



## wwPDB EM Validation Summary Report ⓘ

Nov 12, 2022 – 08:44 PM EST

PDB ID : 6VKT  
EMDB ID : EMD-21229  
Title : Cryo-electron microscopy structures of a gonococcal multidrug efflux pump illuminate a mechanism of erythromycin drug recognition  
Authors : Lyu, M.; Moseng, M.A.  
Deposited on : 2020-01-22  
Resolution : 2.72 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

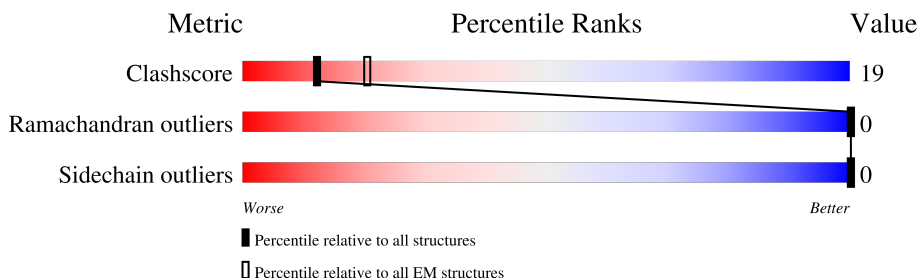
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.72 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1046	
1	B	1046	
1	C	1046	

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
2	PTY	C	1106	-	-	X	-
3	ERY	B	1101	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24331 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1037	Total	C	N	O	S	0	0
			7761	4977	1288	1451	45		
1	B	1043	Total	C	N	O	S	0	0
			7813	5010	1299	1459	45		
1	C	1042	Total	C	N	O	S	0	0
			7806	5006	1298	1457	45		

There are 66 discrepancies between the modelled and reference sequences:

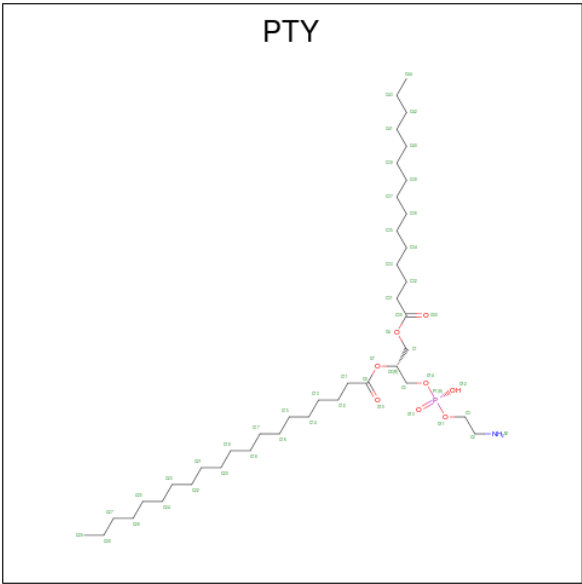
Chain	Residue	Modelled	Actual	Comment	Reference
A	738	VAL	ILE	conflict	UNP A0A4T9VBR9
A	774	GLY	GLU	conflict	UNP A0A4T9VBR9
A	791	SER	LYS	conflict	UNP A0A4T9VBR9
A	794	ILE	VAL	conflict	UNP A0A4T9VBR9
A	800	SER	THR	conflict	UNP A0A4T9VBR9
A	807	GLN	GLU	conflict	UNP A0A4T9VBR9
A	808	MET	ASN	conflict	UNP A0A4T9VBR9
A	821	ALA	SER	conflict	UNP A0A4T9VBR9
A	823	GLU	LYS	conflict	UNP A0A4T9VBR9
A	826	GLY	ALA	conflict	UNP A0A4T9VBR9
A	839	GLU	ALA	conflict	UNP A0A4T9VBR9
A	850	SER	GLY	conflict	UNP A0A4T9VBR9
A	854	LEU	PHE	conflict	UNP A0A4T9VBR9
A	871	ILE	LEU	conflict	UNP A0A4T9VBR9
A	872	ALA	ILE	conflict	UNP A0A4T9VBR9
A	875	ALA	GLY	conflict	UNP A0A4T9VBR9
A	878	ALA	VAL	conflict	UNP A0A4T9VBR9
A	879	VAL	ALA	conflict	UNP A0A4T9VBR9
A	899	LEU	ILE	conflict	UNP A0A4T9VBR9
A	902	MET	ILE	conflict	UNP A0A4T9VBR9
A	907	ALA	ILE	conflict	UNP A0A4T9VBR9
A	1000	GLY	ALA	conflict	UNP A0A4T9VBR9
B	738	VAL	ILE	conflict	UNP A0A4T9VBR9
B	774	GLY	GLU	conflict	UNP A0A4T9VBR9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	791	SER	LYS	conflict	UNP A0A4T9VBR9
B	794	ILE	VAL	conflict	UNP A0A4T9VBR9
B	800	SER	THR	conflict	UNP A0A4T9VBR9
B	807	GLN	GLU	conflict	UNP A0A4T9VBR9
B	808	MET	ASN	conflict	UNP A0A4T9VBR9
B	821	ALA	SER	conflict	UNP A0A4T9VBR9
B	823	GLU	LYS	conflict	UNP A0A4T9VBR9
B	826	GLY	ALA	conflict	UNP A0A4T9VBR9
B	839	GLU	ALA	conflict	UNP A0A4T9VBR9
B	850	SER	GLY	conflict	UNP A0A4T9VBR9
B	854	LEU	PHE	conflict	UNP A0A4T9VBR9
B	871	ILE	LEU	conflict	UNP A0A4T9VBR9
B	872	ALA	ILE	conflict	UNP A0A4T9VBR9
B	875	ALA	GLY	conflict	UNP A0A4T9VBR9
B	878	ALA	VAL	conflict	UNP A0A4T9VBR9
B	879	VAL	ALA	conflict	UNP A0A4T9VBR9
B	899	LEU	ILE	conflict	UNP A0A4T9VBR9
B	902	MET	ILE	conflict	UNP A0A4T9VBR9
B	907	ALA	ILE	conflict	UNP A0A4T9VBR9
B	1000	GLY	ALA	conflict	UNP A0A4T9VBR9
C	738	VAL	ILE	conflict	UNP A0A4T9VBR9
C	774	GLY	GLU	conflict	UNP A0A4T9VBR9
C	791	SER	LYS	conflict	UNP A0A4T9VBR9
C	794	ILE	VAL	conflict	UNP A0A4T9VBR9
C	800	SER	THR	conflict	UNP A0A4T9VBR9
C	807	GLN	GLU	conflict	UNP A0A4T9VBR9
C	808	MET	ASN	conflict	UNP A0A4T9VBR9
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C	823	GLU	LYS	conflict	UNP A0A4T9VBR9
C	826	GLY	ALA	conflict	UNP A0A4T9VBR9
C	839	GLU	ALA	conflict	UNP A0A4T9VBR9
C	850	SER	GLY	conflict	UNP A0A4T9VBR9
C	854	LEU	PHE	conflict	UNP A0A4T9VBR9
C	871	ILE	LEU	conflict	UNP A0A4T9VBR9
C	872	ALA	ILE	conflict	UNP A0A4T9VBR9
C	875	ALA	GLY	conflict	UNP A0A4T9VBR9
C	878	ALA	VAL	conflict	UNP A0A4T9VBR9
C	879	VAL	ALA	conflict	UNP A0A4T9VBR9
C	899	LEU	ILE	conflict	UNP A0A4T9VBR9
C	902	MET	ILE	conflict	UNP A0A4T9VBR9
C	907	ALA	ILE	conflict	UNP A0A4T9VBR9
C	1000	GLY	ALA	conflict	UNP A0A4T9VBR9

- Molecule 2 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



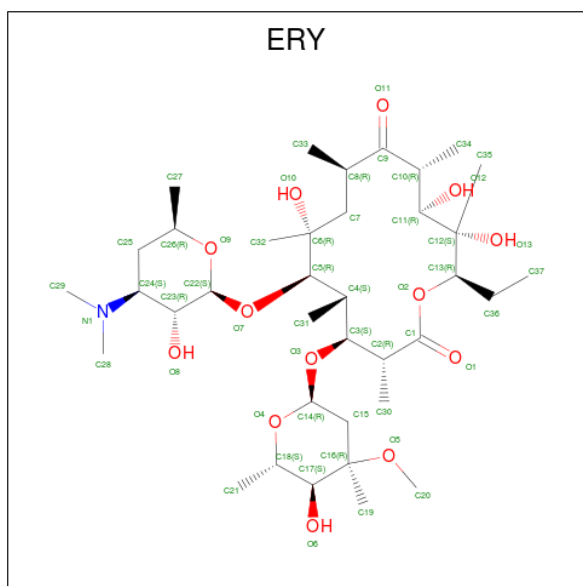
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			264	204	6	48	6	
			Total	C	N	O	P	
			264	204	6	48	6	
			Total	C	N	O	P	
2	A	1	264	204	6	48	6	0
			Total	C	N	O	P	
			264	204	6	48	6	
			Total	C	N	O	P	
			264	204	6	48	6	
2	A	1	Total	C	N	O	P	0
			264	204	6	48	6	
			Total	C	N	O	P	
			264	204	6	48	6	
			Total	C	N	O	P	
2	B	1	322	242	8	64	8	0
			Total	C	N	O	P	
			322	242	8	64	8	
			Total	C	N	O	P	
			322	242	8	64	8	
2	B	1	Total	C	N	O	P	0
			322	242	8	64	8	
			Total	C	N	O	P	
			322	242	8	64	8	
			Total	C	N	O	P	
2	B	1	322	242	8	64	8	0
			Total	C	N	O	P	
			322	242	8	64	8	
			Total	C	N	O	P	
			322	242	8	64	8	

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			322	242	8	64	8	
2	B	1	Total	C	N	O	P	0
			322	242	8	64	8	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	
2	C	1	Total	C	N	O	P	0
			314	246	6	56	6	

- Molecule 3 is ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ) (labeled as "Ligand of Interest" by depositor).

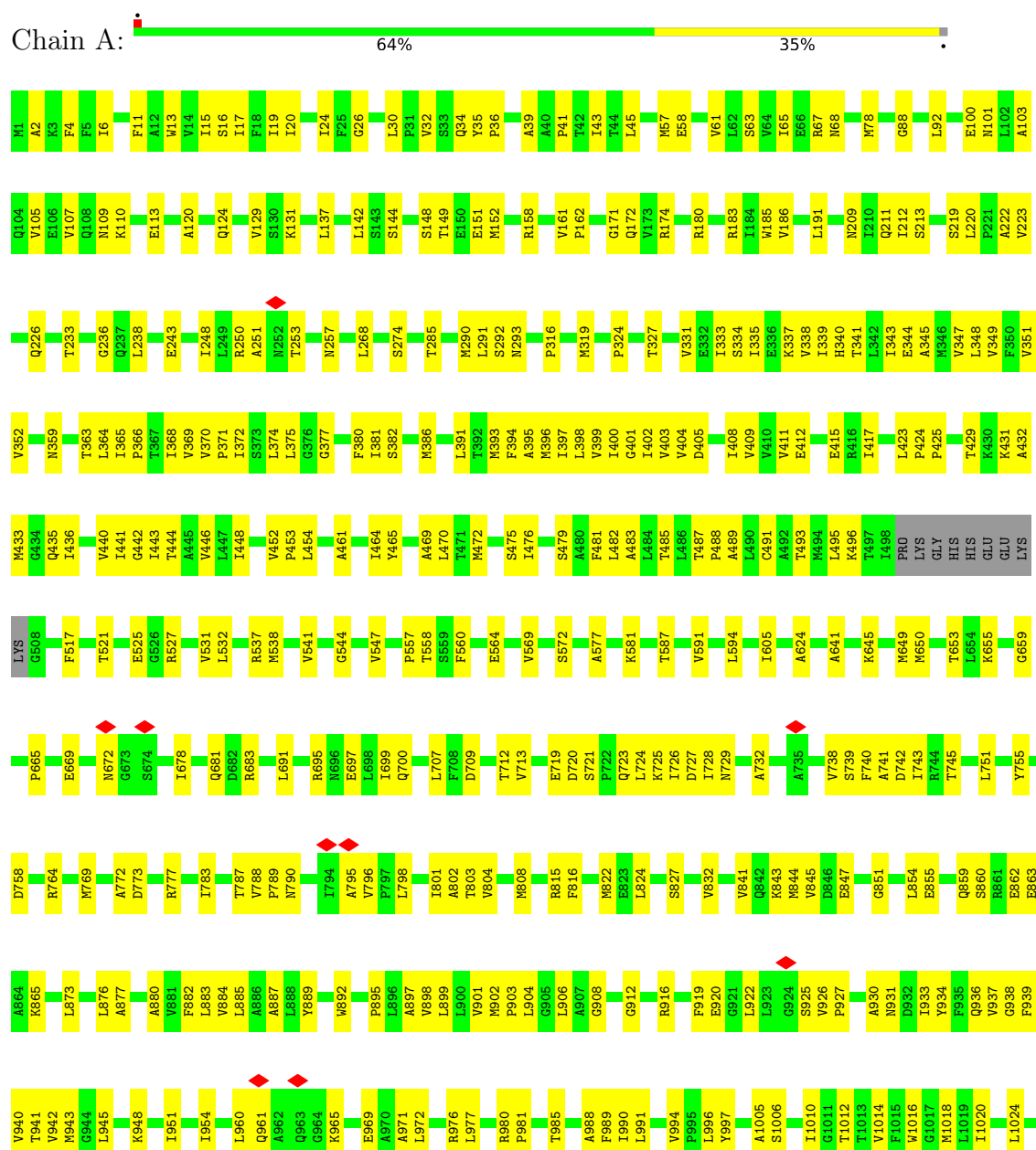


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	B	1	51	37	1	13	0

### 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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Efflux pump membrane transporter

