



Full wwPDB EM Validation Report ⓘ

May 25, 2026 – 04:15 PM JST

PDB ID : 9J8R / pdb_00009j8r
EMDB ID : EMD-61239
Title : MprF from Pseudomonas aeruginosa in GDN micelle, C1 symmetry
Authors : Jha, S.; Vinothkumar, K.R.
Deposited on : 2024-08-21
Resolution : 3.40 Å(reported)
Based on initial model : .

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

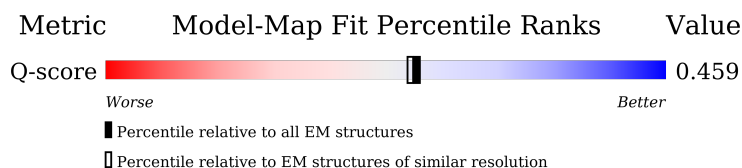
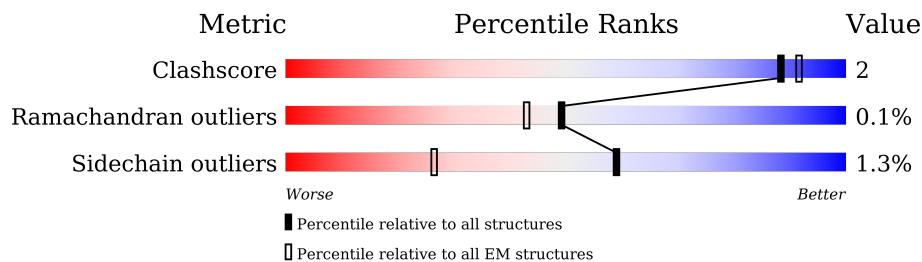
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 ≥ 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	903	
1	B	903	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13056 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 Phosphatidylglycerol lysyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	799	Total	C	N	O	S	0	0
			6145	4020	1069	1035	21		
1	B	799	Total	C	N	O	S	0	0
			6145	4020	1069	1035	21		

There are 44 discrepancies between the modelled and reference sequences:

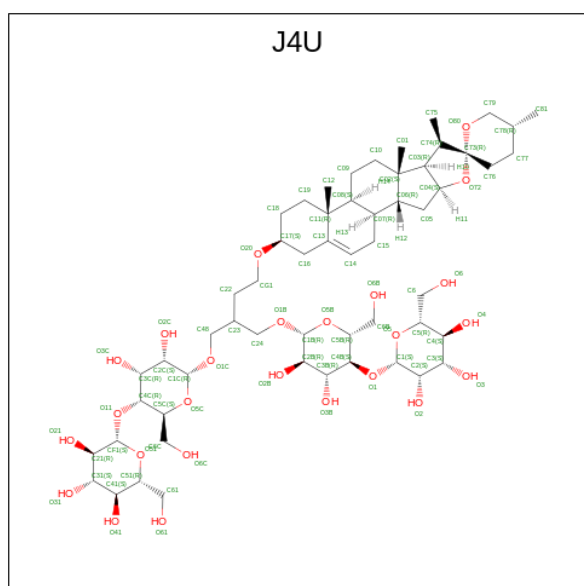
Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q9I537
A	-11	TRP	-	expression tag	UNP Q9I537
A	-10	SER	-	expression tag	UNP Q9I537
A	-9	HIS	-	expression tag	UNP Q9I537
A	-8	PRO	-	expression tag	UNP Q9I537
A	-7	GLN	-	expression tag	UNP Q9I537
A	-6	PHE	-	expression tag	UNP Q9I537
A	-5	GLU	-	expression tag	UNP Q9I537
A	-4	LYS	-	expression tag	UNP Q9I537
A	-3	GLY	-	expression tag	UNP Q9I537
A	-2	GLY	-	expression tag	UNP Q9I537
A	-1	SER	-	expression tag	UNP Q9I537
A	0	GLY	-	expression tag	UNP Q9I537
A	882	ARG	-	expression tag	UNP Q9I537
A	883	ASN	-	expression tag	UNP Q9I537
A	884	SER	-	expression tag	UNP Q9I537
A	885	SER	-	expression tag	UNP Q9I537
A	886	SER	-	expression tag	UNP Q9I537
A	887	VAL	-	expression tag	UNP Q9I537
A	888	ASP	-	expression tag	UNP Q9I537
A	889	ALA	-	expression tag	UNP Q9I537
A	890	LEU	-	expression tag	UNP Q9I537
B	-12	MET	-	initiating methionine	UNP Q9I537
B	-11	TRP	-	expression tag	UNP Q9I537
B	-10	SER	-	expression tag	UNP Q9I537
B	-9	HIS	-	expression tag	UNP Q9I537

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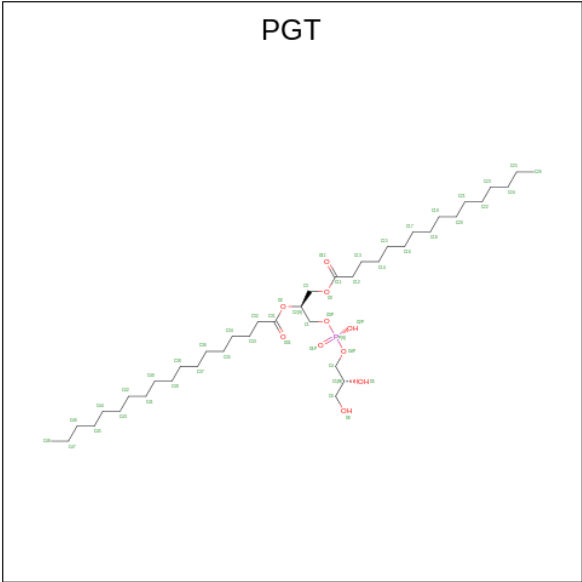
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	PRO	-	expression tag	UNP Q9I537
B	-7	GLN	-	expression tag	UNP Q9I537
B	-6	PHE	-	expression tag	UNP Q9I537
B	-5	GLU	-	expression tag	UNP Q9I537
B	-4	LYS	-	expression tag	UNP Q9I537
B	-3	GLY	-	expression tag	UNP Q9I537
B	-2	GLY	-	expression tag	UNP Q9I537
B	-1	SER	-	expression tag	UNP Q9I537
B	0	GLY	-	expression tag	UNP Q9I537
B	882	ARG	-	expression tag	UNP Q9I537
B	883	ASN	-	expression tag	UNP Q9I537
B	884	SER	-	expression tag	UNP Q9I537
B	885	SER	-	expression tag	UNP Q9I537
B	886	SER	-	expression tag	UNP Q9I537
B	887	VAL	-	expression tag	UNP Q9I537
B	888	ASP	-	expression tag	UNP Q9I537
B	889	ALA	-	expression tag	UNP Q9I537
B	890	LEU	-	expression tag	UNP Q9I537

- Molecule 2 is (2 {R},3 {S},4 {S},5 {S},6 {S})-2-(hydroxymethyl)-6-[(2 {R},3 {S},4 {R},5 {R},6 {R})-2-(hydroxymethyl)-6-[2-[(2 {R},3 {S},4 {R},5 {R},6 {S})-6-(hydroxymethyl)-5-[(2 {S},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4-bis(oxidanyl)oxan-2-yl]oxymethyl]-4-[(1 {R},2 {R},4 {S},5' {R},6 {R},7 {R},8 {R},9 {S},12 {S},13 {R},16 {S})-5',7,9,13-tetramethylspiro[5-oxapentacyclo[10.8.0.0^{2,9}.0^{4,8}.0^{1,3,18}]]icos-18-ene-6,2'-oxane]-16-yl]oxy-butoxy]-4,5-bis(oxidanyl)oxan-3-yl]oxy-oxane-3,4,5-triol (CCD ID: J4U) (formula: C₅₆H₉₂O₂₅).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	32	3	
2	B	1	Total	C	O	0
			35	32	3	

- Molecule 3 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



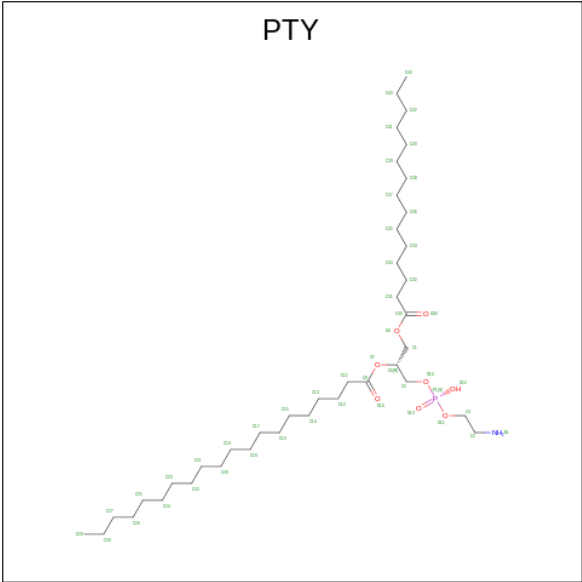
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			33	24	8	1	
3	A	1	Total	C			0
			14	14			
3	A	1	Total	C			0
			14	14			
3	A	1	Total	C			0
			14	14			
3	A	1	Total	C			0
			14	14			
3	A	1	Total	C			0
			17	17			
3	A	1	Total	C			0
			15	15			
3	A	1	Total	C	O		0
			20	18	2		
3	A	1	Total	C	O	P	0
			51	40	10	1	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C			0
			10	10			
3	A	1	Total	C	O	P	0
			51	40	10	1	
3	B	1	Total	C			0
			10	10			
3	B	1	Total	C	O	P	0
			51	40	10	1	
3	B	1	Total	C	O	P	0
			33	24	8	1	
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			14	14			
3	B	1	Total	C			0
			17	17			
3	B	1	Total	C			0
			15	15			
3	B	1	Total	C	O		0
			20	18	2		
3	B	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 4 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).

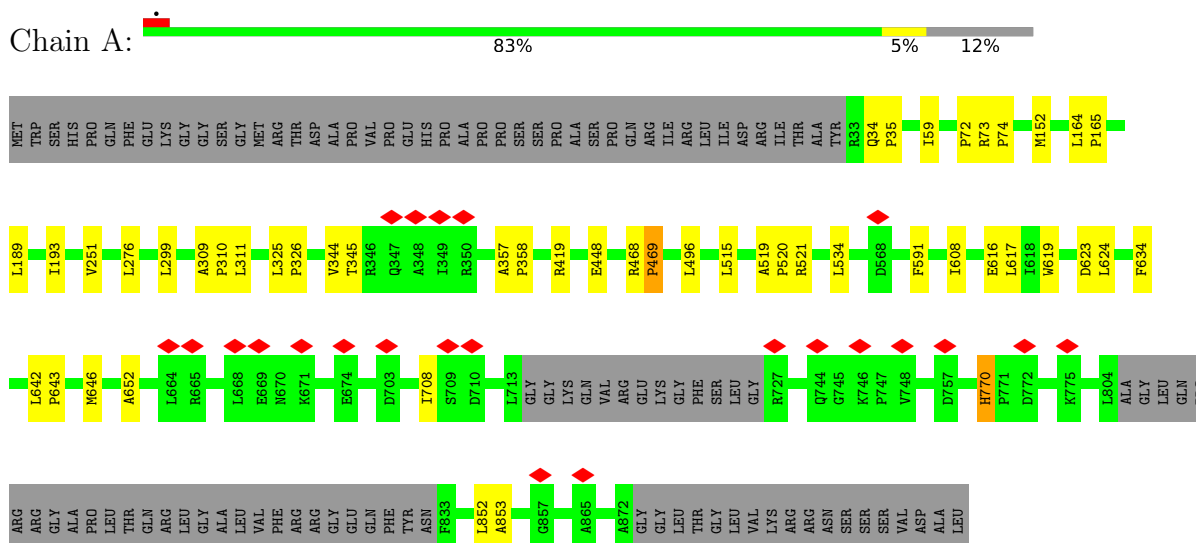


Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	C	0
			15	15	
4	A	1	Total	C	0
			15	15	
4	A	1	Total	C	0
			15	15	
4	A	1	Total	C	0
			15	15	
4	A	1	Total	C	0
			20	20	
4	A	1	Total	C	0
			15	15	
4	B	1	Total	C	0
			15	15	
4	B	1	Total	C	0
			15	15	
4	B	1	Total	C	0
			15	15	
4	B	1	Total	C	0
			20	20	
4	B	1	Total	C	0
			15	15	

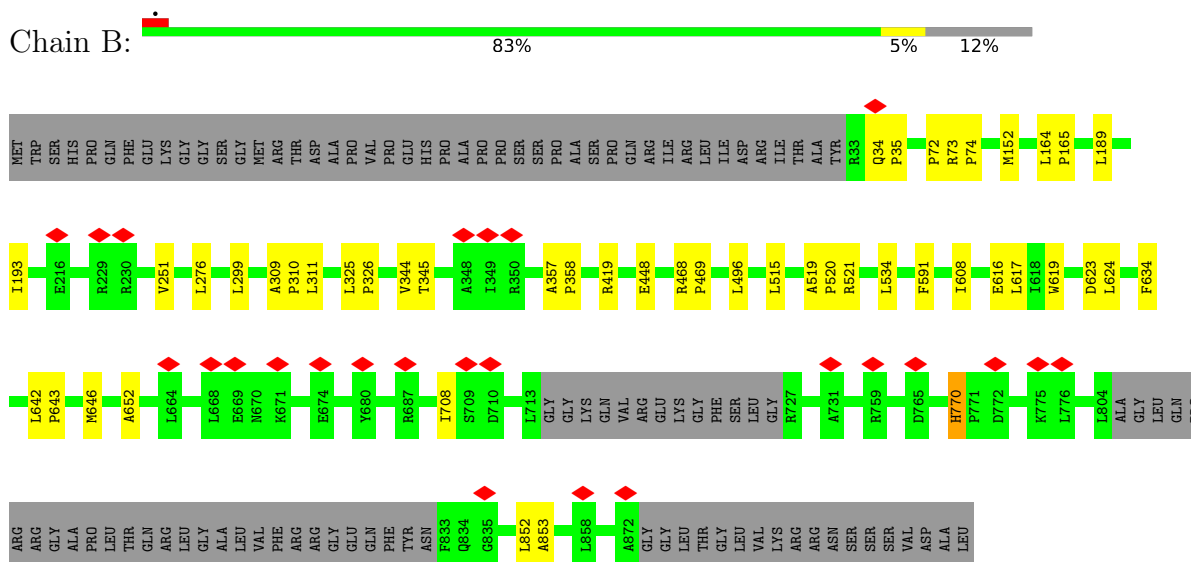
3 Residue-property plots

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: Phosphatidylglycerol lysyltransferase



• Molecule 1: Phosphatidylglycerol lysyltransferase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	109157	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.75	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130841	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	8.144	Depositor
Minimum map value	-5.414	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.116	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGT, J4U, 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	0.45	0/6286	0.79	0/8560
1	B	0.45	0/6286	0.79	0/8560
All	All	0.45	0/12572	0.79	0/17120

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	A	6145	0	6404	23	0
1	B	6145	0	6404	23	0
2	A	35	0	0	0	0
2	B	35	0	0	1	0
3	A	253	0	402	0	0
3	B	253	0	402	1	0
4	A	95	0	169	1	0
4	B	95	0	169	1	0
All	All	13056	0	13950	50	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 2.

