3.0
1	H	249	LYS	2.9
2	L	126[A]	LEU	2.6
3	M	301	HIS	2.6
3	M	105	PHE	2.1
3	M	21	THR	2.1
3	M	110	LYS	2.1
2	L	281	GLY	2.0

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

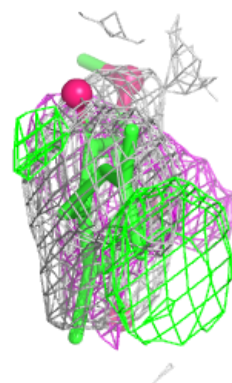
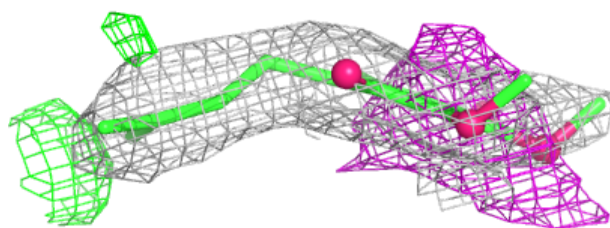
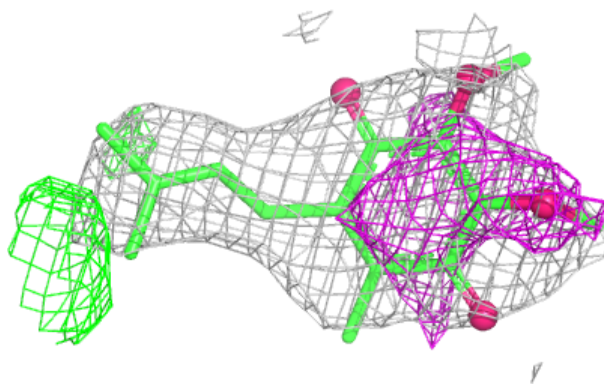
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
8	LDA	M	405	16/16	0.85	0.33	86,97,141,143	0
6	U10	L	303	18/63	0.87	0.26	80,88,94,94	0
11	CDL	M	408	69/100	0.92	0.16	60,81,93,118	0
10	SPO	M	407	42/42	0.93	0.17	58,78,102,109	0
8	LDA	M	404	16/16	0.93	0.20	79,95,115,116	0
7	CL	L	306	1/1	0.95	0.14	92,92,92,92	0
8	LDA	M	403	16/16	0.95	0.18	93,99,106,108	0
5	BPH	L	305	55/65	0.96	0.11	48,59,91,93	0
4	BCL	M	401	51/66	0.96	0.09	43,47,71,74	0
4	BCL	L	304	66/66	0.97	0.09	38,43,77,88	0
4	BCL	L	301	66/66	0.97	0.09	34,40,77,85	0
4	BCL	M	402	66/66	0.97	0.09	41,45,79,99	0
5	BPH	L	302	65/65	0.97	0.08	40,45,65,67	0
9	FE	M	406	1/1	1.00	0.03	42,42,42,42	0

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

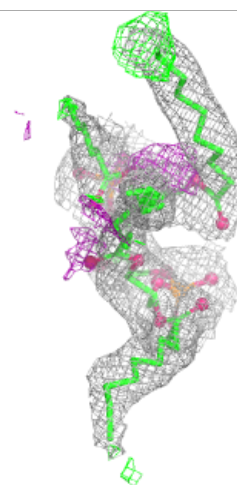
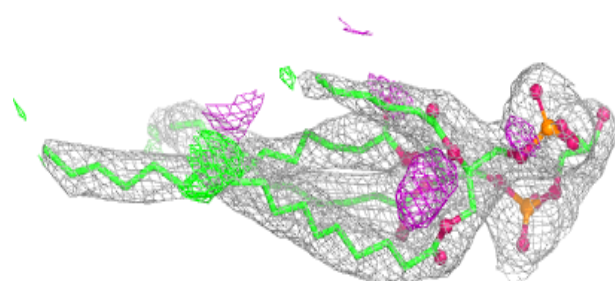
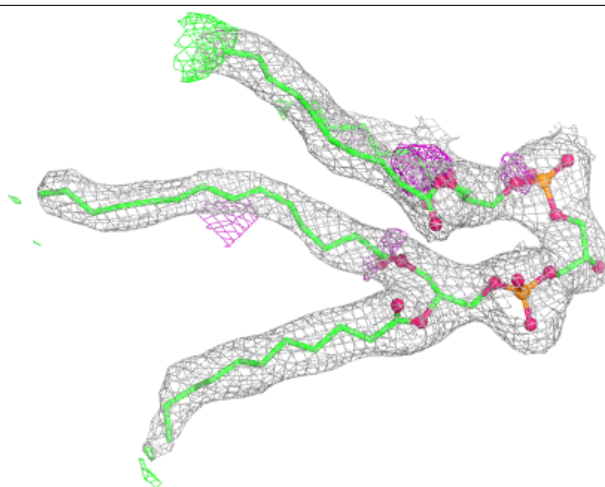
Electron density around U10 L 303:

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



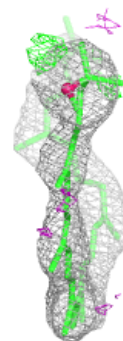
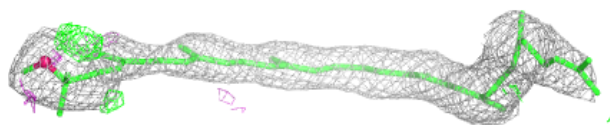
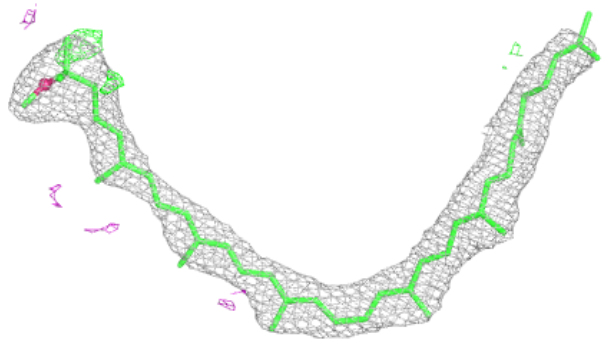
Electron density around CDL M 408:

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

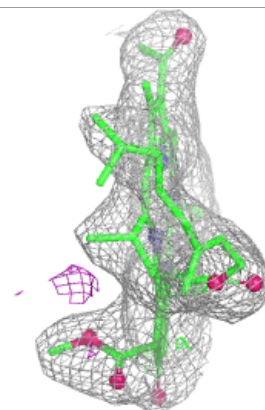
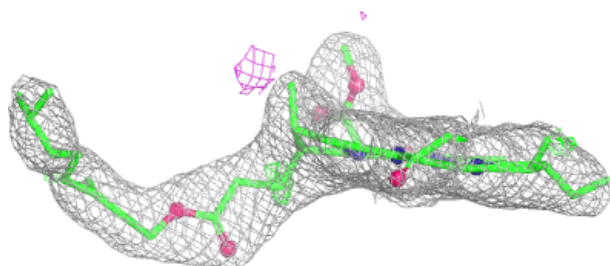
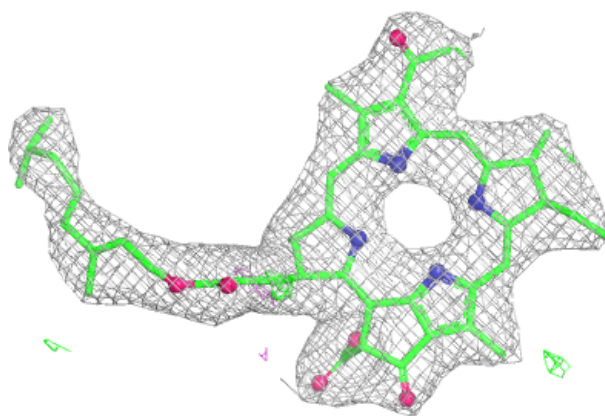


Electron density around SPO M 407:

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

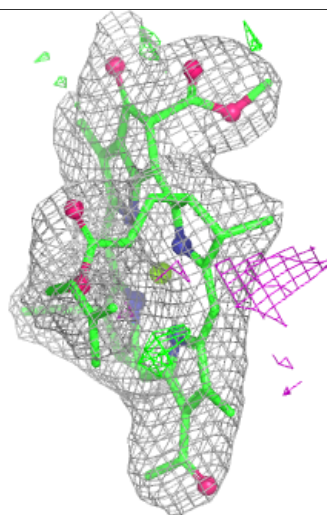
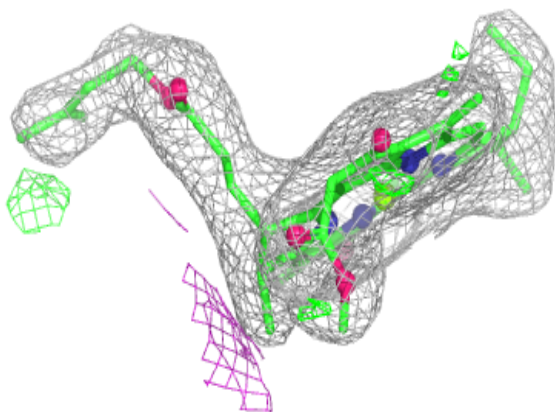
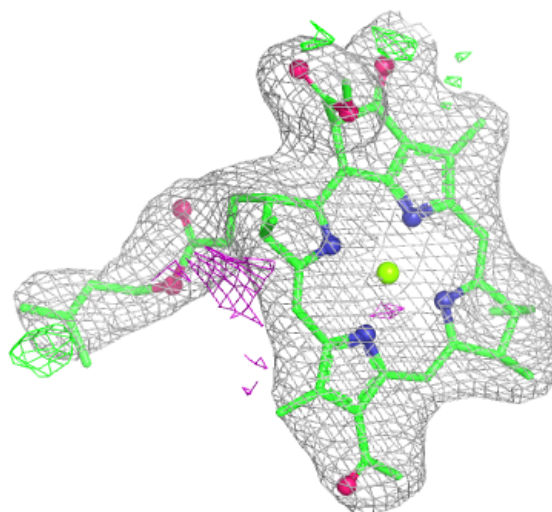
**Electron density around BPH L 305:**

