



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 23, 2021 – 12:06 PM EST

PDB ID : 7MH3
Title : Crystal structure of R. sphaeroides Photosynthetic Reaction Center variant;
Y(M210)3-chlorotyrosine
Authors : Mathews, I.; Weaver, J.B.; Boxer, S.G.
Deposited on : 2021-04-14
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.25
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.25

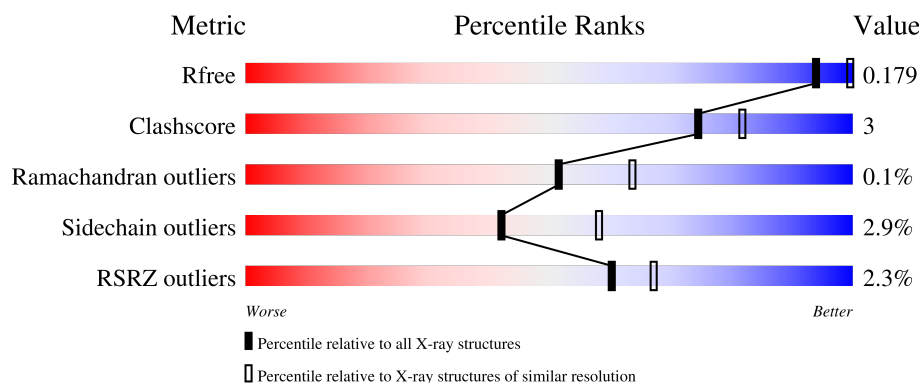
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	<div> <div>2%</div> <div>85%</div> <div>5%</div> <div>10%</div> </div>
2	L	282	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
3	M	308	<div> <div>2%</div> <div>92%</div> <div>6%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BPH	M	407	X	-	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7435 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	240	Total	C	N	O	S	0	1	0
			1841	1178	315	339	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

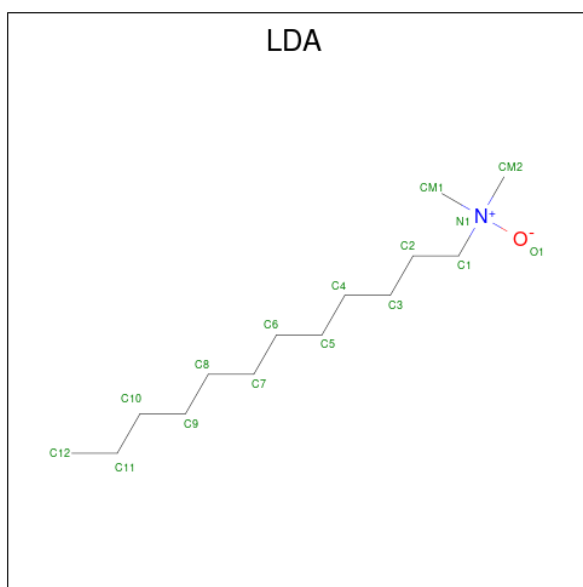
- Molecule 2 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	2	0
			2248	1517	357	366	8			

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

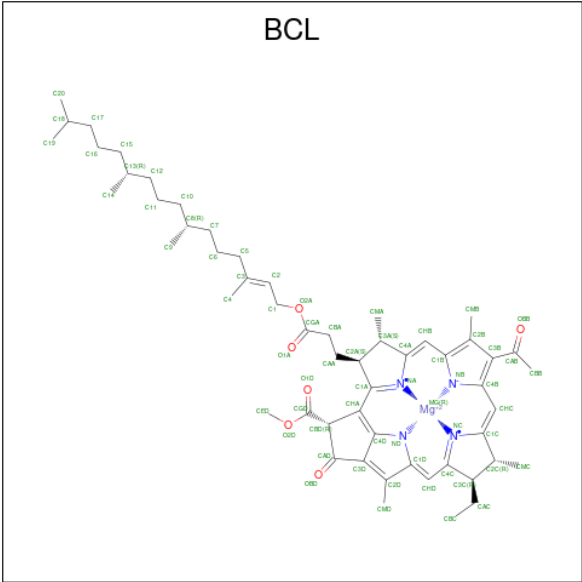
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	M	301	Total	C	Cl	N	O	S	0	0	0
			2405	1604	2	393	396	10			

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



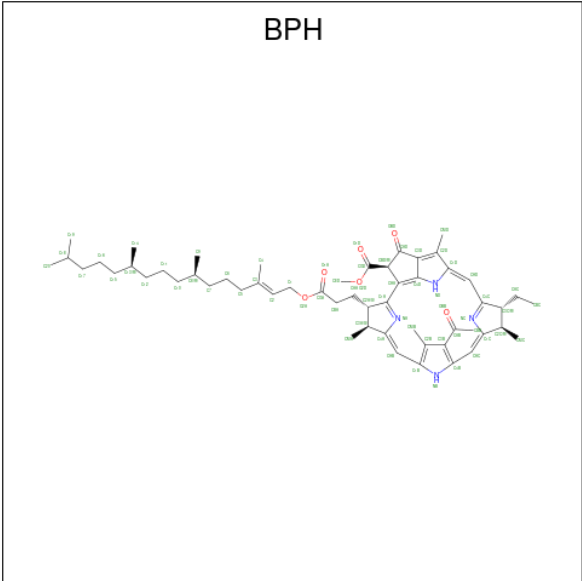
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



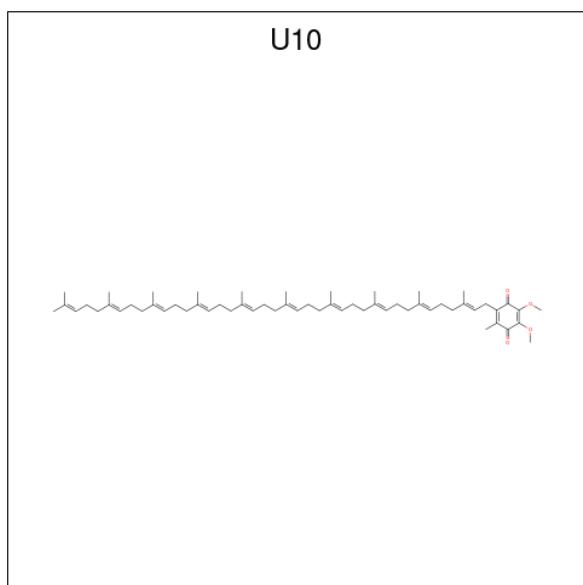
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
5	L	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
5	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆) (labeled as "Ligand of Interest" by depositor).



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
			55	45	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			18	14	4		
7	M	1	Total	C	O	0	0
			48	44	4		

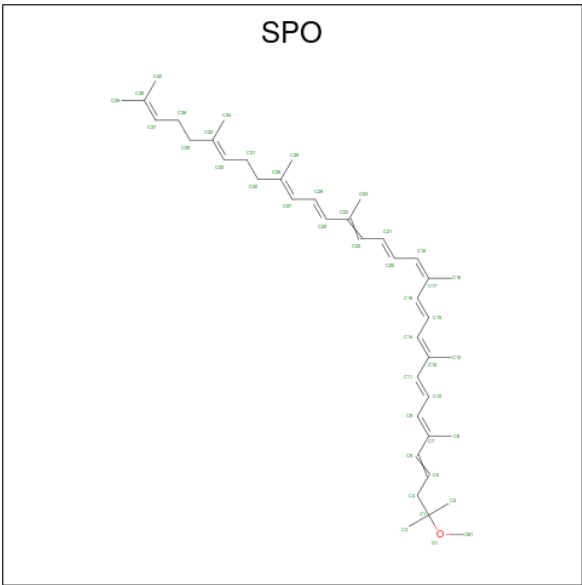
- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

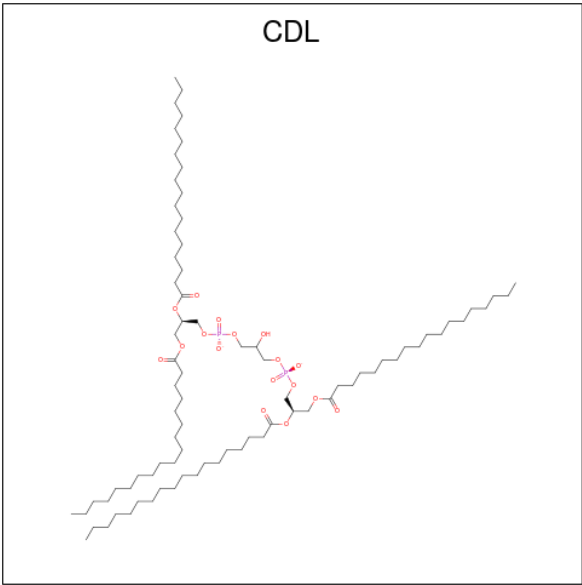
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	M	1	Total	Fe	0	0
			1	1		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



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

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

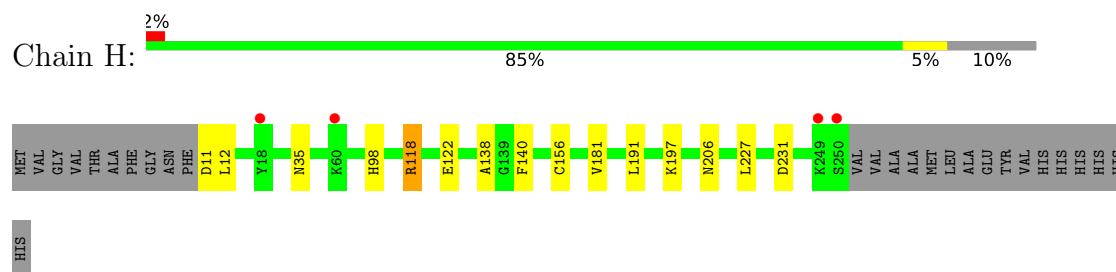
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	H	141	Total 141	O 141	0	0
12	L	73	Total 73	O 73	0	0
12	M	98	Total 99	O 99	0	1

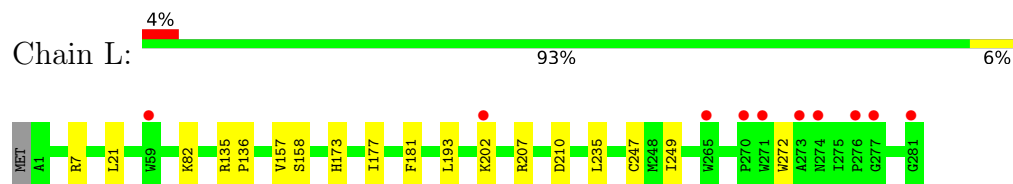
3 Residue-property plots

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

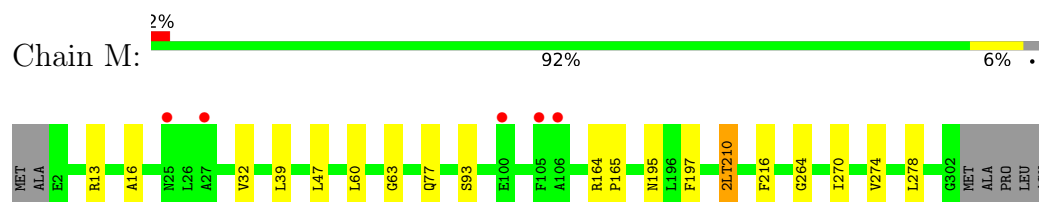
- Molecule 1: Reaction center protein H chain



- 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	141.67Å 141.67Å 187.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.11 – 2.30 39.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.1 (39.11-2.30) 94.2 (39.08-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.157 , 0.174 0.165 , 0.179	Depositor DCC
R_{free} test set	4508 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7435	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPO, U10, LDA, BCL, BPH, CDL, CL, 2LT, 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	H	0.61	0/1890	0.77	0/2571
2	L	0.62	0/2336	0.70	0/3197
3	M	0.62	0/2481	0.72	0/3385
All	All	0.62	0/6707	0.73	0/9153

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.

