



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 10:01 PM UTC

PDB ID : 8W25 / pdb_00008w25
EMDB ID : EMD-43739
Title : Cryo-EM structure of human tankyrase 2 SAM-PARP filament bound to compound, TDI-2804 (focused refinement map).
Authors : Malone, B.F.; Zimmerman, J.L.; Dow, L.E.; Hite, R.K.
Deposited on : 2024-02-20
Resolution : 2.42 Å(reported)
Based on initial model : 8ALY

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 : 2022.3.0, CSD as543be (2022)
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

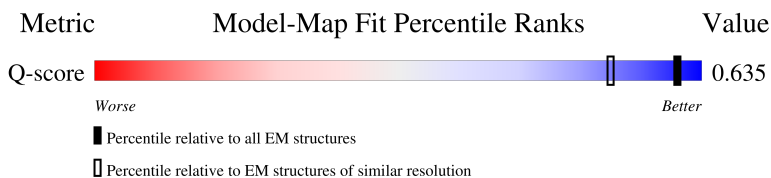
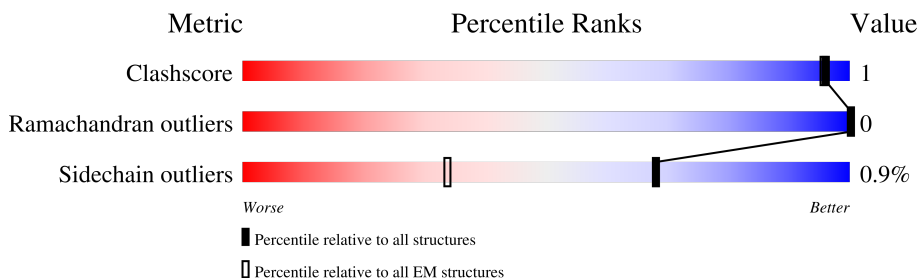
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.42 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	5729 (1.92 - 2.92)

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	D	729	
1	Q	729	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4600 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 Maltose/maltodextrin-binding periplasmic protein,Poly [ADP-ribose] polymerase tankyrase-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	284	Total	C	N	O	S	0	0
			2241	1420	408	400	13		
1	Q	284	Total	C	N	O	S	0	0
			2241	1420	408	400	13		

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	438	MET	-	initiating methionine	UNP P0AEY0
D	439	SER	-	expression tag	UNP P0AEY0
D	440	ALA	-	expression tag	UNP P0AEY0
D	441	TRP	-	expression tag	UNP P0AEY0
D	442	SER	-	expression tag	UNP P0AEY0
D	443	HIS	-	expression tag	UNP P0AEY0
D	444	PRO	-	expression tag	UNP P0AEY0
D	445	GLN	-	expression tag	UNP P0AEY0
D	446	PHE	-	expression tag	UNP P0AEY0
D	447	GLU	-	expression tag	UNP P0AEY0
D	448	LYS	-	expression tag	UNP P0AEY0
D	449	GLY	-	expression tag	UNP P0AEY0
D	450	GLY	-	expression tag	UNP P0AEY0
D	451	GLY	-	expression tag	UNP P0AEY0
D	452	SER	-	expression tag	UNP P0AEY0
D	453	GLY	-	expression tag	UNP P0AEY0
D	454	GLY	-	expression tag	UNP P0AEY0
D	455	GLY	-	expression tag	UNP P0AEY0
D	456	SER	-	expression tag	UNP P0AEY0
D	457	GLY	-	expression tag	UNP P0AEY0
D	458	GLY	-	expression tag	UNP P0AEY0
D	459	SER	-	expression tag	UNP P0AEY0
D	460	ALA	-	expression tag	UNP P0AEY0
D	461	TRP	-	expression tag	UNP P0AEY0
D	462	SER	-	expression tag	UNP P0AEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	463	HIS	-	expression tag	UNP P0AEY0
D	464	PRO	-	expression tag	UNP P0AEY0
D	465	GLN	-	expression tag	UNP P0AEY0
D	466	PHE	-	expression tag	UNP P0AEY0
D	467	GLU	-	expression tag	UNP P0AEY0
D	468	LYS	-	expression tag	UNP P0AEY0
D	469	THR	-	expression tag	UNP P0AEY0
D	470	GLY	-	expression tag	UNP P0AEY0
D	471	SER	-	expression tag	UNP P0AEY0
D	472	MET	-	expression tag	UNP P0AEY0
D	473	GLY	-	expression tag	UNP P0AEY0
D	839	GLU	-	linker	UNP P0AEY0
D	840	LEU	-	linker	UNP P0AEY0
D	841	GLU	-	linker	UNP P0AEY0
D	842	LEU	-	linker	UNP P0AEY0
D	843	GLU	-	linker	UNP P0AEY0
D	844	VAL	-	linker	UNP P0AEY0
D	845	LEU	-	linker	UNP P0AEY0
D	846	PHE	-	linker	UNP P0AEY0
D	847	GLN	-	linker	UNP P0AEY0
D	848	GLY	-	linker	UNP P0AEY0
D	849	PRO	-	linker	UNP P0AEY0
Q	438	MET	-	initiating methionine	UNP P0AEY0
Q	439	SER	-	expression tag	UNP P0AEY0
Q	440	ALA	-	expression tag	UNP P0AEY0
Q	441	TRP	-	expression tag	UNP P0AEY0
Q	442	SER	-	expression tag	UNP P0AEY0
Q	443	HIS	-	expression tag	UNP P0AEY0
Q	444	PRO	-	expression tag	UNP P0AEY0
Q	445	GLN	-	expression tag	UNP P0AEY0
Q	446	PHE	-	expression tag	UNP P0AEY0
Q	447	GLU	-	expression tag	UNP P0AEY0
Q	448	LYS	-	expression tag	UNP P0AEY0
Q	449	GLY	-	expression tag	UNP P0AEY0
Q	450	GLY	-	expression tag	UNP P0AEY0
Q	451	GLY	-	expression tag	UNP P0AEY0
Q	452	SER	-	expression tag	UNP P0AEY0
Q	453	GLY	-	expression tag	UNP P0AEY0
Q	454	GLY	-	expression tag	UNP P0AEY0
Q	455	GLY	-	expression tag	UNP P0AEY0
Q	456	SER	-	expression tag	UNP P0AEY0
Q	457	GLY	-	expression tag	UNP P0AEY0

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	458	GLY	-	expression tag	UNP P0AEY0
Q	459	SER	-	expression tag	UNP P0AEY0
Q	460	ALA	-	expression tag	UNP P0AEY0
Q	461	TRP	-	expression tag	UNP P0AEY0
Q	462	SER	-	expression tag	UNP P0AEY0
Q	463	HIS	-	expression tag	UNP P0AEY0
Q	464	PRO	-	expression tag	UNP P0AEY0
Q	465	GLN	-	expression tag	UNP P0AEY0
Q	466	PHE	-	expression tag	UNP P0AEY0
Q	467	GLU	-	expression tag	UNP P0AEY0
Q	468	LYS	-	expression tag	UNP P0AEY0
Q	469	THR	-	expression tag	UNP P0AEY0
Q	470	GLY	-	expression tag	UNP P0AEY0
Q	471	SER	-	expression tag	UNP P0AEY0
Q	472	MET	-	expression tag	UNP P0AEY0
Q	473	GLY	-	expression tag	UNP P0AEY0
Q	839	GLU	-	linker	UNP P0AEY0
Q	840	LEU	-	linker	UNP P0AEY0
Q	841	GLU	-	linker	UNP P0AEY0
Q	842	LEU	-	linker	UNP P0AEY0
Q	843	GLU	-	linker	UNP P0AEY0
Q	844	VAL	-	linker	UNP P0AEY0
Q	845	LEU	-	linker	UNP P0AEY0
Q	846	PHE	-	linker	UNP P0AEY0
Q	847	GLN	-	linker	UNP P0AEY0
Q	848	GLY	-	linker	UNP P0AEY0
Q	849	PRO	-	linker	UNP P0AEY0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
2	D	1	Total Zn 1 1	0
2	Q	1	Total Zn 1 1	0

- Molecule 3 is N-{2-[4-(2-hydroxypropan-2-yl)phenyl]-4-oxo-1,4-dihydroquinazolin-7-yl}-4-methoxy-6-phenylpyridine-3-carboxamide (CCD ID: A1AE4) (formula: C₃₀H₂₆N₄O₄) (labeled as "Ligand of Interest" by depositor).