All (50) 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:515:LEU:O	1:A:521:ARG:NH2	2.30	0.65
1:A:634:PHE:HB2	1:A:853:ALA:HB3	1.80	0.63
1:B:515:LEU:O	1:B:521:ARG:NH2	2.30	0.63
1:B:634:PHE:HB2	1:B:853:ALA:HB3	1.80	0.62
1:A:591:PHE:CZ	1:A:608:ILE:HD12	2.41	0.56
1:B:642:LEU:HD22	1:B:652:ALA:HB2	1.87	0.56
1:A:642:LEU:N	1:A:643:PRO:HD2	2.21	0.56
1:B:591:PHE:CZ	1:B:608:ILE:HD12	2.41	0.56
1:B:708:ILE:HD12	1:B:770:HIS:CE1	2.42	0.55
1:B:642:LEU:N	1:B:643:PRO:HD2	2.21	0.55
1:A:642:LEU:HD22	1:A:652:ALA:HB2	1.88	0.54
1:A:708:ILE:HD12	1:A:770:HIS:CE1	2.42	0.54
1:A:325:LEU:HB3	1:A:326:PRO:HD3	1.91	0.53
1:B:325:LEU:HB3	1:B:326:PRO:HD3	1.90	0.53
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.92	0.51
1:B:357:ALA:HB3	1:B:358:PRO:HD3	1.93	0.51
1:A:251:VAL:HG11	1:A:276:LEU:HD21	1.92	0.50
1:B:251:VAL:HG11	1:B:276:LEU:HD21	1.92	0.50
1:A:189:LEU:O	1:A:193:ILE:HG12	2.14	0.48
1:B:519:ALA:HB3	1:B:520:PRO:HD3	1.96	0.48
1:B:299:LEU:HD23	1:B:311:LEU:HD23	1.96	0.47
1:A:519:ALA:HB3	1:A:520:PRO:HD3	1.96	0.47
1:A:299:LEU:HD23	1:A:311:LEU:HD23	1.96	0.47
1:B:189:LEU:O	1:B:193:ILE:HG12	2.14	0.47
1:B:309:ALA:HB3	1:B:310:PRO:HD3	1.97	0.46
1:A:496:LEU:C	1:A:496:LEU:HD23	2.40	0.46
1:B:496:LEU:C	1:B:496:LEU:HD23	2.40	0.46
1:A:309:ALA:HB3	1:A:310:PRO:HD3	1.98	0.45
1:A:344:VAL:HG23	1:A:345:THR:HG23	2.00	0.44
4:A:915:PTY:H151	4:A:915:PTY:H182	1.83	0.44
1:A:448:GLU:OE1	1:A:448:GLU:N	2.50	0.43
3:B:904:PGT:H122	3:B:904:PGT:H32	1.71	0.43
1:B:419:ARG:NH1	1:B:623:ASP:OD1	2.51	0.43
1:A:419:ARG:NH1	1:A:623:ASP:OD1	2.52	0.43
1:A:72:PRO:HB2	1:A:74:PRO:HD2	2.02	0.42
1:A:468:ARG:HD2	1:A:619:TRP:CG	2.55	0.42
1:B:468:ARG:HD2	1:B:619:TRP:CG	2.54	0.42
1:A:617:LEU:HD23	1:A:617:LEU:HA	1.91	0.42
1:B:344:VAL:HG23	1:B:345:THR:HG23	2.00	0.42
1:B:617:LEU:HD23	1:B:617:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:N	1:A:165:PRO:CD	2.83	0.41
1:B:72:PRO:HB2	1:B:74:PRO:HD2	2.01	0.41
1:B:164:LEU:N	1:B:165:PRO:CD	2.83	0.41
1:A:34:GLN:N	1:A:35:PRO:HD2	2.36	0.41
1:B:34:GLN:N	1:B:35:PRO:HD2	2.36	0.41
2:B:903:J4U:C01	2:B:903:J4U:C75	2.99	0.40
4:B:917:PTY:H151	4:B:917:PTY:H182	1.80	0.40
1:A:73:ARG:N	1:A:74:PRO:CD	2.84	0.40
1:B:448:GLU:OE1	1:B:448:GLU:N	2.50	0.40
1:B:73:ARG:N	1:B:74:PRO:CD	2.84	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 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	793/903 (88%)	763 (96%)	29 (4%)	1 (0%)	48	78
1	B	793/903 (88%)	763 (96%)	29 (4%)	1 (0%)	48	78
All	All	1586/1806 (88%)	1526 (96%)	58 (4%)	2 (0%)	49	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	469	PRO
1	A	469	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	624/706 (88%)	615 (99%)	9 (1%)	59	70
1	B	624/706 (88%)	617 (99%)	7 (1%)	65	74
All	All	1248/1412 (88%)	1232 (99%)	16 (1%)	59	71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	152	MET
1	A	469	PRO
1	A	534	LEU
1	A	616	GLU
1	A	624	LEU
1	A	646	MET
1	A	770	HIS
1	A	852	LEU
1	B	152	MET
1	B	534	LEU
1	B	616	GLU
1	B	624	LEU
1	B	646	MET
1	B	770	HIS
1	B	852	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	HIS
1	A	393	HIS
1	A	501	GLN
1	A	569	GLN
1	A	844	GLN
1	B	211	HIS
1	B	286	HIS
1	B	501	GLN
1	B	844	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 ⓘ

36 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	$\# Z > 2$
3	PGT	A	909	-	16,16,50	0.08	0	15,15,56	0.04	0
3	PGT	B	902	-	50,50,50	0.26	0	53,56,56	0.37	0
3	PGT	A	911	-	19,19,50	0.33	0	19,19,56	0.16	0
3	PGT	B	906	-	13,13,50	0.08	0	12,12,56	0.06	0
3	PGT	A	918	-	50,50,50	0.27	0	53,56,56	0.36	0
4	PTY	A	905	-	14,14,49	0.09	0	13,13,54	0.07	0
3	PGT	A	910	-	14,14,50	0.08	0	13,13,56	0.06	0
4	PTY	B	917	-	19,19,49	0.12	0	18,18,54	0.15	0
3	PGT	A	907	-	13,13,50	0.08	0	12,12,56	0.07	0
4	PTY	A	913	-	14,14,49	0.11	0	13,13,54	0.09	0
4	PTY	B	915	-	14,14,49	0.10	0	13,13,54	0.09	0
3	PGT	A	902	-	32,32,50	0.34	0	35,37,56	0.43	0
3	PGT	A	917	-	9,9,50	0.11	0	8,8,56	0.08	0
3	PGT	B	911	-	16,16,50	0.08	0	15,15,56	0.04	0
3	PGT	B	912	-	14,14,50	0.08	0	13,13,56	0.06	0
4	PTY	A	915	-	19,19,49	0.12	0	18,18,54	0.14	0
3	PGT	B	914	-	50,50,50	0.26	0	53,56,56	0.30	0
4	PTY	B	916	-	14,14,49	0.10	0	13,13,54	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGT	A	908	-	13,13,50	0.09	0	12,12,56	0.08	0
2	J4U	B	903	-	40,40,90	0.31	0	64,64,138	1.03	3 (4%)
4	PTY	B	918	-	14,14,49	0.09	0	13,13,54	0.08	0
2	J4U	A	901	-	40,40,90	0.32	0	64,64,138	1.05	3 (4%)
4	PTY	A	914	-	14,14,49	0.10	0	13,13,54	0.10	0
3	PGT	B	913	-	19,19,50	0.33	0	19,19,56	0.16	0
4	PTY	A	916	-	14,14,49	0.09	0	13,13,54	0.07	0
3	PGT	A	912	-	50,50,50	0.26	0	53,56,56	0.28	0
3	PGT	B	910	-	13,13,50	0.08	0	12,12,56	0.07	0
3	PGT	A	903	-	13,13,50	0.09	0	12,12,56	0.08	0
4	PTY	B	907	-	14,14,49	0.10	0	13,13,54	0.08	0
3	PGT	B	905	-	13,13,50	0.08	0	12,12,56	0.07	0
4	PTY	A	906	-	14,14,49	0.09	0	13,13,54	0.14	0
3	PGT	B	904	-	32,32,50	0.33	0	35,37,56	0.44	0
4	PTY	B	908	-	14,14,49	0.09	0	13,13,54	0.13	0
3	PGT	A	904	-	13,13,50	0.08	0	12,12,56	0.06	0
3	PGT	B	909	-	13,13,50	0.09	0	12,12,56	0.07	0
3	PGT	B	901	-	9,9,50	0.10	0	8,8,56	0.09	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
3	PGT	A	909	-	-	4/14/14/55	-
3	PGT	B	902	-	-	16/55/55/55	-
3	PGT	A	911	-	-	14/17/17/55	-
3	PGT	B	906	-	-	5/11/11/55	-
3	PGT	A	918	-	-	15/55/55/55	-
4	PTY	A	905	-	-	6/12/12/53	-
3	PGT	A	910	-	-	1/12/12/55	-
4	PTY	B	917	-	-	7/17/17/53	-
3	PGT	A	907	-	-	3/11/11/55	-
4	PTY	A	913	-	-	9/12/12/53	-
4	PTY	B	915	-	-	9/12/12/53	-
3	PGT	A	902	-	-	16/36/36/55	-
3	PGT	A	917	-	-	2/7/7/55	-
3	PGT	B	911	-	-	4/14/14/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGT	B	912	-	-	1/12/12/55	-
4	PTY	A	915	-	-	7/17/17/53	-
3	PGT	B	914	-	-	26/55/55/55	-
4	PTY	B	916	-	-	8/12/12/53	-
3	PGT	A	908	-	-	4/11/11/55	-
2	J4U	B	903	-	-	2/6/94/200	0/6/6/10
4	PTY	B	918	-	-	5/12/12/53	-
2	J4U	A	901	-	-	2/6/94/200	0/6/6/10
4	PTY	A	914	-	-	7/12/12/53	-
3	PGT	B	913	-	-	14/17/17/55	-
4	PTY	A	916	-	-	5/12/12/53	-
3	PGT	A	912	-	-	25/55/55/55	-
3	PGT	B	910	-	-	4/11/11/55	-
3	PGT	A	903	-	-	2/11/11/55	-
4	PTY	B	907	-	-	7/12/12/53	-
3	PGT	B	905	-	-	3/11/11/55	-
4	PTY	A	906	-	-	8/12/12/53	-
3	PGT	B	904	-	-	15/36/36/55	-
4	PTY	B	908	-	-	9/12/12/53	-
3	PGT	A	904	-	-	4/11/11/55	-
3	PGT	B	909	-	-	3/11/11/55	-
3	PGT	B	901	-	-	3/7/7/55	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	J4U	C15-C07-C08	4.71	115.42	109.71
2	B	903	J4U	C15-C07-C08	4.68	115.38	109.71
2	A	901	J4U	C11-C08-C07	3.93	118.63	112.73
2	B	903	J4U	C11-C08-C07	3.79	118.42	112.73
2	A	901	J4U	C07-C15-C14	2.71	116.62	112.73
2	B	903	J4U	C07-C15-C14	2.65	116.53	112.73

There are no chirality outliers.

