



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 24, 2026 – 07:52 am BST

PDB ID : 8C5X / pdb_00008c5x
Title : Double mutant A(L37)C/S(L99)C structure of Photosynthetic Reaction Center From Cereibacter sphaeroides strain RV
Authors : Gabdulkhakov, A.; Selikhanov, G.; Fufina, T.; Vasilieva, L.; Atamas, A.; Uhimchuk, D.
Deposited on : 2023-01-10
Resolution : 2.60 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	:	1.8.4, CSD as541be (2020)
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

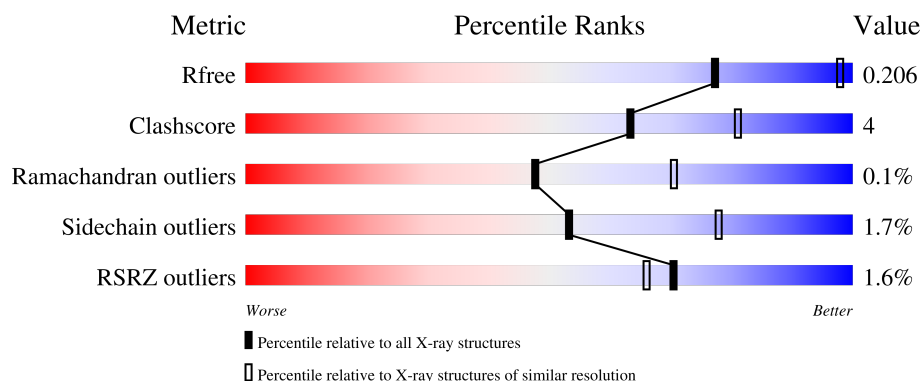
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

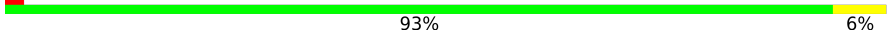
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	242	
2	L	281	
3	M	303	

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
4	LDA	M	412	-	-	-	X
5	UNL	H	303	-	-	-	X
5	UNL	L	306	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 7547 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	3	0
			1848	1183	317	339	9			

- 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
			2245	1516	356	363	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	37	CYS	ALA	engineered mutation	UNP P0C0Y8
L	99	CYS	SER	engineered mutation	UNP P0C0Y8
L	178	THR	SER	conflict	UNP P0C0Y8

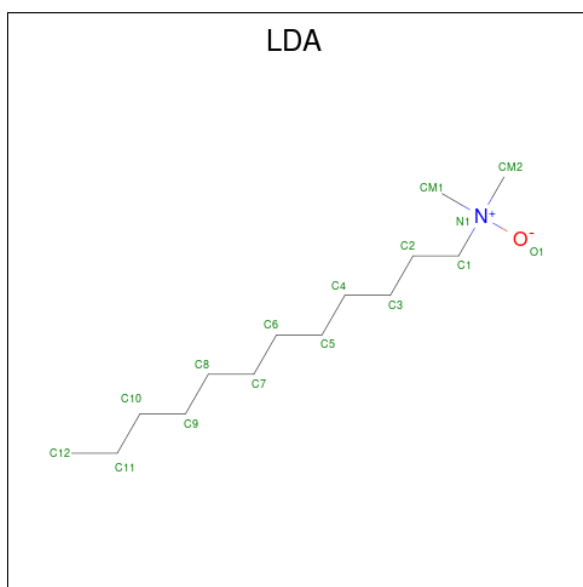
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	2	0
			2425	1621	397	397	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	conflict	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

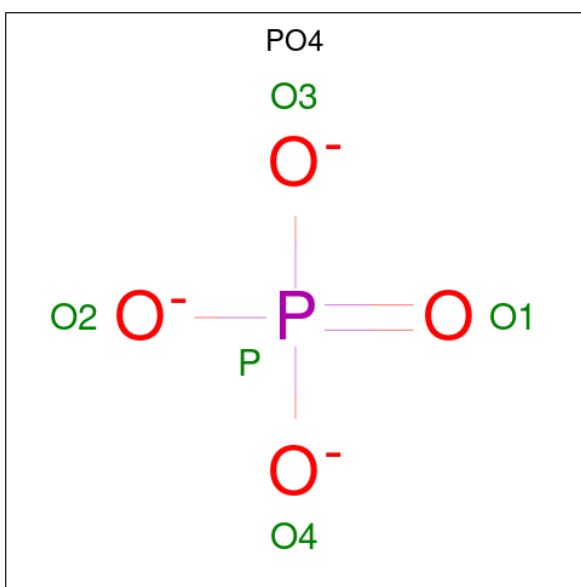


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

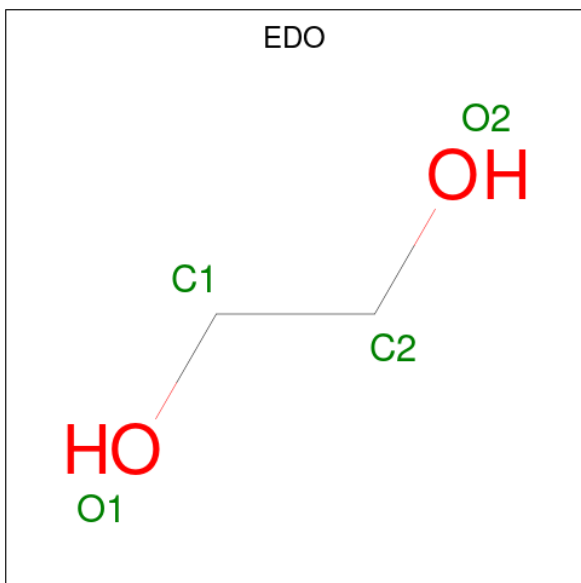
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	4	Total	C	0	0
			51	51		
5	L	3	Total	C	0	0
			37	37		
5	M	3	Total	C	0	0
			39	39		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

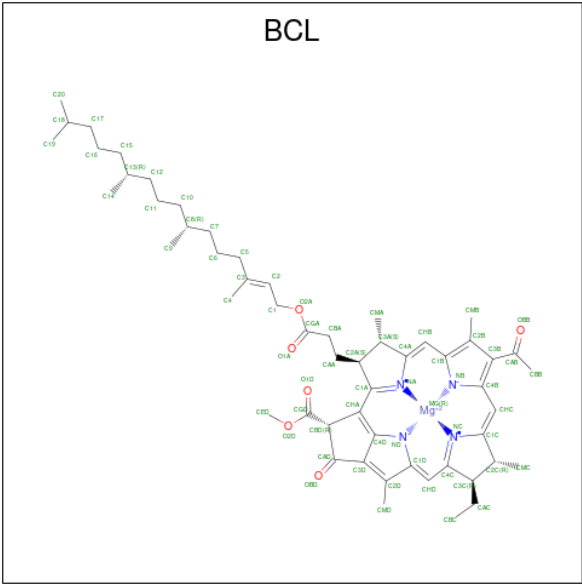


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	H	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	L	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0
7	M	1	Total C O 4 2 2	0	0

- Molecule 8 is POTASSIUM ION (CCD ID: K) (formula: K).

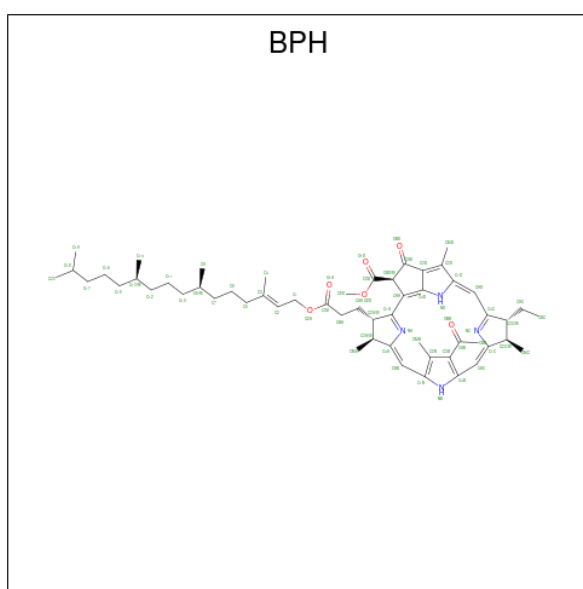
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total K 1 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



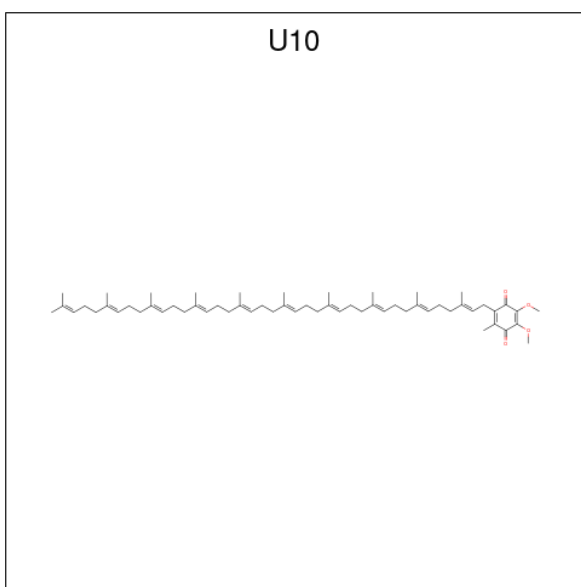
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



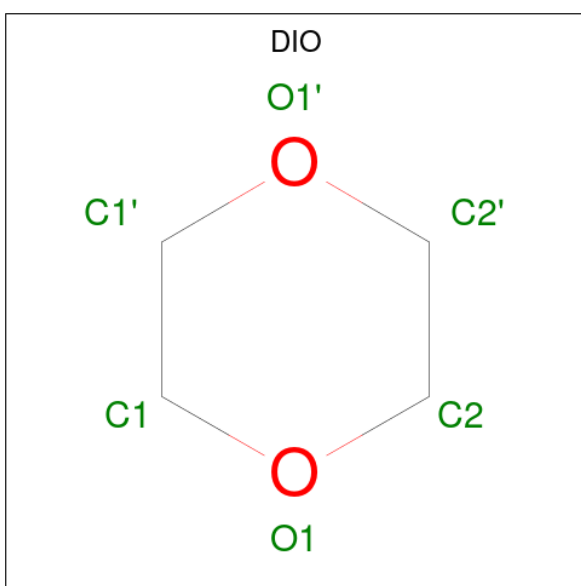
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



