Full wwPDB EM Validation Report ⓘ

Apr 6, 2025 – 01:26 AM JST

PDB ID	:	9IP2 / pdb_00009ip2
EMDB ID	:	EMD-60755
Title	:	Cryo-EM structure of the RNA-dependent RNA polymerase complex from Marburg virus
Authors	:	Li, G.; Du, T.; Wang, J.; Wu, S.; Ru, H.
Deposited on	:	2024-07-10
Resolution	:	2.70 Å(reported)

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:

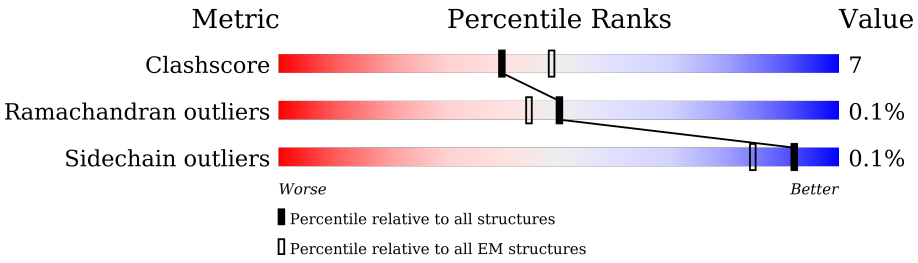
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	2757	42% 7% 51%
2	B	727	28% 70%
2	C	727	8% 91%
2	D	727	96%
2	E	727	96%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13606 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 RNA-directed RNA polymerase L,Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1363	11040	7105	1872	2011	52	0	0

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	489	ALA	LEU	conflict	UNP P31352
A	979	GLY	ARG	conflict	UNP P31352
A	1428	THR	SER	conflict	UNP P31352
A	2332	SER	-	linker	UNP P31352
A	2333	ARG	-	linker	UNP P31352
A	2334	GLU	-	linker	UNP P31352
A	2335	ASN	-	linker	UNP P31352
A	2336	LEU	-	linker	UNP P31352
A	2337	TYR	-	linker	UNP P31352
A	2338	PHE	-	linker	UNP P31352
A	2339	GLN	-	linker	UNP P31352
A	2340	GLY	-	linker	UNP P31352
A	2341	SER	-	linker	UNP P31352
A	2342	GLY	-	linker	UNP P31352
A	2343	TRP	-	linker	UNP P31352
A	2344	SER	-	linker	UNP P31352
A	2345	HIS	-	linker	UNP P31352
A	2346	PRO	-	linker	UNP P31352
A	2347	GLN	-	linker	UNP P31352
A	2348	PHE	-	linker	UNP P31352
A	2349	GLU	-	linker	UNP P31352
A	2350	LYS	-	linker	UNP P31352
A	2351	GLY	-	linker	UNP P31352
A	2352	GLY	-	linker	UNP P31352
A	2353	GLY	-	linker	UNP P31352
A	2354	SER	-	linker	UNP P31352
A	2355	GLY	-	linker	UNP P31352

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2356	GLY	-	linker	UNP P31352
A	2357	GLY	-	linker	UNP P31352
A	2358	SER	-	linker	UNP P31352
A	2359	GLY	-	linker	UNP P31352
A	2360	GLY	-	linker	UNP P31352
A	2361	SER	-	linker	UNP P31352
A	2362	ALA	-	linker	UNP P31352
A	2363	TRP	-	linker	UNP P31352
A	2364	SER	-	linker	UNP P31352
A	2365	HIS	-	linker	UNP P31352
A	2366	PRO	-	linker	UNP P31352
A	2367	GLN	-	linker	UNP P31352
A	2368	PHE	-	linker	UNP P31352
A	2369	GLU	-	linker	UNP P31352
A	2370	LYS	-	linker	UNP P31352
A	2371	GLY	-	linker	UNP P31352
A	2372	SER	-	linker	UNP P31352
A	2373	ALA	-	linker	UNP P31352
A	2374	SER	-	linker	UNP P31352
A	2375	HIS	-	linker	UNP P31352
A	2376	HIS	-	linker	UNP P31352
A	2377	HIS	-	linker	UNP P31352
A	2378	HIS	-	linker	UNP P31352
A	2379	HIS	-	linker	UNP P31352
A	2380	HIS	-	linker	UNP P31352
A	2381	GLY	-	linker	UNP P31352
A	2382	THR	-	linker	UNP P31352
A	2383	LYS	-	linker	UNP P31352
A	2384	THR	-	linker	UNP P31352
A	2749	GLY	-	expression tag	UNP P0AEX9
A	2750	ASP	-	expression tag	UNP P0AEX9
A	2751	TYR	-	expression tag	UNP P0AEX9
A	2752	LYS	-	expression tag	UNP P0AEX9
A	2753	ASP	-	expression tag	UNP P0AEX9
A	2754	ASP	-	expression tag	UNP P0AEX9
A	2755	ASP	-	expression tag	UNP P0AEX9
A	2756	ASP	-	expression tag	UNP P0AEX9
A	2757	LYS	-	expression tag	UNP P0AEX9

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein,Polymerase cofactor VP35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	217	Total	C	N	O	S	0	0
			1649	1048	285	308	8		
2	C	63	Total	C	N	O	S	0	0
			471	301	80	87	3		
2	D	32	Total	C	N	O	S	0	0
			244	156	40	45	3		
2	E	26	Total	C	N	O	S	0	0
			201	128	34	36	3		

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-397	MET	-	initiating methionine	UNP P0AEX9
B	-396	GLY	-	expression tag	UNP P0AEX9
B	-395	SER	-	expression tag	UNP P0AEX9
B	-394	SER	-	expression tag	UNP P0AEX9
B	-393	HIS	-	expression tag	UNP P0AEX9
B	-392	HIS	-	expression tag	UNP P0AEX9
B	-391	HIS	-	expression tag	UNP P0AEX9
B	-390	HIS	-	expression tag	UNP P0AEX9
B	-389	HIS	-	expression tag	UNP P0AEX9
B	-388	HIS	-	expression tag	UNP P0AEX9
B	-387	GLY	-	expression tag	UNP P0AEX9
B	-386	THR	-	expression tag	UNP P0AEX9
B	-385	LYS	-	expression tag	UNP P0AEX9
B	-384	THR	-	expression tag	UNP P0AEX9
B	-19	GLY	-	linker	UNP P0AEX9
B	-18	THR	-	linker	UNP P0AEX9
B	-17	ASP	-	linker	UNP P0AEX9
B	-16	TYR	-	linker	UNP P0AEX9
B	-15	ASP	-	linker	UNP P0AEX9
B	-14	ILE	-	linker	UNP P0AEX9
B	-13	PRO	-	linker	UNP P0AEX9
B	-12	THR	-	linker	UNP P0AEX9
B	-11	THR	-	linker	UNP P0AEX9
B	-10	LEU	-	linker	UNP P0AEX9
B	-9	GLU	-	linker	UNP P0AEX9
B	-8	VAL	-	linker	UNP P0AEX9
B	-7	LEU	-	linker	UNP P0AEX9
B	-6	PHE	-	linker	UNP P0AEX9
B	-5	GLN	-	linker	UNP P0AEX9
B	-4	GLY	-	linker	UNP P0AEX9
B	-3	PRO	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	LEU	-	linker	UNP P0AEX9
B	-1	GLY	-	linker	UNP P0AEX9
B	0	SER	-	linker	UNP P0AEX9
B	296	CYS	SER	conflict	UNP P35259
C	-397	MET	-	initiating methionine	UNP P0AEX9
C	-396	GLY	-	expression tag	UNP P0AEX9
C	-395	SER	-	expression tag	UNP P0AEX9
C	-394	SER	-	expression tag	UNP P0AEX9
C	-393	HIS	-	expression tag	UNP P0AEX9
C	-392	HIS	-	expression tag	UNP P0AEX9
C	-391	HIS	-	expression tag	UNP P0AEX9
C	-390	HIS	-	expression tag	UNP P0AEX9
C	-389	HIS	-	expression tag	UNP P0AEX9
C	-388	HIS	-	expression tag	UNP P0AEX9
C	-387	GLY	-	expression tag	UNP P0AEX9
C	-386	THR	-	expression tag	UNP P0AEX9
C	-385	LYS	-	expression tag	UNP P0AEX9
C	-384	THR	-	expression tag	UNP P0AEX9
C	-19	GLY	-	linker	UNP P0AEX9
C	-18	THR	-	linker	UNP P0AEX9
C	-17	ASP	-	linker	UNP P0AEX9
C	-16	TYR	-	linker	UNP P0AEX9
C	-15	ASP	-	linker	UNP P0AEX9
C	-14	ILE	-	linker	UNP P0AEX9
C	-13	PRO	-	linker	UNP P0AEX9
C	-12	THR	-	linker	UNP P0AEX9
C	-11	THR	-	linker	UNP P0AEX9
C	-10	LEU	-	linker	UNP P0AEX9
C	-9	GLU	-	linker	UNP P0AEX9
C	-8	VAL	-	linker	UNP P0AEX9
C	-7	LEU	-	linker	UNP P0AEX9
C	-6	PHE	-	linker	UNP P0AEX9
C	-5	GLN	-	linker	UNP P0AEX9
C	-4	GLY	-	linker	UNP P0AEX9
C	-3	PRO	-	linker	UNP P0AEX9
C	-2	LEU	-	linker	UNP P0AEX9
C	-1	GLY	-	linker	UNP P0AEX9
C	0	SER	-	linker	UNP P0AEX9
C	296	CYS	SER	conflict	UNP P35259
D	-397	MET	-	initiating methionine	UNP P0AEX9
D	-396	GLY	-	expression tag	UNP P0AEX9
D	-395	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-394	SER	-	expression tag	UNP P0AEX9
D	-393	HIS	-	expression tag	UNP P0AEX9
D	-392	HIS	-	expression tag	UNP P0AEX9
D	-391	HIS	-	expression tag	UNP P0AEX9
D	-390	HIS	-	expression tag	UNP P0AEX9
D	-389	HIS	-	expression tag	UNP P0AEX9
D	-388	HIS	-	expression tag	UNP P0AEX9
D	-387	GLY	-	expression tag	UNP P0AEX9
D	-386	THR	-	expression tag	UNP P0AEX9
D	-385	LYS	-	expression tag	UNP P0AEX9
D	-384	THR	-	expression tag	UNP P0AEX9
D	-19	GLY	-	linker	UNP P0AEX9
D	-18	THR	-	linker	UNP P0AEX9
D	-17	ASP	-	linker	UNP P0AEX9
D	-16	TYR	-	linker	UNP P0AEX9
D	-15	ASP	-	linker	UNP P0AEX9
D	-14	ILE	-	linker	UNP P0AEX9
D	-13	PRO	-	linker	UNP P0AEX9
D	-12	THR	-	linker	UNP P0AEX9
D	-11	THR	-	linker	UNP P0AEX9
D	-10	LEU	-	linker	UNP P0AEX9
D	-9	GLU	-	linker	UNP P0AEX9
D	-8	VAL	-	linker	UNP P0AEX9
D	-7	LEU	-	linker	UNP P0AEX9
D	-6	PHE	-	linker	UNP P0AEX9
D	-5	GLN	-	linker	UNP P0AEX9
D	-4	GLY	-	linker	UNP P0AEX9
D	-3	PRO	-	linker	UNP P0AEX9
D	-2	LEU	-	linker	UNP P0AEX9
D	-1	GLY	-	linker	UNP P0AEX9
D	0	SER	-	linker	UNP P0AEX9
D	296	CYS	SER	conflict	UNP P35259
E	-397	MET	-	initiating methionine	UNP P0AEX9
E	-396	GLY	-	expression tag	UNP P0AEX9
E	-395	SER	-	expression tag	UNP P0AEX9
E	-394	SER	-	expression tag	UNP P0AEX9
E	-393	HIS	-	expression tag	UNP P0AEX9
E	-392	HIS	-	expression tag	UNP P0AEX9
E	-391	HIS	-	expression tag	UNP P0AEX9
E	-390	HIS	-	expression tag	UNP P0AEX9
E	-389	HIS	-	expression tag	UNP P0AEX9
E	-388	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-387	GLY	-	expression tag	UNP P0AEX9
E	-386	THR	-	expression tag	UNP P0AEX9
E	-385	LYS	-	expression tag	UNP P0AEX9
E	-384	THR	-	expression tag	UNP P0AEX9
E	-19	GLY	-	linker	UNP P0AEX9
E	-18	THR	-	linker	UNP P0AEX9
E	-17	ASP	-	linker	UNP P0AEX9
E	-16	TYR	-	linker	UNP P0AEX9
E	-15	ASP	-	linker	UNP P0AEX9
E	-14	ILE	-	linker	UNP P0AEX9
E	-13	PRO	-	linker	UNP P0AEX9
E	-12	THR	-	linker	UNP P0AEX9
E	-11	THR	-	linker	UNP P0AEX9
E	-10	LEU	-	linker	UNP P0AEX9
E	-9	GLU	-	linker	UNP P0AEX9
E	-8	VAL	-	linker	UNP P0AEX9
E	-7	LEU	-	linker	UNP P0AEX9
E	-6	PHE	-	linker	UNP P0AEX9
E	-5	GLN	-	linker	UNP P0AEX9
E	-4	GLY	-	linker	UNP P0AEX9
E	-3	PRO	-	linker	UNP P0AEX9
E	-2	LEU	-	linker	UNP P0AEX9
E	-1	GLY	-	linker	UNP P0AEX9
E	0	SER	-	linker	UNP P0AEX9
E	296	CYS	SER	conflict	UNP P35259