All (275) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	J4U	C22-CG1-O20-C17
2	B	903	J4U	C22-CG1-O20-C17
3	A	902	PGT	C1-O3P-P-O1P
3	A	902	PGT	C1-O3P-P-O4P
3	A	902	PGT	O11-C11-O3-C3
3	A	902	PGT	C12-C11-O3-C3
3	A	912	PGT	C1-O3P-P-O1P
3	A	912	PGT	C1-O3P-P-O2P
3	A	912	PGT	C4-O4P-P-O1P
3	A	912	PGT	C4-O4P-P-O2P
3	A	918	PGT	O11-C11-O3-C3
3	A	918	PGT	C12-C11-O3-C3
3	B	902	PGT	O11-C11-O3-C3
3	B	902	PGT	C12-C11-O3-C3
3	B	904	PGT	C1-O3P-P-O1P
3	B	904	PGT	C1-O3P-P-O4P
3	B	904	PGT	O11-C11-O3-C3
3	B	904	PGT	C12-C11-O3-C3
3	B	914	PGT	C1-O3P-P-O1P
3	B	914	PGT	C1-O3P-P-O2P
3	B	914	PGT	C4-O4P-P-O1P
3	B	914	PGT	C4-O4P-P-O2P
4	A	915	PTY	C11-C12-C13-C14
4	B	917	PTY	C11-C12-C13-C14
4	A	915	PTY	C25-C26-C27-C28
4	B	917	PTY	C13-C14-C15-C16
4	B	917	PTY	C25-C26-C27-C28
4	A	915	PTY	C13-C14-C15-C16
3	B	902	PGT	C31-C32-C33-C34
3	B	913	PGT	C41-C42-C43-C44
3	A	918	PGT	C31-C32-C33-C34
3	A	911	PGT	C41-C42-C43-C44
4	B	917	PTY	C15-C16-C17-C18
3	B	914	PGT	C34-C35-C36-C37
3	A	912	PGT	C1-O3P-P-O4P
3	A	912	PGT	C4-O4P-P-O3P
3	B	914	PGT	C1-O3P-P-O4P
3	B	914	PGT	C4-O4P-P-O3P
4	A	915	PTY	C15-C16-C17-C18
3	A	912	PGT	C34-C35-C36-C37
3	A	911	PGT	C40-C41-C42-C43
3	A	911	PGT	C36-C37-C38-C39
3	A	918	PGT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	B	902	PGT	C12-C13-C14-C15
4	A	916	PTY	C8-C11-C12-C13
4	B	915	PTY	C13-C14-C15-C16
3	A	918	PGT	C36-C37-C38-C39
3	B	913	PGT	C36-C37-C38-C39
4	A	913	PTY	C13-C14-C15-C16
3	B	913	PGT	C40-C41-C42-C43
4	B	916	PTY	C15-C16-C17-C18
3	A	918	PGT	C32-C33-C34-C35
3	A	902	PGT	C33-C34-C35-C36
3	B	905	PGT	C38-C39-C40-C41
4	A	914	PTY	C15-C16-C17-C18
3	A	903	PGT	C38-C39-C40-C41
3	B	904	PGT	C33-C34-C35-C36
3	A	903	PGT	C33-C34-C35-C36
3	B	905	PGT	C33-C34-C35-C36
3	B	913	PGT	C31-C32-C33-C34
3	A	912	PGT	C20-C21-C22-C23
3	B	902	PGT	C35-C36-C37-C38
3	B	914	PGT	C20-C21-C22-C23
4	A	913	PTY	C12-C13-C14-C15
4	A	913	PTY	C16-C17-C18-C19
4	B	915	PTY	C16-C17-C18-C19
3	A	911	PGT	C38-C39-C40-C41
3	A	912	PGT	C42-C43-C44-C45
3	B	902	PGT	C36-C37-C38-C39
3	B	913	PGT	C38-C39-C40-C41
4	B	915	PTY	C12-C13-C14-C15
4	B	918	PTY	C17-C18-C19-C20
3	A	911	PGT	C31-C32-C33-C34
3	B	902	PGT	C32-C33-C34-C35
3	B	914	PGT	C42-C43-C44-C45
4	A	916	PTY	C17-C18-C19-C20
3	A	918	PGT	C35-C36-C37-C38
4	A	905	PTY	C19-C20-C21-C22
4	B	918	PTY	C8-C11-C12-C13
4	B	907	PTY	C19-C20-C21-C22
3	A	911	PGT	C44-C45-C46-C47
3	B	913	PGT	C44-C45-C46-C47
4	A	906	PTY	C21-C22-C23-C24
4	A	916	PTY	C13-C14-C15-C16
3	A	902	PGT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	B	908	PTY	C21-C22-C23-C24
3	B	904	PGT	C12-C13-C14-C15
4	A	913	PTY	C15-C16-C17-C18
4	B	918	PTY	C13-C14-C15-C16
3	A	911	PGT	C32-C33-C34-C35
3	B	904	PGT	C11-C12-C13-C14
3	B	913	PGT	C32-C33-C34-C35
4	B	915	PTY	C15-C16-C17-C18
4	A	906	PTY	C12-C13-C14-C15
4	A	915	PTY	C16-C17-C18-C19
4	B	918	PTY	C15-C16-C17-C18
4	B	908	PTY	C12-C13-C14-C15
4	B	917	PTY	C16-C17-C18-C19
3	A	912	PGT	O2-C2-C3-O3
3	B	914	PGT	O2-C2-C3-O3
3	A	902	PGT	C11-C12-C13-C14
4	A	906	PTY	C14-C15-C16-C17
4	A	916	PTY	C15-C16-C17-C18
3	A	918	PGT	C37-C38-C39-C40
3	B	901	PGT	C33-C34-C35-C36
3	A	918	PGT	O3P-C1-C2-C3
3	B	902	PGT	C37-C38-C39-C40
3	A	917	PGT	C33-C34-C35-C36
4	B	908	PTY	C14-C15-C16-C17
3	A	909	PGT	C45-C46-C47-C48
3	B	906	PGT	C32-C33-C34-C35
3	A	904	PGT	C32-C33-C34-C35
3	A	918	PGT	C15-C16-C17-C18
3	B	911	PGT	C45-C46-C47-C48
3	A	912	PGT	C23-C24-C25-C26
4	B	907	PTY	C20-C21-C22-C23
3	B	914	PGT	C23-C24-C25-C26
4	A	905	PTY	C20-C21-C22-C23
3	B	902	PGT	C15-C16-C17-C18
3	B	901	PGT	C38-C39-C40-C41
4	B	917	PTY	C26-C27-C28-C29
4	A	915	PTY	C26-C27-C28-C29
3	B	902	PGT	C16-C17-C18-C19
4	A	913	PTY	C11-C12-C13-C14
4	A	905	PTY	C17-C18-C19-C20
4	B	915	PTY	C11-C12-C13-C14
3	A	918	PGT	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
3	B	902	PGT	C34-C35-C36-C37
4	A	914	PTY	C13-C14-C15-C16
4	B	907	PTY	C17-C18-C19-C20
3	A	902	PGT	O3P-C1-C2-C3
3	B	902	PGT	O3P-C1-C2-C3
3	B	904	PGT	O3P-C1-C2-C3
4	B	916	PTY	C17-C18-C19-C20
3	A	904	PGT	C33-C34-C35-C36
3	A	911	PGT	C33-C34-C35-C36
4	B	916	PTY	C13-C14-C15-C16
3	A	902	PGT	C1-C2-C3-O3
3	A	912	PGT	C1-C2-C3-O3
3	B	904	PGT	C1-C2-C3-O3
3	B	914	PGT	C1-C2-C3-O3
4	A	914	PTY	C17-C18-C19-C20
3	B	906	PGT	C33-C34-C35-C36
3	A	917	PGT	C38-C39-C40-C41
3	B	909	PGT	C40-C41-C42-C43
3	A	918	PGT	O3P-C1-C2-O2
3	A	904	PGT	C36-C37-C38-C39
4	A	906	PTY	C18-C19-C20-C21
4	B	908	PTY	C18-C19-C20-C21
3	B	906	PGT	C36-C37-C38-C39
3	B	913	PGT	C33-C34-C35-C36
4	B	916	PTY	C16-C17-C18-C19
3	A	918	PGT	C34-C35-C36-C37
3	A	907	PGT	C40-C41-C42-C43
4	A	906	PTY	C19-C20-C21-C22
4	B	916	PTY	C19-C20-C21-C22
3	B	913	PGT	C34-C35-C36-C37
3	B	902	PGT	C43-C44-C45-C46
4	B	908	PTY	C19-C20-C21-C22
3	A	902	PGT	O3P-C1-C2-O2
3	B	902	PGT	O3P-C1-C2-O2
3	B	904	PGT	O3P-C1-C2-O2
4	A	914	PTY	C19-C20-C21-C22
3	A	902	PGT	O2-C2-C3-O3
3	B	904	PGT	O2-C2-C3-O3
4	A	914	PTY	C16-C17-C18-C19
2	A	901	J4U	C23-C22-CG1-O20
2	B	903	J4U	C23-C22-CG1-O20
3	A	912	PGT	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
3	A	918	PGT	C43-C44-C45-C46
4	B	907	PTY	C18-C19-C20-C21
3	B	904	PGT	C16-C17-C18-C19
3	B	914	PGT	C36-C37-C38-C39
3	A	912	PGT	C2-C1-O3P-P
3	B	914	PGT	C2-C1-O3P-P
3	A	912	PGT	C36-C37-C38-C39
3	B	913	PGT	C35-C36-C37-C38
3	A	912	PGT	C16-C17-C18-C19
4	A	905	PTY	C18-C19-C20-C21
4	A	905	PTY	C11-C12-C13-C14
3	A	907	PGT	C32-C33-C34-C35
4	B	907	PTY	C11-C12-C13-C14
3	A	912	PGT	C22-C23-C24-C25
3	B	914	PGT	C39-C40-C41-C42
3	B	906	PGT	C40-C41-C42-C43
4	A	905	PTY	C13-C14-C15-C16
3	B	914	PGT	C16-C17-C18-C19
3	A	904	PGT	C40-C41-C42-C43
3	A	912	PGT	C13-C14-C15-C16
3	A	911	PGT	C35-C36-C37-C38
3	A	902	PGT	C16-C17-C18-C19
3	B	909	PGT	C32-C33-C34-C35
4	B	907	PTY	C13-C14-C15-C16
3	B	914	PGT	C13-C14-C15-C16
3	A	911	PGT	C34-C35-C36-C37
4	B	915	PTY	C20-C21-C22-C23
3	B	909	PGT	C42-C43-C44-C45
4	A	913	PTY	C21-C22-C23-C24
3	A	909	PGT	C44-C45-C46-C47
4	A	916	PTY	C14-C15-C16-C17
3	A	908	PGT	C39-C40-C41-C42
3	B	911	PGT	C44-C45-C46-C47
4	B	915	PTY	C21-C22-C23-C24
4	A	913	PTY	C20-C21-C22-C23
4	B	915	PTY	C19-C20-C21-C22
3	A	911	PGT	C39-C40-C41-C42
3	A	909	PGT	C32-C33-C34-C35
4	A	913	PTY	C19-C20-C21-C22
3	B	910	PGT	C39-C40-C41-C42
3	A	907	PGT	C42-C43-C44-C45
3	A	908	PGT	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
3	B	914	PGT	C41-C42-C43-C44
3	A	909	PGT	C43-C44-C45-C46
4	A	913	PTY	C17-C18-C19-C20
4	B	918	PTY	C14-C15-C16-C17
3	B	910	PGT	C36-C37-C38-C39
3	B	914	PGT	C22-C23-C24-C25
4	B	915	PTY	C17-C18-C19-C20
3	B	911	PGT	C43-C44-C45-C46
3	A	908	PGT	C36-C37-C38-C39
3	A	912	PGT	C12-C13-C14-C15
3	B	911	PGT	C32-C33-C34-C35
3	B	910	PGT	C37-C38-C39-C40
3	A	912	PGT	C33-C34-C35-C36
3	A	911	PGT	C42-C43-C44-C45
3	B	914	PGT	C35-C36-C37-C38
3	B	913	PGT	C39-C40-C41-C42
3	A	912	PGT	C35-C36-C37-C38
3	A	911	PGT	O2-C31-C32-C33
3	B	914	PGT	C12-C13-C14-C15
3	B	913	PGT	O31-C31-C32-C33
3	B	913	PGT	O2-C31-C32-C33
3	A	902	PGT	O2-C31-C32-C33
3	A	902	PGT	C13-C14-C15-C16
3	A	912	PGT	O2-C31-C32-C33
3	A	912	PGT	C41-C42-C43-C44
3	B	914	PGT	C33-C34-C35-C36
4	A	906	PTY	C15-C16-C17-C18
4	B	908	PTY	C15-C16-C17-C18
3	A	911	PGT	O31-C31-C32-C33
3	A	910	PGT	C37-C38-C39-C40
4	B	916	PTY	C8-C11-C12-C13
3	B	904	PGT	O2-C31-C32-C33
3	B	910	PGT	C42-C43-C44-C45
3	B	914	PGT	O2-C31-C32-C33
4	B	916	PTY	C12-C13-C14-C15
4	A	906	PTY	C13-C14-C15-C16
4	B	908	PTY	C16-C17-C18-C19
4	A	906	PTY	C16-C17-C18-C19
3	B	902	PGT	O2-C31-C32-C33
4	A	914	PTY	C8-C11-C12-C13
4	A	914	PTY	C12-C13-C14-C15
3	B	914	PGT	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	908	PTY	C13-C14-C15-C16
4	B	917	PTY	C22-C23-C24-C25
3	B	912	PGT	C37-C38-C39-C40
3	B	905	PGT	C40-C41-C42-C43
3	B	901	PGT	C36-C37-C38-C39
3	B	914	PGT	O31-C31-C32-C33
3	A	912	PGT	O31-C31-C32-C33
4	B	907	PTY	C8-C11-C12-C13
3	A	902	PGT	C15-C16-C17-C18
3	B	904	PGT	O31-C31-C32-C33
4	B	916	PTY	C21-C22-C23-C24
3	A	902	PGT	O31-C31-C32-C33
3	B	902	PGT	O31-C31-C32-C33
3	B	904	PGT	C13-C14-C15-C16
4	B	908	PTY	C17-C18-C19-C20
4	A	915	PTY	C22-C23-C24-C25
3	A	908	PGT	C42-C43-C44-C45
3	A	912	PGT	C38-C39-C40-C41
3	B	913	PGT	C42-C43-C44-C45
3	B	914	PGT	C38-C39-C40-C41
3	B	906	PGT	C35-C36-C37-C38
3	A	918	PGT	O2-C31-C32-C33