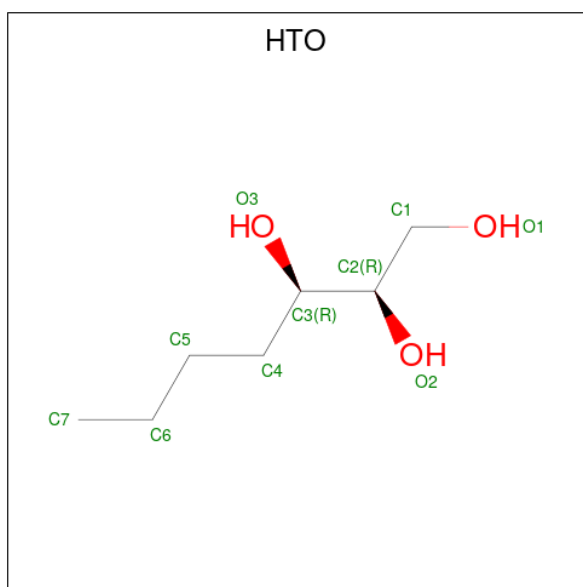
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			48	44	4		
11	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 12 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



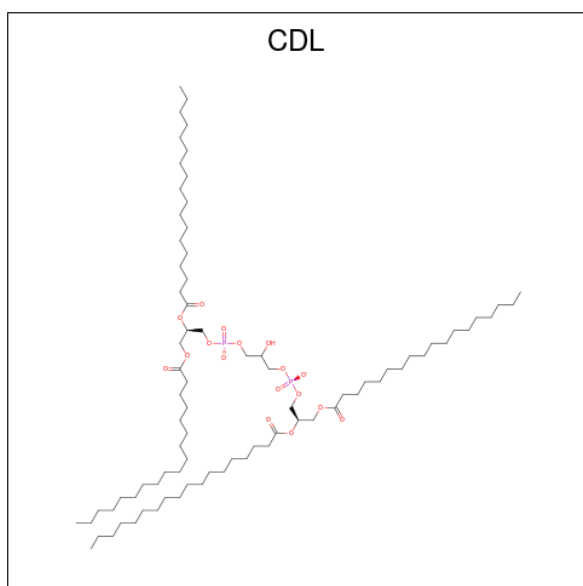
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	L	1	Total	C	O	0	0
			6	4	2		

- Molecule 13 is HEPTANE-1,2,3-TRIOL (CCD ID: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

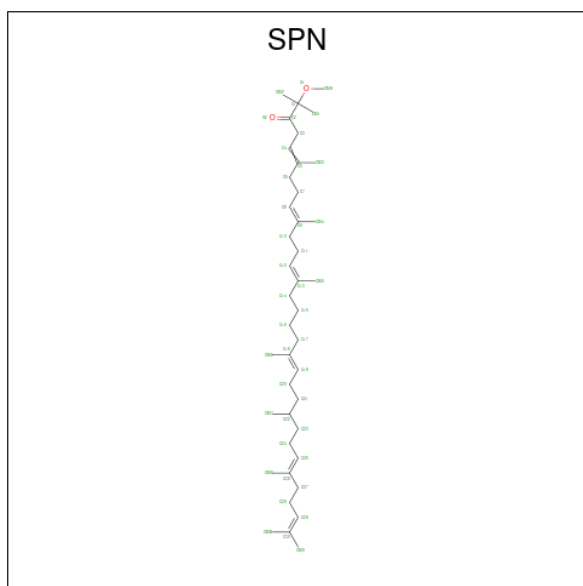


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 15 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 16 is SPEROIDENONE (CCD ID: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	43	Total	O	0	0
			43	43		
17	L	22	Total	O	0	0
			22	22		
17	M	41	Total	O	0	0
			41	41		

3 Residue-property plots [i](#)

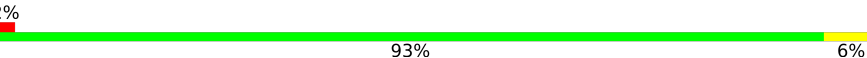
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

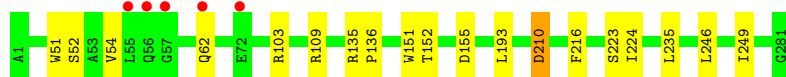
- Molecule 1: Reaction center protein H chain

Chain H:  89% 10%

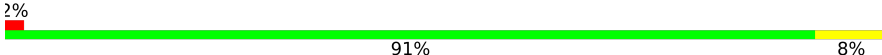


- Molecule 2: Reaction center protein L chain

Chain L:  93% 6%



- Molecule 3: Reaction center protein M chain

Chain M:  91% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.85Å 139.85Å 186.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.89 – 2.60 29.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.89-2.60) 99.9 (29.89-2.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.186 , 0.207 0.189 , 0.206	Depositor DCC
R_{free} test set	3351 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7547	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: DIO, HTO, U10, BCL, BPH, K, SPN, CDL, PO4, EDO, UNL, LDA, 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	0.39	0/1905	0.57	0/2590
2	L	0.40	0/2336	0.57	0/3197
3	M	0.38	0/2524	0.54	0/3445
All	All	0.39	0/6765	0.56	0/9232

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1848	0	1866	17	0
2	L	2245	0	2204	11	0
3	M	2425	0	2345	17	0
4	H	16	0	31	2	0
4	M	96	0	186	6	0
5	H	51	0	0	0	0
5	L	37	0	0	1	0
5	M	39	0	0	0	0
6	H	5	0	0	0	0
6	L	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	10	0	0	0	0
7	H	12	0	18	2	0
7	L	12	0	18	0	0
7	M	8	0	12	0	0
8	H	1	0	0	0	0
9	L	132	0	148	0	0
9	M	132	0	148	3	0
10	L	65	0	76	0	0
10	M	65	0	76	2	0
11	L	48	0	63	3	0
11	M	48	0	63	2	0
12	L	6	0	8	0	0
13	L	10	0	16	0	0
14	M	81	0	106	6	0
15	M	1	0	0	0	0
16	M	43	0	70	7	0
17	H	43	0	0	0	0
17	L	22	0	0	1	0
17	M	41	0	0	0	0
All	All	7547	0	7454	59	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 4.

The worst 5 of 59 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:H:301:LDA:H121	4:M:408:LDA:H91	1.63	0.78
3:M:34:PRO:HA	4:M:412:LDA:H101	1.75	0.68
2:L:62:GLN:OE1	2:L:151:TRP:NE1	2.28	0.66
3:M:161:GLY:HA3	16:M:407:SPN:H201	1.78	0.65
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.80	0.63

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	241/242 (100%)	238 (99%)	3 (1%)	0	100	100
2	L	281/281 (100%)	268 (95%)	12 (4%)	1 (0%)	30	51
3	M	302/303 (100%)	291 (96%)	11 (4%)	0	100	100
All	All	824/826 (100%)	797 (97%)	26 (3%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	52	SER

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	198/197 (100%)	195 (98%)	3 (2%)	57	80
2	L	223/221 (101%)	220 (99%)	3 (1%)	61	82
3	M	238/237 (100%)	233 (98%)	5 (2%)	47	73
All	All	659/655 (101%)	648 (98%)	11 (2%)	53	78

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	62	SER
3	M	182	HIS

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Mol	Chain	Res	Type
3	M	274	VAL
3	M	265	ILE
2	L	216	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	129	ASN
2	L	258	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 43 ligands modelled in this entry, 10 are unknown and 2 are monoatomic - leaving 31 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	$\# Z > 2$
7	EDO	H	308	-	3,3,3	0.60	0	2,2,2	0.13	0
4	LDA	M	420	-	12,15,15	2.07	1 (8%)	14,17,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	M	419	-	3,3,3	0.55	0	2,2,2	0.28	0
13	HTO	L	312	-	9,9,9	0.47	0	10,10,10	1.11	1 (10%)
7	EDO	L	309	-	3,3,3	0.52	0	2,2,2	0.30	0
16	SPN	M	407	-	40,42,42	0.38	0	50,52,52	0.70	0
6	PO4	H	306	-	4,4,4	0.86	0	6,6,6	0.49	0
14	CDL	M	401	-	80,80,99	0.47	1 (1%)	86,92,111	0.37	0
6	PO4	M	416	-	4,4,4	0.98	0	6,6,6	0.47	0
9	BCL	M	402	3	69,74,74	1.28	8 (11%)	83,115,115	1.57	15 (18%)
7	EDO	L	310	-	3,3,3	0.43	0	2,2,2	0.50	0
10	BPH	M	404	-	59,70,70	1.24	5 (8%)	61,101,101	2.10	13 (21%)
12	DIO	L	308	-	6,6,6	0.50	0	6,6,6	0.08	0
7	EDO	L	311	-	3,3,3	0.48	0	2,2,2	0.64	0
7	EDO	H	309	-	3,3,3	0.50	0	2,2,2	0.32	0
9	BCL	L	302	2	69,74,74	1.34	10 (14%)	83,115,115	1.46	12 (14%)
4	LDA	M	408	-	12,15,15	2.14	1 (8%)	14,17,17	0.44	0
9	BCL	L	301	2	69,74,74	1.35	8 (11%)	83,115,115	1.42	11 (13%)
4	LDA	H	301	-	12,15,15	1.94	1 (8%)	14,17,17	0.54	0
11	U10	L	304	-	48,48,63	2.58	12 (25%)	58,61,79	2.10	22 (37%)
9	BCL	M	403	3	69,74,74	1.34	8 (11%)	83,115,115	1.40	8 (9%)
4	LDA	M	412	-	12,15,15	2.01	1 (8%)	14,17,17	0.44	0
6	PO4	M	417	-	4,4,4	0.70	0	6,6,6	0.50	0
7	EDO	H	307	-	3,3,3	0.61	0	2,2,2	0.24	0
7	EDO	M	418	-	3,3,3	0.52	0	2,2,2	0.61	0
11	U10	M	406	-	48,48,63	2.66	13 (27%)	58,61,79	1.80	16 (27%)
6	PO4	L	313	-	4,4,4	0.72	0	6,6,6	0.57	0
4	LDA	M	410	-	12,15,15	2.11	1 (8%)	14,17,17	0.67	0
4	LDA	M	411	-	12,15,15	2.08	1 (8%)	14,17,17	0.50	0
10	BPH	L	303	-	59,70,70	1.32	8 (13%)	61,101,101	2.12	10 (16%)
4	LDA	M	409	-	12,15,15	1.98	1 (8%)	14,17,17	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	H	308	-	-	0/1/1/1	-
4	LDA	M	420	-	-	10/13/13/13	-
7	EDO	M	419	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	HTO	L	312	-	-	4/10/10/10	-
7	EDO	L	309	-	-	0/1/1/1	-
16	SPN	M	407	-	-	13/50/51/51	-
14	CDL	M	401	-	-	34/91/91/110	-
9	BCL	M	402	3	-	7/41/137/137	-
7	EDO	L	310	-	-	0/1/1/1	-
10	BPH	M	404	-	-	9/37/105/105	0/5/6/6
12	DIO	L	308	-	-	-	0/1/1/1
7	EDO	L	311	-	-	1/1/1/1	-
7	EDO	H	309	-	-	0/1/1/1	-
9	BCL	L	302	2	-	1/41/137/137	-
4	LDA	M	408	-	-	4/13/13/13	-
9	BCL	L	301	2	-	2/41/137/137	-
4	LDA	H	301	-	-	8/13/13/13	-
11	U10	L	304	-	-	16/45/69/87	0/1/1/1
9	BCL	M	403	3	-	2/41/137/137	-
4	LDA	M	412	-	-	4/13/13/13	-
7	EDO	H	307	-	-	0/1/1/1	-
7	EDO	M	418	-	-	0/1/1/1	-
11	U10	M	406	-	-	10/45/69/87	0/1/1/1
4	LDA	M	410	-	-	4/13/13/13	-
4	LDA	M	411	-	-	6/13/13/13	-
10	BPH	L	303	-	-	3/37/105/105	0/5/6/6
4	LDA	M	409	-	-	5/13/13/13	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	410	LDA	O1-N1	-7.25	1.25	1.42
4	M	408	LDA	O1-N1	-7.21	1.25	1.42
4	M	411	LDA	O1-N1	-7.14	1.25	1.42
4	M	420	LDA	O1-N1	-7.09	1.25	1.42
4	M	412	LDA	O1-N1	-6.86	1.26	1.42