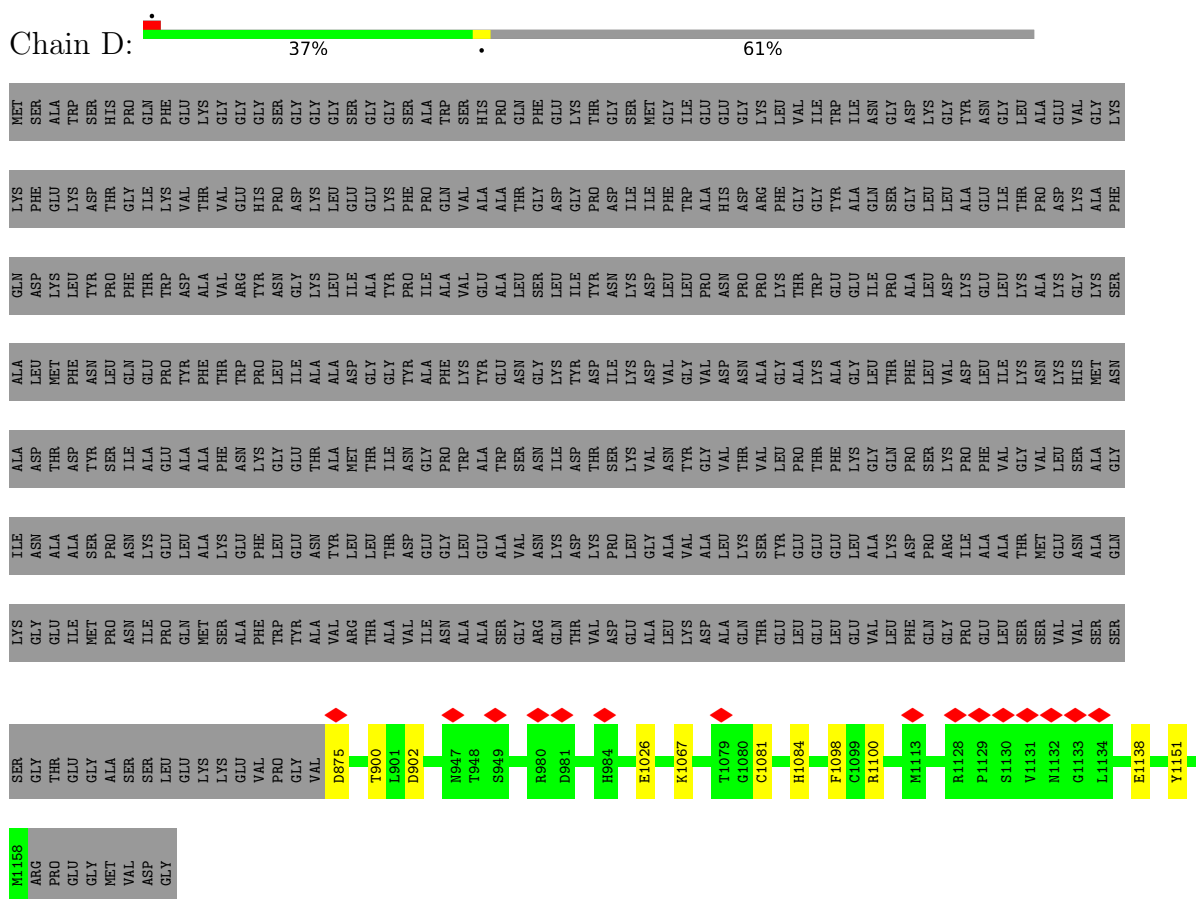
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	AltConf
4	D	23	Total O 23 23	0
4	Q	17	Total O 17 17	0

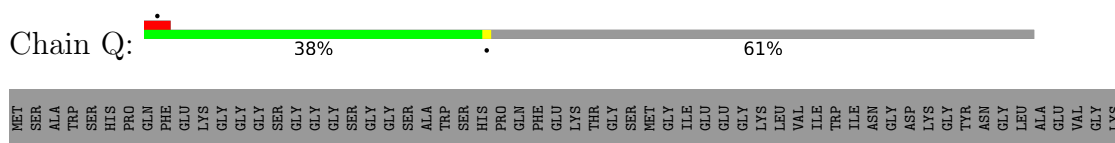
3 Residue-property plots

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: Maltose/maltodextrin-binding periplasmic protein,Poly [ADP-ribose] polymerase tankyrase-2



- Molecule 1: Maltose/maltodextrin-binding periplasmic protein,Poly [ADP-ribose] polymerase tankyrase-2



W1158	ARG	SER	LYS	ILE	ALA	ALA	ALA	GLN	LYS
PRO	GLU	GLY	GLY	ASN	ASP	LEU	THR	ASP	PHE
GLU	ILE	GLU	ILE	ALA	THR	PHE	LEU	LYS	GLU
MET	GLY	GLY	MET	SER	ASP	TYR	THR	ASP	THR
VAL	MET	ALA	PRO	ASN	ILE	SER	GLN	PHE	GLY
ASP	VAL	SER	ASN	LYS	GLU	ASN	THR	VAL	ARG
GLY	GLY	VAL	PHE	ALA	THR	GLU	GLU	HIS	GLU
		PRO	THR	TYR	GLY	ASN	PRO	ASP	PRO
		VAL	VAL	ALA	THR	ALA	LYS	LYS	VAL
		D876	VAL	VAL	ARG	THR	LEU	ILE	LEU
		I878	ALA	THR	THR	LEU	MET	ASP	ALA
		E888	ILE	VAL	ASN	GLY	TYR	PRO	GLY
		R896	ASN	ILE	GLY	PRO	PHE	ALA	GLN
		L904	ALA	ALA	LEU	TRP	LYS	VAL	VAL
		G916	SER	GLY	ALA	TRP	GLU	ALA	ALA
		N947	ARG	GLN	ILE	ASN	GLY	SER	THR
		T948	THR	THR	ASP	ASP	TYR	ILE	GLY
		S949	VAL	VAL	LYS	LYS	ASP	PRO	PRO
		G950	GLU	GLU	LEU	LEU	LYS	ILE	ASN
		S951	ALA	ALA	GLY	VAL	ASP	ASP	ILE
		D957	LEU	LYS	ALA	ASN	PHE	LEU	PHE
		D961	ASP	ASP	GLY	VAL	TRP	PRO	ALA
		D962	ALA	ALA	LEU	VAL	ALA	ASN	HIS
		K963	GLN	THR	LYS	THR	PRO	PRO	ARG
		R980	GLU	LEU	TYR	LEU	GLY	LYS	PHE
		L995	GLU	GLU	SER	PHE	THR	THR	GLY
		K996	VAL	VAL	LYS	GLN	GLU	PRO	ALA
		K1003	LEU	PHE	ASP	PRO	LYS	ALA	GLY
		N1022	GLN	GLY	ARG	SER	LEU	LEU	LEU
		I1091	PRO	PRO	ILE	LYS	VAL	ASP	ALA
		R1126	GLU	GLU	PHE	LEU	LEU	GLU	LYS
		P1129	LEU	LEU	ALA	VAL	ILE	GLU	ALA
		S1130	SER	SER	ALA	THR	GLY	LYS	ILE
		V1131	THR	THR	THR	VAL	ASN	ALA	PRO
		N1132	SER	SER	MET	LEU	LYS	ASP	THR
		G1133	VAL	VAL	GLU	SER	LYS	GLY	ASP
		L1134	SER	SER	ALA	ALA	LYS	LYS	LYS
					GLN	GLY	ALA	ALA	PHE

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-52.4°, rise=13.6 Å, axial sym=D1	Depositor
Number of segments used	1310954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	55.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.653	Depositor
Minimum map value	-1.864	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	422.912, 422.912, 422.912	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1AE4, ZN

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	D	0.13	0/2294	0.29	0/3088
1	Q	0.13	0/2294	0.27	0/3088
All	All	0.13	0/4588	0.28	0/6176

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	D	2241	0	2168	6	0
1	Q	2241	0	2168	3	0
2	D	1	0	0	0	0
2	Q	1	0	0	0	0
3	D	38	0	0	0	0
3	Q	38	0	0	0	0
4	D	23	0	0	0	0
4	Q	17	0	0	0	0
All	All	4600	0	4336	8	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 1.

