



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:01 AM UTC

PDB ID : 9ARV / pdb_00009arv
EMDB ID : EMD-43795
Title : CryoEM structure of AMETA-A3
Authors : Huang, W.; Sang, Z.; Taylor, D.
Deposited on : 2024-02-23
Resolution : 3.60 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:

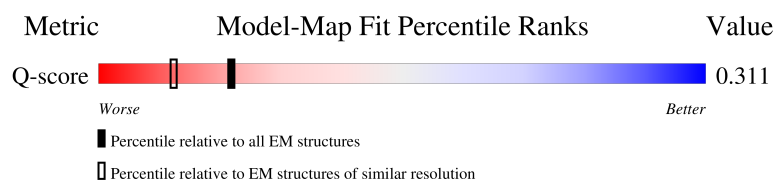
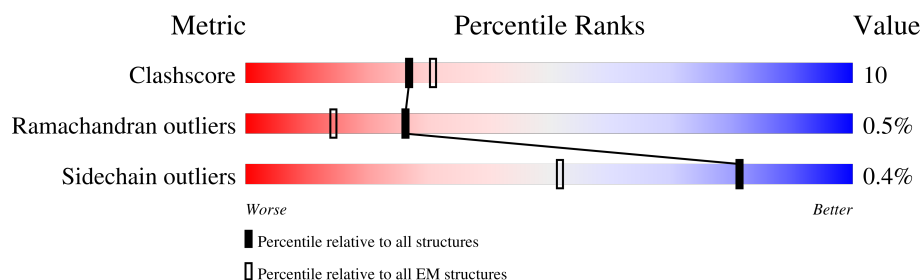
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	
1	B	375	
1	C	375	
1	D	375	

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Mol	Chain	Length	Quality of chain
1	E	375	43%18%39%
1	L	375	44%15%41%
1	M	375	45%15%39%
1	N	375	42%18%39%
1	O	375	49%11%39%
1	P	375	53%10%37%
2	J	167	43%8%49%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 36630 atoms, of which 18110 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 Isoform 1 of Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	235	Total	C	H	N	O	S	0	0
			3589	1143	1770	307	360	9		
1	B	230	Total	C	H	N	O	S	0	0
			3525	1122	1741	302	352	8		
1	C	228	Total	C	H	N	O	S	0	0
			3499	1114	1730	300	347	8		
1	D	229	Total	C	H	N	O	S	0	0
			3511	1118	1734	301	350	8		
1	E	228	Total	C	H	N	O	S	0	0
			3499	1114	1730	300	347	8		
1	L	223	Total	C	H	N	O	S	0	0
			3436	1095	1701	295	338	7		
1	M	227	Total	C	H	N	O	S	0	0
			3489	1111	1726	299	345	8		
1	N	227	Total	C	H	N	O	S	0	0
			3488	1111	1725	299	345	8		
1	O	228	Total	C	H	N	O	S	0	0
			3499	1114	1730	300	347	8		
1	P	235	Total	C	H	N	O	S	0	0
			3590	1143	1771	307	360	9		

