Full wwPDB EM Validation Report ⓘ

Jul 22, 2025 – 10:31 AM EDT

PDB ID	:	9MZH / pdb_00009mzh
EMDB ID	:	EMD-45896
Title	:	Cryo-EM structure of the Nipah virus polymerase containing the connecting domain
Authors	:	Chen, Z.H.; Liang, B.
Deposited on	:	2025-01-23
Resolution	:	2.99 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:

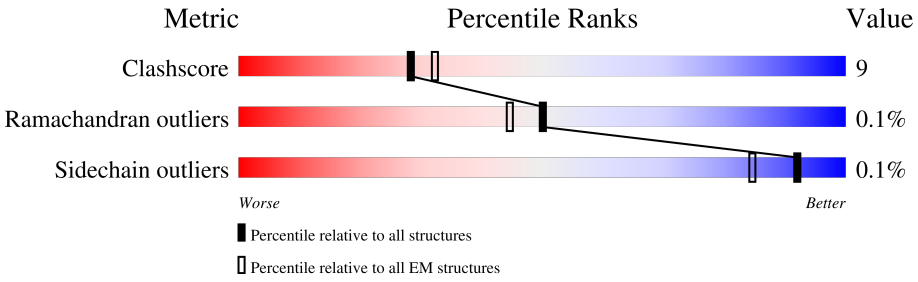
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 2.99 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	B	759	95%
1	C	759	94%
1	D	759	95%
1	E	759	5% 93%
1	G	759	5% 5% 93%
2	A	2270	12% 44% 10% 46%
2	H	2270	95%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12643 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	41	Total	C	N	O	S	0	0
			309	197	52	57	3		
1	C	47	Total	C	N	O	S	0	0
			355	224	63	65	3		
1	D	38	Total	C	N	O	S	0	0
			292	187	48	54	3		
1	E	54	Total	C	N	O	S	0	0
			421	270	70	78	3		
1	G	54	Total	C	N	O	S	0	0
			434	265	76	92	1		

There are 250 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-49	MET	-	initiating methionine	UNP Q9IK91
B	-48	LYS	-	expression tag	UNP Q9IK91
B	-47	SER	-	expression tag	UNP Q9IK91
B	-46	SER	-	expression tag	UNP Q9IK91
B	-45	TRP	-	expression tag	UNP Q9IK91
B	-44	SER	-	expression tag	UNP Q9IK91
B	-43	HIS	-	expression tag	UNP Q9IK91
B	-42	PRO	-	expression tag	UNP Q9IK91
B	-41	GLN	-	expression tag	UNP Q9IK91
B	-40	PHE	-	expression tag	UNP Q9IK91
B	-39	GLU	-	expression tag	UNP Q9IK91
B	-38	LYS	-	expression tag	UNP Q9IK91
B	-37	GLY	-	expression tag	UNP Q9IK91
B	-36	ALA	-	expression tag	UNP Q9IK91
B	-35	MET	-	expression tag	UNP Q9IK91
B	-34	THR	-	expression tag	UNP Q9IK91
B	-33	GLY	-	expression tag	UNP Q9IK91
B	-32	TRP	-	expression tag	UNP Q9IK91
B	-31	SER	-	expression tag	UNP Q9IK91
B	-30	HIS	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-29	PRO	-	expression tag	UNP Q9IK91
B	-28	GLN	-	expression tag	UNP Q9IK91
B	-27	PHE	-	expression tag	UNP Q9IK91
B	-26	GLU	-	expression tag	UNP Q9IK91
B	-25	LYS	-	expression tag	UNP Q9IK91
B	-24	GLY	-	expression tag	UNP Q9IK91
B	-23	SER	-	expression tag	UNP Q9IK91
B	-22	SER	-	expression tag	UNP Q9IK91
B	-21	ALA	-	expression tag	UNP Q9IK91
B	-20	SER	-	expression tag	UNP Q9IK91
B	-19	TRP	-	expression tag	UNP Q9IK91
B	-18	SER	-	expression tag	UNP Q9IK91
B	-17	HIS	-	expression tag	UNP Q9IK91
B	-16	PRO	-	expression tag	UNP Q9IK91
B	-15	GLN	-	expression tag	UNP Q9IK91
B	-14	PHE	-	expression tag	UNP Q9IK91
B	-13	GLU	-	expression tag	UNP Q9IK91
B	-12	LYS	-	expression tag	UNP Q9IK91
B	-11	GLY	-	expression tag	UNP Q9IK91
B	-10	ALA	-	expression tag	UNP Q9IK91
B	-9	GLU	-	expression tag	UNP Q9IK91
B	-8	ASN	-	expression tag	UNP Q9IK91
B	-7	LEU	-	expression tag	UNP Q9IK91
B	-6	TYR	-	expression tag	UNP Q9IK91
B	-5	PHE	-	expression tag	UNP Q9IK91
B	-4	GLN	-	expression tag	UNP Q9IK91
B	-3	SER	-	expression tag	UNP Q9IK91
B	-2	ASN	-	expression tag	UNP Q9IK91
B	-1	GLY	-	expression tag	UNP Q9IK91
B	0	SER	-	expression tag	UNP Q9IK91
C	-49	MET	-	initiating methionine	UNP Q9IK91
C	-48	LYS	-	expression tag	UNP Q9IK91
C	-47	SER	-	expression tag	UNP Q9IK91
C	-46	SER	-	expression tag	UNP Q9IK91
C	-45	TRP	-	expression tag	UNP Q9IK91
C	-44	SER	-	expression tag	UNP Q9IK91
C	-43	HIS	-	expression tag	UNP Q9IK91
C	-42	PRO	-	expression tag	UNP Q9IK91
C	-41	GLN	-	expression tag	UNP Q9IK91
C	-40	PHE	-	expression tag	UNP Q9IK91
C	-39	GLU	-	expression tag	UNP Q9IK91
C	-38	LYS	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-37	GLY	-	expression tag	UNP Q9IK91
C	-36	ALA	-	expression tag	UNP Q9IK91
C	-35	MET	-	expression tag	UNP Q9IK91
C	-34	THR	-	expression tag	UNP Q9IK91
C	-33	GLY	-	expression tag	UNP Q9IK91
C	-32	TRP	-	expression tag	UNP Q9IK91
C	-31	SER	-	expression tag	UNP Q9IK91
C	-30	HIS	-	expression tag	UNP Q9IK91
C	-29	PRO	-	expression tag	UNP Q9IK91
C	-28	GLN	-	expression tag	UNP Q9IK91
C	-27	PHE	-	expression tag	UNP Q9IK91
C	-26	GLU	-	expression tag	UNP Q9IK91
C	-25	LYS	-	expression tag	UNP Q9IK91
C	-24	GLY	-	expression tag	UNP Q9IK91
C	-23	SER	-	expression tag	UNP Q9IK91
C	-22	SER	-	expression tag	UNP Q9IK91
C	-21	ALA	-	expression tag	UNP Q9IK91
C	-20	SER	-	expression tag	UNP Q9IK91
C	-19	TRP	-	expression tag	UNP Q9IK91
C	-18	SER	-	expression tag	UNP Q9IK91
C	-17	HIS	-	expression tag	UNP Q9IK91
C	-16	PRO	-	expression tag	UNP Q9IK91
C	-15	GLN	-	expression tag	UNP Q9IK91
C	-14	PHE	-	expression tag	UNP Q9IK91
C	-13	GLU	-	expression tag	UNP Q9IK91
C	-12	LYS	-	expression tag	UNP Q9IK91
C	-11	GLY	-	expression tag	UNP Q9IK91
C	-10	ALA	-	expression tag	UNP Q9IK91
C	-9	GLU	-	expression tag	UNP Q9IK91
C	-8	ASN	-	expression tag	UNP Q9IK91
C	-7	LEU	-	expression tag	UNP Q9IK91
C	-6	TYR	-	expression tag	UNP Q9IK91
C	-5	PHE	-	expression tag	UNP Q9IK91
C	-4	GLN	-	expression tag	UNP Q9IK91
C	-3	SER	-	expression tag	UNP Q9IK91
C	-2	ASN	-	expression tag	UNP Q9IK91
C	-1	GLY	-	expression tag	UNP Q9IK91
C	0	SER	-	expression tag	UNP Q9IK91
D	-49	MET	-	initiating methionine	UNP Q9IK91
D	-48	LYS	-	expression tag	UNP Q9IK91
D	-47	SER	-	expression tag	UNP Q9IK91
D	-46	SER	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-45	TRP	-	expression tag	UNP Q9IK91
D	-44	SER	-	expression tag	UNP Q9IK91
D	-43	HIS	-	expression tag	UNP Q9IK91
D	-42	PRO	-	expression tag	UNP Q9IK91
D	-41	GLN	-	expression tag	UNP Q9IK91
D	-40	PHE	-	expression tag	UNP Q9IK91
D	-39	GLU	-	expression tag	UNP Q9IK91
D	-38	LYS	-	expression tag	UNP Q9IK91
D	-37	GLY	-	expression tag	UNP Q9IK91
D	-36	ALA	-	expression tag	UNP Q9IK91
D	-35	MET	-	expression tag	UNP Q9IK91
D	-34	THR	-	expression tag	UNP Q9IK91
D	-33	GLY	-	expression tag	UNP Q9IK91
D	-32	TRP	-	expression tag	UNP Q9IK91
D	-31	SER	-	expression tag	UNP Q9IK91
D	-30	HIS	-	expression tag	UNP Q9IK91
D	-29	PRO	-	expression tag	UNP Q9IK91
D	-28	GLN	-	expression tag	UNP Q9IK91
D	-27	PHE	-	expression tag	UNP Q9IK91
D	-26	GLU	-	expression tag	UNP Q9IK91
D	-25	LYS	-	expression tag	UNP Q9IK91
D	-24	GLY	-	expression tag	UNP Q9IK91
D	-23	SER	-	expression tag	UNP Q9IK91
D	-22	SER	-	expression tag	UNP Q9IK91
D	-21	ALA	-	expression tag	UNP Q9IK91
D	-20	SER	-	expression tag	UNP Q9IK91
D	-19	TRP	-	expression tag	UNP Q9IK91
D	-18	SER	-	expression tag	UNP Q9IK91
D	-17	HIS	-	expression tag	UNP Q9IK91
D	-16	PRO	-	expression tag	UNP Q9IK91
D	-15	GLN	-	expression tag	UNP Q9IK91
D	-14	PHE	-	expression tag	UNP Q9IK91
D	-13	GLU	-	expression tag	UNP Q9IK91
D	-12	LYS	-	expression tag	UNP Q9IK91
D	-11	GLY	-	expression tag	UNP Q9IK91
D	-10	ALA	-	expression tag	UNP Q9IK91
D	-9	GLU	-	expression tag	UNP Q9IK91
D	-8	ASN	-	expression tag	UNP Q9IK91
D	-7	LEU	-	expression tag	UNP Q9IK91
D	-6	TYR	-	expression tag	UNP Q9IK91
D	-5	PHE	-	expression tag	UNP Q9IK91
D	-4	GLN	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	SER	-	expression tag	UNP Q9IK91
D	-2	ASN	-	expression tag	UNP Q9IK91
D	-1	GLY	-	expression tag	UNP Q9IK91
D	0	SER	-	expression tag	UNP Q9IK91
E	-49	MET	-	initiating methionine	UNP Q9IK91
E	-48	LYS	-	expression tag	UNP Q9IK91
E	-47	SER	-	expression tag	UNP Q9IK91
E	-46	SER	-	expression tag	UNP Q9IK91
E	-45	TRP	-	expression tag	UNP Q9IK91
E	-44	SER	-	expression tag	UNP Q9IK91
E	-43	HIS	-	expression tag	UNP Q9IK91
E	-42	PRO	-	expression tag	UNP Q9IK91
E	-41	GLN	-	expression tag	UNP Q9IK91
E	-40	PHE	-	expression tag	UNP Q9IK91
E	-39	GLU	-	expression tag	UNP Q9IK91
E	-38	LYS	-	expression tag	UNP Q9IK91
E	-37	GLY	-	expression tag	UNP Q9IK91
E	-36	ALA	-	expression tag	UNP Q9IK91
E	-35	MET	-	expression tag	UNP Q9IK91
E	-34	THR	-	expression tag	UNP Q9IK91
E	-33	GLY	-	expression tag	UNP Q9IK91
E	-32	TRP	-	expression tag	UNP Q9IK91
E	-31	SER	-	expression tag	UNP Q9IK91
E	-30	HIS	-	expression tag	UNP Q9IK91
E	-29	PRO	-	expression tag	UNP Q9IK91
E	-28	GLN	-	expression tag	UNP Q9IK91
E	-27	PHE	-	expression tag	UNP Q9IK91
E	-26	GLU	-	expression tag	UNP Q9IK91
E	-25	LYS	-	expression tag	UNP Q9IK91
E	-24	GLY	-	expression tag	UNP Q9IK91
E	-23	SER	-	expression tag	UNP Q9IK91
E	-22	SER	-	expression tag	UNP Q9IK91
E	-21	ALA	-	expression tag	UNP Q9IK91
E	-20	SER	-	expression tag	UNP Q9IK91
E	-19	TRP	-	expression tag	UNP Q9IK91
E	-18	SER	-	expression tag	UNP Q9IK91
E	-17	HIS	-	expression tag	UNP Q9IK91
E	-16	PRO	-	expression tag	UNP Q9IK91
E	-15	GLN	-	expression tag	UNP Q9IK91
E	-14	PHE	-	expression tag	UNP Q9IK91
E	-13	GLU	-	expression tag	UNP Q9IK91
E	-12	LYS	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	GLY	-	expression tag	UNP Q9IK91
E	-10	ALA	-	expression tag	UNP Q9IK91
E	-9	GLU	-	expression tag	UNP Q9IK91
E	-8	ASN	-	expression tag	UNP Q9IK91
E	-7	LEU	-	expression tag	UNP Q9IK91
E	-6	TYR	-	expression tag	UNP Q9IK91
E	-5	PHE	-	expression tag	UNP Q9IK91
E	-4	GLN	-	expression tag	UNP Q9IK91
E	-3	SER	-	expression tag	UNP Q9IK91
E	-2	ASN	-	expression tag	UNP Q9IK91
E	-1	GLY	-	expression tag	UNP Q9IK91
E	0	SER	-	expression tag	UNP Q9IK91
G	-49	MET	-	initiating methionine	UNP Q9IK91
G	-48	LYS	-	expression tag	UNP Q9IK91
G	-47	SER	-	expression tag	UNP Q9IK91
G	-46	SER	-	expression tag	UNP Q9IK91
G	-45	TRP	-	expression tag	UNP Q9IK91
G	-44	SER	-	expression tag	UNP Q9IK91
G	-43	HIS	-	expression tag	UNP Q9IK91
G	-42	PRO	-	expression tag	UNP Q9IK91
G	-41	GLN	-	expression tag	UNP Q9IK91
G	-40	PHE	-	expression tag	UNP Q9IK91
G	-39	GLU	-	expression tag	UNP Q9IK91
G	-38	LYS	-	expression tag	UNP Q9IK91
G	-37	GLY	-	expression tag	UNP Q9IK91
G	-36	ALA	-	expression tag	UNP Q9IK91
G	-35	MET	-	expression tag	UNP Q9IK91
G	-34	THR	-	expression tag	UNP Q9IK91
G	-33	GLY	-	expression tag	UNP Q9IK91
G	-32	TRP	-	expression tag	UNP Q9IK91
G	-31	SER	-	expression tag	UNP Q9IK91
G	-30	HIS	-	expression tag	UNP Q9IK91
G	-29	PRO	-	expression tag	UNP Q9IK91
G	-28	GLN	-	expression tag	UNP Q9IK91
G	-27	PHE	-	expression tag	UNP Q9IK91
G	-26	GLU	-	expression tag	UNP Q9IK91
G	-25	LYS	-	expression tag	UNP Q9IK91
G	-24	GLY	-	expression tag	UNP Q9IK91
G	-23	SER	-	expression tag	UNP Q9IK91
G	-22	SER	-	expression tag	UNP Q9IK91
G	-21	ALA	-	expression tag	UNP Q9IK91
G	-20	SER	-	expression tag	UNP Q9IK91