All (8) 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:D:900:THR:OG1	1:D:902:ASP:OD1	1.91	0.89
1:D:1081:CYS:SG	1:D:1084:HIS:HB2	2.40	0.61
1:D:1100:ARG:NH2	1:Q:1022:ASN:O	2.40	0.52
1:Q:878:ILE:HD11	1:Q:904:LEU:HD22	1.99	0.44
1:Q:957:ASP:OD2	1:Q:957:ASP:N	2.50	0.44
1:D:1067:LYS:HE3	1:D:1138:GLU:OE1	2.17	0.43
1:D:1098:PHE:HB3	1:D:1151:TYR:HB2	2.03	0.41
1:D:1026:GLU:OE1	1:D:1100:ARG:HD3	2.22	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	D	282/729 (39%)	277 (98%)	5 (2%)	0	100	100
1	Q	282/729 (39%)	280 (99%)	2 (1%)	0	100	100
All	All	564/1458 (39%)	557 (99%)	7 (1%)	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	D	231/596 (39%)	230 (100%)	1 (0%)	84	92
1	Q	231/596 (39%)	228 (99%)	3 (1%)	61	78
All	All	462/1192 (39%)	458 (99%)	4 (1%)	68	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	875	ASP
1	Q	888	GLU
1	Q	947	ASN
1	Q	996	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	918	ASN
1	D	922	HIS
1	D	937	GLN
1	D	1048	HIS
1	D	1084	HIS
1	D	1109	GLN
1	Q	880	GLN
1	Q	937	GLN
1	Q	947	ASN
1	Q	1002	ASN
1	Q	1070	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	A1AE4	Q	1202	-	42,42,42	2.19	13 (30%)	58,61,61	1.24	7 (12%)
3	A1AE4	D	1202	-	42,42,42	2.21	12 (28%)	58,61,61	1.24	7 (12%)

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	A1AE4	Q	1202	-	-	7/24/24/24	0/5/5/5
3	A1AE4	D	1202	-	-	7/24/24/24	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	A1AE4	O23-C22	9.94	1.40	1.23
3	Q	1202	A1AE4	O23-C22	9.83	1.40	1.23
3	D	1202	A1AE4	C15-N17	3.54	1.46	1.35
3	Q	1202	A1AE4	C15-N17	3.53	1.46	1.35
3	D	1202	A1AE4	C29-C25	3.09	1.53	1.47
3	Q	1202	A1AE4	C29-C25	3.07	1.53	1.47
3	D	1202	A1AE4	O38-C35	-2.99	1.40	1.44
3	Q	1202	A1AE4	C09-C07	2.94	1.53	1.49
3	D	1202	A1AE4	C09-C07	2.93	1.53	1.49
3	D	1202	A1AE4	C21-C22	-2.91	1.43	1.48
3	Q	1202	A1AE4	O38-C35	-2.90	1.40	1.44
3	Q	1202	A1AE4	C21-C22	-2.87	1.43	1.48
3	Q	1202	A1AE4	C22-N24	-2.85	1.33	1.38
3	D	1202	A1AE4	C22-N24	-2.85	1.33	1.38
3	D	1202	A1AE4	C21-C27	-2.73	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1202	A1AE4	C21-C27	-2.63	1.37	1.41
3	Q	1202	A1AE4	C25-N26	-2.51	1.32	1.36
3	D	1202	A1AE4	C25-N26	-2.45	1.32	1.36
3	D	1202	A1AE4	C28-C27	2.43	1.43	1.39
3	Q	1202	A1AE4	C28-C27	2.36	1.43	1.39
3	D	1202	A1AE4	O02-C03	2.28	1.40	1.37
3	Q	1202	A1AE4	O02-C03	2.28	1.40	1.37
3	D	1202	A1AE4	C18-N17	2.27	1.46	1.41
3	Q	1202	A1AE4	C18-N17	2.24	1.46	1.41
3	Q	1202	A1AE4	O16-C15	-2.07	1.18	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1202	A1AE4	C03-C04-C15	-4.18	118.70	126.24
3	Q	1202	A1AE4	C03-C04-C15	-4.09	118.87	126.24
3	D	1202	A1AE4	C05-N06-C07	2.55	121.25	117.93
3	D	1202	A1AE4	C05-C04-C03	2.54	119.49	117.16
3	Q	1202	A1AE4	C05-C04-C03	2.52	119.47	117.16
3	Q	1202	A1AE4	O02-C03-C04	2.42	120.07	116.55
3	D	1202	A1AE4	C04-C05-N06	-2.40	120.94	124.32
3	D	1202	A1AE4	O02-C03-C04	2.40	120.04	116.55
3	Q	1202	A1AE4	C05-N06-C07	2.35	120.98	117.93
3	Q	1202	A1AE4	C08-C07-C09	-2.31	118.69	121.82
3	Q	1202	A1AE4	C04-C05-N06	-2.30	121.09	124.32
3	D	1202	A1AE4	C27-C21-C22	-2.28	117.65	120.11
3	Q	1202	A1AE4	C27-C21-C22	-2.19	117.74	120.11
3	D	1202	A1AE4	C08-C07-C09	-2.12	118.94	121.82

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1202	A1AE4	C31-C32-C35-C37
3	D	1202	A1AE4	C33-C32-C35-C37
3	Q	1202	A1AE4	C31-C32-C35-C36
3	Q	1202	A1AE4	C33-C32-C35-C36
3	Q	1202	A1AE4	C03-C04-C15-O16
3	D	1202	A1AE4	C05-C04-C15-N17
3	D	1202	A1AE4	C31-C32-C35-O38
3	D	1202	A1AE4	C33-C32-C35-O38
3	Q	1202	A1AE4	C31-C32-C35-O38

Continued on next page...

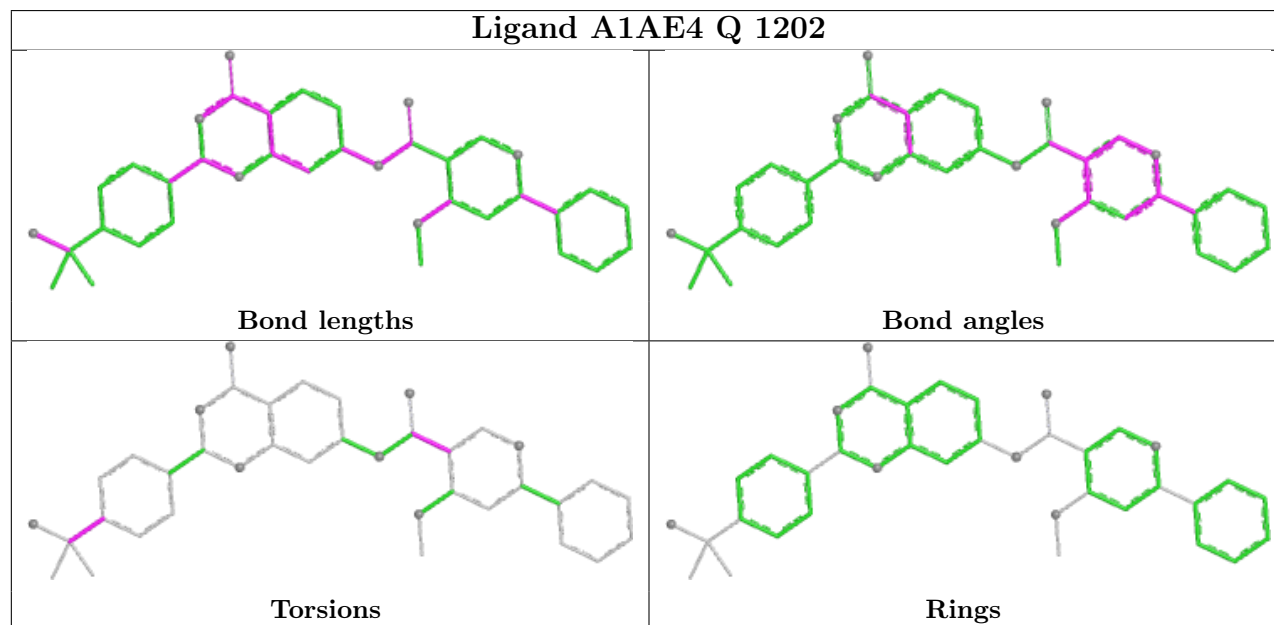
Continued from previous page...