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	303	BPH	C4D-CHA-CBD	-12.35	102.93	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	404	BPH	C4D-CHA-CBD	-10.34	103.84	108.52
9	M	402	BCL	CHD-C1D-ND	-5.55	119.35	124.45
11	L	304	U10	C1M-C1-C6	-5.38	115.62	124.40
9	L	301	BCL	CHD-C1D-ND	-5.06	119.80	124.45

There are no chirality outliers.

5 of 143 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	M	408	LDA	C2-C1-N1-CM1
4	M	409	LDA	C2-C1-N1-O1
4	M	409	LDA	C2-C1-N1-CM1

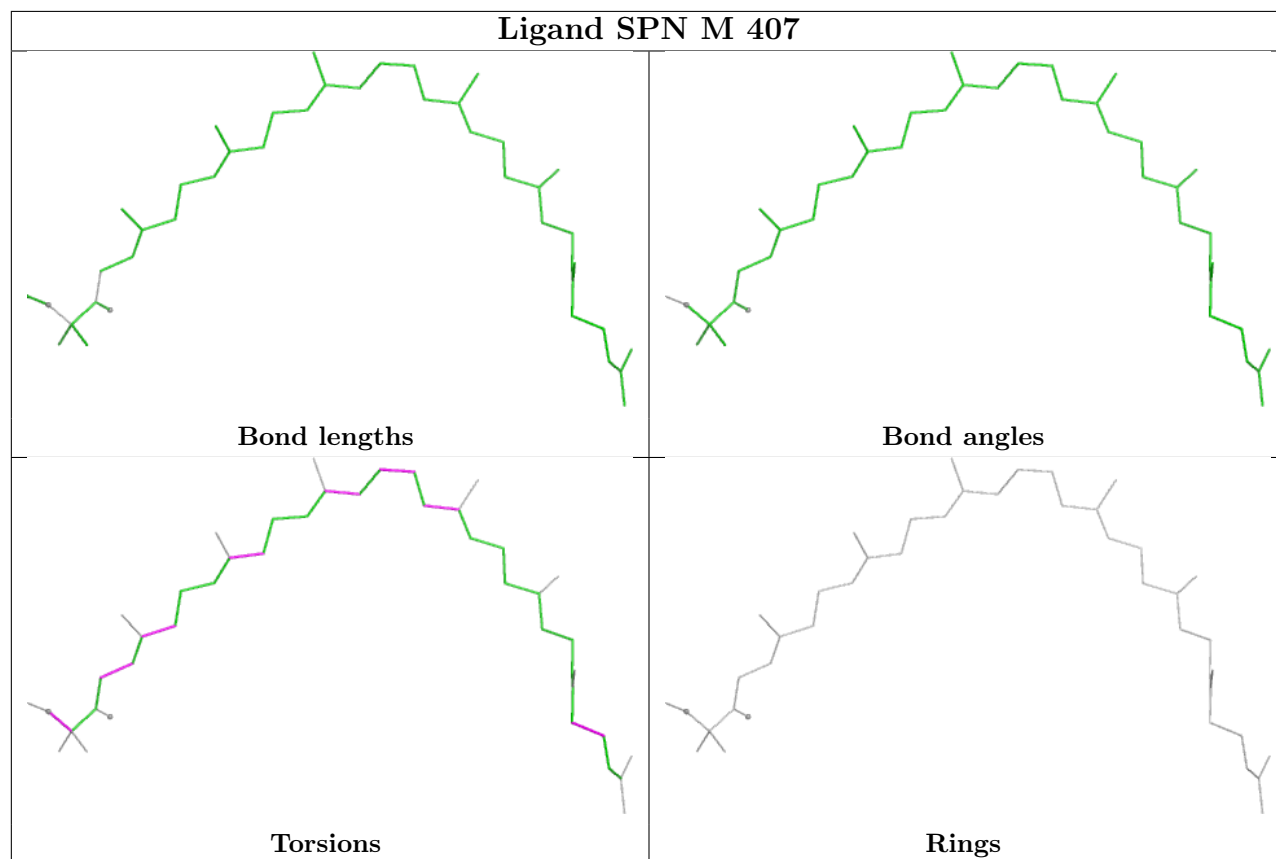
There are no ring outliers.

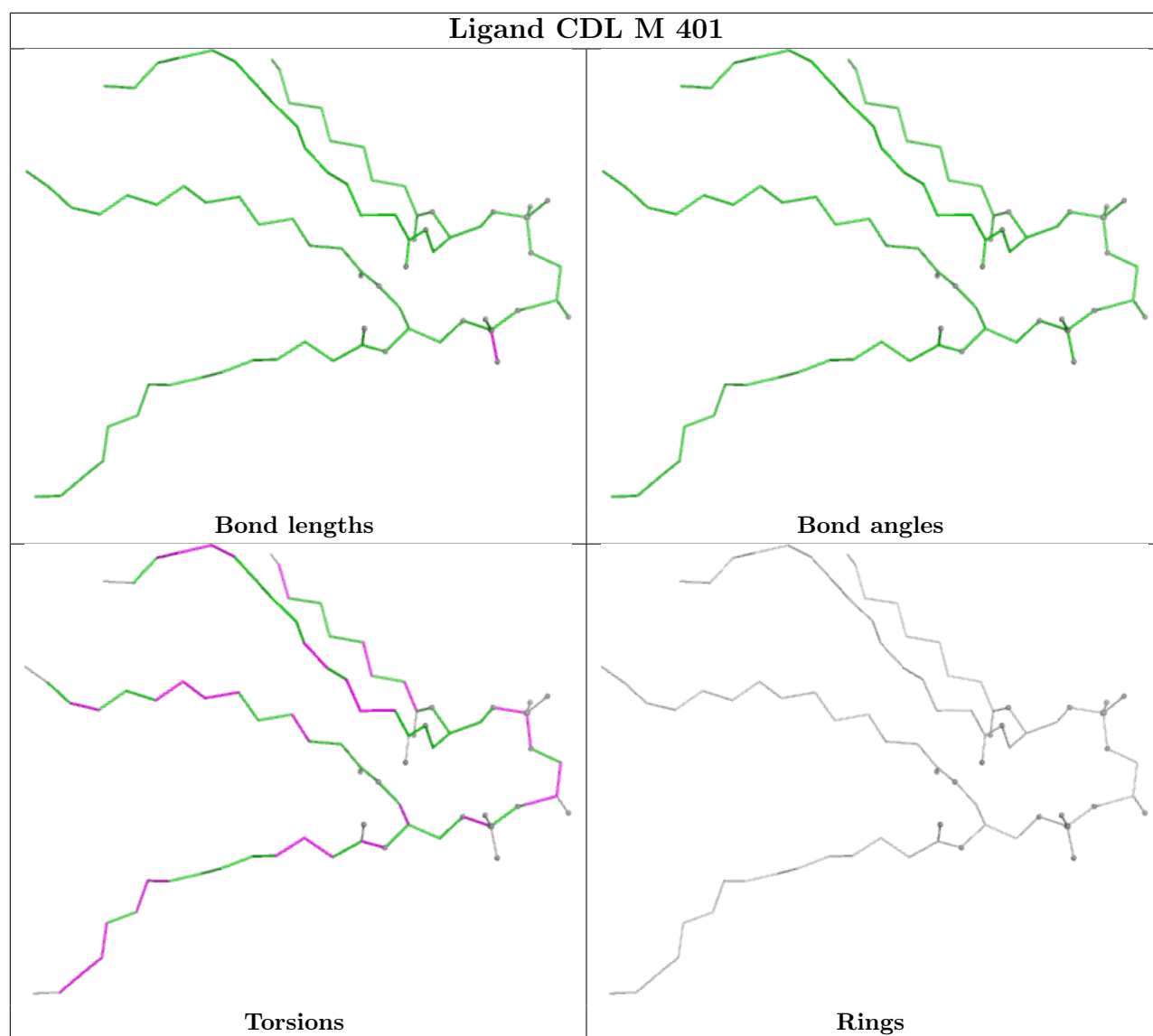
13 monomers are involved in 30 short contacts:

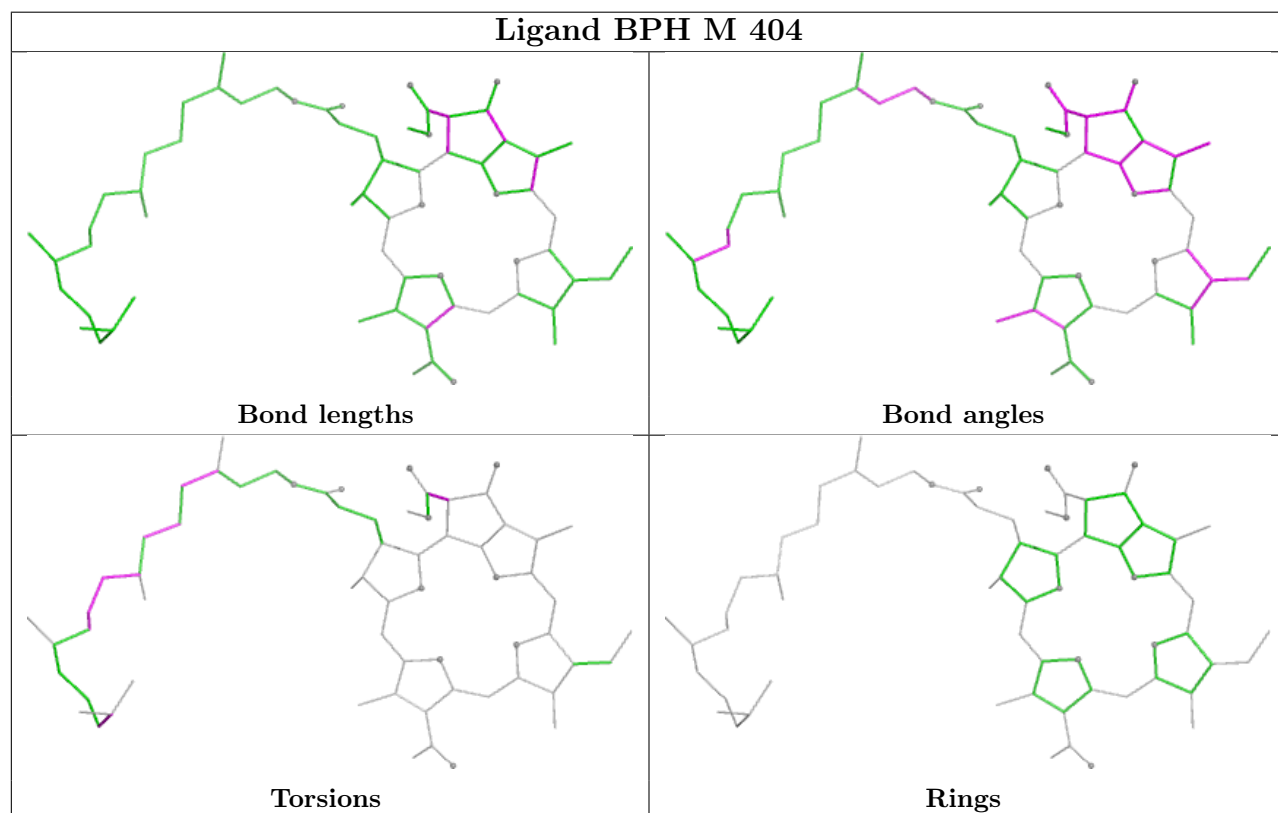
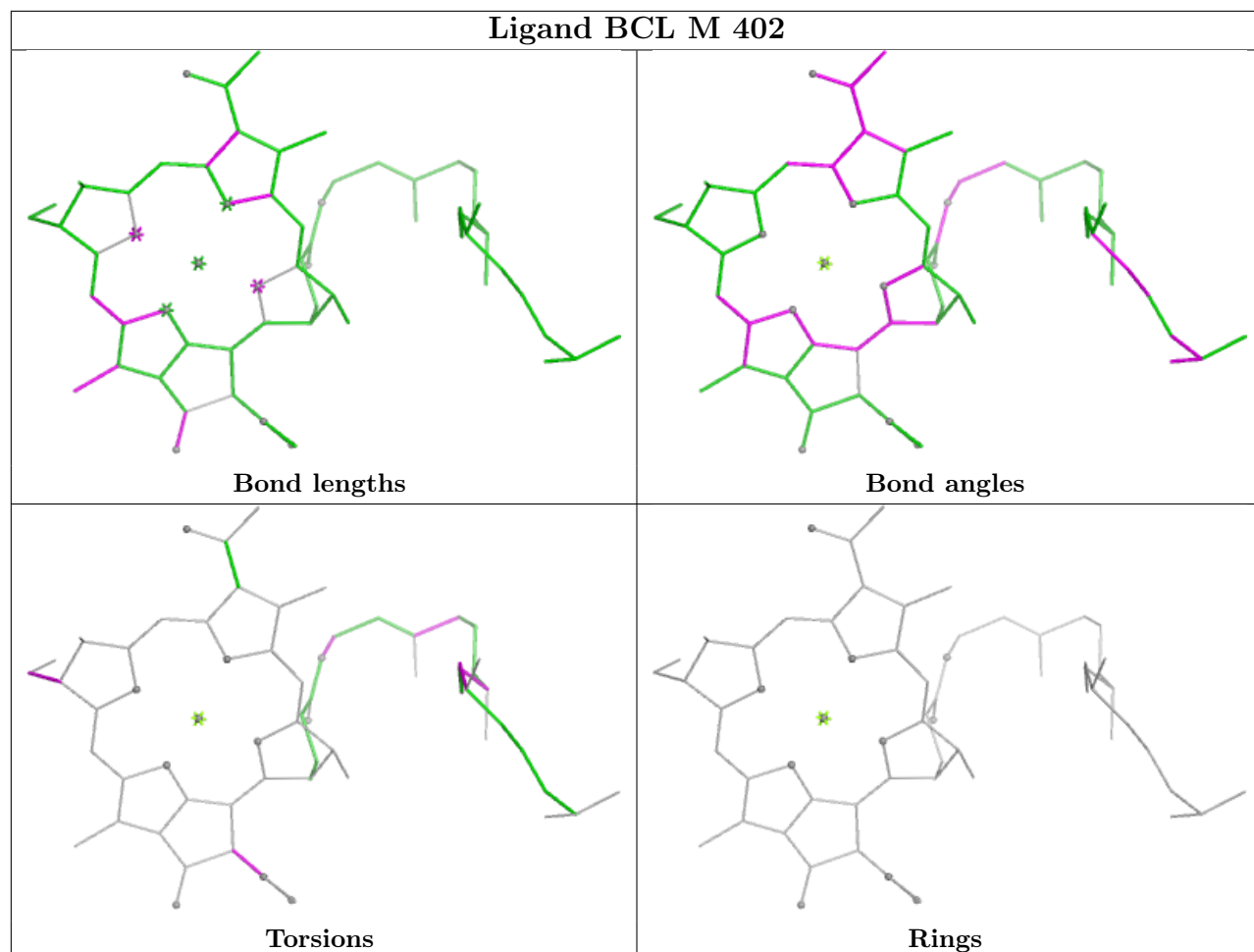
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	420	LDA	1	0
16	M	407	SPN	7	0
14	M	401	CDL	6	0
9	M	402	BCL	2	0
10	M	404	BPH	2	0
4	M	408	LDA	2	0
4	H	301	LDA	2	0
11	L	304	U10	3	0
9	M	403	BCL	1	0
4	M	412	LDA	2	0
7	H	307	EDO	2	0
11	M	406	U10	2	0
4	M	410	LDA	1	0

