



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 01:35 pm BST

PDB ID : 30WC / pdb_000030wc
EMDB ID : EMD-58108
Title : Structure of E. coli WbaP in complex with a megabody in the presence of UDP-Gal processed in C2 symmetry
Authors : Weckener, M.; Le Bas, A.; Ward, P.N.; Harrison, P.J.; Naismith, J.H.
Deposited on : 2026-05-14
Resolution : 3.00 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 : 1.8.4, 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

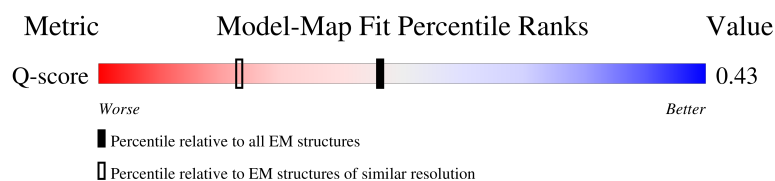
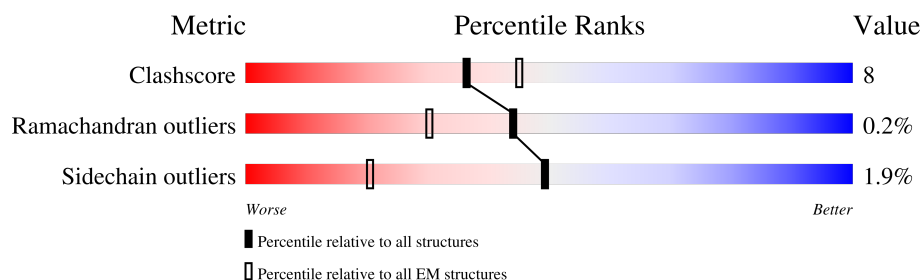
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	496	<div> <div>17%</div> <div>74%</div> <div>14%</div> <div>•</div> <div>12%</div> </div>
1	B	496	<div> <div>17%</div> <div>77%</div> <div>10%</div> <div>12%</div> </div>
2	C	524	<div> <div>5%</div> <div>18%</div> <div>•</div> <div>78%</div> </div>
2	D	524	<div> <div>5%</div> <div>18%</div> <div>•</div> <div>78%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18039 atoms, of which 9028 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 Undecaprenyl-phosphate galactose phosphotransferase WbaP.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	436	Total	C	H	N	O	S	0	0
			7183	2328	3628	602	610	15		
1	B	436	Total	C	H	N	O	S	0	0
			7183	2328	3628	602	610	15		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ARG	LYS	conflict	UNP A0A6D1CLM9
A	8	VAL	ILE	conflict	UNP A0A6D1CLM9
A	9	SER	GLY	conflict	UNP A0A6D1CLM9
A	11	SER	THR	conflict	UNP A0A6D1CLM9
A	13	THR	ALA	conflict	UNP A0A6D1CLM9
A	15	ALA	VAL	conflict	UNP A0A6D1CLM9
A	17	VAL	SER	conflict	UNP A0A6D1CLM9
A	22	LEU	PHE	conflict	UNP A0A6D1CLM9
A	23	THR	VAL	conflict	UNP A0A6D1CLM9
A	30	LEU	VAL	conflict	UNP A0A6D1CLM9
A	32	VAL	LEU	conflict	UNP A0A6D1CLM9
A	34	SER	ALA	conflict	UNP A0A6D1CLM9
A	35	LEU	VAL	conflict	UNP A0A6D1CLM9
A	36	THR	SER	conflict	UNP A0A6D1CLM9
A	37	LEU	MET	conflict	UNP A0A6D1CLM9
A	38	GLU	THR	conflict	UNP A0A6D1CLM9
A	39	HIS	ASP	conflict	UNP A0A6D1CLM9
A	41	GLN	GLU	conflict	UNP A0A6D1CLM9
A	42	GLN	THR	conflict	UNP A0A6D1CLM9
A	46	GLN	GLY	conflict	UNP A0A6D1CLM9
A	47	ASP	GLU	conflict	UNP A0A6D1CLM9
A	49	ILE	LEU	conflict	UNP A0A6D1CLM9
A	50	GLU	ASP	conflict	UNP A0A6D1CLM9
A	51	GLY	THR	conflict	UNP A0A6D1CLM9
A	54	GLY	LEU	conflict	UNP A0A6D1CLM9
A	57	TRP	LEU	conflict	UNP A0A6D1CLM9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	82	PHE	TYR	conflict	UNP A0A6D1CLM9
A	92	VAL	ILE	conflict	UNP A0A6D1CLM9
A	96	ILE	VAL	conflict	UNP A0A6D1CLM9
A	99	VAL	MET	conflict	UNP A0A6D1CLM9
A	101	ILE	VAL	conflict	UNP A0A6D1CLM9
A	102	ILE	MET	conflict	UNP A0A6D1CLM9
A	116	MET	LEU	conflict	UNP A0A6D1CLM9
A	119	VAL	LEU	conflict	UNP A0A6D1CLM9
A	120	PHE	LEU	conflict	UNP A0A6D1CLM9
A	122	ALA	VAL	conflict	UNP A0A6D1CLM9
A	123	ALA	PHE	conflict	UNP A0A6D1CLM9
A	128	LEU	ALA	conflict	UNP A0A6D1CLM9
A	131	THR	GLY	conflict	UNP A0A6D1CLM9
A	132	ALA	THR	conflict	UNP A0A6D1CLM9
A	134	TYR	TRP	conflict	UNP A0A6D1CLM9
A	135	ILE	CYS	conflict	UNP A0A6D1CLM9
A	138	SER	LYS	conflict	UNP A0A6D1CLM9
A	139	LEU	ILE	conflict	UNP A0A6D1CLM9
A	141	LEU	PHE	conflict	UNP A0A6D1CLM9
A	143	MET	LEU	conflict	UNP A0A6D1CLM9
A	156	HIS	ILE	conflict	UNP A0A6D1CLM9
A	163	ASN	TYR	conflict	UNP A0A6D1CLM9
A	166	ASN	ARG	conflict	UNP A0A6D1CLM9
A	171	ASN	LYS	conflict	UNP A0A6D1CLM9
A	172	VAL	ILE	conflict	UNP A0A6D1CLM9
A	176	VAL	ILE	conflict	UNP A0A6D1CLM9
A	178	VAL	SER	conflict	UNP A0A6D1CLM9
A	179	ASP	GLY	conflict	UNP A0A6D1CLM9
A	180	ASP	SER	conflict	UNP A0A6D1CLM9
A	?	-	ALA	deletion	UNP A0A6D1CLM9
A	?	-	SER	deletion	UNP A0A6D1CLM9
A	183	ASN	THR	conflict	UNP A0A6D1CLM9
A	184	GLY	HIS	conflict	UNP A0A6D1CLM9
A	185	SER	GLY	conflict	UNP A0A6D1CLM9
A	186	LYS	THR	conflict	UNP A0A6D1CLM9
A	187	ASN	ASP	conflict	UNP A0A6D1CLM9
A	188	THR	VAL	conflict	UNP A0A6D1CLM9
A	190	ASP	ASN	conflict	UNP A0A6D1CLM9
A	191	SER	GLY	conflict	UNP A0A6D1CLM9
A	192	VAL	ILE	conflict	UNP A0A6D1CLM9
A	193	GLN	GLU	conflict	UNP A0A6D1CLM9
A	196	SER	LYS	conflict	UNP A0A6D1CLM9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	VAL	ALA	conflict	UNP A0A6D1CLM9
A	198	ASP	SER	conflict	UNP A0A6D1CLM9
A	200	THR	ASP	conflict	UNP A0A6D1CLM9
A	203	THR	GLU	conflict	UNP A0A6D1CLM9
A	204	THR	SER	conflict	UNP A0A6D1CLM9
A	205	VAL	ILE	conflict	UNP A0A6D1CLM9
A	208	HIS	ARG	conflict	UNP A0A6D1CLM9
A	218	HIS	THR	conflict	UNP A0A6D1CLM9
A	219	GLN	GLU	conflict	UNP A0A6D1CLM9
A	222	ILE	THR	conflict	UNP A0A6D1CLM9
A	233	ARG	LYS	conflict	UNP A0A6D1CLM9
A	247	MET	VAL	conflict	UNP A0A6D1CLM9
A	269	GLN	HIS	conflict	UNP A0A6D1CLM9
A	278	ALA	ILE	conflict	UNP A0A6D1CLM9
A	279	LEU	ILE	conflict	UNP A0A6D1CLM9
A	282	ALA	LEU	conflict	UNP A0A6D1CLM9
A	285	ILE	VAL	conflict	UNP A0A6D1CLM9
A	290	SER	GLY	conflict	UNP A0A6D1CLM9
A	293	ILE	PHE	conflict	UNP A0A6D1CLM9
A	294	VAL	ILE	conflict	UNP A0A6D1CLM9
A	298	VAL	LEU	conflict	UNP A0A6D1CLM9
A	300	LEU	ILE	conflict	UNP A0A6D1CLM9
A	304	GLN	TYR	conflict	UNP A0A6D1CLM9
A	312	SER	PRO	conflict	UNP A0A6D1CLM9
A	323	GLY	ASN	conflict	UNP A0A6D1CLM9
A	345	ARG	ASN	conflict	UNP A0A6D1CLM9
A	348	GLU	ALA	conflict	UNP A0A6D1CLM9
A	349	ASN	THR	conflict	UNP A0A6D1CLM9
A	351	PRO	ASP	conflict	UNP A0A6D1CLM9
A	352	LYS	SER	conflict	UNP A0A6D1CLM9
A	354	LYS	ARG	conflict	UNP A0A6D1CLM9
A	355	ALA	HIS	conflict	UNP A0A6D1CLM9
A	358	ASP	GLU	conflict	UNP A0A6D1CLM9
A	359	ALA	MET	conflict	UNP A0A6D1CLM9
A	365	ASP	ASN	conflict	UNP A0A6D1CLM9
A	375	PHE	LEU	conflict	UNP A0A6D1CLM9
A	416	ASP	ALA	conflict	UNP A0A6D1CLM9
A	421	ILE	SER	conflict	UNP A0A6D1CLM9
A	466	ILE	THR	conflict	UNP A0A6D1CLM9
A	467	GLY	THR	conflict	UNP A0A6D1CLM9
A	472	LYS	ARG	conflict	UNP A0A6D1CLM9
A	477	LEU	-	expression tag	UNP A0A6D1CLM9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	478	GLU	-	expression tag	UNP A0A6D1CLM9
A	479	GLU	-	expression tag	UNP A0A6D1CLM9
A	480	ASN	-	expression tag	UNP A0A6D1CLM9
A	481	LEU	-	expression tag	UNP A0A6D1CLM9
A	482	TYR	-	expression tag	UNP A0A6D1CLM9
A	483	PHE	-	expression tag	UNP A0A6D1CLM9
A	484	GLN	-	expression tag	UNP A0A6D1CLM9
A	485	GLY	-	expression tag	UNP A0A6D1CLM9
A	486	ALA	-	expression tag	UNP A0A6D1CLM9
A	487	HIS	-	expression tag	UNP A0A6D1CLM9
A	488	HIS	-	expression tag	UNP A0A6D1CLM9
A	489	HIS	-	expression tag	UNP A0A6D1CLM9
A	490	HIS	-	expression tag	UNP A0A6D1CLM9
A	491	HIS	-	expression tag	UNP A0A6D1CLM9
A	492	HIS	-	expression tag	UNP A0A6D1CLM9
A	493	HIS	-	expression tag	UNP A0A6D1CLM9
A	494	HIS	-	expression tag	UNP A0A6D1CLM9
A	495	HIS	-	expression tag	UNP A0A6D1CLM9
A	496	HIS	-	expression tag	UNP A0A6D1CLM9
B	6	ARG	LYS	conflict	UNP A0A6D1CLM9
B	8	VAL	ILE	conflict	UNP A0A6D1CLM9
B	9	SER	GLY	conflict	UNP A0A6D1CLM9
B	11	SER	THR	conflict	UNP A0A6D1CLM9
B	13	THR	ALA	conflict	UNP A0A6D1CLM9
B	15	ALA	VAL	conflict	UNP A0A6D1CLM9
B	17	VAL	SER	conflict	UNP A0A6D1CLM9
B	22	LEU	PHE	conflict	UNP A0A6D1CLM9
B	23	THR	VAL	conflict	UNP A0A6D1CLM9
B	30	LEU	VAL	conflict	UNP A0A6D1CLM9
B	32	VAL	LEU	conflict	UNP A0A6D1CLM9
B	34	SER	ALA	conflict	UNP A0A6D1CLM9
B	35	LEU	VAL	conflict	UNP A0A6D1CLM9
B	36	THR	SER	conflict	UNP A0A6D1CLM9
B	37	LEU	MET	conflict	UNP A0A6D1CLM9
B	38	GLU	THR	conflict	UNP A0A6D1CLM9
B	39	HIS	ASP	conflict	UNP A0A6D1CLM9
B	41	GLN	GLU	conflict	UNP A0A6D1CLM9
B	42	GLN	THR	conflict	UNP A0A6D1CLM9
B	46	GLN	GLY	conflict	UNP A0A6D1CLM9
B	47	ASP	GLU	conflict	UNP A0A6D1CLM9
B	49	ILE	LEU	conflict	UNP A0A6D1CLM9
B	50	GLU	ASP	conflict	UNP A0A6D1CLM9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	51	GLY	THR	conflict	UNP A0A6D1CLM9
B	54	GLY	LEU	conflict	UNP A0A6D1CLM9
B	57	TRP	LEU	conflict	UNP A0A6D1CLM9
B	82	PHE	TYR	conflict	UNP A0A6D1CLM9
B	92	VAL	ILE	conflict	UNP A0A6D1CLM9
B	96	ILE	VAL	conflict	UNP A0A6D1CLM9
B	99	VAL	MET	conflict	UNP A0A6D1CLM9
B	101	ILE	VAL	conflict	UNP A0A6D1CLM9
B	102	ILE	MET	conflict	UNP A0A6D1CLM9
B	116	MET	LEU	conflict	UNP A0A6D1CLM9
B	119	VAL	LEU	conflict	UNP A0A6D1CLM9
B	120	PHE	LEU	conflict	UNP A0A6D1CLM9
B	122	ALA	VAL	conflict	UNP A0A6D1CLM9
B	123	ALA	PHE	conflict	UNP A0A6D1CLM9
B	128	LEU	ALA	conflict	UNP A0A6D1CLM9
B	131	THR	GLY	conflict	UNP A0A6D1CLM9
B	132	ALA	THR	conflict	UNP A0A6D1CLM9
B	134	TYR	TRP	conflict	UNP A0A6D1CLM9
B	135	ILE	CYS	conflict	UNP A0A6D1CLM9
B	138	SER	LYS	conflict	UNP A0A6D1CLM9
B	139	LEU	ILE	conflict	UNP A0A6D1CLM9
B	141	LEU	PHE	conflict	UNP A0A6D1CLM9
B	143	MET	LEU	conflict	UNP A0A6D1CLM9
B	156	HIS	ILE	conflict	UNP A0A6D1CLM9
B	163	ASN	TYR	conflict	UNP A0A6D1CLM9
B	166	ASN	ARG	conflict	UNP A0A6D1CLM9
B	171	ASN	LYS	conflict	UNP A0A6D1CLM9
B	172	VAL	ILE	conflict	UNP A0A6D1CLM9
B	176	VAL	ILE	conflict	UNP A0A6D1CLM9
B	178	VAL	SER	conflict	UNP A0A6D1CLM9
B	179	ASP	GLY	conflict	UNP A0A6D1CLM9
B	180	ASP	SER	conflict	UNP A0A6D1CLM9
B	?	-	ALA	deletion	UNP A0A6D1CLM9
B	?	-	SER	deletion	UNP A0A6D1CLM9
B	183	ASN	THR	conflict	UNP A0A6D1CLM9
B	184	GLY	HIS	conflict	UNP A0A6D1CLM9
B	185	SER	GLY	conflict	UNP A0A6D1CLM9
B	186	LYS	THR	conflict	UNP A0A6D1CLM9
B	187	ASN	ASP	conflict	UNP A0A6D1CLM9
B	188	THR	VAL	conflict	UNP A0A6D1CLM9
B	190	ASP	ASN	conflict	UNP A0A6D1CLM9
B	191	SER	GLY	conflict	UNP A0A6D1CLM9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	192	VAL	ILE	conflict	UNP A0A6D1CLM9
B	193	GLN	GLU	conflict	UNP A0A6D1CLM9
B	196	SER	LYS	conflict	UNP A0A6D1CLM9
B	197	VAL	ALA	conflict	UNP A0A6D1CLM9
B	198	ASP	SER	conflict	UNP A0A6D1CLM9
B	200	THR	ASP	conflict	UNP A0A6D1CLM9
B	203	THR	GLU	conflict	UNP A0A6D1CLM9
B	204	THR	SER	conflict	UNP A0A6D1CLM9
B	205	VAL	ILE	conflict	UNP A0A6D1CLM9
B	208	HIS	ARG	conflict	UNP A0A6D1CLM9
B	218	HIS	THR	conflict	UNP A0A6D1CLM9
B	219	GLN	GLU	conflict	UNP A0A6D1CLM9
B	222	ILE	THR	conflict	UNP A0A6D1CLM9
B	233	ARG	LYS	conflict	UNP A0A6D1CLM9
B	247	MET	VAL	conflict	UNP A0A6D1CLM9
B	269	GLN	HIS	conflict	UNP A0A6D1CLM9
B	278	ALA	ILE	conflict	UNP A0A6D1CLM9
B	279	LEU	ILE	conflict	UNP A0A6D1CLM9
B	282	ALA	LEU	conflict	UNP A0A6D1CLM9
B	285	ILE	VAL	conflict	UNP A0A6D1CLM9
B	290	SER	GLY	conflict	UNP A0A6D1CLM9
B	293	ILE	PHE	conflict	UNP A0A6D1CLM9
B	294	VAL	ILE	conflict	UNP A0A6D1CLM9
B	298	VAL	LEU	conflict	UNP A0A6D1CLM9
B	300	LEU	ILE	conflict	UNP A0A6D1CLM9
B	304	GLN	TYR	conflict	UNP A0A6D1CLM9
B	312	SER	PRO	conflict	UNP A0A6D1CLM9
B	323	GLY	ASN	conflict	UNP A0A6D1CLM9
B	345	ARG	ASN	conflict	UNP A0A6D1CLM9
B	348	GLU	ALA	conflict	UNP A0A6D1CLM9
B	349	ASN	THR	conflict	UNP A0A6D1CLM9
B	351	PRO	ASP	conflict	UNP A0A6D1CLM9
B	352	LYS	SER	conflict	UNP A0A6D1CLM9
B	354	LYS	ARG	conflict	UNP A0A6D1CLM9
B	355	ALA	HIS	conflict	UNP A0A6D1CLM9
B	358	ASP	GLU	conflict	UNP A0A6D1CLM9
B	359	ALA	MET	conflict	UNP A0A6D1CLM9
B	365	ASP	ASN	conflict	UNP A0A6D1CLM9
B	375	PHE	LEU	conflict	UNP A0A6D1CLM9
B	416	ASP	ALA	conflict	UNP A0A6D1CLM9
B	421	ILE	SER	conflict	UNP A0A6D1CLM9
B	466	ILE	THR	conflict	UNP A0A6D1CLM9