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

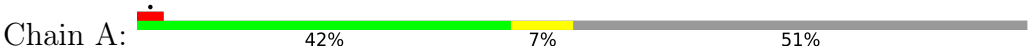
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0

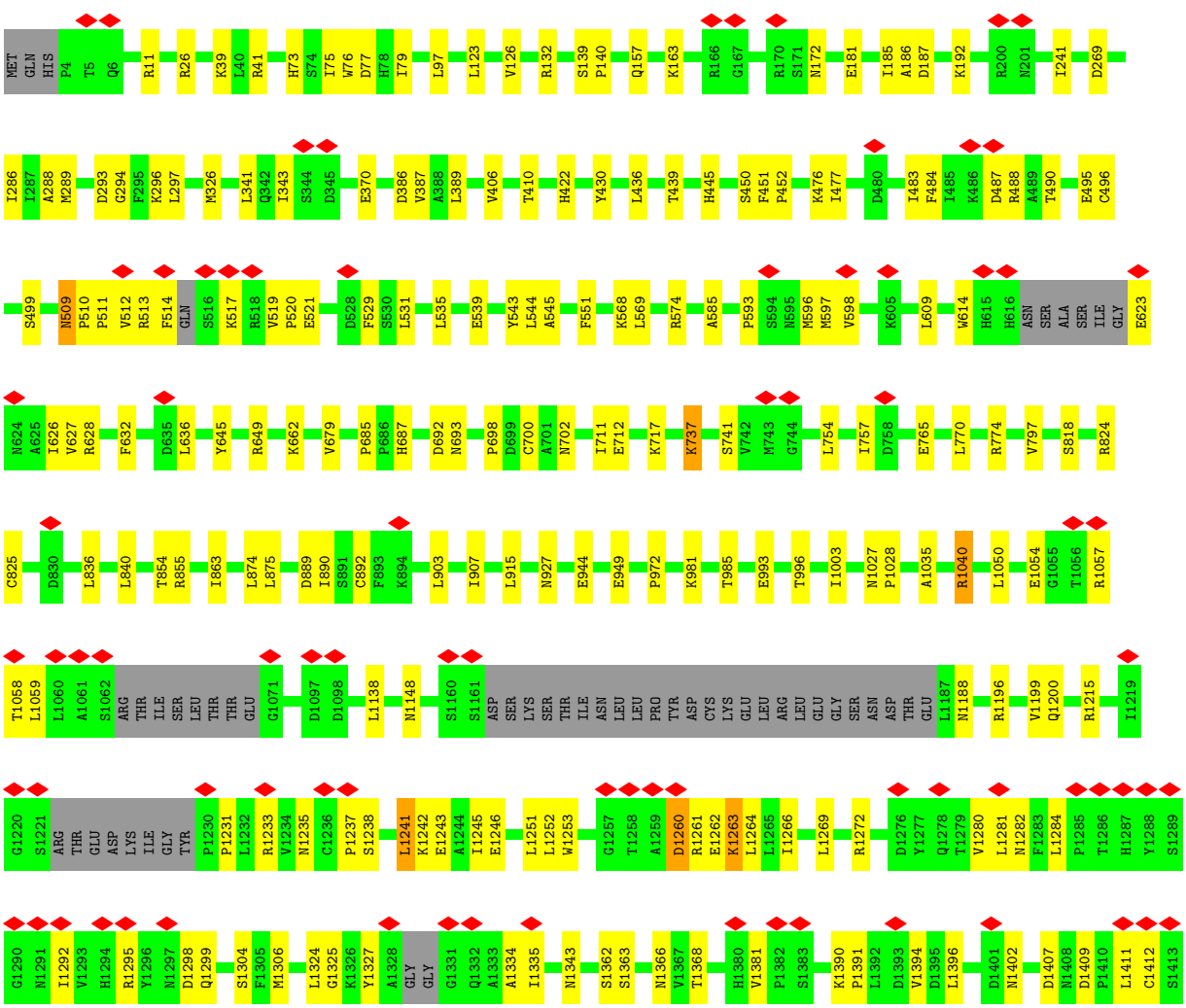
3 Residue-property plots (i)

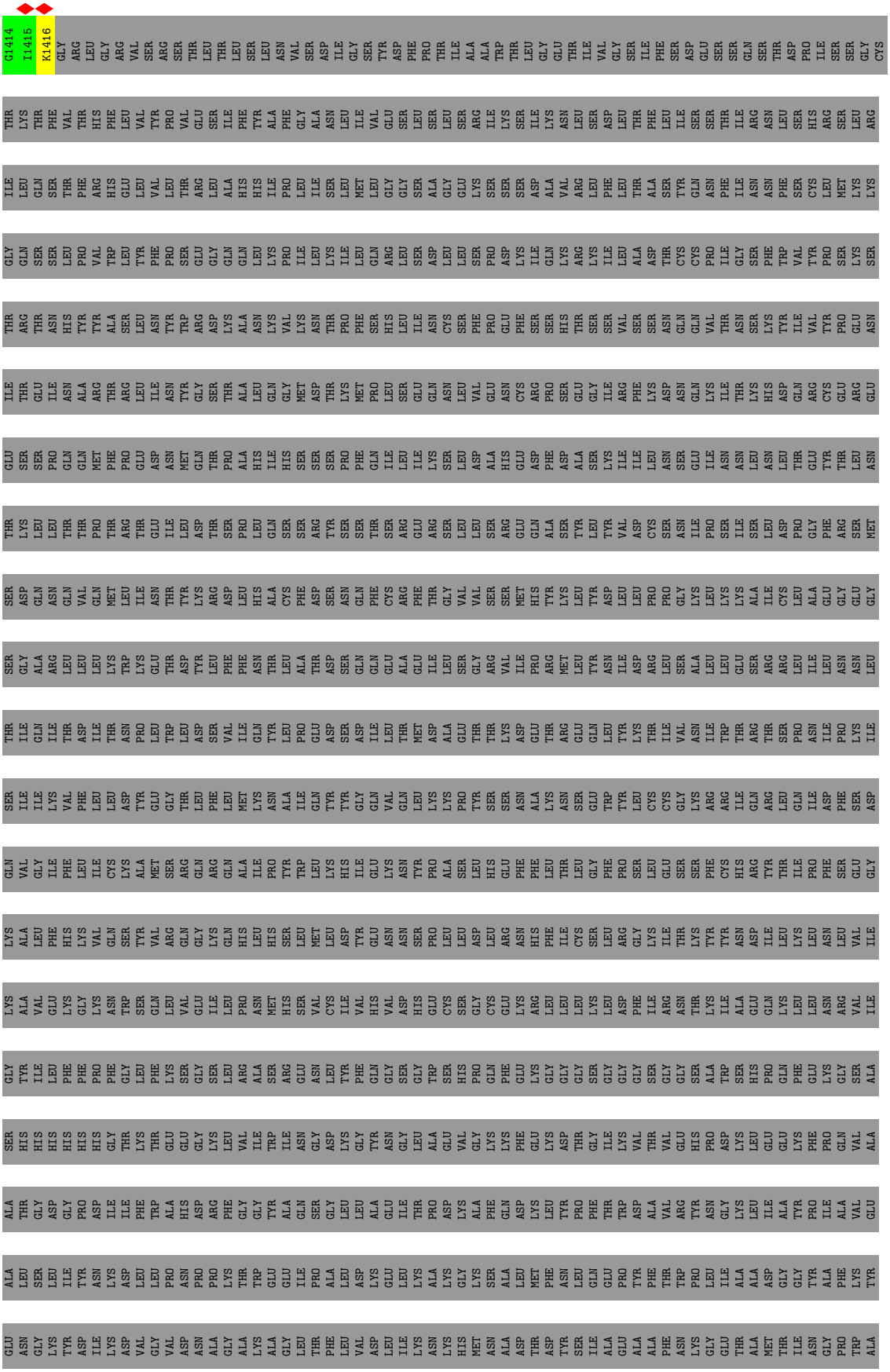
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

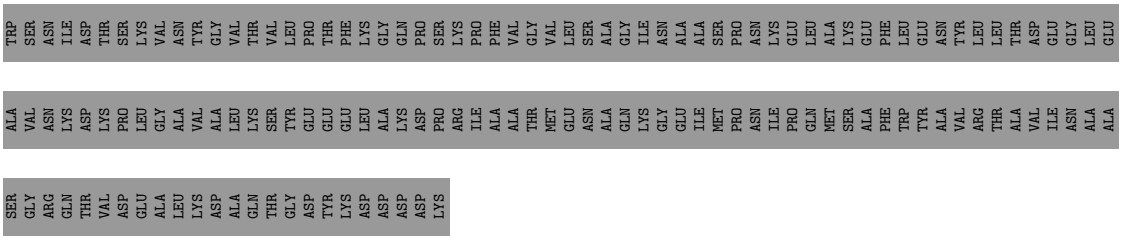
• Molecule 1: RNA-directed RNA polymerase L,Maltose/maltodextrin-binding periplasmic protein

Chain A:



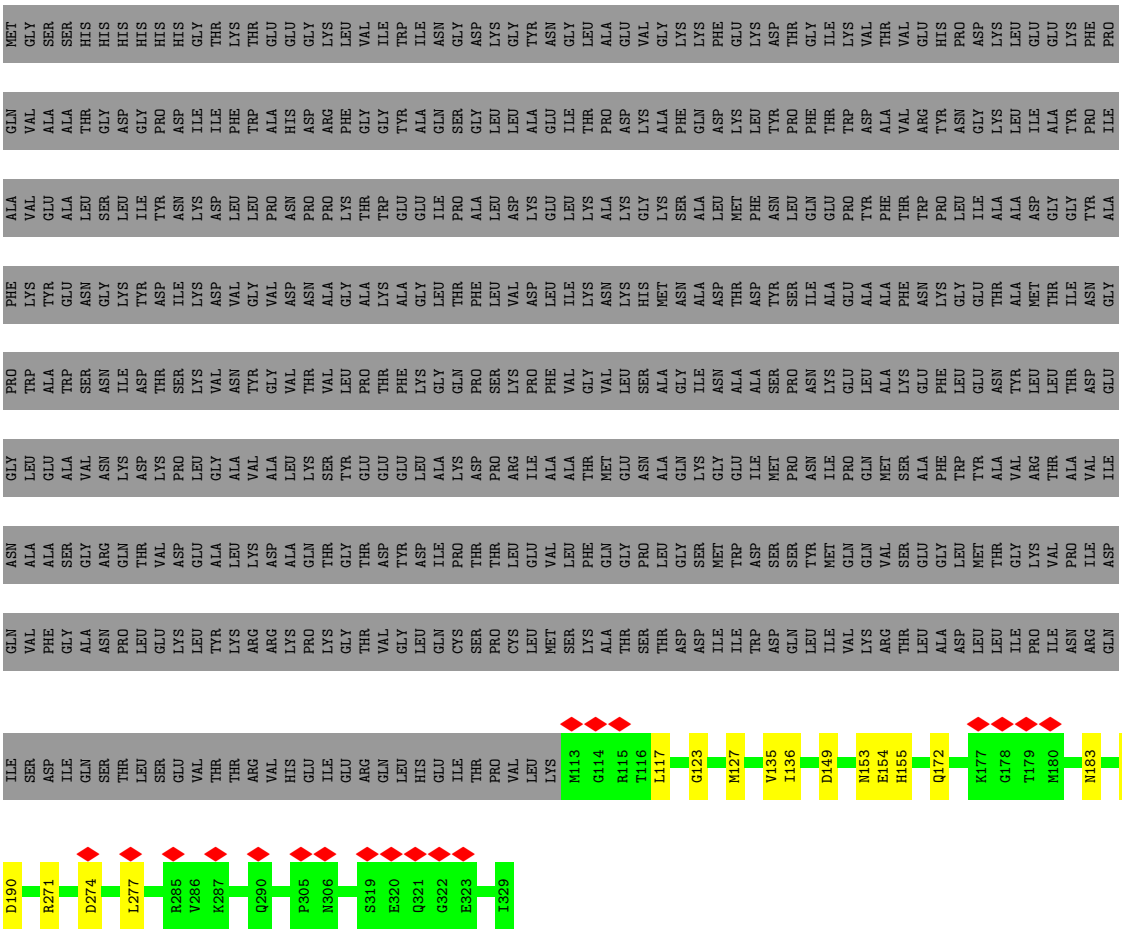



G1414
I1415
K1416



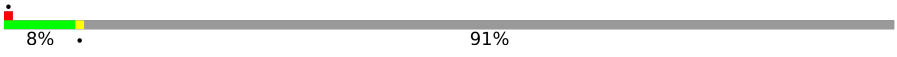
• Molecule 2: Maltose/maltodextrin-binding periplasmic protein,Polymerase cofactor VP35