There are 270 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P01871
A	2	SER	-	expression tag	UNP P01871
A	3	ARG	-	expression tag	UNP P01871
A	4	GLY	-	expression tag	UNP P01871
A	5	VAL	-	expression tag	UNP P01871
A	6	PRO	-	expression tag	UNP P01871
A	7	HIS	-	expression tag	UNP P01871
A	8	ILE	-	expression tag	UNP P01871
A	9	VAL	-	expression tag	UNP P01871
A	10	MET	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	-	expression tag	UNP P01871
A	12	ASP	-	expression tag	UNP P01871
A	13	ALA	-	expression tag	UNP P01871
A	14	TYR	-	expression tag	UNP P01871
A	15	LYS	-	expression tag	UNP P01871
A	16	ARG	-	expression tag	UNP P01871
A	17	TYR	-	expression tag	UNP P01871
A	18	LYS	-	expression tag	UNP P01871
A	19	GLY	-	expression tag	UNP P01871
A	20	GLY	-	expression tag	UNP P01871
A	21	GLY	-	expression tag	UNP P01871
A	22	GLY	-	expression tag	UNP P01871
A	23	SER	-	expression tag	UNP P01871
A	24	ILE	-	expression tag	UNP P01871
A	25	ASP	-	expression tag	UNP P01871
A	26	THR	-	expression tag	UNP P01871
A	27	THR	-	expression tag	UNP P01871
B	1	GLY	-	expression tag	UNP P01871
B	2	SER	-	expression tag	UNP P01871
B	3	ARG	-	expression tag	UNP P01871
B	4	GLY	-	expression tag	UNP P01871
B	5	VAL	-	expression tag	UNP P01871
B	6	PRO	-	expression tag	UNP P01871
B	7	HIS	-	expression tag	UNP P01871
B	8	ILE	-	expression tag	UNP P01871
B	9	VAL	-	expression tag	UNP P01871
B	10	MET	-	expression tag	UNP P01871
B	11	VAL	-	expression tag	UNP P01871
B	12	ASP	-	expression tag	UNP P01871
B	13	ALA	-	expression tag	UNP P01871
B	14	TYR	-	expression tag	UNP P01871
B	15	LYS	-	expression tag	UNP P01871
B	16	ARG	-	expression tag	UNP P01871
B	17	TYR	-	expression tag	UNP P01871
B	18	LYS	-	expression tag	UNP P01871
B	19	GLY	-	expression tag	UNP P01871
B	20	GLY	-	expression tag	UNP P01871
B	21	GLY	-	expression tag	UNP P01871
B	22	GLY	-	expression tag	UNP P01871
B	23	SER	-	expression tag	UNP P01871
B	24	ILE	-	expression tag	UNP P01871
B	25	ASP	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	THR	-	expression tag	UNP P01871
B	27	THR	-	expression tag	UNP P01871
C	1	GLY	-	expression tag	UNP P01871
C	2	SER	-	expression tag	UNP P01871
C	3	ARG	-	expression tag	UNP P01871
C	4	GLY	-	expression tag	UNP P01871
C	5	VAL	-	expression tag	UNP P01871
C	6	PRO	-	expression tag	UNP P01871
C	7	HIS	-	expression tag	UNP P01871
C	8	ILE	-	expression tag	UNP P01871
C	9	VAL	-	expression tag	UNP P01871
C	10	MET	-	expression tag	UNP P01871
C	11	VAL	-	expression tag	UNP P01871
C	12	ASP	-	expression tag	UNP P01871
C	13	ALA	-	expression tag	UNP P01871
C	14	TYR	-	expression tag	UNP P01871
C	15	LYS	-	expression tag	UNP P01871
C	16	ARG	-	expression tag	UNP P01871
C	17	TYR	-	expression tag	UNP P01871
C	18	LYS	-	expression tag	UNP P01871
C	19	GLY	-	expression tag	UNP P01871
C	20	GLY	-	expression tag	UNP P01871
C	21	GLY	-	expression tag	UNP P01871
C	22	GLY	-	expression tag	UNP P01871
C	23	SER	-	expression tag	UNP P01871
C	24	ILE	-	expression tag	UNP P01871
C	25	ASP	-	expression tag	UNP P01871
C	26	THR	-	expression tag	UNP P01871
C	27	THR	-	expression tag	UNP P01871
D	1	GLY	-	expression tag	UNP P01871
D	2	SER	-	expression tag	UNP P01871
D	3	ARG	-	expression tag	UNP P01871
D	4	GLY	-	expression tag	UNP P01871
D	5	VAL	-	expression tag	UNP P01871
D	6	PRO	-	expression tag	UNP P01871
D	7	HIS	-	expression tag	UNP P01871
D	8	ILE	-	expression tag	UNP P01871
D	9	VAL	-	expression tag	UNP P01871
D	10	MET	-	expression tag	UNP P01871
D	11	VAL	-	expression tag	UNP P01871
D	12	ASP	-	expression tag	UNP P01871
D	13	ALA	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
D	14	TYR	-	expression tag	UNP P01871
D	15	LYS	-	expression tag	UNP P01871
D	16	ARG	-	expression tag	UNP P01871
D	17	TYR	-	expression tag	UNP P01871
D	18	LYS	-	expression tag	UNP P01871
D	19	GLY	-	expression tag	UNP P01871
D	20	GLY	-	expression tag	UNP P01871
D	21	GLY	-	expression tag	UNP P01871
D	22	GLY	-	expression tag	UNP P01871
D	23	SER	-	expression tag	UNP P01871
D	24	ILE	-	expression tag	UNP P01871
D	25	ASP	-	expression tag	UNP P01871
D	26	THR	-	expression tag	UNP P01871
D	27	THR	-	expression tag	UNP P01871
E	1	GLY	-	expression tag	UNP P01871
E	2	SER	-	expression tag	UNP P01871
E	3	ARG	-	expression tag	UNP P01871
E	4	GLY	-	expression tag	UNP P01871
E	5	VAL	-	expression tag	UNP P01871
E	6	PRO	-	expression tag	UNP P01871
E	7	HIS	-	expression tag	UNP P01871
E	8	ILE	-	expression tag	UNP P01871
E	9	VAL	-	expression tag	UNP P01871
E	10	MET	-	expression tag	UNP P01871
E	11	VAL	-	expression tag	UNP P01871
E	12	ASP	-	expression tag	UNP P01871
E	13	ALA	-	expression tag	UNP P01871
E	14	TYR	-	expression tag	UNP P01871
E	15	LYS	-	expression tag	UNP P01871
E	16	ARG	-	expression tag	UNP P01871
E	17	TYR	-	expression tag	UNP P01871
E	18	LYS	-	expression tag	UNP P01871
E	19	GLY	-	expression tag	UNP P01871
E	20	GLY	-	expression tag	UNP P01871
E	21	GLY	-	expression tag	UNP P01871
E	22	GLY	-	expression tag	UNP P01871
E	23	SER	-	expression tag	UNP P01871
E	24	ILE	-	expression tag	UNP P01871
E	25	ASP	-	expression tag	UNP P01871
E	26	THR	-	expression tag	UNP P01871
E	27	THR	-	expression tag	UNP P01871