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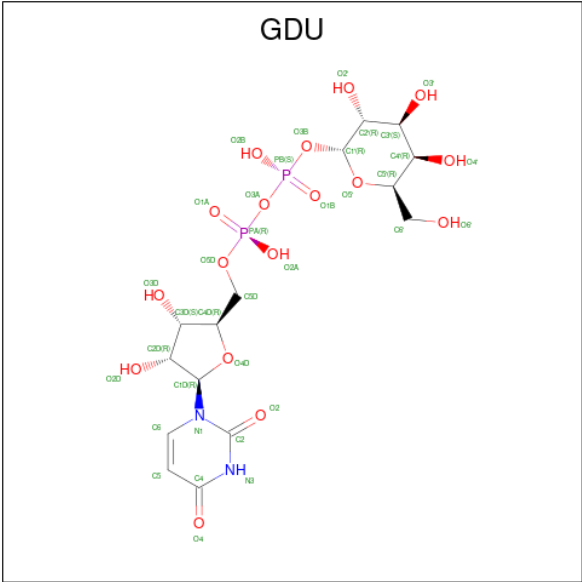
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Chain	Residue	Modelled	Actual	Comment	Reference
B	467	GLY	THR	conflict	UNP A0A6D1CLM9
B	472	LYS	ARG	conflict	UNP A0A6D1CLM9
B	477	LEU	-	expression tag	UNP A0A6D1CLM9
B	478	GLU	-	expression tag	UNP A0A6D1CLM9
B	479	GLU	-	expression tag	UNP A0A6D1CLM9
B	480	ASN	-	expression tag	UNP A0A6D1CLM9
B	481	LEU	-	expression tag	UNP A0A6D1CLM9
B	482	TYR	-	expression tag	UNP A0A6D1CLM9
B	483	PHE	-	expression tag	UNP A0A6D1CLM9
B	484	GLN	-	expression tag	UNP A0A6D1CLM9
B	485	GLY	-	expression tag	UNP A0A6D1CLM9
B	486	ALA	-	expression tag	UNP A0A6D1CLM9
B	487	HIS	-	expression tag	UNP A0A6D1CLM9
B	488	HIS	-	expression tag	UNP A0A6D1CLM9
B	489	HIS	-	expression tag	UNP A0A6D1CLM9
B	490	HIS	-	expression tag	UNP A0A6D1CLM9
B	491	HIS	-	expression tag	UNP A0A6D1CLM9
B	492	HIS	-	expression tag	UNP A0A6D1CLM9
B	493	HIS	-	expression tag	UNP A0A6D1CLM9
B	494	HIS	-	expression tag	UNP A0A6D1CLM9
B	495	HIS	-	expression tag	UNP A0A6D1CLM9
B	496	HIS	-	expression tag	UNP A0A6D1CLM9

- Molecule 2 is a protein called Megabody.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	117	Total	C	H	N	O	S	0	0
			1802	583	876	157	181	5		
2	D	117	Total	C	H	N	O	S	0	0
			1801	583	876	156	181	5		

- Molecule 3 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (CCD ID: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂) (labeled as "Ligand of Interest" by depositor).