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



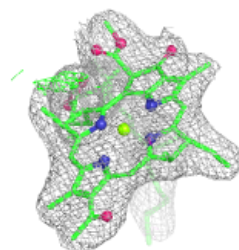
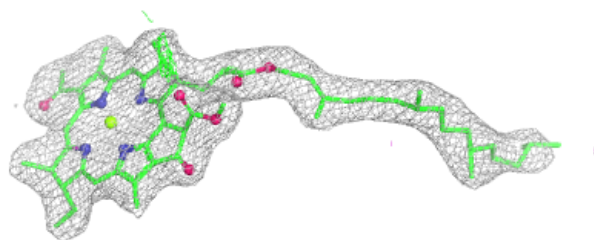
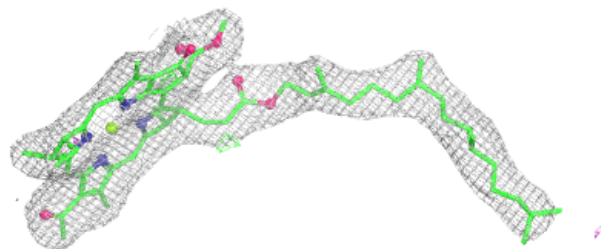
Electron density around BCL M 401:

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



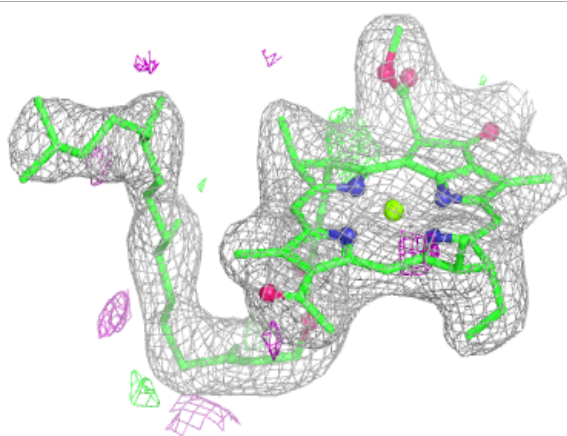
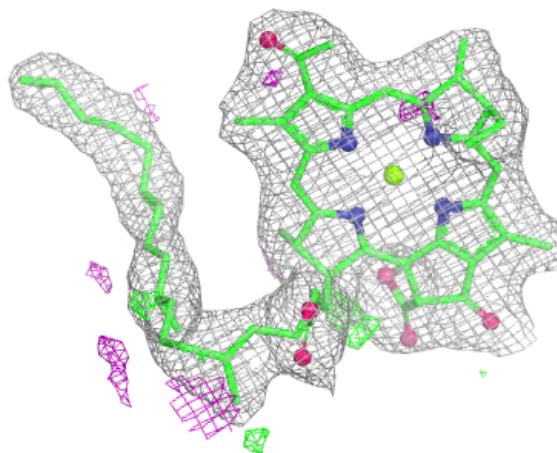
Electron density around BCL L 304:

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



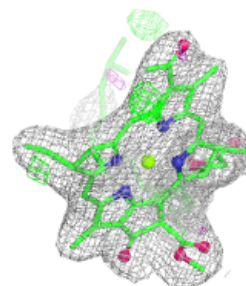
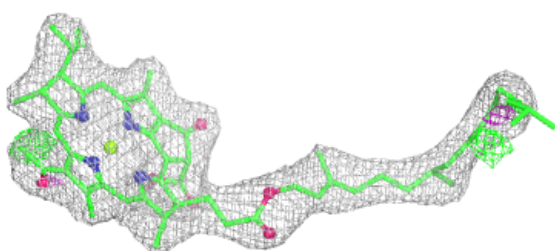
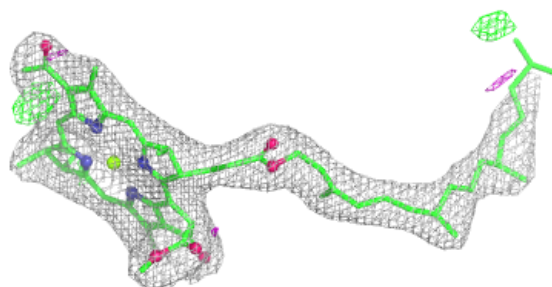
Electron density around BCL L 301:

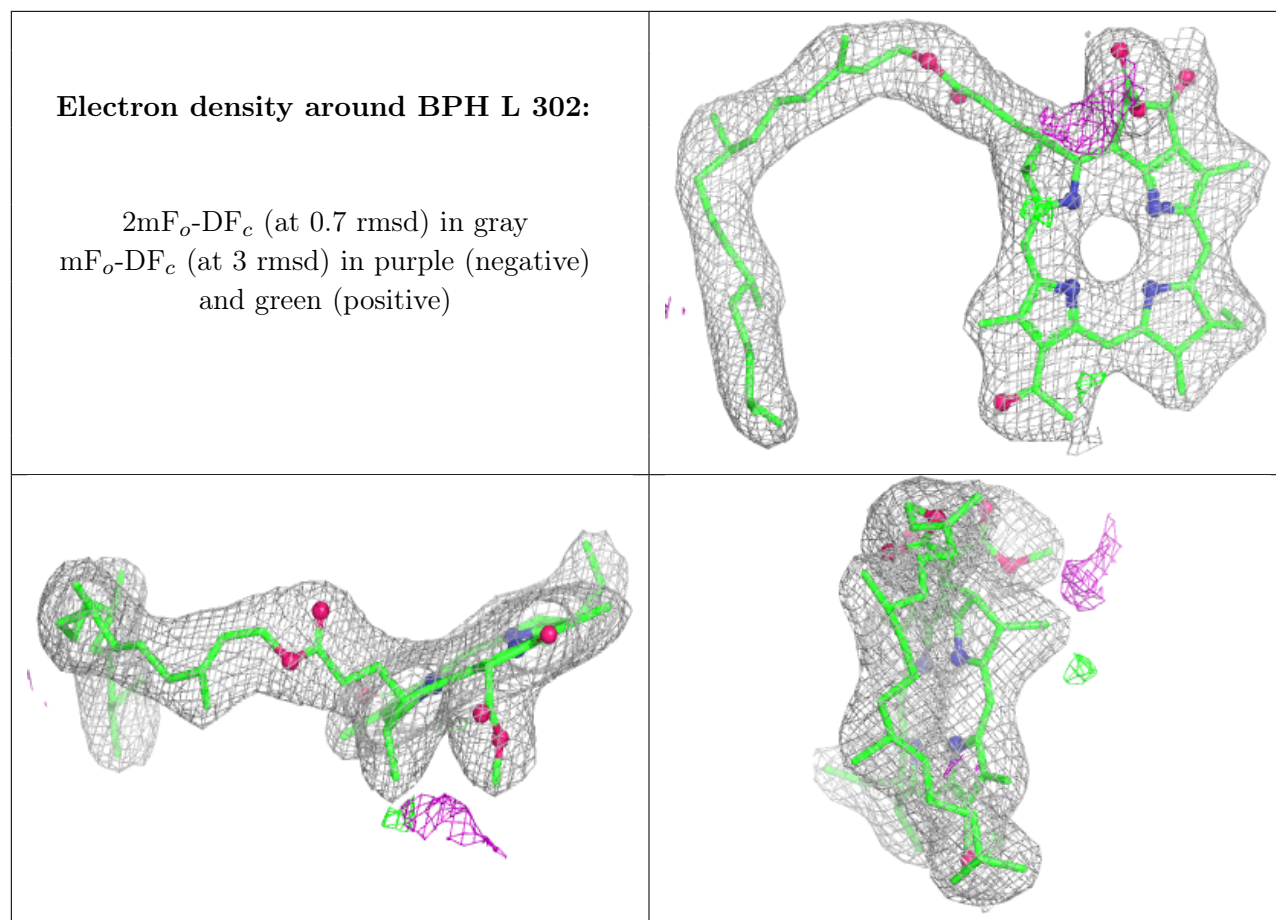
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCL M 402:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.