L	1	GLY	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
L	2	SER	-	expression tag	UNP P01871
L	3	ARG	-	expression tag	UNP P01871
L	4	GLY	-	expression tag	UNP P01871
L	5	VAL	-	expression tag	UNP P01871
L	6	PRO	-	expression tag	UNP P01871
L	7	HIS	-	expression tag	UNP P01871
L	8	ILE	-	expression tag	UNP P01871
L	9	VAL	-	expression tag	UNP P01871
L	10	MET	-	expression tag	UNP P01871
L	11	VAL	-	expression tag	UNP P01871
L	12	ASP	-	expression tag	UNP P01871
L	13	ALA	-	expression tag	UNP P01871
L	14	TYR	-	expression tag	UNP P01871
L	15	LYS	-	expression tag	UNP P01871
L	16	ARG	-	expression tag	UNP P01871
L	17	TYR	-	expression tag	UNP P01871
L	18	LYS	-	expression tag	UNP P01871
L	19	GLY	-	expression tag	UNP P01871
L	20	GLY	-	expression tag	UNP P01871
L	21	GLY	-	expression tag	UNP P01871
L	22	GLY	-	expression tag	UNP P01871
L	23	SER	-	expression tag	UNP P01871
L	24	ILE	-	expression tag	UNP P01871
L	25	ASP	-	expression tag	UNP P01871
L	26	THR	-	expression tag	UNP P01871
L	27	THR	-	expression tag	UNP P01871
M	1	GLY	-	expression tag	UNP P01871
M	2	SER	-	expression tag	UNP P01871
M	3	ARG	-	expression tag	UNP P01871
M	4	GLY	-	expression tag	UNP P01871
M	5	VAL	-	expression tag	UNP P01871
M	6	PRO	-	expression tag	UNP P01871
M	7	HIS	-	expression tag	UNP P01871
M	8	ILE	-	expression tag	UNP P01871
M	9	VAL	-	expression tag	UNP P01871
M	10	MET	-	expression tag	UNP P01871
M	11	VAL	-	expression tag	UNP P01871
M	12	ASP	-	expression tag	UNP P01871
M	13	ALA	-	expression tag	UNP P01871
M	14	TYR	-	expression tag	UNP P01871
M	15	LYS	-	expression tag	UNP P01871
M	16	ARG	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
M	17	TYR	-	expression tag	UNP P01871
M	18	LYS	-	expression tag	UNP P01871
M	19	GLY	-	expression tag	UNP P01871
M	20	GLY	-	expression tag	UNP P01871
M	21	GLY	-	expression tag	UNP P01871
M	22	GLY	-	expression tag	UNP P01871
M	23	SER	-	expression tag	UNP P01871
M	24	ILE	-	expression tag	UNP P01871
M	25	ASP	-	expression tag	UNP P01871
M	26	THR	-	expression tag	UNP P01871
M	27	THR	-	expression tag	UNP P01871
N	1	GLY	-	expression tag	UNP P01871
N	2	SER	-	expression tag	UNP P01871
N	3	ARG	-	expression tag	UNP P01871
N	4	GLY	-	expression tag	UNP P01871
N	5	VAL	-	expression tag	UNP P01871
N	6	PRO	-	expression tag	UNP P01871
N	7	HIS	-	expression tag	UNP P01871
N	8	ILE	-	expression tag	UNP P01871
N	9	VAL	-	expression tag	UNP P01871
N	10	MET	-	expression tag	UNP P01871
N	11	VAL	-	expression tag	UNP P01871
N	12	ASP	-	expression tag	UNP P01871
N	13	ALA	-	expression tag	UNP P01871
N	14	TYR	-	expression tag	UNP P01871
N	15	LYS	-	expression tag	UNP P01871
N	16	ARG	-	expression tag	UNP P01871
N	17	TYR	-	expression tag	UNP P01871
N	18	LYS	-	expression tag	UNP P01871
N	19	GLY	-	expression tag	UNP P01871
N	20	GLY	-	expression tag	UNP P01871
N	21	GLY	-	expression tag	UNP P01871
N	22	GLY	-	expression tag	UNP P01871
N	23	SER	-	expression tag	UNP P01871
N	24	ILE	-	expression tag	UNP P01871
N	25	ASP	-	expression tag	UNP P01871
N	26	THR	-	expression tag	UNP P01871
N	27	THR	-	expression tag	UNP P01871
O	1	GLY	-	expression tag	UNP P01871
O	2	SER	-	expression tag	UNP P01871
O	3	ARG	-	expression tag	UNP P01871
O	4	GLY	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
O	5	VAL	-	expression tag	UNP P01871
O	6	PRO	-	expression tag	UNP P01871
O	7	HIS	-	expression tag	UNP P01871
O	8	ILE	-	expression tag	UNP P01871
O	9	VAL	-	expression tag	UNP P01871
O	10	MET	-	expression tag	UNP P01871
O	11	VAL	-	expression tag	UNP P01871
O	12	ASP	-	expression tag	UNP P01871
O	13	ALA	-	expression tag	UNP P01871
O	14	TYR	-	expression tag	UNP P01871
O	15	LYS	-	expression tag	UNP P01871
O	16	ARG	-	expression tag	UNP P01871
O	17	TYR	-	expression tag	UNP P01871
O	18	LYS	-	expression tag	UNP P01871
O	19	GLY	-	expression tag	UNP P01871
O	20	GLY	-	expression tag	UNP P01871
O	21	GLY	-	expression tag	UNP P01871
O	22	GLY	-	expression tag	UNP P01871
O	23	SER	-	expression tag	UNP P01871
O	24	ILE	-	expression tag	UNP P01871
O	25	ASP	-	expression tag	UNP P01871
O	26	THR	-	expression tag	UNP P01871
O	27	THR	-	expression tag	UNP P01871
P	1	GLY	-	expression tag	UNP P01871
P	2	SER	-	expression tag	UNP P01871
P	3	ARG	-	expression tag	UNP P01871
P	4	GLY	-	expression tag	UNP P01871
P	5	VAL	-	expression tag	UNP P01871
P	6	PRO	-	expression tag	UNP P01871
P	7	HIS	-	expression tag	UNP P01871
P	8	ILE	-	expression tag	UNP P01871
P	9	VAL	-	expression tag	UNP P01871
P	10	MET	-	expression tag	UNP P01871
P	11	VAL	-	expression tag	UNP P01871
P	12	ASP	-	expression tag	UNP P01871
P	13	ALA	-	expression tag	UNP P01871
P	14	TYR	-	expression tag	UNP P01871
P	15	LYS	-	expression tag	UNP P01871
P	16	ARG	-	expression tag	UNP P01871
P	17	TYR	-	expression tag	UNP P01871
P	18	LYS	-	expression tag	UNP P01871
P	19	GLY	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
P	20	GLY	-	expression tag	UNP P01871
P	21	GLY	-	expression tag	UNP P01871
P	22	GLY	-	expression tag	UNP P01871
P	23	SER	-	expression tag	UNP P01871
P	24	ILE	-	expression tag	UNP P01871
P	25	ASP	-	expression tag	UNP P01871
P	26	THR	-	expression tag	UNP P01871
P	27	THR	-	expression tag	UNP P01871