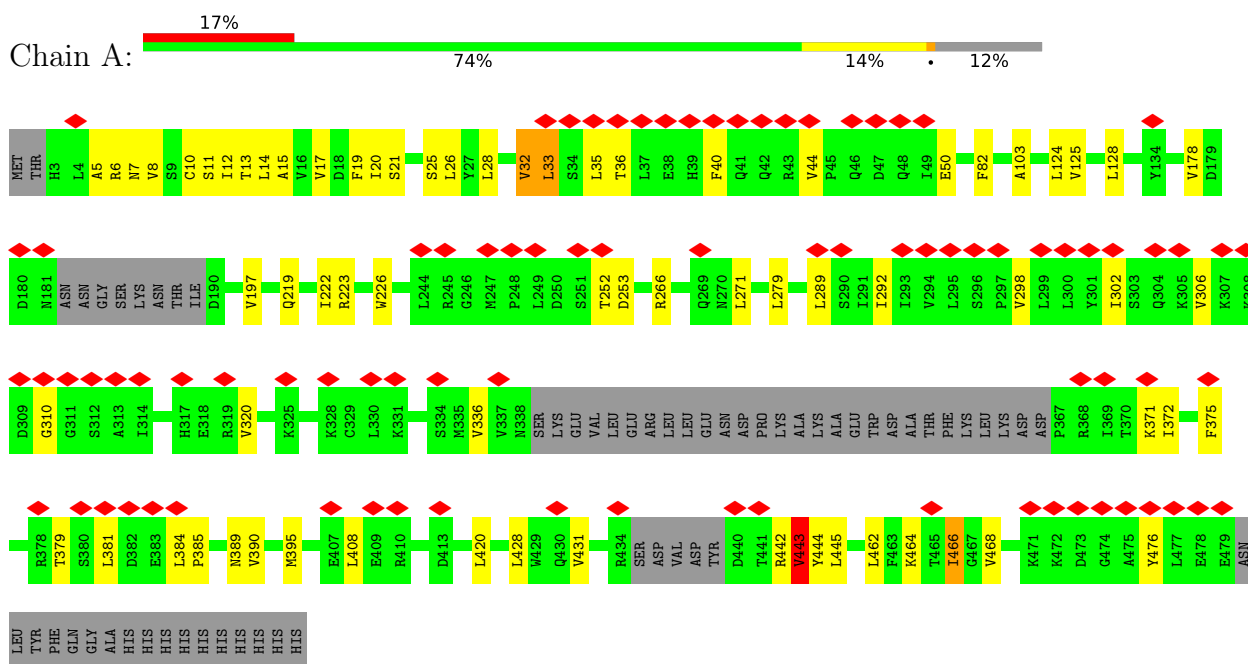


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
3	A	1	35	9	10	2	12	2	0
3	B	1	35	9	10	2	12	2	0

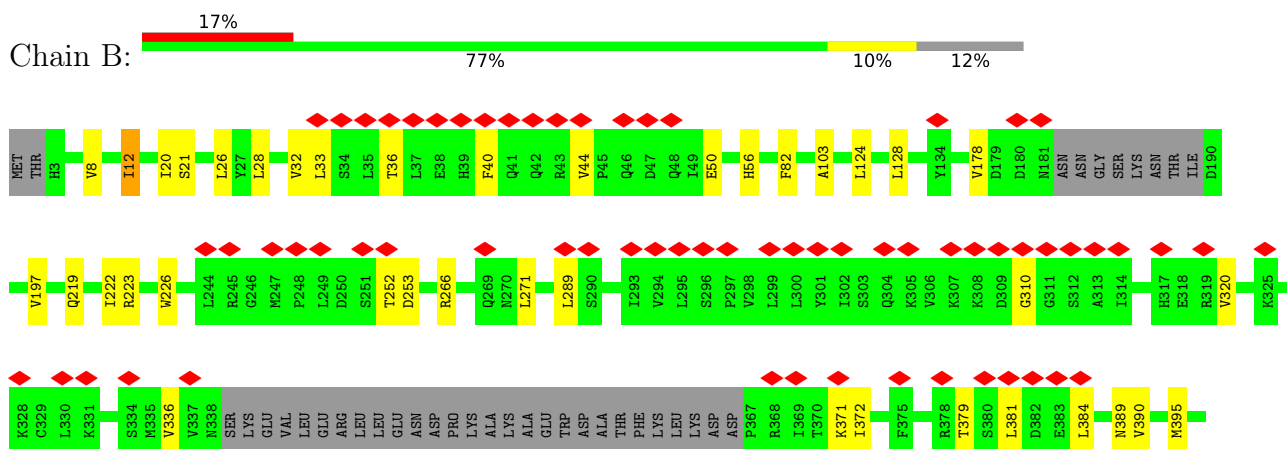
3 Residue-property plots

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: Undecaprenyl-phosphate galactose phosphotransferase WbaP



- Molecule 1: Undecaprenyl-phosphate galactose phosphotransferase WbaP



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	492904	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.029	Depositor
Map size (Å)	336.896, 336.896, 336.896	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.658, 0.658, 0.658	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.13	0/3642	0.29	0/4937
1	B	0.13	0/3642	0.30	0/4937
2	C	0.18	0/949	0.46	0/1283
2	D	0.18	0/948	0.48	0/1281
All	All	0.14	0/9181	0.34	0/12438

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 [i](#)

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	3555	3628	3624	61	0
1	B	3555	3628	3624	51	0
2	C	926	876	877	20	0
2	D	925	876	873	20	0
3	A	25	10	10	0	0
3	B	25	10	10	0	0
All	All	9011	9028	9018	138	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 8.

All (138) 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:431:VAL:HG11	1:A:464:LYS:HG2	1.64	0.79
1:B:431:VAL:HG11	1:B:464:LYS:HG2	1.64	0.78
1:B:431:VAL:HG13	1:B:468:VAL:HG21	1.69	0.73
1:A:462:LEU:O	1:A:466:ILE:HG23	1.90	0.72
1:B:462:LEU:O	1:B:466:ILE:HG23	1.89	0.72
2:C:445:TYR:CD1	2:C:449:VAL:HG11	2.26	0.71
1:B:197:VAL:HG11	2:D:489:SER:CB	2.22	0.70
1:A:197:VAL:HG11	2:C:489:SER:CB	2.22	0.70
2:D:445:TYR:CD1	2:D:449:VAL:HG11	2.28	0.68
1:B:40:PHE:O	1:B:44:VAL:HG22	1.96	0.66
1:B:28:LEU:O	1:B:32:VAL:HG13	1.97	0.65
2:D:464:LEU:HD23	2:D:465:TYR:N	2.12	0.65
1:A:32:VAL:O	1:A:36:THR:HG23	1.97	0.65
1:A:103:ALA:HB2	1:B:103:ALA:HB2	1.79	0.63
1:A:197:VAL:HG11	2:C:489:SER:HB2	1.82	0.62
1:A:431:VAL:HG13	1:A:468:VAL:HG21	1.82	0.61
2:D:5:VAL:HG23	2:D:408:THR:CG2	2.31	0.61
1:B:197:VAL:HG11	2:D:489:SER:HB2	1.84	0.60
1:B:8:VAL:O	1:B:12:ILE:HD12	2.01	0.60
1:A:219:GLN:HB3	1:A:222:ILE:HD12	1.84	0.60
1:A:40:PHE:O	1:A:44:VAL:HG22	2.02	0.59
1:A:8:VAL:O	1:A:12:ILE:HD12	2.03	0.59
1:B:222:ILE:HD11	2:D:490:TYR:CZ	2.39	0.58
2:D:4:LEU:HD11	2:D:481:CYS:HB3	1.84	0.57
2:D:437:MET:HE1	2:D:490:TYR:CE1	2.39	0.57
1:B:219:GLN:HB3	1:B:222:ILE:HD12	1.86	0.57
1:A:320:VAL:HG11	1:A:408:LEU:CD1	2.35	0.57
1:A:222:ILE:HD11	2:C:490:TYR:CE1	2.40	0.56
2:C:464:LEU:HD23	2:C:465:TYR:N	2.22	0.55
1:A:222:ILE:HD11	2:C:490:TYR:CZ	2.41	0.55
2:D:421:TRP:HE1	2:D:464:LEU:HD22	1.72	0.55
1:B:222:ILE:HD11	2:D:490:TYR:CE1	2.42	0.54
1:A:103:ALA:HB2	1:B:103:ALA:CB	2.37	0.54
1:A:103:ALA:CB	1:B:103:ALA:HB2	2.37	0.54
1:B:320:VAL:HG11	1:B:408:LEU:CD1	2.37	0.53
1:A:390:VAL:HG22	1:A:395:MET:HB3	1.91	0.53
1:B:252:THR:HG21	1:B:266:ARG:O	2.09	0.53
2:C:409:ALA:HB2	2:C:414:PHE:CD2	2.45	0.52
2:C:436:ILE:HG23	2:C:436:ILE:O	2.09	0.52
1:A:252:THR:HG21	1:A:266:ARG:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD21	1:B:128:LEU:HD22	1.93	0.51
2:D:436:ILE:HG23	2:D:436:ILE:O	2.10	0.51
1:A:124:LEU:HD21	1:A:128:LEU:HD22	1.93	0.51
1:A:28:LEU:O	1:A:32:VAL:HG13	2.11	0.50
2:C:421:TRP:HE1	2:C:464:LEU:HD22	1.76	0.50
1:B:390:VAL:HG22	1:B:395:MET:HB3	1.93	0.49
1:A:44:VAL:O	1:A:44:VAL:HG23	2.12	0.49
1:B:32:VAL:O	1:B:36:THR:HG23	2.12	0.49
2:C:464:LEU:HD23	2:C:464:LEU:C	2.37	0.49
1:B:320:VAL:HG11	1:B:408:LEU:HD11	1.93	0.49
1:A:320:VAL:HG11	1:A:408:LEU:HD12	1.94	0.49
2:D:472:LYS:N	2:D:472:LYS:HD2	2.28	0.49
2:D:5:VAL:HG23	2:D:408:THR:HG22	1.94	0.48
1:A:442:ARG:O	1:A:443:VAL:C	2.56	0.48
2:C:4:LEU:HD11	2:C:481:CYS:HB3	1.95	0.48
1:A:428:LEU:HD23	1:A:445:LEU:HD23	1.95	0.48
1:A:33:LEU:HD21	1:A:40:PHE:HB2	1.95	0.48
2:C:407:CYS:O	2:C:463:THR:HG23	2.14	0.48
2:C:472:LYS:N	2:C:472:LYS:HD2	2.28	0.47
1:A:371:LYS:O	1:A:372:ILE:HB	2.14	0.47
1:B:371:LYS:O	1:B:372:ILE:HB	2.14	0.47
1:B:384:LEU:H	1:B:384:LEU:HD22	1.79	0.47
1:A:384:LEU:H	1:A:384:LEU:HD22	1.80	0.47
1:B:44:VAL:HG23	1:B:44:VAL:O	2.14	0.47
1:B:442:ARG:O	1:B:444:TYR:N	2.48	0.47
2:C:445:TYR:CE1	2:C:449:VAL:HG11	2.49	0.47
1:B:428:LEU:HD23	1:B:445:LEU:HD23	1.95	0.47
1:A:12:ILE:O	1:A:13:THR:C	2.58	0.47
2:C:437:MET:HE1	2:C:490:TYR:CE1	2.49	0.47
1:B:26:LEU:HD12	1:B:56:HIS:CG	2.49	0.46
1:B:124:LEU:HD23	1:B:124:LEU:O	2.16	0.46
1:B:33:LEU:C	1:B:33:LEU:HD23	2.39	0.46
1:B:442:ARG:O	1:B:443:VAL:C	2.58	0.46
1:A:124:LEU:HD23	1:A:124:LEU:O	2.16	0.46
2:C:409:ALA:HB3	2:C:462:ASN:HB3	1.98	0.46
2:D:409:ALA:HB2	2:D:414:PHE:CD2	2.50	0.46
2:D:445:TYR:OH	2:D:455:ILE:HG22	2.16	0.46
1:A:178:VAL:CG1	1:A:222:ILE:HD13	2.45	0.46
1:B:8:VAL:HG22	1:B:12:ILE:CD1	2.46	0.46
2:D:464:LEU:HD23	2:D:464:LEU:C	2.40	0.46
1:A:20:ILE:O	1:A:21:SER:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:THR:HB	1:B:381:LEU:HD23	1.98	0.45
1:A:384:LEU:HB2	1:A:385:PRO:HD3	1.98	0.45
2:D:4:LEU:C	2:D:4:LEU:HD13	2.42	0.45
1:A:82:PHE:CE1	1:B:253:ASP:OD1	2.71	0.44
2:D:468:MET:HA	2:D:468:MET:HE2	1.98	0.44
1:A:5:ALA:O	1:A:6:ARG:C	2.59	0.44
1:A:320:VAL:HG11	1:A:408:LEU:HD11	1.98	0.44
1:A:428:LEU:HD21	1:A:445:LEU:HG	2.00	0.44
1:B:428:LEU:HD21	1:B:445:LEU:HG	1.99	0.44
1:A:8:VAL:HG22	1:A:12:ILE:CD1	2.47	0.44
1:A:271:LEU:HD12	1:A:271:LEU:O	2.18	0.44
1:B:447:ALA:O	1:B:450:VAL:HG12	2.18	0.44
1:A:14:LEU:O	1:A:17:VAL:HG12	2.18	0.44
1:B:20:ILE:O	1:B:21:SER:C	2.60	0.44
2:C:476:THR:O	2:C:476:THR:HG22	2.18	0.44
1:B:178:VAL:CG1	1:B:222:ILE:HD13	2.47	0.44
1:B:271:LEU:HD12	1:B:271:LEU:O	2.18	0.44
1:B:26:LEU:HD23	1:B:26:LEU:O	2.17	0.43
1:A:222:ILE:O	1:A:223:ARG:C	2.62	0.43
1:A:442:ARG:O	1:A:444:TYR:N	2.51	0.43
1:B:310:GLY:HA2	1:B:336:VAL:HG13	2.00	0.43
1:A:253:ASP:OD1	1:B:82:PHE:CE1	2.71	0.43
1:A:310:GLY:HA2	1:A:336:VAL:HG13	2.00	0.42
1:A:5:ALA:O	1:A:8:VAL:HG12	2.19	0.42
1:A:21:SER:OG	1:A:125:VAL:HG22	2.18	0.42
1:B:222:ILE:O	1:B:223:ARG:C	2.62	0.42
1:A:25:SER:O	1:A:26:LEU:C	2.62	0.42
1:B:197:VAL:HG11	2:D:489:SER:HB3	2.00	0.42
1:A:11:SER:O	1:A:12:ILE:C	2.60	0.42
1:A:379:THR:HB	1:A:381:LEU:HD23	2.01	0.42
1:A:14:LEU:O	1:A:15:ALA:C	2.63	0.42
1:A:222:ILE:HG22	1:A:226:TRP:HD1	1.84	0.42
1:A:6:ARG:O	1:A:7:ASN:C	2.63	0.42
1:A:389:ASN:OD1	1:A:389:ASN:C	2.62	0.42
1:A:32:VAL:O	1:A:35:LEU:HD12	2.20	0.41
1:A:50:GLU:OE1	1:A:50:GLU:C	2.62	0.41
1:B:222:ILE:HG22	1:B:226:TRP:HD1	1.85	0.41
1:B:389:ASN:OD1	1:B:389:ASN:C	2.64	0.41
2:D:446:ALA:HB3	2:D:449:VAL:HG23	2.03	0.41
1:A:10:CYS:O	1:A:11:SER:C	2.64	0.41
1:B:26:LEU:HD12	1:B:56:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:O	1:A:20:ILE:C	2.64	0.41
1:A:13:THR:O	1:A:14:LEU:C	2.64	0.41
1:B:26:LEU:HD23	1:B:26:LEU:C	2.46	0.41
1:B:252:THR:O	1:B:253:ASP:C	2.63	0.41
1:A:302:ILE:O	1:A:306:VAL:HG12	2.21	0.41
1:A:443:VAL:HG23	1:A:444:TYR:H	1.86	0.41
1:B:381:LEU:HD13	1:B:384:LEU:HD21	2.02	0.41
1:B:443:VAL:HG23	1:B:444:TYR:H	1.86	0.41
1:A:375:PHE:HD1	1:A:476:TYR:HH	1.69	0.40
1:B:395:MET:HE3	1:B:423:PRO:HB2	2.04	0.40
1:A:124:LEU:HD23	1:A:124:LEU:C	2.47	0.40
2:C:4:LEU:C	2:C:4:LEU:HD13	2.46	0.40
1:A:289:LEU:O	1:A:292:ILE:HG22	2.21	0.40
1:B:50:GLU:C	1:B:50:GLU:OE2	2.64	0.40
2:C:2:VAL:O	2:C:2:VAL:HG23	2.21	0.40
2:C:421:TRP:CD1	2:C:466:LEU:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	428/496 (86%)	399 (93%)	28 (6%)	1 (0%)	43	76
1	B	428/496 (86%)	406 (95%)	21 (5%)	1 (0%)	43	76
2	C	113/524 (22%)	100 (88%)	13 (12%)	0	100	100
2	D	113/524 (22%)	99 (88%)	14 (12%)	0	100	100
All	All	1082/2040 (53%)	1004 (93%)	76 (7%)	2 (0%)	44	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	VAL
1	B	443	VAL