There are no bond angle outliers.

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	1841	0	1844	8	0
2	L	2248	0	2200	10	0
3	M	2405	0	2310	13	0
4	H	16	0	31	0	0
4	M	64	0	124	0	0
5	L	183	0	189	10	0
5	M	66	0	74	7	0
6	L	65	0	76	4	0
6	M	55	0	53	6	0
7	L	18	0	15	4	0
7	M	48	0	63	0	0
8	L	1	0	0	0	0
9	M	1	0	0	0	0
10	M	42	0	60	1	0
11	M	69	0	82	0	0
12	H	141	0	0	1	0
12	L	73	0	0	0	0
12	M	99	0	0	0	0
All	All	7435	0	7121	45	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 (45) 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)
6:L:302:BPH:HBB3	6:L:302:BPH:HHC	1.62	0.80
5:L:301:BCL:HBB2	5:L:301:BCL:HHC	1.69	0.74
3:M:16:ALA:HB1	3:M:32:VAL:HG11	1.73	0.70
7:L:303:U10:O5	7:L:303:U10:H8	1.95	0.66
6:L:302:BPH:HBB2	3:M:210:2LT:HB2	1.80	0.63
3:M:197:PHE:CZ	5:M:401:BCL:HBB2	2.35	0.61
5:L:304:BCL:HBB3	5:L:304:BCL:HMB1	1.87	0.57
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.24	0.55
5:L:304:BCL:HMB1	5:L:304:BCL:CBB	2.37	0.55
3:M:197:PHE:HZ	5:M:401:BCL:HBB2	1.72	0.54
2:L:181:PHE:CD2	6:M:407:BPH:HBB1	2.44	0.53
2:L:157:VAL:HG11	5:M:401:BCL:HBB1	1.91	0.53
7:L:303:U10:O2	7:L:303:U10:H3M3	2.08	0.52
3:M:270:ILE:O	3:M:274:VAL:HG13	2.08	0.52
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.92	0.52
5:L:305:BCL:HHC	5:L:305:BCL:HBB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:301:BCL:ND	3:M:210:2LT:CL2	2.80	0.51
2:L:181:PHE:HB3	6:M:407:BPH:HBB2	1.92	0.50
6:M:407:BPH:HHD	6:M:407:BPH:HBC3	1.93	0.50
1:H:35:ASN:OD1	3:M:264:GLY:HA3	2.13	0.49
1:H:140:PHE:HA	3:M:13:ARG:O	2.12	0.49
1:H:118:ARG:NH2	12:H:401:HOH:O	2.34	0.48
5:L:305:BCL:HHC	5:L:305:BCL:CBB	2.43	0.48
7:L:303:U10:O5	7:L:303:U10:C8	2.61	0.48
2:L:181:PHE:HB3	6:M:407:BPH:CBB	2.44	0.48
6:M:407:BPH:HBB3	6:M:407:BPH:HHC	1.95	0.47
5:L:305:BCL:HBB3	5:M:401:BCL:H41	1.97	0.46
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.64	0.46
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.97	0.46
6:L:302:BPH:HHC	6:L:302:BPH:CBB	2.39	0.46
5:L:301:BCL:HHC	5:L:301:BCL:CBB	2.44	0.45
3:M:164:ARG:HB3	3:M:165:PRO:HD3	1.99	0.44
2:L:249:ILE:HD12	2:L:249:ILE:HA	1.92	0.44
6:L:302:BPH:HBB1	3:M:210:2LT:CD2	2.48	0.44
1:H:122:GLU:HB2	1:H:227:LEU:HD21	2.00	0.43
2:L:193:LEU:HD23	7:L:303:U10:C2	2.49	0.43
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.54	0.43
3:M:63:GLY:HA3	6:M:407:BPH:H5C1	2.01	0.42
5:M:401:BCL:HAA2	5:M:401:BCL:HBD	2.01	0.42
3:M:197:PHE:CE1	5:M:401:BCL:HBB2	2.54	0.42
5:L:304:BCL:H192	5:L:304:BCL:H161	1.96	0.42
5:M:401:BCL:HBB3	5:M:401:BCL:HHC	2.02	0.42
3:M:77:GLN:HE22	3:M:93:SER:H	1.67	0.41
1:H:156:CYS:HB3	1:H:206:ASN:O	2.21	0.41
5:L:305:BCL:CBB	10:M:409:SPO:H243	2.51	0.40

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	H	239/266 (90%)	236 (99%)	3 (1%)	0	100	100
2	L	281/282 (100%)	276 (98%)	5 (2%)	0	100	100
3	M	298/308 (97%)	288 (97%)	9 (3%)	1 (0%)	41	50
All	All	818/856 (96%)	800 (98%)	17 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	195	ASN

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	196/215 (91%)	191 (97%)	5 (3%)	46	63
2	L	222/221 (100%)	213 (96%)	9 (4%)	30	43
3	M	235/240 (98%)	230 (98%)	5 (2%)	53	70
All	All	653/676 (97%)	634 (97%)	19 (3%)	42	58

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	11	ASP
1	H	12	LEU
1	H	118	ARG
1	H	197	LYS
1	H	231	ASP
2	L	21	LEU
2	L	82	LYS
2	L	158	SER
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	235	LEU

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Mol	Chain	Res	Type
2	L	247	CYS
2	L	272	TRP
3	M	39	LEU
3	M	47	LEU
3	M	60	LEU
3	M	216	PHE
3	M	278	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
2	L	183	ASN
3	M	77	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
3	2LT	M	210	3	13,14,15	0.99	0	16,19,21	1.91	4 (25%)

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
3	2LT	M	210	3	-	2/5/6/8	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	210	2LT	CB-CG-CD1	4.35	127.91	120.44
3	M	210	2LT	CB-CG-CD2	-3.76	113.98	120.44
3	M	210	2LT	CZ-CE2-CL2	2.41	121.81	118.78
3	M	210	2LT	CZ-CE1-CL1	2.14	121.47	118.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	210	2LT	CA-CB-CG-CD1
3	M	210	2LT	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	210	2LT	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
5	BCL	M	401	-	58,74,74	1.53	8 (13%)	69,115,115	1.62	16 (23%)
6	BPH	L	302	-	64,70,70	0.51	0	76,101,101	0.85	4 (5%)
4	LDA	M	403	-	12,15,15	0.13	0	14,17,17	0.29	0
6	BPH	M	407	-	54,60,70	0.61	0	64,89,101	0.85	2 (3%)
4	LDA	H	301	-	12,15,15	0.14	0	14,17,17	0.26	0
5	BCL	L	304	-	58,74,74	1.53	8 (13%)	69,115,115	1.47	14 (20%)
5	BCL	L	301	-	58,74,74	1.51	8 (13%)	69,115,115	1.70	14 (20%)
5	BCL	L	305	-	43,59,74	1.81	9 (20%)	51,97,115	1.78	14 (27%)
7	U10	M	408	-	48,48,63	0.63	1 (2%)	58,61,79	0.53	0
11	CDL	M	410	-	68,68,99	0.36	0	74,80,111	0.45	0
10	SPO	M	409	-	40,41,41	1.59	8 (20%)	47,50,50	1.22	7 (14%)
4	LDA	M	404	-	12,15,15	0.14	0	14,17,17	0.20	0
4	LDA	M	402	-	12,15,15	0.20	0	14,17,17	0.27	0
4	LDA	M	405	-	12,15,15	0.18	0	14,17,17	0.18	0
7	U10	L	303	-	18,18,63	0.97	2 (11%)	22,25,79	0.89	2 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	M	401	-	-	2/37/137/137	-
6	BPH	L	302	-	-	9/54/105/105	0/5/6/6
10	SPO	M	409	-	-	6/47/47/47	-
4	LDA	M	403	-	-	4/13/13/13	-
6	BPH	M	407	-	1/1/16/22	11/42/93/105	0/5/6/6
4	LDA	H	301	-	-	6/13/13/13	-
5	BCL	L	304	-	-	3/37/137/137	-
5	BCL	L	301	-	-	2/37/137/137	-
5	BCL	L	305	-	-	2/19/119/137	-
7	U10	M	408	-	-	8/45/69/87	0/1/1/1
11	CDL	M	410	-	-	25/79/79/110	-
4	LDA	M	405	-	-	4/13/13/13	-
4	LDA	M	402	-	-	5/13/13/13	-
4	LDA	M	404	-	-	4/13/13/13	-
7	U10	L	303	-	-	5/9/33/87	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	304	BCL	O2D-CGD	4.87	1.45	1.33
5	M	401	BCL	O2D-CGD	4.86	1.45	1.33
5	M	401	BCL	OBD-CAD	4.84	1.29	1.22
5	L	305	BCL	C3D-C2D	4.72	1.47	1.39
5	L	301	BCL	O2D-CGD	4.60	1.44	1.33
5	L	304	BCL	C3B-C2B	4.54	1.47	1.39
5	L	301	BCL	C3D-C2D	4.45	1.47	1.39
5	L	305	BCL	O2A-CGA	4.44	1.46	1.33
5	L	305	BCL	C3B-C2B	4.40	1.47	1.39
5	L	304	BCL	OBD-CAD	4.39	1.28	1.22
5	L	305	BCL	O2D-CGD	4.37	1.43	1.33
5	M	401	BCL	C3D-C2D	4.32	1.47	1.39
5	L	305	BCL	OBD-CAD	4.27	1.28	1.22
10	M	409	SPO	C9-C7	4.24	1.41	1.35
5	L	301	BCL	OBD-CAD	4.24	1.28	1.22
5	L	301	BCL	O2A-CGA	4.16	1.45	1.33
5	M	401	BCL	C3B-C2B	4.15	1.46	1.39
5	L	304	BCL	O2A-CGA	4.01	1.45	1.33
5	L	304	BCL	C3D-C2D	3.87	1.46	1.39
10	M	409	SPO	C19-C17	3.78	1.40	1.35
5	M	401	BCL	O2A-CGA	3.68	1.44	1.33
5	L	301	BCL	C3B-C2B	3.60	1.45	1.39
10	M	409	SPO	C14-C12	3.49	1.40	1.35
10	M	409	SPO	C22-C23	3.09	1.39	1.35
5	L	304	BCL	C2D-C1D	2.85	1.49	1.42
5	M	401	BCL	C2D-C1D	2.82	1.49	1.42
5	L	301	BCL	C2D-C1D	2.71	1.48	1.42
10	M	409	SPO	C25-C23	-2.64	1.40	1.45
7	L	303	U10	C3-C2	-2.61	1.41	1.48
10	M	409	SPO	C16-C17	-2.60	1.40	1.45
5	L	305	BCL	C2D-C1D	2.58	1.48	1.42
10	M	409	SPO	C11-C12	-2.46	1.40	1.45
5	L	301	BCL	C1B-CHB	2.39	1.47	1.41
5	M	401	BCL	C4B-CHC	2.38	1.47	1.41
5	L	305	BCL	C1B-CHB	2.33	1.47	1.41
5	M	401	BCL	C1B-CHB	2.33	1.47	1.41
5	L	304	BCL	C1B-CHB	2.30	1.47	1.41
5	L	304	BCL	C4B-CHC	2.24	1.47	1.41
7	M	408	U10	C6-C1	2.23	1.39	1.35
5	L	305	BCL	C4B-CHC	2.21	1.47	1.41
5	L	301	BCL	MG-NA	-2.19	2.01	2.06
7	L	303	U10	C4-C5	-2.15	1.42	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	305	BCL	MG-NA	-2.15	2.01	2.06
10	M	409	SPO	C6-C7	-2.05	1.41	1.45