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-19	TRP	-	expression tag	UNP Q9IK91
G	-18	SER	-	expression tag	UNP Q9IK91
G	-17	HIS	-	expression tag	UNP Q9IK91
G	-16	PRO	-	expression tag	UNP Q9IK91
G	-15	GLN	-	expression tag	UNP Q9IK91
G	-14	PHE	-	expression tag	UNP Q9IK91
G	-13	GLU	-	expression tag	UNP Q9IK91
G	-12	LYS	-	expression tag	UNP Q9IK91
G	-11	GLY	-	expression tag	UNP Q9IK91
G	-10	ALA	-	expression tag	UNP Q9IK91
G	-9	GLU	-	expression tag	UNP Q9IK91
G	-8	ASN	-	expression tag	UNP Q9IK91
G	-7	LEU	-	expression tag	UNP Q9IK91
G	-6	TYR	-	expression tag	UNP Q9IK91
G	-5	PHE	-	expression tag	UNP Q9IK91
G	-4	GLN	-	expression tag	UNP Q9IK91
G	-3	SER	-	expression tag	UNP Q9IK91
G	-2	ASN	-	expression tag	UNP Q9IK91
G	-1	GLY	-	expression tag	UNP Q9IK91
G	0	SER	-	expression tag	UNP Q9IK91

- Molecule 2 is a protein called RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	121	Total	C	N	O	S	0	0
			979	634	158	182	5		
2	A	1220	Total	C	N	O	S	0	0
			9853	6288	1686	1813	66		

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-25	MET	-	expression tag	UNP Q997F0
H	-24	LYS	-	expression tag	UNP Q997F0
H	-23	SER	-	expression tag	UNP Q997F0
H	-22	SER	-	expression tag	UNP Q997F0
H	-21	HIS	-	expression tag	UNP Q997F0
H	-20	HIS	-	expression tag	UNP Q997F0
H	-19	HIS	-	expression tag	UNP Q997F0
H	-18	HIS	-	expression tag	UNP Q997F0
H	-17	HIS	-	expression tag	UNP Q997F0
H	-16	HIS	-	expression tag	UNP Q997F0

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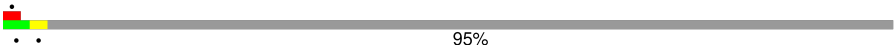
Chain	Residue	Modelled	Actual	Comment	Reference
H	-15	HIS	-	expression tag	UNP Q997F0
H	-14	HIS	-	expression tag	UNP Q997F0
H	-13	HIS	-	expression tag	UNP Q997F0
H	-12	HIS	-	expression tag	UNP Q997F0
H	-11	GLY	-	expression tag	UNP Q997F0
H	-10	SER	-	expression tag	UNP Q997F0
H	-9	SER	-	expression tag	UNP Q997F0
H	-8	GLU	-	expression tag	UNP Q997F0
H	-7	ASN	-	expression tag	UNP Q997F0
H	-6	LEU	-	expression tag	UNP Q997F0
H	-5	TYR	-	expression tag	UNP Q997F0
H	-4	PHE	-	expression tag	UNP Q997F0
H	-3	GLN	-	expression tag	UNP Q997F0
H	-2	SER	-	expression tag	UNP Q997F0
H	-1	GLY	-	expression tag	UNP Q997F0
H	0	SER	-	expression tag	UNP Q997F0
A	-25	MET	-	expression tag	UNP Q997F0
A	-24	LYS	-	expression tag	UNP Q997F0
A	-23	SER	-	expression tag	UNP Q997F0
A	-22	SER	-	expression tag	UNP Q997F0
A	-21	HIS	-	expression tag	UNP Q997F0
A	-20	HIS	-	expression tag	UNP Q997F0
A	-19	HIS	-	expression tag	UNP Q997F0
A	-18	HIS	-	expression tag	UNP Q997F0
A	-17	HIS	-	expression tag	UNP Q997F0
A	-16	HIS	-	expression tag	UNP Q997F0
A	-15	HIS	-	expression tag	UNP Q997F0
A	-14	HIS	-	expression tag	UNP Q997F0
A	-13	HIS	-	expression tag	UNP Q997F0
A	-12	HIS	-	expression tag	UNP Q997F0
A	-11	GLY	-	expression tag	UNP Q997F0
A	-10	SER	-	expression tag	UNP Q997F0
A	-9	SER	-	expression tag	UNP Q997F0
A	-8	GLU	-	expression tag	UNP Q997F0
A	-7	ASN	-	expression tag	UNP Q997F0
A	-6	LEU	-	expression tag	UNP Q997F0
A	-5	TYR	-	expression tag	UNP Q997F0
A	-4	PHE	-	expression tag	UNP Q997F0
A	-3	GLN	-	expression tag	UNP Q997F0
A	-2	SER	-	expression tag	UNP Q997F0
A	-1	GLY	-	expression tag	UNP Q997F0
A	0	SER	-	expression tag	UNP Q997F0

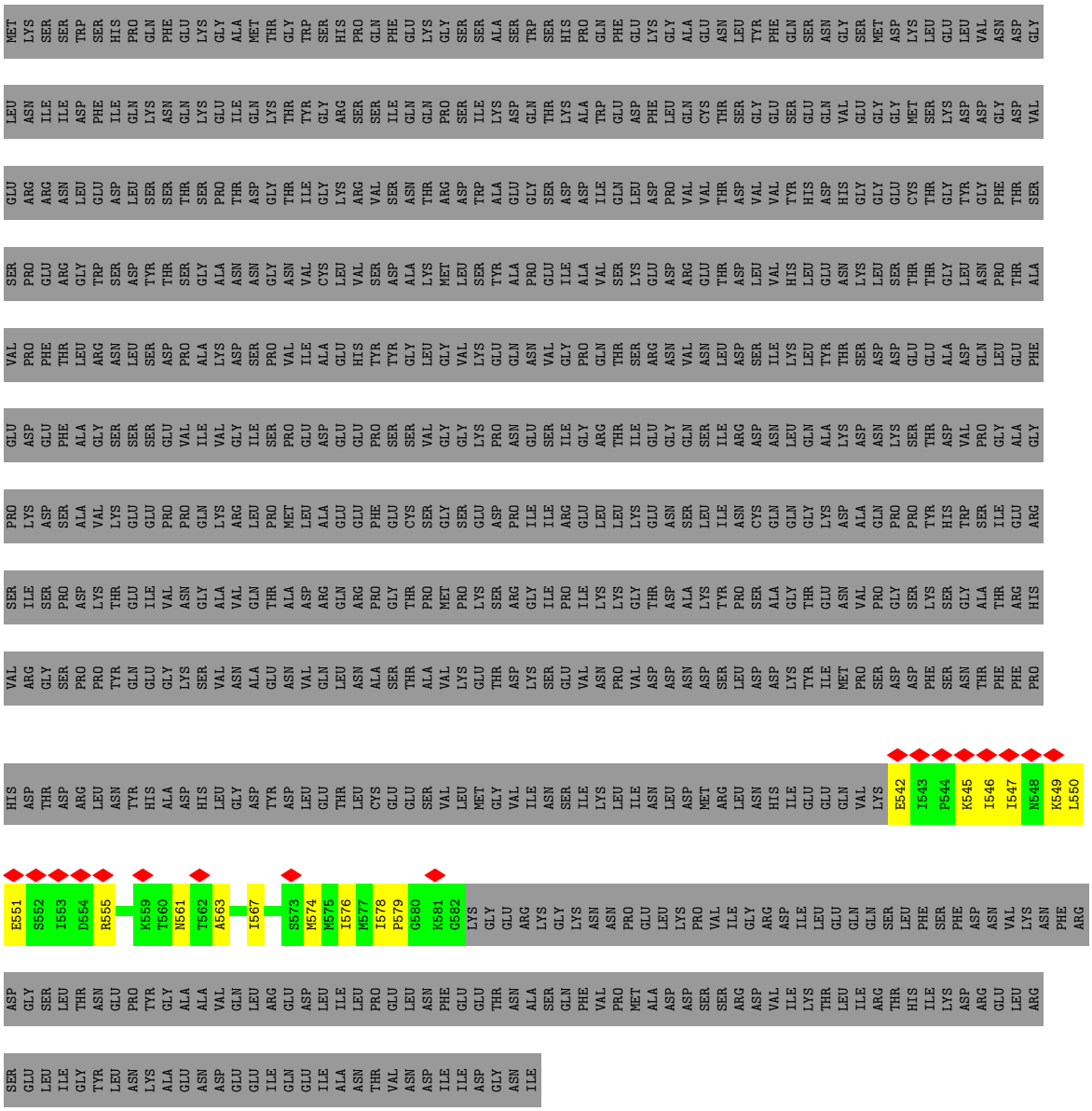
3 Residue-property plots (i)

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: Phosphoprotein

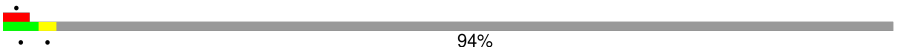
Chain B:

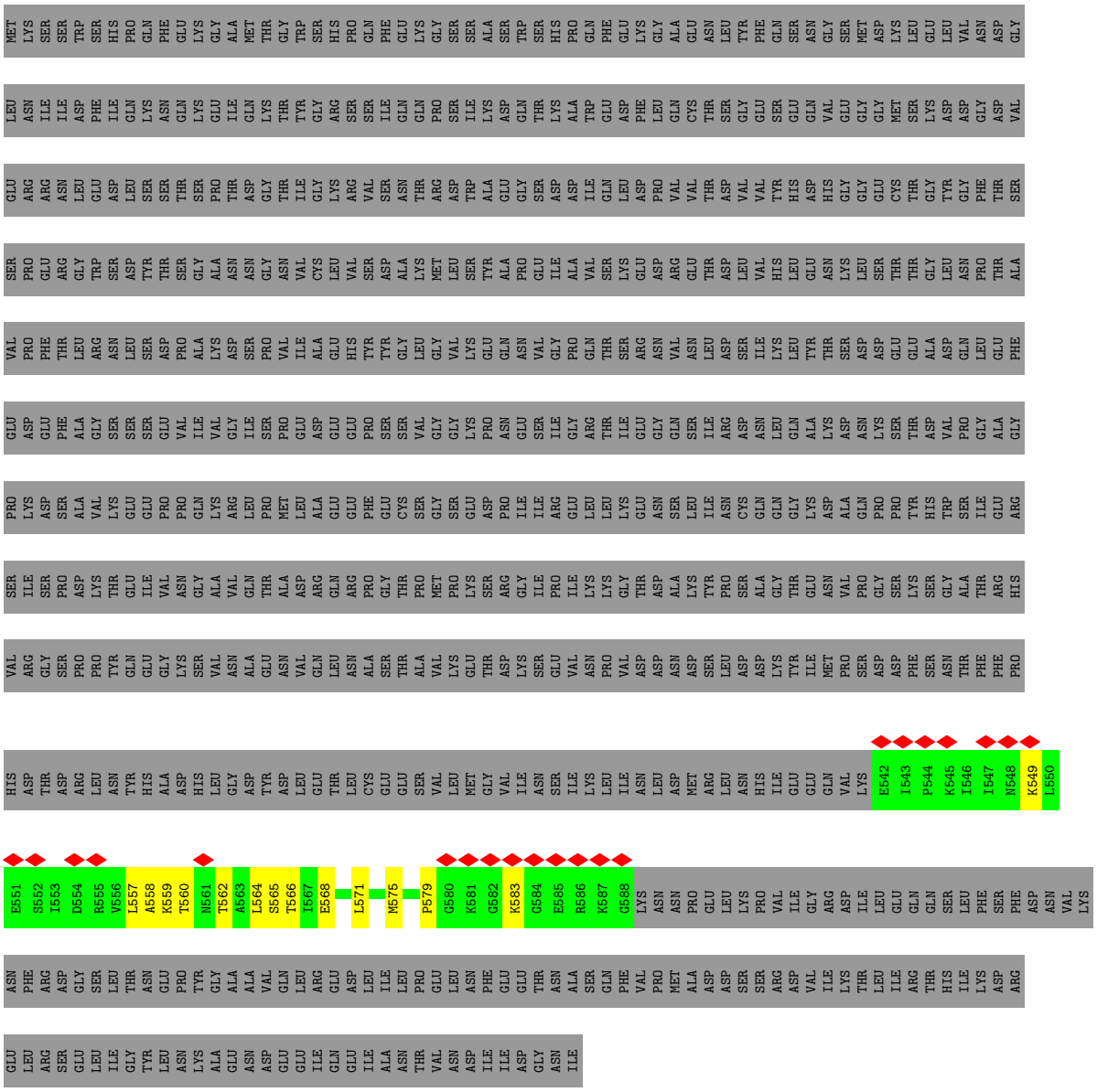




• Molecule 1: Phosphoprotein

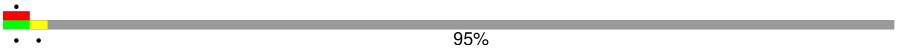
Chain C:

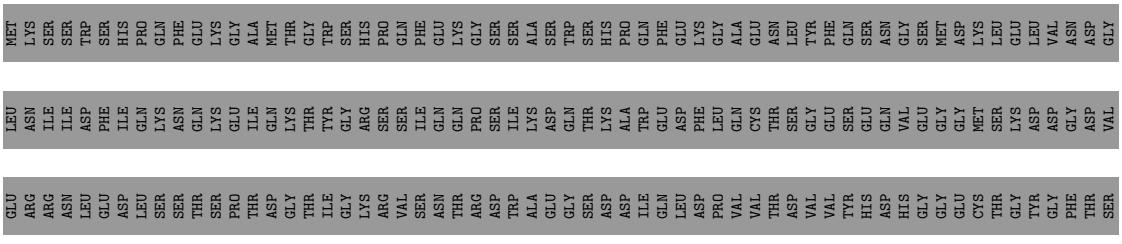


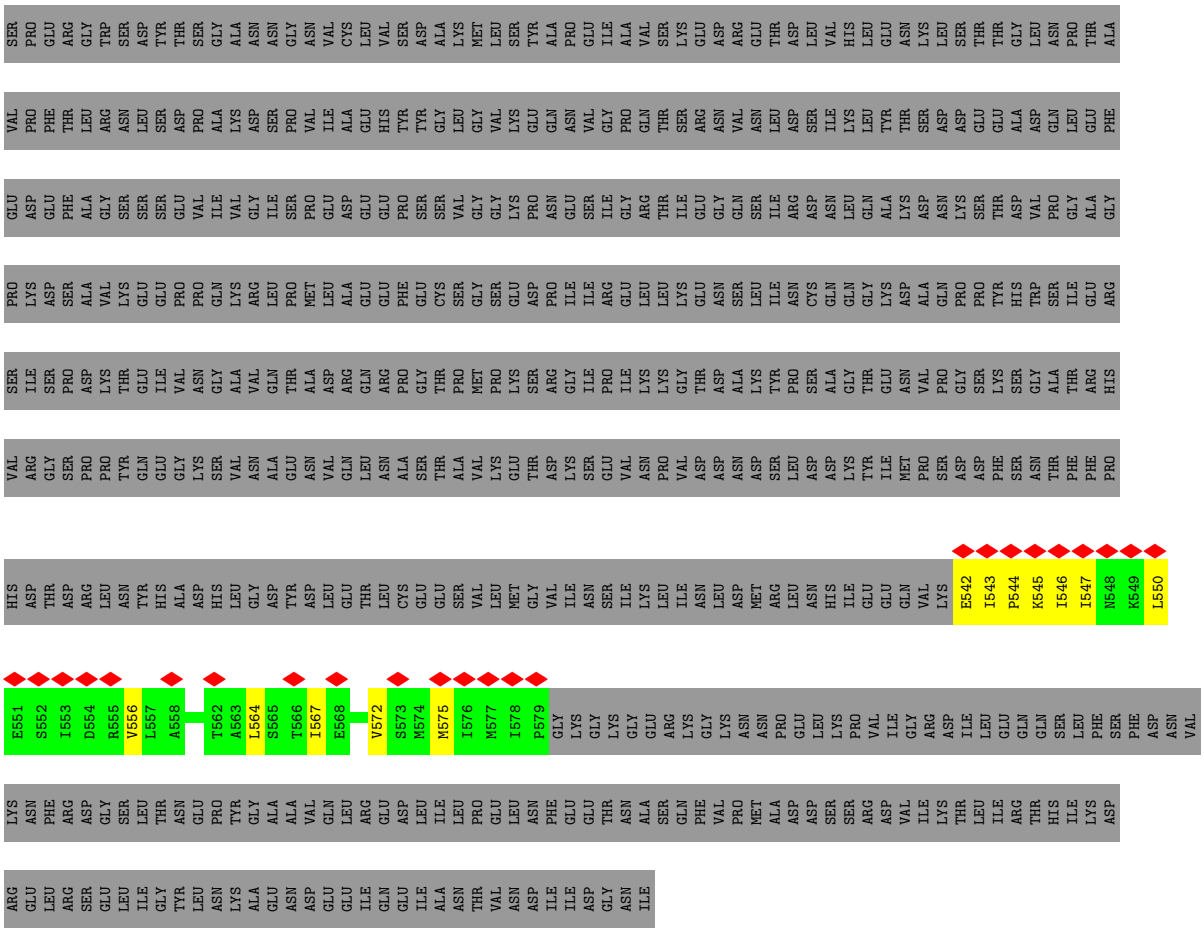


• Molecule 1: Phosphoprotein

Chain D:

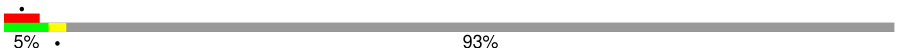


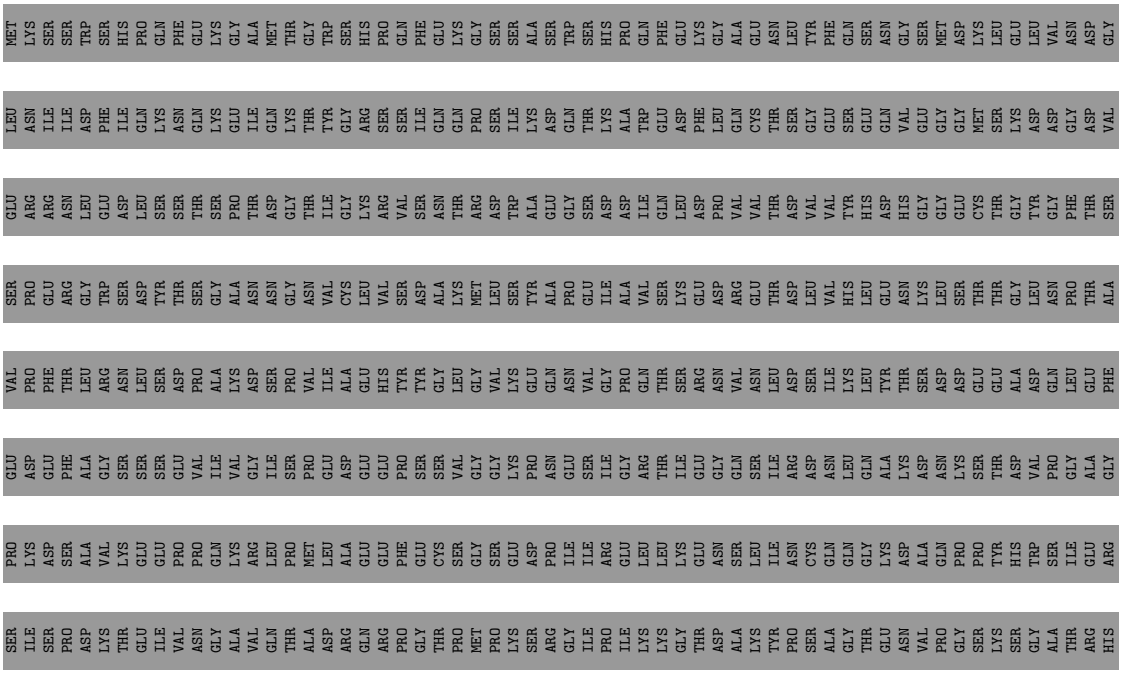


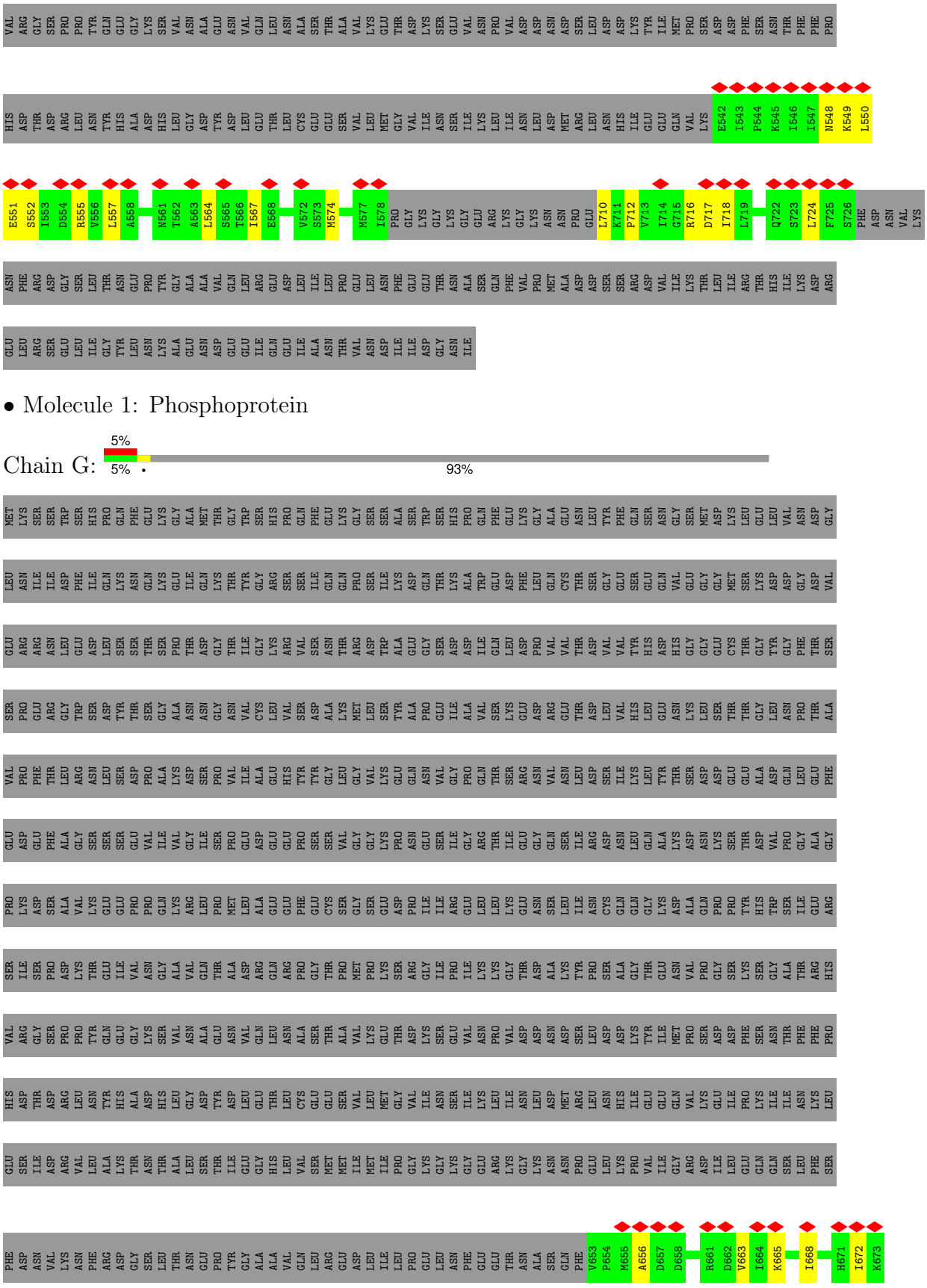


• Molecule 1: Phosphoprotein

Chain E:

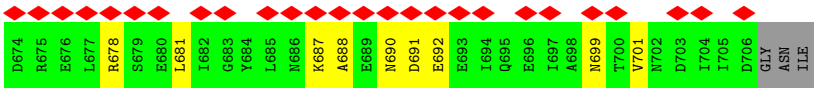






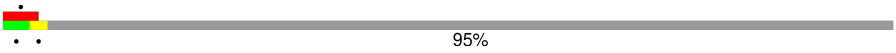
- Molecule 1: Phosphoprotein

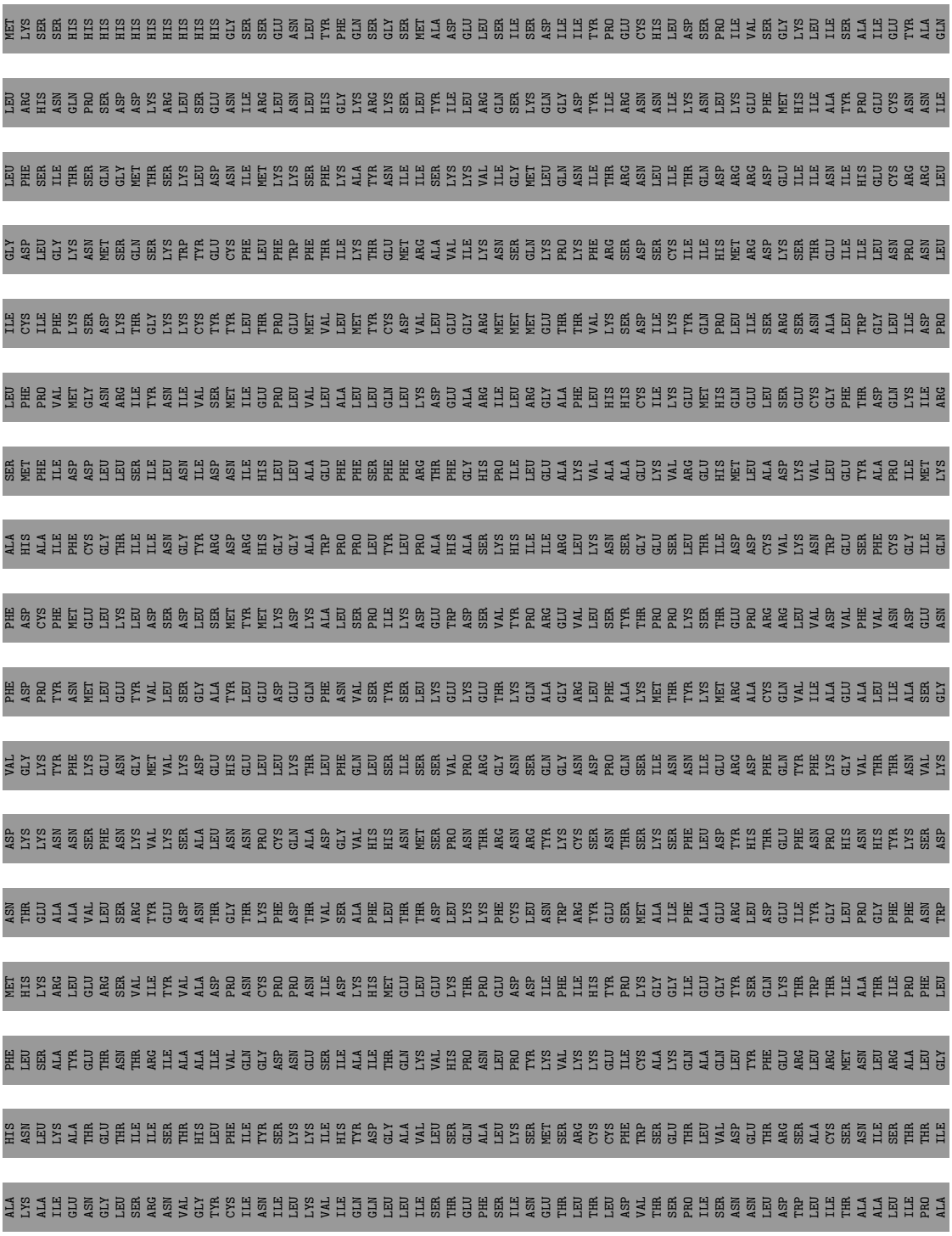
Chain G:

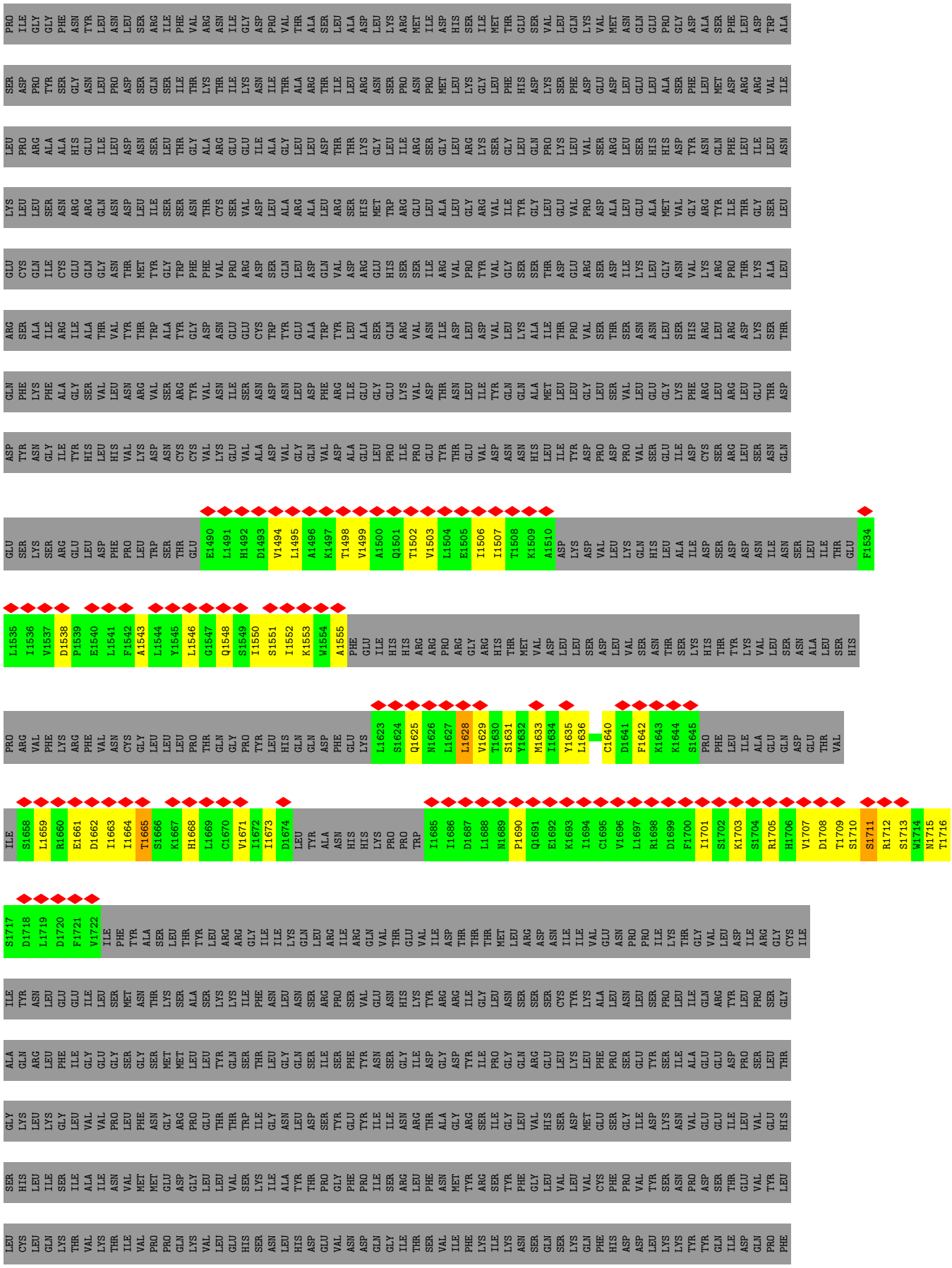


• Molecule 2: RNA-directed RNA polymerase L

Chain H:



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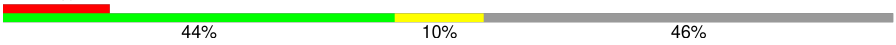
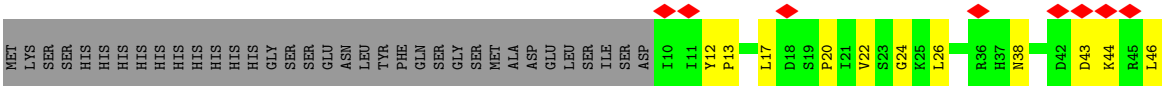
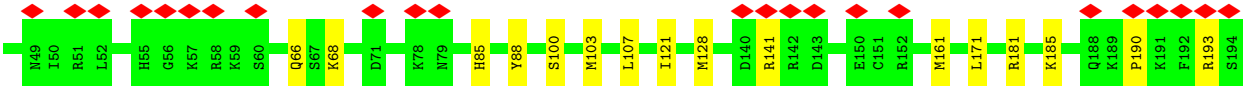
SER ASP PRO TYR SER GLY ASN LEU PRO ASP SER GLN SER ILE THR LYS THR ILE LYS ASN ILE THR ALA ARG THR ILE LEU ARG ASN GLY PRO ASN PRO MET LEU LYS GLY LEU PHE HIS SER ASP LYS SER PHE ASP GLU ASP LEU GLU GLU LEU ALA SER PHE LEU MET ASP ARG ARG VAL ILE
LEU PRO ARG ALA ALA HIS GLU ILE LEU ASP ASN SER LEU THR GLY ALA ARG GLU GLU ILE ALA GLY LEU LEU ASP THR THR LYS GLY LEU ILE ARG GLU ALA LEU SER HIS HIS ASP TYR ASN GLN PHE LEU ILE ASN
LYS LEU LEU SER ASN ARG ARG GLN ASN ASP LEU ILE SER SER ASN THR CYS SER VAL ASP LEU ALA ARG ALA LEU ARG SER HIS MET TRP ARG GLU LEU ILE ARG GLU LEU ALA LEU GLY ARG TYR ILE THR GLY SER LEU
GLU CYS GLN ILE CYS GLU GLN GLY ASN THR MET TYR GLY TRP PHE PHE VAL PRO ARG ASP SER GLN LEU ASP GLN VAL ASP ARG GLU HIS SER SER ILE ARG LEU GLY ASN VAL LYS LYS LEU ALA
ARG SER ALA ILE ARG ILE ALA THR VAL TYR THR THR TRP ALA TYR GLY ASP ASN GLU GLU CYS TRP TYR GLU ALA TRP TYR LEU ASP PHE ARG ILE GLU GLY GLU LYS VAL ASN ILE ASP LEU VAL LEU LYS ALA ILE THR PRO VAL SER ASP ILE LYS LEU ARG LEU ARG ASP LYS SER THR
GLN PHE LYS PHE ALA GLY SER VAL LEU ASN ARG VAL SER ARG TYR VAL ASN LEU ASP PHE ARG ILE GLU GLY GLU LYS VAL ASP THR ASN LEU ILE TYR GLN GLN ALA MET LEU LEU LEU GLY LEU SER VAL LEU GLU GLY GLY LYS PHE ARG LEU ARG LEU GLU THR ASP
ASP TYR ASN GLY ILE TYR HIS LEU HIS VAL LYS ASP ASN CYS CYS VAL LYS GLU VAL ALA ASP VAL GLY GLN VAL ASP ALA GLU LEU PRO ILE PRO GLU TYR THR GLU VAL ASP ASN ASN HIS LEU ILE TYR ASP PRO ASP PRO VAL SER GLU ILE ASP CYS SER ARG LEU SER ASN GLN
GLU SER LYS SER ARG GLU LEU ASP PHE PRO LEU TRP SER THR GLU E1490 L1491 H1492 D1493 V1494 L1495 A1496 K1497 T1498 V1499 A1500 Q1501 T1502 V1503 L1504 E1505 I1506 I1507 T1508 K1509 A1510 ASP LYS ASP VAL LEU LYS GLN HIS LEU ALA ILE ASP SER ASP ASP ASN ILE ASN SER LEU ILE THR GLU F1534
L1535 I1536 V1537 D1538 P1539 E1540 L1541 F1542 A1543 L1544 Y1545 L1546 G1547 Q1548 S1549 I1550 S1551 I1552 K1553 W1554 A1555 PHE GLU ILE HIS HIS ARG ARG PRO ARG GLY ARG HIS THR MET VAL ASP LEU LEU SER ASP LEU VAL SER ASN THR SER LYS HIS THR TYR LYS VAL LEU SER ASN ALA LEU SER HIS
PRO ARG VAL PHE LYS ARG PHE VAL ASN CYS GLY LEU LEU LEU PRO THR GLN GLY PRO TYR LEU HIS GLN GLN ASP PHE GLU LYS L1623 S1624 Q1625 N1626 L1627 L1628 V1629 T1630 S1631 Y1632 M1633 I1634 Y1635 L1636 C1640 D1641 F1642 K1643 K1644 S1645 PRO PHE LEU ILE ALA GLU GLN ASP GLU THR VAL
ILE S1658 L1659 R1660 E1661 D1662 I1663 I1664 T1665 S1666 K1667 H1668 L1669 C1670 V1671 I1672 I1673 D1674 LEU TYR ALA ASN HIS HIS LYS PRO PRO TRP I1685 I1686 D1687 L1688 M1689 P1690 Q1691 E1692 K1693 I1694 C1695 V1696 L1697 R1698 D1699 F1700 I1701 S1702 K1703 S1704 R1705 H1706 V1707 D1708 T1709 S1710 S1711 R1712 S1713 W1714 N1715 T1716
S1717 D1718 L1719 D1720 F1721 V1722 ILE PHE TYR ALA SER LEU THR TYR LEU ARG ARG GLY ILE ILE LYS GLN LEU ARG ILE ARG GLN VAL THR GLU VAL ILE ASP THR THR THR MET LEU ARG ASP ASN ILE ILE VAL GLU ASN PRO PRO ILE LYS THR GLY VAL LEU ASP ILE ARG GLY CYS ILE
ILE TYR ASN LEU GLU GLU ILE LEU SER MET ASN THR LYS SER ALA SER LYS LYS ILE PHE ASN LEU ASN SER ARG PRO SER VAL GLU ASN HIS LYS TYR ARG ARG ILE GLY LEU ASN SER SER SER CYS TYR TYR LYS ALA LEU ASN LEU SER PRO LEU ILE GLN ARG TYR LEU PRO SER GLY
ALA GLN ARG LEU PHE ILE GLY GLU GLY SER GLY SER MET MET LEU LEU TYR TYR GLN SER THR LEU GLY GLN SER ILE SER SER PHE TYR ASN SER GLY ILE ASP GLY ASP TYR ILE PRO GLY GLN ARG GLU LEU LYS LEU PHE PRO SER GLU GLU ASP PRO SER LEU THR
GLY LYS LEU LYS GLY VAL VAL PRO LEU PHE ASN GLY ARG PRO GLU THR TRP ILE GLY ASN LEU ASP TYR SER TYR GLU TYR ILE ILE ASN ARG THR ALA GLY ARG SER ILE GLY LEU VAL HIS SER ASP MET GLU SER GLY ILE ASP LYS ASN VAL GLU GLU ILE LEU VAL GLU HIS
SER HIS LEU ILE SER ILE ALA ILE ASN LEU VAL MET MET GLU ASP GLY LEU LEU VAL SER LYS ILE ALA TYR THR PRO GLY PHE PRO ILE SER ARG LEU PHE ASN MET TYR ARG SER ILE TYR PHE GLY LEU VAL LEU VAL CYS PHE PRO VAL TYR SER ASN PRO ASP SER THR GLU VAL TYR LEU
LEU CYS LEU GLN LYS THR ILE VAL LYS THR VAL LEU GLU HIS SER ASN LEU HIS ASP GLU VAL ASN ASP GLN GLY ILE THR SER VAL ILE PHE LYS ILE LYS ASN SER GLN SER LYS GLN PHE HIS ASP ASP LEU LYS LYS TYR TYR GLN ILE ASP GLN PRO PHE

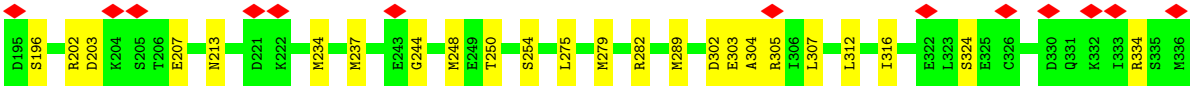
• Molecule 2: RNA-directed RNA polymerase L

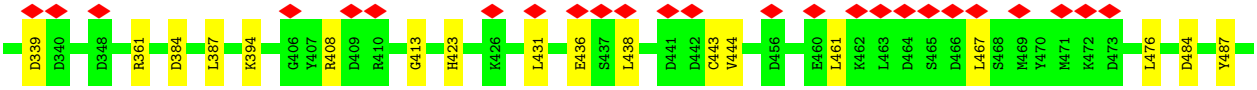
Chain A:

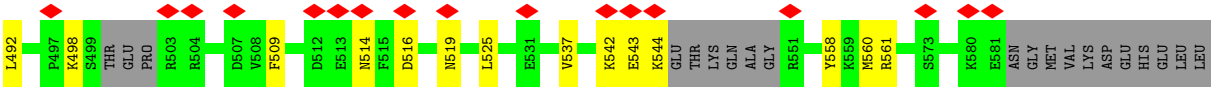


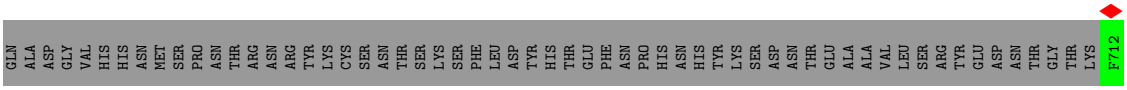


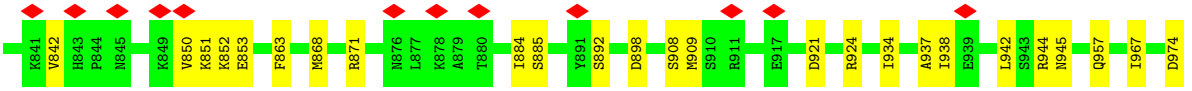


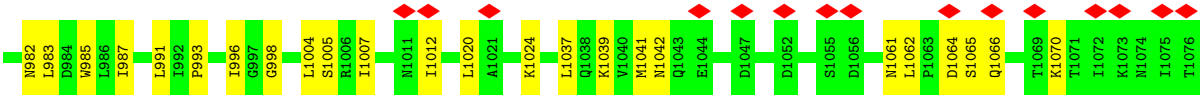


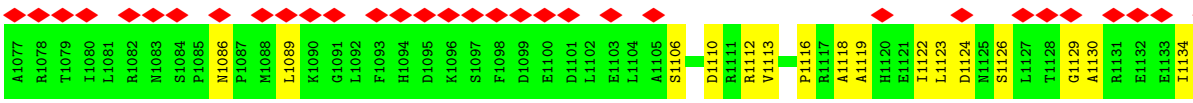


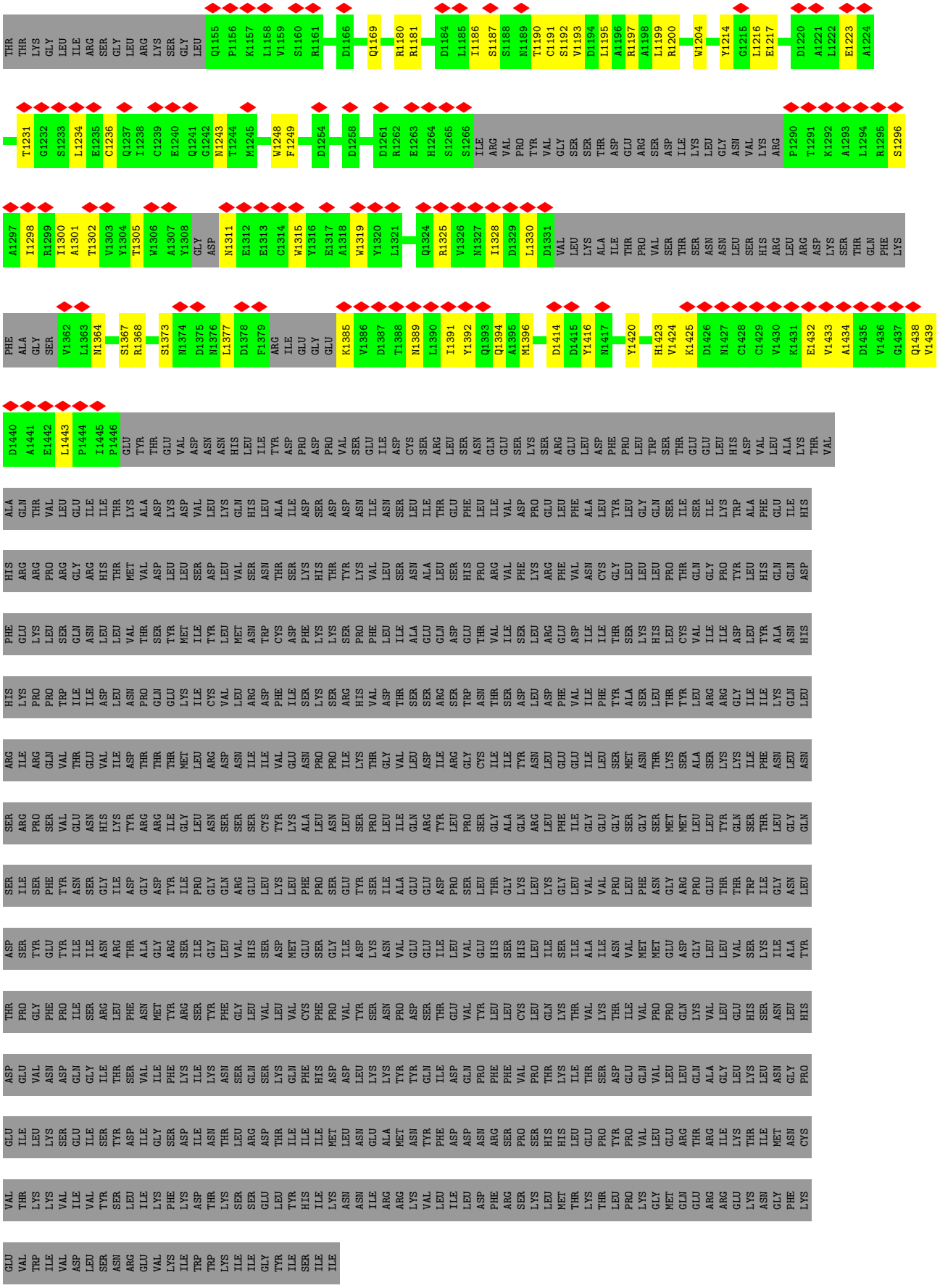











THR THR LYS GLY LEU ILE ARG SER GLY LEU LYS ARG LEU GLU ILE ILE ARG LEU ILE ILE ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68791	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 ($e^-/Å^2$)	52.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.481	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	322.56, 322.56, 322.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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	B	0.14	0/311	0.32	0/417
1	C	0.15	0/357	0.39	0/475
1	D	0.14	0/294	0.33	0/396
1	E	0.09	0/423	0.24	0/567
1	G	0.09	0/436	0.24	0/588
2	A	0.09	0/10054	0.26	1/13581 (0.0%)
2	H	0.12	0/993	0.35	0/1341
All	All	0.10	0/12868	0.27	1/17365 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	788	ASP	CB-CA-C	-5.13	109.15	116.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	309	0	340	18	0
1	C	355	0	391	16	0
1	D	292	0	321	11	0
1	E	421	0	458	16	0
1	G	434	0	431	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	9853	0	9891	156	0
2	H	979	0	1000	33	0
All	All	12643	0	12832	237	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 9.