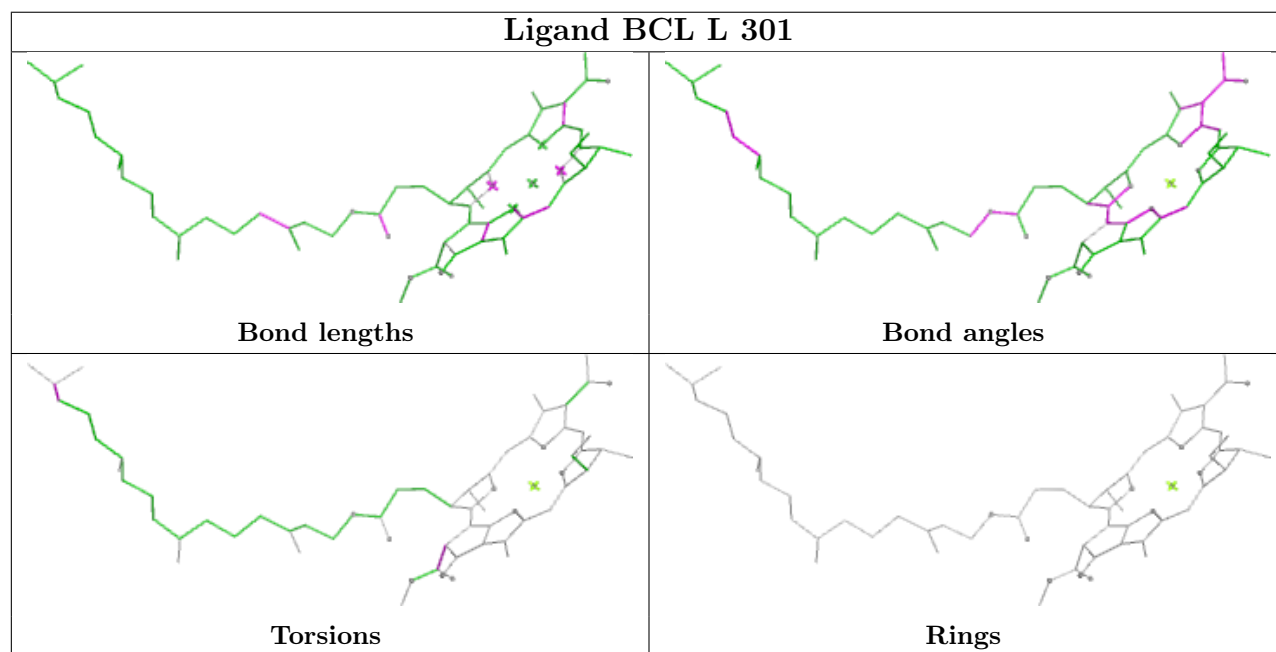
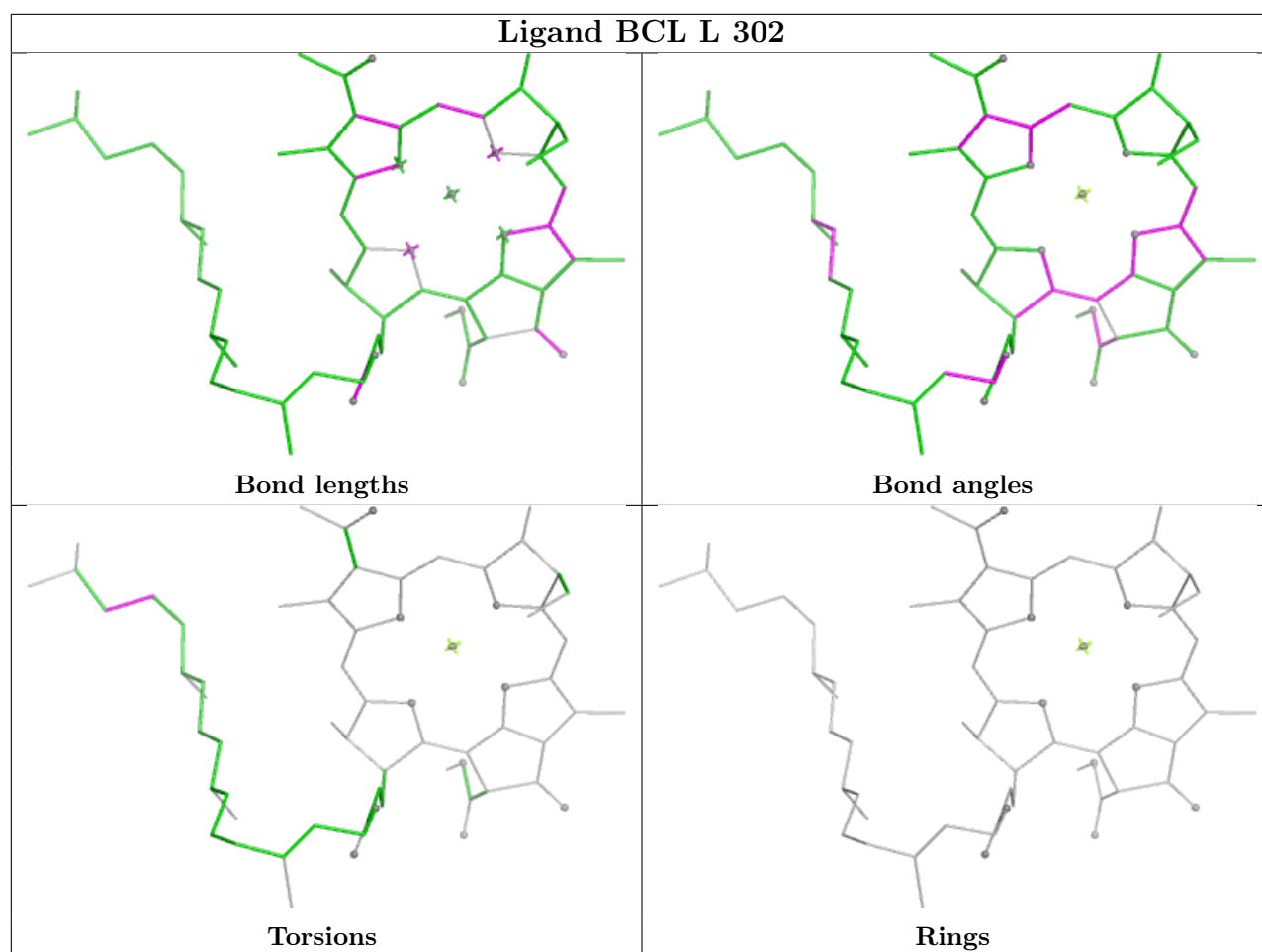
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

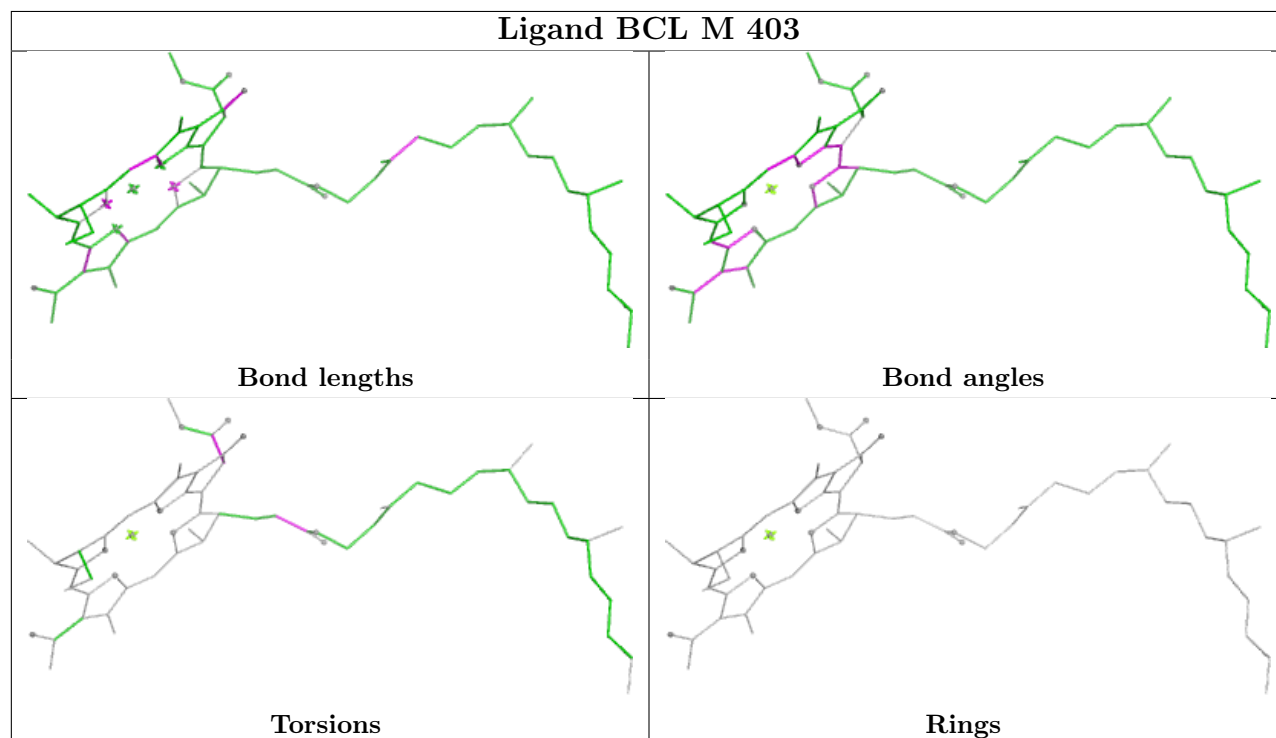
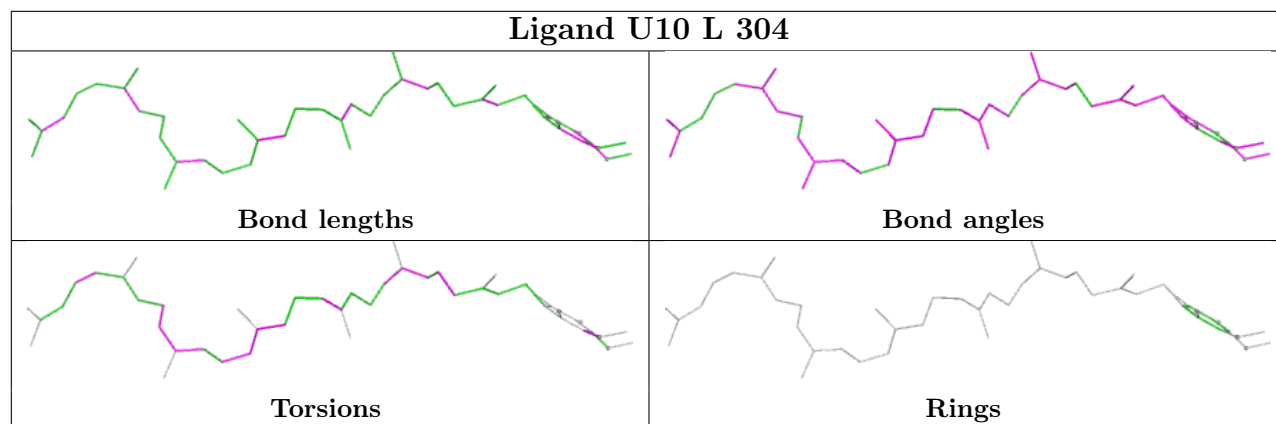
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