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	301	BCL	O2D-CGD-CBD	5.27	120.63	111.27
5	L	301	BCL	C1C-NC-C4C	-4.86	104.52	106.71
5	M	401	BCL	C1C-NC-C4C	-4.64	104.62	106.71
5	L	305	BCL	O2D-CGD-CBD	4.55	119.36	111.27
5	L	301	BCL	C4C-CHD-C1D	-4.50	119.24	125.88
5	L	301	BCL	CHD-C4C-NC	4.18	129.72	125.08
5	L	304	BCL	C3C-C4C-CHD	-4.16	114.50	123.39
5	M	401	BCL	C3C-C4C-CHD	-4.15	114.52	123.39
5	L	305	BCL	C3C-C4C-CHD	-4.13	114.58	123.39
5	L	301	BCL	C3C-C4C-CHD	-4.03	114.78	123.39
5	L	304	BCL	C1C-NC-C4C	-3.93	104.94	106.71
5	L	305	BCL	C1C-NC-C4C	-3.88	104.96	106.71
5	L	305	BCL	CHD-C4C-NC	3.81	129.30	125.08
5	M	401	BCL	O2D-CGD-CBD	3.65	117.75	111.27
6	L	302	BPH	C1C-NC-C4C	-3.59	107.38	110.54
5	L	304	BCL	CHD-C4C-NC	3.54	129.01	125.08
5	M	401	BCL	O2D-CGD-O1D	-3.52	116.96	123.84
5	M	401	BCL	CHD-C4C-NC	3.27	128.71	125.08
5	M	401	BCL	C4C-CHD-C1D	-3.26	121.06	125.88
5	L	305	BCL	C4C-CHD-C1D	-3.19	121.18	125.88
5	L	304	BCL	CHB-C4A-NA	3.19	128.92	124.51
5	L	301	BCL	CHB-C4A-NA	3.07	128.76	124.51
5	L	304	BCL	C4C-CHD-C1D	-3.06	121.37	125.88
5	L	305	BCL	CMB-C2B-C3B	3.05	130.39	124.68
5	L	301	BCL	CHC-C1C-NC	3.03	128.71	124.51
5	L	304	BCL	C4-C3-C5	3.03	120.36	115.27
5	M	401	BCL	C4B-C3B-CAB	2.89	132.71	127.13
5	L	301	BCL	C4A-NA-C1A	2.76	107.95	106.71
5	M	401	BCL	O2A-CGA-CBA	2.72	120.45	111.91
5	L	305	BCL	O2D-CGD-O1D	-2.66	118.64	123.84
5	L	301	BCL	O2D-CGD-O1D	-2.66	118.65	123.84
5	M	401	BCL	CED-O2D-CGD	2.63	121.88	115.94
5	L	305	BCL	C1-C2-C3	-2.62	122.52	126.75
5	L	304	BCL	CHC-C1C-NC	2.61	128.12	124.51
5	L	304	BCL	C4B-CHC-C1C	-2.58	125.01	130.12
5	M	401	BCL	CHB-C4A-NA	2.57	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	304	BCL	CMB-C2B-C3B	2.55	129.46	124.68
5	L	305	BCL	C1-O2A-CGA	2.55	123.12	116.44
5	L	305	BCL	CHB-C4A-NA	2.54	128.02	124.51
5	L	305	BCL	CHC-C1C-NC	2.45	127.91	124.51
10	M	409	SPO	C13-C12-C14	-2.44	119.50	122.92
7	L	303	U10	C7-C6-C5	2.41	121.38	118.48
5	L	305	BCL	C4B-CHC-C1C	-2.36	125.44	130.12
5	L	304	BCL	O2A-CGA-O1A	-2.33	117.71	123.59
10	M	409	SPO	C21-C20-C19	2.33	128.24	123.47
6	M	407	BPH	CHD-C4C-NC	-2.32	122.45	125.20
10	M	409	SPO	C21-C22-C23	2.30	130.59	127.31
5	L	305	BCL	O2A-CGA-CBA	2.29	119.10	111.91
5	L	304	BCL	O2A-CGA-CBA	2.26	118.99	111.91
5	M	401	BCL	CHC-C1C-NC	2.25	127.63	124.51
6	M	407	BPH	C1B-NB-C4B	2.25	110.75	106.51
5	L	304	BCL	C1B-CHB-C4A	-2.24	125.69	130.12
10	M	409	SPO	C10-C9-C7	2.23	130.50	127.31
10	M	409	SPO	C8-C7-C9	-2.23	119.80	122.92
5	M	401	BCL	CMB-C2B-C3B	2.20	128.78	124.68
5	M	401	BCL	CAD-C3D-C4D	2.18	109.69	108.47
6	L	302	BPH	C1B-NB-C4B	2.14	110.55	106.51
6	L	302	BPH	C4D-CHA-C1A	-2.14	125.24	130.51
5	L	301	BCL	C4B-CHC-C1C	-2.14	125.88	130.12
5	M	401	BCL	C4A-NA-C1A	2.13	107.67	106.71
10	M	409	SPO	C18-C17-C19	-2.13	119.94	122.92
6	L	302	BPH	CHD-C4C-NC	-2.12	122.68	125.20
5	L	305	BCL	C1B-CHB-C4A	-2.11	125.94	130.12
5	L	301	BCL	C1B-CHB-C4A	-2.10	125.95	130.12
5	L	301	BCL	C4-C3-C5	2.10	118.80	115.27
5	M	401	BCL	O2A-CGA-O1A	-2.09	118.31	123.59
5	L	304	BCL	O2D-CGD-CBD	2.08	114.97	111.27
10	M	409	SPO	C24-C23-C22	-2.07	120.02	122.92
5	L	304	BCL	C2A-C1A-CHA	-2.07	120.24	123.86
5	L	301	BCL	CMB-C2B-C3B	2.07	128.54	124.68
5	M	401	BCL	C2A-C1A-CHA	-2.06	120.26	123.86
7	L	303	U10	C1M-C1-C6	-2.05	121.06	124.40
5	L	301	BCL	O2A-CGA-CBA	2.04	118.31	111.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	M	407	BPH	C8