All (237) 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)
2:A:324:SER:OG	2:A:334:ARG:NH1	2.14	0.81
2:A:993:PRO:HD2	2:A:996:ILE:HD11	1.68	0.74
2:A:868:MET:SD	2:A:871:ARG:NH2	2.61	0.74
2:A:1062:LEU:HB2	2:A:1065:SER:HB3	1.70	0.73
2:A:1066:GLN:HE21	2:A:1070:LYS:HE2	1.56	0.71
1:B:542:GLU:HB3	1:B:545:LYS:HG2	1.74	0.69
1:C:557:LEU:HD11	1:D:556:VAL:HG11	1.74	0.68
2:A:1249:PHE:HB2	2:A:1420:TYR:HB3	1.77	0.67
2:H:1705:ARG:NH1	2:H:1716:THR:OG1	2.28	0.67
2:H:1709:THR:HG23	2:A:1180:ARG:HH12	1.60	0.66
1:B:549:LYS:HD2	1:E:550:LEU:HD23	1.76	0.66
2:A:1391:ILE:HB	2:A:1394:GLN:HB2	1.76	0.66
1:B:549:LYS:NZ	1:E:551:GLU:OE1	2.27	0.66
2:A:17:LEU:HD22	2:A:237:MET:HB2	1.78	0.64
1:G:699:ASN:OD1	2:A:305:ARG:NH2	2.31	0.64
2:H:1710:SER:O	2:H:1712:ARG:N	2.30	0.64
2:A:88:TYR:HE1	2:A:237:MET:HE1	1.63	0.63
1:E:574:MET:HG3	1:E:712:PRO:HB3	1.81	0.63
2:A:1130:ALA:O	2:A:1134:ILE:HD12	1.98	0.63
1:B:561:ASN:OD1	1:C:560:THR:OG1	2.14	0.62
2:H:1543:ALA:O	2:H:1631:SER:OG	2.11	0.62
2:A:26:LEU:HD22	2:A:234:MET:HE1	1.81	0.62
1:B:574:MET:HA	1:E:712:PRO:HD2	1.80	0.62
1:B:579:PRO:HG2	1:E:718:ILE:HD11	1.81	0.62
1:C:568:GLU:HG3	1:D:567:ILE:HD11	1.80	0.62
2:A:431:LEU:HD22	2:A:436:GLU:HB3	1.82	0.61
2:H:1495:LEU:O	2:H:1499:VAL:HG23	2.01	0.61
2:A:1112:ARG:NH1	2:A:1438:GLN:O	2.34	0.61
2:A:755:MET:HE1	2:A:801:TYR:HB3	1.84	0.60
1:C:579:PRO:HG2	1:E:716:ARG:HD3	1.82	0.60
2:H:1551:SER:O	2:H:1555:ALA:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1673:ILE:HD11	2:H:1701:ILE:HG12	1.84	0.59
2:H:1552:ILE:HD13	2:H:1668:HIS:HB2	1.84	0.59
1:C:583:LYS:NZ	2:A:744:GLU:OE2	2.36	0.59
1:G:665:LYS:NZ	2:A:339:ASP:OD2	2.35	0.59
2:A:898:ASP:O	2:A:1368:ARG:NH1	2.35	0.59
2:H:1662:ASP:HB2	2:H:1690:PRO:HG3	1.84	0.59
2:A:1301:ALA:O	2:A:1305:THR:HG23	2.02	0.59
2:A:842:VAL:HG21	2:A:851:LYS:HG2	1.85	0.58
1:G:668:ILE:HD13	1:G:681:LEU:HB3	1.86	0.58
2:A:719:LEU:HD11	2:A:863:PHE:HB2	1.84	0.58
2:A:509:PHE:O	2:A:1086:ASN:ND2	2.37	0.57
2:A:1223:GLU:O	2:A:1425:LYS:NZ	2.36	0.57
1:D:572:VAL:HA	1:D:575:MET:HE2	1.86	0.57
2:A:1214:TYR:OH	2:A:1433:VAL:O	2.21	0.57
2:A:161:MET:HE2	2:A:957:GLN:HE22	1.70	0.57
1:E:724:LEU:HD23	1:E:724:LEU:H	1.70	0.56
2:A:185:LYS:NZ	2:A:967:ILE:O	2.38	0.56
1:C:558:ALA:O	1:C:562:THR:HG23	2.05	0.56
2:A:983:LEU:O	2:A:987:ILE:HD12	2.04	0.56
2:H:1502:THR:O	2:H:1506:ILE:HB	2.06	0.56
2:A:1243:ASN:ND2	2:A:1424:VAL:O	2.39	0.56
2:A:938:ILE:HA	2:A:942:LEU:HB3	1.88	0.56
2:A:909:MET:HE1	2:A:934:ILE:HD13	1.87	0.55
2:A:1064:ASP:O	2:A:1169:GLN:NE2	2.38	0.55
2:H:1494:VAL:O	2:H:1498:THR:HG23	2.05	0.55
2:A:467:LEU:HD11	2:A:1089:LEU:HB3	1.89	0.55
2:A:384:ASP:OD1	2:A:384:ASP:N	2.39	0.55
2:A:487:TYR:HB2	2:A:492:LEU:HD11	1.88	0.55
2:H:1548:GLN:HG3	2:H:1635:TYR:CZ	2.42	0.55
2:A:982:ASN:HB3	2:A:985:TRP:HB2	1.90	0.54
2:A:121:ILE:HG21	2:A:987:ILE:HG21	1.88	0.54
2:A:1432:GLU:OE1	2:A:1434:ALA:N	2.40	0.54
1:G:690:ASN:HD21	1:G:692:GLU:HB2	1.71	0.54
2:H:1499:VAL:O	2:H:1503:VAL:HG23	2.08	0.54
2:A:728:LEU:O	2:A:731:ARG:NH1	2.40	0.53
2:A:1298:ILE:O	2:A:1302:THR:HG22	2.07	0.53
1:B:561:ASN:HD21	1:C:559:LYS:HG3	1.73	0.53
2:A:43:ASP:HB3	2:A:46:LEU:HB3	1.90	0.53
2:A:22:VAL:HG12	2:A:24:GLY:H	1.73	0.53
2:A:88:TYR:CE1	2:A:237:MET:HE1	2.44	0.53
2:A:476:LEU:HD13	2:A:558:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1633:MET:HE2	2:H:1633:MET:HA	1.91	0.53
2:A:312:LEU:O	2:A:316:ILE:HG13	2.09	0.52
2:A:1414:ASP:N	2:A:1414:ASP:OD1	2.42	0.52
2:A:1197:ARG:HG3	2:A:1217:GLU:HG2	1.92	0.52
1:B:550:LEU:HD23	1:C:549:LYS:HZ2	1.75	0.52
2:A:1112:ARG:HG3	2:A:1439:VAL:HG12	1.93	0.51
2:A:408:ARG:HE	2:A:413:GLY:HA2	1.74	0.51
2:A:924:ARG:NH1	2:A:998:GLY:O	2.41	0.51
2:A:324:SER:HG	2:A:334:ARG:NH1	2.07	0.51
1:G:668:ILE:O	1:G:672:ILE:HB	2.11	0.51
2:A:244:GLY:O	2:A:248:MET:HG3	2.10	0.51
2:A:484:ASP:OD2	2:A:778:HIS:ND1	2.43	0.51
2:A:1041:MET:HG2	2:A:1199:LEU:HD13	1.91	0.51
1:D:544:PRO:HA	1:D:547:ILE:HG12	1.91	0.51
1:D:550:LEU:HB3	1:E:549:LYS:HZ1	1.76	0.50
2:A:1042:ASN:ND2	2:A:1181:ARG:O	2.39	0.50
1:C:559:LYS:O	1:C:559:LYS:HD3	2.10	0.50
1:C:571:LEU:HD22	1:D:567:ILE:HG23	1.93	0.50
1:E:548:ASN:OD1	1:E:549:LYS:N	2.44	0.50
2:A:303:GLU:HB3	2:A:852:LYS:HG3	1.94	0.50
2:A:1311:ASN:OD1	2:A:1438:GLN:NE2	2.45	0.50
2:H:1642:PHE:HA	2:H:1715:ASN:HD22	1.75	0.50
2:A:811:ILE:HD11	2:A:829:VAL:HG11	1.94	0.50
2:H:1708:ASP:O	2:H:1711:SER:OG	2.29	0.49
2:H:1710:SER:HG	2:H:1713:SER:HG	1.58	0.49
2:A:498:LYS:HE3	2:A:498:LYS:HA	1.92	0.49
2:A:1392:TYR:O	2:A:1396:MET:HG2	2.11	0.49
1:B:567:ILE:HD13	1:E:567:ILE:HG22	1.94	0.49
2:A:13:PRO:HG2	2:A:181:ARG:HG2	1.95	0.49
1:B:551:GLU:O	1:B:555:ARG:HG3	2.12	0.49
2:A:516:ASP:HB3	2:A:519:ASN:HB2	1.94	0.49
1:E:552:SER:HA	1:E:555:ARG:HE	1.77	0.49
2:A:100:SER:OG	2:A:203:ASP:OD2	2.31	0.49
2:H:1705:ARG:O	2:H:1711:SER:OG	2.29	0.48
1:G:672:ILE:O	1:G:678:ARG:NH1	2.46	0.48
1:B:563:ALA:O	1:B:567:ILE:HG13	2.13	0.48
2:A:908:SER:HB2	2:A:937:ALA:HB2	1.95	0.48
2:A:1005:SER:HB2	2:A:1012:ILE:HD12	1.95	0.48
2:A:850:VAL:HA	2:A:853:GLU:HG2	1.94	0.48
2:A:1192:SER:OG	2:A:1223:GLU:OE1	2.19	0.48
2:A:302:ASP:OD2	2:A:885:SER:OG	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1122:ILE:O	2:A:1126:SER:HB3	2.14	0.48
1:E:717:ASP:OD1	1:E:717:ASP:N	2.46	0.48
1:G:656:ALA:N	1:G:691:ASP:OD1	2.44	0.47
2:H:1668:HIS:O	2:H:1671:VAL:HG12	2.14	0.47
2:A:1296:SER:O	2:A:1300:ILE:HG13	2.14	0.47
1:G:663:VAL:HG22	2:A:312:LEU:HG	1.96	0.47
1:D:545:LYS:HE2	1:D:545:LYS:HA	1.95	0.47
2:A:190:PRO:HA	2:A:193:ARG:HH12	1.79	0.47
2:A:788:ASP:HB3	2:A:789:ILE:H	1.51	0.47
1:B:563:ALA:HB3	1:E:564:LEU:HD13	1.96	0.47
2:H:1640:CYS:HB3	2:A:974:ASP:OD2	2.14	0.47
1:B:578:ILE:HD11	2:A:733:GLU:HB2	1.96	0.47
2:A:141:ARG:N	2:A:141:ARG:HD2	2.31	0.46
2:A:12:TYR:HD2	2:A:921:ASP:H	1.64	0.46
2:A:1110:ASP:HB3	2:A:1443:LEU:HD13	1.97	0.46
1:C:564:LEU:HD21	1:D:564:LEU:HD22	1.97	0.46
2:H:1659:LEU:H	2:H:1659:LEU:HD23	1.81	0.46
2:A:1123:LEU:O	2:A:1129:GLY:N	2.45	0.46
2:A:987:ILE:HG23	2:A:991:LEU:HD13	1.97	0.46
2:A:107:LEU:HG	2:A:171:LEU:HD22	1.97	0.46
2:A:742:LEU:HD11	2:A:808:ILE:HD11	1.97	0.46
2:H:1663:ILE:HG22	2:H:1664:ILE:HG23	1.97	0.46
2:A:1364:ASN:ND2	2:A:1368:ARG:HB3	2.30	0.46
2:A:44:LYS:HB2	2:A:44:LYS:HE2	1.69	0.46
2:A:408:ARG:HB3	2:A:408:ARG:CZ	2.46	0.46
2:A:1037:LEU:HG	2:A:1041:MET:HE2	1.98	0.46
1:B:547:ILE:HD12	1:B:547:ILE:HA	1.82	0.45
2:A:542:LYS:HA	2:A:542:LYS:HD2	1.76	0.45
2:A:758:ARG:HA	2:A:758:ARG:HH11	1.81	0.45
2:A:1385:LYS:HB2	2:A:1385:LYS:HE2	1.71	0.45
2:A:361:ARG:HH12	2:A:544:LYS:HB3	1.82	0.45
2:A:394:LYS:HD3	2:A:444:VAL:HG13	1.98	0.45
1:B:576:ILE:HB	2:A:387:LEU:HB2	1.99	0.45
2:A:1200:ARG:NH1	2:A:1217:GLU:OE2	2.49	0.45
1:D:546:ILE:HD12	1:D:547:ILE:HD13	1.99	0.45
2:A:944:ARG:HB3	2:A:1007:ILE:HD12	1.98	0.45
2:H:1551:SER:O	2:H:1555:ALA:CB	2.63	0.45
2:A:1066:GLN:NE2	2:A:1070:LYS:HE2	2.29	0.45
2:A:525:LEU:HD21	2:A:748:LEU:HB3	1.98	0.45
2:A:1118:ALA:O	2:A:1122:ILE:HD13	2.17	0.45
2:A:1122:ILE:HG13	2:A:1300:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1248:TRP:HE3	2:A:1373:SER:HB3	1.81	0.45
2:A:181:ARG:NH2	2:A:921:ASP:OD1	2.50	0.44
2:A:1236:CYS:SG	2:A:1423:HIS:HE1	2.40	0.44
2:A:1039:LYS:HB2	2:A:1039:LYS:HE3	1.69	0.44
2:A:275:LEU:HB3	2:A:279:MET:HG3	1.98	0.44
2:A:1020:LEU:HD13	2:A:1195:LEU:HB3	1.99	0.44
2:A:1113:VAL:HB	2:A:1439:VAL:HG11	2.00	0.44
1:G:687:LYS:HG3	1:G:688:ALA:H	1.82	0.44
2:A:282:ARG:HE	2:A:282:ARG:HB3	1.66	0.44
2:A:909:MET:HE3	2:A:942:LEU:HD22	1.99	0.44
2:A:66:GLN:OE1	2:A:213:ASN:ND2	2.39	0.44
2:A:128:MET:HE3	2:A:1004:LEU:HD21	1.99	0.44
2:A:275:LEU:O	2:A:279:MET:HB2	2.17	0.44
2:A:1389:ASN:OD1	2:A:1389:ASN:N	2.42	0.44
1:G:687:LYS:HG3	1:G:688:ALA:N	2.33	0.44
2:A:560:MET:HE3	2:A:560:MET:HA	1.99	0.44
2:A:1061:ASN:HB2	2:A:1204:TRP:CE2	2.53	0.44
1:D:542:GLU:N	1:D:542:GLU:OE1	2.50	0.44
2:A:543:GLU:OE1	2:A:544:LYS:NZ	2.51	0.44
2:A:945:ASN:OD1	2:A:945:ASN:N	2.51	0.44
2:A:20:PRO:HD3	2:A:543:GLU:HB3	2.00	0.43
2:H:1546:LEU:HD21	2:H:1628:LEU:HD12	1.99	0.43
2:H:1546:LEU:O	2:H:1550:ILE:HG12	2.18	0.43
2:A:12:TYR:CD1	2:A:185:LYS:HD2	2.53	0.43
2:A:1193:VAL:HG13	2:A:1217:GLU:HB3	1.99	0.43
2:H:1701:ILE:O	2:H:1705:ARG:HG3	2.19	0.43
1:E:710:LEU:HD23	1:E:710:LEU:HA	1.84	0.43
2:A:719:LEU:HG	2:A:884:ILE:HG12	2.01	0.43
1:B:545:LYS:HG3	1:B:546:ILE:N	2.32	0.43
2:H:1636:LEU:HD23	2:H:1636:LEU:HA	1.83	0.43
2:A:1130:ALA:HB2	2:A:1325:ARG:HH12	1.82	0.43
2:H:1507:ILE:HD12	2:H:1507:ILE:HA	1.87	0.43
2:A:1315:TRP:HE1	2:A:1330:LEU:HD23	1.82	0.43
2:A:289:MET:HE3	2:A:289:MET:HB3	1.78	0.43
2:A:461:LEU:HD21	2:A:748:LEU:HD21	1.99	0.43
2:A:1319:TRP:NE1	2:A:1328:ILE:O	2.47	0.43
2:A:1364:ASN:OD1	2:A:1367:SER:OG	2.36	0.43
2:A:250:THR:O	2:A:254:SER:OG	2.30	0.43
2:A:758:ARG:O	2:A:758:ARG:NH1	2.52	0.43
2:A:1024:LYS:HB3	2:A:1024:LYS:HE2	1.79	0.42
2:A:1187:SER:O	2:A:1190:THR:OG1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:892:SER:O	2:A:892:SER:OG	2.33	0.42
2:A:1119:ALA:O	2:A:1123:LEU:HD13	2.19	0.42
2:A:103:MET:HE3	2:A:203:ASP:HB2	2.01	0.42
2:A:826:ALA:HB3	2:A:837:ALA:HB3	2.01	0.42
2:A:202:ARG:HH11	2:A:207:GLU:HG2	1.84	0.42
2:A:1234:LEU:HD23	2:A:1234:LEU:H	1.85	0.42
2:H:1703:LYS:O	2:H:1707:VAL:HG23	2.20	0.42
1:B:574:MET:HB2	1:E:712:PRO:HG2	2.02	0.42
1:D:543:ILE:HB	1:D:544:PRO:HD3	2.01	0.42
2:A:103:MET:HE2	2:A:103:MET:HB3	1.96	0.42
2:H:1625:GLN:O	2:H:1629:VAL:HG12	2.19	0.42
2:A:68:LYS:HD2	2:A:196:SER:HB3	2.01	0.42
2:A:304:ALA:HB3	2:A:307:LEU:HB2	2.01	0.41
1:C:559:LYS:HD3	1:C:559:LYS:C	2.45	0.41
2:A:758:ARG:HA	2:A:758:ARG:HD2	1.88	0.41
2:A:1106:SER:O	2:A:1110:ASP:HB2	2.20	0.41
2:A:829:VAL:HG23	2:A:834:GLU:HG3	2.01	0.41
2:A:1116:PRO:HG2	2:A:1216:LEU:HD11	2.01	0.41
2:H:1661:GLU:HA	2:H:1665:THR:HG22	2.01	0.41
1:C:575:MET:HE2	1:C:575:MET:HB3	1.88	0.41
1:G:687:LYS:HE2	1:G:687:LYS:HB2	1.84	0.41
2:A:38:ASN:ND2	2:A:85:HIS:O	2.42	0.41
2:A:1191:CYS:SG	2:A:1192:SER:N	2.93	0.41
2:A:1377:LEU:HD23	2:A:1392:TYR:CD1	2.55	0.41
1:E:557:LEU:HD12	1:E:557:LEU:HA	1.88	0.41
1:G:665:LYS:HE3	1:G:665:LYS:HB2	1.78	0.41
1:G:668:ILE:HD11	1:G:701:VAL:HG11	2.03	0.41
2:A:438:LEU:HD13	2:A:443:CYS:SG	2.61	0.41
2:A:514:ASN:OD1	2:A:514:ASN:N	2.53	0.41
2:A:737:ILE:HD12	2:A:737:ILE:HA	1.86	0.41
2:A:1186:ILE:C	2:A:1186:ILE:HD12	2.46	0.41
2:A:1124:ASP:HA	2:A:1129:GLY:HA3	2.03	0.41
2:A:1305:THR:HG21	2:A:1315:TRP:HZ3	1.86	0.41
2:H:1553:LYS:HA	2:H:1553:LYS:HD2	1.71	0.40
2:A:181:ARG:HH22	2:A:921:ASP:CG	2.29	0.40
1:C:562:THR:O	1:C:566:THR:HG22	2.21	0.40
2:A:561:ARG:HA	2:A:561:ARG:HD3	1.90	0.40
2:H:1538:ASP:N	2:H:1538:ASP:OD1	2.54	0.40
2:A:537:VAL:HG13	2:A:764:ILE:HG12	2.03	0.40
1:B:550:LEU:HD23	1:C:549:LYS:NZ	2.36	0.40
1:C:565:SER:HB3	2:A:423:HIS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1231:THR:HB	2:A:1416:TYR:CE1	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	B	39/759 (5%)	37 (95%)	2 (5%)	0	100	100
1	C	45/759 (6%)	44 (98%)	1 (2%)	0	100	100
1	D	36/759 (5%)	35 (97%)	1 (3%)	0	100	100
1	E	50/759 (7%)	50 (100%)	0	0	100	100
1	G	52/759 (7%)	49 (94%)	3 (6%)	0	100	100
2	A	1200/2270 (53%)	1167 (97%)	33 (3%)	0	100	100
2	H	111/2270 (5%)	104 (94%)	6 (5%)	1 (1%)	14	49
All	All	1533/8335 (18%)	1486 (97%)	46 (3%)	1 (0%)	50	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	1711	SER