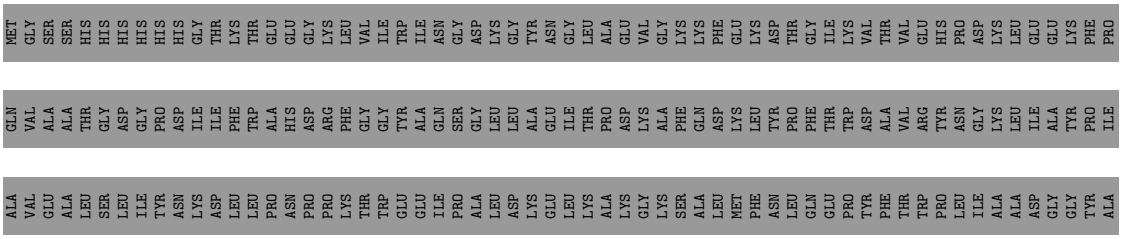
Chain B:

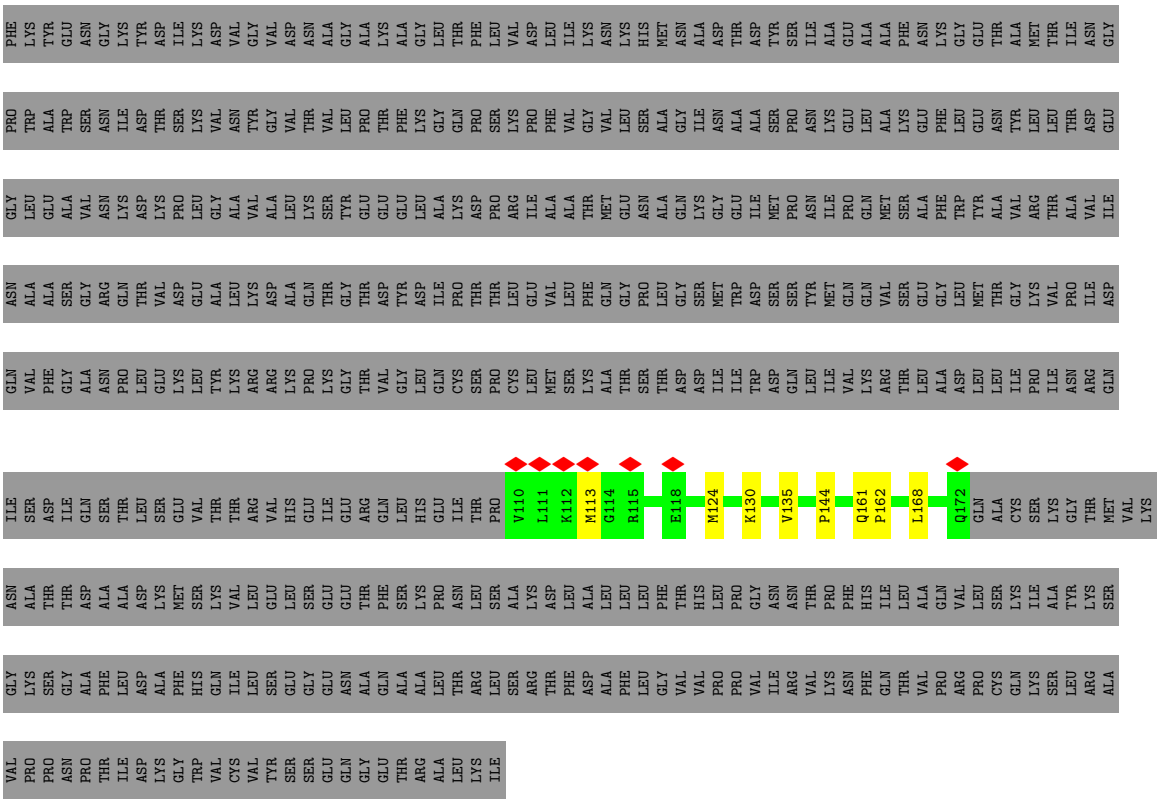


• Molecule 2: Maltose/maltodextrin-binding periplasmic protein,Polymerase cofactor VP35

Chain C:

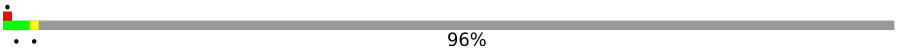


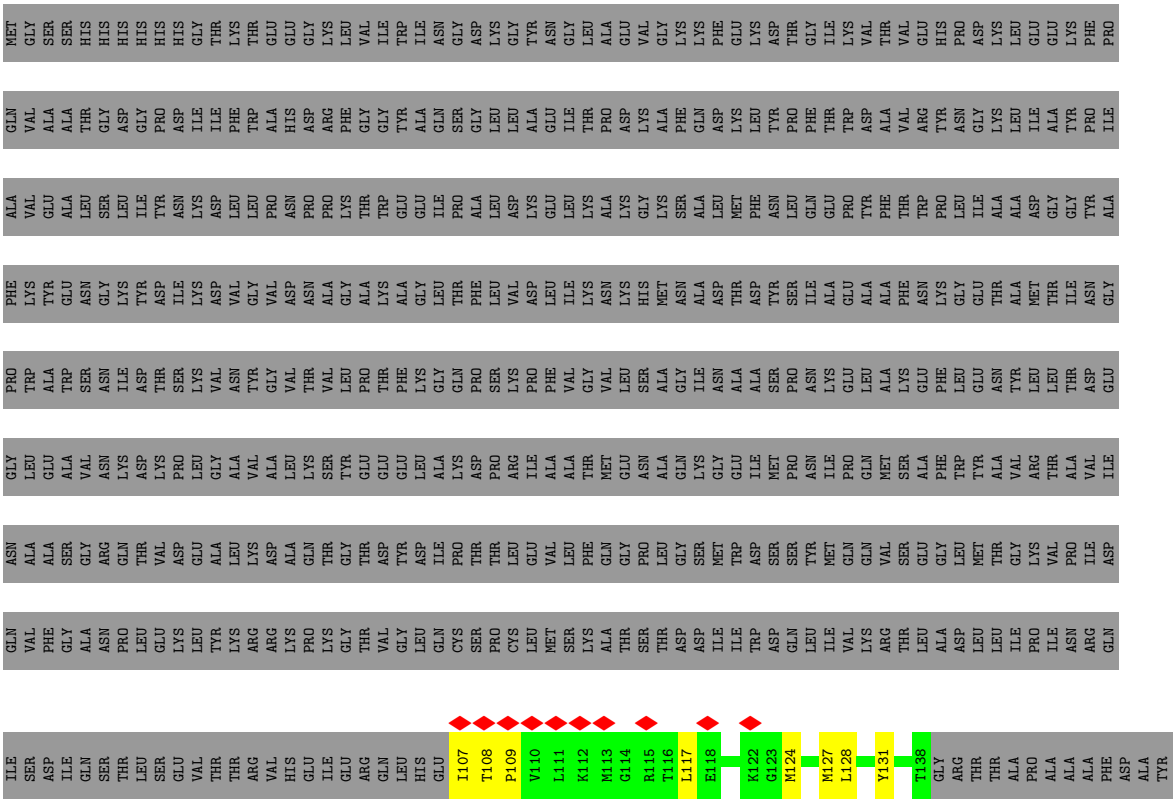


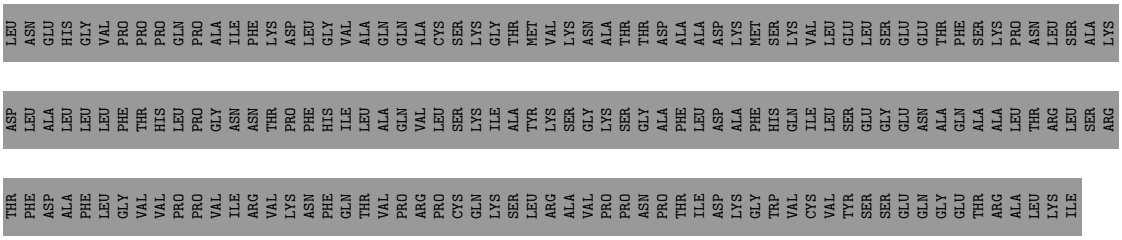


• Molecule 2: Maltose/maltodextrin-binding periplasmic protein,Polymerase cofactor VP35

Chain D:

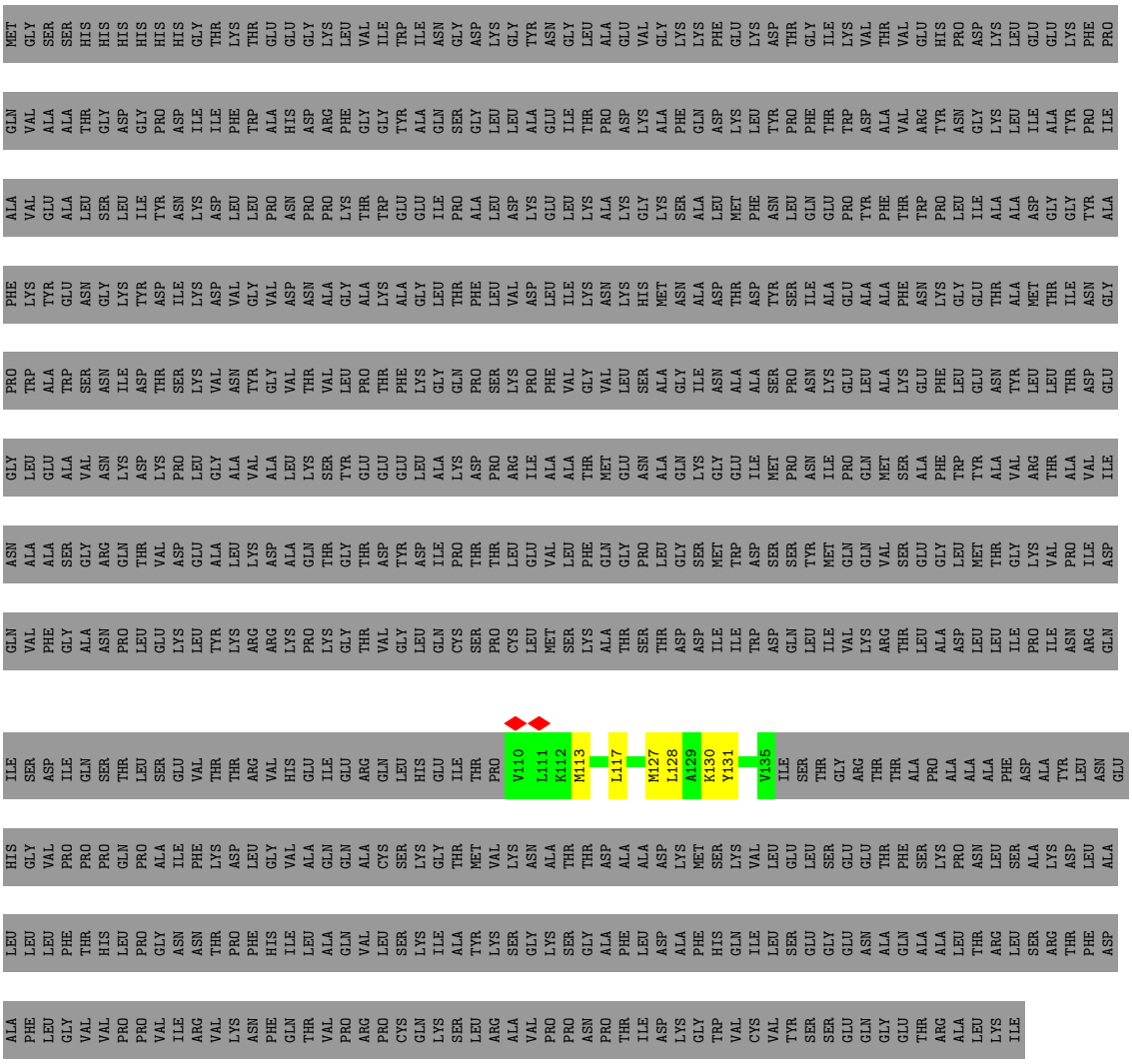






• Molecule 2: Maltose/maltodextrin-binding periplasmic protein,Polymerase cofactor VP35