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	301	LDA	C2-C1-N1-O1
4	H	301	LDA	C2-C1-N1-CM1
4	H	301	LDA	C2-C1-N1-CM2
4	M	403	LDA	N1-C1-C2-C3
6	M	407	BPH	C4B-C3B-CAB-CBB
6	M	407	BPH	C4B-C3B-CAB-OB
7	L	303	U10	C1-C6-C7-C8
7	L	303	U10	C5-C6-C7-C8
7	M	408	U10	C32-C33-C34-C35
7	M	408	U10	C32-C33-C34-C36
11	M	410	CDL	CB2-OB2-PB2-OB3
7	M	408	U10	C24-C26-C27-C28
7	M	408	U10	C29-C31-C32-C33
7	L	303	U10	C7-C8-C9-C10
11	M	410	CDL	CA3-OA5-PA1-OA2
6	M	407	BPH	C5-C6-C7-C8
11	M	410	CDL	CA7-C31-C32-C33
4	H	301	LDA	C6-C7-C8-C9
11	M	410	CDL	C33-C34-C35-C36
5	L	301	BCL	C15-C16-C17-C18
4	M	404	LDA	C6-C7-C8-C9
6	M	407	BPH	O2A-C1-C2-C3
4	M	405	LDA	C1-C2-C3-C4
4	M	403	LDA	C1-C2-C3-C4
7	L	303	U10	C7-C8-C9-C11
4	M	404	LDA	C4-C5-C6-C7
11	M	410	CDL	C71-C72-C73-C74
11	M	410	CDL	C11-CA5-OA6-CA4
4	M	404	LDA	C1-C2-C3-C4
11	M	410	CDL	OA7-CA5-OA6-CA4
11	M	410	CDL	C39-C40-C41-C42
4	H	301	LDA	C11-C10-C9-C8
4	M	402	LDA	C1-C2-C3-C4
4	M	404	LDA	C9-C10-C11-C12
4	H	301	LDA	C9-C10-C11-C12
10	M	409	SPO	C4-C1-O1-CM1
11	M	410	CDL	C36-C37-C38-C39
5	L	304	BCL	C15-C16-C17-C18
11	M	410	CDL	C11-C12-C13-C14
10	M	409	SPO	C3-C1-O1-CM1
4	M	402	LDA	C4-C5-C6-C7
6	L	302	BPH	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
4	M	405	LDA	C9-C10-C11-C12
4	M	402	LDA	C11-C10-C9-C8
11	M	410	CDL	C17-C18-C19-C20
6	M	407	BPH	C4-C3-C5-C6
7	M	408	U10	C31-C32-C33-C34
4	M	405	LDA	C3-C4-C5-C6
5	L	305	BCL	C4C-C3C-CAC-CBC
6	M	407	BPH	C4C-C3C-CAC-CBC
6	M	407	BPH	C2-C3-C5-C6
5	M	401	BCL	C13-C15-C16-C17
4	M	405	LDA	C6-C7-C8-C9
6	M	407	BPH	C6-C7-C8-C9
6	M	407	BPH	C6-C7-C8-C10
10	M	409	SPO	C34-C33-C35-C36
11	M	410	CDL	CA3-OA5-PA1-OA3
10	M	409	SPO	C1-C4-C5-C6
6	M	407	BPH	C2C-C3C-CAC-CBC
4	M	402	LDA	C2-C3-C4-C5
11	M	410	CDL	C72-C71-CB7-OB8
4	M	403	LDA	C5-C6-C7-C8
7	L	303	U10	C5-C4-O4-C4M
11	M	410	CDL	C31-C32-C33-C34
10	M	409	SPO	C32-C33-C35-C36
10	M	409	SPO	C2-C1-O1-CM1
11	M	410	CDL	CB2-OB2-PB2-OB5
6	L	302	BPH	C4-C3-C5-C6
11	M	410	CDL	C72-C73-C74-C75
5	L	304	BCL	C2A-CAA-CBA-CGA
11	M	410	CDL	C13-C14-C15-C16
6	L	302	BPH	C5-C6-C7-C8
4	M	403	LDA	C6-C7-C8-C9
6	L	302	BPH	C14-C13-C15-C16
7	M	408	U10	C3-C4-O4-C4M
6	L	302	BPH	C2-C3-C5-C6
6	L	302	BPH	C4B-C3B-CAB-OB
7	M	408	U10	C30-C29-C31-C32
5	L	304	BCL	CAD-CBD-CGD-O2D
5	L	305	BCL	CAD-CBD-CGD-O2D
6	L	302	BPH	CAD-CBD-CGD-O2D
6	M	407	BPH	CAD-CBD-CGD-O2D
11	M	410	CDL	OA5-CA3-CA4-OA6
6	L	302	BPH	O2A-C1-C2-C3

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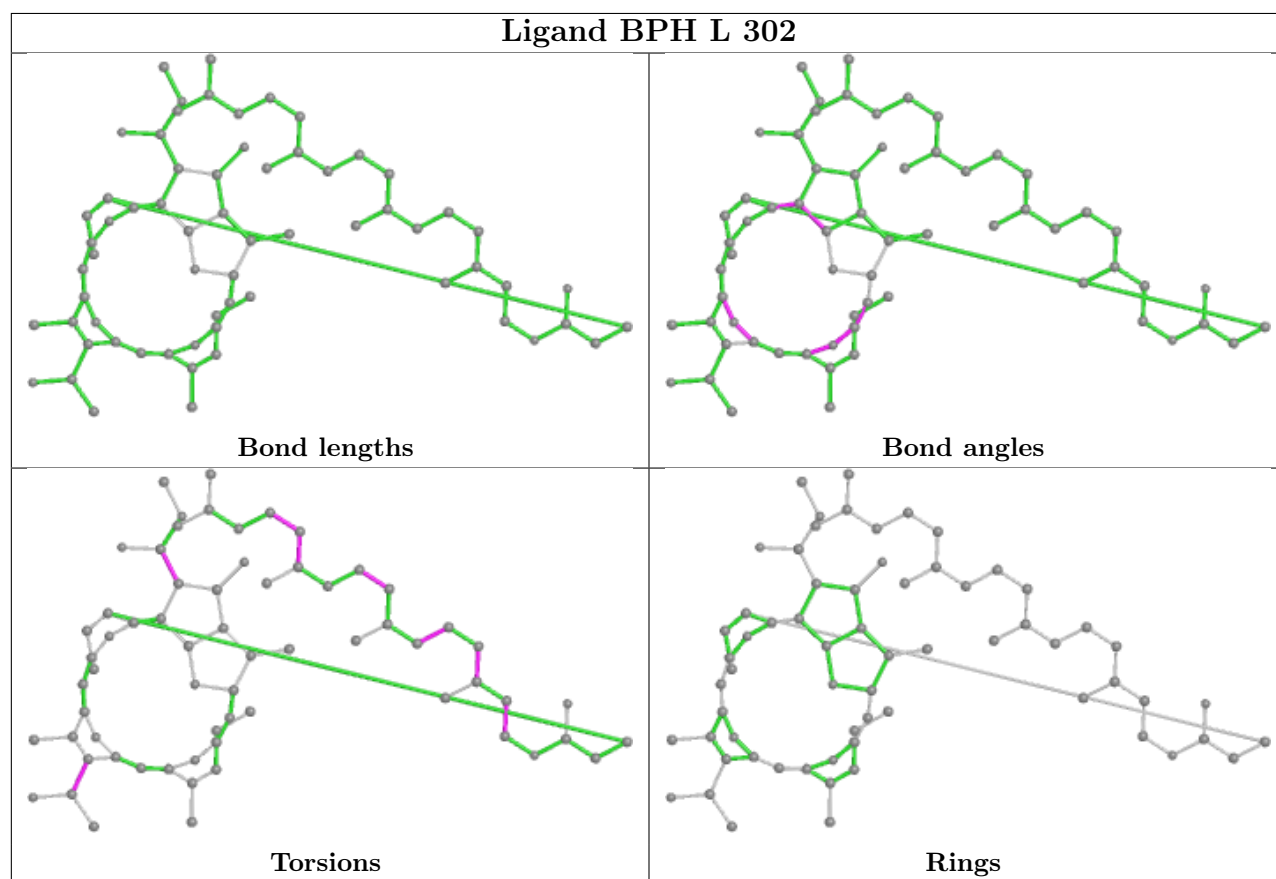
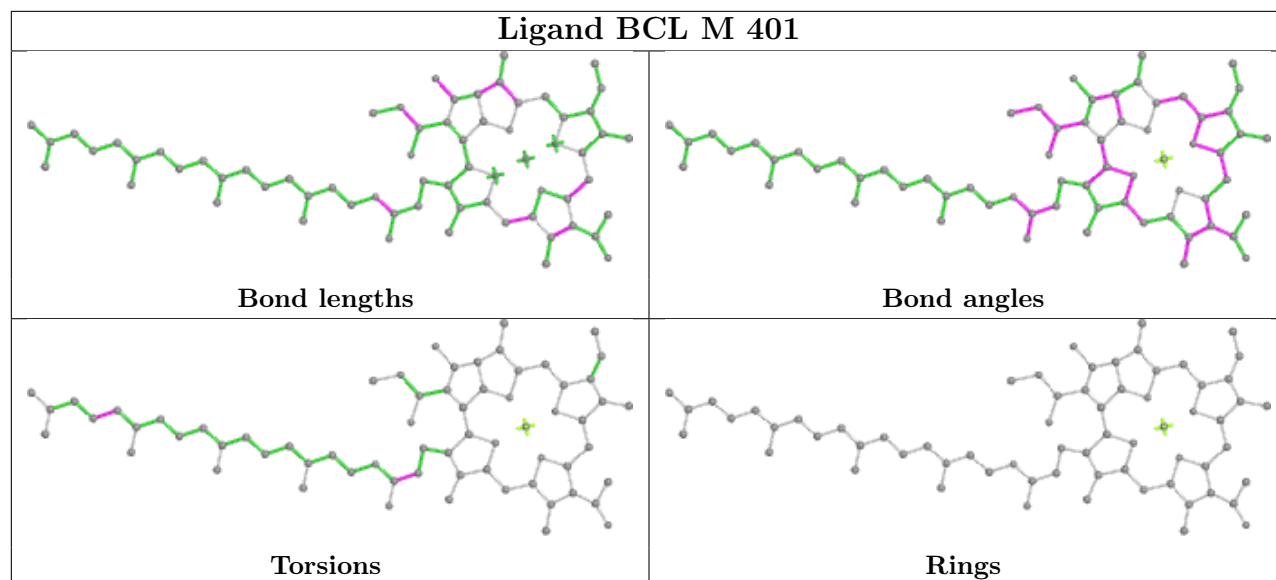
Mol	Chain	Res	Type	Atoms
6	L	302	BPH	C8-C10-C11-C12
5	L	301	BCL	CHA-CBD-CGD-O1D
11	M	410	CDL	OA5-CA3-CA4-CA6
11	M	410	CDL	C32-C31-CA7-OA8
11	M	410	CDL	C15-C16-C17-C18
11	M	410	CDL	C52-C51-CB5-OB6
11	M	410	CDL	C32-C31-CA7-OA9
11	M	410	CDL	CB2-OB2-PB2-OB4
11	M	410	CDL	C52-C51-CB5-OB7
7	M	408	U10	C5-C4-O4-C4M
4	M	402	LDA	C7-C8-C9-C10
5	M	401	BCL	CAA-CBA-CGA-O2A