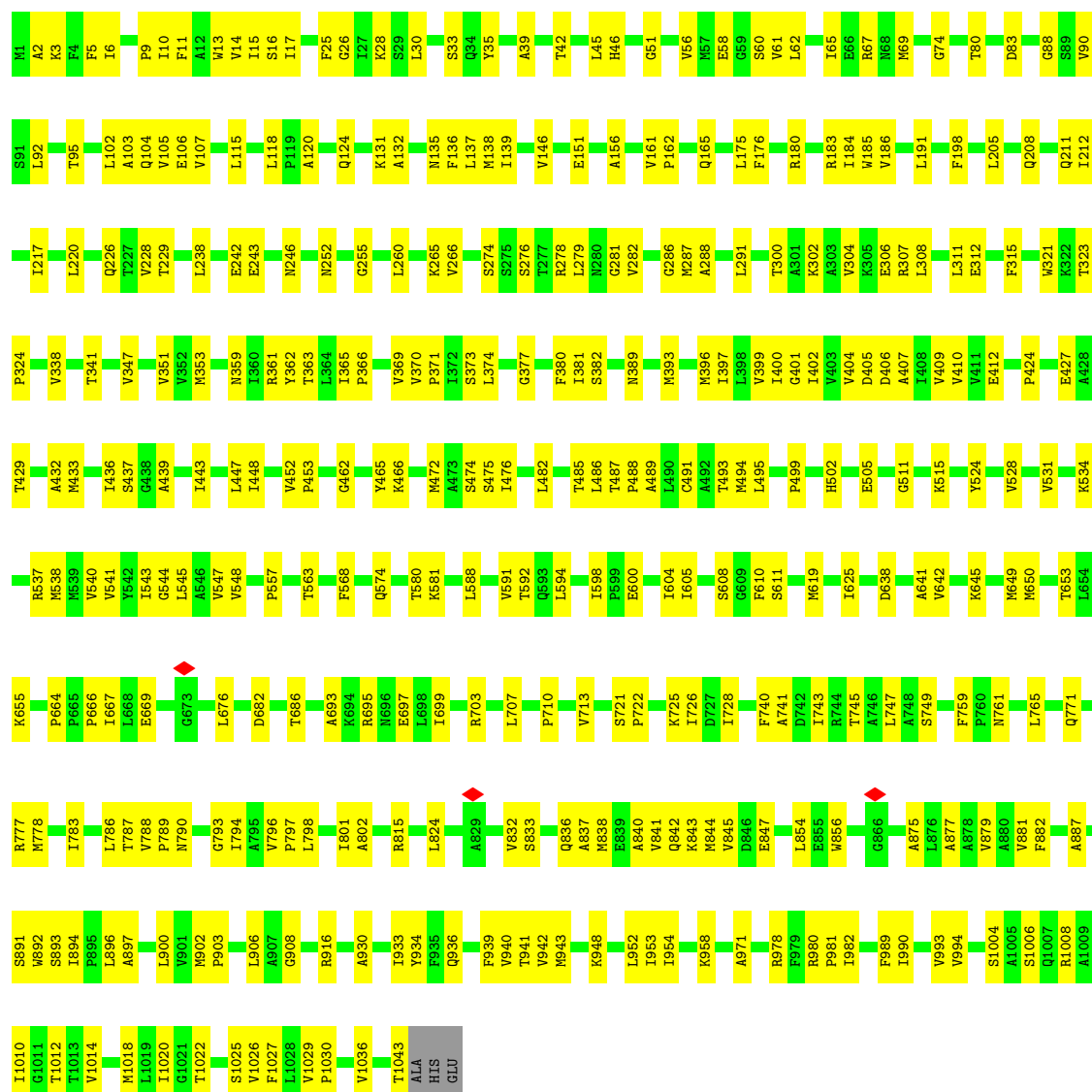




V1029  
P1030  
L1031  
F1032  
V1036  
E1042  
T1043  
A1044  
H1045  
E1046

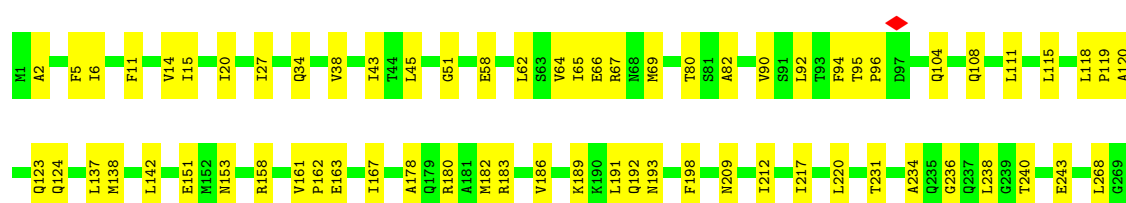
● Molecule 1: Efflux pump membrane transporter

Chain B:  67% 32%



● Molecule 1: Efflux pump membrane transporter

Chain C:  68% 31%



V1029	G938	A837	L724	M618	P488	F394	M270
P1030	Y942	M838	R730	M619	M494	A395	E271
Y1033	K948	E839	A741	A620		M396	D272
K1041	A840	A840	A741	F623	E504	I397	Y273
E1042	Q842	Q842	R744	A624	E505	L398	S274
THR	K843	K843	T745	I625	K506	V399	T285
ALA	M844	M844		R632	G511	V403	L291
HIS	V845	V845	A748	R632	K515	V404	L291
GLU	D846	D846	S749	S637		D405	M298
	E847	E847		D638	E525	D406	A407
	L854	L854	S752		G526	T408	K302
	E855	E855	S753	A641	R527	V409	E306
	M856	M856	D758	V642		V410	R307
	Q961	Q961		K645	V531	V411	L308
	R861	R861	M761		L532	E412	N413
	A875	A875	R764	M650	R533	V414	M321
	R879	R879		T653	K534	M433	P324
	F882	F882	V768	L654	R537	I436	K329
	L883	L883	V770		M538		F330
	V884	V884	Q771	I660	M539	V440	V331
	A886	A886	A772	A661	V540	I441	E332
	A887	A887	D774	V662	V541	G442	I333
	L888	L888	G774	P664	F542	I443	S334
	Y889	Y889	M778		I543	T444	I335
			Q779	I667	L545	A445	E336
			P780	L668	A546	V446	K337
				E669	V547	L447	V338
			L784	L676	V550	V452	F350
			T787	S677	F551	P453	
			V788	I678		L454	Y354
			P789	M679	R555	A455	I355
				L680	L556	F356	F356
			A795	Q681	P557	L357	L357
			V796		E564	Q358	Q358
			P797	T686		N359	N359
			V804	A690	F568	I360	I360
				R695	V569	R361	R361
			E811		V573	Y362	Y362
			Q812	L698	A577	L364	L364
			G818	K701	G578	I365	I365
			M822	L707	A579	P366	P366
			E823	F708	T580	T367	T367
			S827		K581	V370	V370
			P828		L588	P371	P371
			A829	S711		I381	I381
			I933	T712	V591	M386	M386
			Y934		L594	L484	L484
			F935	L718		T485	T485
			Q936	E719		L486	L486
			V937			T392	T392
						M393	M393

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1507208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	45.425	Depositor
Minimum map value	-21.501	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.0	Depositor
Map size ( $\text{\AA}$ )	378.0, 378.0, 378.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERY, PTY

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	A	0.25	0/7900	0.41	0/10719
1	B	0.25	0/7955	0.40	0/10792
1	C	0.25	0/7948	0.40	0/10782
All	All	0.25	0/23803	0.41	0/32293

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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	ARG	Sidechain
1	B	67	ARG	Sidechain
1	C	744	ARG	Sidechain

## 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	A	7761	0	7927	324	0
1	B	7813	0	7986	297	0
1	C	7806	0	7979	259	0
2	A	264	0	378	36	0
2	B	322	0	440	45	0
2	C	314	0	441	46	0
3	B	51	0	67	41	0
All	All	24331	0	25218	945	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 19.

The worst 5 of 945 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)
1:A:961:GLN:HG3	1:A:1046:GLU:OE2	1.33	1.26
2:C:1101:PTY:HC11	2:C:1106:PTY:C1	1.71	1.18
2:C:1101:PTY:HC11	2:C:1106:PTY:HC11	1.24	1.14
1:B:176:PHE:CG	3:B:1101:ERY:H26	1.85	1.11
1:B:176:PHE:CD2	3:B:1101:ERY:H26	1.85	1.11

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 PDB entries followed by that with respect to all EM entries.

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	A	1033/1046 (99%)	1002 (97%)	31 (3%)	0	100	100
1	B	1041/1046 (100%)	1018 (98%)	23 (2%)	0	100	100
1	C	1040/1046 (99%)	1013 (97%)	27 (3%)	0	100	100
All	All	3114/3138 (99%)	3033 (97%)	81 (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 PDB entries followed by that with respect to all EM entries.

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	A	829/837 (99%)	829 (100%)	0	100	100
1	B	835/837 (100%)	835 (100%)	0	100	100
1	C	834/837 (100%)	834 (100%)	0	100	100
All	All	2498/2511 (100%)	2498 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	681	GLN
1	C	762	GLN
1	B	211	GLN
1	B	165	GLN
1	C	869	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 ligands are 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$
2	PTY	C	1109	-	14,14,49	2.04	2 (14%)	14,14,54	1.06	1 (7%)
2	PTY	C	1105	-	34,34,49	1.11	2 (5%)	37,39,54	1.08	2 (5%)
2	PTY	B	1109	-	43,43,49	0.98	2 (4%)	46,48,54	1.11	2 (4%)
2	PTY	C	1108	-	14,14,49	1.20	1 (7%)	14,14,54	1.05	0
3	ERY	B	1101	-	53,53,53	0.92	1 (1%)	82,82,82	1.52	13 (15%)
2	PTY	B	1107	-	49,49,49	0.97	2 (4%)	52,54,54	1.11	4 (7%)
2	PTY	C	1107	-	49,49,49	0.89	2 (4%)	52,54,54	1.02	2 (3%)
2	PTY	A	1103	-	44,44,49	0.94	2 (4%)	47,49,54	1.07	2 (4%)
2	PTY	B	1103	-	35,35,49	1.07	2 (5%)	38,40,54	1.21	3 (7%)
2	PTY	B	1106	-	34,34,49	1.10	2 (5%)	37,39,54	1.12	2 (5%)
2	PTY	C	1104	-	31,31,49	1.15	2 (6%)	34,36,54	1.12	2 (5%)
2	PTY	B	1108	-	34,34,49	1.11	2 (5%)	37,39,54	1.32	3 (8%)
2	PTY	C	1103	-	40,40,49	0.97	2 (5%)	43,45,54	1.20	3 (6%)
2	PTY	C	1106	-	37,37,49	1.08	3 (8%)	39,39,54	1.26	3 (7%)
2	PTY	A	1101	-	47,47,49	0.95	2 (4%)	50,52,54	1.05	3 (6%)
2	PTY	A	1105	-	43,43,49	0.97	2 (4%)	46,48,54	1.06	2 (4%)
2	PTY	B	1104	-	40,40,49	0.91	2 (5%)	43,45,54	1.27	4 (9%)
2	PTY	A	1102	-	44,44,49	0.93	2 (4%)	47,49,54	1.14	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PTY	A	1106	-	40,40,49	0.99	2 (5%)	43,45,54	1.10	1 (2%)
2	PTY	A	1104	-	40,40,49	1.00	2 (5%)	43,45,54	1.16	5 (11%)
2	PTY	B	1102	-	36,36,49	1.02	2 (5%)	39,41,54	1.07	3 (7%)
2	PTY	C	1101	-	45,45,49	0.94	2 (4%)	48,50,54	1.08	3 (6%)
2	PTY	B	1105	-	43,43,49	1.00	2 (4%)	46,48,54	1.15	3 (6%)
2	PTY	C	1102	-	40,40,49	0.98	2 (5%)	43,45,54	1.09	3 (6%)