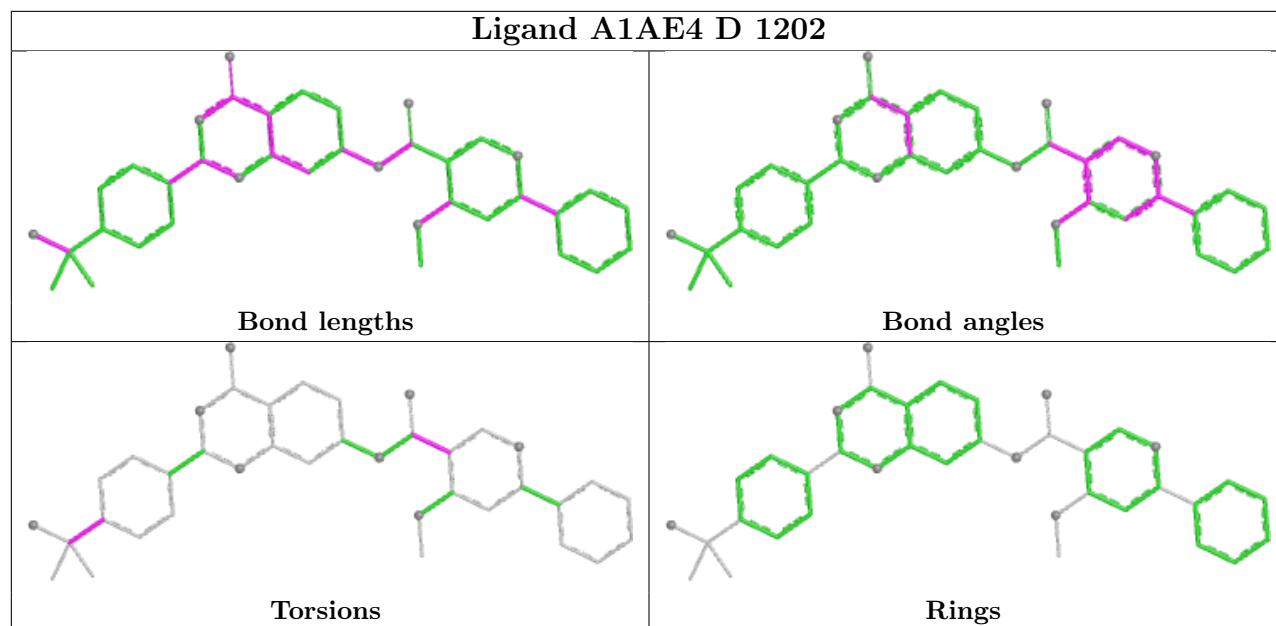
Mol	Chain	Res	Type	Atoms
3	Q	1202	A1AE4	C33-C32-C35-O38
3	D	1202	A1AE4	C03-C04-C15-O16
3	Q	1202	A1AE4	C03-C04-C15-N17
3	D	1202	A1AE4	C03-C04-C15-N17
3	Q	1202	A1AE4	C05-C04-C15-N17

There are no ring outliers.

No monomer is involved in short contacts.

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.

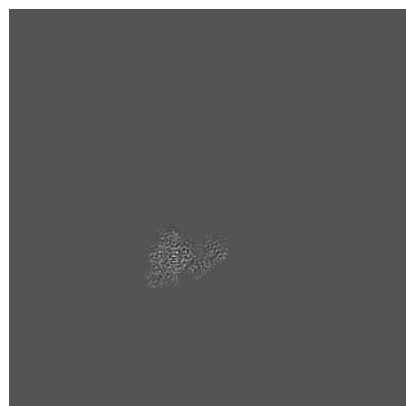
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43739. These allow visual inspection of the internal detail of the map and identification of artifacts.

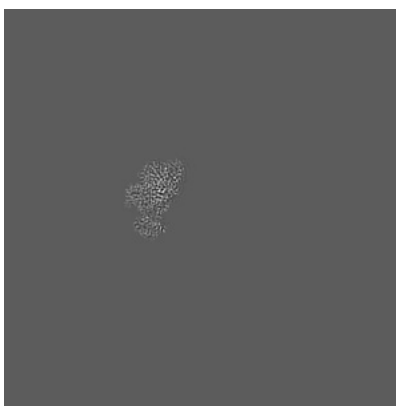
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

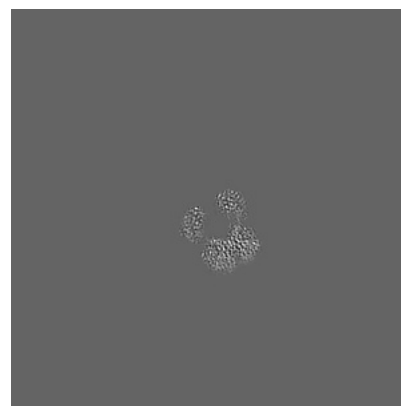
6.1.1 Primary map



X

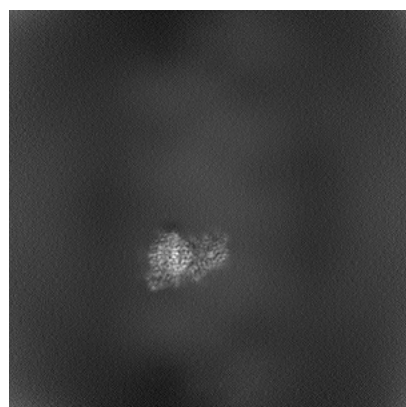


Y

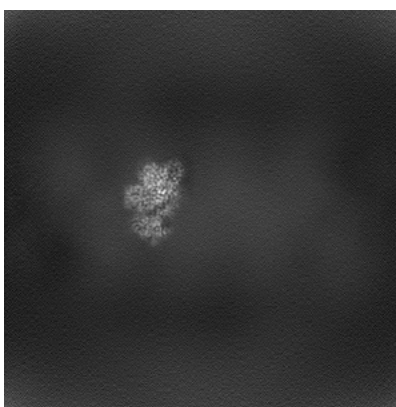


Z

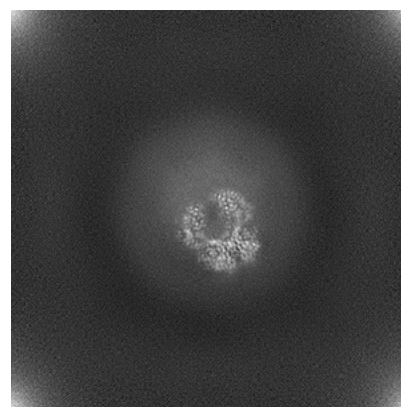
6.1.2 Raw map



X



Y

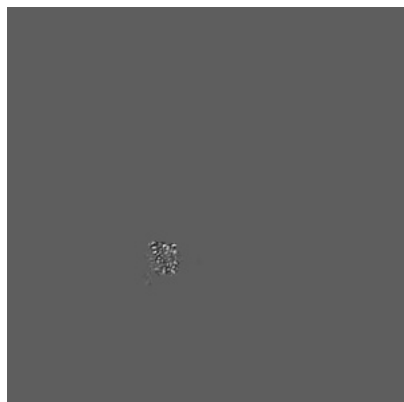


Z

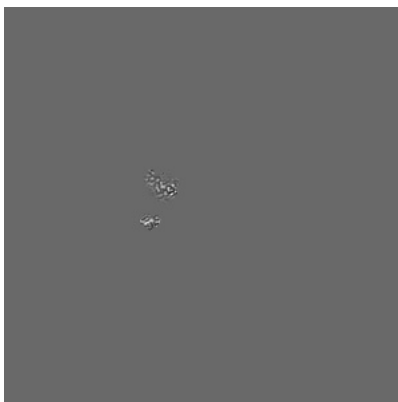
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

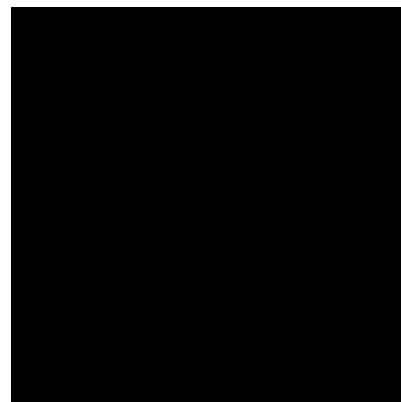
6.2.1 Primary map



X Index: 256

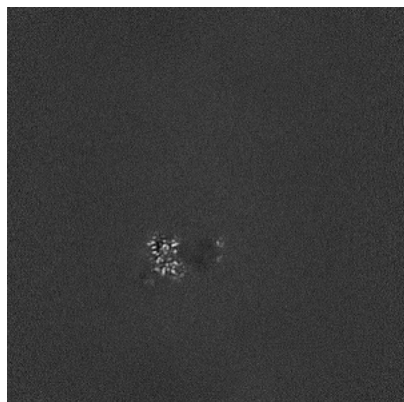


Y Index: 256



Z Index: 256

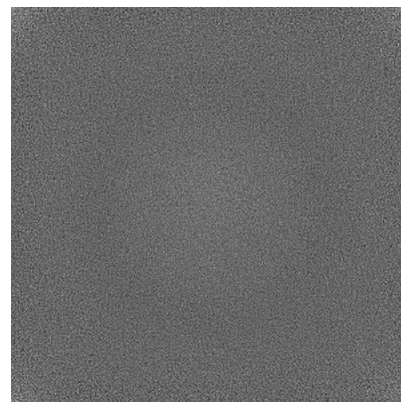
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