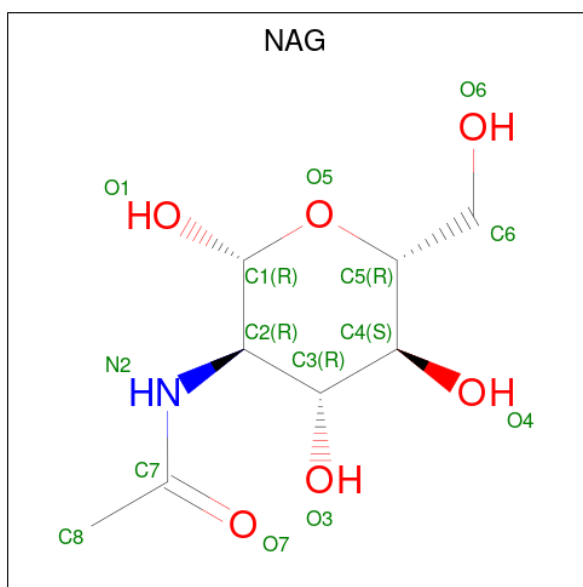
- Molecule 2 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	86	Total	C	H	N	O	S	0	0
			1370	430	687	119	127	7		

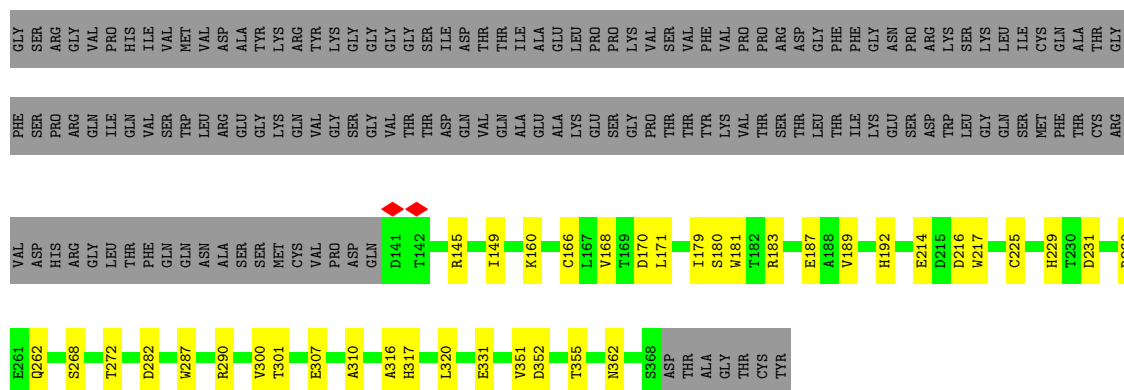
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	164	HIS	-	expression tag	UNP P01591
J	165	HIS	-	expression tag	UNP P01591
J	166	HIS	-	expression tag	UNP P01591
J	167	HIS	-	expression tag	UNP P01591
J	168	HIS	-	expression tag	UNP P01591
J	169	HIS	-	expression tag	UNP P01591
J	170	HIS	-	expression tag	UNP P01591
J	171	HIS	-	expression tag	UNP P01591