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
2	PTY	C	1109	-	-	5/12/12/53	-
2	PTY	C	1105	-	-	16/38/38/53	-
2	PTY	B	1109	-	-	21/47/47/53	-
2	PTY	C	1108	-	-	2/12/12/53	-
3	ERY	B	1101	-	-	38/72/107/107	0/3/3/3
2	PTY	B	1107	-	-	22/53/53/53	-
2	PTY	C	1107	-	-	17/53/53/53	-
2	PTY	A	1103	-	-	19/48/48/53	-
2	PTY	B	1103	-	-	9/39/39/53	-
2	PTY	B	1106	-	-	7/38/38/53	-
2	PTY	C	1104	-	-	9/35/35/53	-
2	PTY	B	1108	-	-	18/38/38/53	-
2	PTY	C	1103	-	-	9/44/44/53	-
2	PTY	C	1106	-	-	12/38/38/53	-
2	PTY	A	1101	-	-	17/51/51/53	-
2	PTY	A	1105	-	-	19/47/47/53	-
2	PTY	B	1104	-	-	17/44/44/53	-
2	PTY	A	1102	-	-	10/48/48/53	-
2	PTY	A	1106	-	-	12/44/44/53	-
2	PTY	A	1104	-	-	19/44/44/53	-
2	PTY	B	1102	-	-	15/40/40/53	-
2	PTY	C	1101	-	-	16/49/49/53	-
2	PTY	B	1105	-	-	15/47/47/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTY	C	1102	-	-	13/44/44/53	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1109	PTY	O10-C8	7.18	1.45	1.22
3	B	1101	ERY	O2-C1	4.99	1.45	1.34
2	B	1107	PTY	O4-C30	4.66	1.47	1.33
2	C	1108	PTY	O4-C30	4.45	1.45	1.30
2	B	1105	PTY	O4-C30	4.31	1.45	1.33

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1104	PTY	O7-C8-C11	5.12	122.54	111.50
2	B	1107	PTY	O7-C8-C11	4.67	121.57	111.50
2	A	1103	PTY	O7-C8-C11	4.66	121.55	111.50
2	A	1102	PTY	O7-C8-C11	4.61	121.43	111.50
2	B	1109	PTY	O7-C8-C11	4.47	121.14	111.50

There are no chirality outliers.

5 of 357 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	PTY	N1-C2-C3-O11
2	A	1101	PTY	C3-O11-P1-O13
2	A	1103	PTY	N1-C2-C3-O11
2	A	1103	PTY	C3-O11-P1-O13
2	A	1104	PTY	O10-C8-O7-C6

There are no ring outliers.

24 monomers are involved in 157 short contacts:

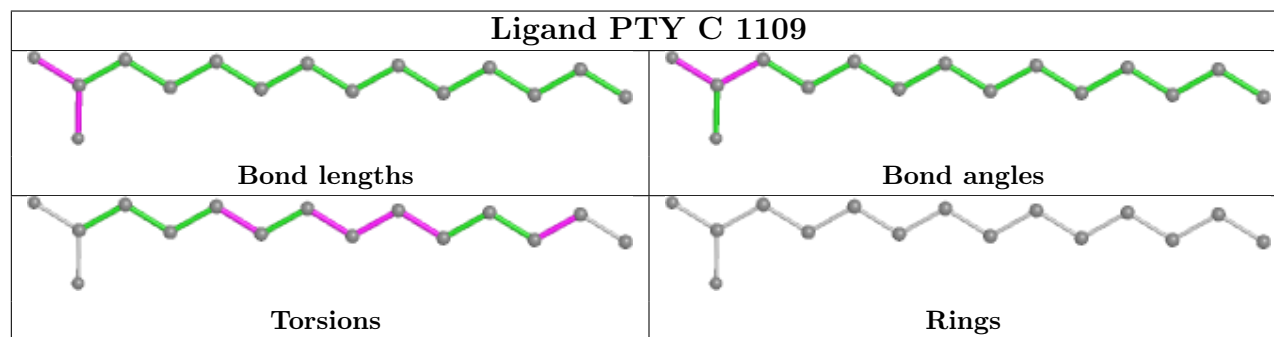
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1109	PTY	3	0
2	C	1105	PTY	9	0
2	B	1109	PTY	2	0
2	C	1108	PTY	3	0
3	B	1101	ERY	41	0
2	B	1107	PTY	2	0
2	C	1107	PTY	5	0