Chain E: 96%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	319722	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 ($e^-/Å^2$)	52.52	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.513	Depositor
Minimum map value	-1.361	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.225	Depositor
Map size (Å)	272.32, 272.32, 272.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.851, 0.851, 0.851	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: 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	A	0.60	3/11316 (0.0%)	0.79	17/15345 (0.1%)
2	B	0.45	0/1684	0.65	2/2283 (0.1%)
2	C	0.53	1/481 (0.2%)	0.78	1/652 (0.2%)
2	D	0.42	0/246	0.72	0/329
2	E	0.51	0/202	0.92	1/267 (0.4%)
All	All	0.58	4/13929 (0.0%)	0.78	21/18876 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	700	CYS	CB-SG	-5.90	1.72	1.81
1	A	892	CYS	CB-SG	-5.16	1.73	1.81
2	C	135	VAL	CB-CG2	-5.07	1.42	1.52
1	A	825	CYS	CB-SG	-5.02	1.73	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1241	LEU	CB-CG-CD2	-14.48	86.39	111.00
1	A	737	LYS	CD-CE-NZ	-9.40	90.07	111.70
1	A	26	ARG	CG-CD-NE	-8.97	92.95	111.80
2	C	113	MET	CB-CG-SD	-8.82	85.94	112.40
2	E	127	MET	CA-CB-CG	8.26	127.35	113.30
1	A	97	LEU	CA-CB-CG	8.23	134.24	115.30
1	A	1324	LEU	CA-CB-CG	8.06	133.84	115.30
1	A	1241	LEU	CB-CG-CD1	7.27	123.36	111.00
1	A	1306	MET	CB-CG-SD	-7.26	90.62	112.40
2	B	127	MET	CA-CB-CG	6.87	124.97	113.30
1	A	1263	LYS	CG-CD-CE	-6.86	91.31	111.90
1	A	41	ARG	CG-CD-NE	6.58	125.61	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1260	ASP	CB-CA-C	6.39	123.17	110.40
1	A	531	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	774	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	636	LEU	CB-CG-CD2	-5.90	100.96	111.00
2	B	127	MET	CB-CG-SD	5.46	128.78	112.40
1	A	774	ARG	CD-NE-CZ	5.45	131.24	123.60
1	A	1040	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	1263	LYS	CA-CB-CG	-5.19	101.99	113.40
1	A	1411	LEU	CA-CB-CG	5.11	127.05	115.30

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	11040	0	10944	154	0
2	B	1649	0	1679	13	0
2	C	471	0	479	5	0
2	D	244	0	264	12	0
2	E	201	0	216	10	0
3	A	1	0	0	0	0
All	All	13606	0	13582	187	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 7.