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

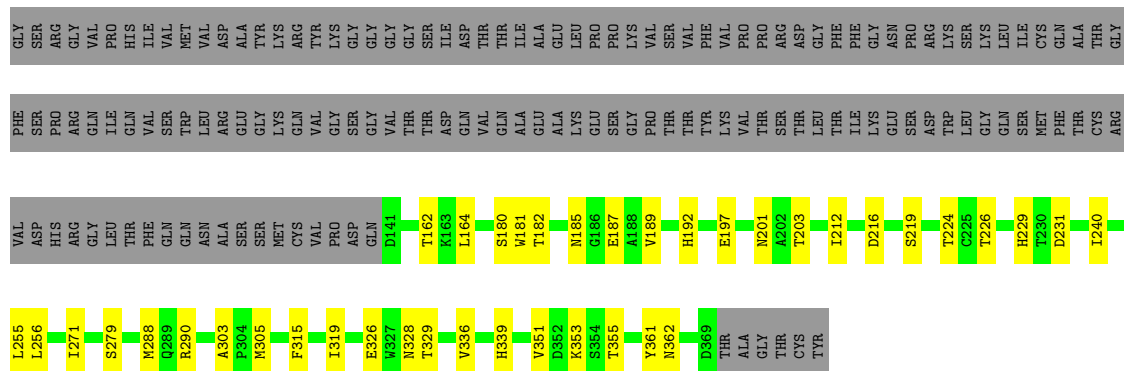


Mol	Chain	Residues	Atoms					AltConf
3	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	D	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	M	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	N	1	Total	C	H	N	O	0
			27	8	13	1	5	
3	O	1	Total	C	H	N	O	0
			27	8	13	1	5	