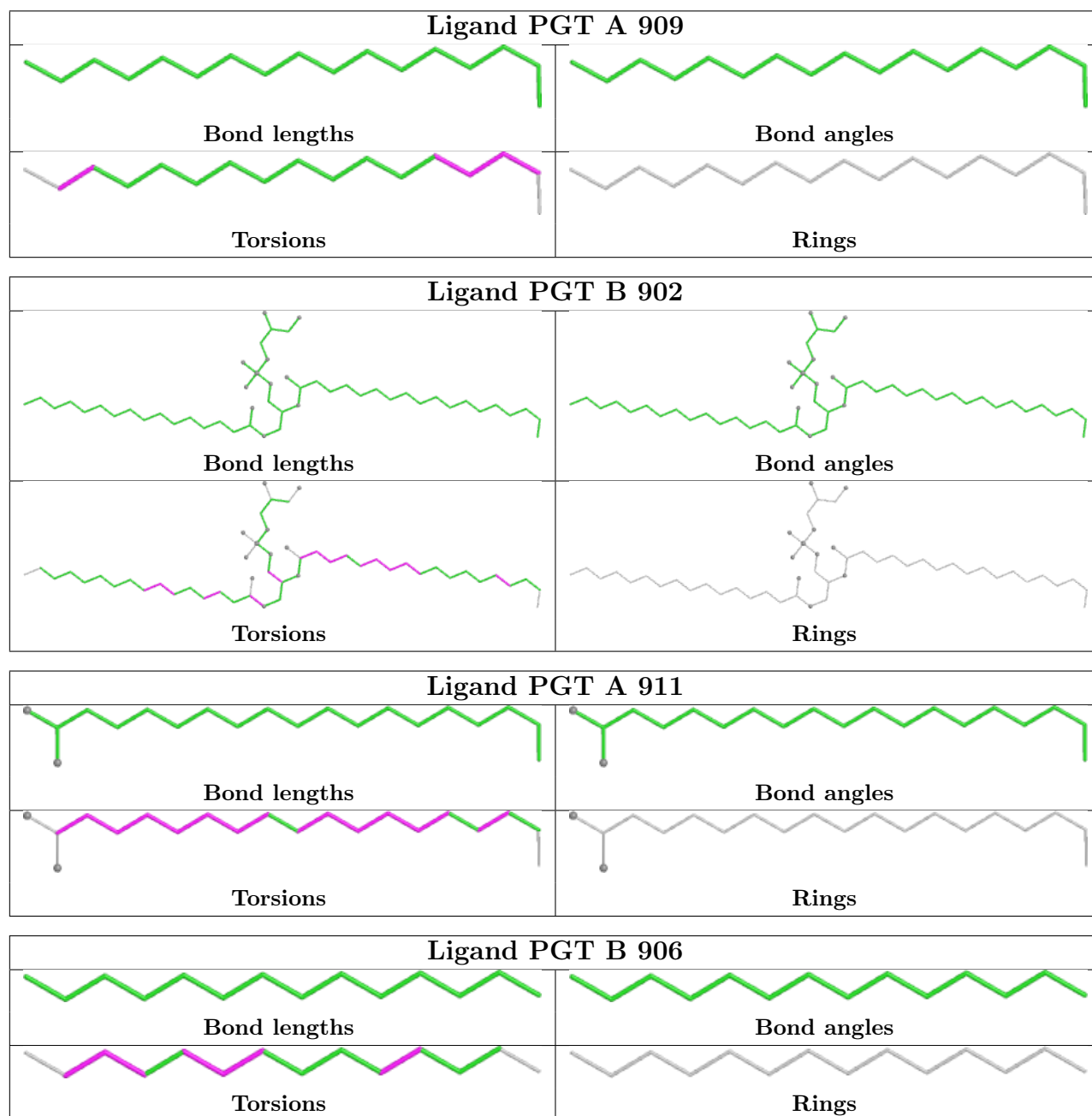
There are no ring outliers.

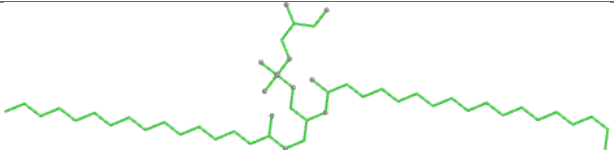
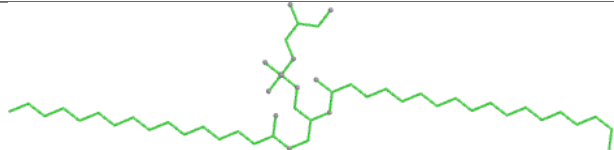
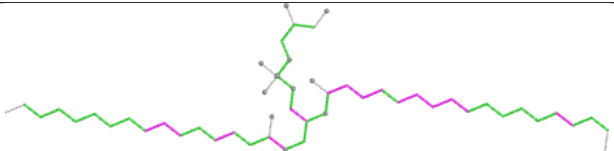
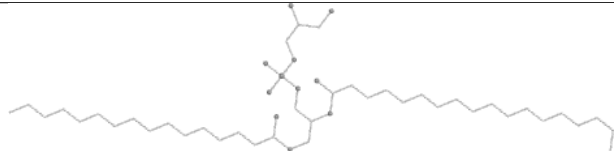
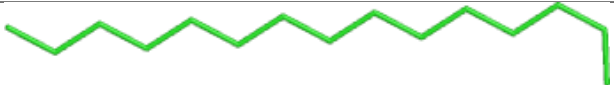
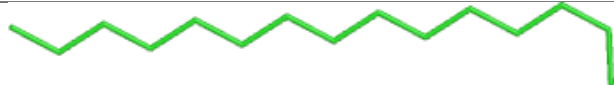
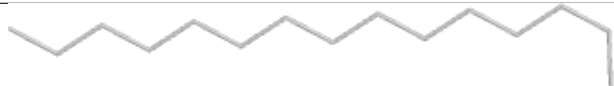
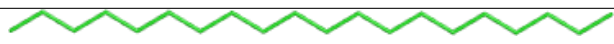
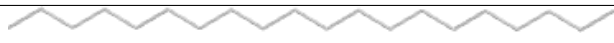
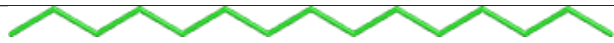
4 monomers are involved in 4 short contacts:

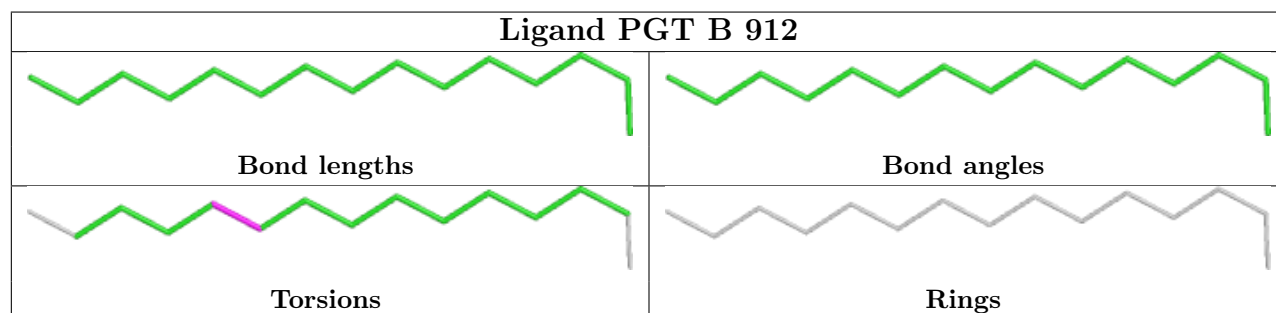
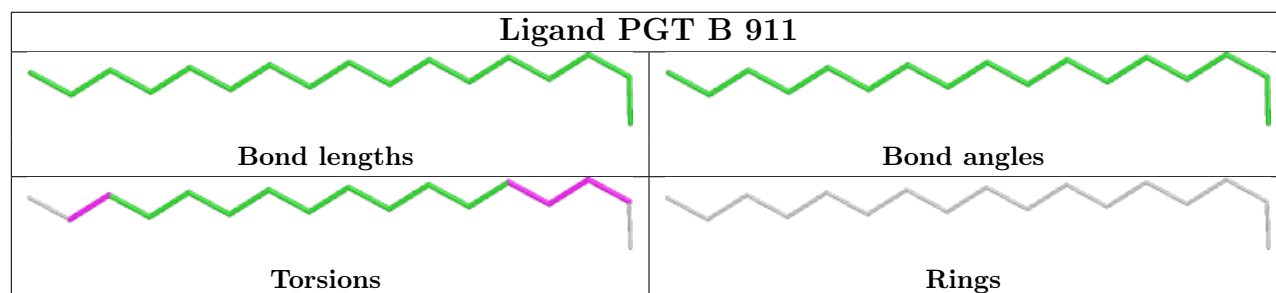
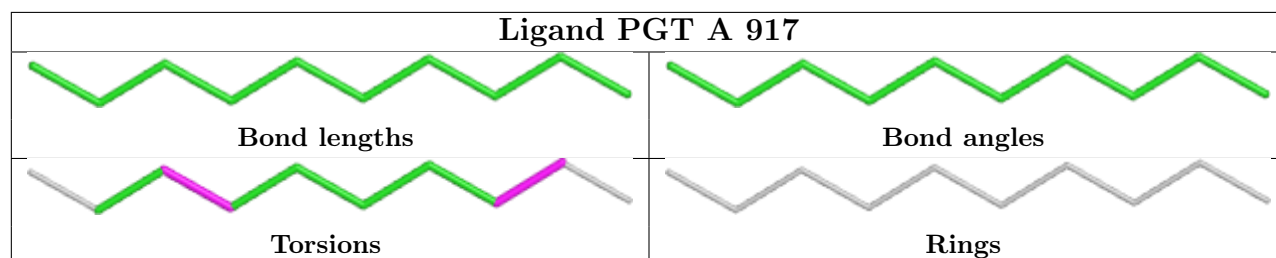
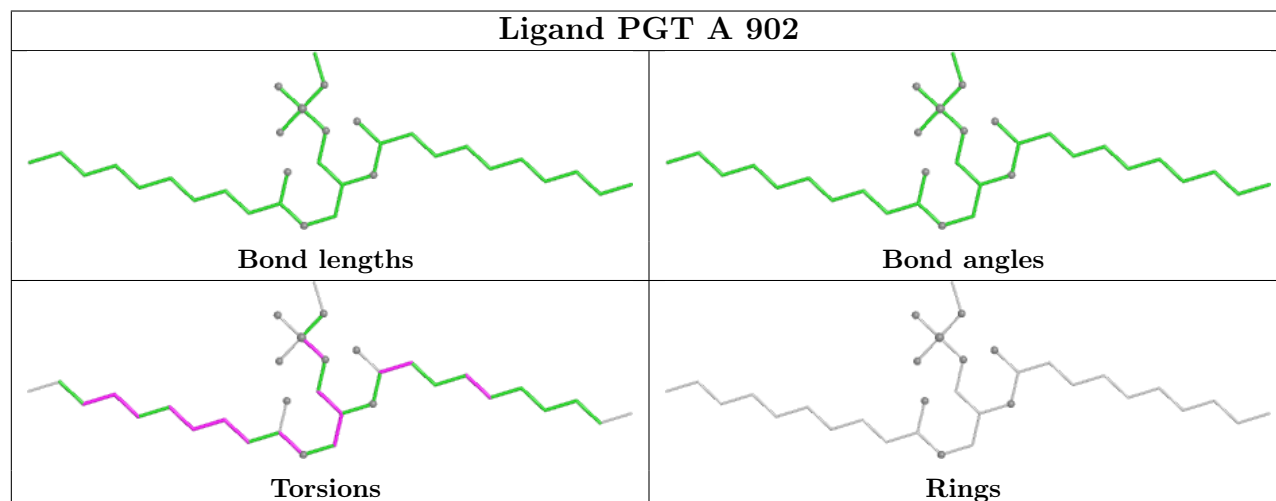
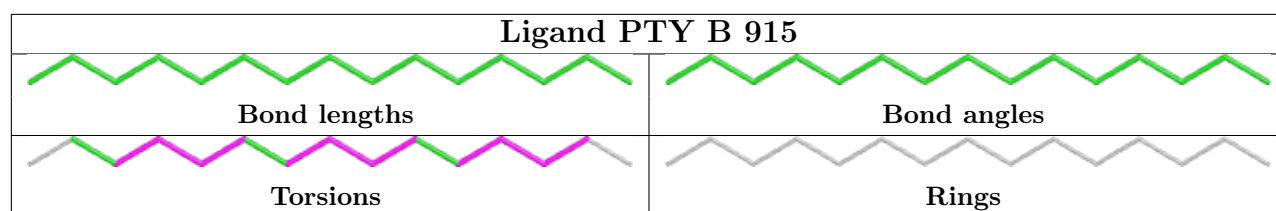
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	917	PTY	1	0
4	A	915	PTY	1	0
2	B	903	J4U	1	0
3	B	904	PGT	1	0

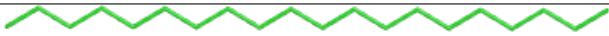
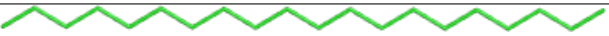
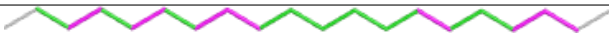
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