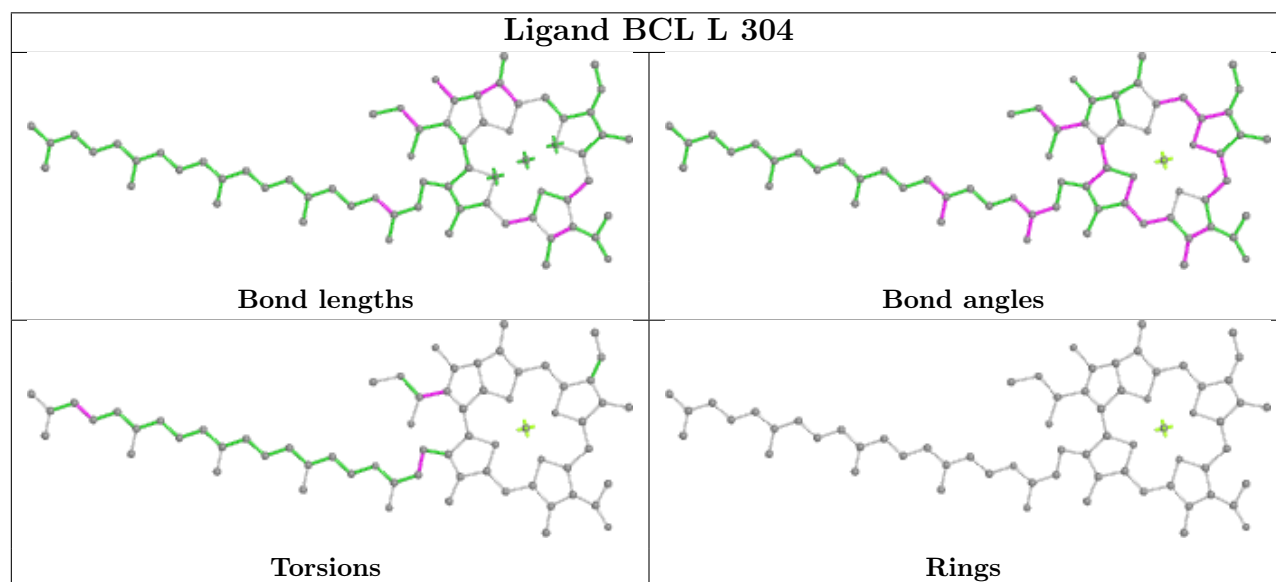
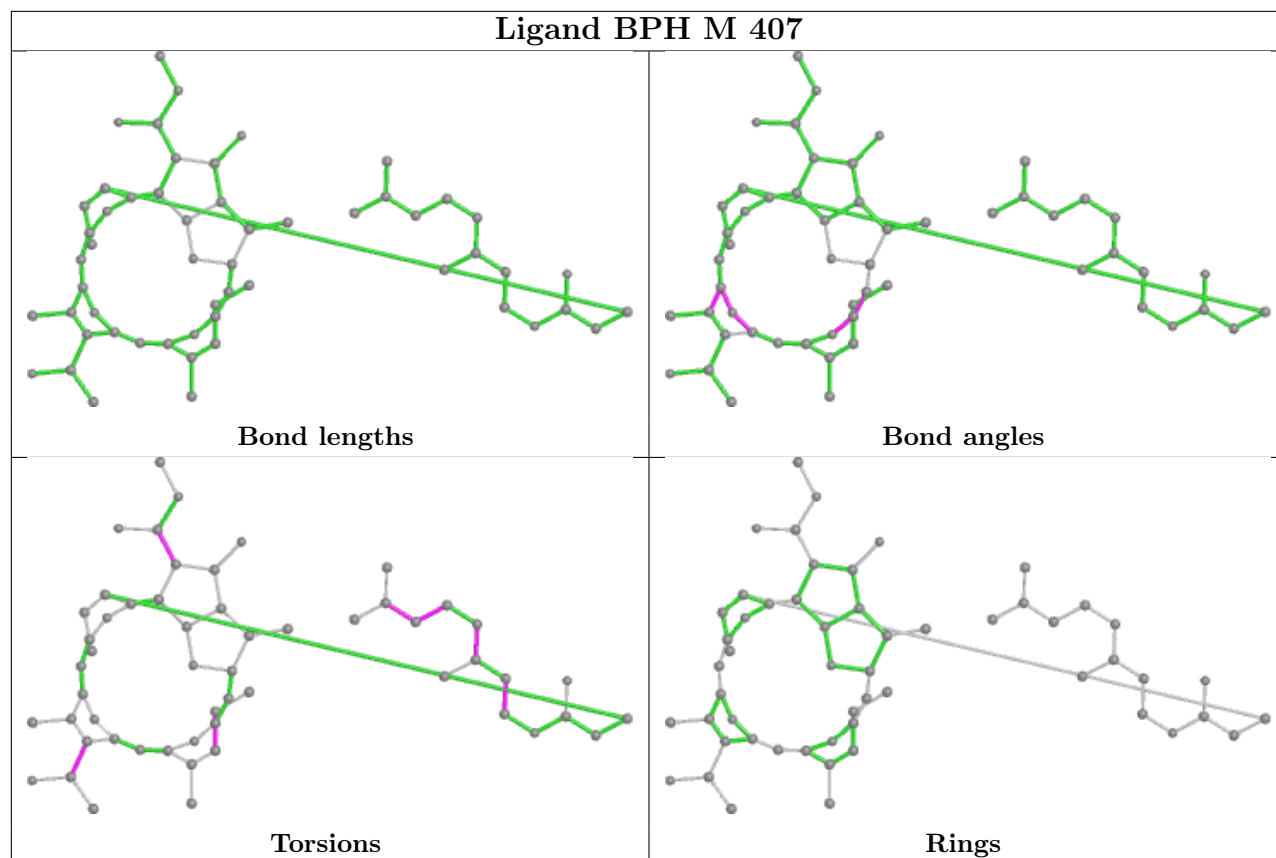
There are no ring outliers.

8 monomers are involved in 30 short contacts:

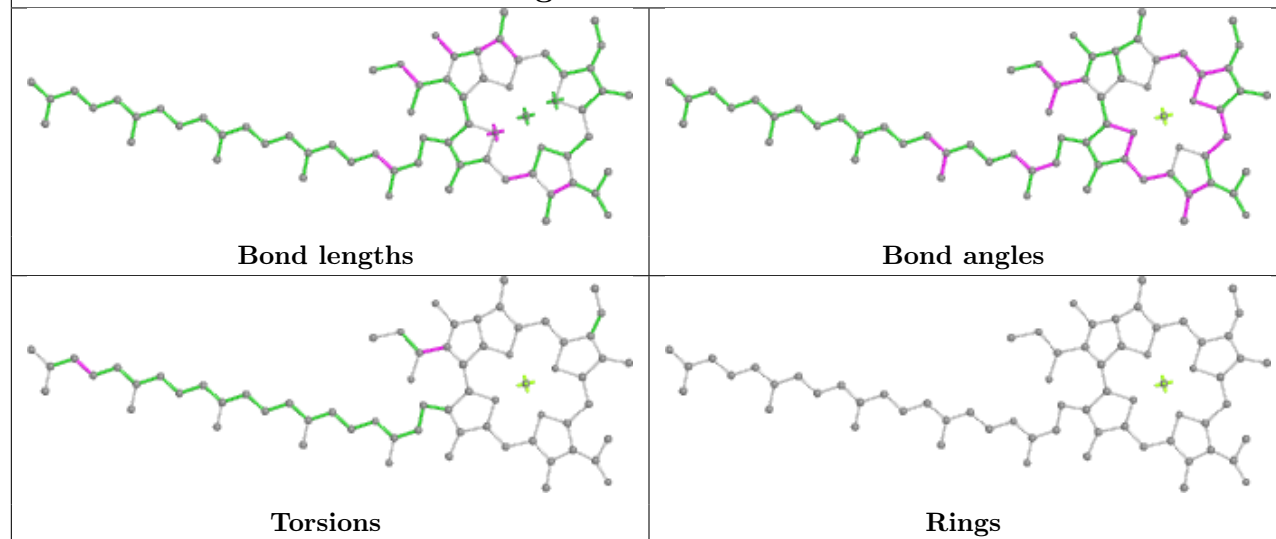
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	401	BCL	7	0
6	L	302	BPH	4	0
6	M	407	BPH	6	0
5	L	304	BCL	3	0
5	L	301	BCL	3	0
5	L	305	BCL	4	0
10	M	409	SPO	1	0
7	L	303	U10	4	0

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.