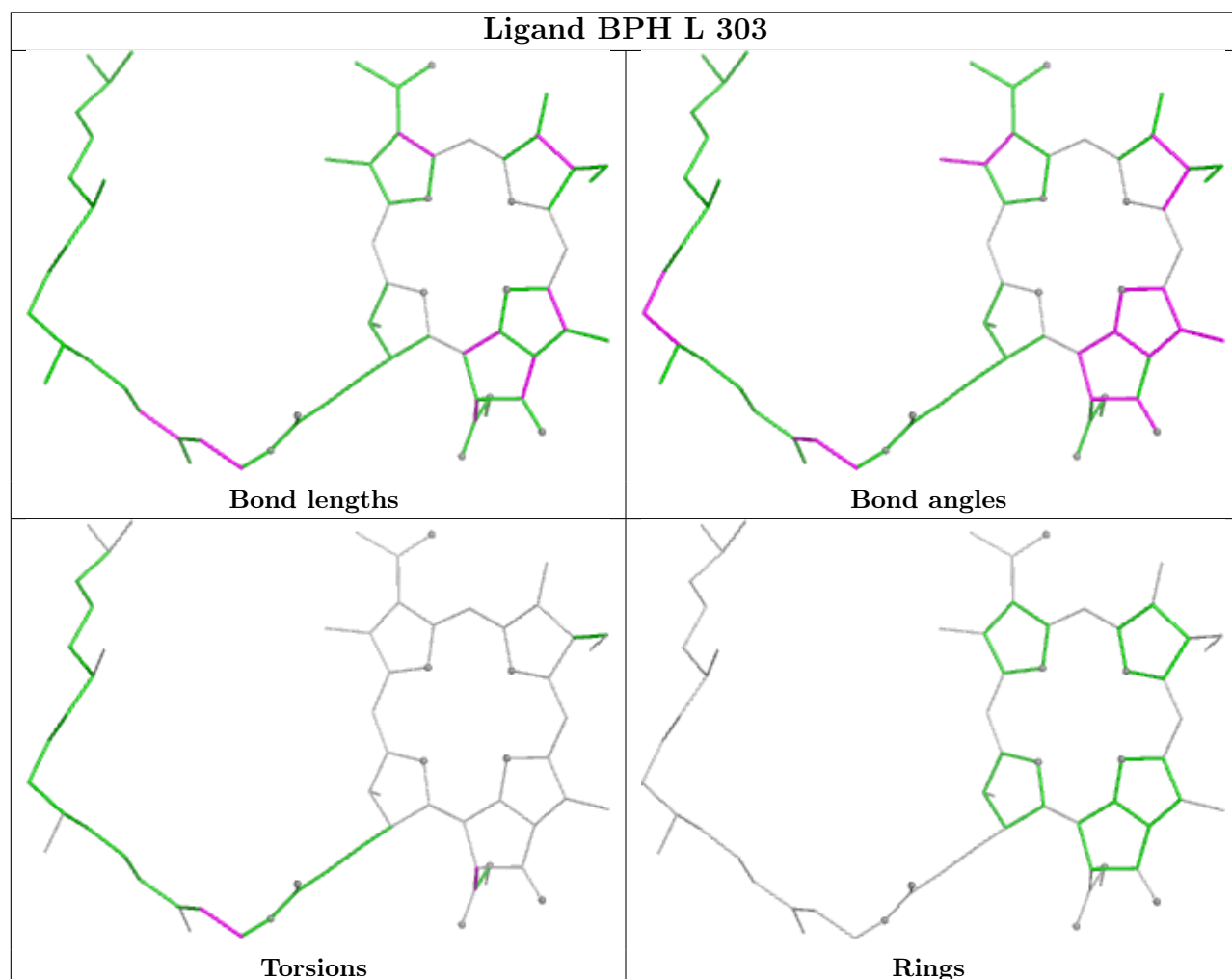
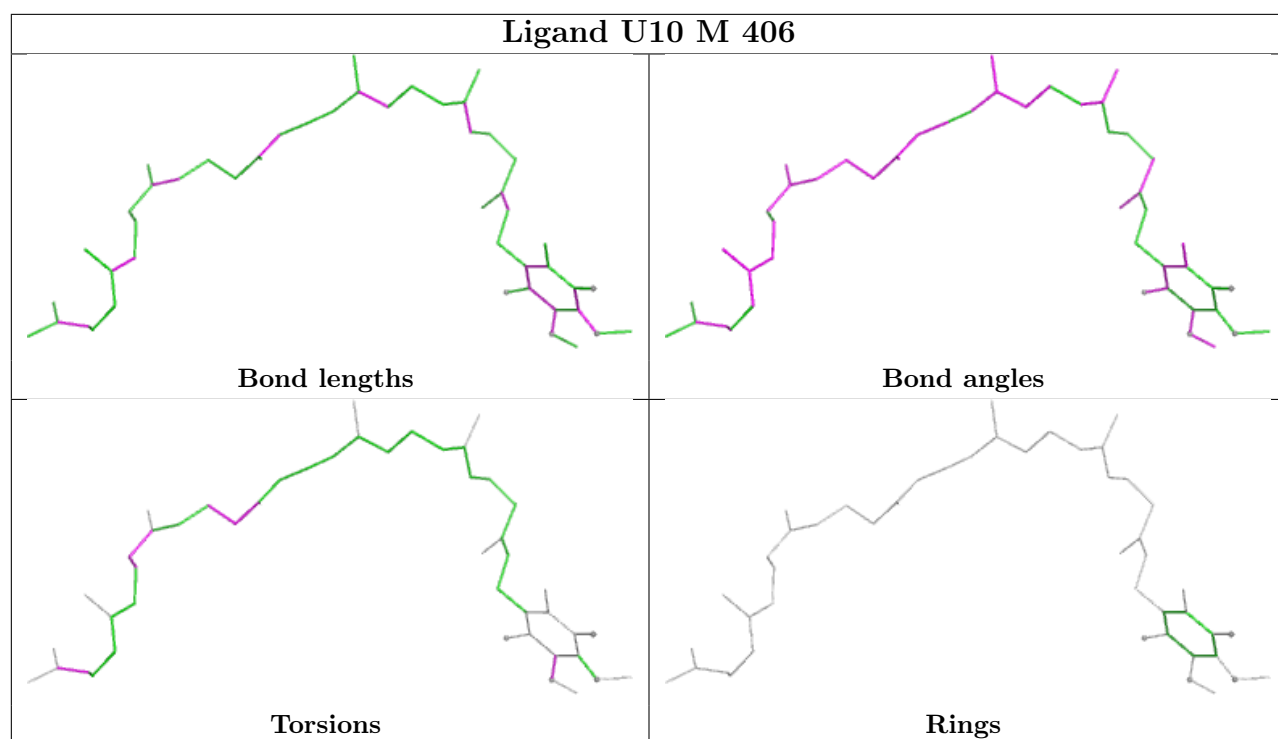












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	H	240/242 (99%)	-0.49	1 (0%) 88 86	26, 47, 61, 87	3 (1%)
2	L	281/281 (100%)	-0.23	5 (1%) 67 63	26, 48, 75, 105	2 (0%)
3	M	302/303 (99%)	-0.31	7 (2%) 61 55	25, 49, 70, 95	2 (0%)
All	All	823/826 (99%)	-0.33	13 (1%) 70 66	25, 48, 70, 105	7 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	188	ASN	3.1
2	L	56	GLN	3.0
3	M	302	GLY	3.0
3	M	1	ALA	3.0
1	H	250	SER	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](#)

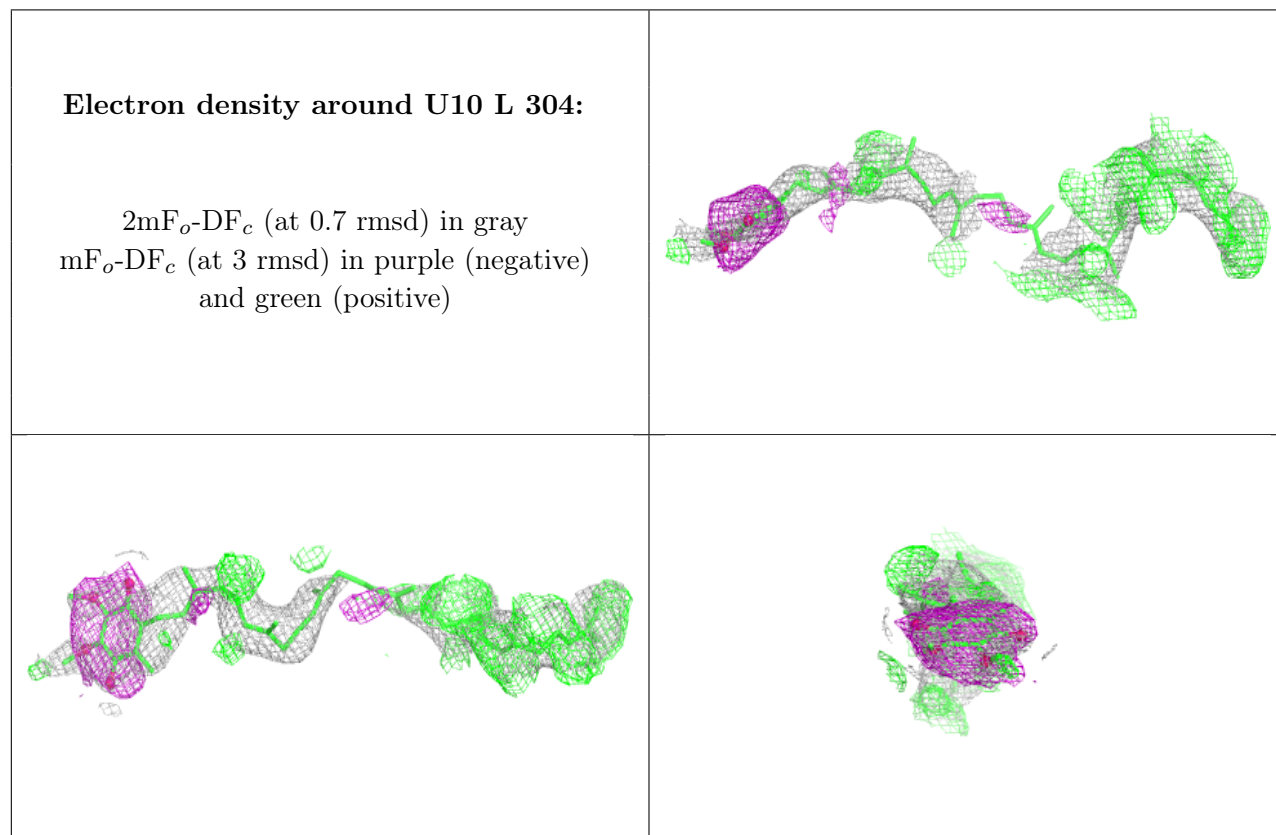
There are no oligosaccharides in this entry.

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.