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	385/439 (88%)	378 (98%)	7 (2%)	51	77
1	B	385/439 (88%)	381 (99%)	4 (1%)	68	84
2	C	99/436 (23%)	96 (97%)	3 (3%)	36	69
2	D	98/436 (22%)	94 (96%)	4 (4%)	27	61
All	All	967/1750 (55%)	949 (98%)	18 (2%)	49	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	33	LEU
1	A	279	LEU
1	A	298	VAL
1	A	420	LEU
1	A	443	VAL
1	A	466	ILE
1	B	12	ILE
1	B	289	LEU
1	B	443	VAL
1	B	466	ILE
2	C	452	ARG
2	C	475	ASP
2	C	497	ARG
2	D	5	VAL
2	D	407	CYS
2	D	452	ARG
2	D	475	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	167	ASN
1	A	412	ASN
1	B	73	HIS
1	B	167	ASN
1	B	412	ASN
1	B	452	ASN
2	D	509	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 [i](#)

2 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	GDU	B	501	-	24,26,38	3.75	13 (54%)	37,40,58	1.54	5 (13%)
3	GDU	A	501	-	24,26,38	3.75	13 (54%)	37,40,58	1.53	5 (13%)

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	GDU	B	501	-	-	6/16/32/59	0/2/2/3
3	GDU	A	501	-	-	6/16/32/59	0/2/2/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	GDU	C2-N1	7.25	1.50	1.38
3	A	501	GDU	C2-N1	7.25	1.50	1.38
3	A	501	GDU	O4D-C4D	7.04	1.60	1.45
3	B	501	GDU	O4D-C4D	7.04	1.60	1.45
3	A	501	GDU	C2-N3	6.98	1.50	1.38
3	B	501	GDU	C2-N3	6.97	1.50	1.38
3	B	501	GDU	C3D-C4D	-6.91	1.35	1.53
3	A	501	GDU	C3D-C4D	-6.90	1.35	1.53
3	A	501	GDU	C6-C5	5.64	1.48	1.35
3	B	501	GDU	C6-C5	5.64	1.48	1.35
3	A	501	GDU	O4D-C1D	-4.69	1.30	1.42
3	B	501	GDU	O4D-C1D	-4.68	1.30	1.42
3	A	501	GDU	PB-O3B	4.20	1.71	1.54
3	B	501	GDU	PB-O3B	4.19	1.71	1.54
3	B	501	GDU	C4-N3	4.05	1.45	1.38
3	A	501	GDU	C4-N3	4.04	1.45	1.38
3	B	501	GDU	O4-C4	-3.02	1.18	1.24
3	A	501	GDU	O4-C4	-3.02	1.18	1.24
3	B	501	GDU	C6-N1	2.91	1.45	1.38
3	A	501	GDU	C6-N1	2.91	1.45	1.38
3	A	501	GDU	O2D-C2D	-2.75	1.36	1.43
3	B	501	GDU	O2D-C2D	-2.75	1.36	1.43
3	B	501	GDU	C5-C4	2.69	1.49	1.43
3	A	501	GDU	C5-C4	2.69	1.49	1.43
3	B	501	GDU	O3D-C3D	2.52	1.48	1.43
3	A	501	GDU	O3D-C3D	2.51	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	GDU	C4-N3-C2	-5.16	119.77	126.58
3	A	501	GDU	C4-N3-C2	-5.16	119.78	126.58
3	B	501	GDU	N3-C2-N1	3.69	119.79	114.89
3	A	501	GDU	N3-C2-N1	3.69	119.78	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	GDU	C5-C4-N3	3.29	119.76	114.84
3	A	501	GDU	C5-C4-N3	3.29	119.76	114.84
3	A	501	GDU	O4-C4-C5	-2.87	120.11	125.16
3	B	501	GDU	O4-C4-C5	-2.87	120.12	125.16
3	B	501	GDU	PA-O3A-PB	-2.76	123.34	132.83
3	A	501	GDU	PA-O3A-PB	-2.76	123.36	132.83

There are no chirality outliers.

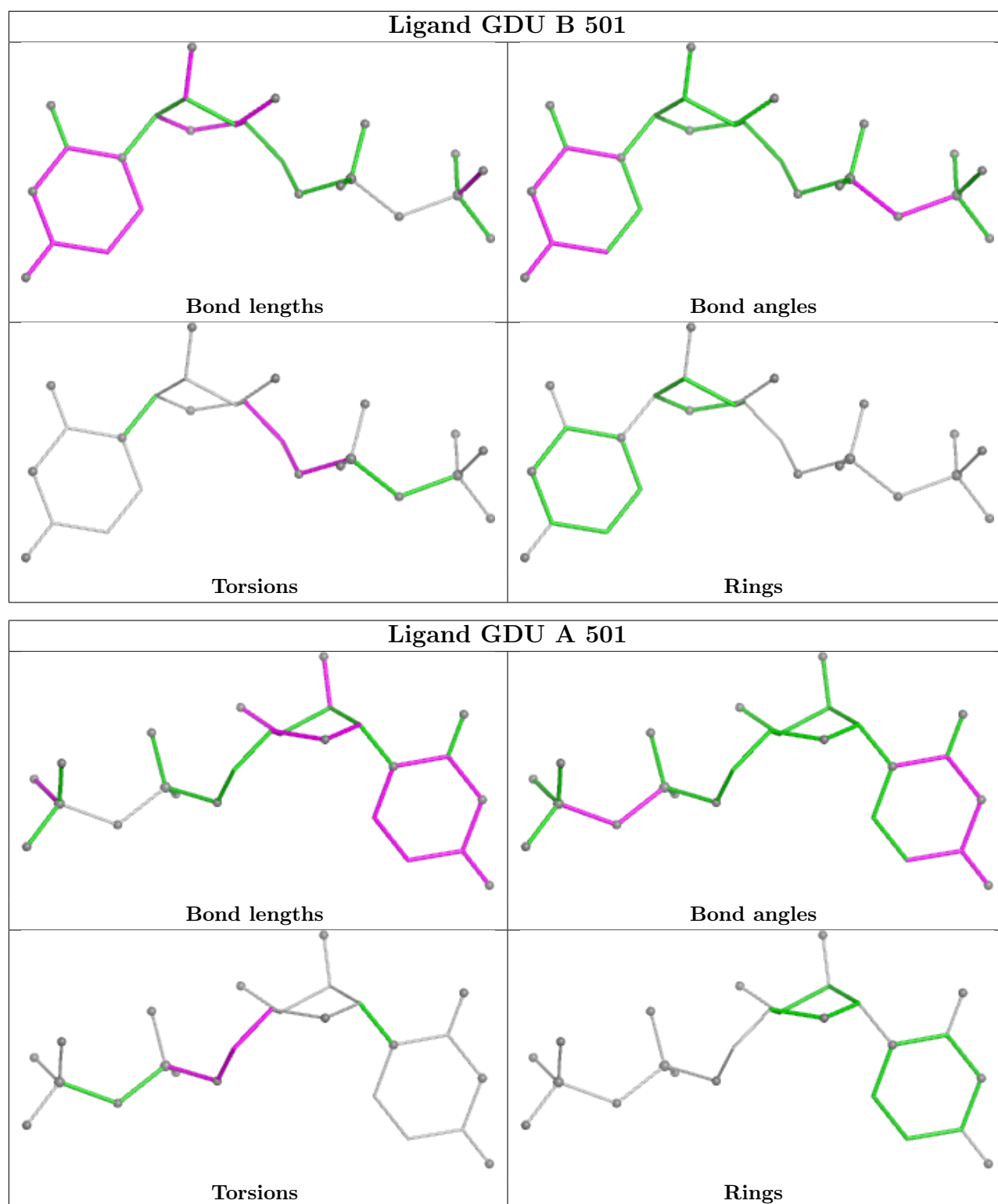
All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GDU	C5D-O5D-PA-O1A
3	B	501	GDU	C5D-O5D-PA-O1A
3	A	501	GDU	C3D-C4D-C5D-O5D
3	B	501	GDU	C3D-C4D-C5D-O5D
3	A	501	GDU	O4D-C4D-C5D-O5D
3	B	501	GDU	O4D-C4D-C5D-O5D
3	A	501	GDU	C4D-C5D-O5D-PA
3	B	501	GDU	C4D-C5D-O5D-PA
3	A	501	GDU	C5D-O5D-PA-O3A
3	B	501	GDU	C5D-O5D-PA-O3A
3	A	501	GDU	C5D-O5D-PA-O2A
3	B	501	GDU	C5D-O5D-PA-O2A