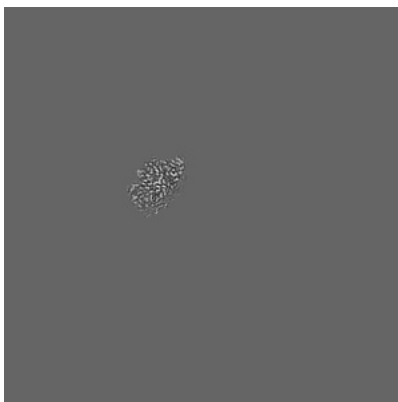
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

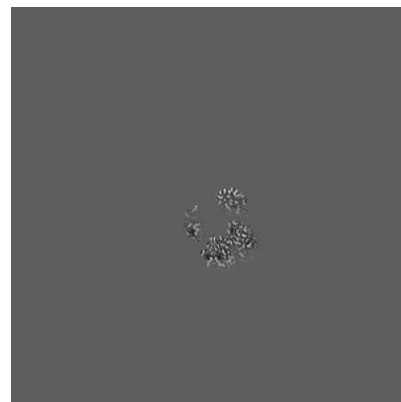
6.3.1 Primary map



X Index: 278

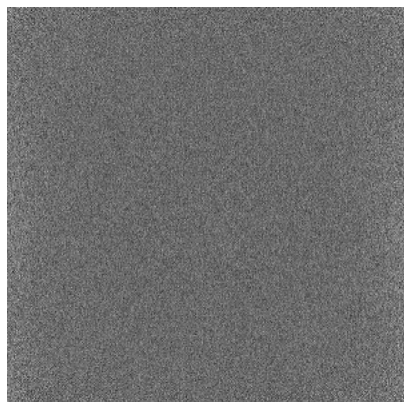


Y Index: 210

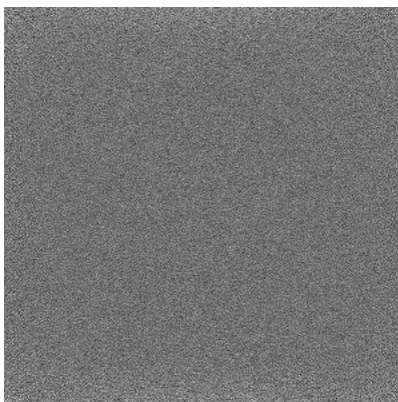


Z Index: 198

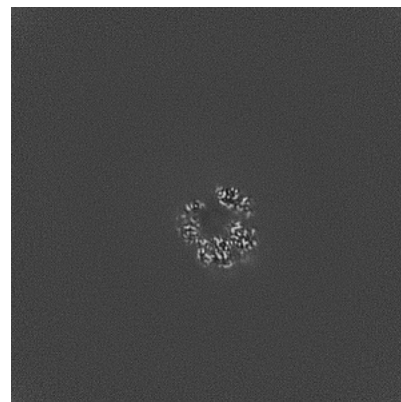
6.3.2 Raw map



X Index: 0



Y Index: 0

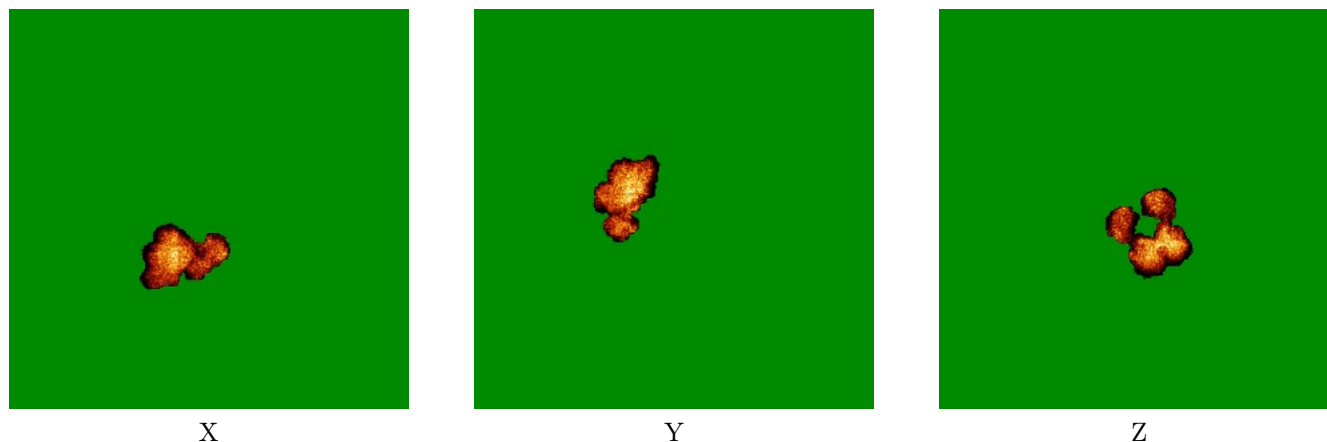


Z Index: 196

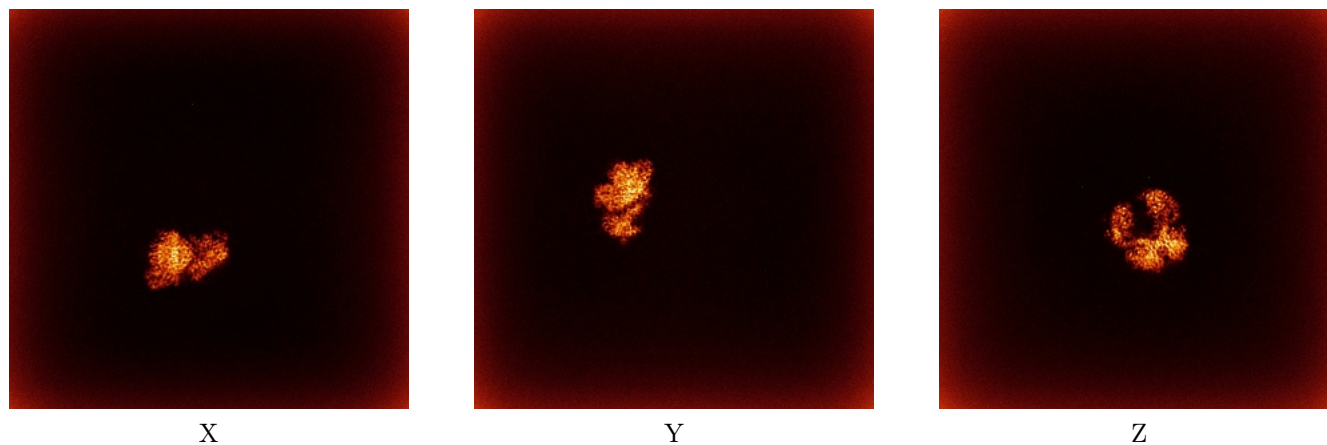
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

6.4.1 Primary map



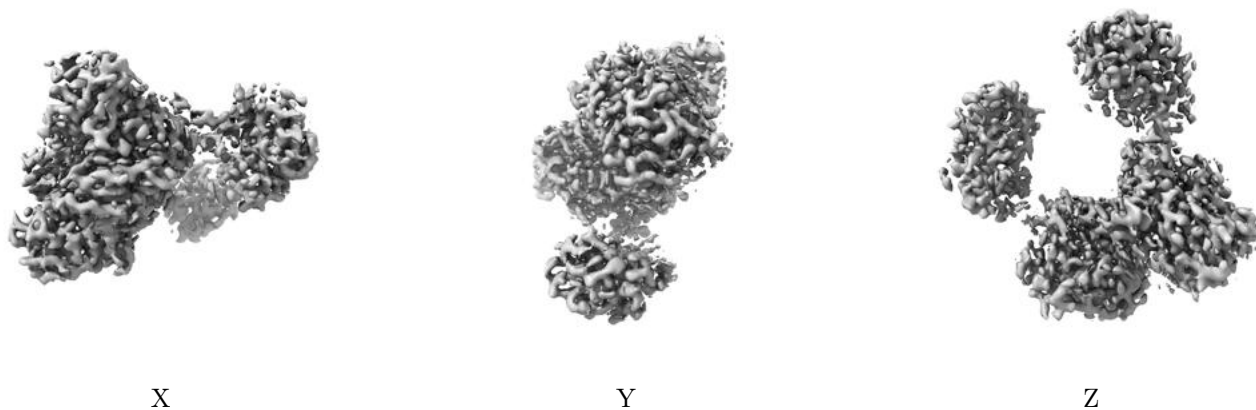
6.4.2 Raw map



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.