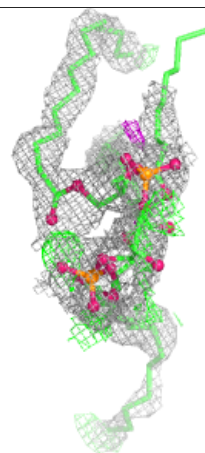
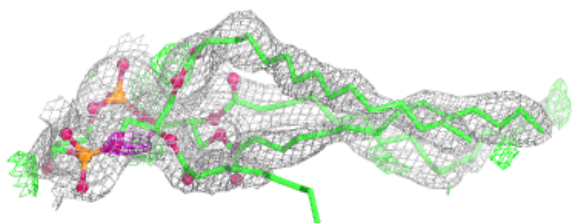
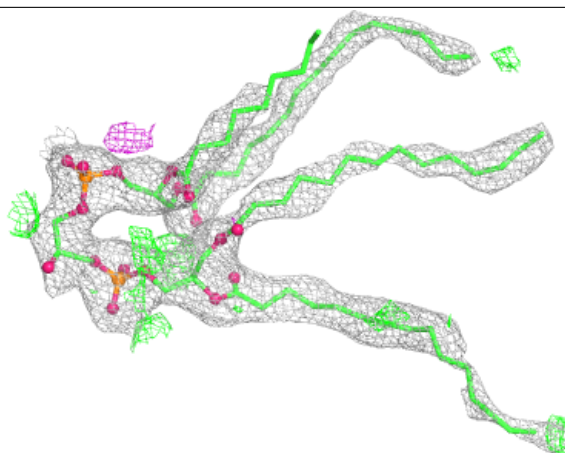
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LDA	M	412	16/16	0.44	0.51	81,108,126,131	0
5	UNL	H	303	12/-	0.57	0.40	85,89,96,99	0
5	UNL	L	306	15/-	0.60	0.40	47,64,81,85	0
11	U10	L	304	48/63	0.61	0.37	43,71,109,123	0
5	UNL	H	305	15/-	0.63	0.29	69,73,94,96	0
5	UNL	H	304	12/-	0.68	0.29	76,81,104,105	0
5	UNL	H	302	12/-	0.68	0.29	73,79,86,86	0
4	LDA	M	420	16/16	0.72	0.28	68,77,117,120	0
5	UNL	M	415	12/-	0.74	0.40	58,84,94,94	0
5	UNL	M	413	15/-	0.76	0.35	53,72,87,91	0
4	LDA	M	410	16/16	0.79	0.23	59,69,94,107	0
5	UNL	M	414	12/-	0.81	0.29	62,71,81,83	0
13	HTO	L	312	10/10	0.82	0.21	63,75,86,89	0
12	DIO	L	308	6/6	0.83	0.24	92,94,95,101	0
4	LDA	M	409	16/16	0.84	0.19	60,68,84,86	0
4	LDA	M	411	16/16	0.85	0.24	73,79,95,98	0
7	EDO	H	307	4/4	0.85	0.21	61,67,73,74	0
7	EDO	H	309	4/4	0.85	0.23	61,64,75,83	0
6	PO4	H	306	5/5	0.87	0.17	80,88,92,94	0
6	PO4	M	417	5/5	0.88	0.12	47,47,61,68	5
7	EDO	L	311	4/4	0.89	0.19	53,58,62,64	0
14	CDL	M	401	81/100	0.89	0.21	42,64,80,87	81
4	LDA	M	408	16/16	0.90	0.15	39,60,73,78	0
10	BPH	M	404	65/65	0.90	0.13	38,49,107,122	0
5	UNL	L	305	12/-	0.90	0.17	61,66,73,74	0
5	UNL	L	307	10/-	0.91	0.22	53,74,80,82	0
11	U10	M	406	48/63	0.92	0.12	33,47,68,78	0
6	PO4	L	313	5/5	0.92	0.16	71,84,104,110	0
4	LDA	H	301	16/16	0.92	0.15	66,74,80,82	0
7	EDO	L	309	4/4	0.92	0.17	61,65,70,73	0
7	EDO	H	308	4/4	0.93	0.17	47,48,50,65	0
6	PO4	M	416	5/5	0.93	0.08	77,78,84,89	0
7	EDO	M	418	4/4	0.93	0.15	47,48,51,54	0
16	SPN	M	407	43/43	0.94	0.12	41,56,70,86	0
9	BCL	M	402	66/66	0.95	0.10	35,48,85,95	0
7	EDO	L	310	4/4	0.96	0.15	47,48,52,56	0
10	BPH	L	303	65/65	0.97	0.07	33,41,53,57	0
9	BCL	L	302	66/66	0.97	0.07	35,43,56,69	0
7	EDO	M	419	4/4	0.97	0.08	43,46,49,50	0
9	BCL	M	403	66/66	0.97	0.08	36,46,66,80	0
9	BCL	L	301	66/66	0.98	0.07	36,45,52,55	0
8	K	H	310	1/1	0.99	0.06	50,50,50,50	0
15	FE	M	405	1/1	1.00	0.02	39,39,39,39	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.

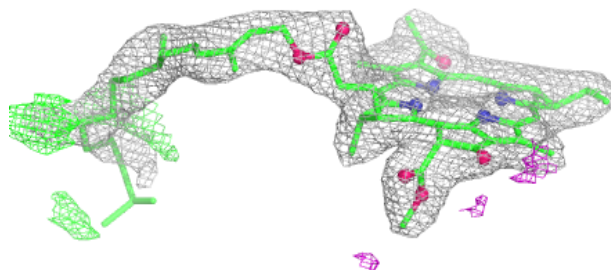
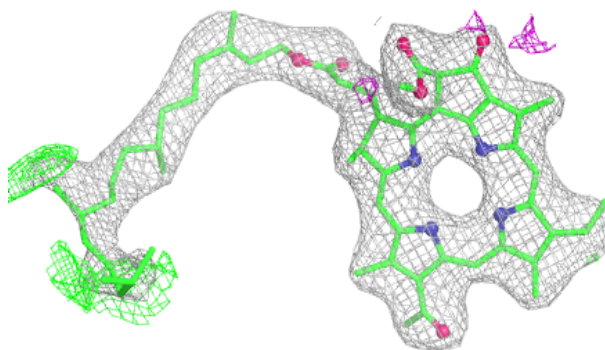


Electron density around CDL M 401:

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

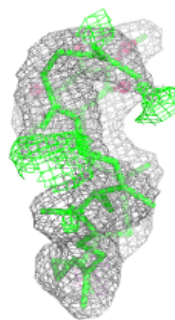
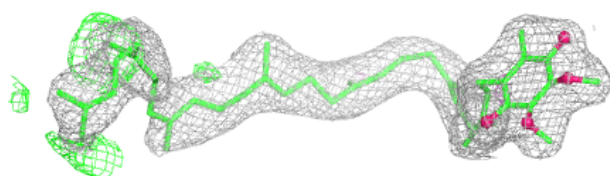
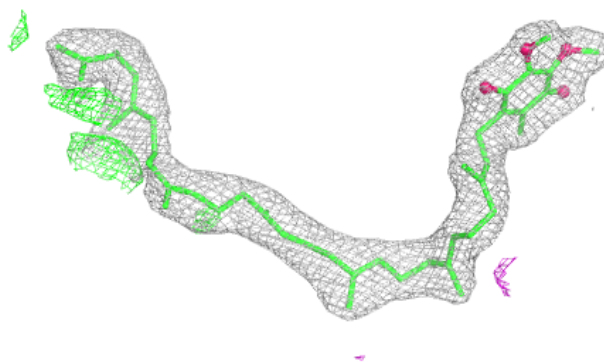
**Electron density around BPH M 404:**

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

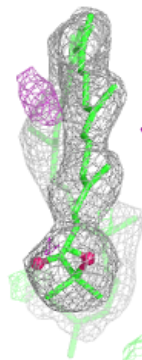
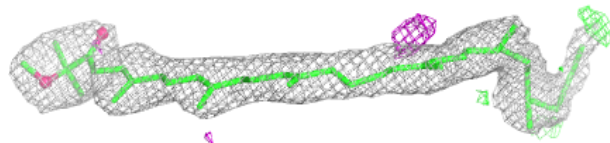
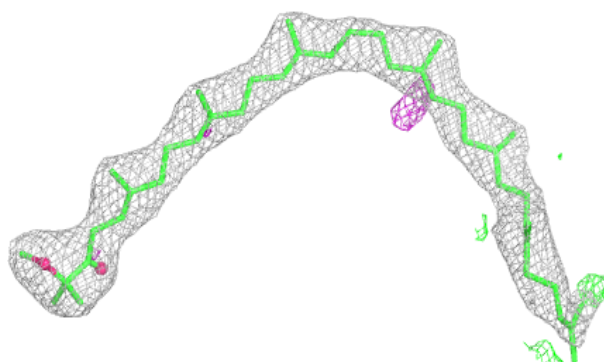


Electron density around U10 M 406:

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

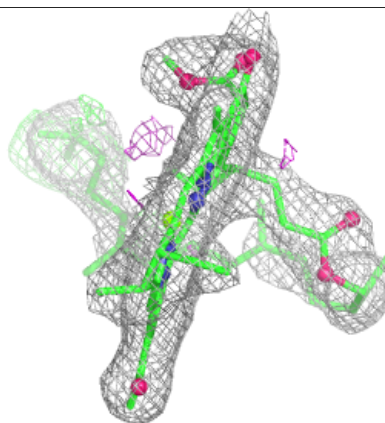
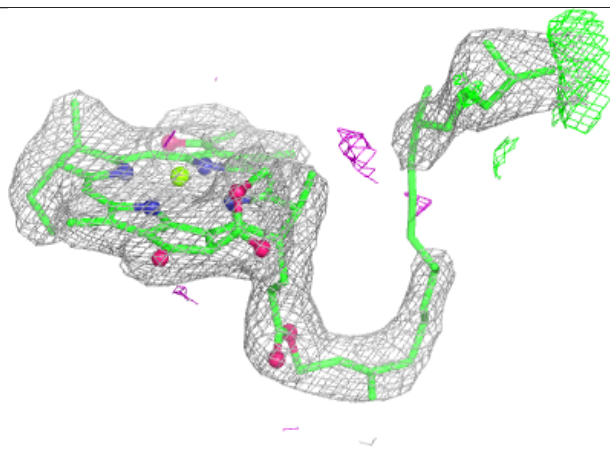
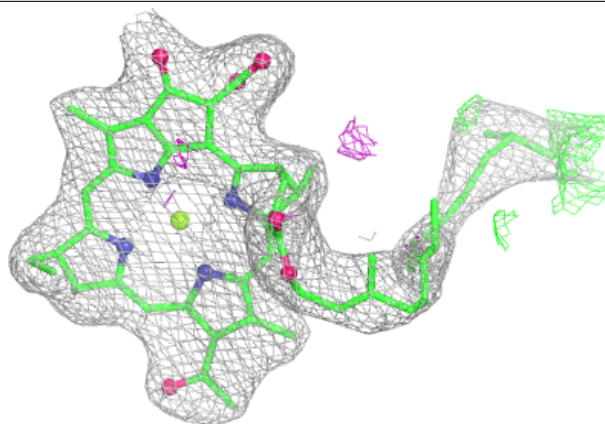
**Electron density around SPN M 407:**