All (187) 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:609:LEU:CD1	1:A:623:GLU:HG3	1.66	1.24
1:A:609:LEU:HD13	1:A:623:GLU:HG3	1.28	1.11
1:A:539:GLU:OE2	1:A:662:LYS:O	1.71	1.05
1:A:1040:ARG:NH1	1:A:1246:GLU:OE1	1.96	0.99
1:A:609:LEU:HD11	1:A:623:GLU:HG3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:113:MET:HA	2:E:113:MET:CE	2.01	0.90
2:D:108:THR:N	2:D:109:PRO:CD	2.34	0.89
1:A:623:GLU:N	1:A:623:GLU:OE1	2.08	0.86
1:A:614:TRP:HE3	1:A:737:LYS:NZ	1.77	0.83
1:A:1260:ASP:O	1:A:1263:LYS:NZ	2.12	0.81
1:A:614:TRP:HE3	1:A:737:LYS:HZ1	1.28	0.78
1:A:488:ARG:HB2	1:A:519:VAL:HG21	1.65	0.78
1:A:1262:GLU:HG2	1:A:1266:ILE:HD11	1.67	0.77
1:A:1252:LEU:HD22	1:A:1261:ARG:HD3	1.67	0.76
1:A:496:CYS:HB3	1:A:512:VAL:HG13	1.69	0.74
1:A:499:SER:HG	1:A:514:PHE:HD1	1.33	0.74
1:A:535:LEU:O	1:A:539:GLU:HG2	1.87	0.73
1:A:1253:TRP:CH2	1:A:1292:ILE:HA	2.21	0.73
2:C:161:GLN:N	2:C:162:PRO:HD3	2.03	0.73
1:A:609:LEU:HD13	1:A:623:GLU:CG	2.14	0.73
1:A:1263:LYS:H	1:A:1263:LYS:HZ2	1.38	0.72
1:A:1281:LEU:HA	1:A:1284:LEU:HD23	1.70	0.72
2:D:107:ILE:C	2:D:109:PRO:HD2	2.09	0.71
1:A:509:ASN:N	1:A:509:ASN:HD22	1.89	0.69
1:A:593:PRO:HG2	1:A:596:MET:HE2	1.75	0.68
1:A:487:ASP:HA	1:A:520:PRO:HD3	1.76	0.68
2:D:108:THR:N	2:D:109:PRO:HD3	2.09	0.67
1:A:626:ILE:HD11	1:A:757:ILE:HA	1.77	0.67
2:D:107:ILE:N	2:D:109:PRO:HD2	2.11	0.66
1:A:1243:GLU:OE1	1:A:1272:ARG:NH2	2.29	0.66
1:A:609:LEU:CD1	1:A:623:GLU:CG	2.61	0.65
2:E:113:MET:HA	2:E:113:MET:HE1	1.79	0.65
1:A:77:ASP:HB2	1:A:288:ALA:HB2	1.79	0.64
1:A:1138:LEU:HD11	1:A:1343:ASN:HB3	1.80	0.64
1:A:1199:VAL:HG12	1:A:1200:GLN:HG2	1.81	0.62
1:A:1262:GLU:O	1:A:1266:ILE:HD12	1.99	0.62
1:A:1260:ASP:CG	1:A:1263:LYS:HZ1	2.03	0.62
2:D:108:THR:N	2:D:109:PRO:HD2	2.15	0.62
1:A:628:ARG:HH22	1:A:765:GLU:HG2	1.64	0.62
1:A:687:HIS:ND1	1:A:702:ASN:OD1	2.33	0.60
1:A:944:GLU:HG2	1:A:949:GLU:OE2	2.02	0.60
1:A:1269:LEU:HD11	1:A:1280:VAL:HG21	1.82	0.60
1:A:1238:SER:OG	1:A:1407:ASP:OD2	2.19	0.59
1:A:628:ARG:NH2	1:A:765:GLU:OE2	2.36	0.59
1:A:645:TYR:O	1:A:649:ARG:HG3	2.02	0.59
1:A:293:ASP:O	1:A:296:LYS:N	2.26	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:HD23	2:E:113:MET:HG3	1.85	0.58
1:A:490:THR:OG1	1:A:517:LYS:O	2.22	0.57
1:A:1050:LEU:O	1:A:1054:GLU:HG3	2.05	0.57
1:A:75:ILE:HG22	1:A:79:ILE:HG13	1.85	0.57
2:C:130:LYS:HD3	2:D:131:TYR:CZ	2.40	0.57
2:C:161:GLN:N	2:C:162:PRO:CD	2.67	0.56
1:A:495:GLU:O	1:A:512:VAL:HG11	2.06	0.56
1:A:39:LYS:HD2	1:A:685:PRO:HG2	1.88	0.56
1:A:484:PHE:HA	1:A:488:ARG:HH22	1.70	0.56
2:D:107:ILE:C	2:D:109:PRO:CD	2.73	0.56
1:A:609:LEU:HD11	1:A:623:GLU:CG	2.30	0.55
1:A:1292:ILE:H	1:A:1292:ILE:HD12	1.71	0.55
1:A:496:CYS:HB3	1:A:512:VAL:CG1	2.37	0.54
1:A:693:ASN:HD21	1:A:698:PRO:HD3	1.71	0.54
1:A:1409:ASP:OD2	1:A:1412:CYS:HB3	2.07	0.54
1:A:488:ARG:CB	1:A:519:VAL:HG21	2.36	0.54
1:A:1362:SER:OG	1:A:1363:SER:N	2.41	0.54
2:D:124:MET:O	2:D:128:LEU:HD23	2.08	0.54
1:A:551:PHE:CZ	1:A:711:ILE:HD13	2.44	0.53
2:B:183:ASN:OD1	2:B:186:THR:HG23	2.08	0.53
1:A:341:LEU:HD12	1:A:343:ILE:HD11	1.90	0.52
1:A:692:ASP:N	1:A:692:ASP:OD1	2.42	0.52
2:B:172:GLN:NE2	2:B:190:ASP:OD2	2.38	0.52
2:D:107:ILE:CA	2:D:109:PRO:HD2	2.40	0.52
1:A:496:CYS:CB	1:A:512:VAL:HG13	2.37	0.51
2:B:271:ARG:HH11	2:B:271:ARG:HG3	1.74	0.51
1:A:711:ILE:HG22	1:A:712:GLU:H	1.75	0.51
1:A:597:MET:HB3	1:A:741:SER:HB2	1.92	0.51
1:A:1188:ASN:ND2	1:A:1325:GLY:HA3	2.25	0.51
1:A:1260:ASP:CG	1:A:1263:LYS:NZ	2.65	0.50
1:A:818:SER:HB2	1:A:854:THR:HB	1.92	0.50
1:A:499:SER:O	1:A:513:ARG:NH2	2.45	0.50
1:A:1027:ASN:HB3	1:A:1028:PRO:HD3	1.93	0.49
1:A:1148:ASN:HB3	1:A:1368:THR:CG2	2.42	0.49
1:A:1148:ASN:HB3	1:A:1368:THR:HG22	1.92	0.49
1:A:1241:LEU:HD12	1:A:1245:ILE:HG12	1.93	0.49
1:A:903:LEU:O	1:A:907:ILE:HG12	2.13	0.49
1:A:593:PRO:HG2	1:A:596:MET:CE	2.42	0.49
1:A:627:VAL:HG22	1:A:754:LEU:HD23	1.94	0.49
1:A:509:ASN:N	1:A:509:ASN:ND2	2.60	0.49
1:A:1237:PRO:O	1:A:1242:LYS:NZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LYS:HG3	1:A:477:ILE:HD12	1.94	0.48
1:A:1263:LYS:HG3	1:A:1264:LEU:N	2.27	0.48
1:A:1196:ARG:NH2	1:A:1366:ASN:HB3	2.28	0.48
1:A:1252:LEU:CD2	1:A:1261:ARG:HD3	2.40	0.48
1:A:73:HIS:O	1:A:76:TRP:HB3	2.13	0.48
1:A:436:LEU:HD22	1:A:436:LEU:N	2.29	0.47
2:D:117:LEU:HD11	2:E:117:LEU:HD13	1.96	0.47
1:A:389:LEU:HD11	1:A:679:VAL:HG23	1.96	0.47
2:D:127:MET:HE2	2:E:128:LEU:HD21	1.97	0.47
1:A:927:ASN:HB2	1:A:1304:SER:HB3	1.97	0.47
1:A:1231:PRO:HG2	1:A:1282:ASN:O	2.14	0.47
1:A:1260:ASP:OD1	1:A:1263:LYS:NZ	2.32	0.47
2:B:183:ASN:H	2:B:186:THR:HG1	1.61	0.47
1:A:854:THR:OG1	1:A:855:ARG:N	2.48	0.47
2:E:113:MET:HA	2:E:113:MET:HE2	1.93	0.47
2:B:154:GLU:OE1	2:B:155:HIS:CD2	2.68	0.46
1:A:770:LEU:HD23	1:A:770:LEU:HA	1.77	0.46
1:A:181:GLU:OE1	1:A:192:LYS:HD3	2.16	0.46
1:A:1263:LYS:HB3	1:A:1263:LYS:HE3	1.60	0.46
1:A:1260:ASP:O	1:A:1263:LYS:HG2	2.16	0.46
1:A:293:ASP:O	1:A:294:GLY:C	2.51	0.46
1:A:737:LYS:HA	1:A:737:LYS:HD3	1.61	0.46
1:A:993:GLU:O	1:A:996:THR:HG22	2.16	0.45
1:A:139:SER:HB3	1:A:140:PRO:HD3	1.97	0.45
1:A:1260:ASP:OD2	1:A:1263:LYS:HE2	2.17	0.45
1:A:569:LEU:H	1:A:574:ARG:HH21	1.65	0.45
2:E:113:MET:CE	2:E:113:MET:CA	2.86	0.45
1:A:499:SER:OG	1:A:514:PHE:HD1	1.96	0.45
1:A:972:PRO:HG3	1:A:1035:ALA:HB2	1.98	0.44
1:A:711:ILE:HG22	1:A:712:GLU:N	2.33	0.44
2:B:136:ILE:HD11	2:E:130:LYS:NZ	2.33	0.44
2:D:127:MET:HE2	2:D:127:MET:HB2	1.63	0.44
1:A:614:TRP:HE3	1:A:737:LYS:HZ3	1.62	0.44
2:B:123:GLY:HA3	2:C:124:MET:SD	2.58	0.44
1:A:597:MET:HG2	1:A:598:VAL:N	2.32	0.44
1:A:445:HIS:HB3	1:A:450:SER:O	2.18	0.44
1:A:510:PRO:HA	1:A:511:PRO:HD3	1.86	0.44
1:A:185:ILE:HG13	1:A:186:ALA:H	1.83	0.43
1:A:1057:ARG:O	1:A:1058:THR:HG22	2.18	0.43
1:A:241:ILE:HD13	1:A:241:ILE:HA	1.81	0.43
1:A:439:THR:O	1:A:439:THR:OG1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:LEU:HD12	1:A:915:LEU:HD22	1.99	0.43
2:B:183:ASN:O	2:B:186:THR:OG1	2.36	0.43
1:A:157:GLN:HG3	1:A:874:LEU:HD11	2.00	0.43
1:A:514:PHE:O	1:A:514:PHE:CG	2.71	0.43
1:A:1260:ASP:CG	1:A:1263:LYS:HE2	2.38	0.43
1:A:172:ASN:N	1:A:172:ASN:OD1	2.52	0.43
2:B:274:ASP:HA	2:B:277:LEU:HD23	2.01	0.43
1:A:614:TRP:CE3	1:A:737:LYS:NZ	2.60	0.43
1:A:297:LEU:HA	1:A:297:LEU:HD23	1.80	0.42
1:A:11:ARG:HH11	1:A:824:ARG:NH2	2.17	0.42
1:A:1381:VAL:HG23	1:A:1381:VAL:O	2.19	0.42
1:A:495:GLU:O	1:A:512:VAL:CG1	2.66	0.42
2:B:135:VAL:HB	2:E:131:TYR:CZ	2.55	0.42
1:A:341:LEU:HB2	1:A:343:ILE:HG13	2.01	0.42
1:A:981:LYS:NZ	1:A:985:THR:OG1	2.36	0.42
1:A:529:PHE:O	1:A:529:PHE:CD2	2.73	0.42
1:A:889:ASP:OD1	1:A:890:ILE:N	2.53	0.42
1:A:123:LEU:HB2	1:A:126:VAL:CG2	2.49	0.42
1:A:568:LYS:HE3	1:A:568:LYS:HB2	1.87	0.42
1:A:543:TYR:O	1:A:545:ALA:N	2.53	0.42
1:A:875:LEU:HA	1:A:875:LEU:HD23	1.64	0.42
1:A:1233:ARG:O	1:A:1416:LYS:HB3	2.19	0.42
2:C:144:PRO:HG2	2:C:168:LEU:HD13	2.02	0.42
1:A:326:MET:CE	1:A:326:MET:HA	2.50	0.41
1:A:649:ARG:HH11	1:A:649:ARG:HD2	1.69	0.41
1:A:514:PHE:CD2	1:A:514:PHE:C	2.91	0.41
1:A:1394:VAL:HG12	1:A:1396:LEU:HD12	2.01	0.41
2:B:149:ASP:OD1	2:B:153:ASN:ND2	2.53	0.41
1:A:289:MET:HE3	1:A:289:MET:HB2	1.94	0.41
1:A:1295:ARG:HH21	1:A:1335:ILE:HG13	1.85	0.41
1:A:836:LEU:HD12	1:A:836:LEU:HA	1.72	0.41
1:A:521:GLU:N	1:A:521:GLU:OE1	2.54	0.41
1:A:543:TYR:C	1:A:545:ALA:H	2.23	0.41
1:A:1390:LYS:HD3	1:A:1391:PRO:HD2	2.02	0.41
2:B:271:ARG:HG3	2:B:271:ARG:NH1	2.35	0.41
2:E:128:LEU:HD23	2:E:128:LEU:HA	1.89	0.41
1:A:269:ASP:O	1:A:370:GLU:HG3	2.20	0.41
1:A:422:HIS:NE2	1:A:430:TYR:HB3	2.36	0.41
1:A:1003:ILE:HG23	1:A:1402:ASN:ND2	2.36	0.41
1:A:1251:LEU:O	1:A:1251:LEU:HD23	2.21	0.41
1:A:386:ASP:OD1	1:A:387:VAL:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:585:ALA:HB2	1:A:717:LYS:HE2	2.03	0.41
1:A:626:ILE:CD1	1:A:757:ILE:HA	2.49	0.41
1:A:632:PHE:HB3	1:A:797:VAL:HG22	2.03	0.41
1:A:1215:ARG:HH11	1:A:1215:ARG:HD2	1.74	0.41
1:A:132:ARG:HH21	1:A:132:ARG:HD3	1.74	0.41
1:A:163:LYS:HE2	1:A:187:ASP:OD1	2.21	0.41
1:A:1327:TYR:HA	1:A:1334:ALA:HB2	2.02	0.40
1:A:483:ILE:H	1:A:483:ILE:HG12	1.63	0.40
1:A:514:PHE:CZ	1:A:517:LYS:HD2	2.57	0.40
1:A:286:ILE:HD13	1:A:286:ILE:HG21	1.83	0.40
1:A:451:PHE:CD2	1:A:452:PRO:HD2	2.56	0.40
1:A:662:LYS:HE3	1:A:662:LYS:HB3	1.92	0.40
1:A:863:ILE:HD13	1:A:863:ILE:HA	1.91	0.40
1:A:1003:ILE:HG23	1:A:1402:ASN:HD22	1.87	0.40
1:A:1057:ARG:C	1:A:1059:LEU:H	2.24	0.40
1:A:1235:ASN:OD1	1:A:1416:LYS:HD2	2.21	0.40
1:A:406:VAL:O	1:A:410:THR:HG22	2.22	0.40
1:A:1298:ASP:OD1	1:A:1299:GLN:N	2.55	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	1349/2757 (49%)	1288 (96%)	60 (4%)	1 (0%)	48 73
2	B	215/727 (30%)	211 (98%)	4 (2%)	0	100 100
2	C	61/727 (8%)	60 (98%)	1 (2%)	0	100 100
2	D	30/727 (4%)	29 (97%)	1 (3%)	0	100 100
2	E	24/727 (3%)	24 (100%)	0	0	100 100
All	All	1679/5665 (30%)	1612 (96%)	66 (4%)	1 (0%)	50 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	LEU

5.3.2 Protein sidechains (i)

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	1225/2455 (50%)	1224 (100%)	1 (0%)	92 98
2	B	179/603 (30%)	179 (100%)	0	100 100
2	C	49/603 (8%)	49 (100%)	0	100 100
2	D	28/603 (5%)	28 (100%)	0	100 100
2	E	22/603 (4%)	22 (100%)	0	100 100
All	All	1503/4867 (31%)	1502 (100%)	1 (0%)	92 98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	509	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	509	ASN
1	A	624	ASN
1	A	1156	GLN
1	A	1188	ASN
2	B	155	HIS
2	B	173	GLN
2	C	161	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

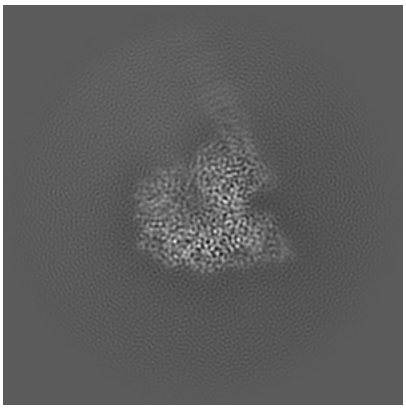
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60755. These allow visual inspection of the internal detail of the map and identification of artifacts.

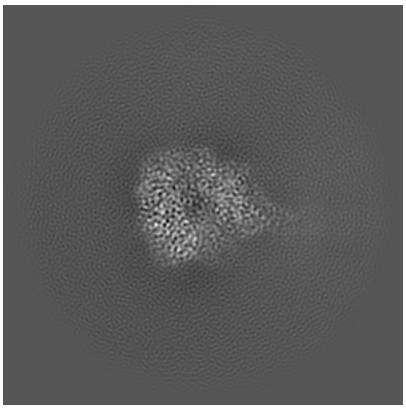
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

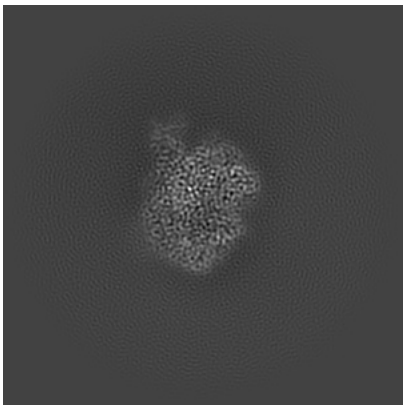
6.1.1 Primary map



X

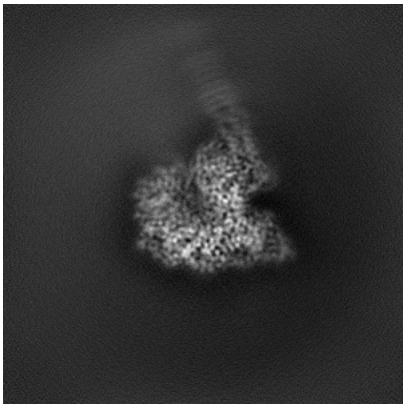


Y

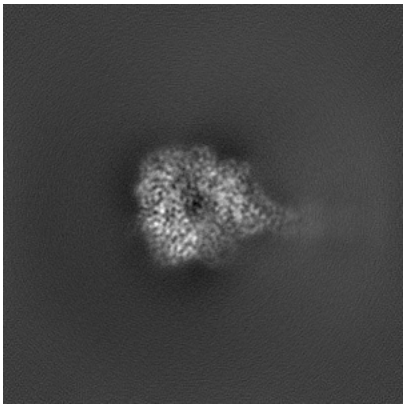


Z

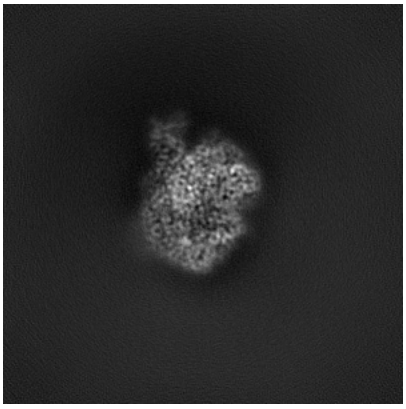
6.1.2 Raw map



X



Y

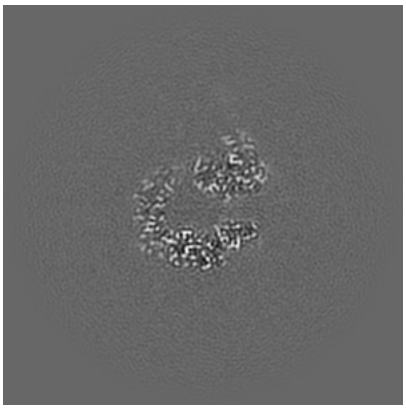


Z

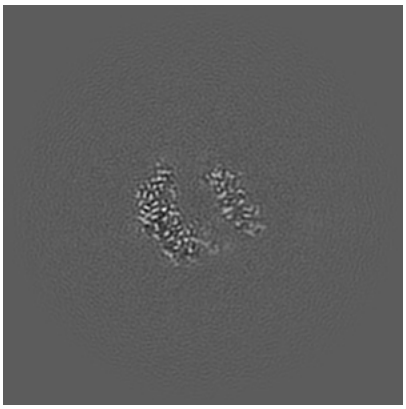
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