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

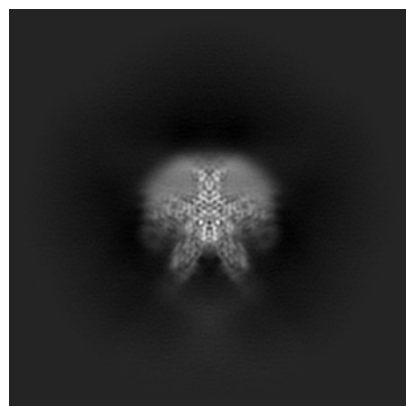
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-58108. These allow visual inspection of the internal detail of the map and identification of artifacts.

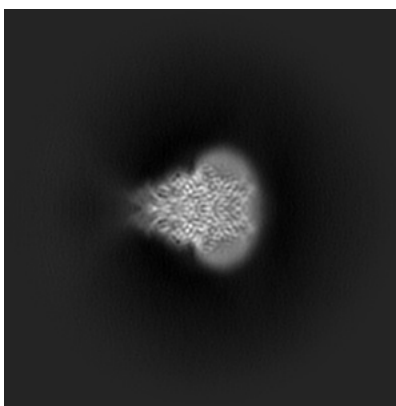
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

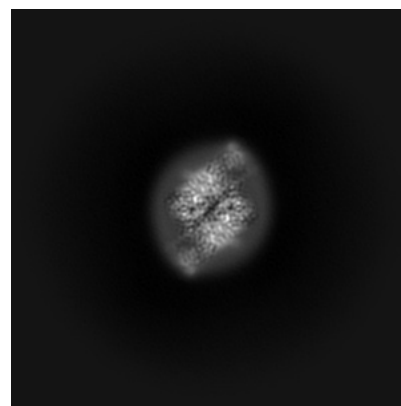
6.1.1 Primary map



X

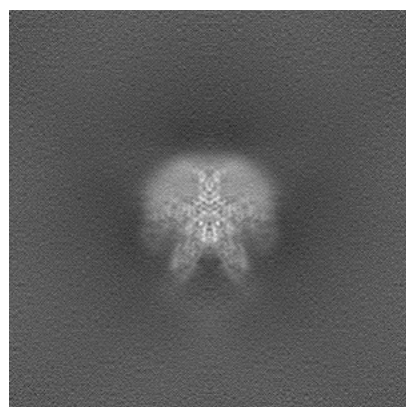


Y

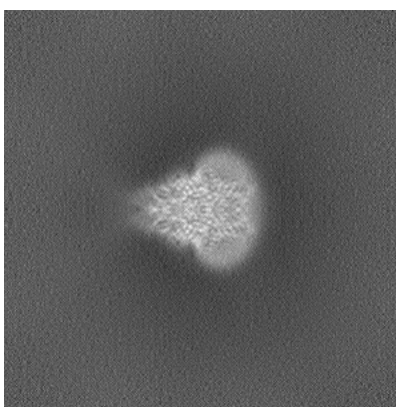


Z

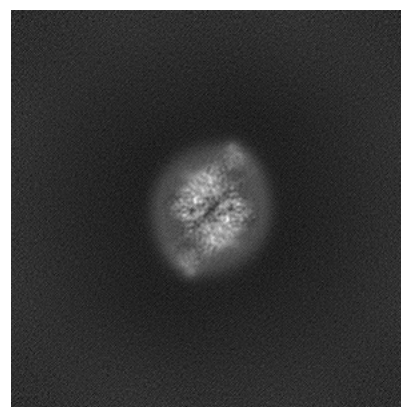
6.1.2 Raw map



X



Y

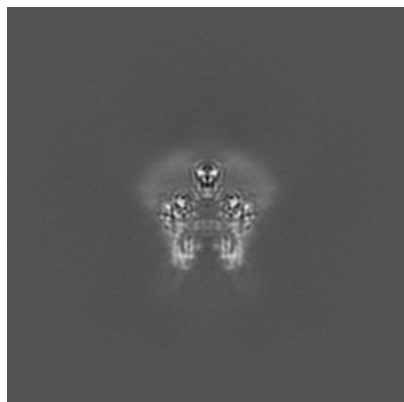


Z

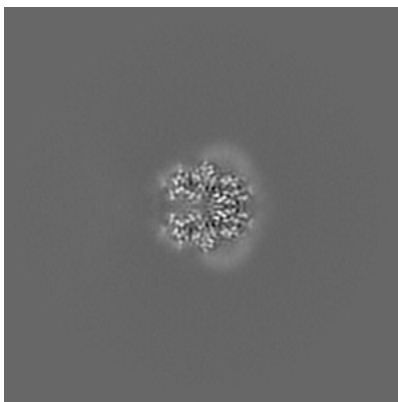
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

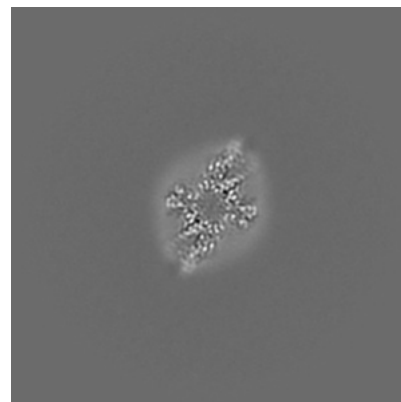
6.2.1 Primary map



X Index: 256

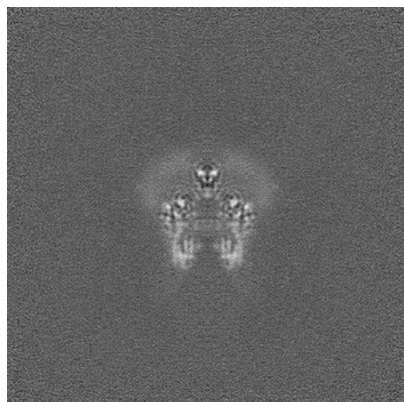


Y Index: 256

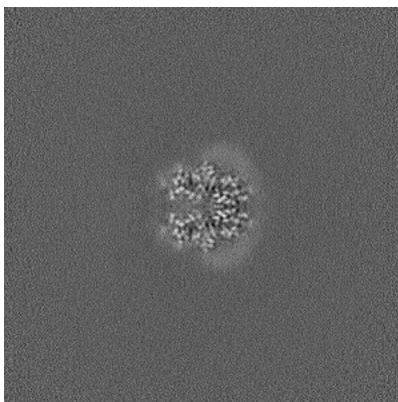


Z Index: 256

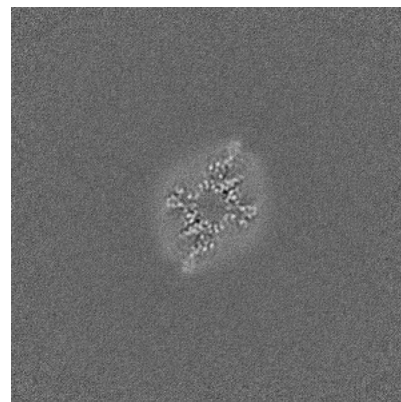
6.2.2 Raw map



X Index: 256



Y Index: 256

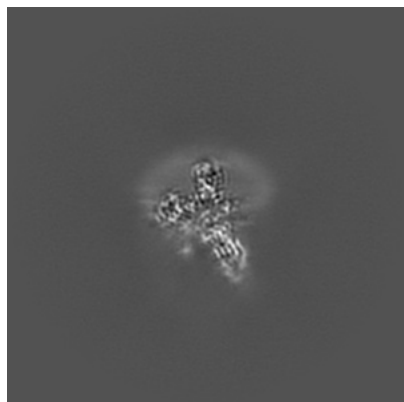


Z Index: 256

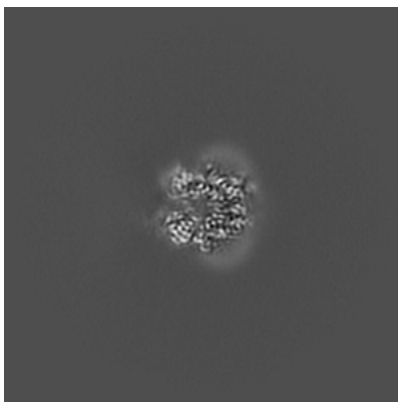
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