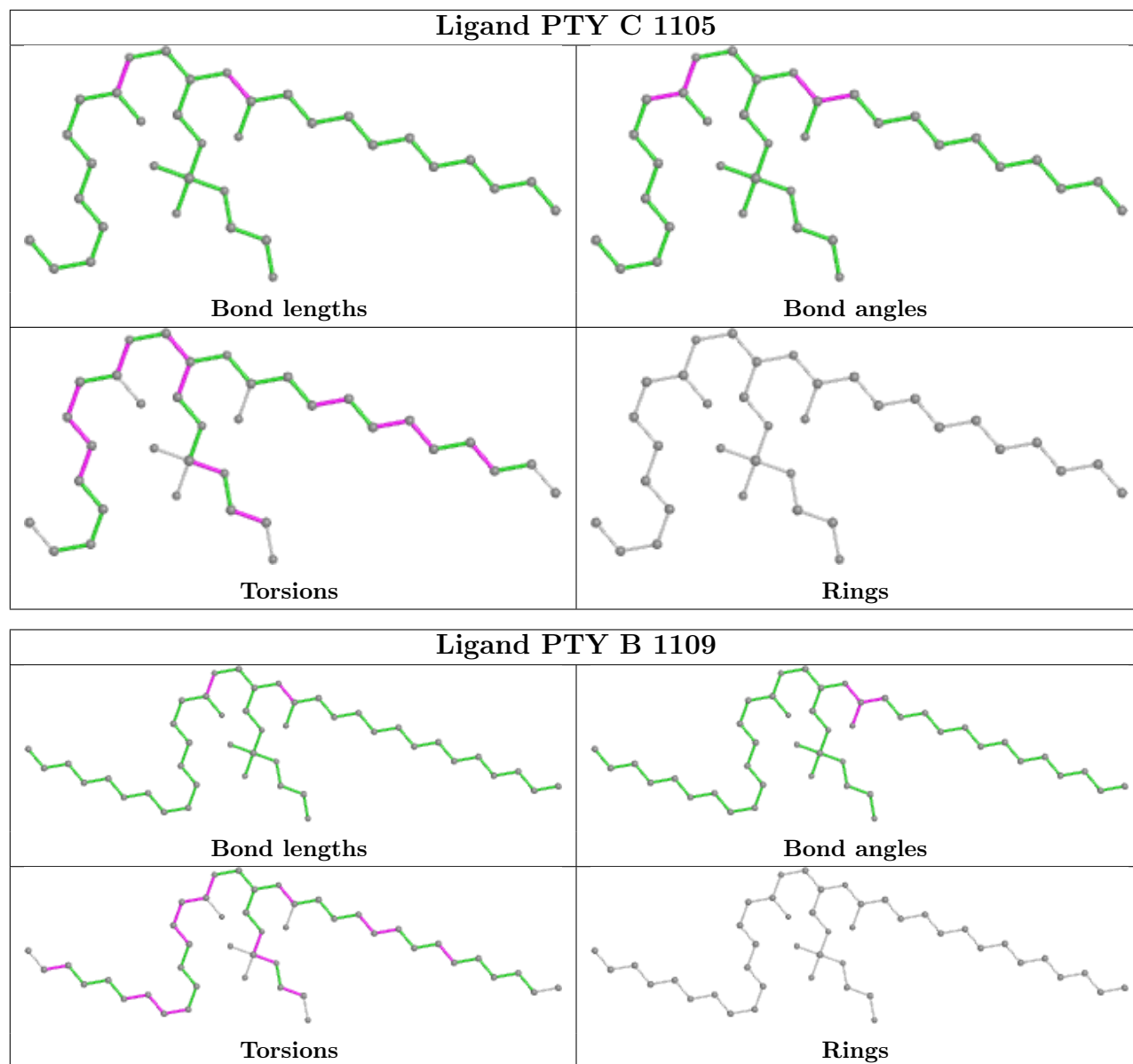
*Continued on next page...*

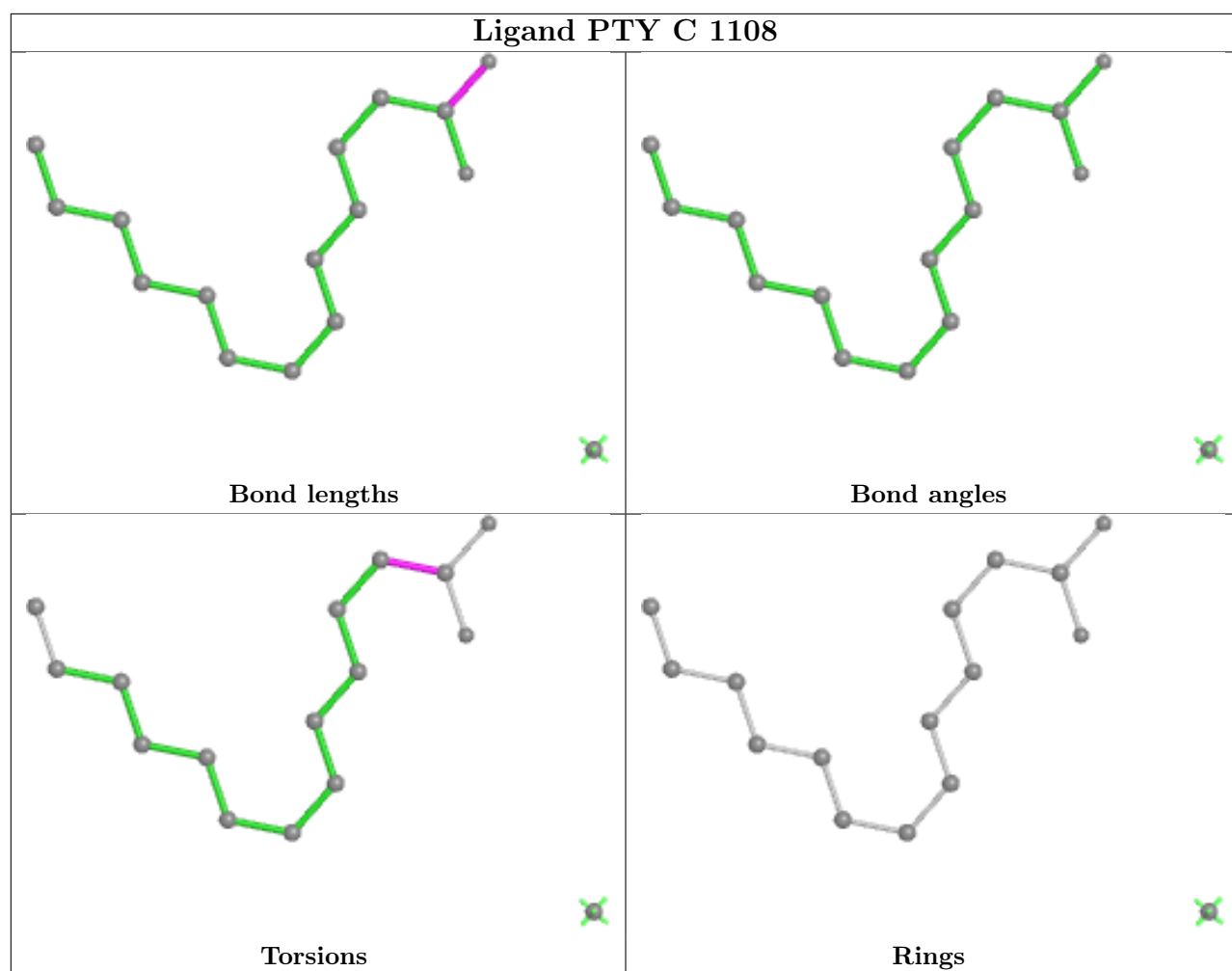
*Continued from previous page...*

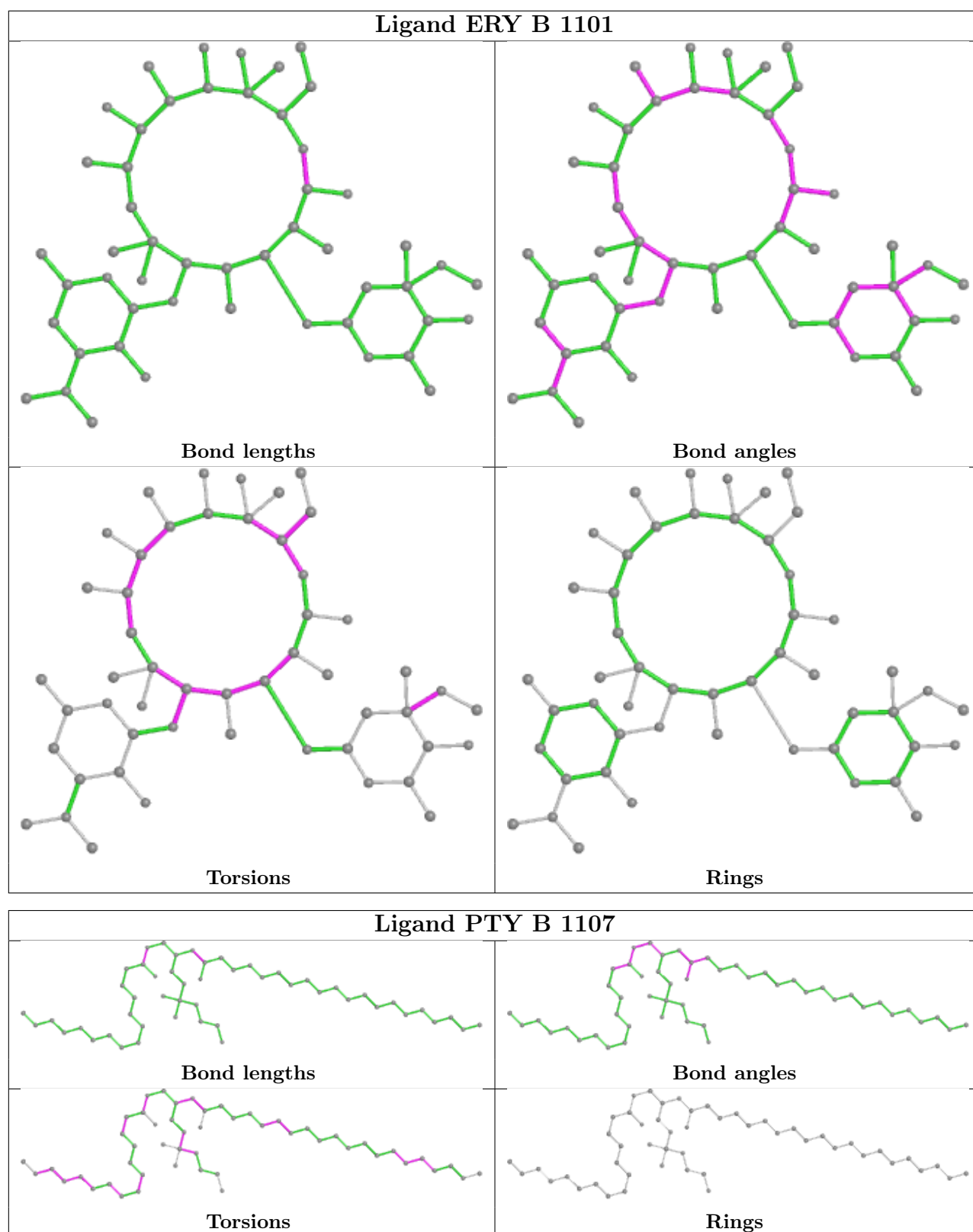
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	PTY	9	0
2	B	1103	PTY	8	0
2	B	1106	PTY	12	0
2	C	1104	PTY	2	0
2	B	1108	PTY	7	0
2	C	1103	PTY	2	0
2	C	1106	PTY	21	0
2	A	1101	PTY	4	0
2	A	1105	PTY	9	0
2	B	1104	PTY	12	0
2	A	1102	PTY	4	0
2	A	1106	PTY	7	0
2	A	1104	PTY	7	0
2	B	1102	PTY	1	0
2	C	1101	PTY	20	0
2	B	1105	PTY	8	0
2	C	1102	PTY	1	0

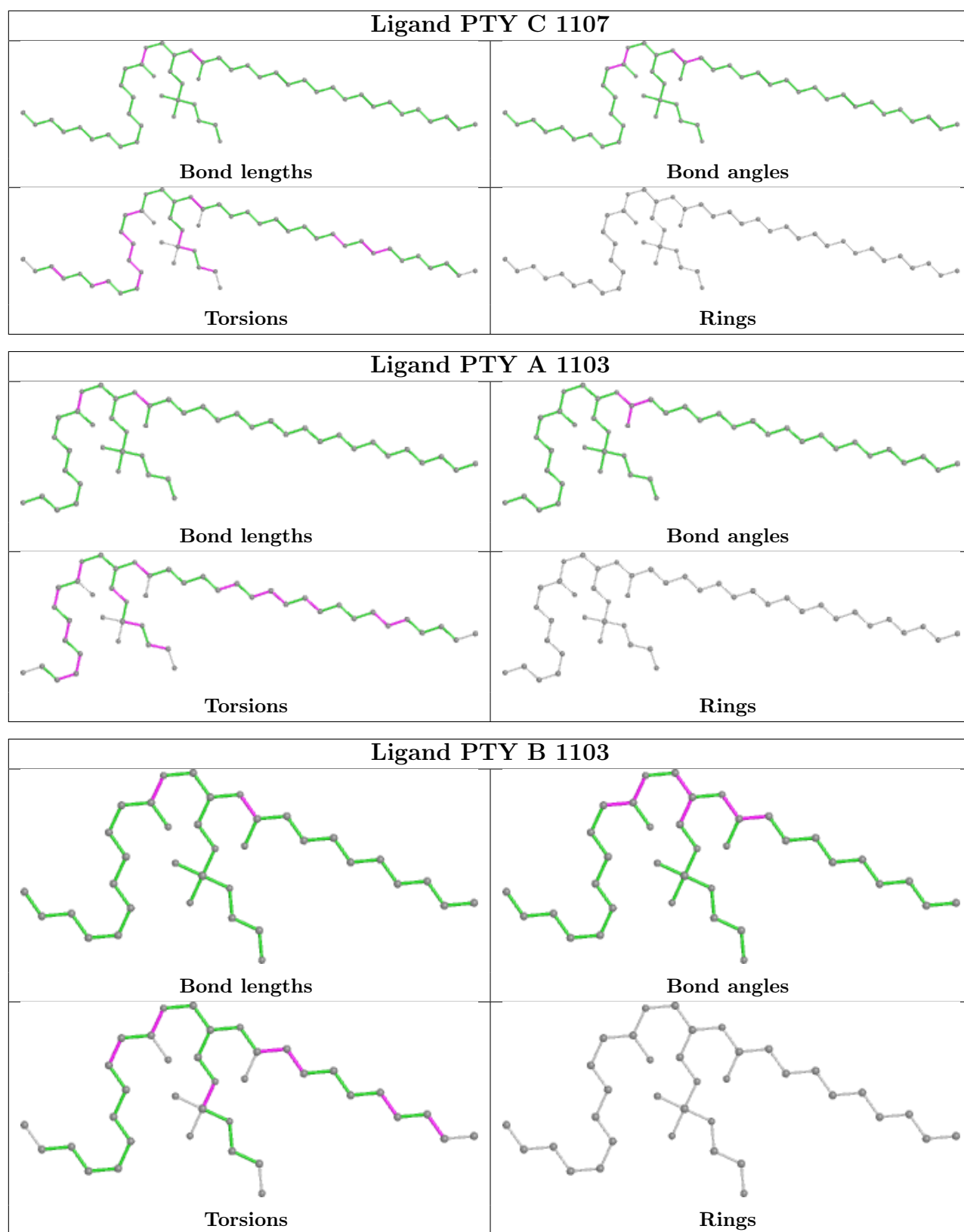
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

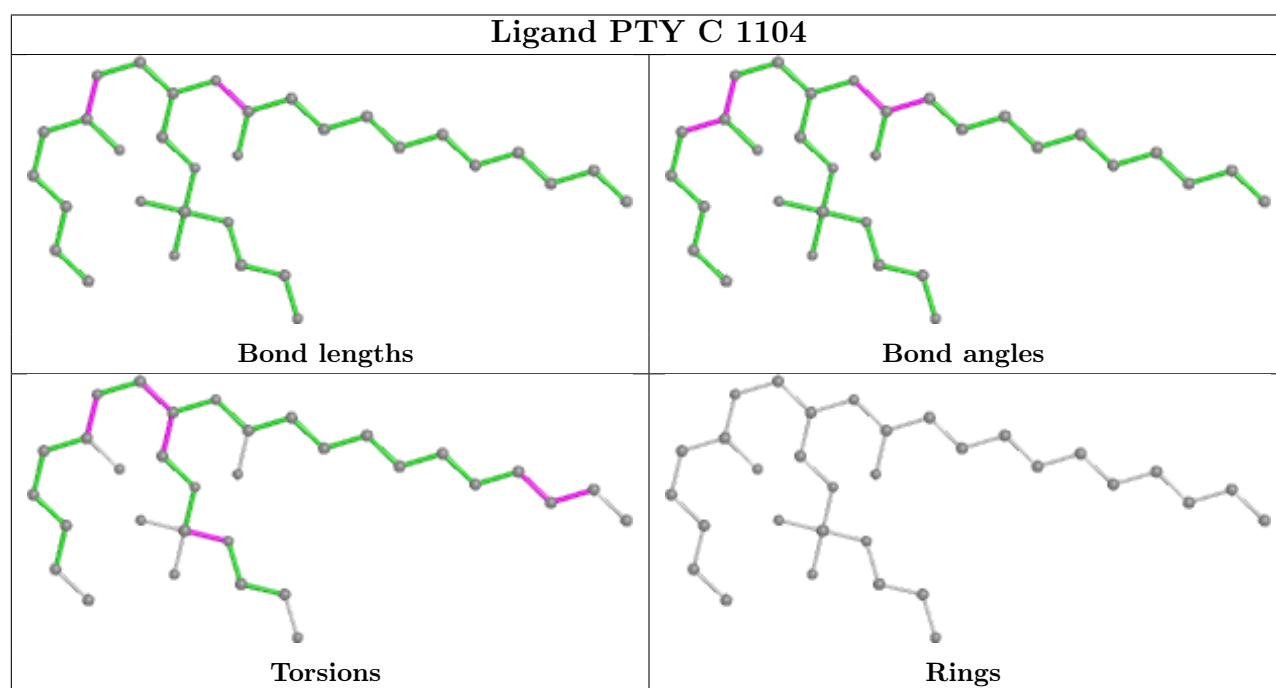
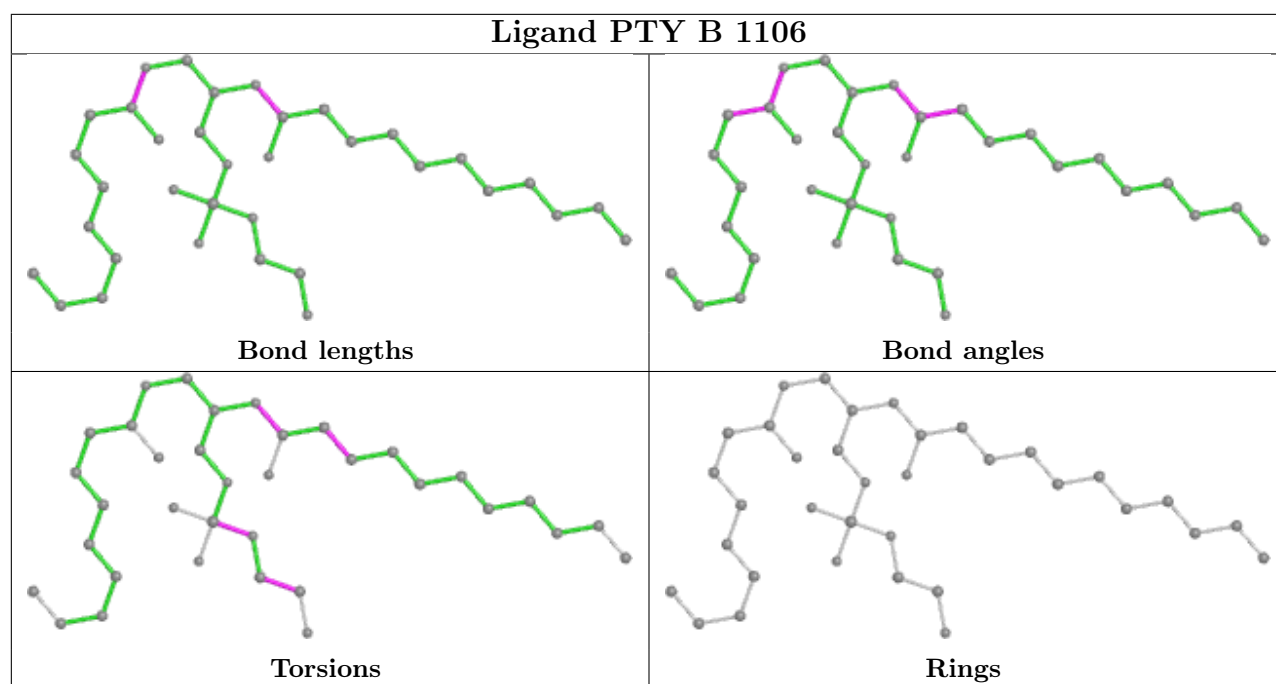