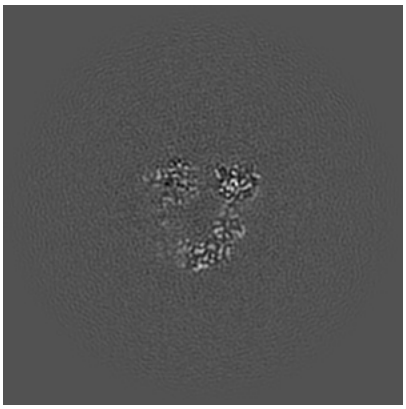
6.2.1 Primary map



X Index: 160

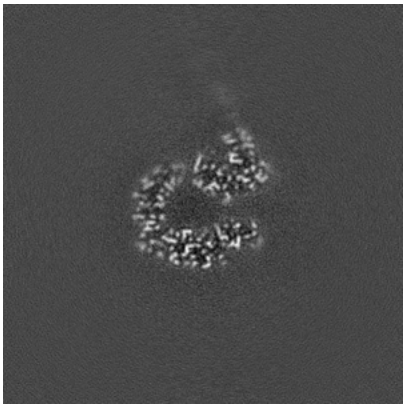


Y Index: 160

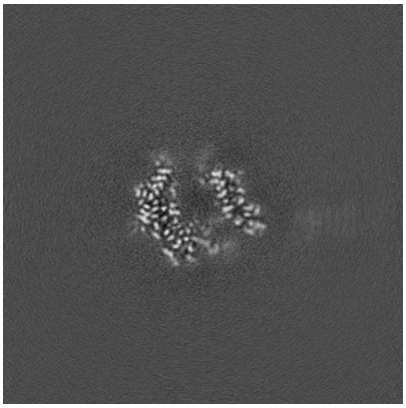


Z Index: 160

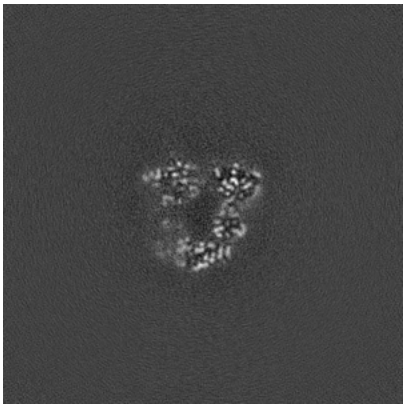
6.2.2 Raw map



X Index: 160



Y Index: 160

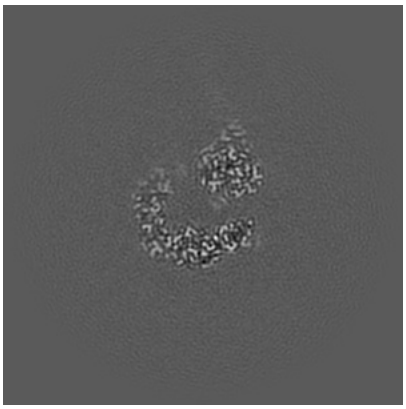


Z Index: 160

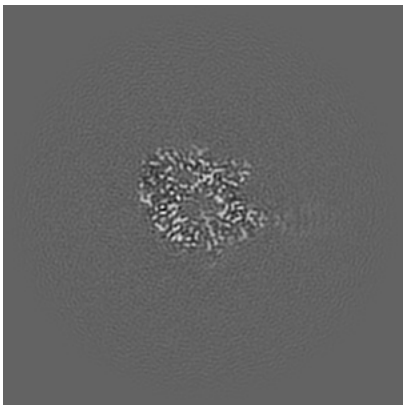
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

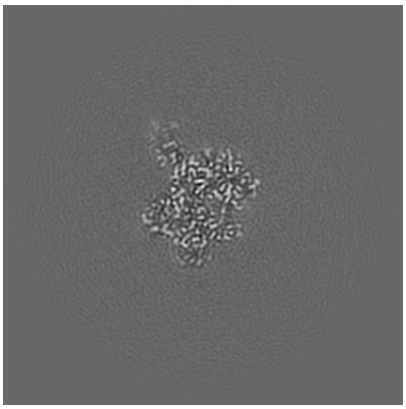
6.3.1 Primary map



X Index: 155

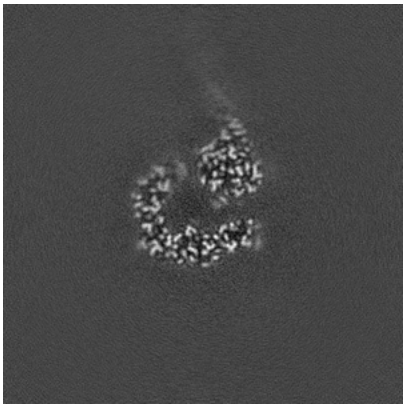


Y Index: 173

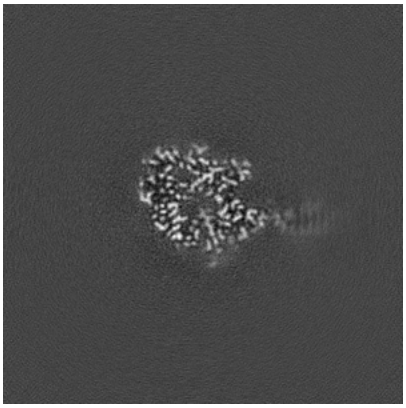


Z Index: 132

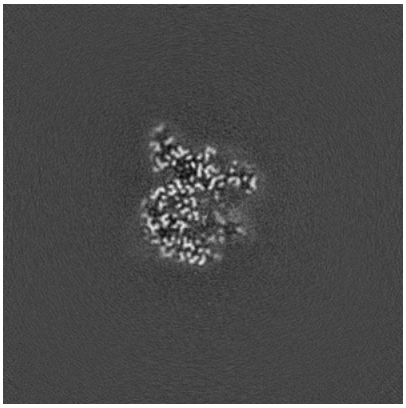
6.3.2 Raw map



X Index: 155



Y Index: 173

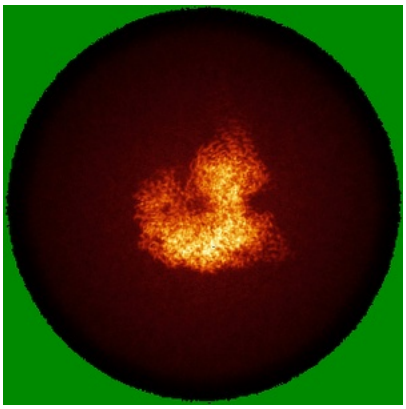


Z Index: 139

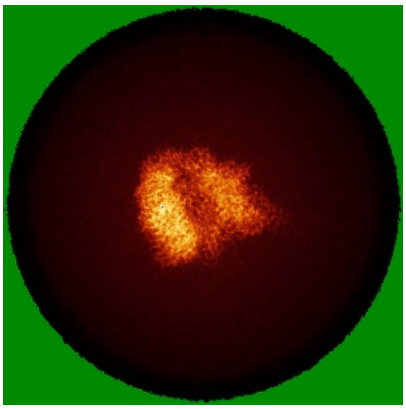
The images above show the largest variance slices of the map in three orthogonal directions.

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

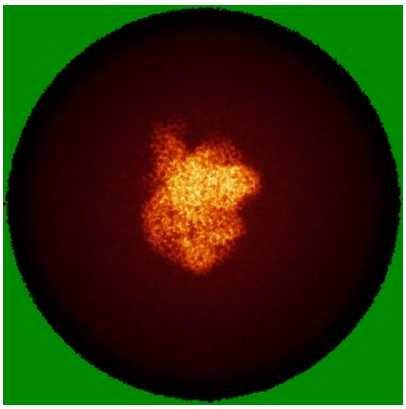
6.4.1 Primary map



X

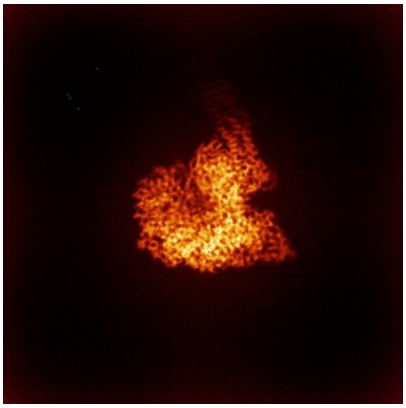


Y

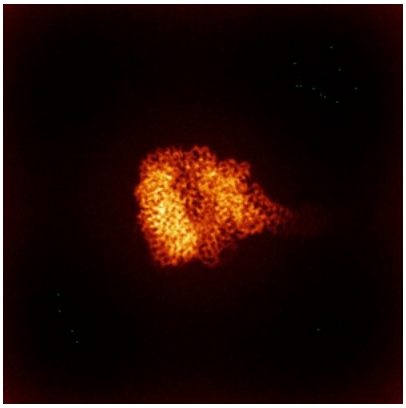


Z

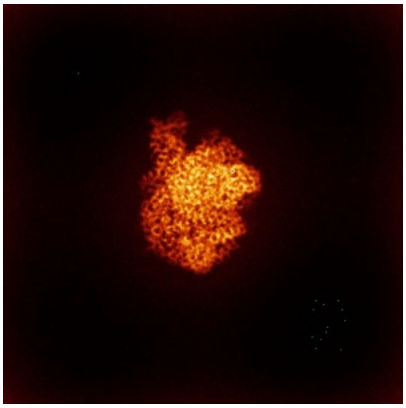
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.225. 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

X Y Z

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.