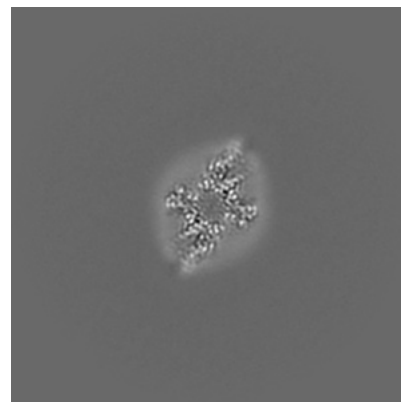
6.3.1 Primary map



X Index: 244

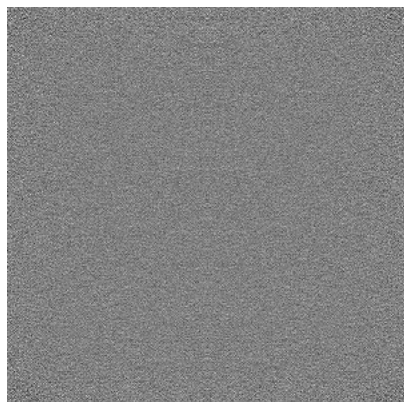


Y Index: 263

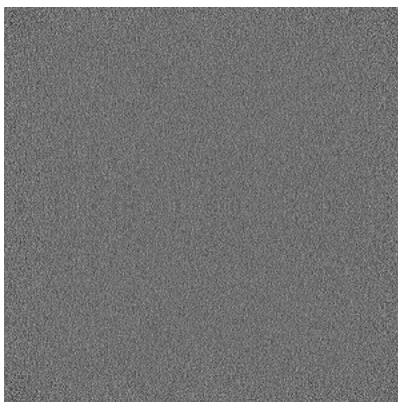


Z Index: 257

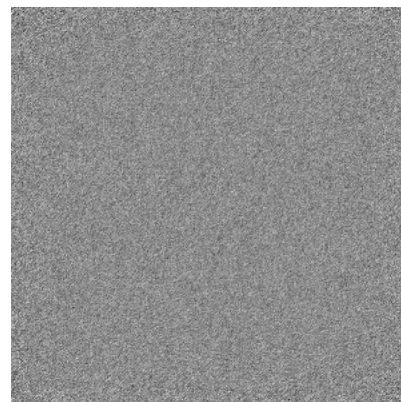
6.3.2 Raw map



X Index: 0



Y Index: 0

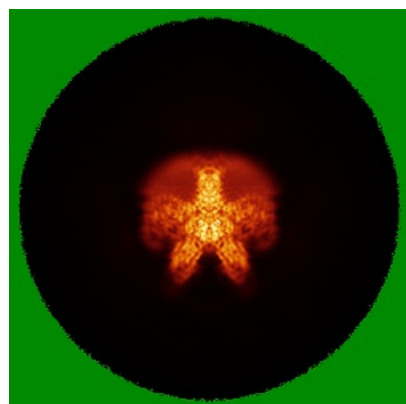


Z Index: 511

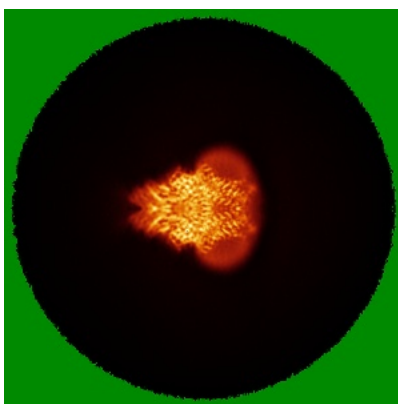
The images above show the largest variance slices of the map in three orthogonal directions.

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

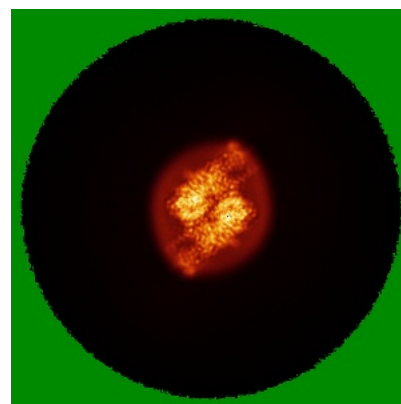
6.4.1 Primary map



X

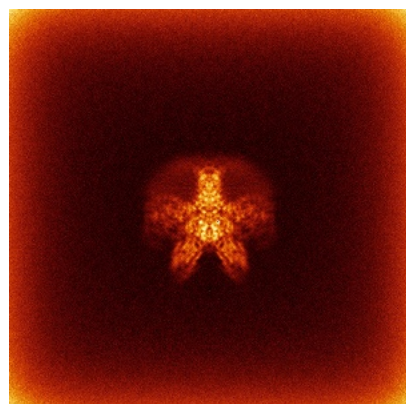


Y

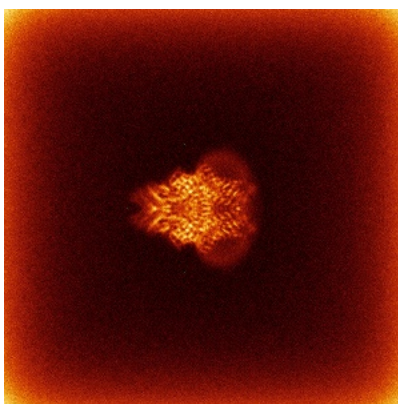


Z

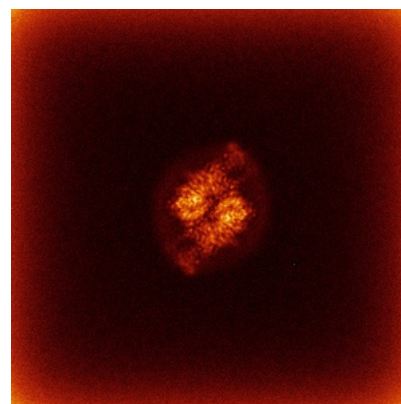
6.4.2 Raw map



X



Y

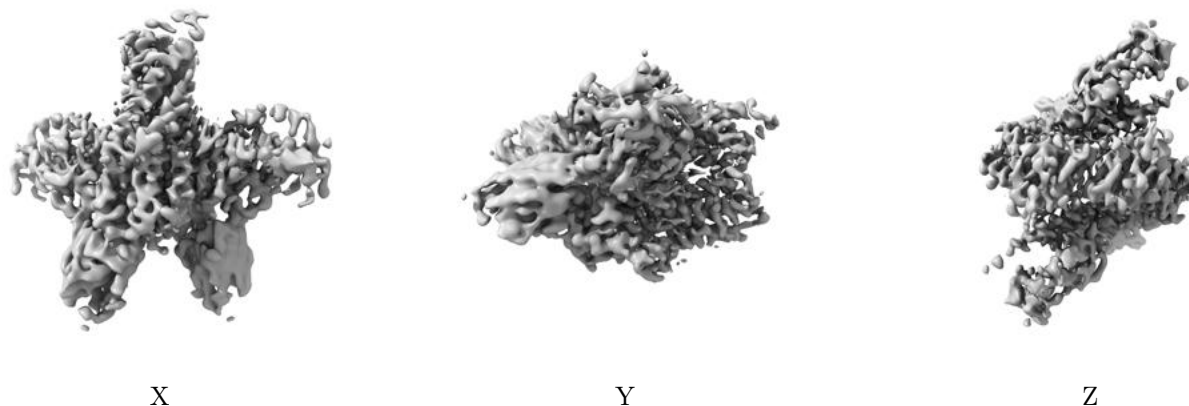


Z

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.

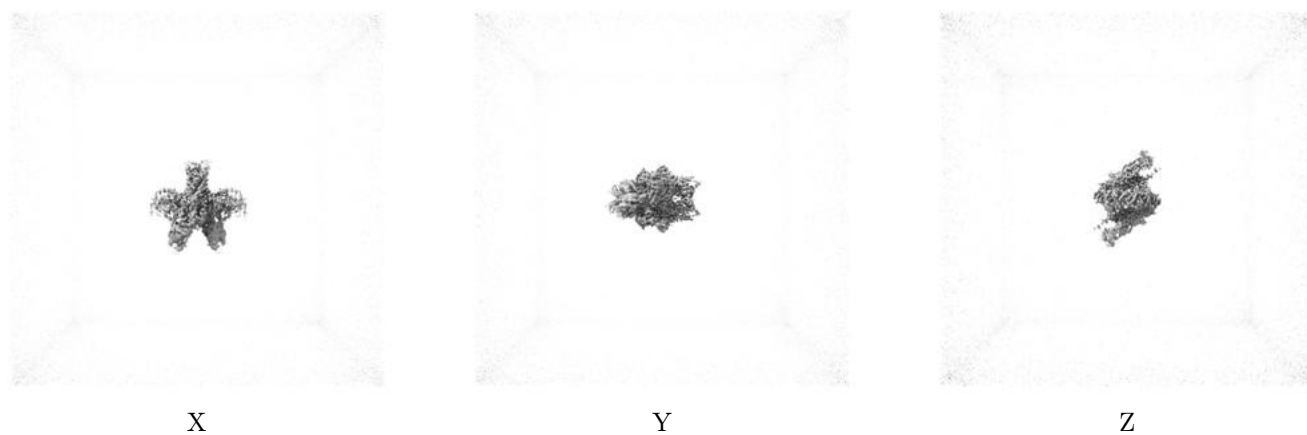
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.029. 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.

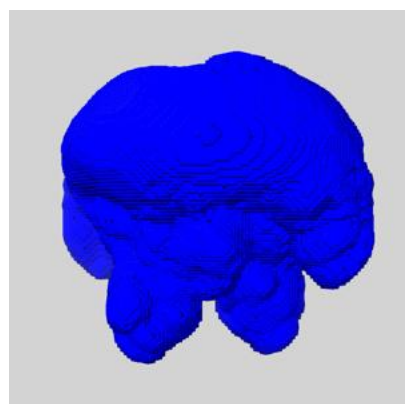
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

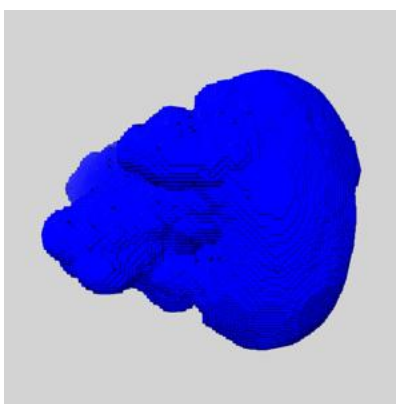
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

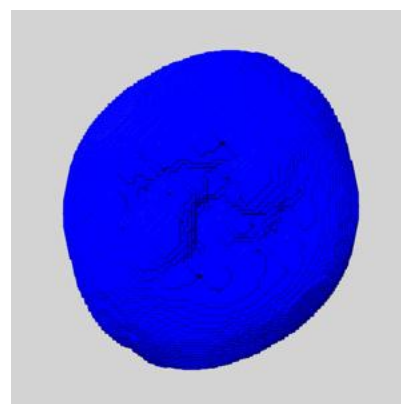
6.6.1 emd_58108_msk_1.map [i](#)