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	B	36/667 (5%)	36 (100%)	0	100 100
1	C	40/667 (6%)	40 (100%)	0	100 100
1	D	35/667 (5%)	35 (100%)	0	100 100
1	E	50/667 (8%)	50 (100%)	0	100 100
1	G	50/667 (8%)	50 (100%)	0	100 100
2	A	1098/2070 (53%)	1098 (100%)	0	100 100
2	H	115/2070 (6%)	113 (98%)	2 (2%)	56 81
All	All	1424/7475 (19%)	1422 (100%)	2 (0%)	92 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	1628	LEU
2	H	1665	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	570	HIS
1	E	722	GLN
2	A	149	HIS
2	A	163	GLN
2	A	321	GLN
2	A	380	HIS
2	A	860	GLN
2	A	904	GLN
2	A	951	ASN
2	A	982	ASN
2	A	1003	ASN
2	A	1066	GLN
2	A	1165	HIS
2	A	1394	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

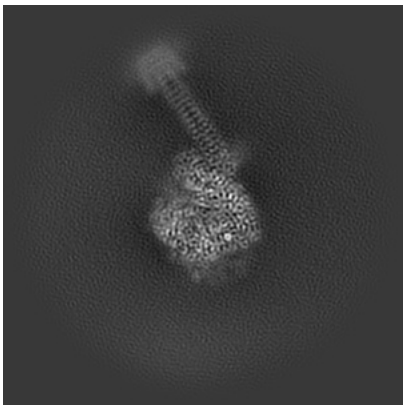
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45896. These allow visual inspection of the internal detail of the map and identification of artifacts.

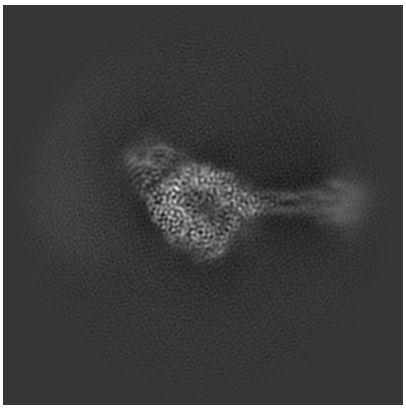
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

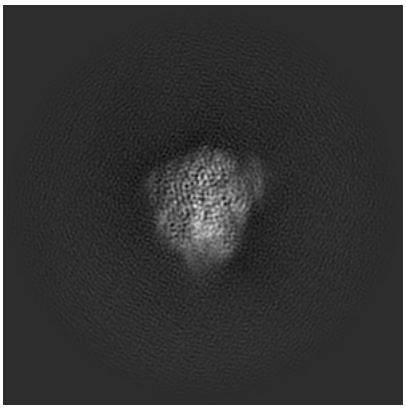
6.1.1 Primary map



X

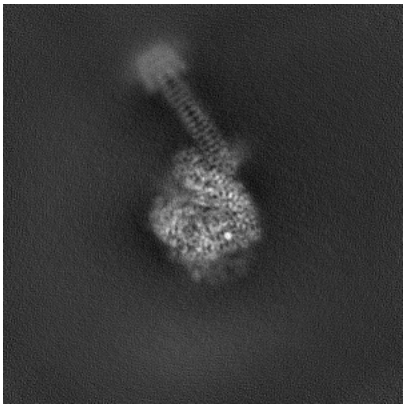


Y

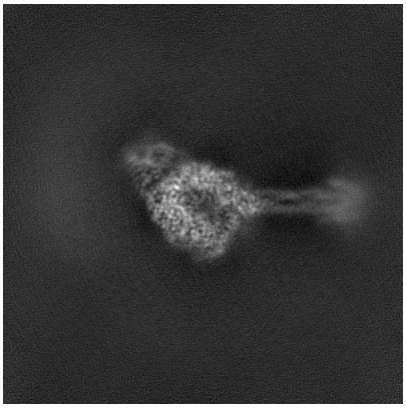


Z

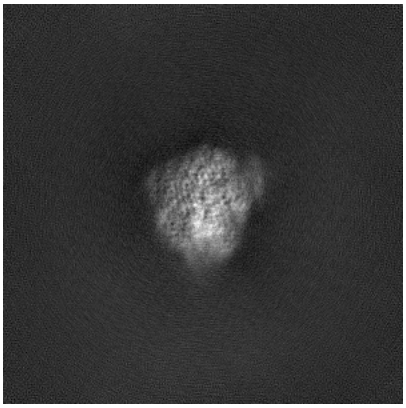
6.1.2 Raw map



X



Y

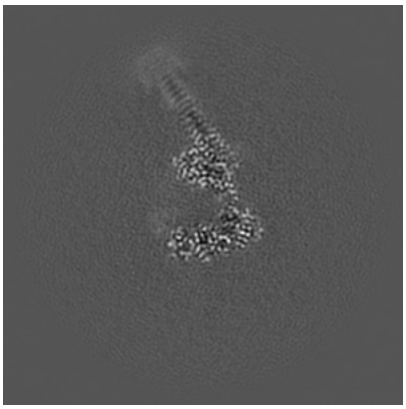


Z

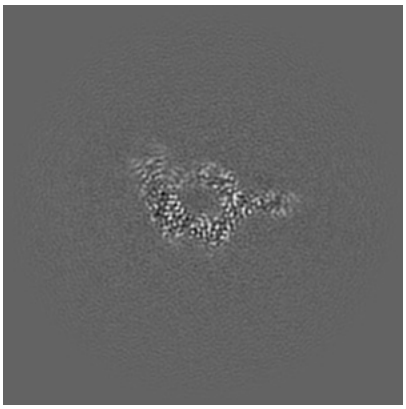
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

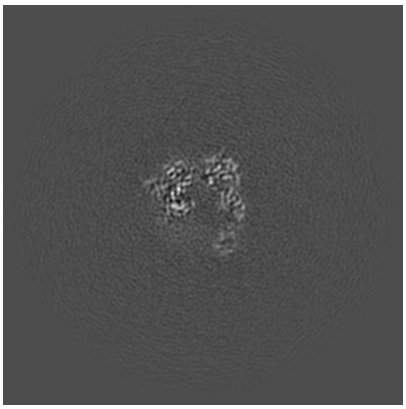
6.2.1 Primary map



X Index: 192

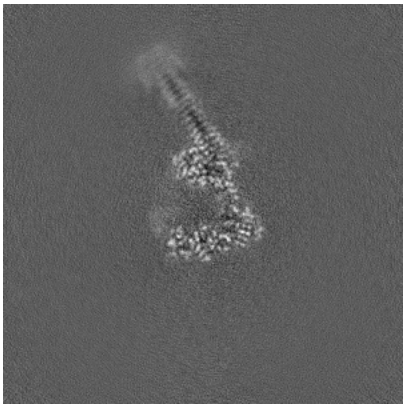


Y Index: 192

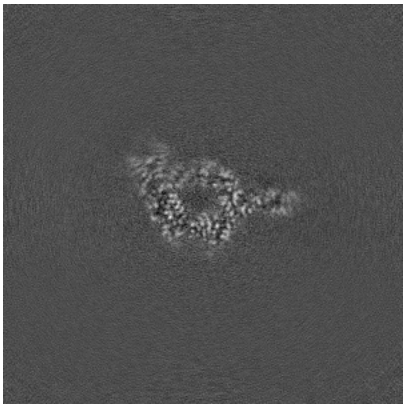


Z Index: 192

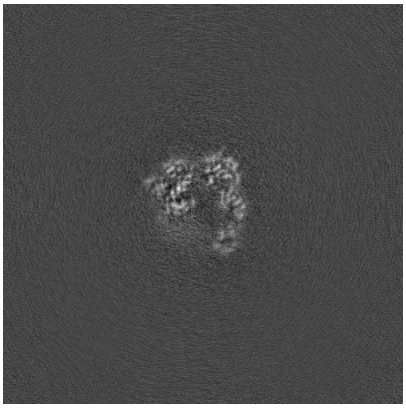
6.2.2 Raw map



X Index: 192



Y Index: 192

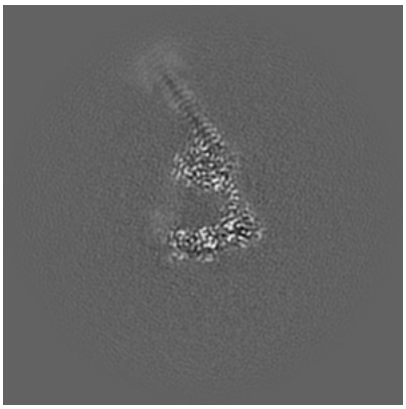


Z Index: 192

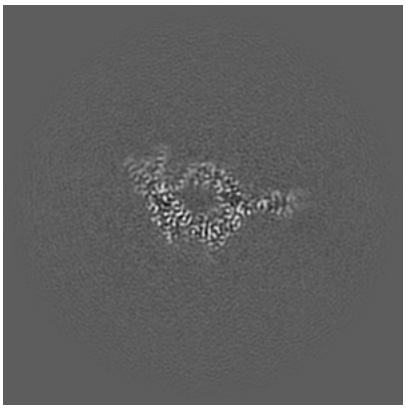
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