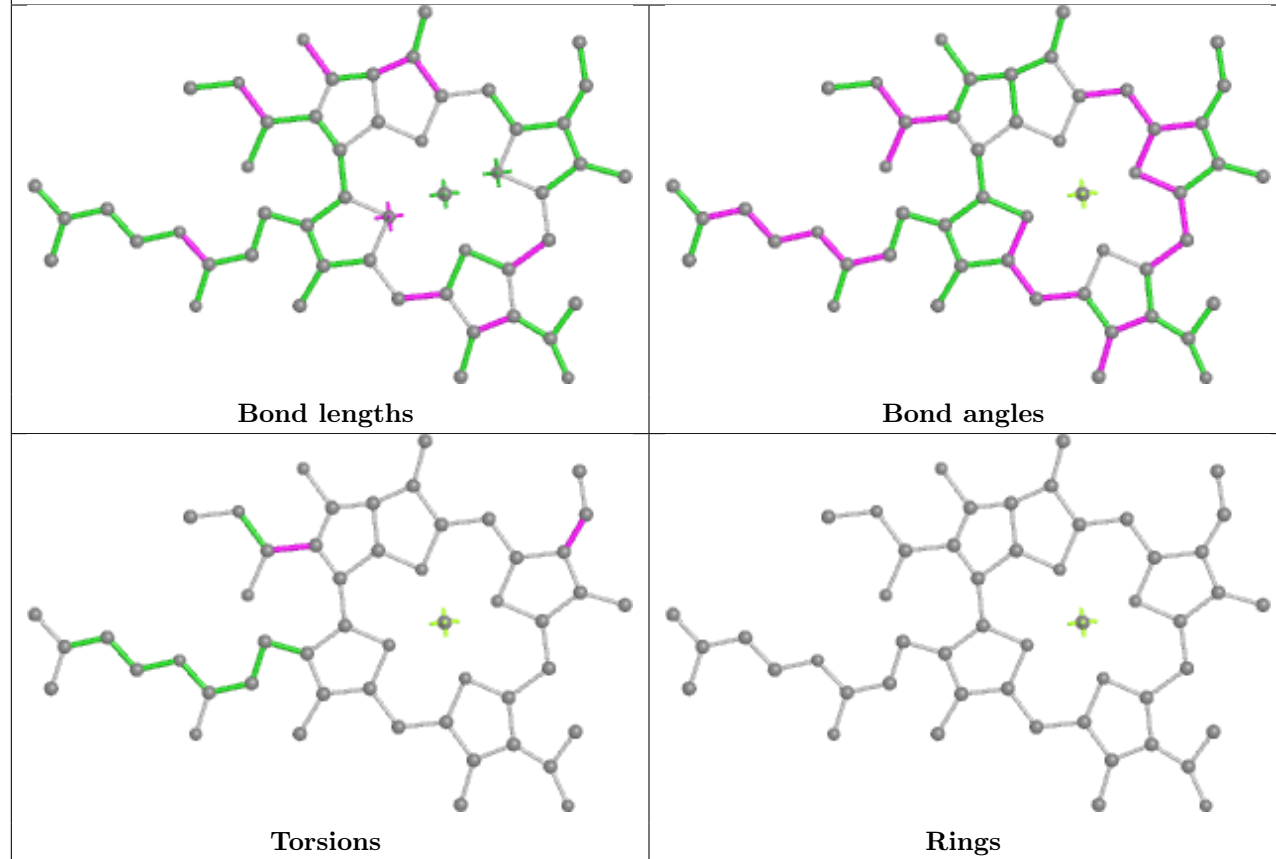




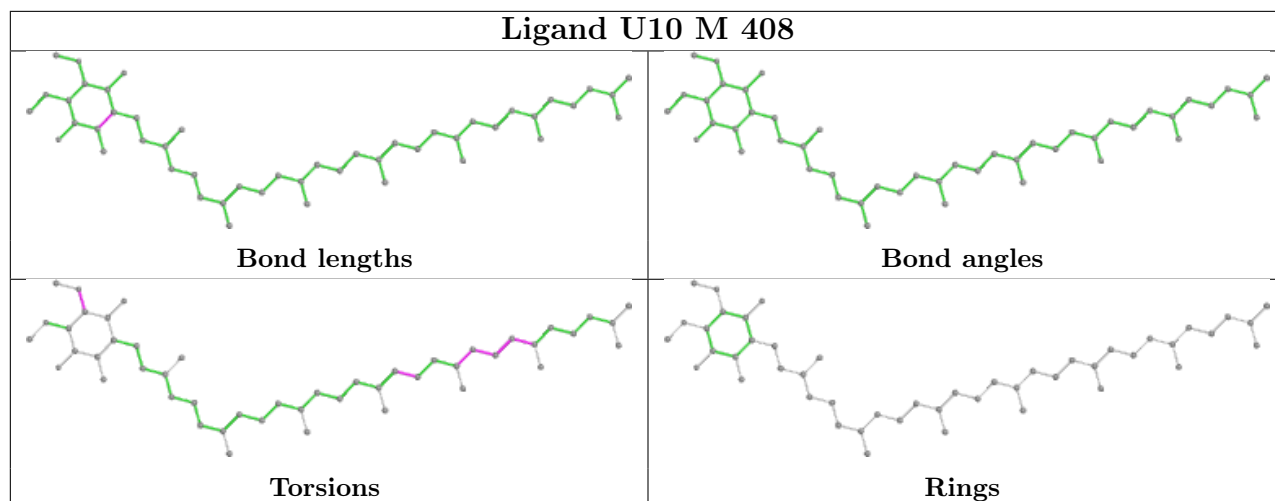
Ligand BCL L 301



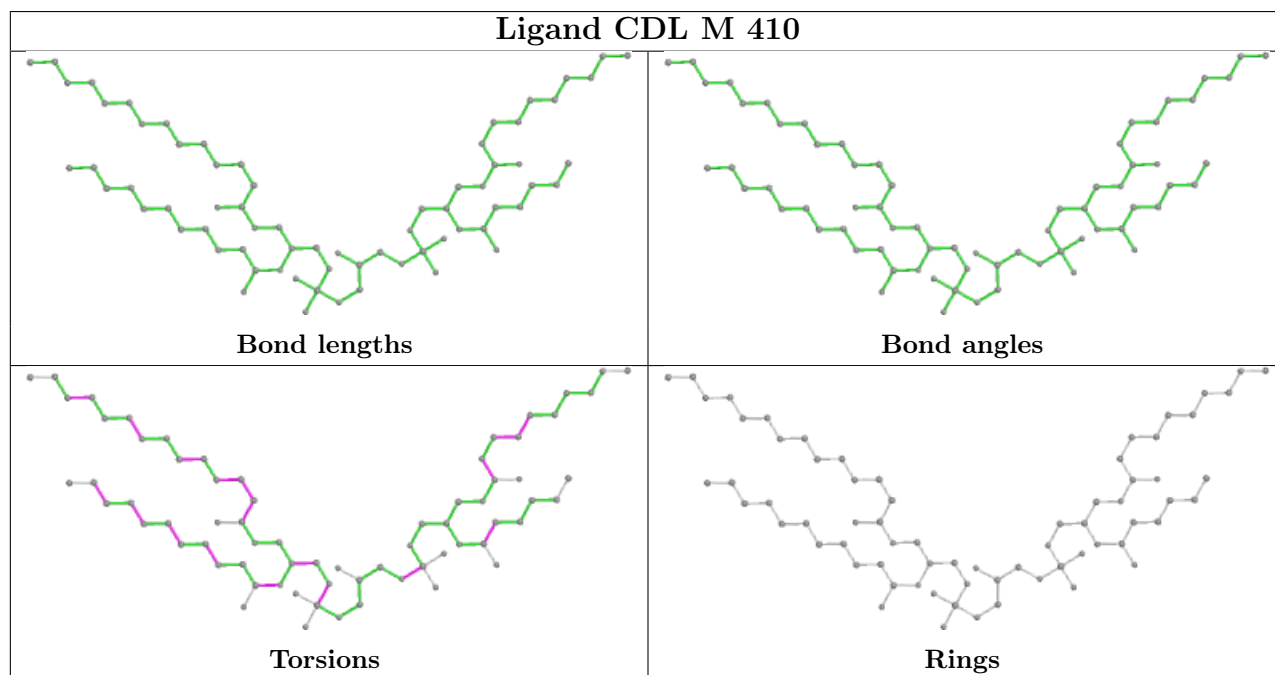
Ligand BCL L 305

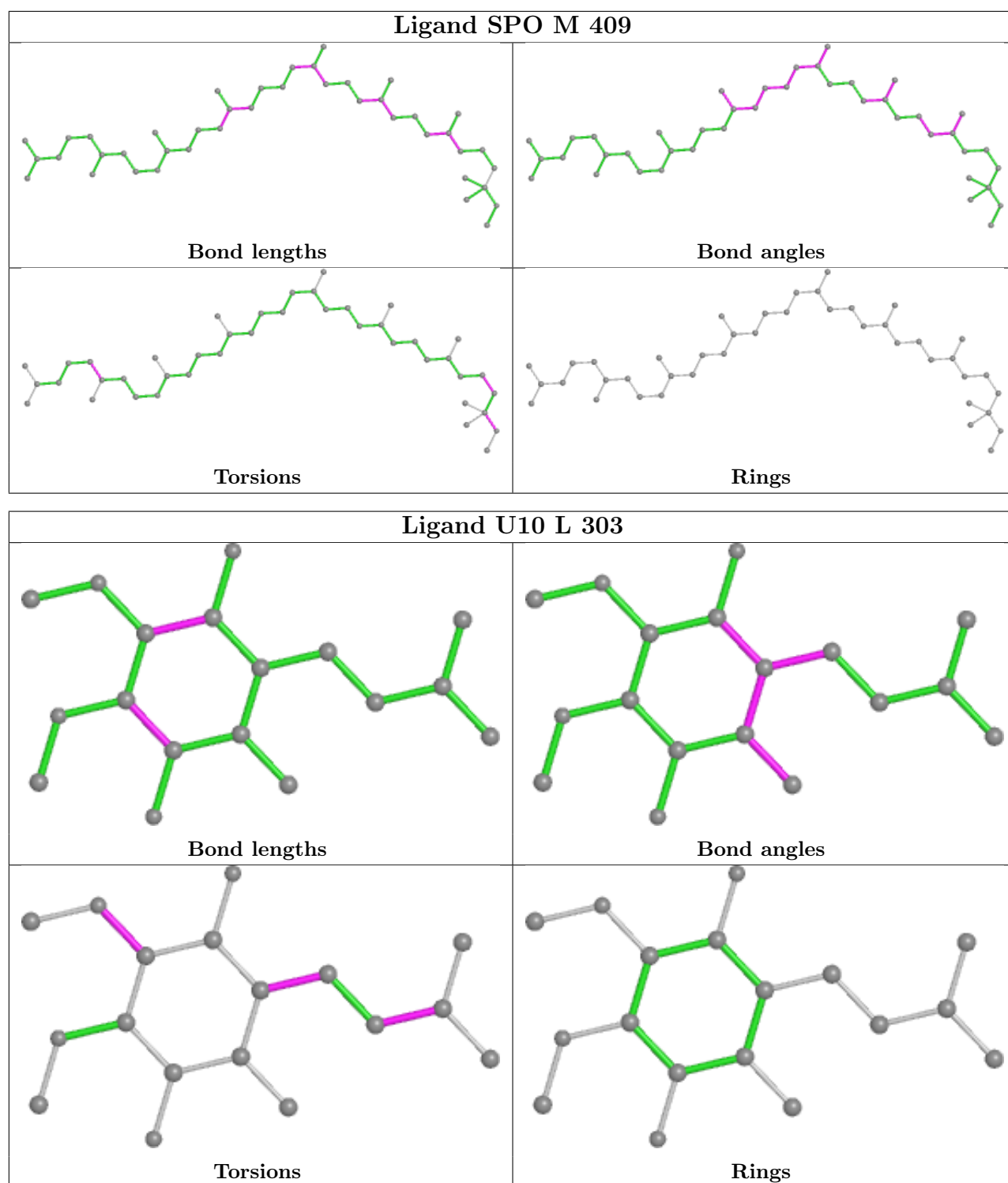


Ligand U10 M 408



Ligand CDL M 410





5.7 Other polymers [i](#)

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	240/266 (90%)	-0.58	4 (1%) 70 76	32, 45, 66, 106	0
2	L	281/282 (99%)	-0.34	10 (3%) 42 49	30, 41, 77, 94	0
3	M	300/308 (97%)	-0.25	5 (1%) 70 76	28, 45, 80, 98	0
All	All	821/856 (95%)	-0.38	19 (2%) 60 67	28, 44, 74, 106	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	59	TRP	4.4
2	L	276	PRO	4.1
3	M	105	PHE	4.0
2	L	281	GLY	3.2
2	L	273	ALA	2.9
2	L	277	GLY	2.8
2	L	274	ASN	2.7
3	M	25	ASN	2.7
2	L	271	TRP	2.6
3	M	27	ALA	2.4
1	H	250	SER	2.4
3	M	106	ALA	2.4
1	H	18[A]	TYR	2.3
2	L	265	TRP	2.2
3	M	100	GLU	2.2
2	L	202	LYS	2.2
1	H	249	LYS	2.1
2	L	270	PRO	2.1
1	H	60	LYS	2.0