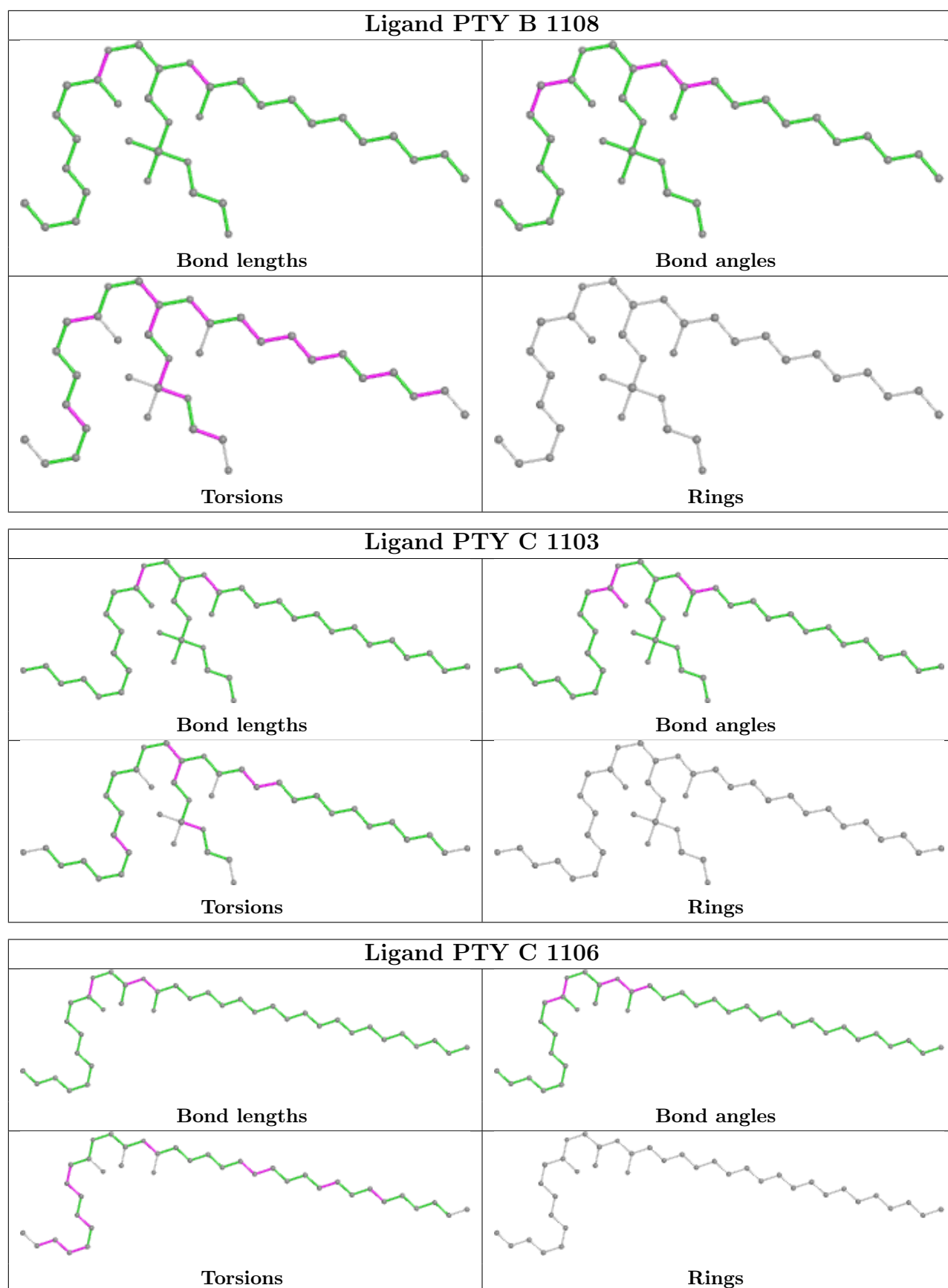




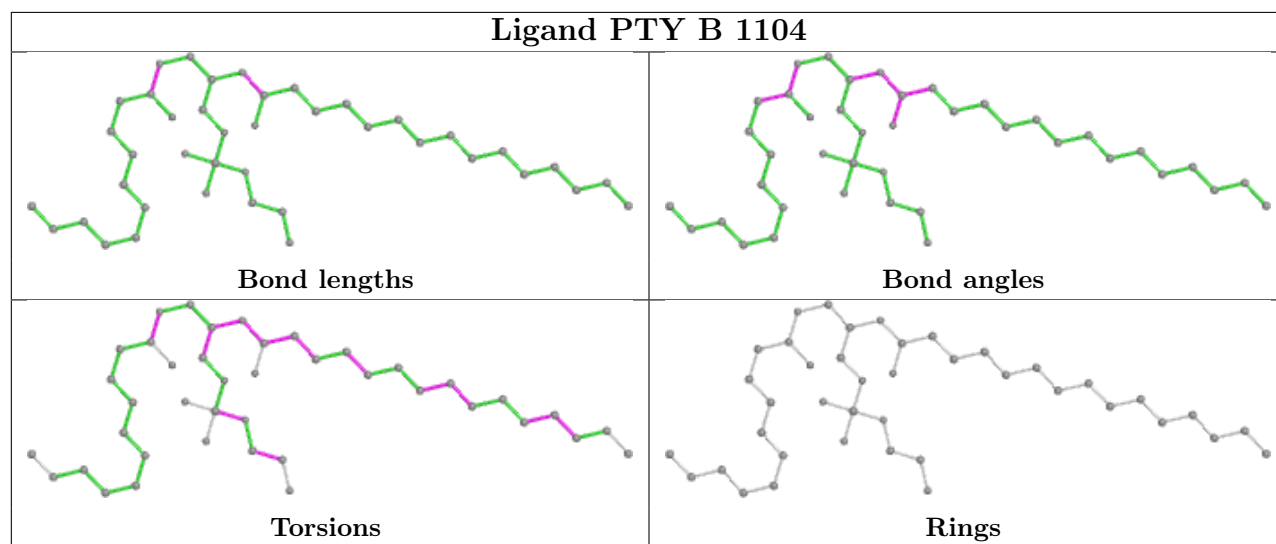
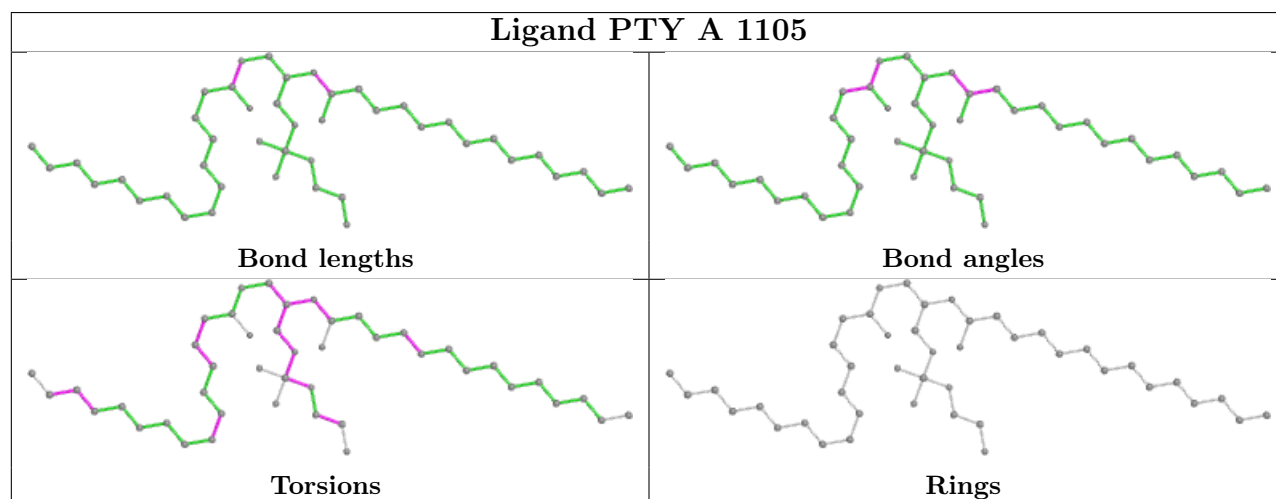
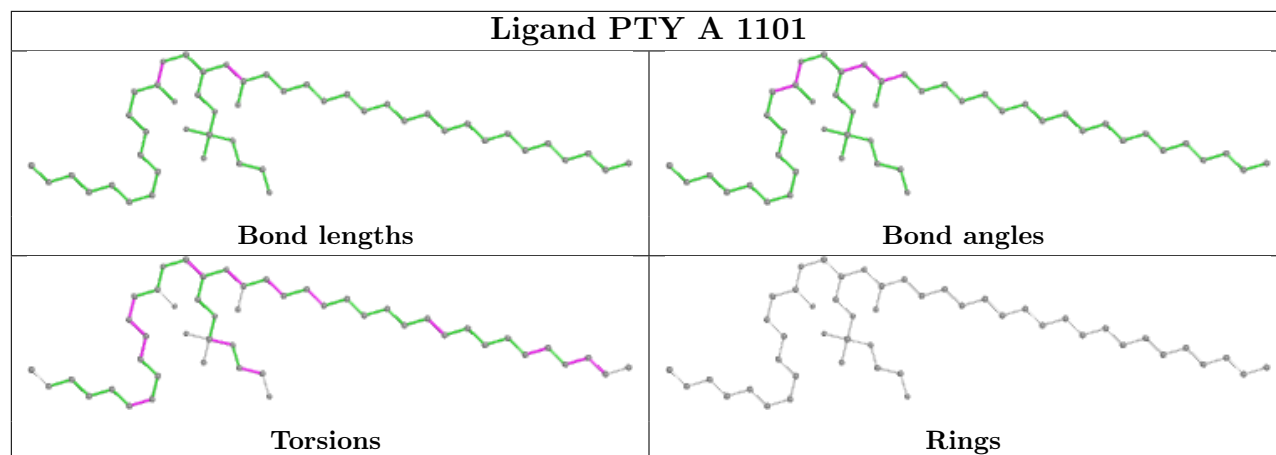