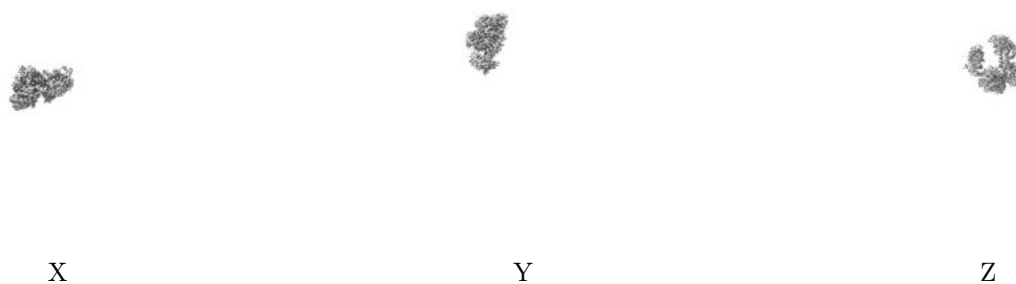
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

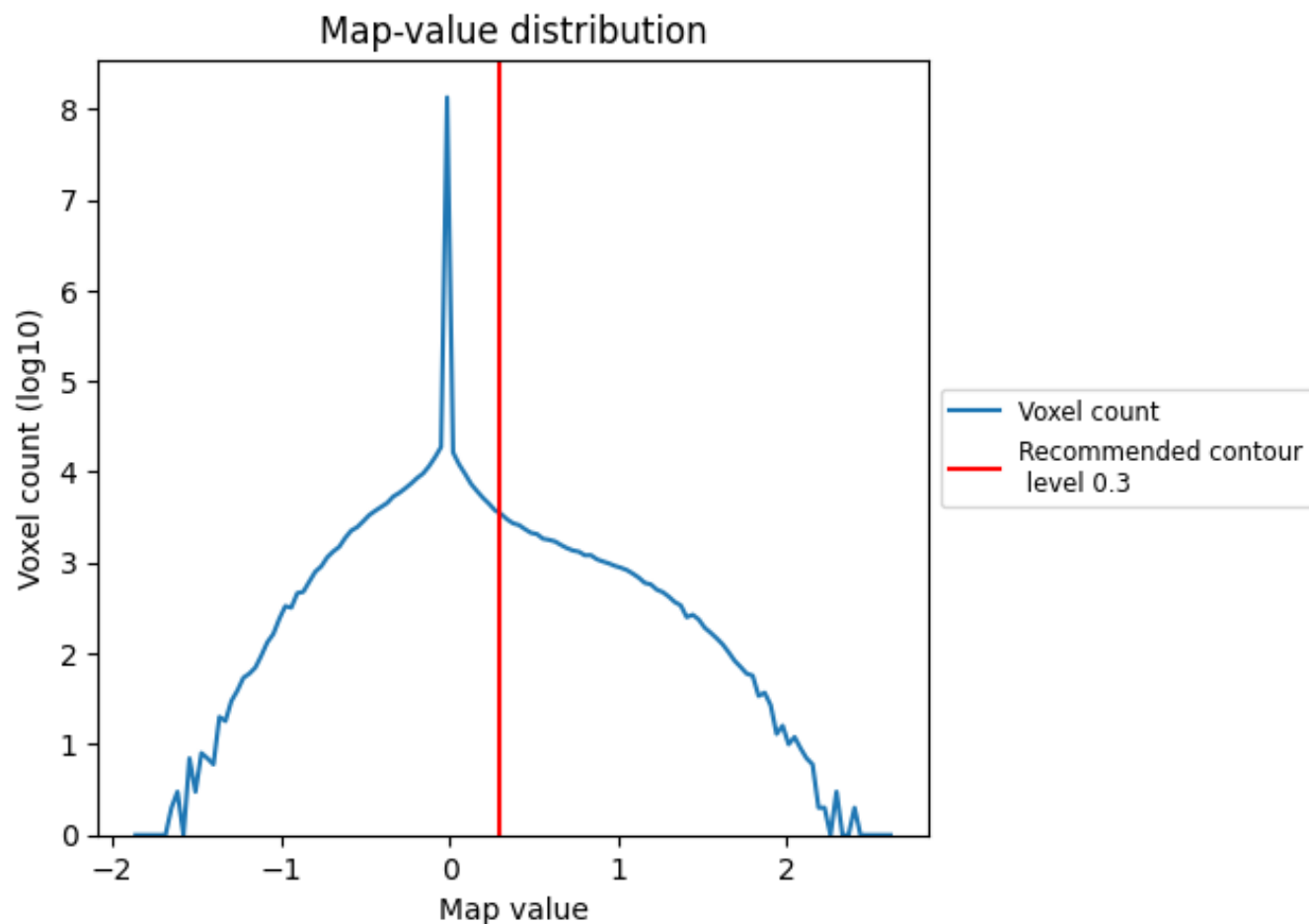
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

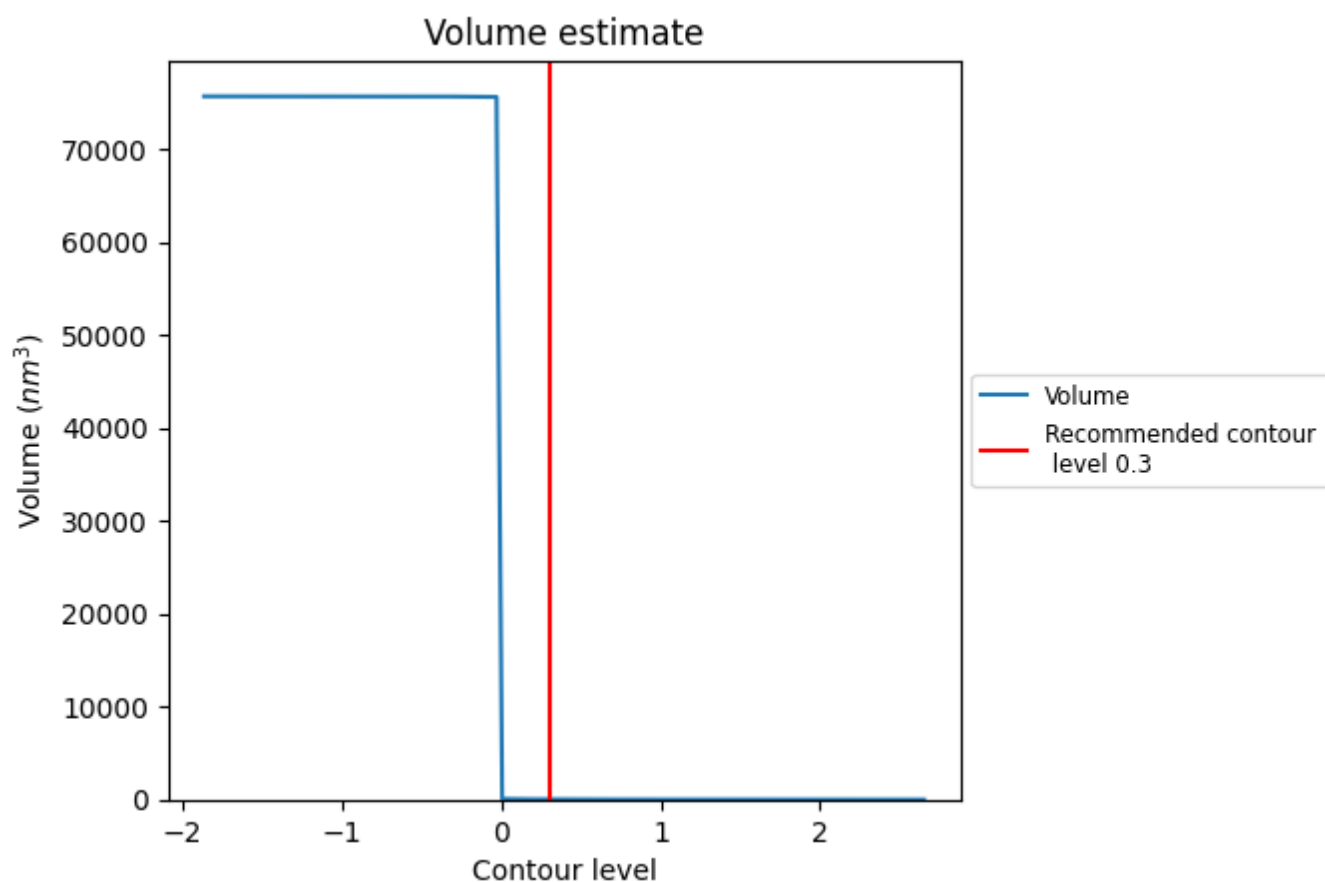
This section contains the results of statistical analysis of the map.

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.