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

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(Å ²)	Q<0.9
3	2LT	M	210	14/15	0.98	0.14	30,31,33,36	2

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

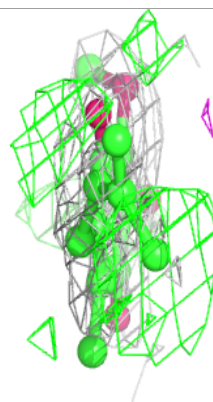
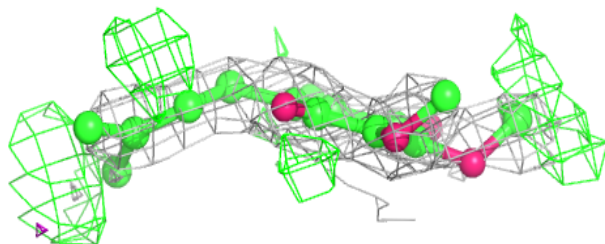
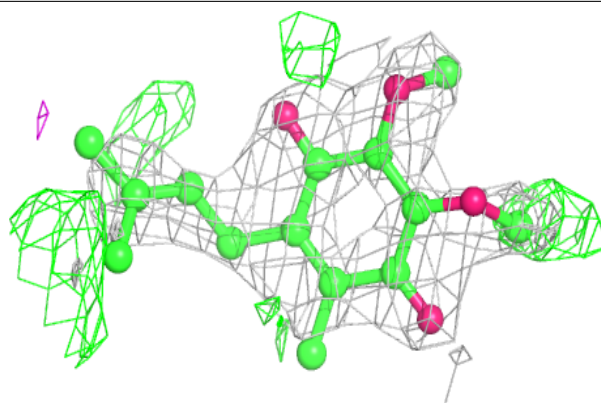
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LDA	M	405	16/16	0.55	0.25	92,98,130,133	0
4	LDA	M	404	16/16	0.68	0.30	97,108,120,120	0
4	LDA	M	403	16/16	0.80	0.30	79,87,119,120	0
4	LDA	M	402	16/16	0.85	0.22	74,79,86,87	0
7	U10	L	303	18/63	0.87	0.42	31,35,39,40	18
4	LDA	H	301	16/16	0.90	0.17	62,73,88,91	0
10	SPO	M	409	42/42	0.90	0.17	43,61,84,89	0
11	CDL	M	410	69/100	0.91	0.18	52,77,94,111	0
8	CL	L	306	1/1	0.93	0.05	81,81,81,81	0
7	U10	M	408	48/63	0.94	0.18	31,46,94,98	0
6	BPH	M	407	55/65	0.95	0.14	39,43,86,88	0
5	BCL	M	401	66/66	0.97	0.15	30,35,66,85	0
6	BPH	L	302	65/65	0.97	0.11	27,32,47,49	0
5	BCL	L	301	66/66	0.97	0.11	30,34,72,78	0
5	BCL	L	304	66/66	0.97	0.13	30,33,54,67	0
5	BCL	L	305	51/66	0.98	0.12	32,35,62,66	0
9	FE	M	406	1/1	0.99	0.10	29,29,29,29	0

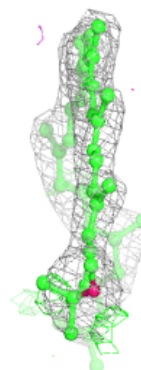
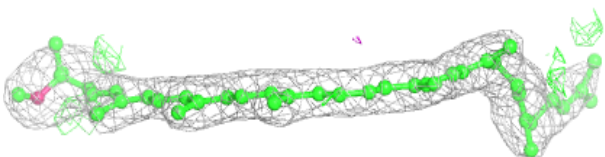
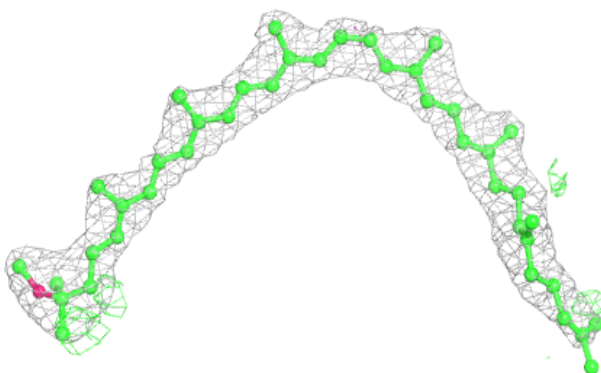
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

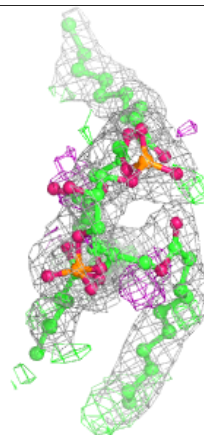
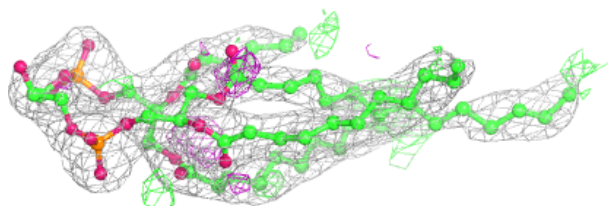
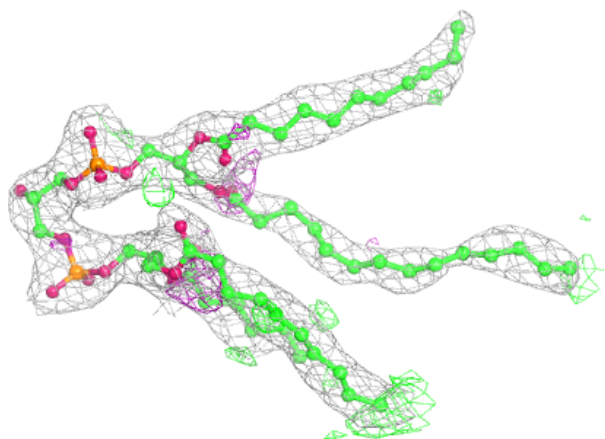
**Electron density around SPO M 409:**

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

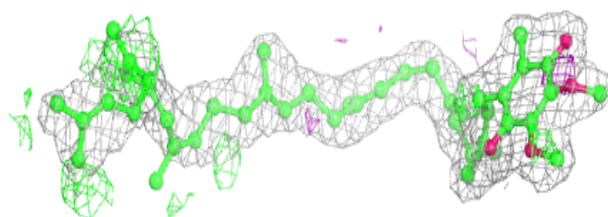
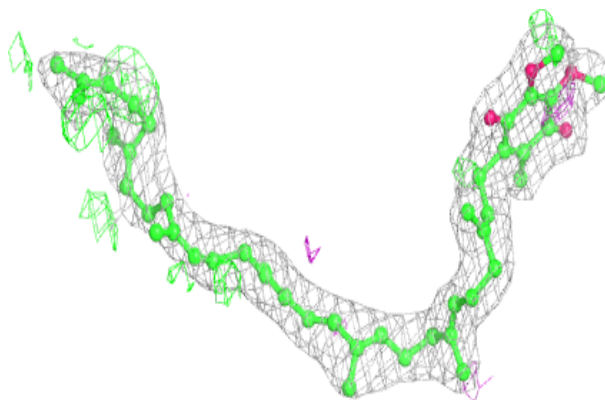


Electron density around CDL M 410:

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

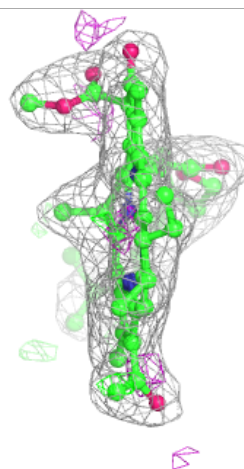
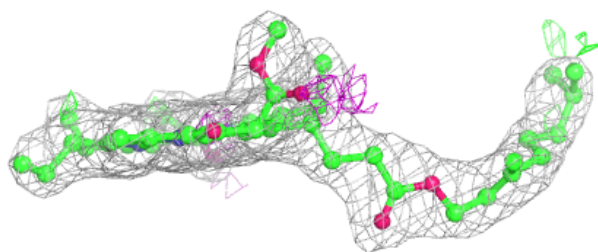
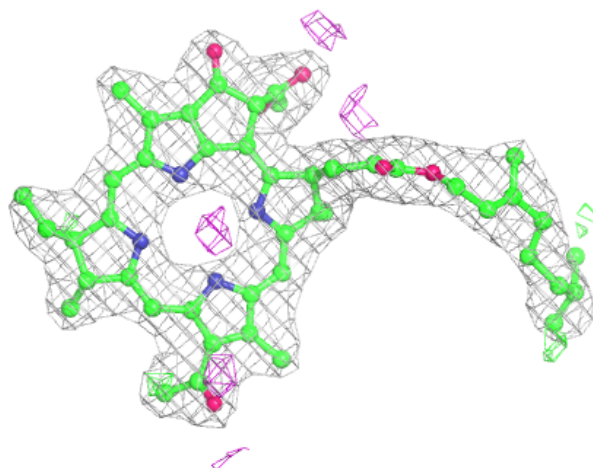
**Electron density around U10 M 408:**