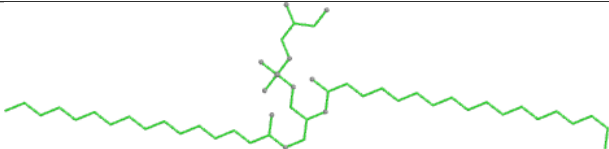
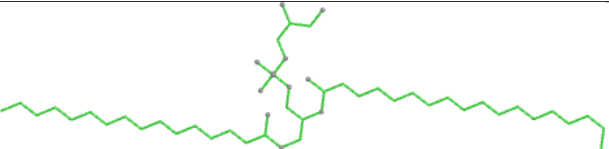
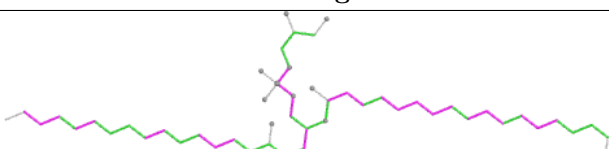
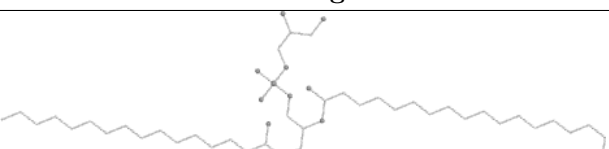
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

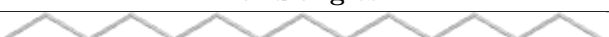


Ligand PGT A 918			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand PTY A 905			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand PGT A 910			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand PTY B 917			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand PGT A 907			
 Bond lengths		 Bond angles	
 Torsions		 Rings	
Ligand PTY A 913			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

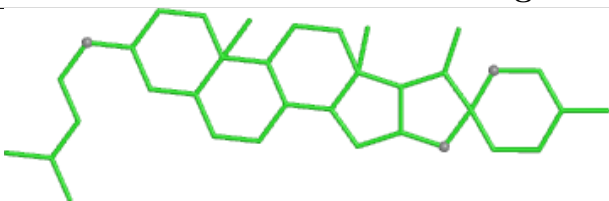
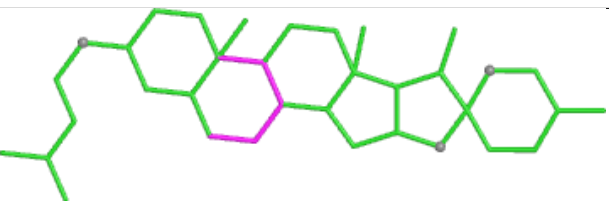
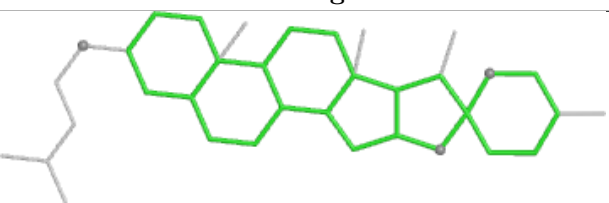


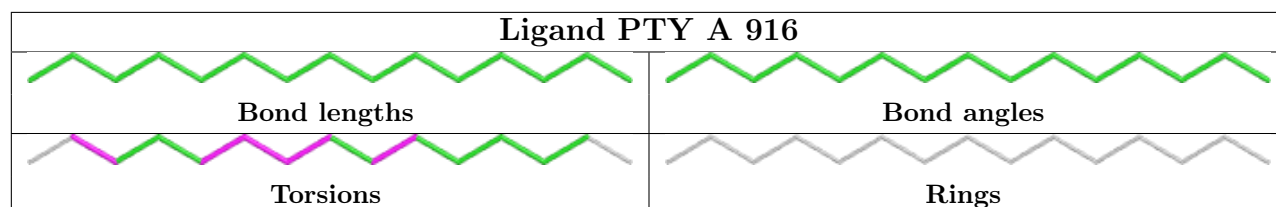
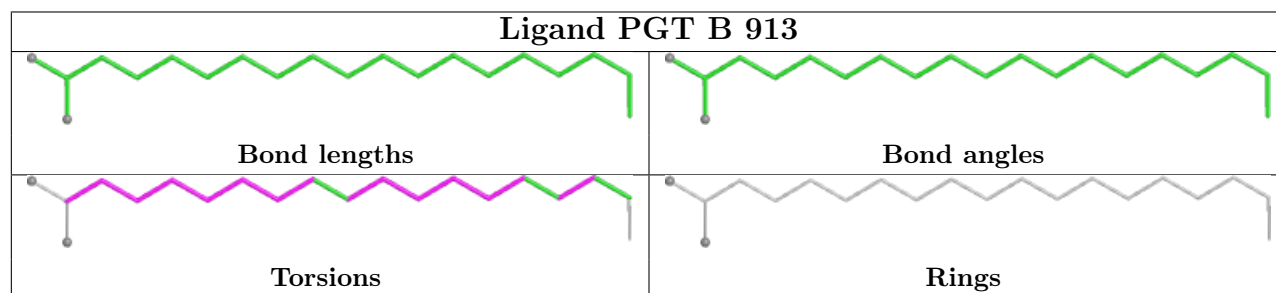
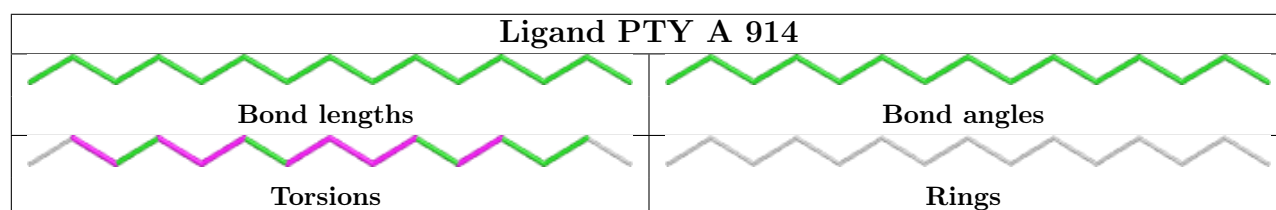
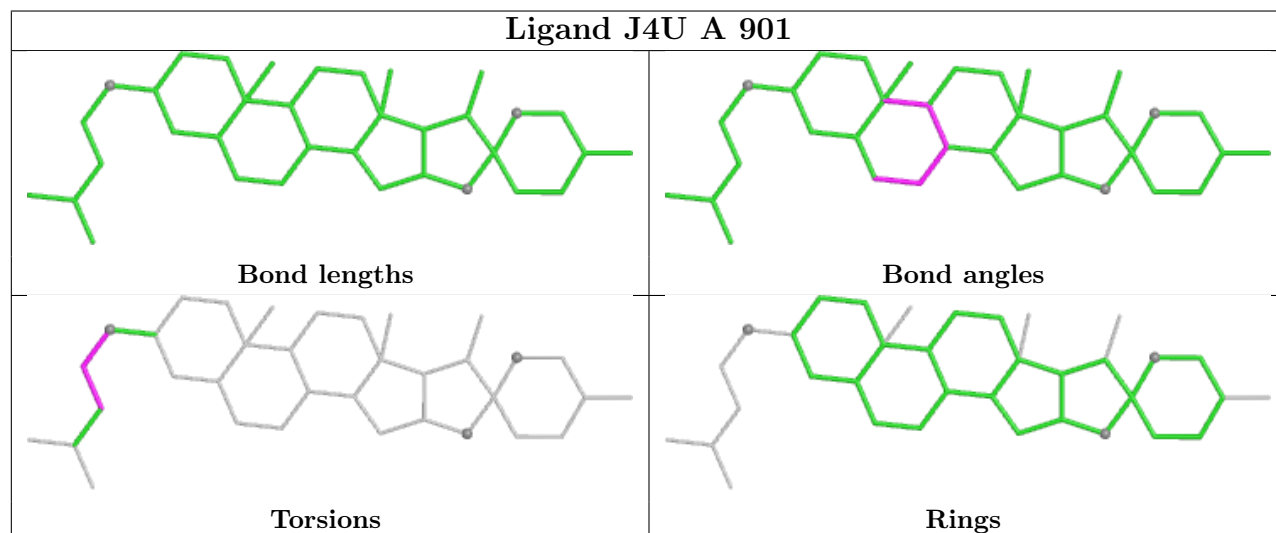
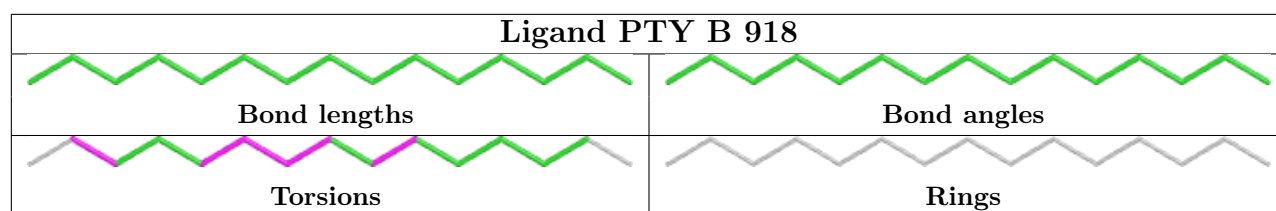
Ligand PTY A 915	
 Bond lengths	 Bond angles
 Torsions	 Rings

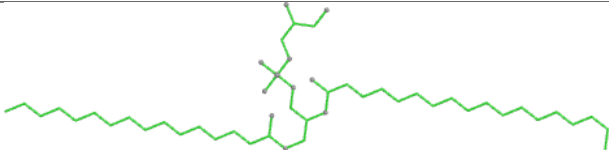
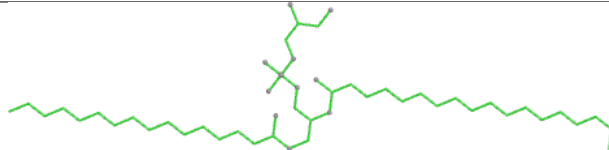
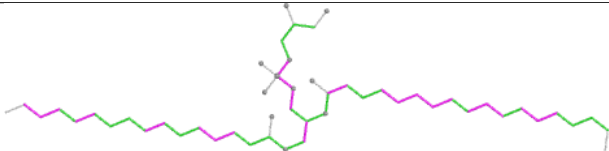
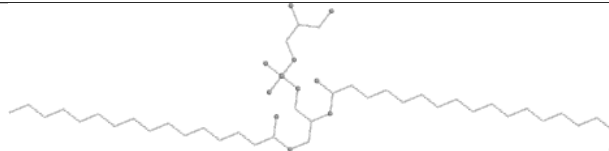
Ligand PGT B 914	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY B 916	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGT A 908	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand J4U B 903	
 Bond lengths	 Bond angles
 Torsions	 Rings



Ligand PGT A 912			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

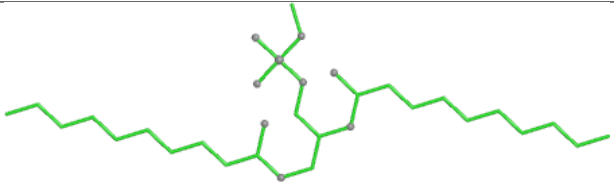
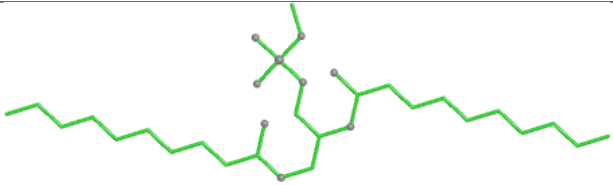
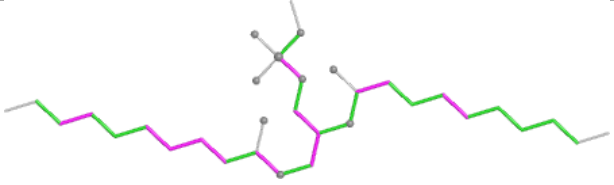
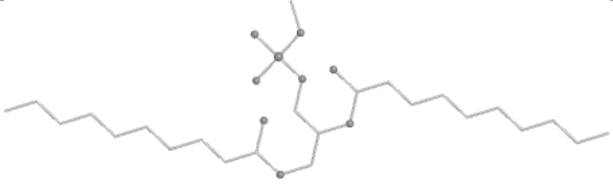
Ligand PGT B 910			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PGT A 903			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

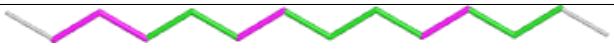
Ligand PTY B 907			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

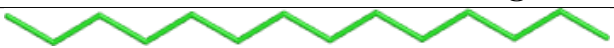
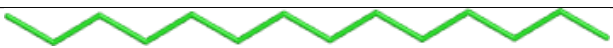
Ligand PGT B 905			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PTY A 906			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PGT B 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PTY B 908	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGT A 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGT B 909	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGT B 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

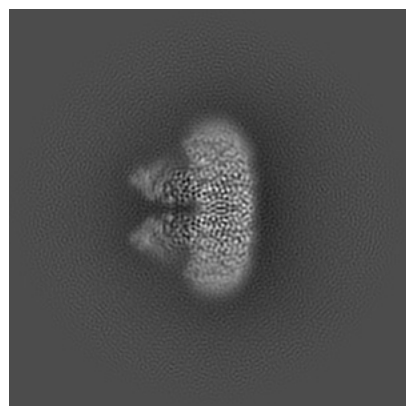
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61239. These allow visual inspection of the internal detail of the map and identification of artifacts.