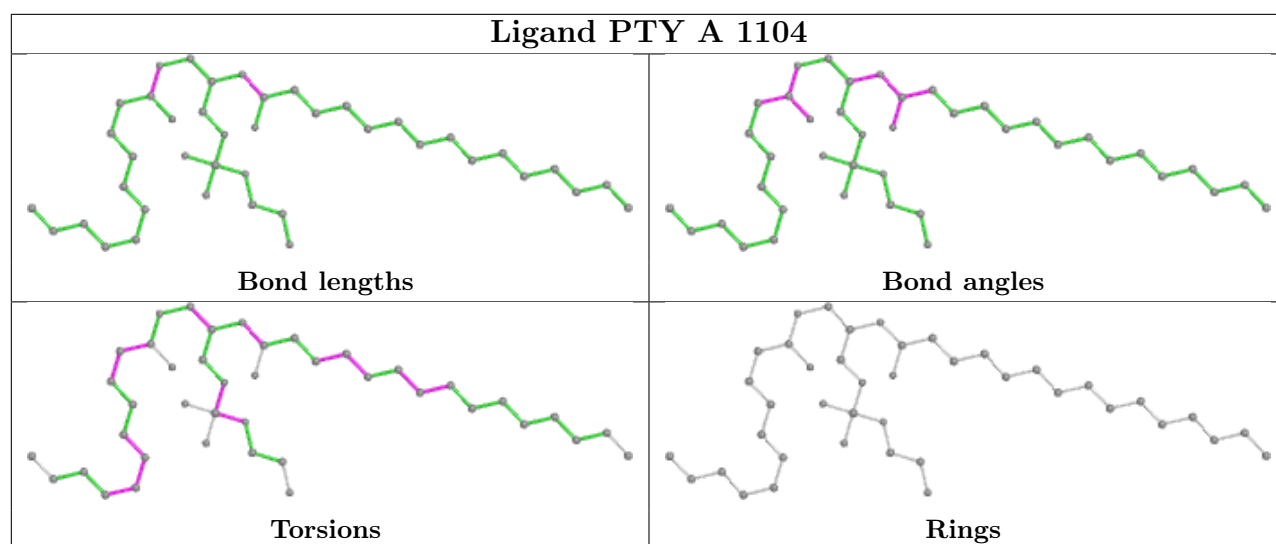
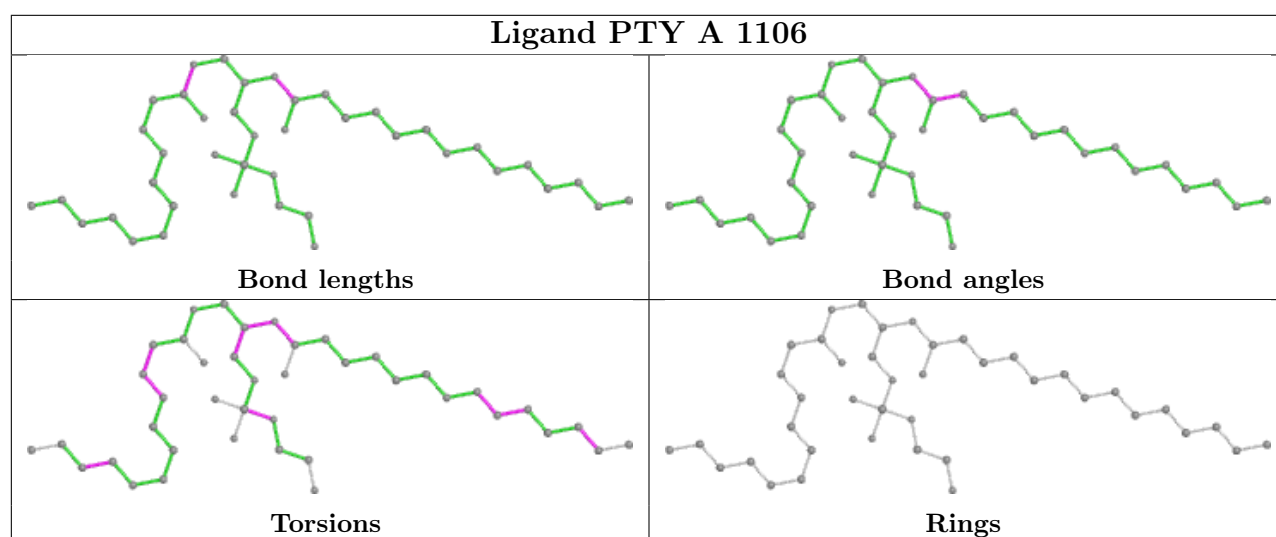
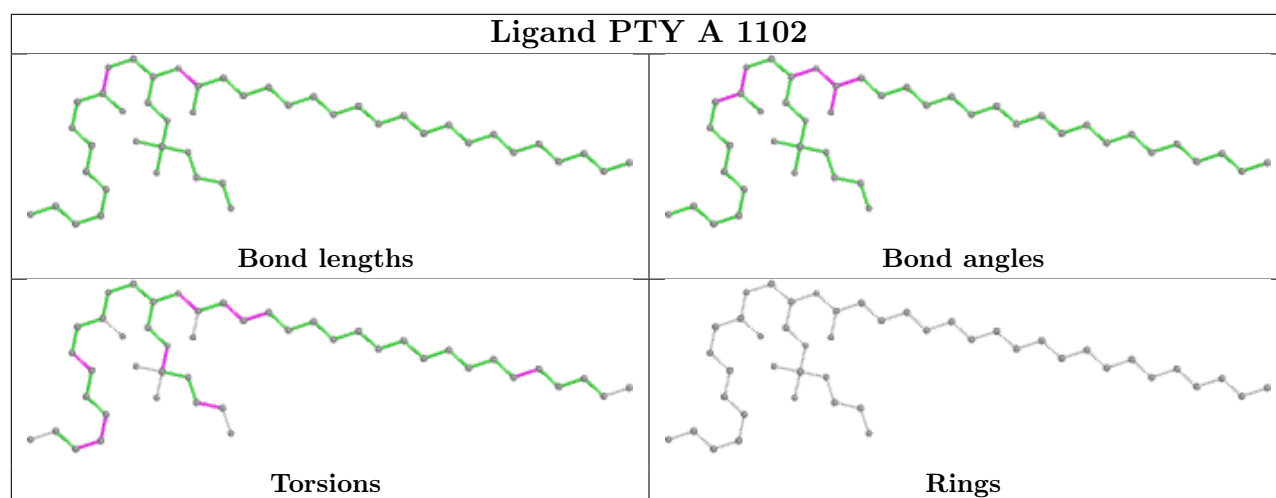


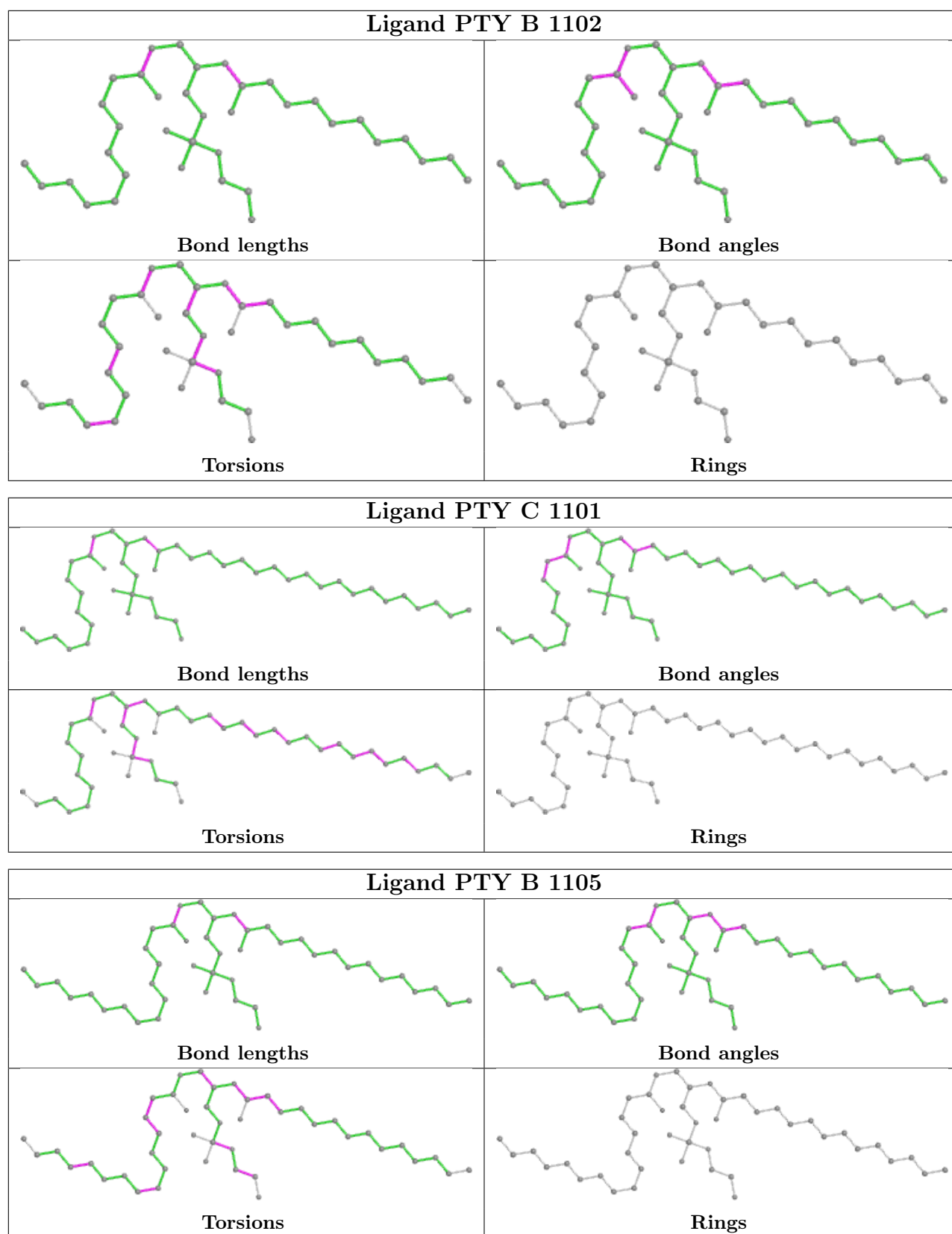


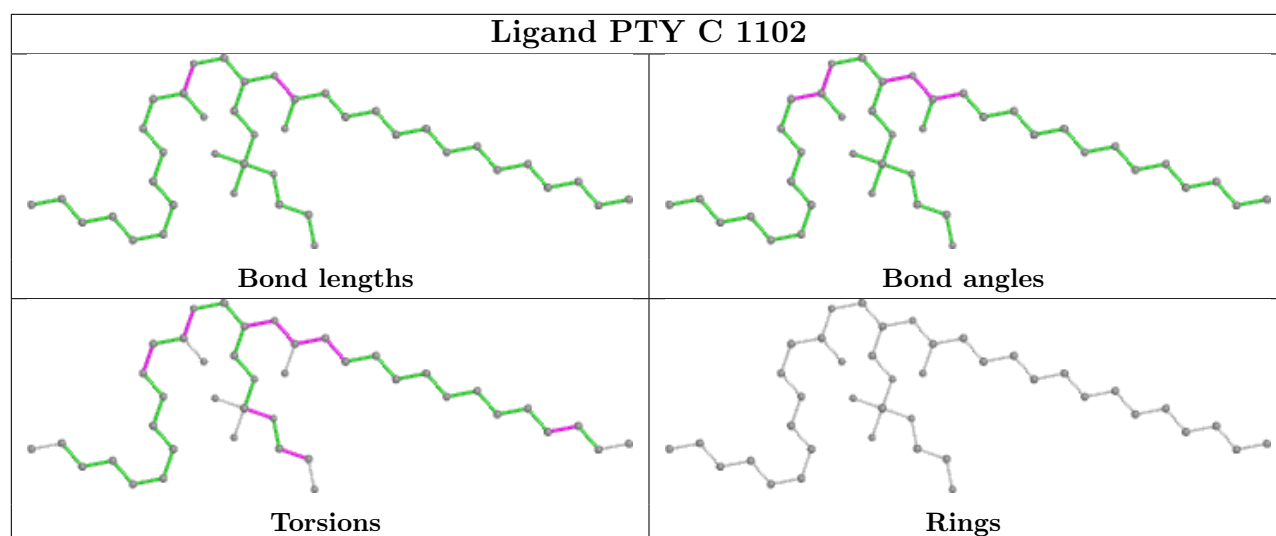












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

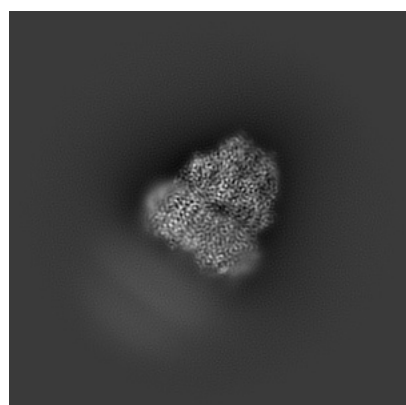
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21229. These allow visual inspection of the internal detail of the map and identification of artifacts.