X



Y

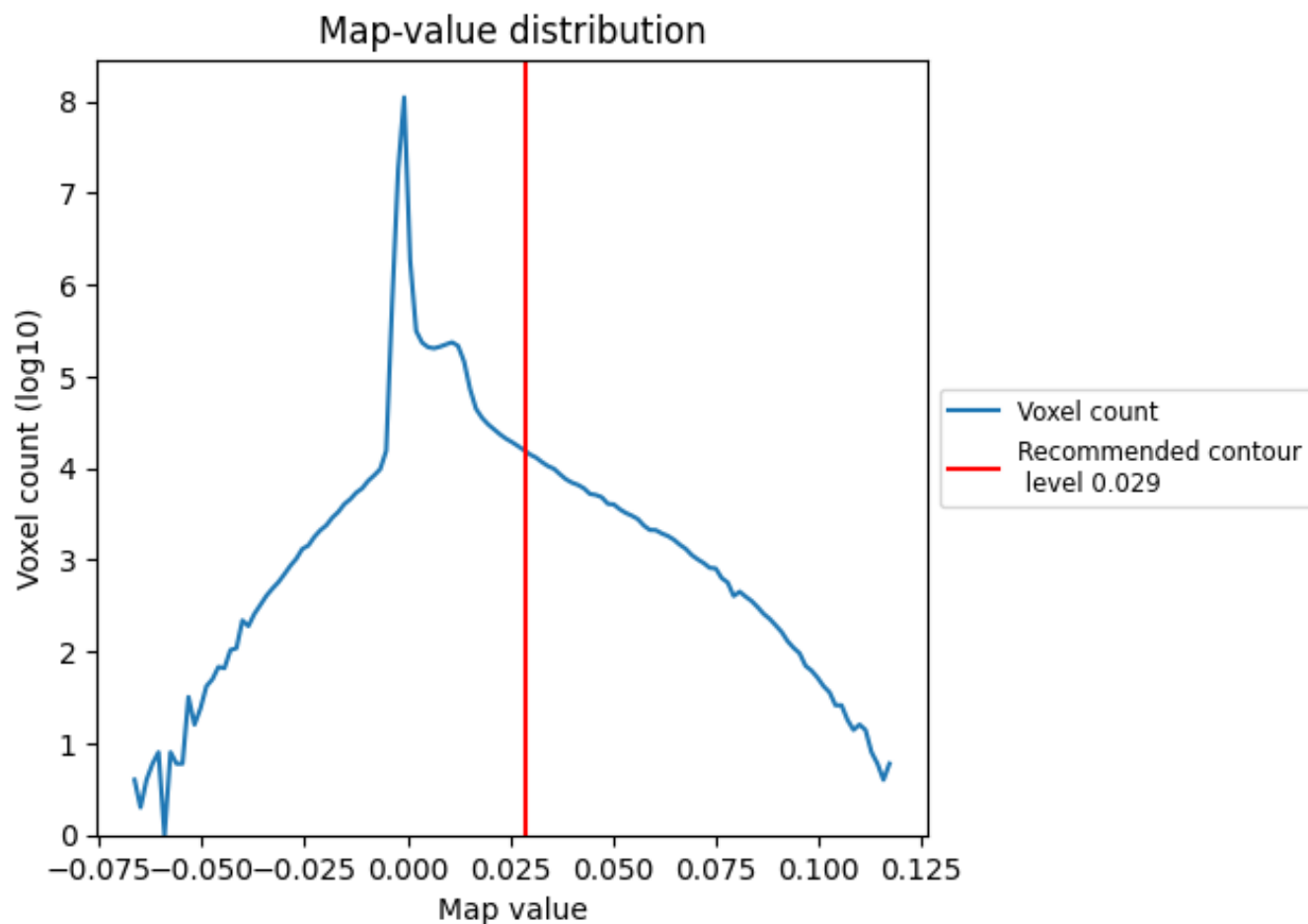


Z

7 Map analysis [i](#)

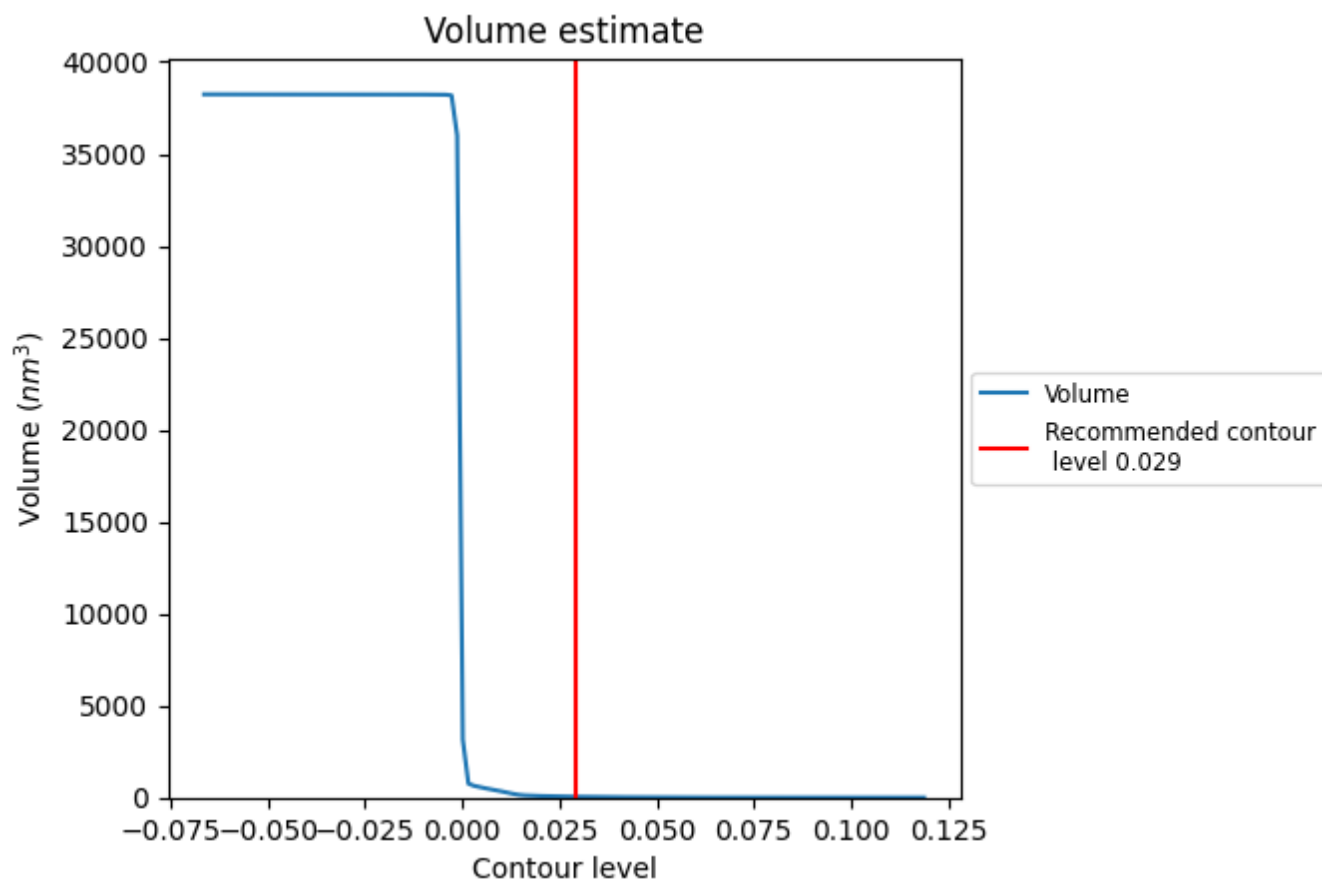
This section contains the results of statistical analysis of the map.

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.

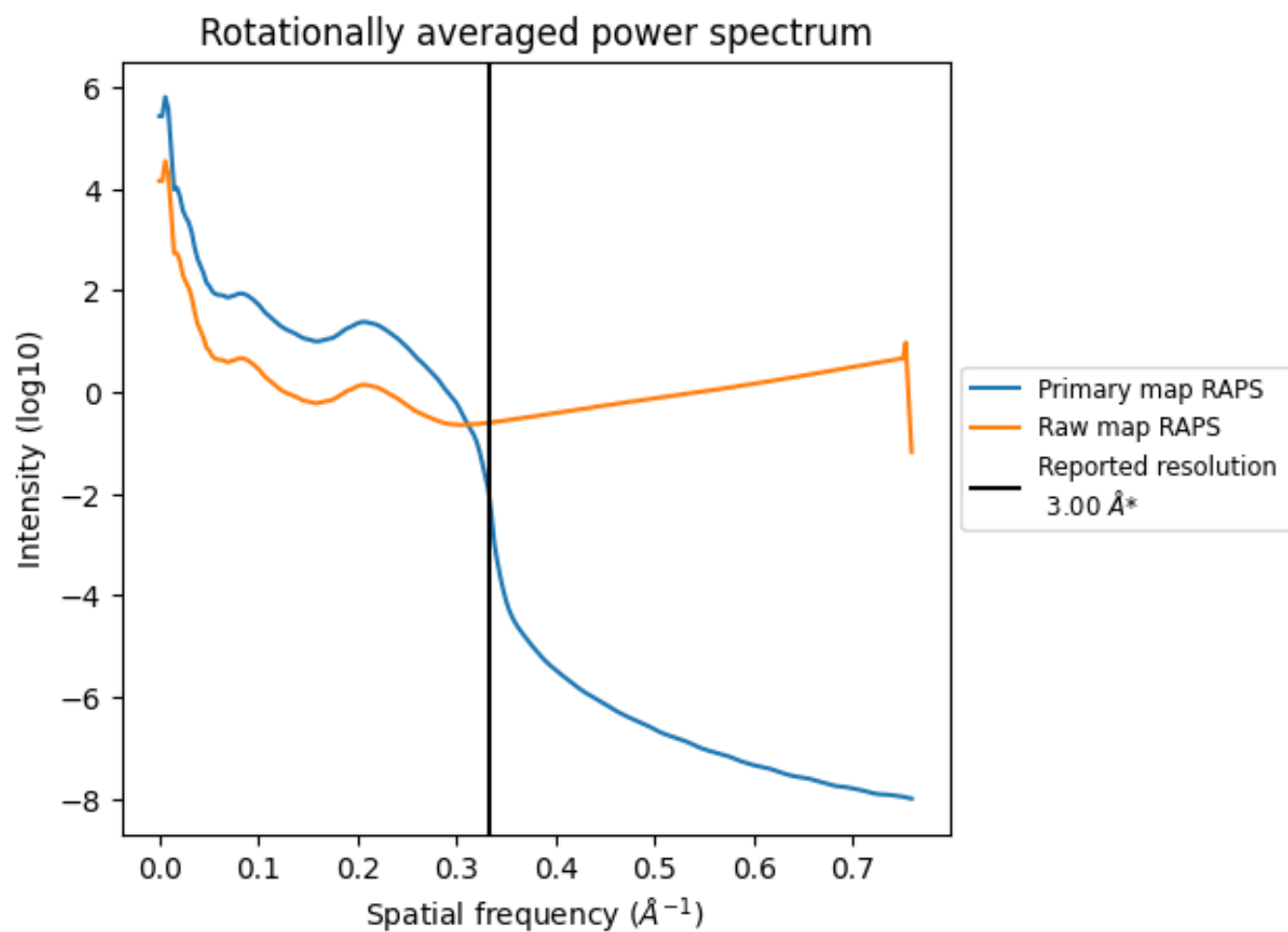
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm^3 ; this corresponds to an approximate mass of 42 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 ⓘ