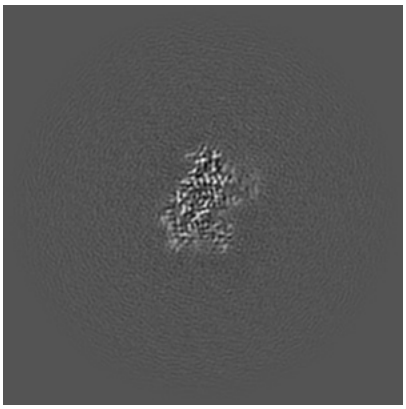
6.3.1 Primary map



X Index: 194

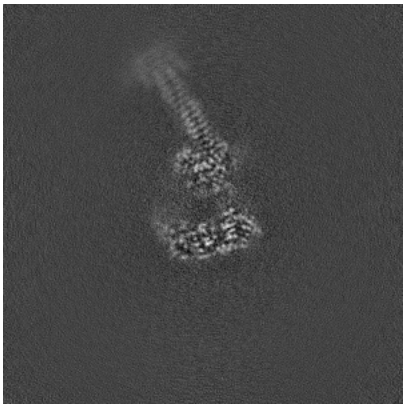


Y Index: 190

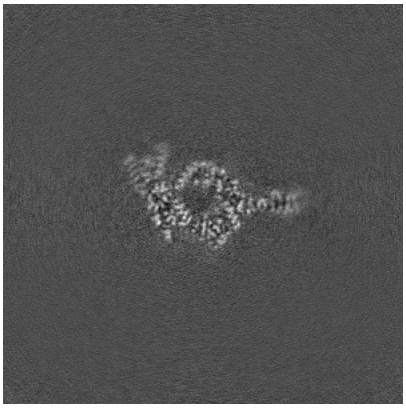


Z Index: 163

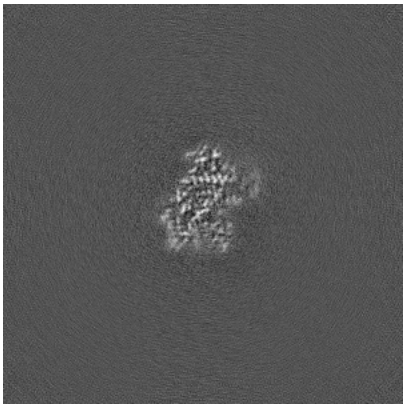
6.3.2 Raw map



X Index: 188



Y Index: 189

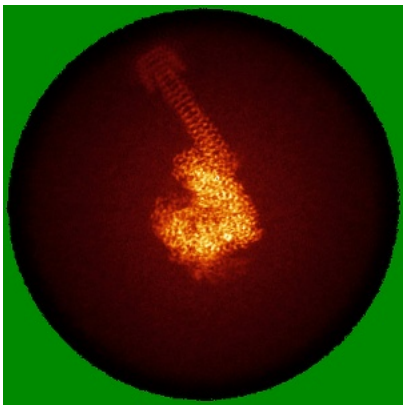


Z Index: 163

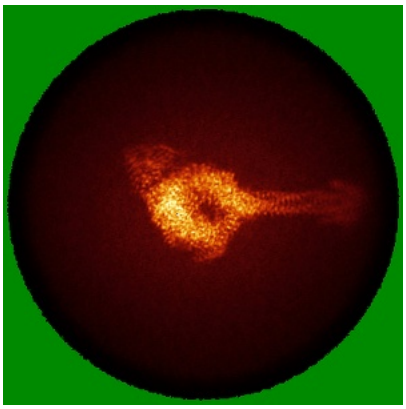
The images above show the largest variance slices of the map in three orthogonal directions.

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

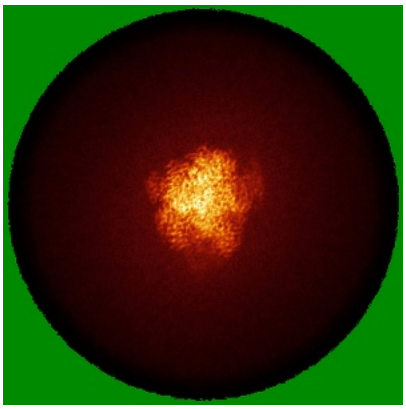
6.4.1 Primary map



X

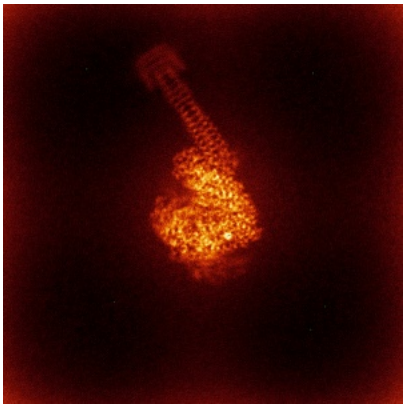


Y

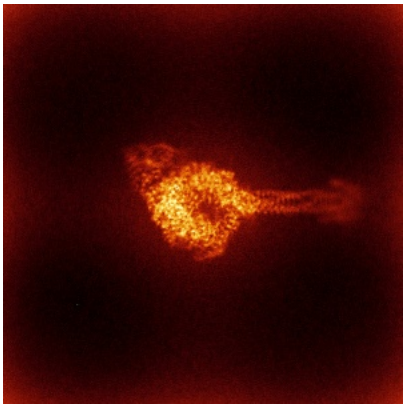


Z

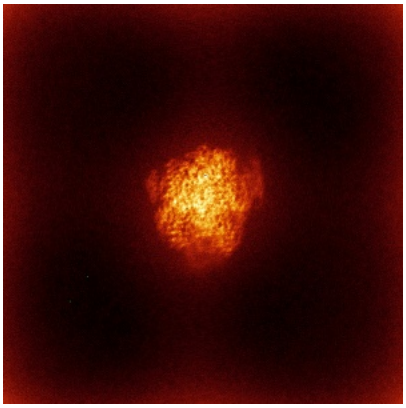
6.4.2 Raw map



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 0.1. 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.

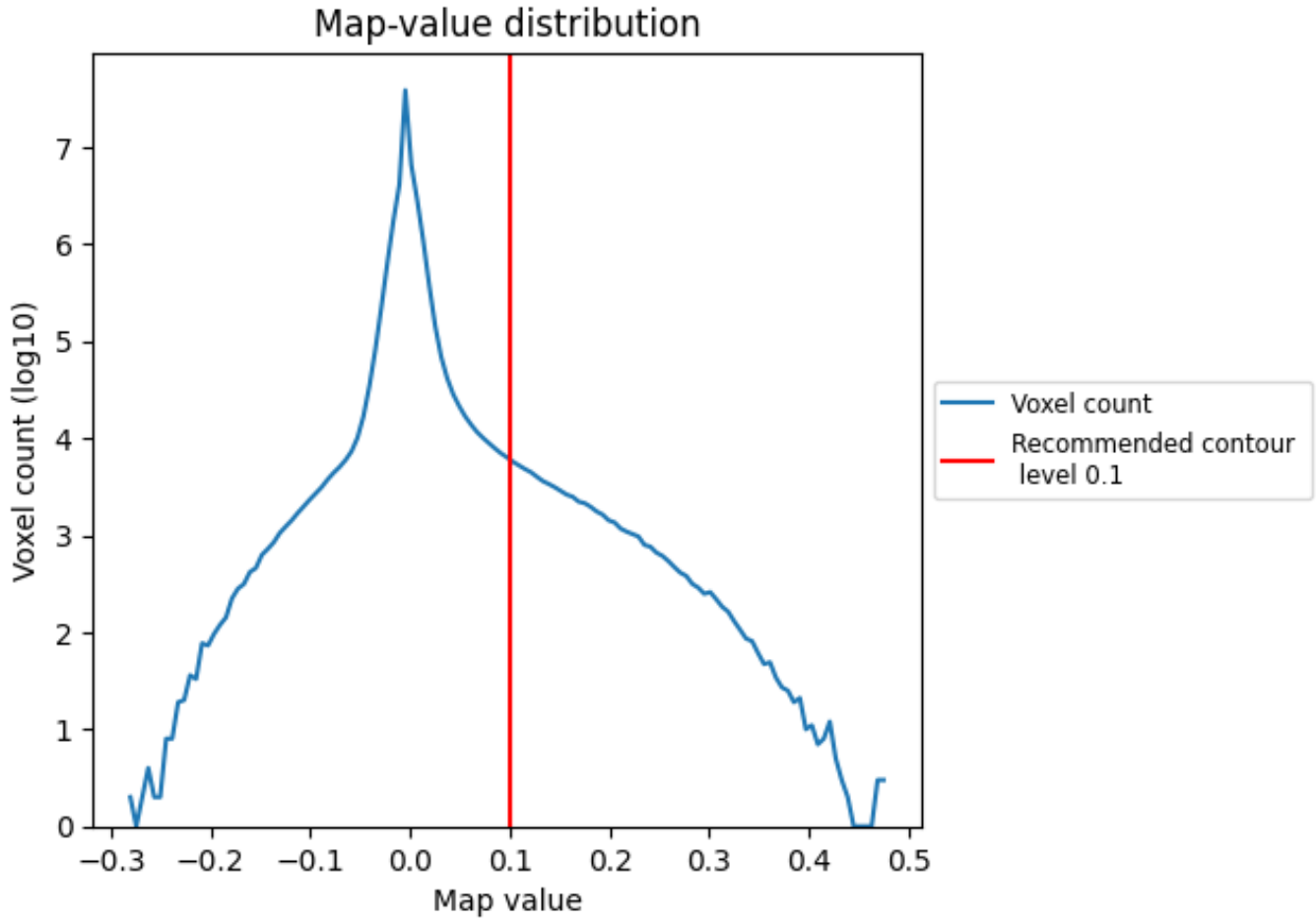
6.6 Mask visualisation (i)

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

7 Map analysis

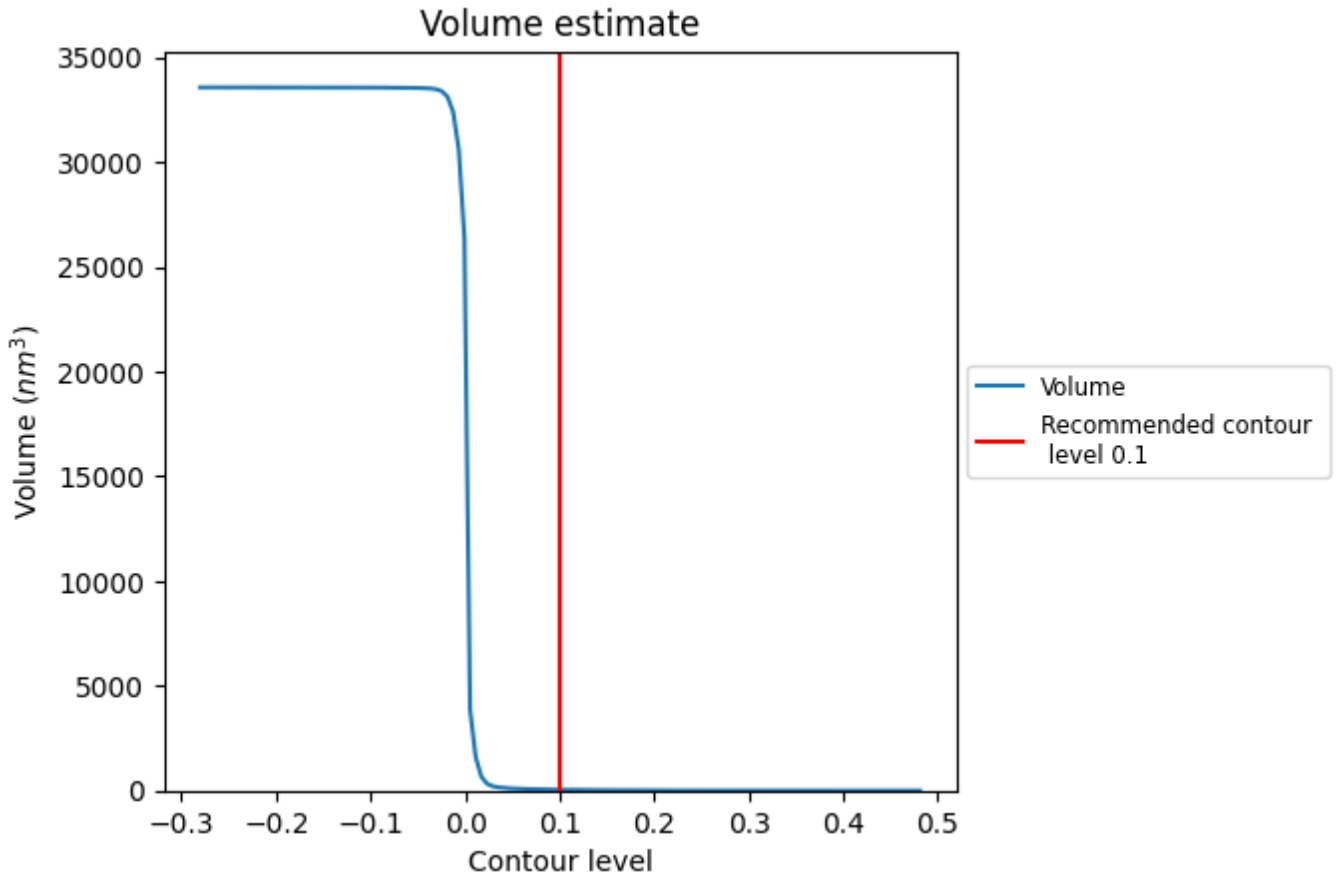
This section contains the results of statistical analysis of the map.

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.