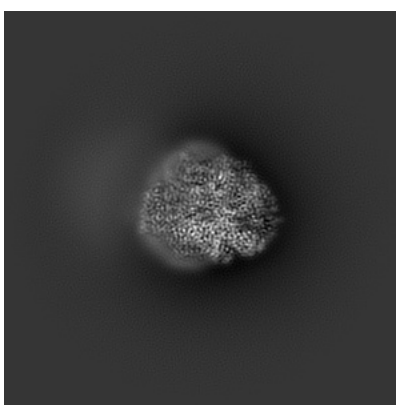
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

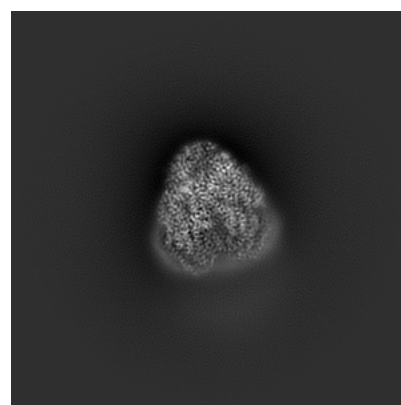
#### 6.1.1 Primary map



X



Y

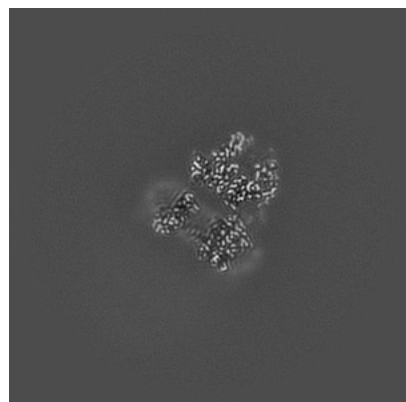


Z

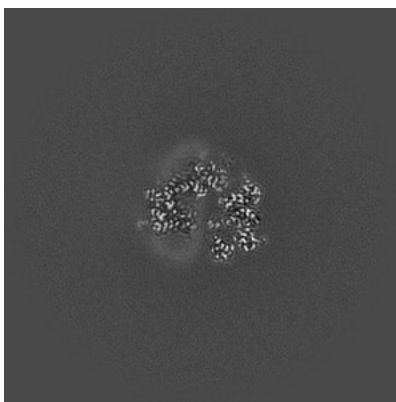
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

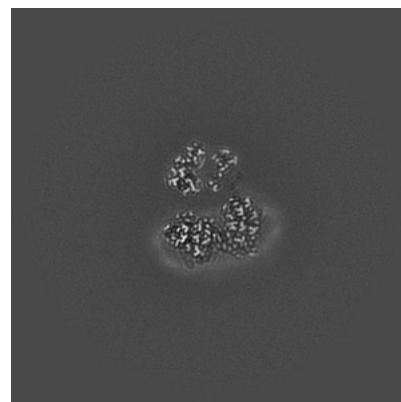
#### 6.2.1 Primary map



X Index: 175



Y Index: 175

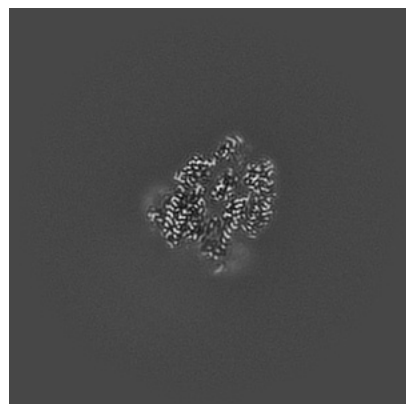


Z Index: 175

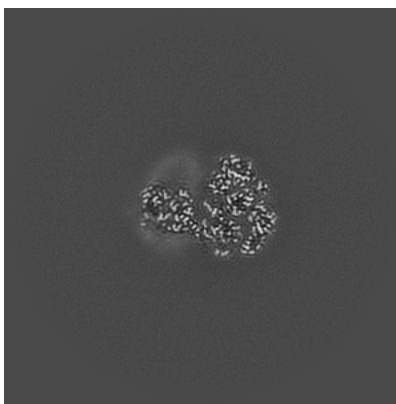
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

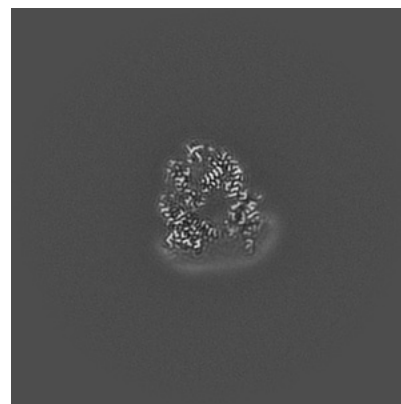
### 6.3.1 Primary map



X Index: 155



Y Index: 190

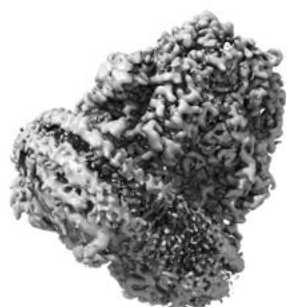


Z Index: 183

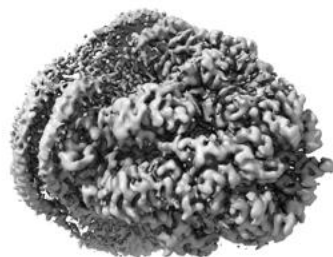
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

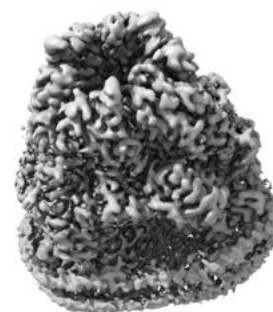
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

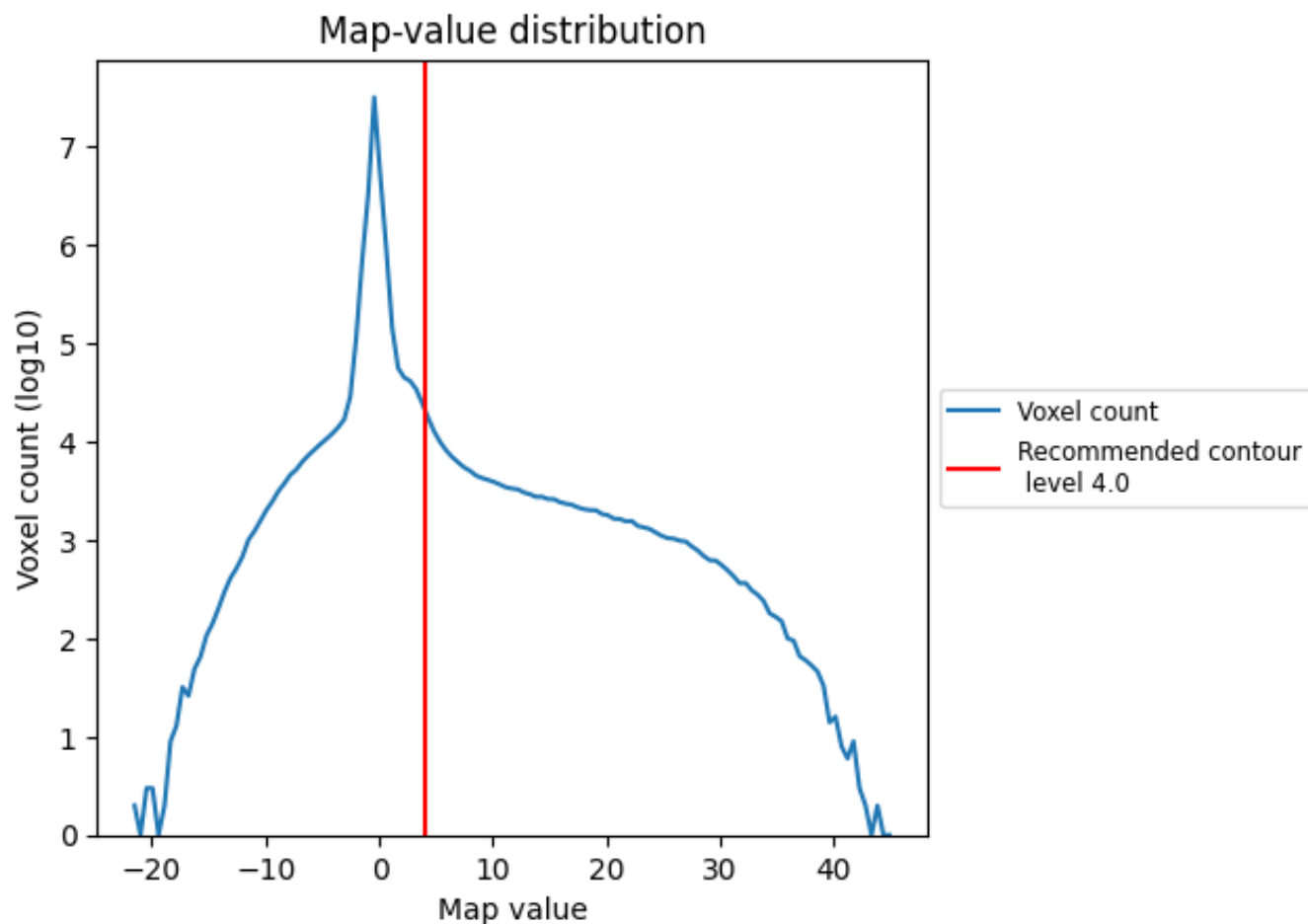
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

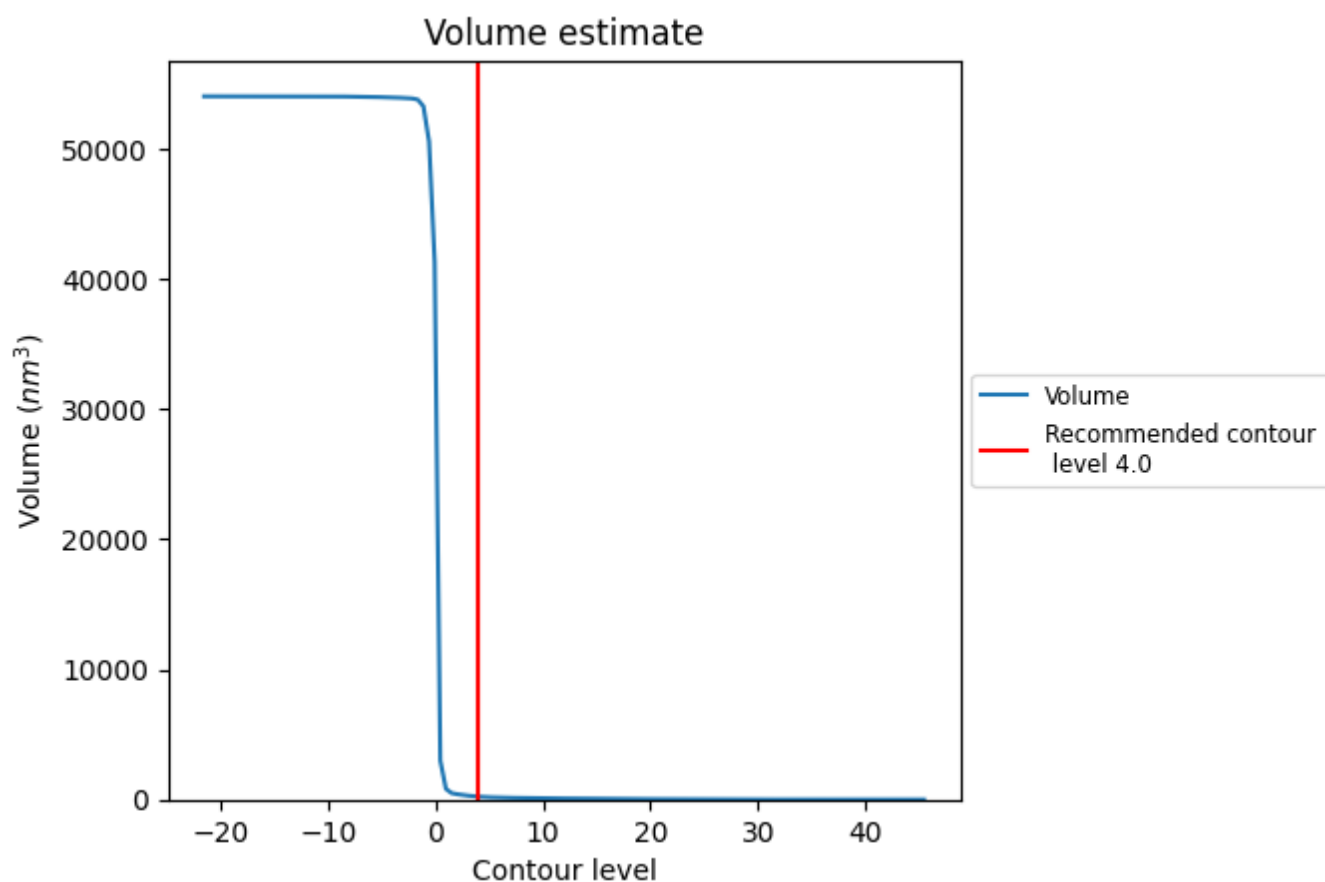
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