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



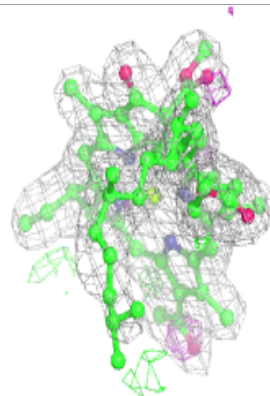
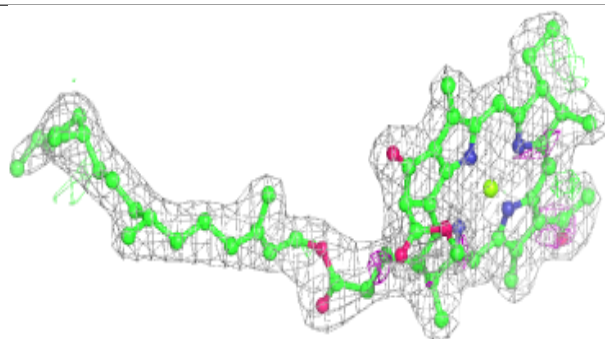
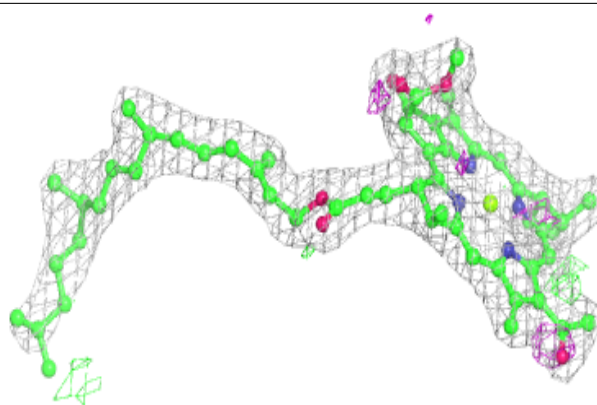
Electron density around BPH M 407:

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and green (positive)

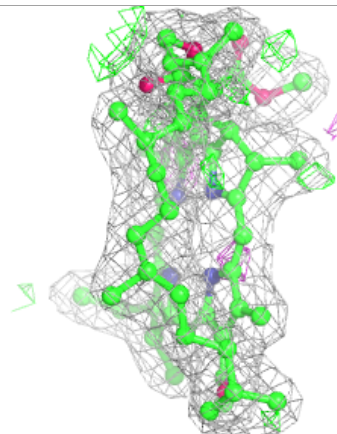
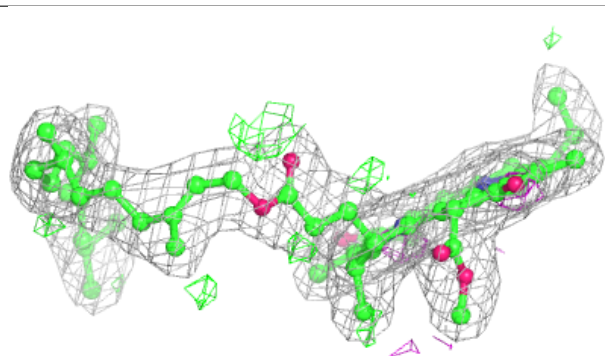
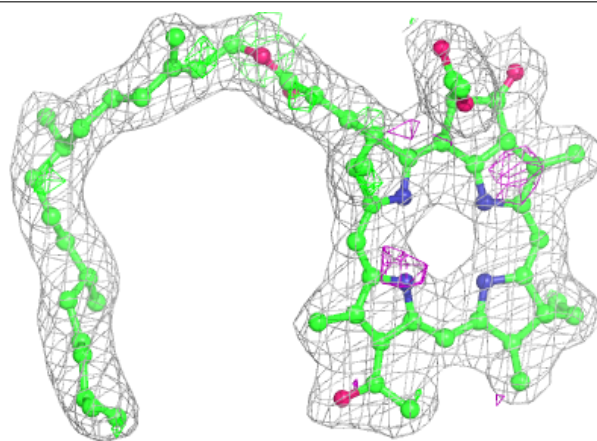


Electron density around BCL M 401:

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and green (positive)

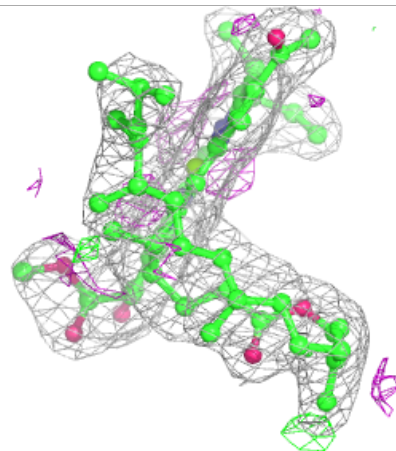
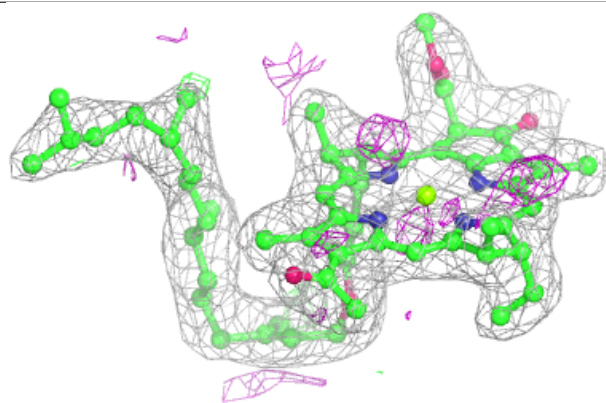
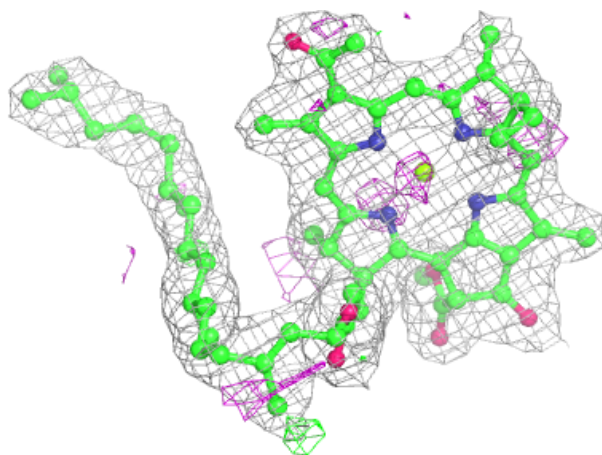
**Electron density around BPH L 302:**

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



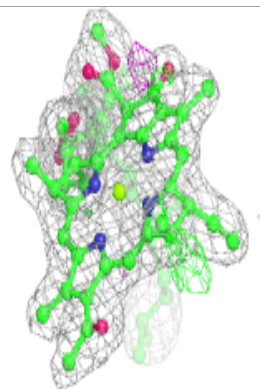
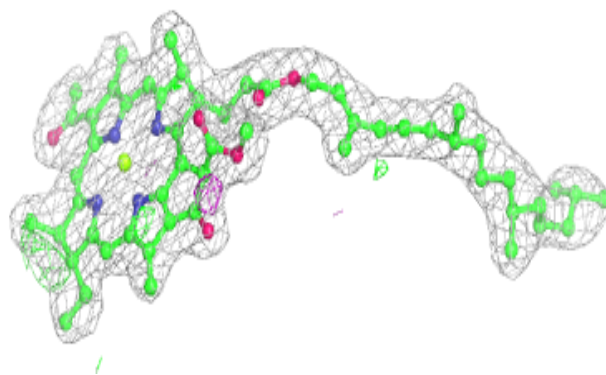
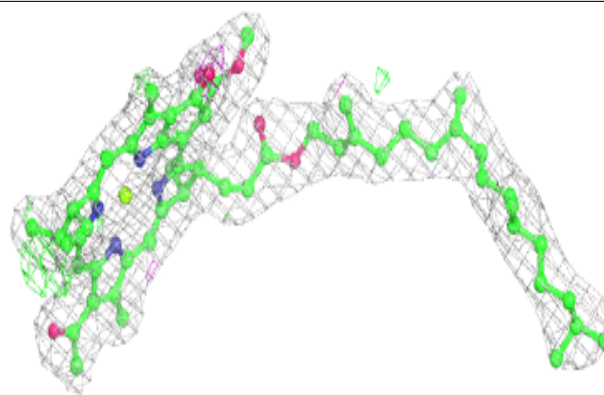
Electron density around BCL L 301:

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



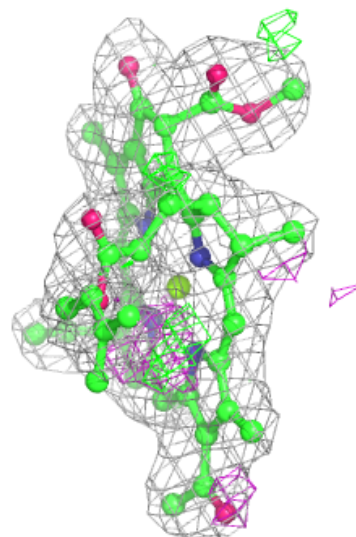
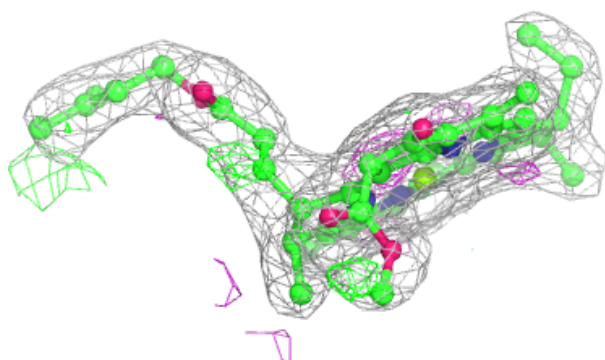
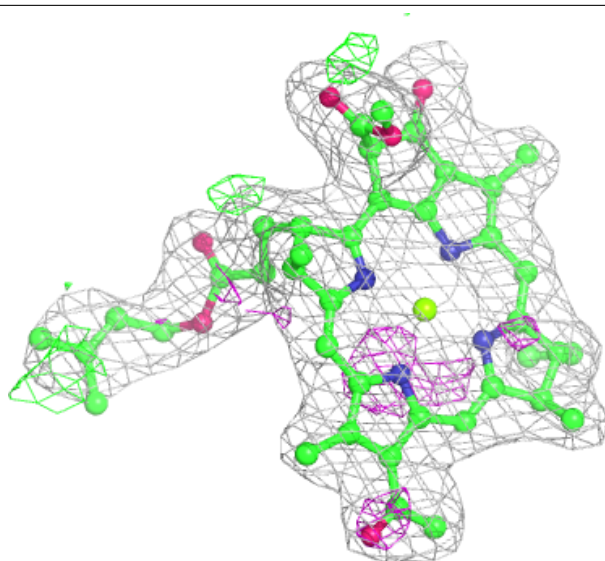
Electron density around BCL L 304:

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



Electron density around BCL L 305:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.