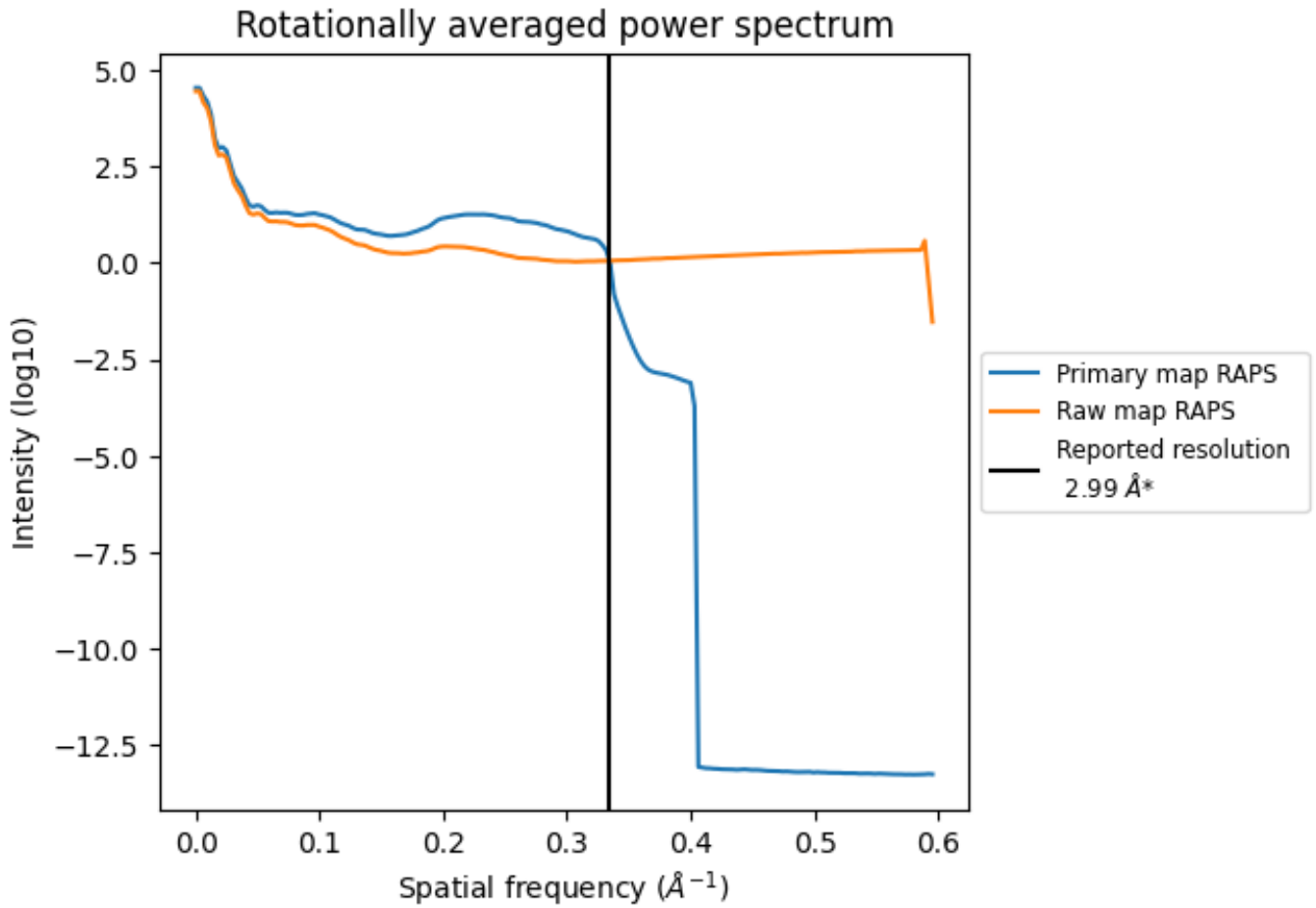
7.2 Volume estimate (i)



The volume at the recommended contour level is 41 nm^3; this corresponds to an approximate mass of 37 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)

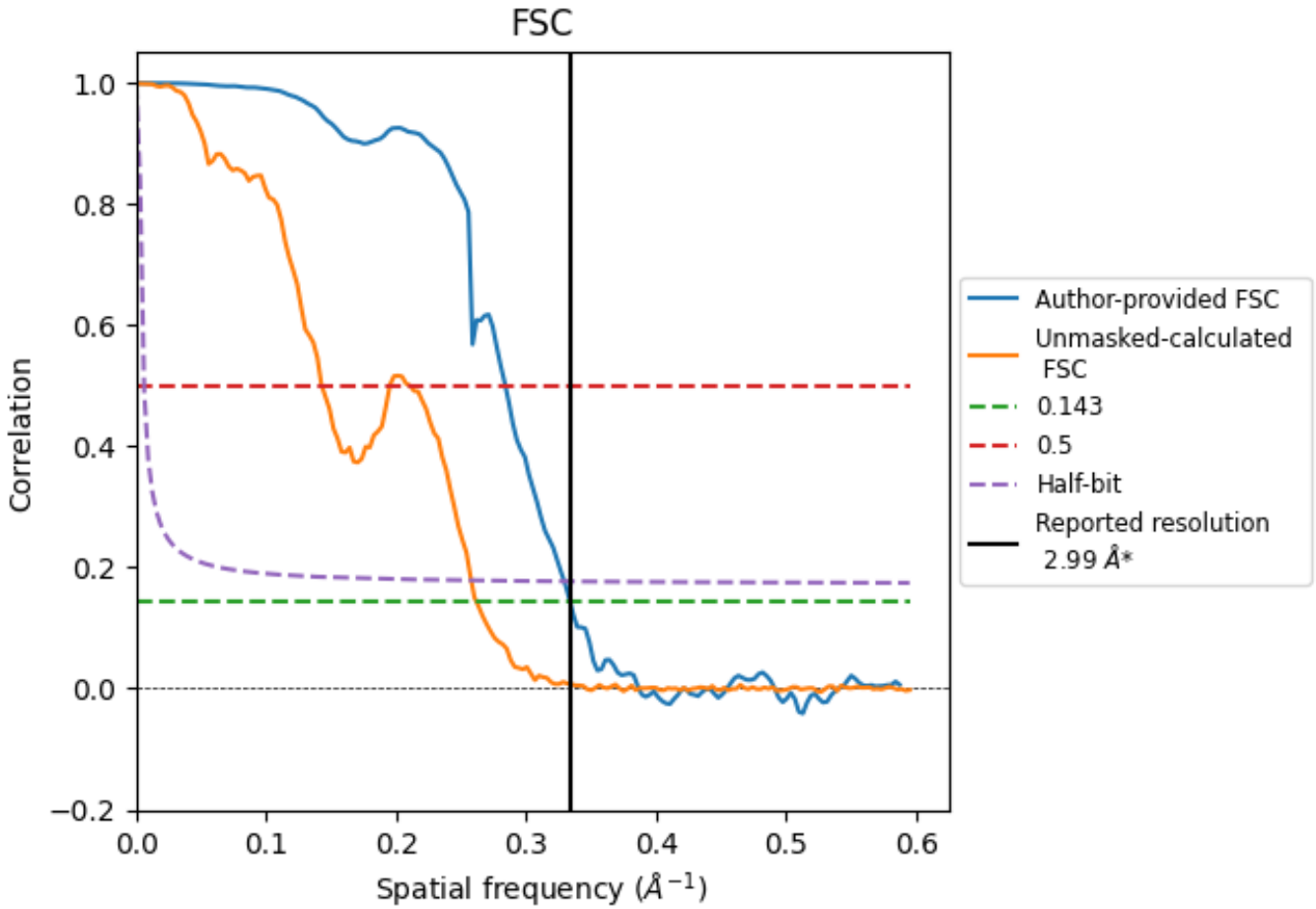


*Reported resolution corresponds to spatial frequency of 0.334 $Å^{-1}$

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 0.334 Å^{-1}

8.2 Resolution estimates (i)

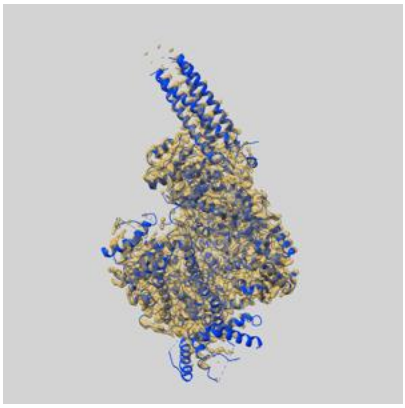
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.52	3.03
Unmasked-calculated*	3.82	7.00	3.88

*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 3.82 differs from the reported value 2.99 by more than 10 %

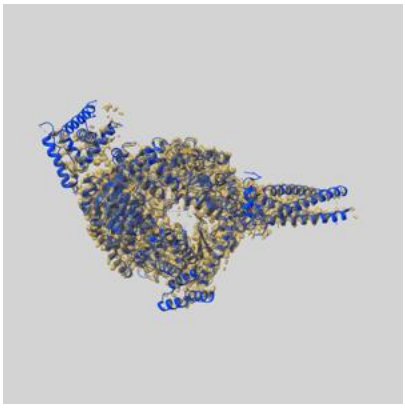
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45896 and PDB model 9MZH. Per-residue inclusion information can be found in section 3 on page 11.

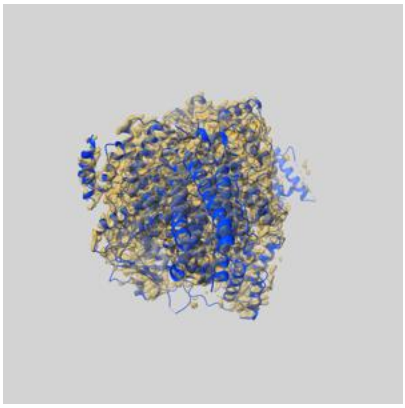
9.1 Map-model overlay



X



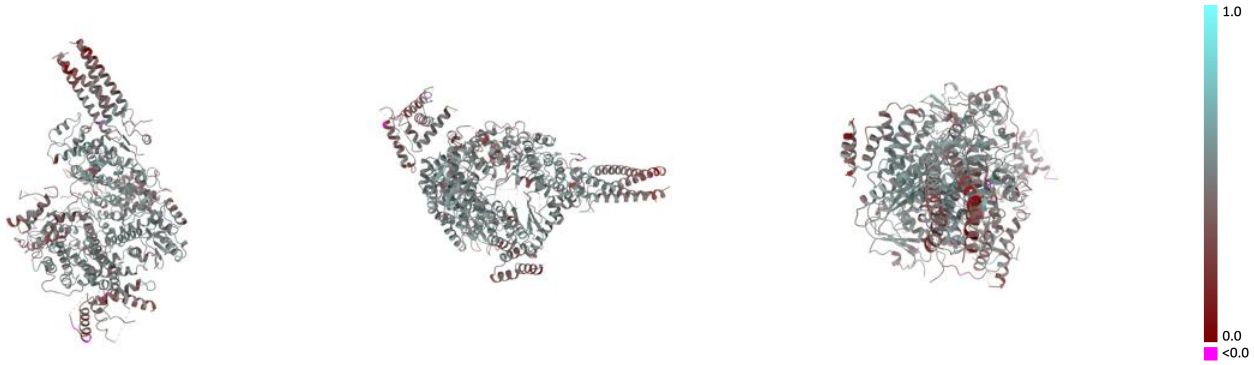
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

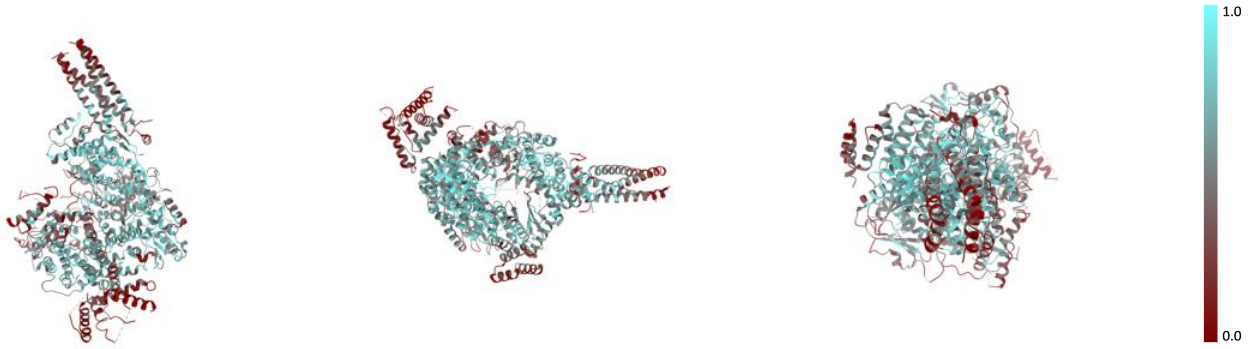
9.2 Q-score mapped to coordinate model (i)



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.

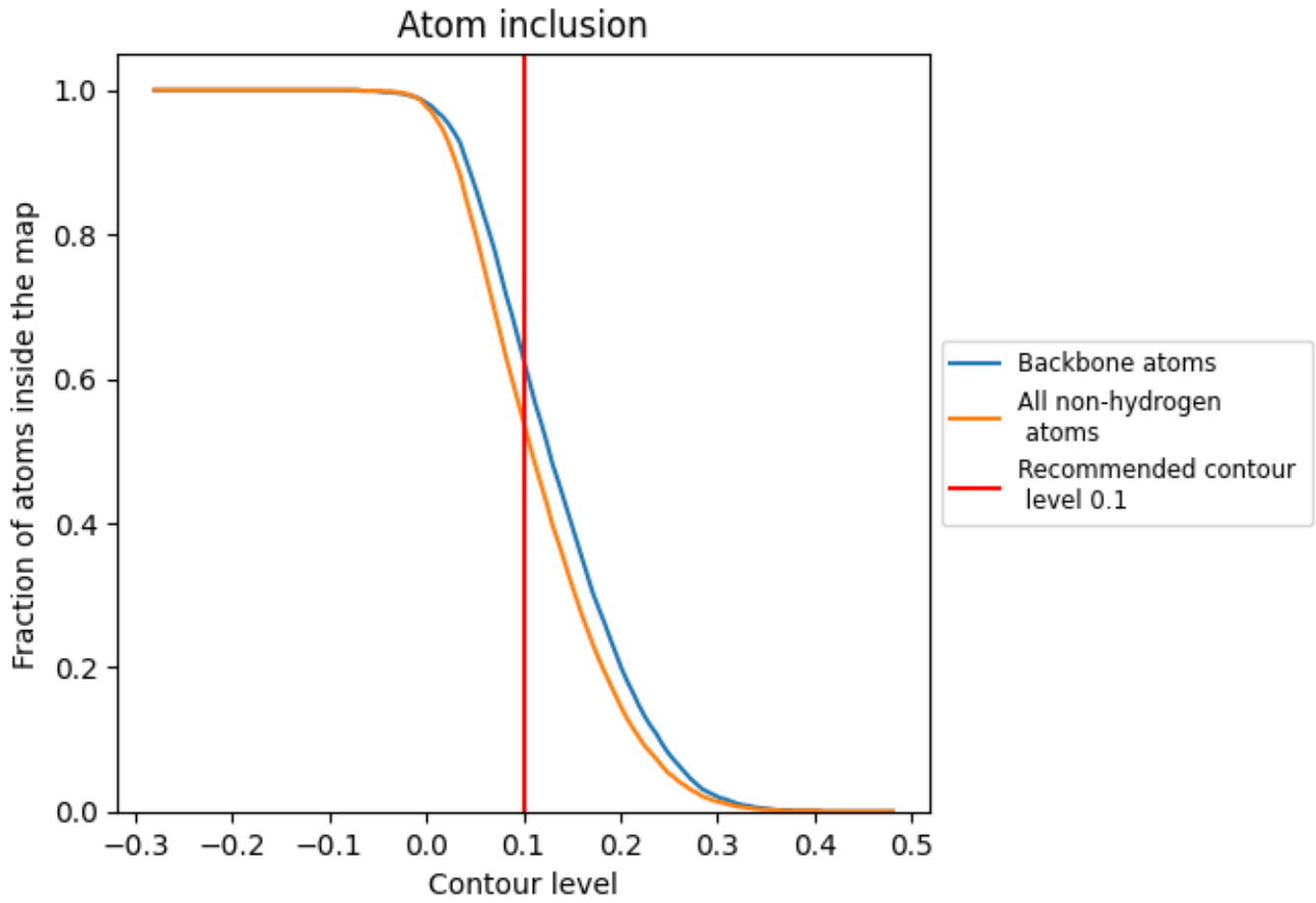
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 54% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5410	0.4720
A	0.6120	0.4930
B	0.4300	0.4360
C	0.4240	0.4110
D	0.3100	0.3760
E	0.3410	0.4030
G	0.2800	0.3950
H	0.1800	0.3890