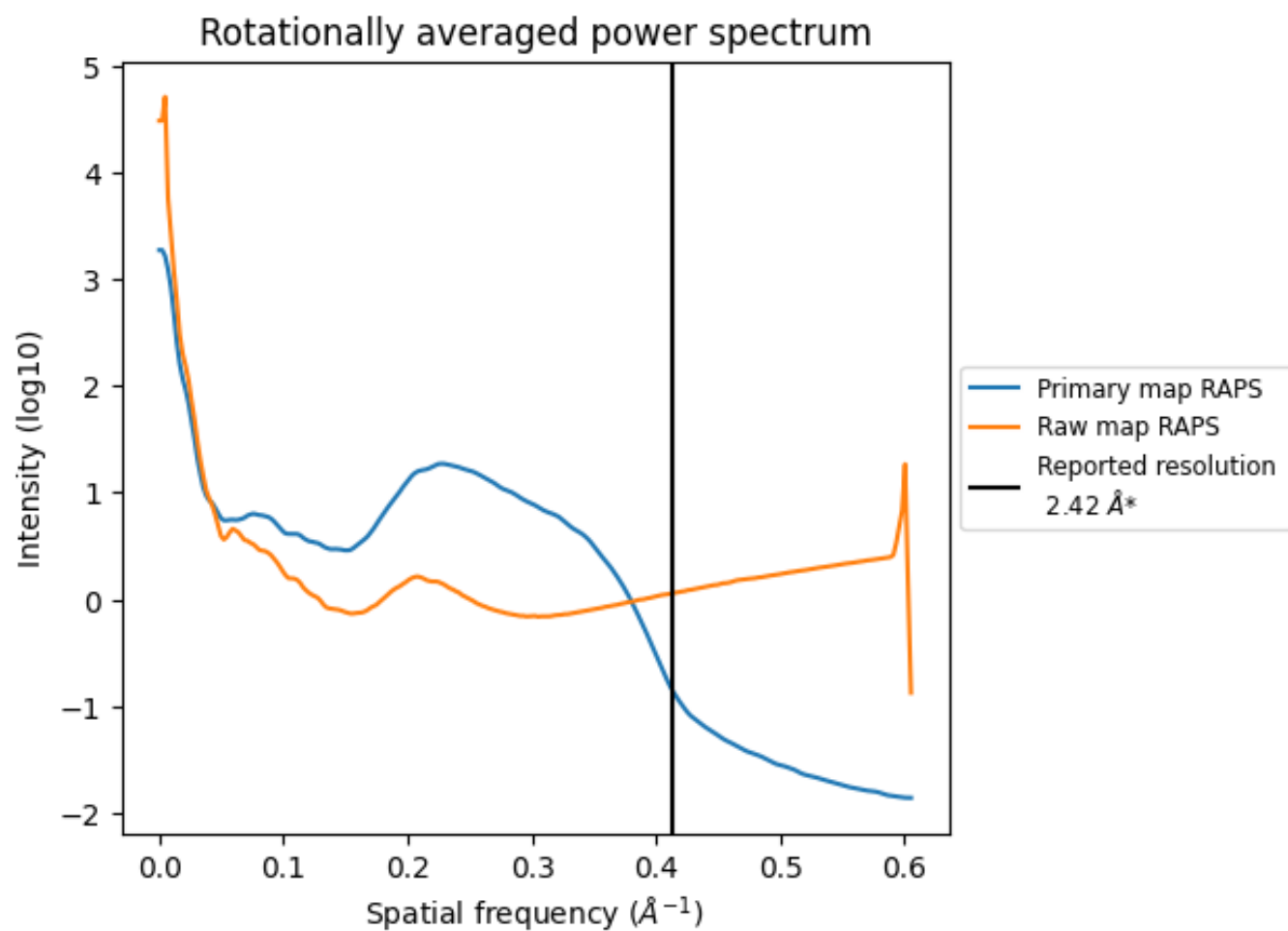
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25 nm³; this corresponds to an approximate mass of 23 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 ⓘ

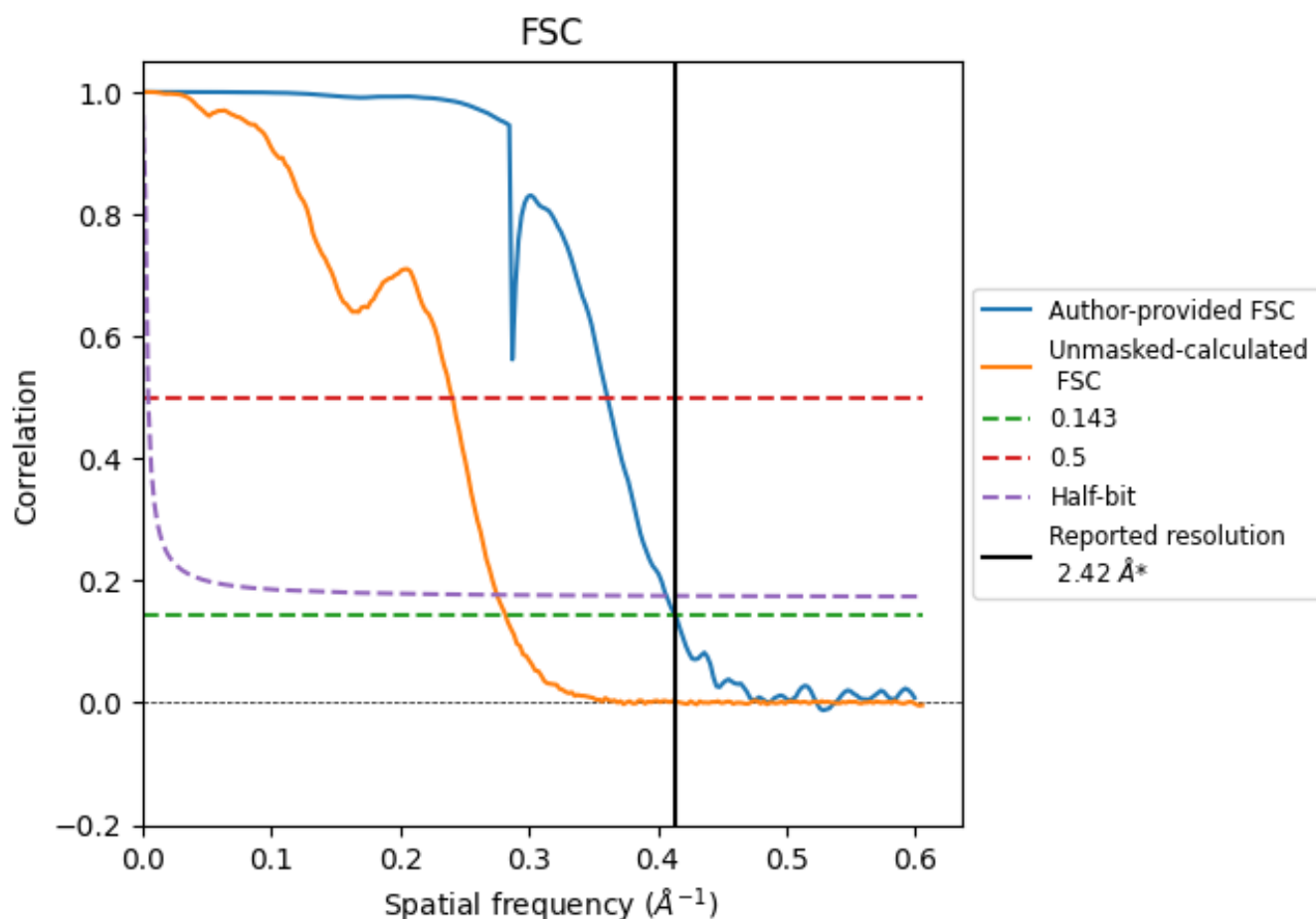


*Reported resolution corresponds to spatial frequency of 0.413 $\text{\AA}^{-1}$

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 0.413 Å⁻¹

8.2 Resolution estimates [i](#)

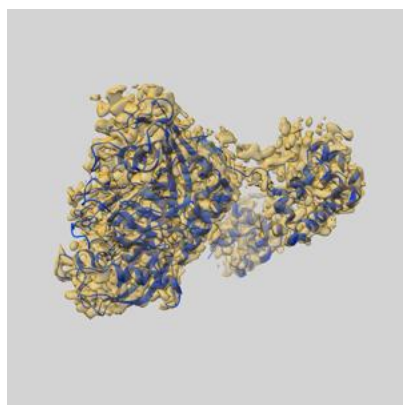
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	2.42	2.77	2.46
Unmasked-calculated*	3.55	4.15	3.63

*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 3.55 differs from the reported value 2.42 by more than 10 %