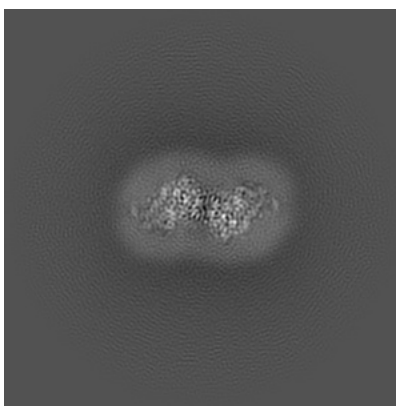
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

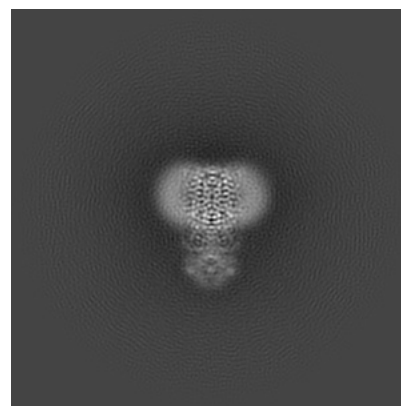
6.1.1 Primary map



X

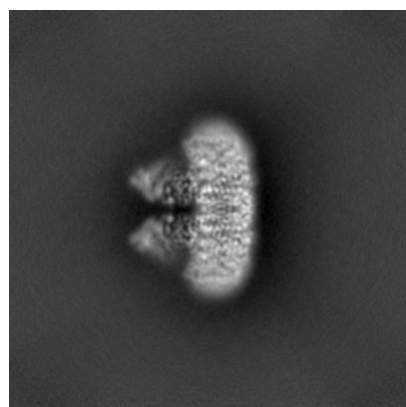


Y

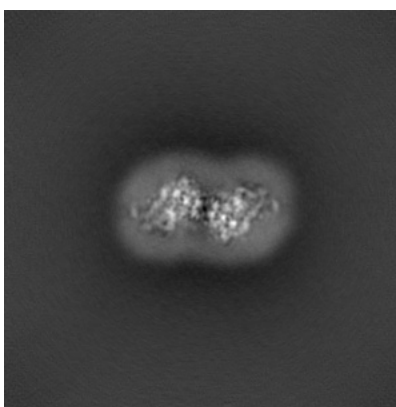


Z

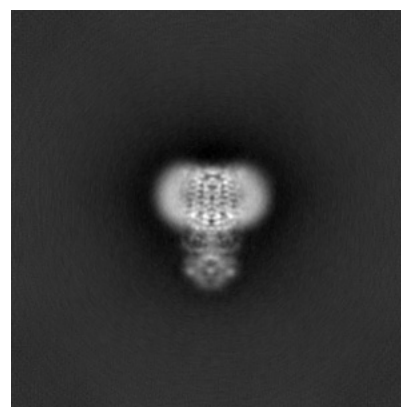
6.1.2 Raw map



X



Y

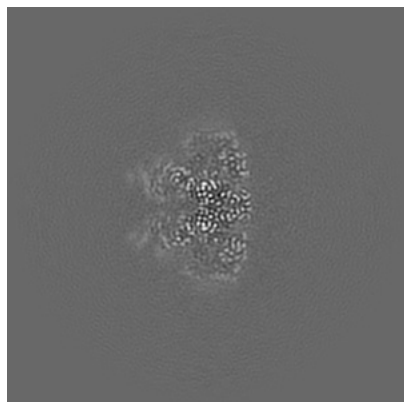


Z

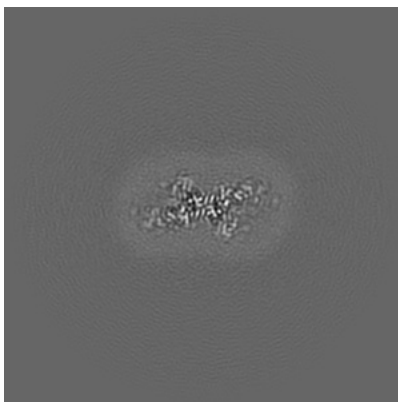
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

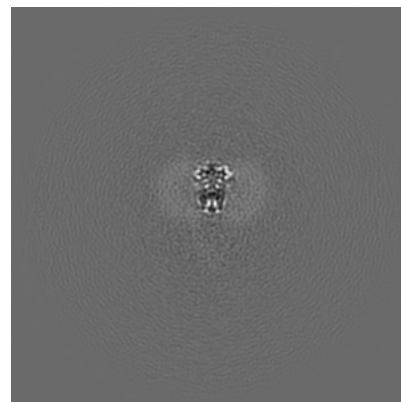
6.2.1 Primary map



X Index: 160

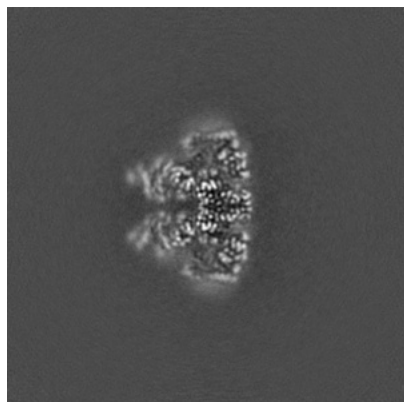


Y Index: 160

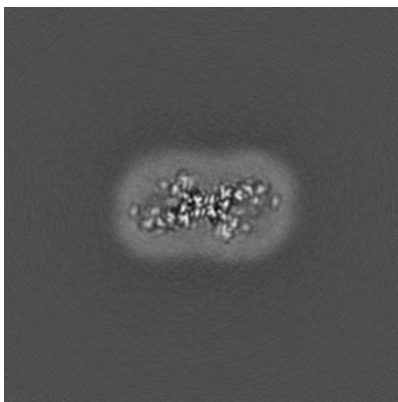


Z Index: 160

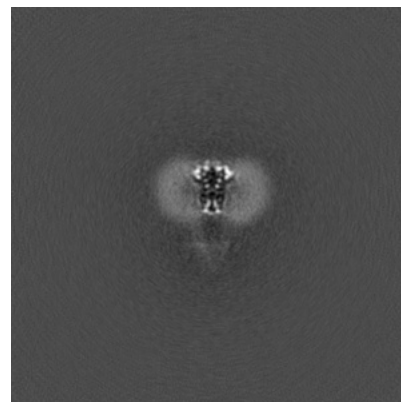
6.2.2 Raw map



X Index: 160



Y Index: 160

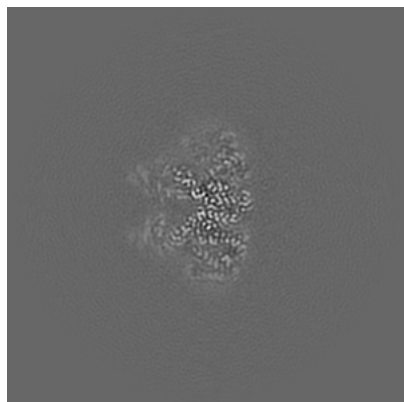


Z Index: 160

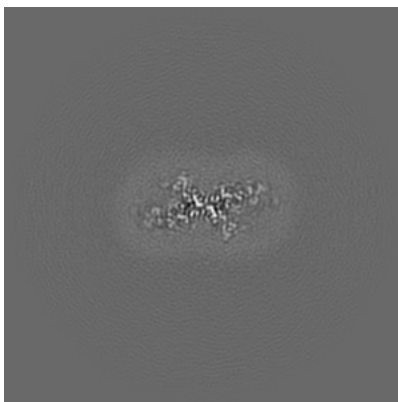
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

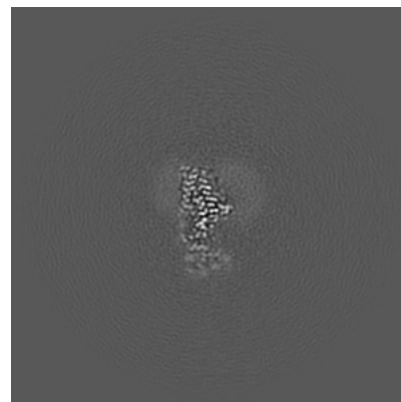
6.3.1 Primary map



X Index: 158

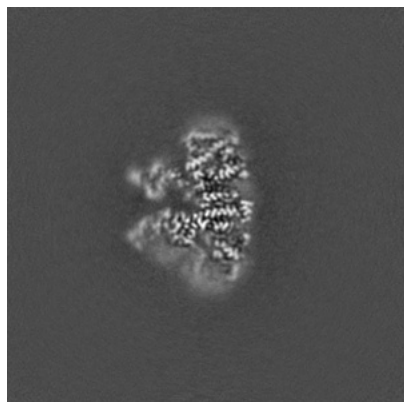


Y Index: 159

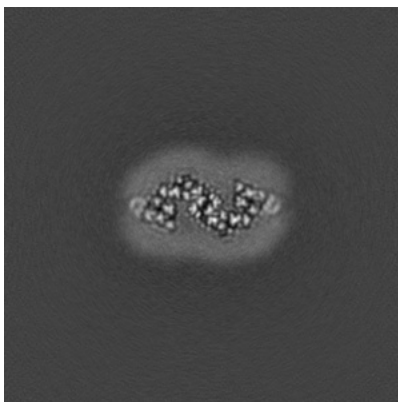


Z Index: 175

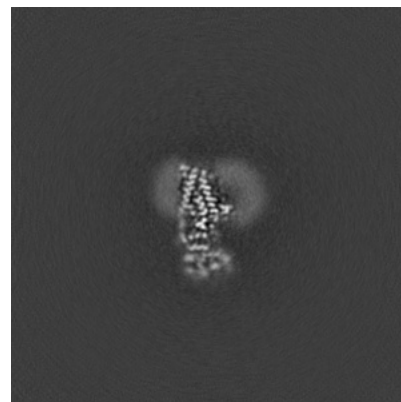
6.3.2 Raw map



X Index: 165



Y Index: 181

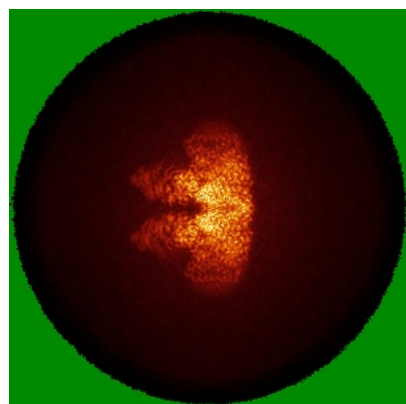


Z Index: 175

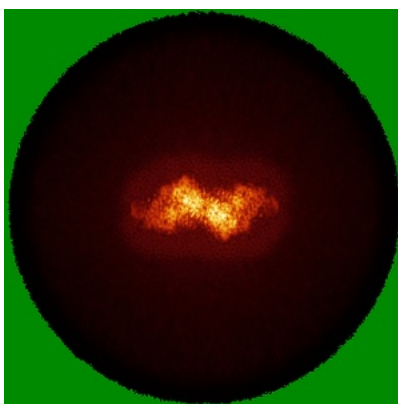
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