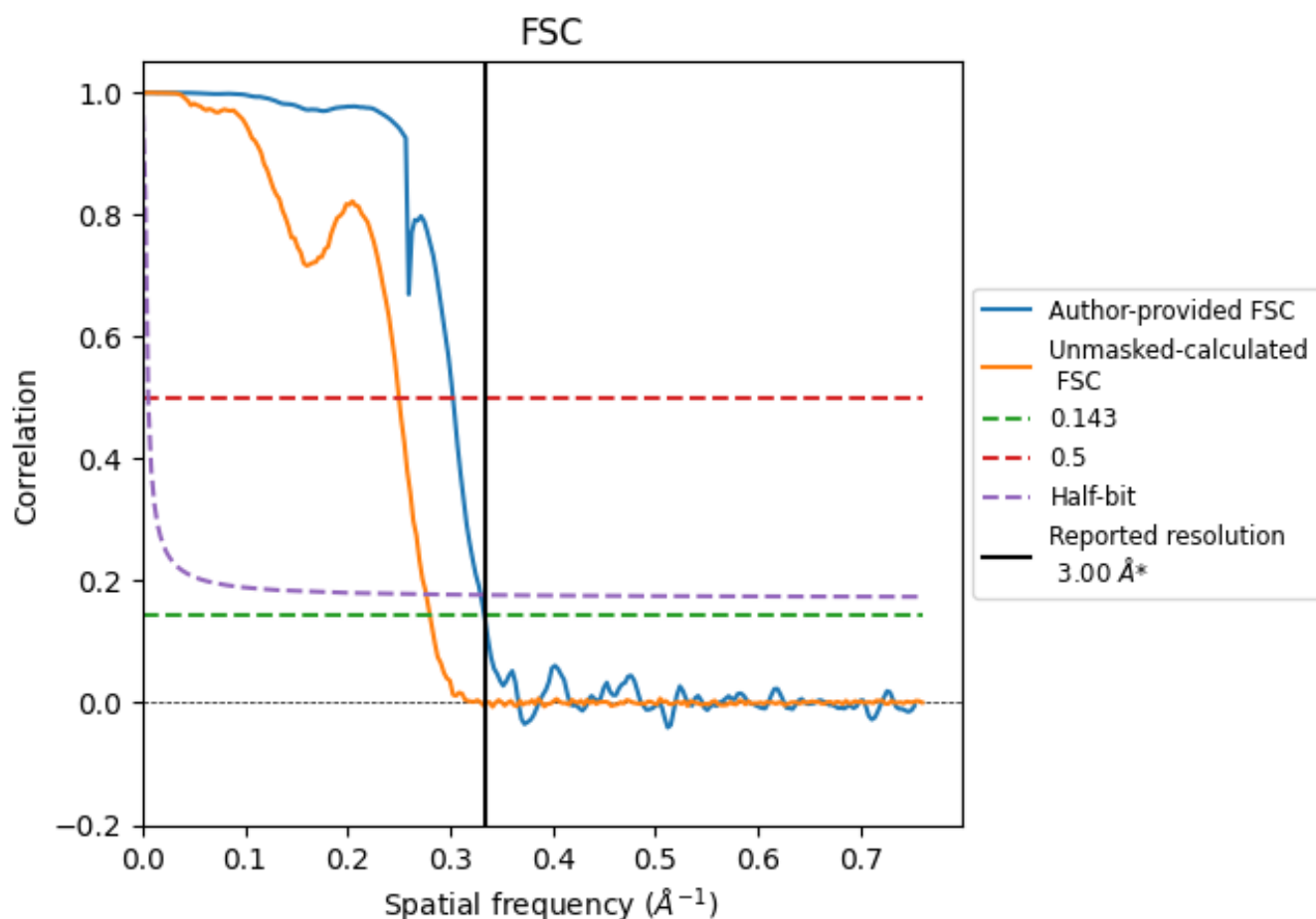


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

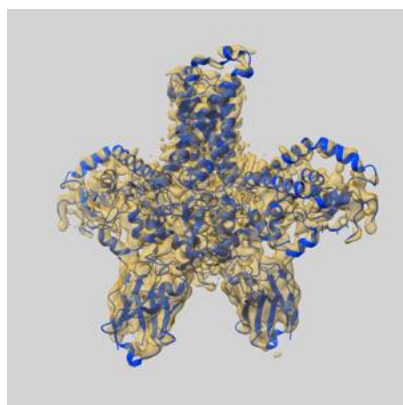
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.00	3.30	3.03
Unmasked-calculated*	3.57	4.00	3.61

*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 3.57 differs from the reported value 3.0 by more than 10 %

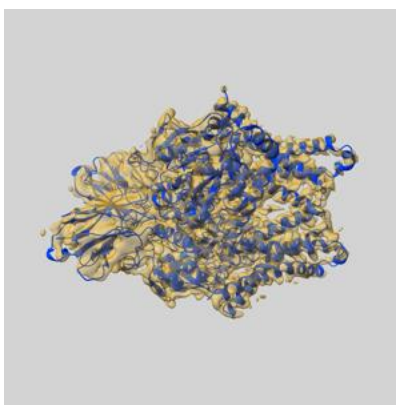
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-58108 and PDB model 30WC. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

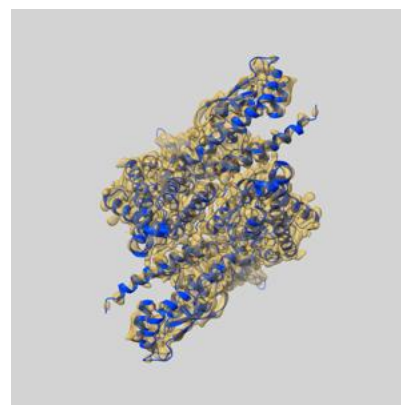
9.1 Map-model overlay [i](#)



X



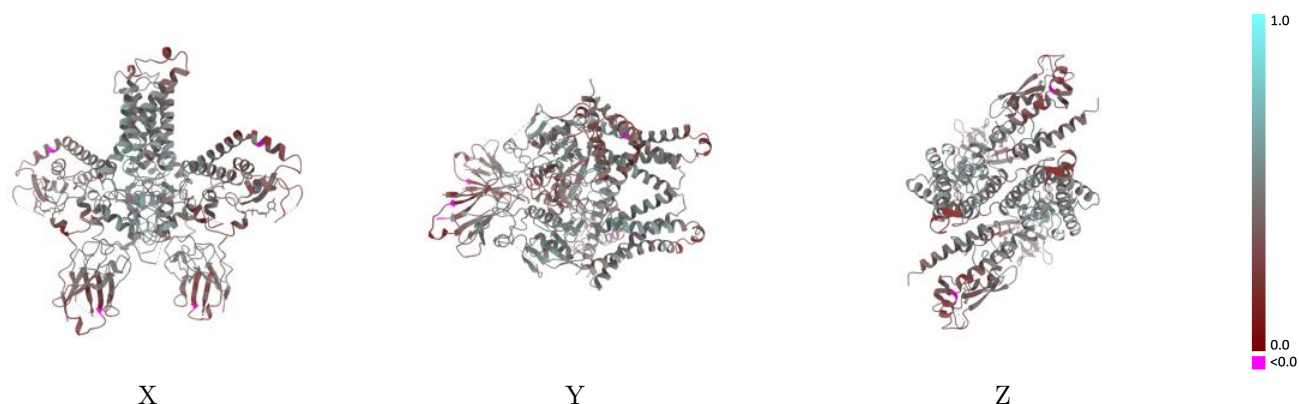
Y



Z

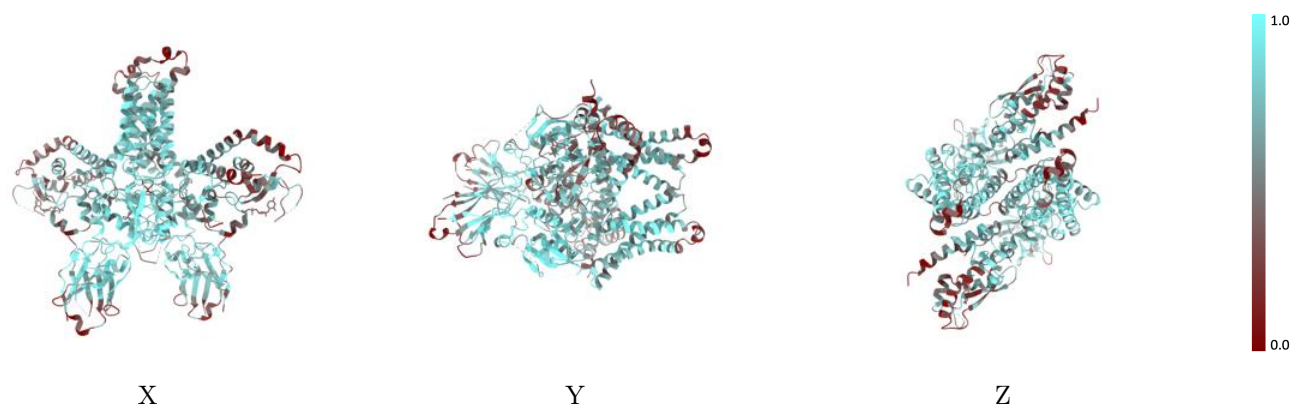
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



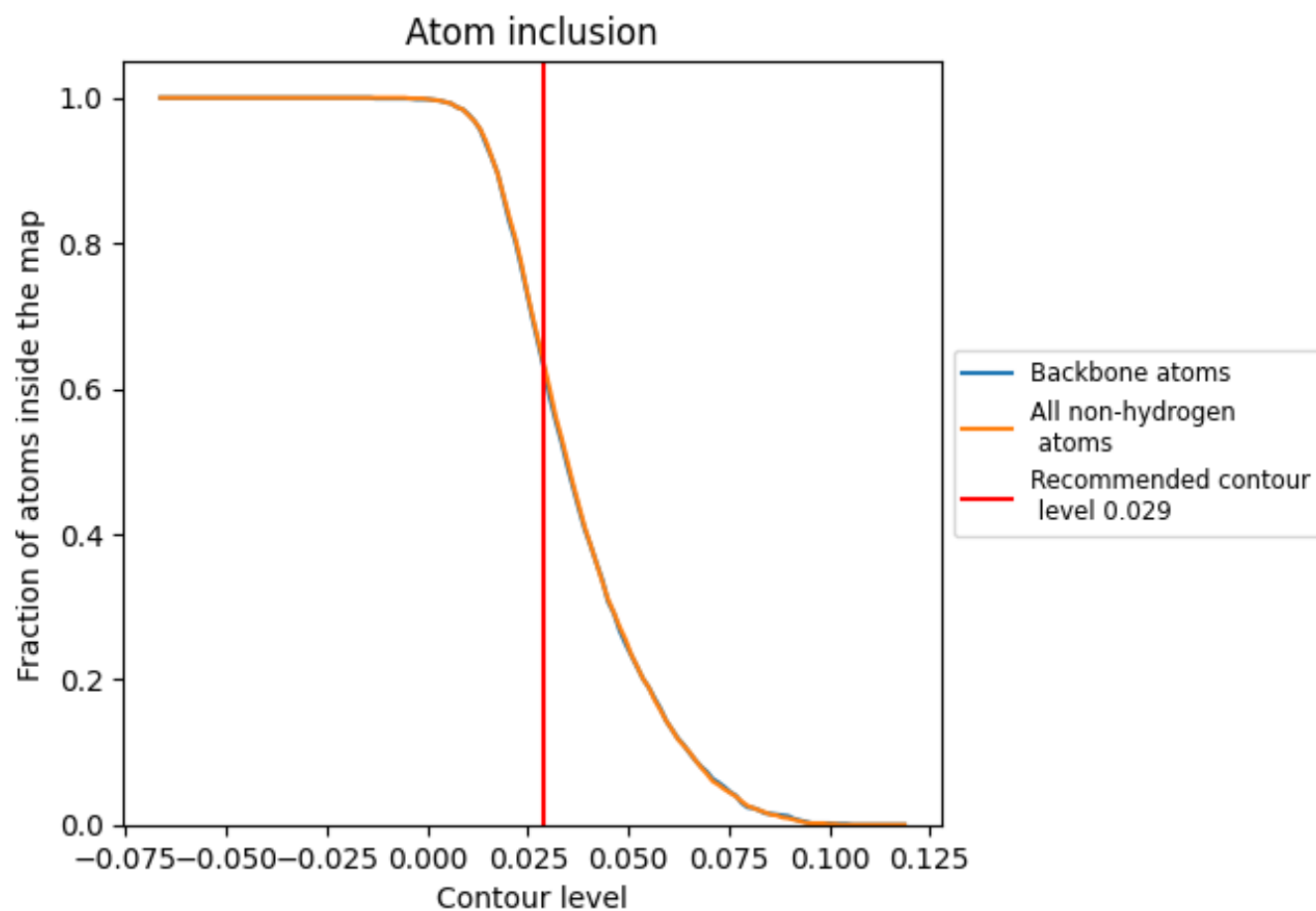
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 64% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6350	<div></div> 0.4300
A	<div></div> 0.6460	<div></div> 0.4430
B	<div></div> 0.6460	<div></div> 0.4430
C	<div></div> 0.6670	<div></div> 0.3820
D	<div></div> 0.6730	<div></div> 0.3810