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



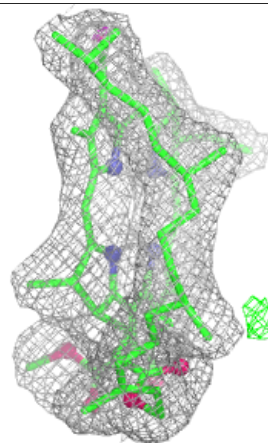
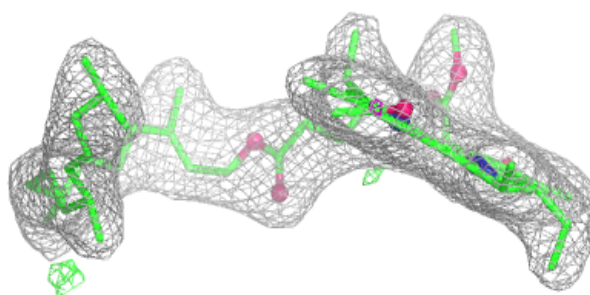
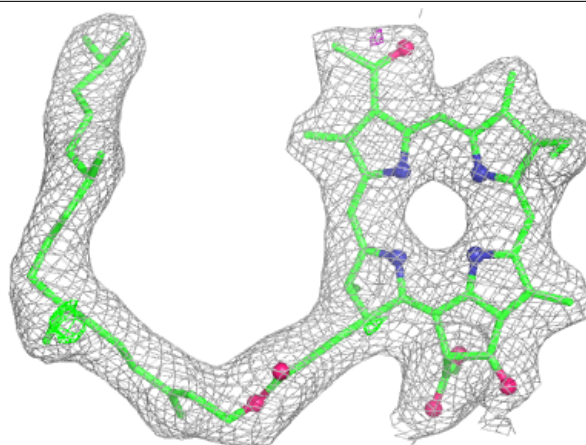
Electron density around BCL M 402:

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



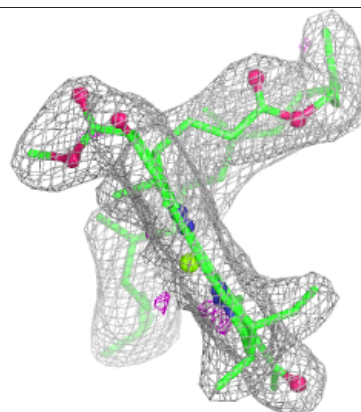
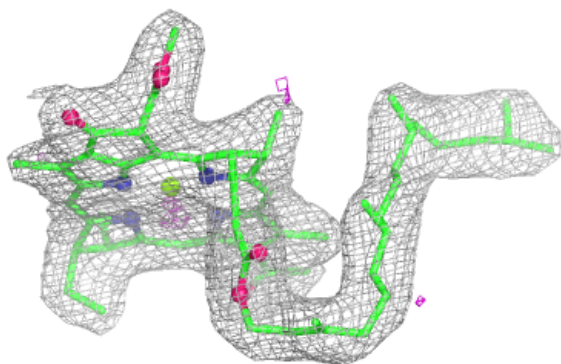
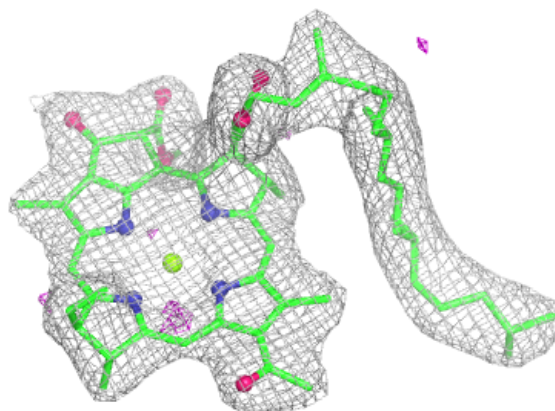
Electron density around BPH L 303:

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

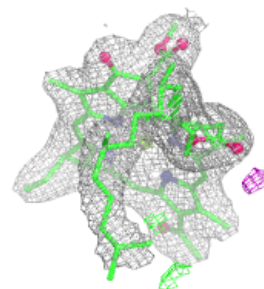
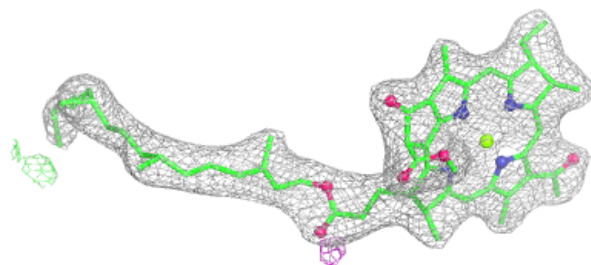
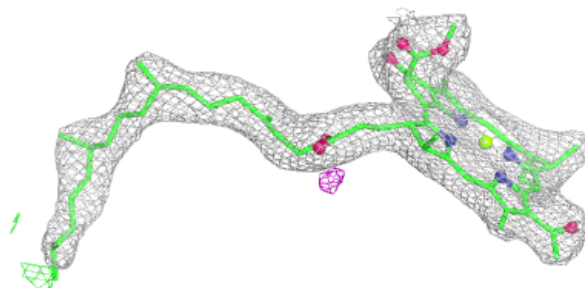


Electron density around BCL L 302:

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

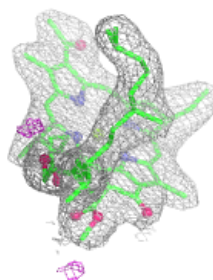
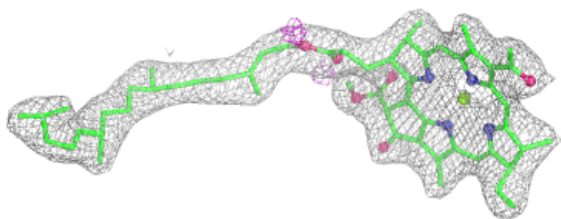
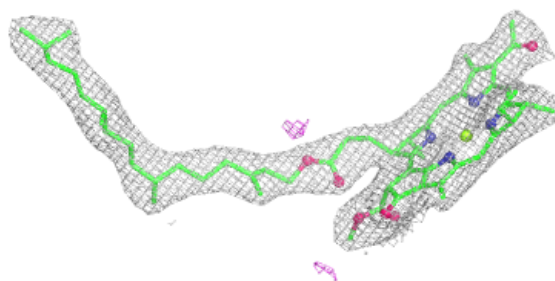
**Electron density around BCL M 403:**

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



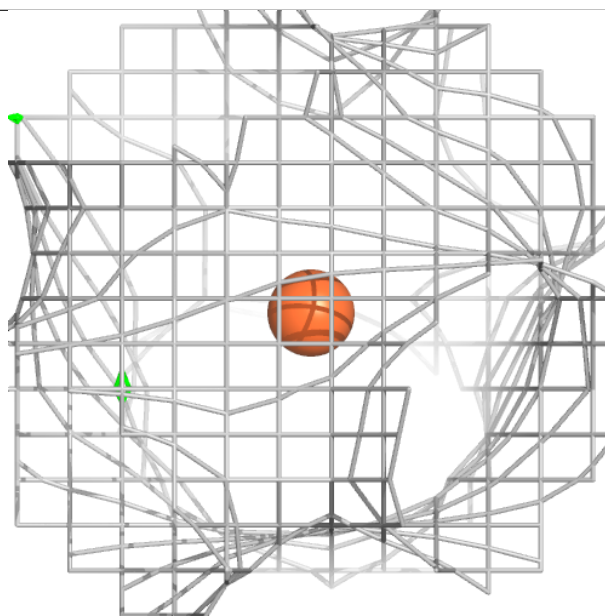
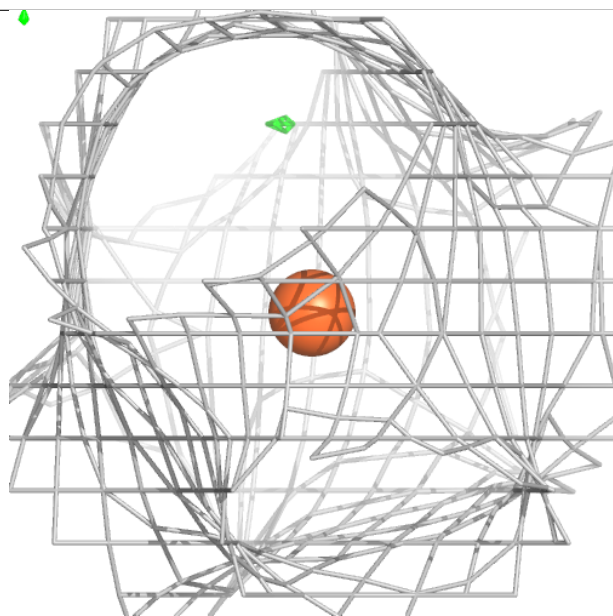
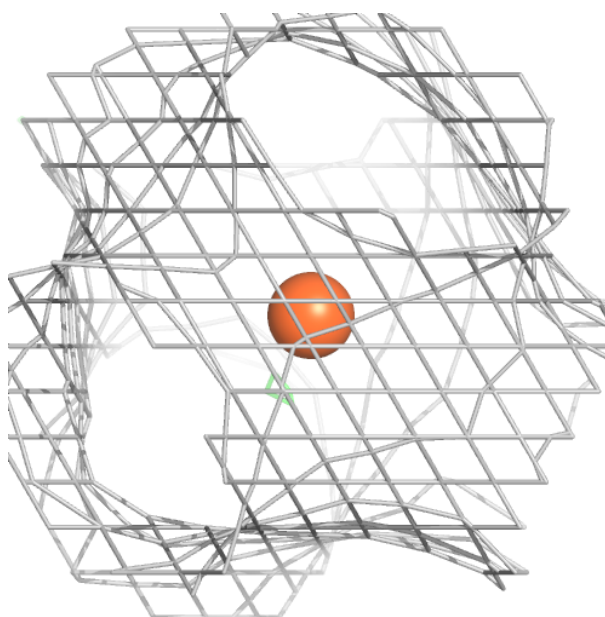
Electron density around BCL L 301:

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



Electron density around FE M 405:

$2mF_o-DF_c$ (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.