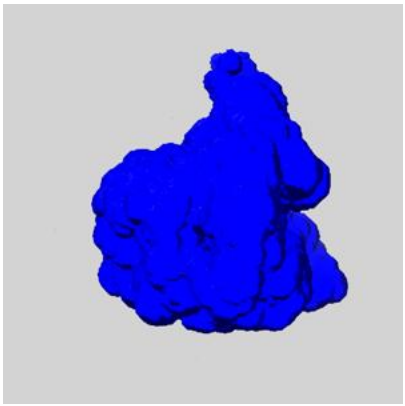
6.6 Mask visualisation

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

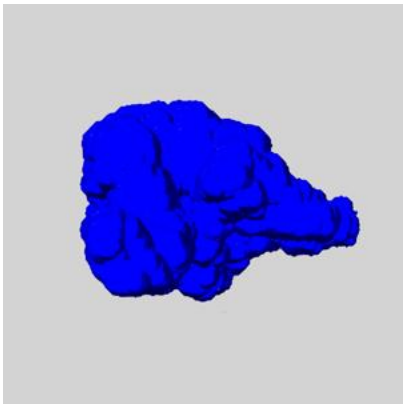
A mask typically either:

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

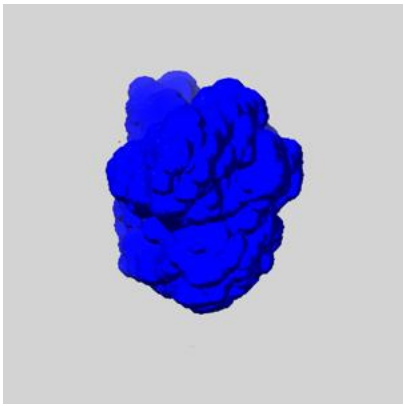
6.6.1 emd_60755_msk_1.map



X



Y

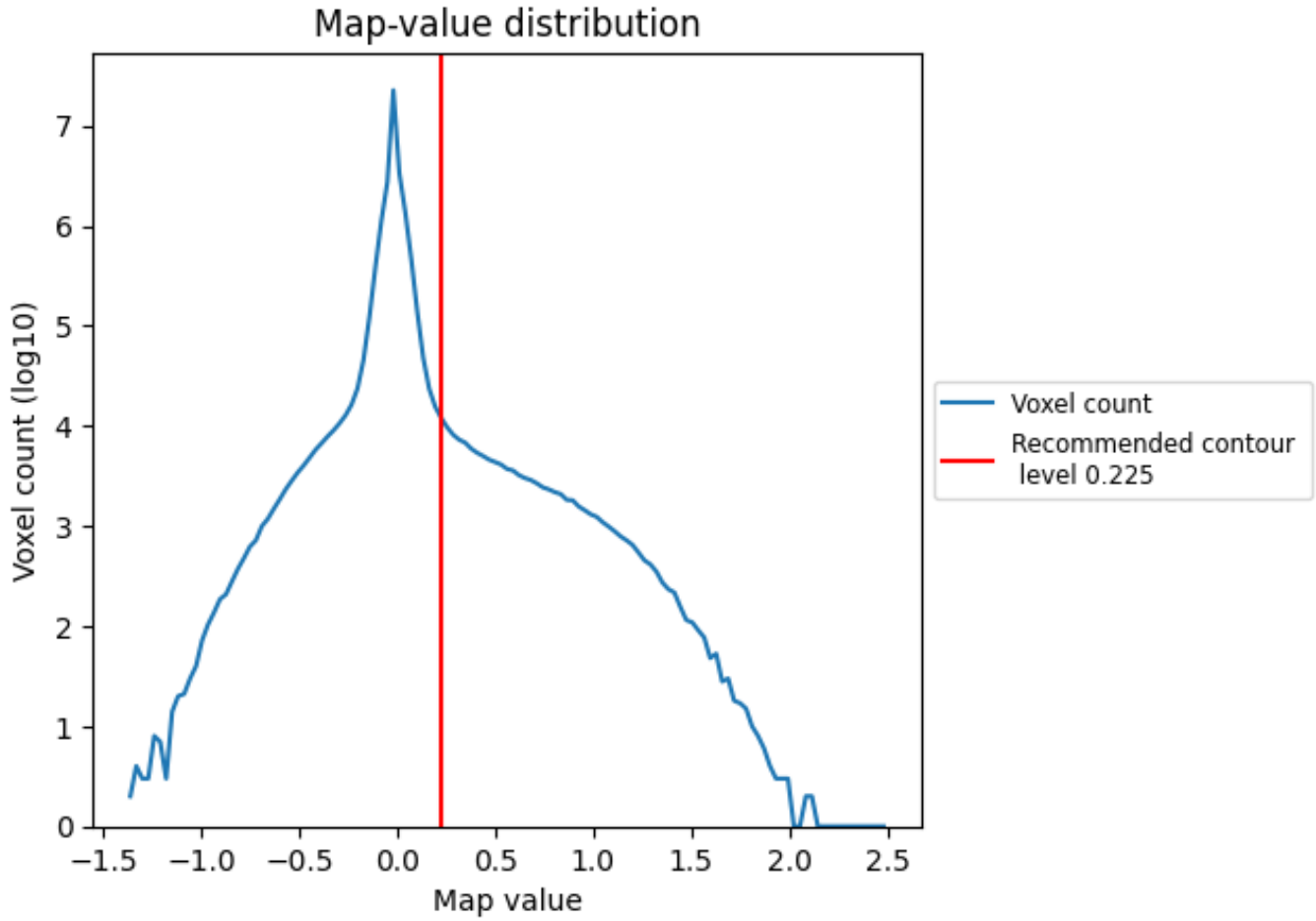


Z

7 Map analysis

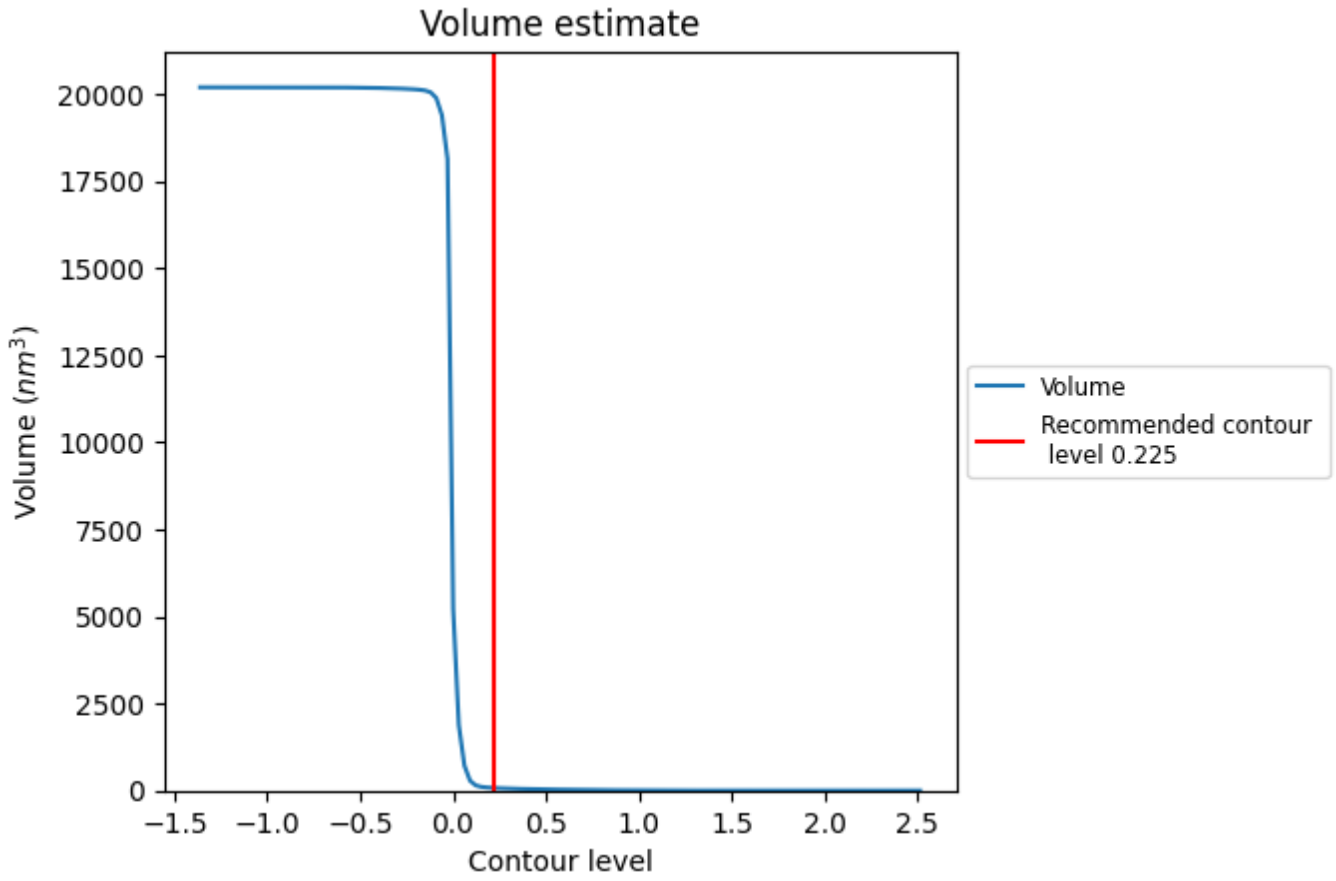
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

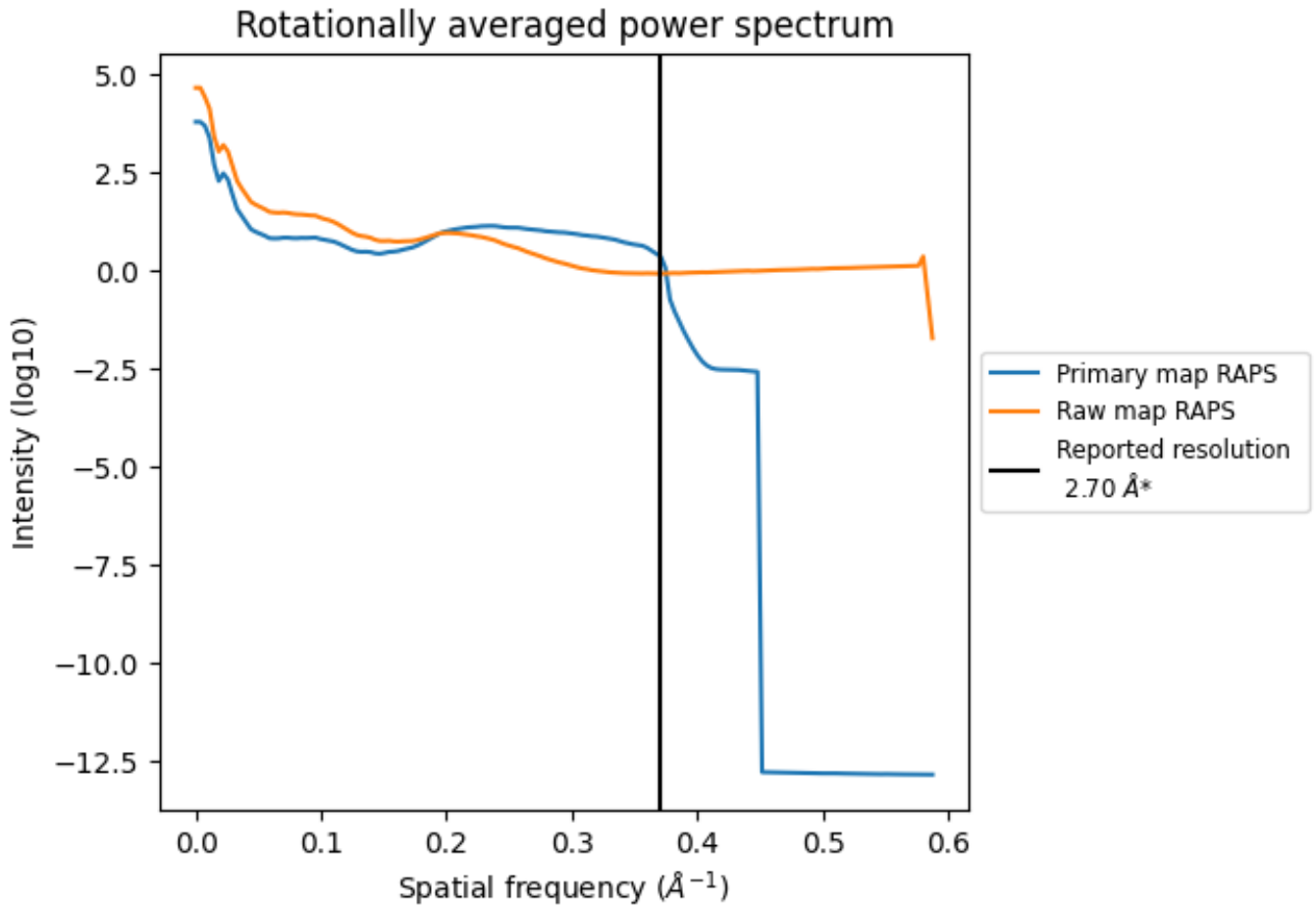
7.2 Volume estimate



The volume at the recommended contour level is 74 nm^3; this corresponds to an approximate mass of 67 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 (i)