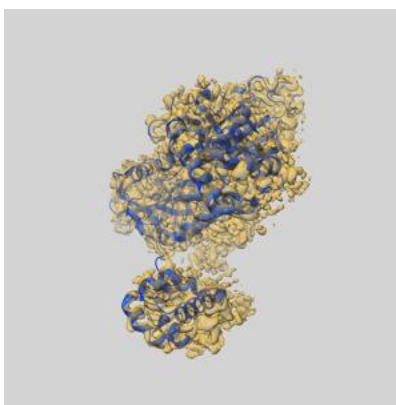
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43739 and PDB model 8W25. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

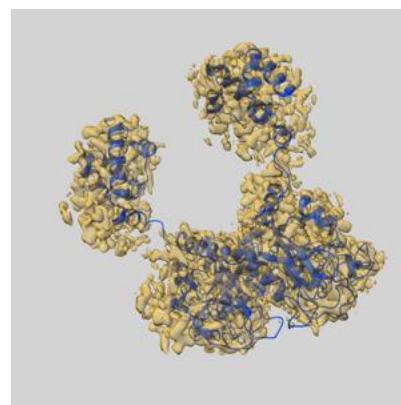
9.1 Map-model overlay [i](#)



X



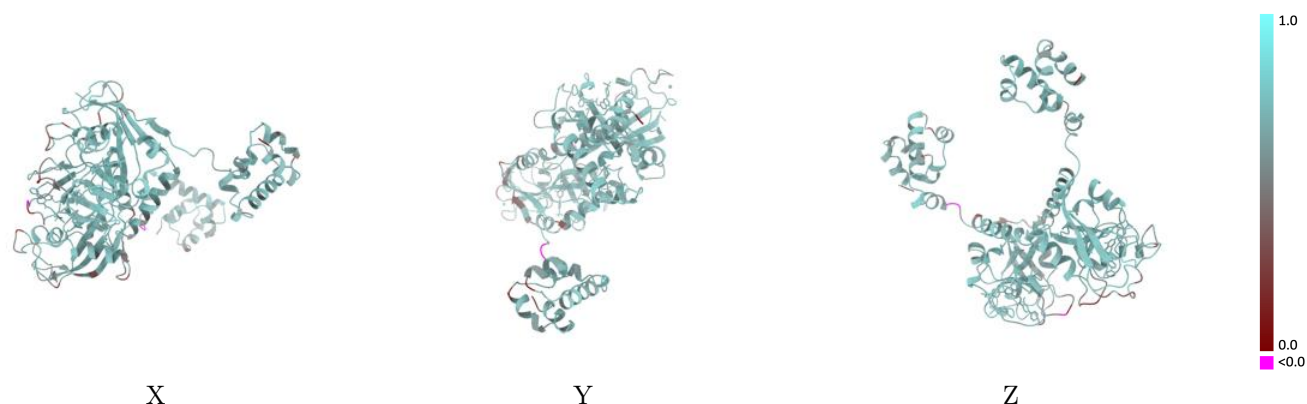
Y



Z

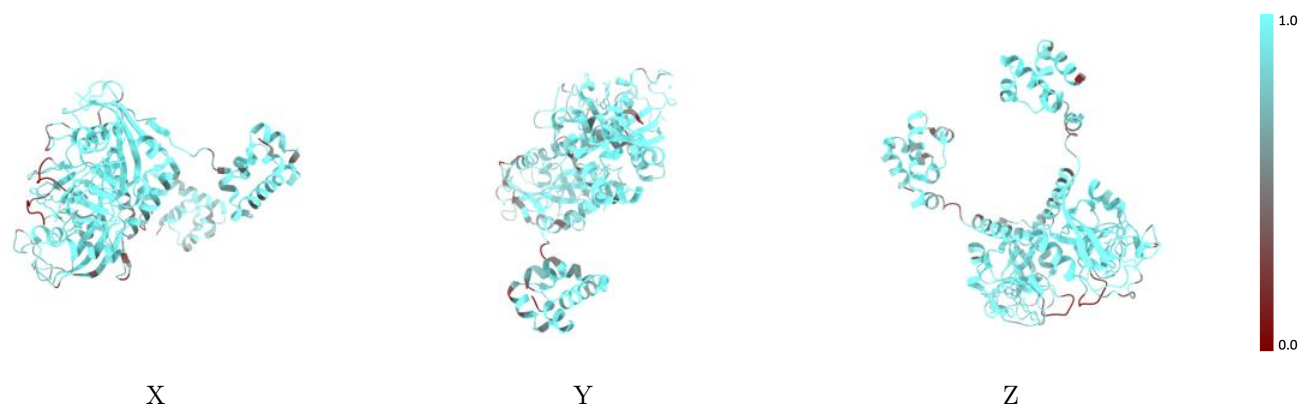
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



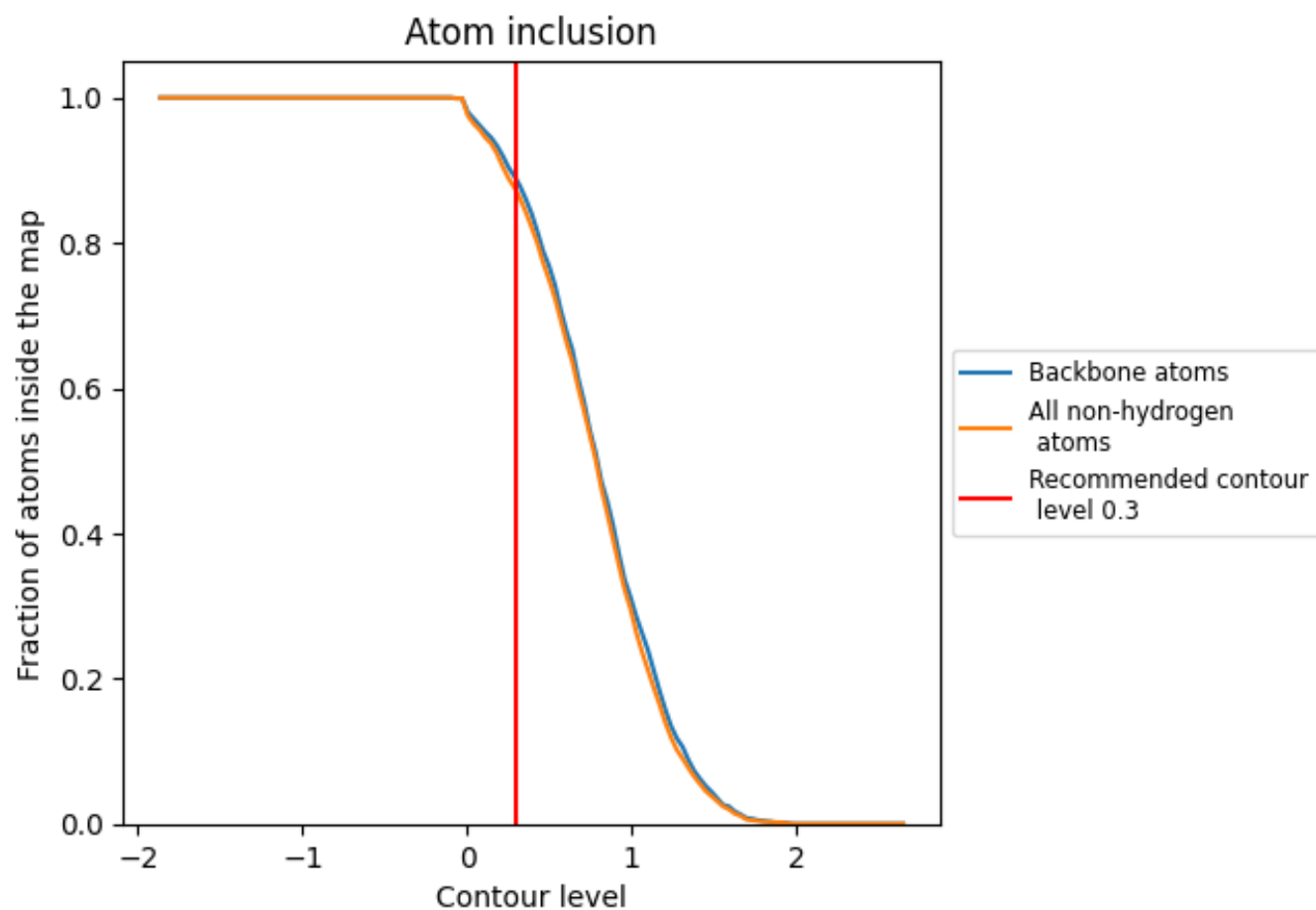
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8720	0.6350
D	0.8940	0.6470
Q	0.8540	0.6230