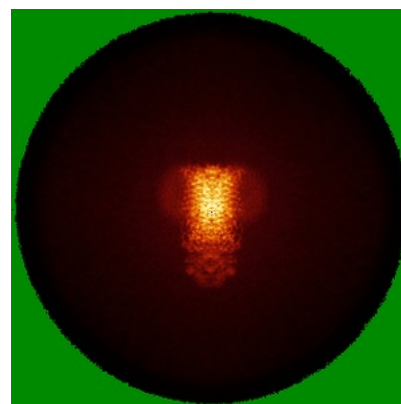
6.4.1 Primary map



X

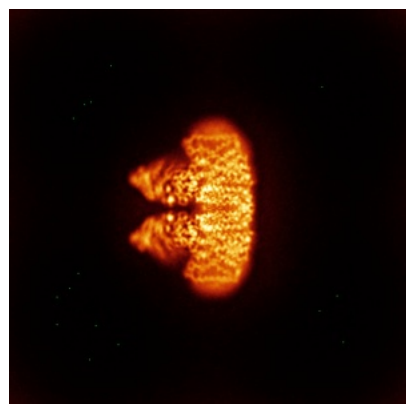


Y

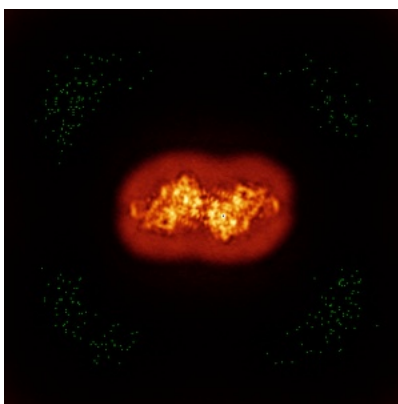


Z

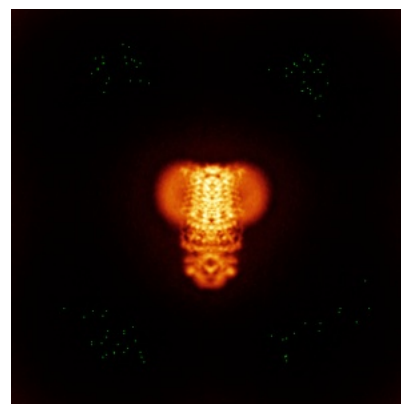
6.4.2 Raw map



X



Y

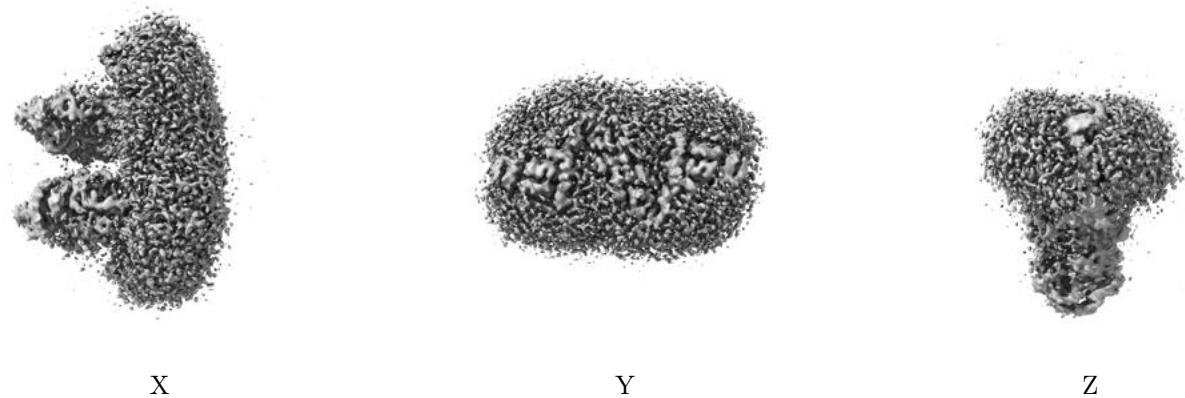


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

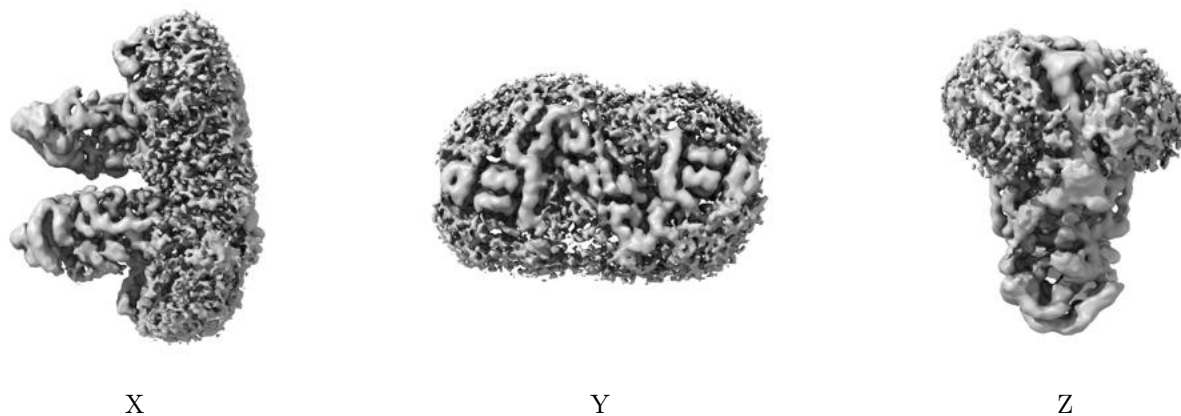
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

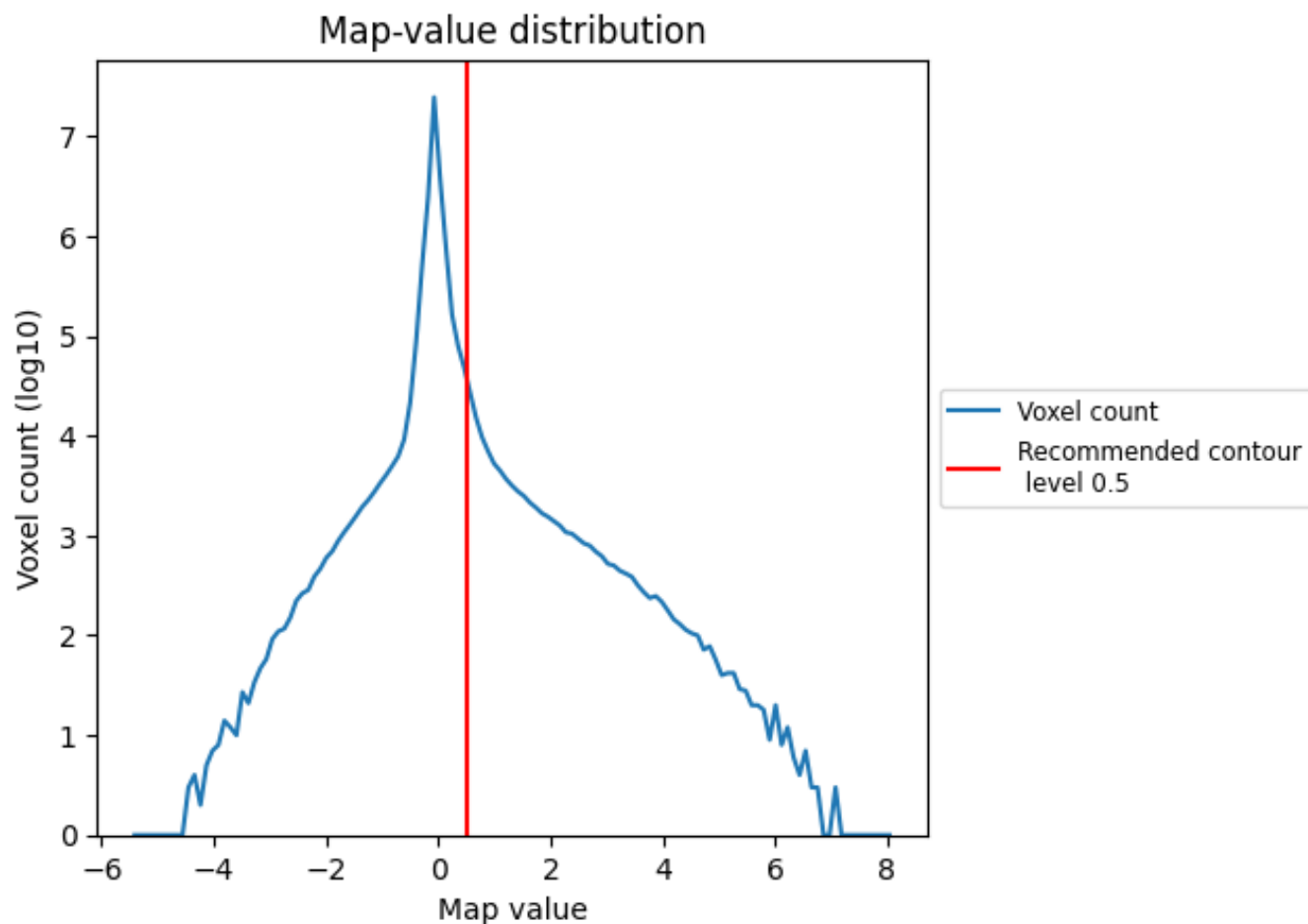
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

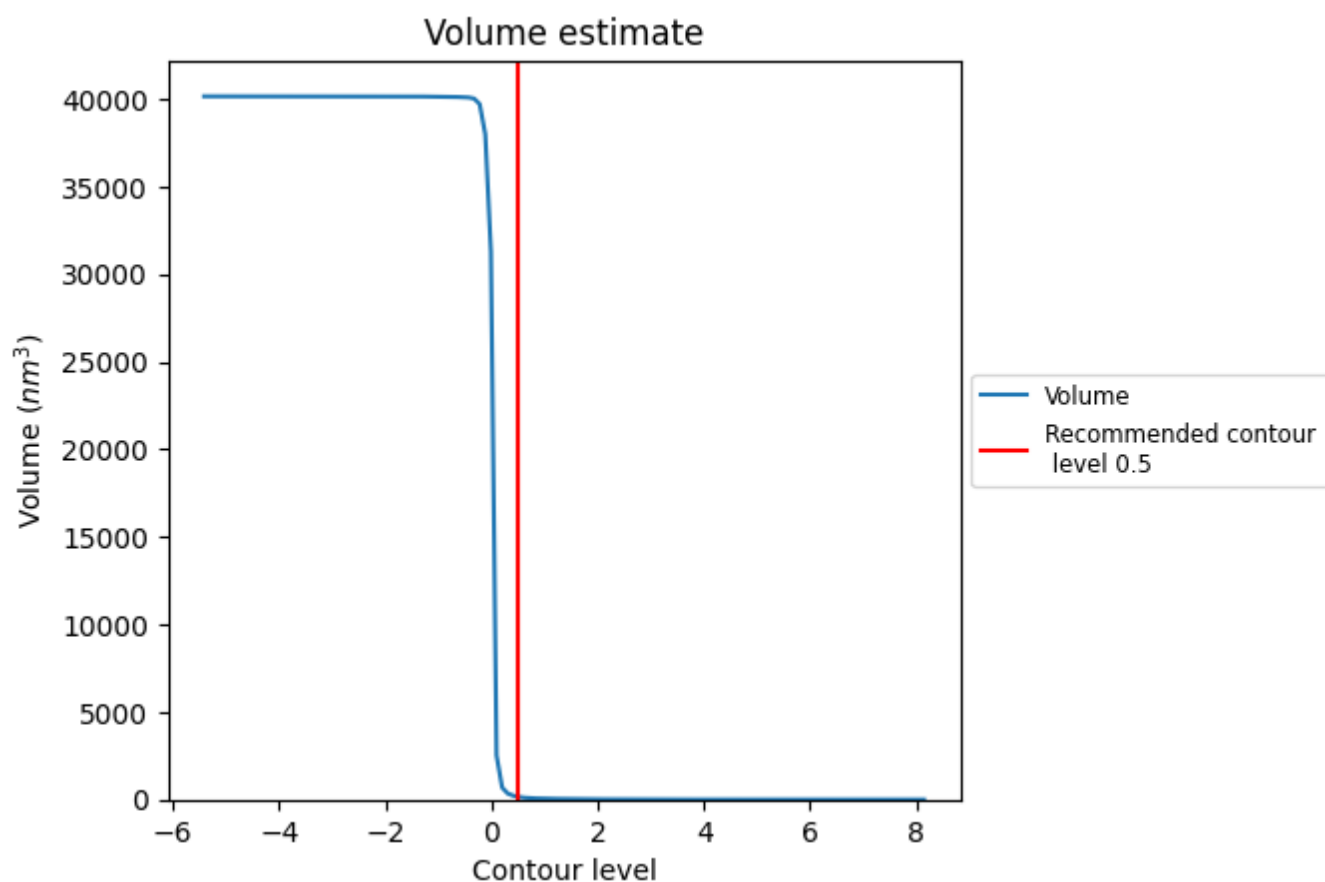
This section contains the results of statistical analysis of the map.

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.

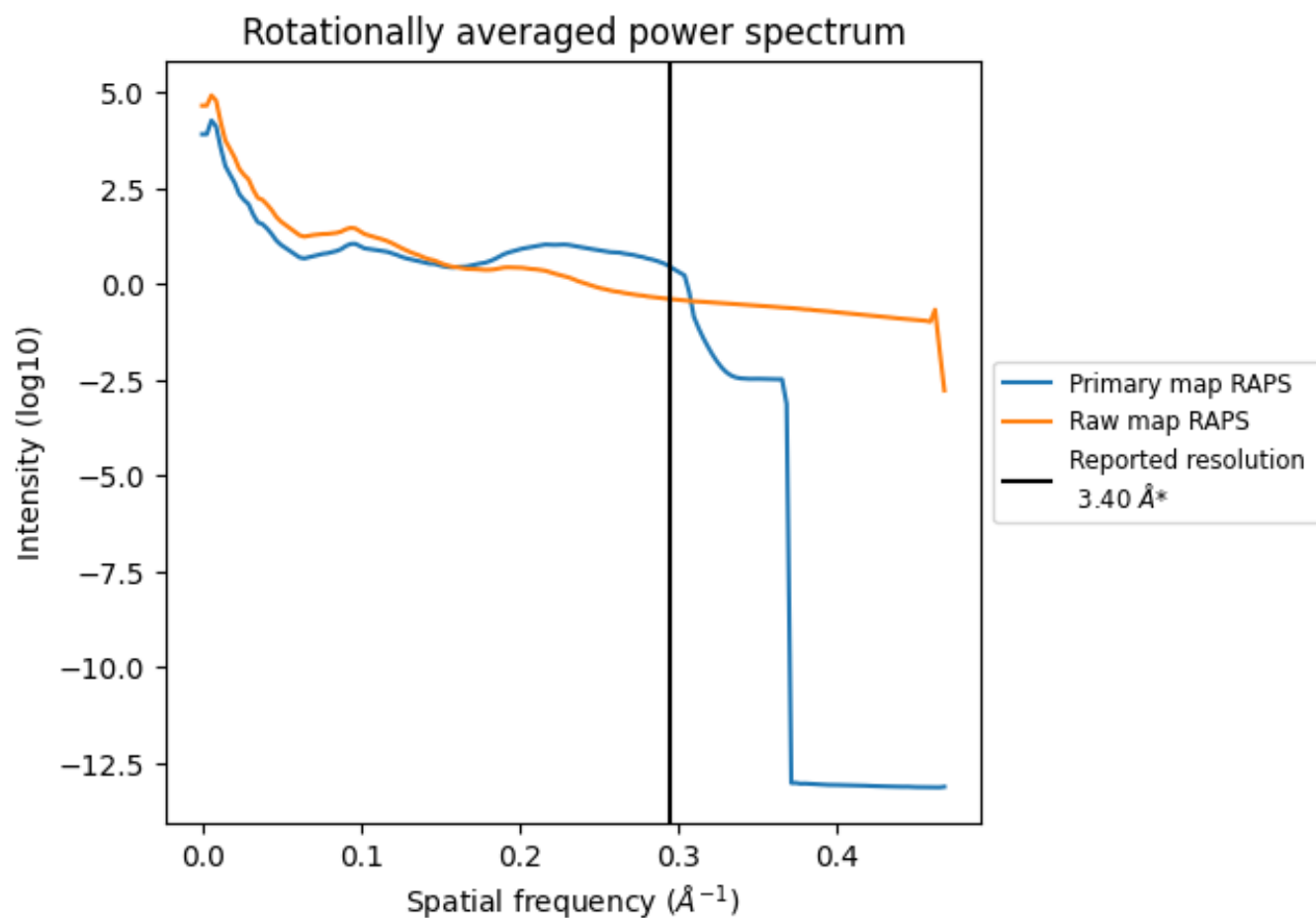
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm^3 ; this corresponds to an approximate mass of 144 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 ⓘ