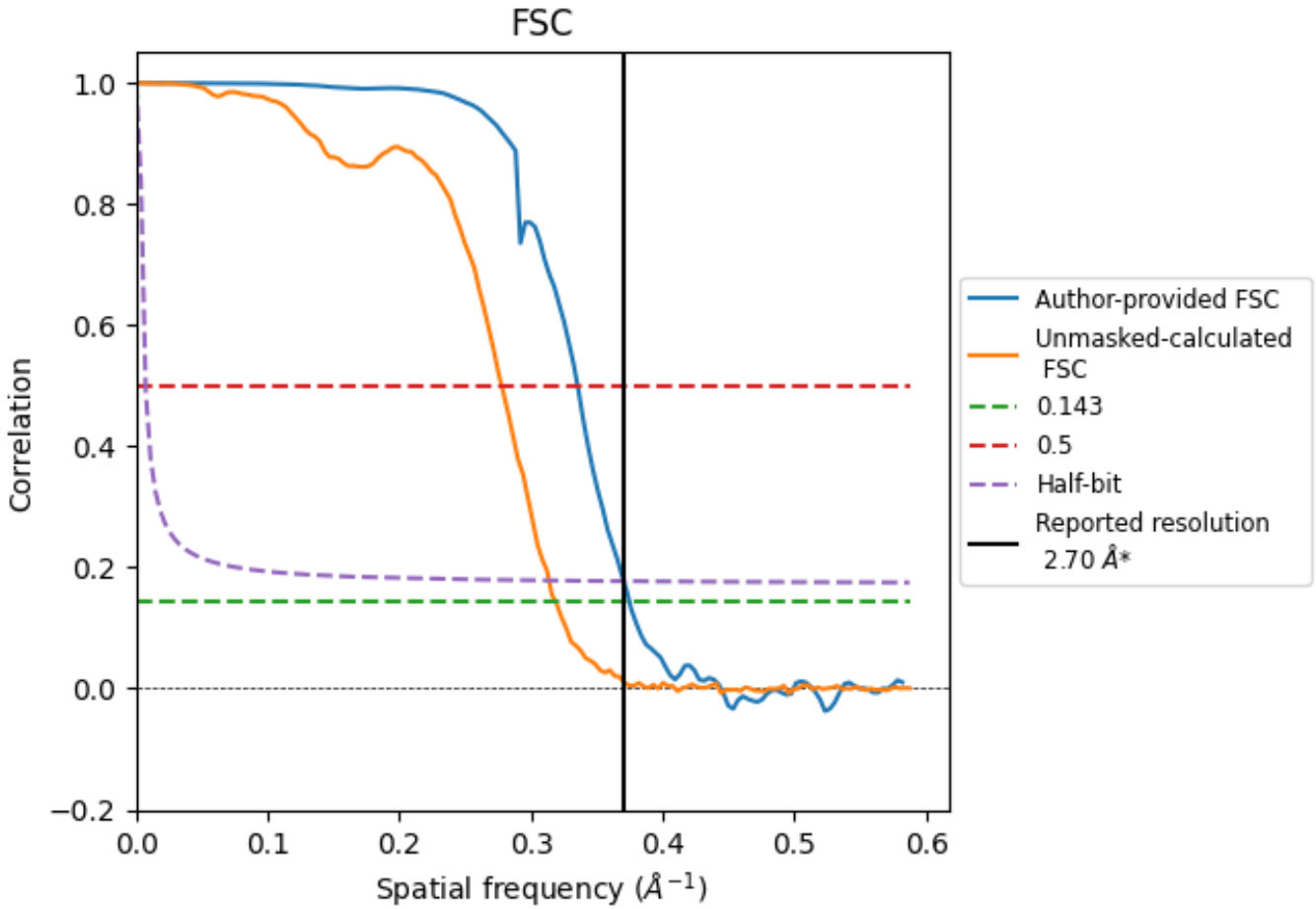


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

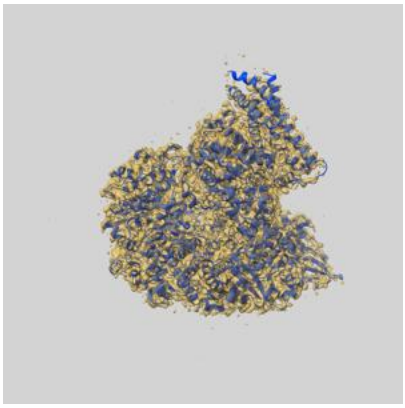
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	2.98	2.70
Unmasked-calculated*	3.14	3.60	3.19

*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 3.14 differs from the reported value 2.7 by more than 10 %

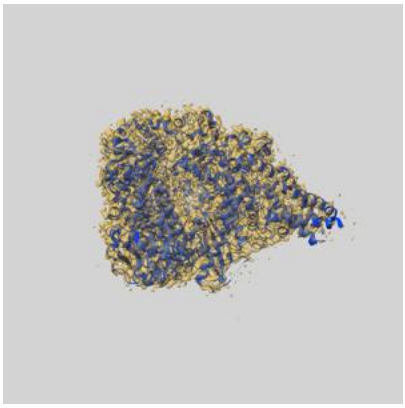
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60755 and PDB model 9IP2. Per-residue inclusion information can be found in section 3 on page 9.

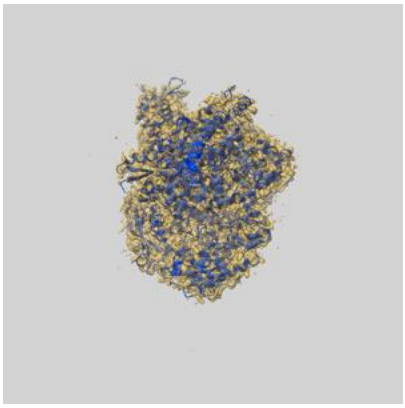
9.1 Map-model overlay



X



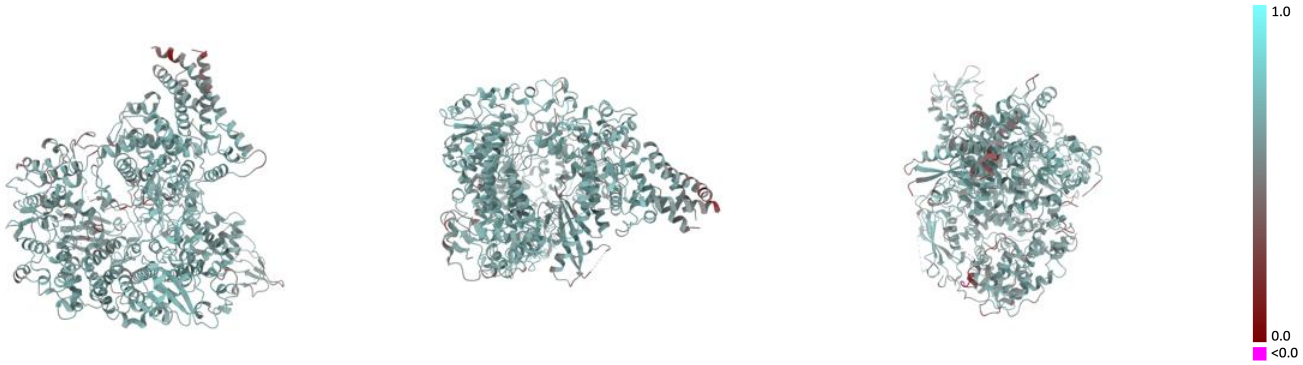
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.225 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.

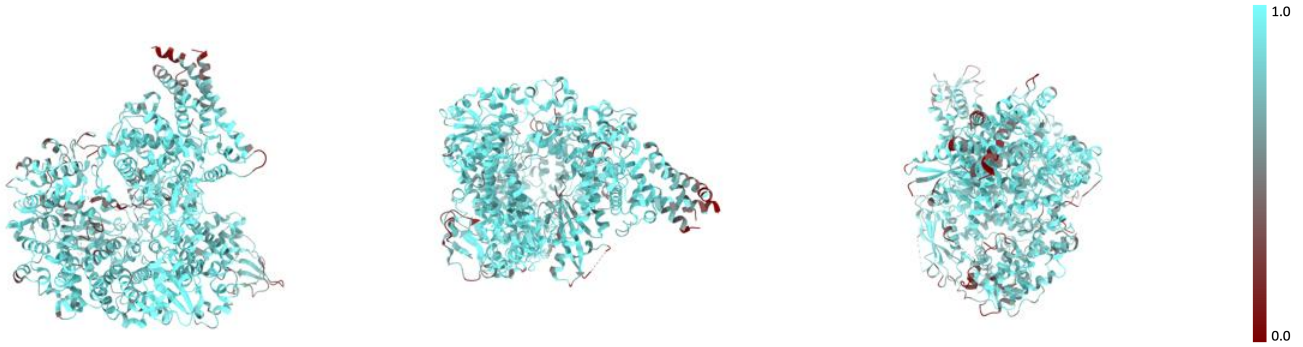
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

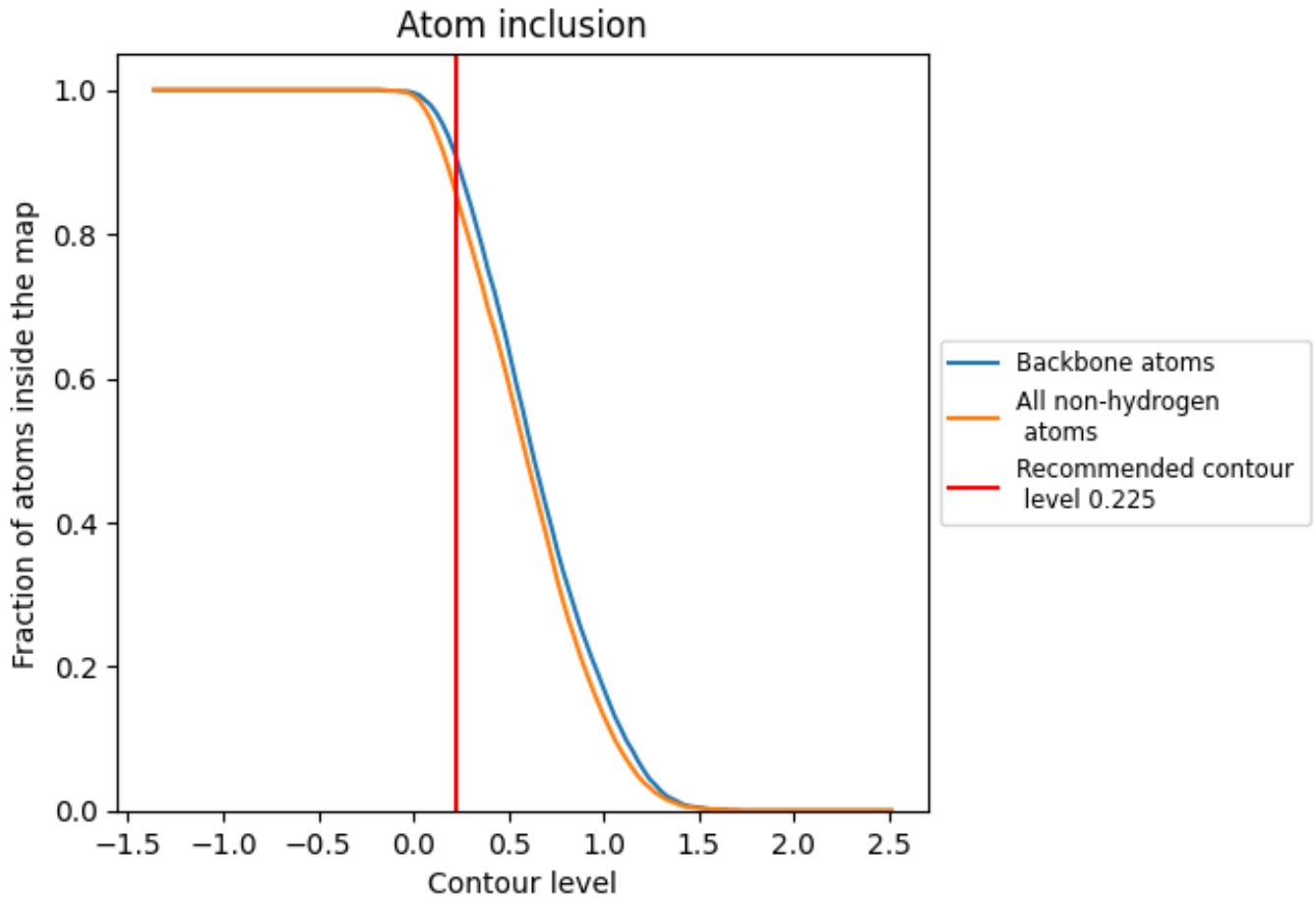
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.225).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.225) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.6050
A	0.8750	0.6110
B	0.8100	0.5900
C	0.7930	0.5870
D	0.5770	0.4850
E	0.6970	0.5500