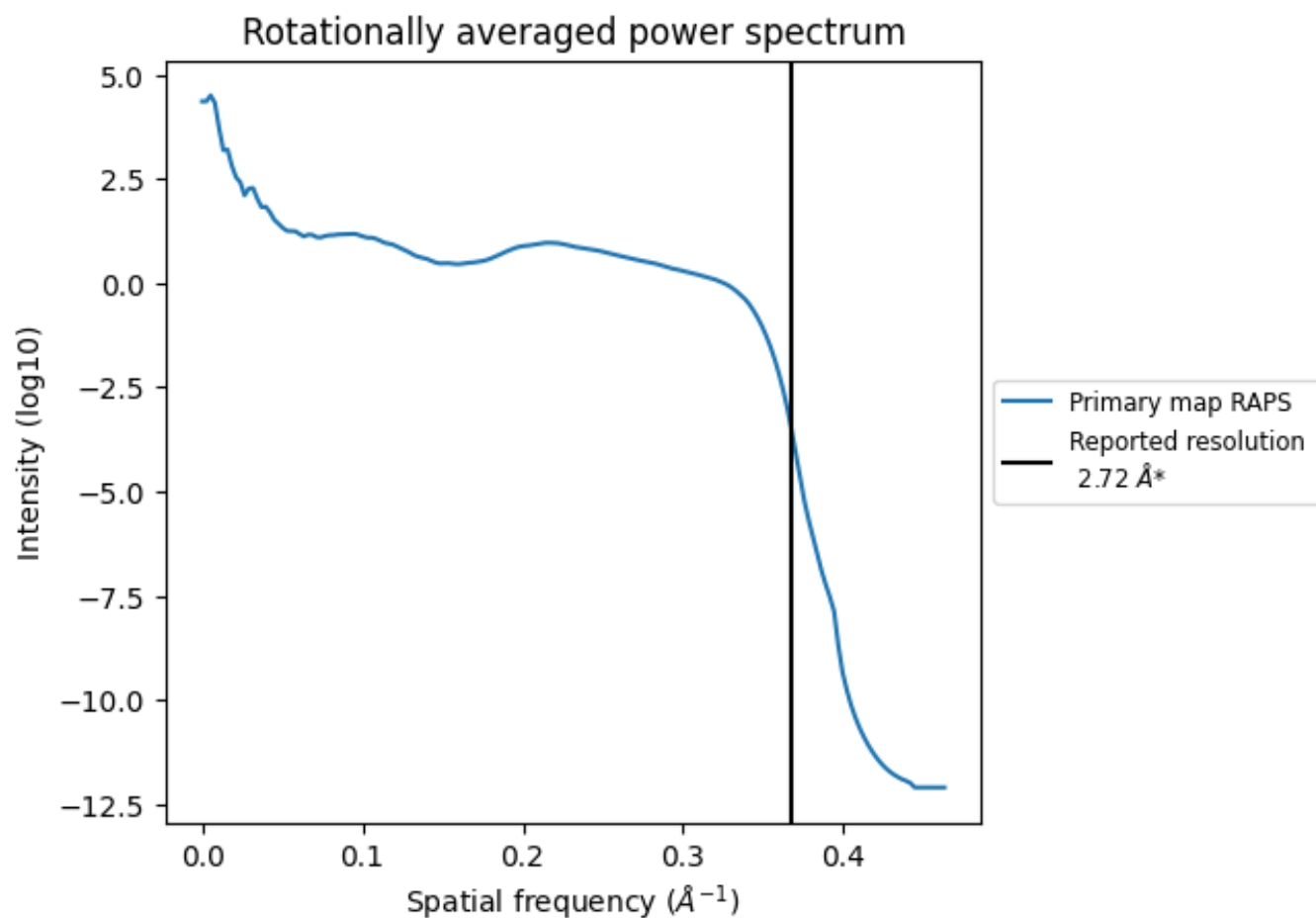
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224  $\text{nm}^3$ ; this corresponds to an approximate mass of 202 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.368 Å<sup>-1</sup>

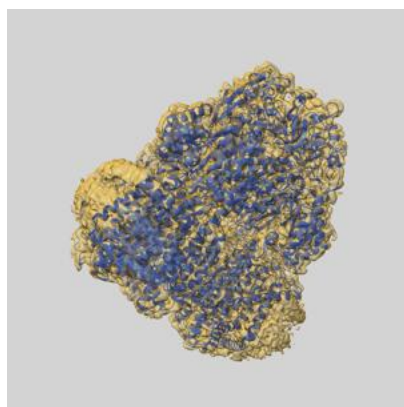
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

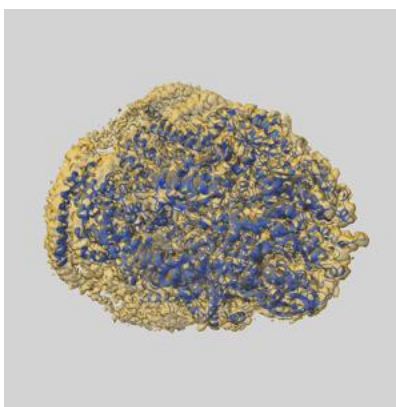
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21229 and PDB model 6VKT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

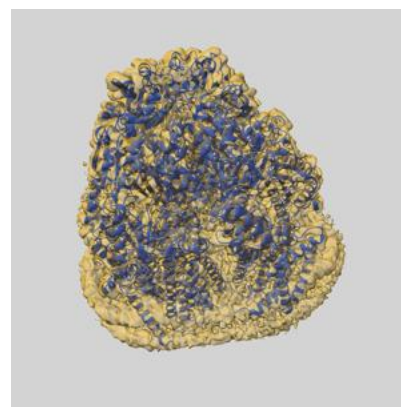
### 9.1 Map-model overlay [i](#)



X



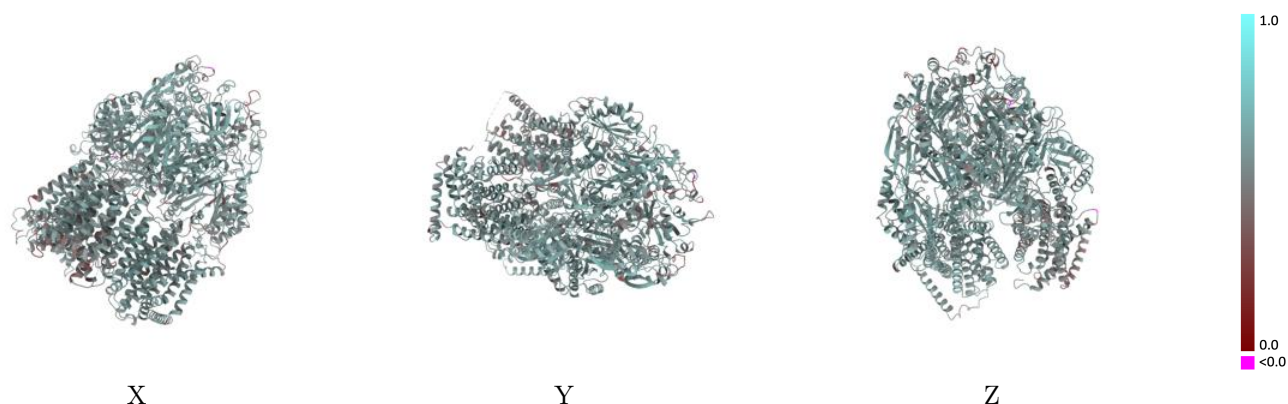
Y



Z

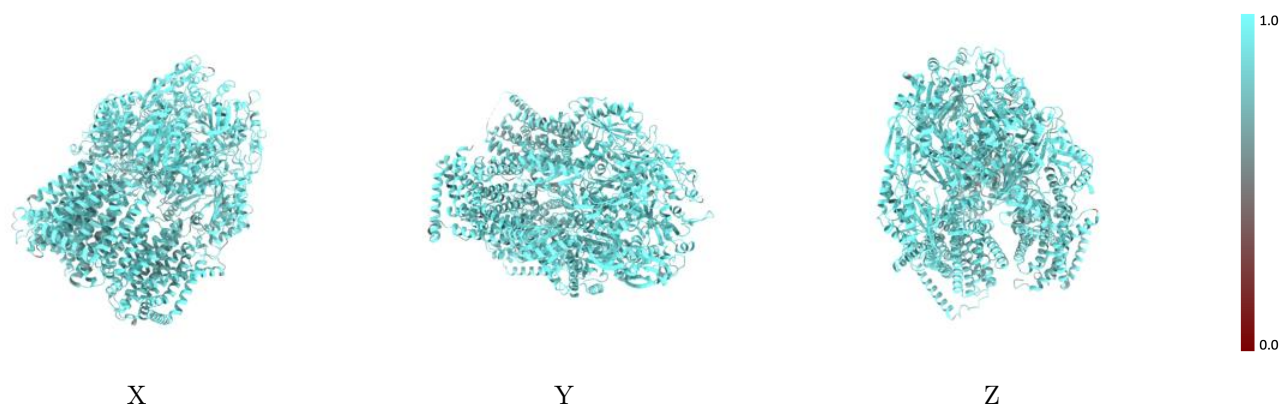
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



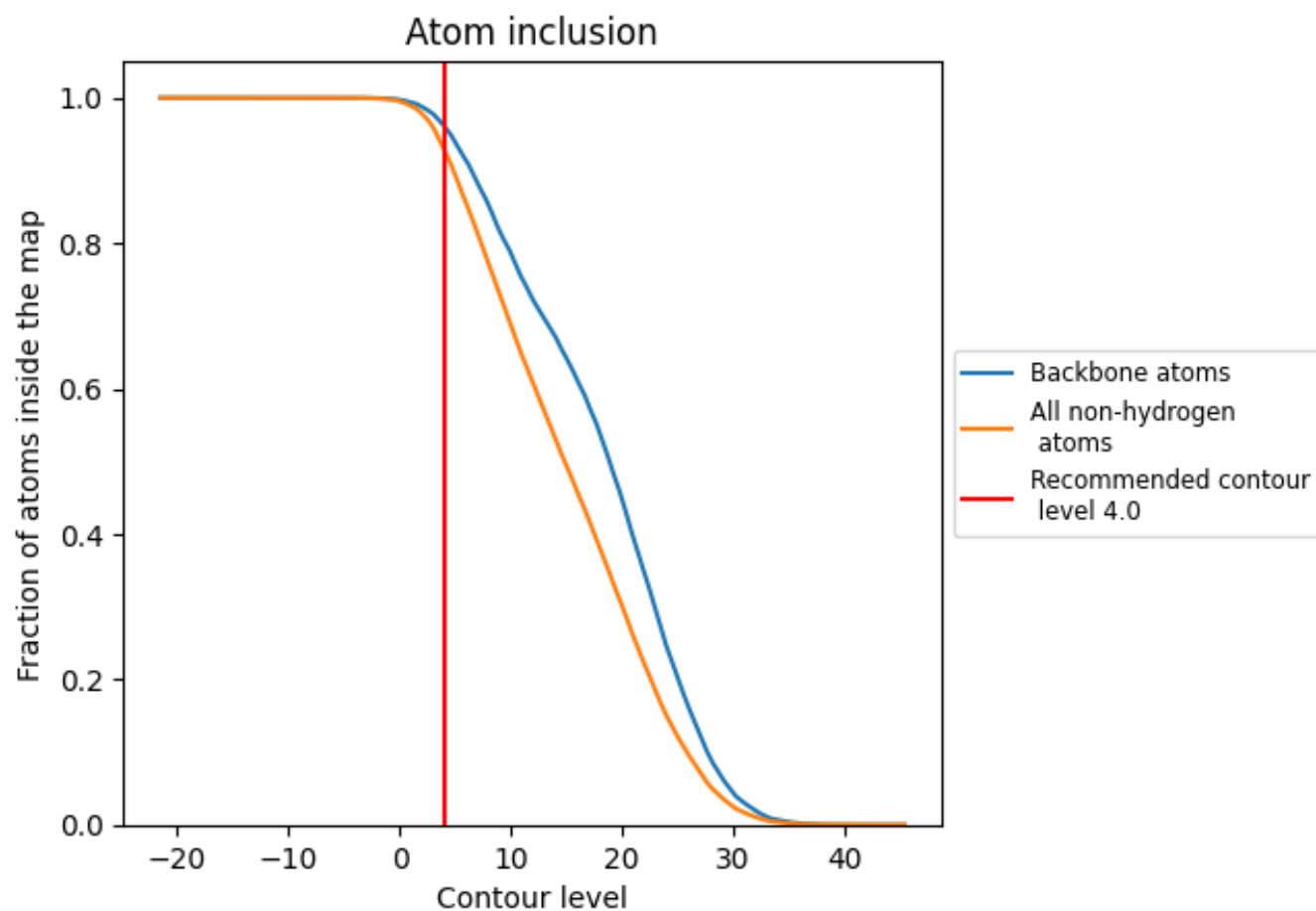
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9292	<div><div></div></div> 0.5660
A	<div><div></div></div> 0.9173	<div><div></div></div> 0.5510
B	<div><div></div></div> 0.9272	<div><div></div></div> 0.5650
C	<div><div></div></div> 0.9431	<div><div></div></div> 0.5840