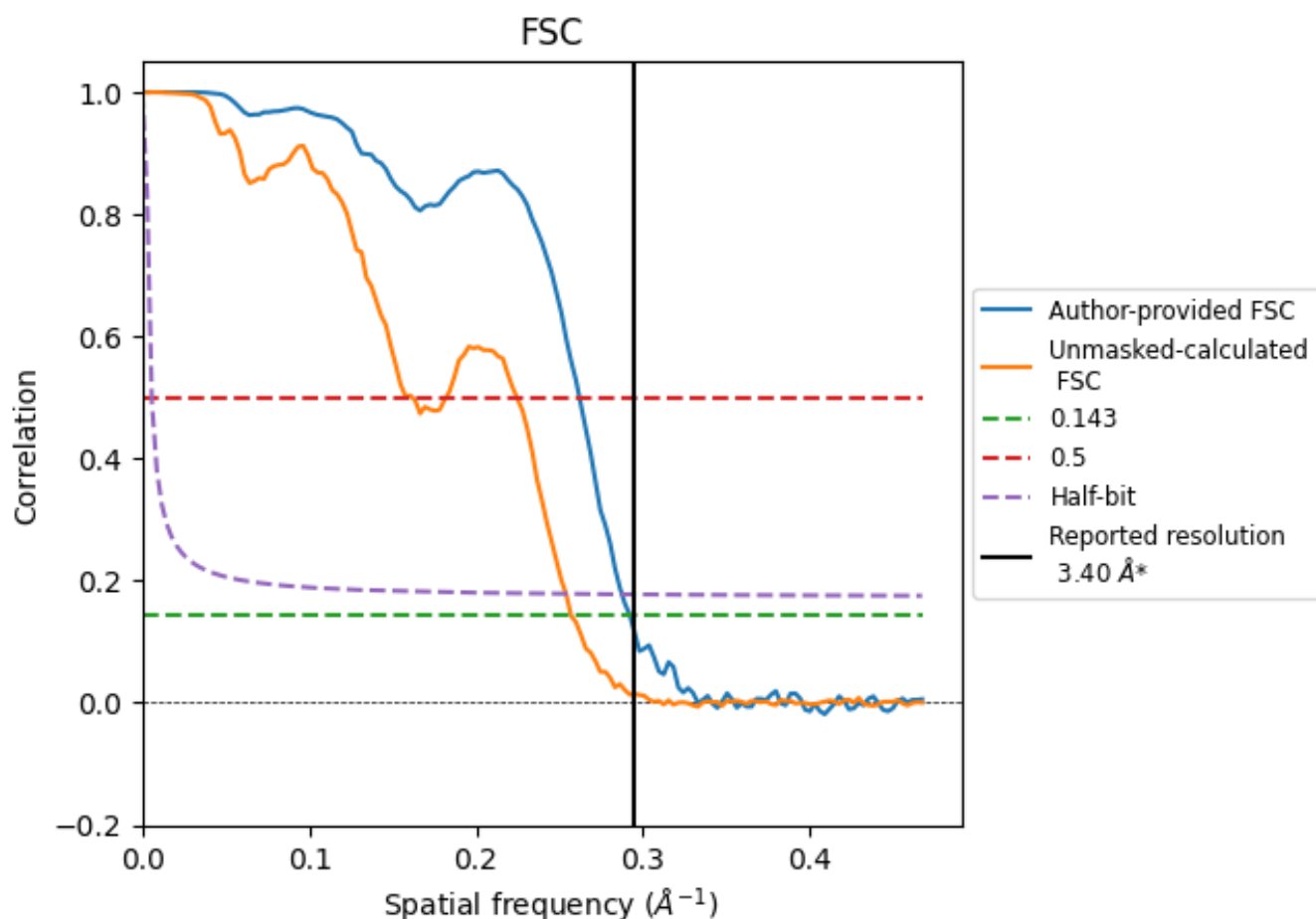


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

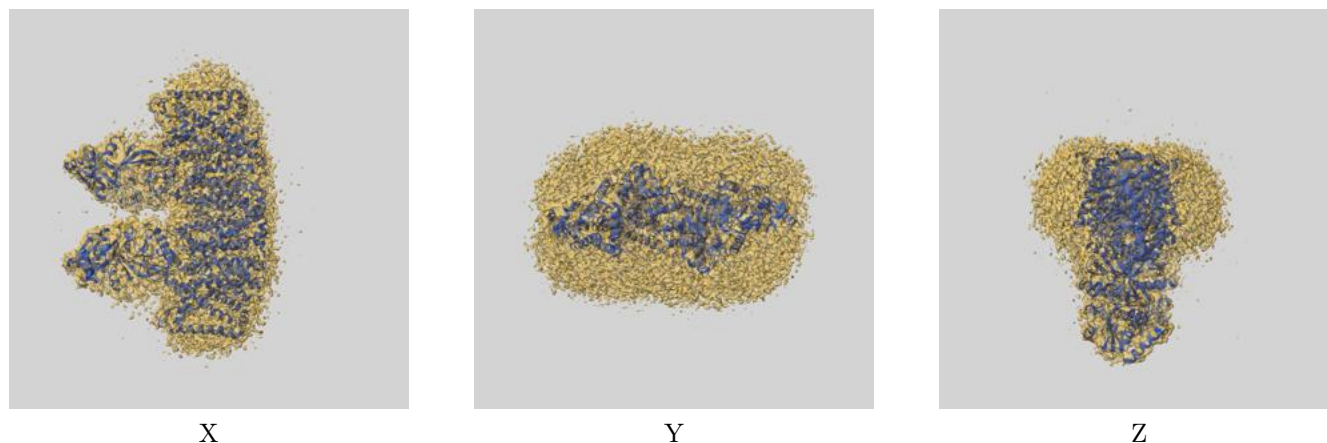
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	3.82	3.48
Unmasked-calculated*	3.89	6.18	3.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

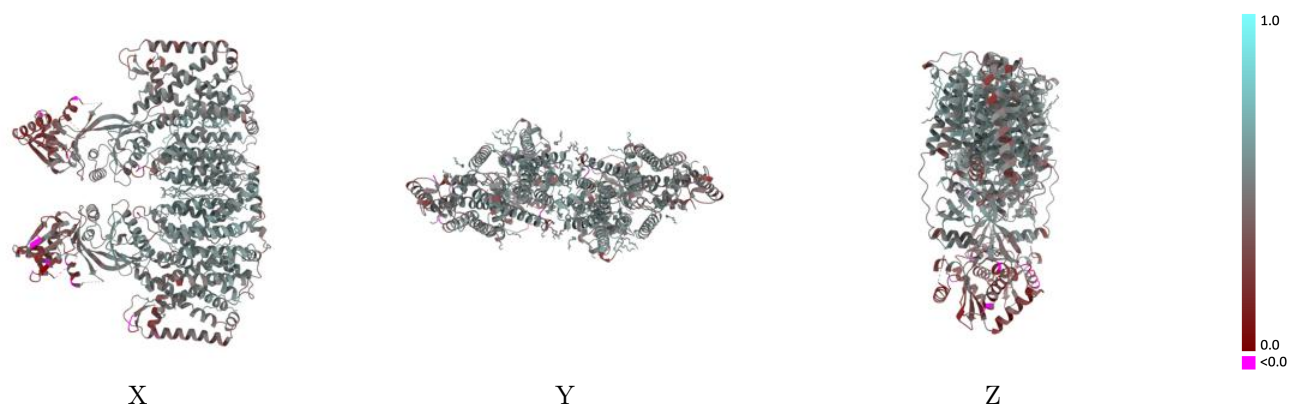
This section contains information regarding the fit between EMDB map EMD-61239 and PDB model 9J8R. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



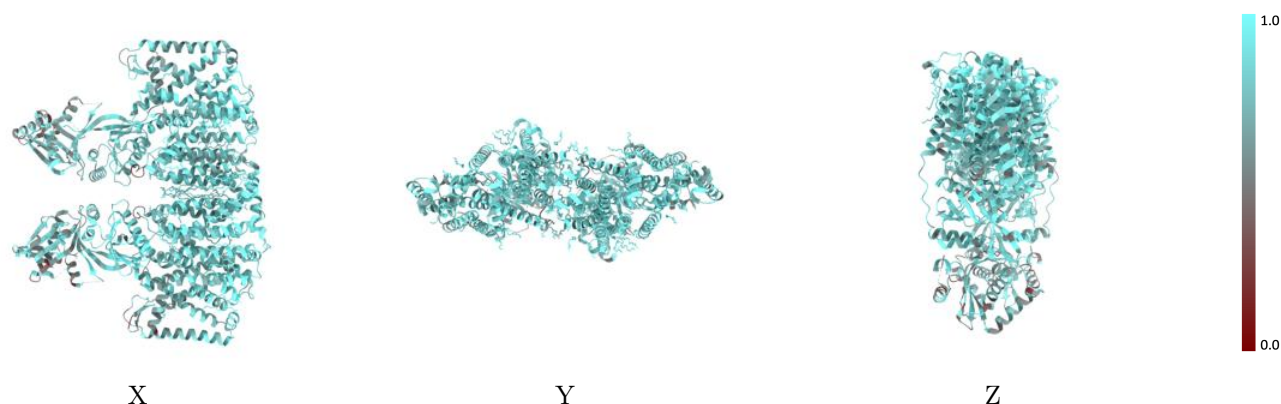
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



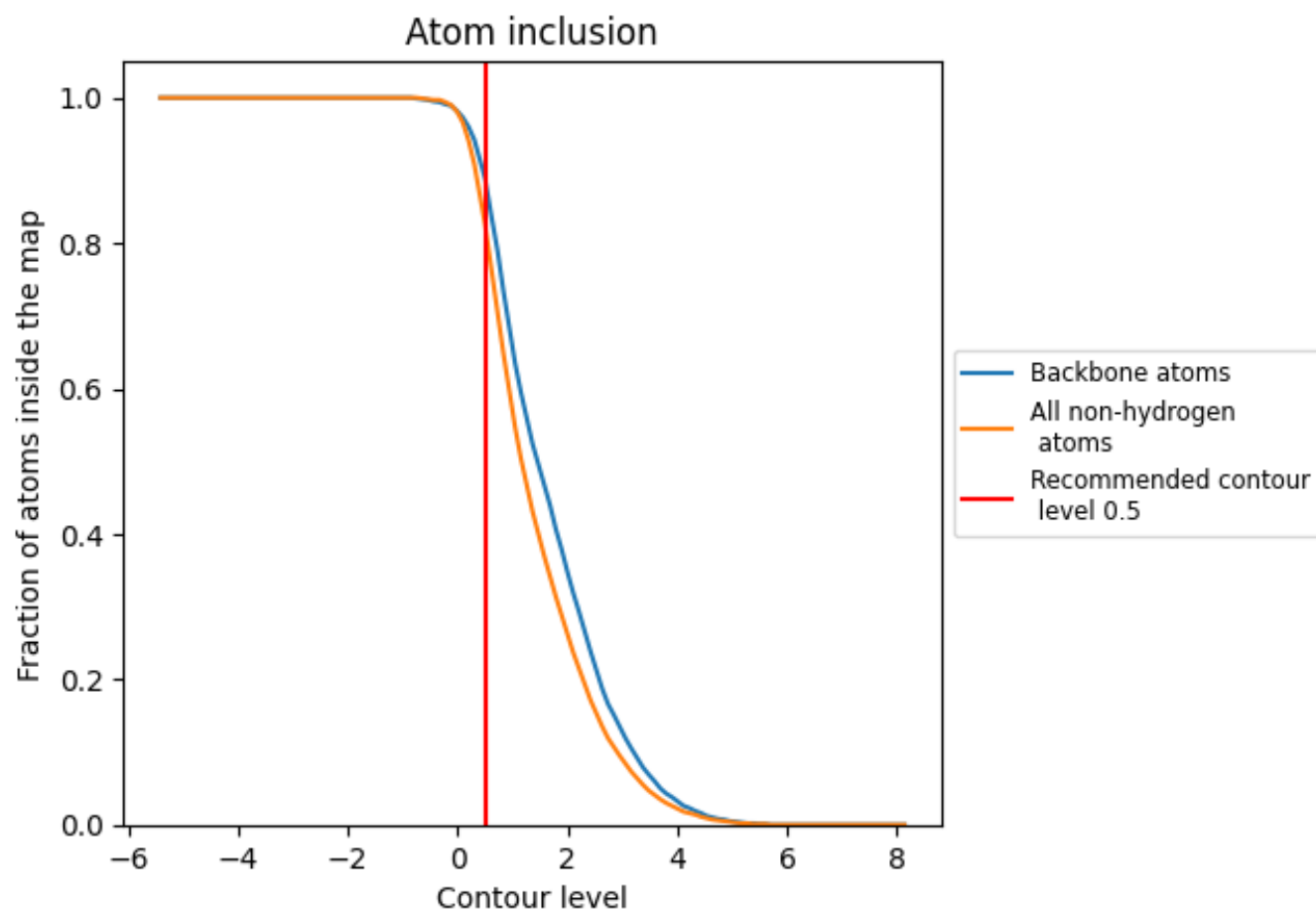
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8260	0.4590
A	0.8280	0.4610
B	0.8230	0.4570