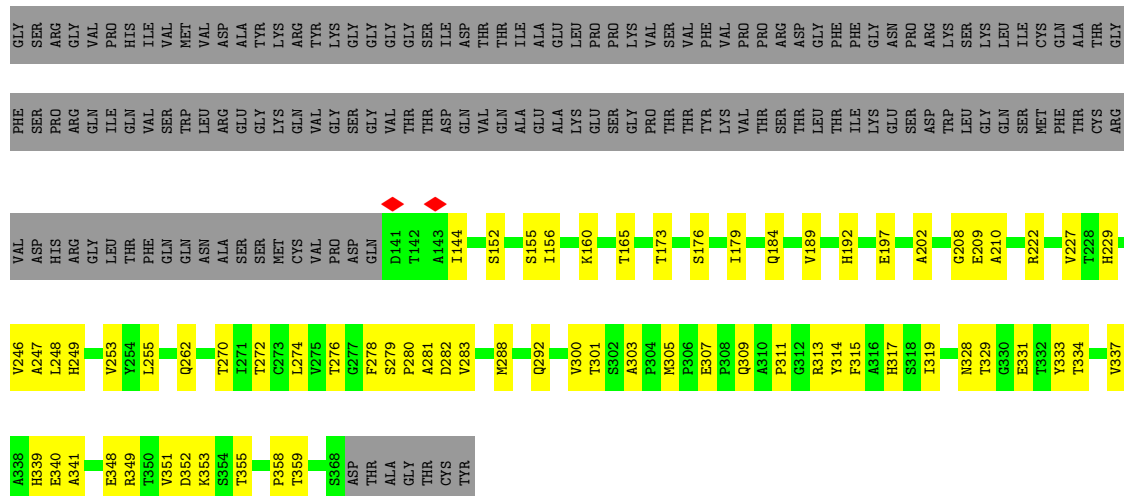
• Molecule 1: Isoform 1 of Immunoglobulin heavy constant mu

Chain D: 50% 11% 39%



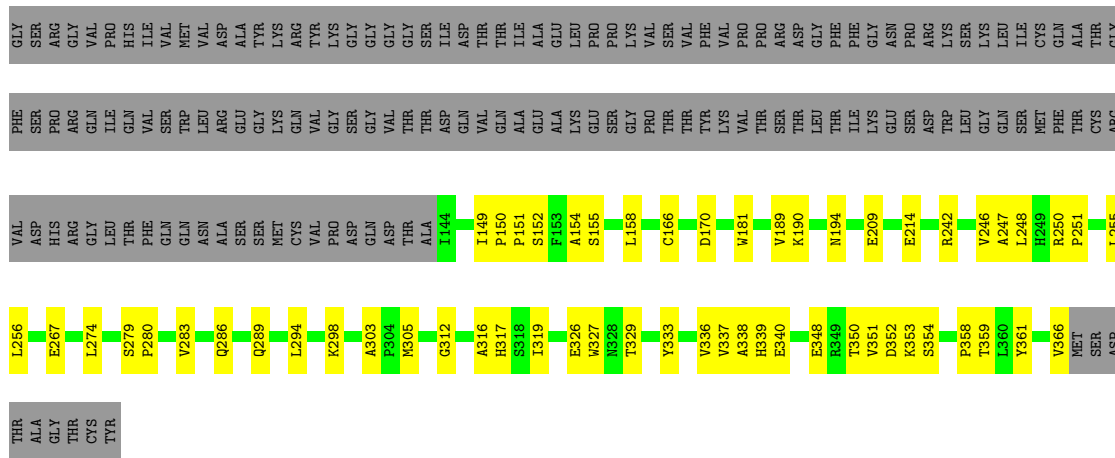
• Molecule 1: Isoform 1 of Immunoglobulin heavy constant mu

Chain E: 43% 18% 39%

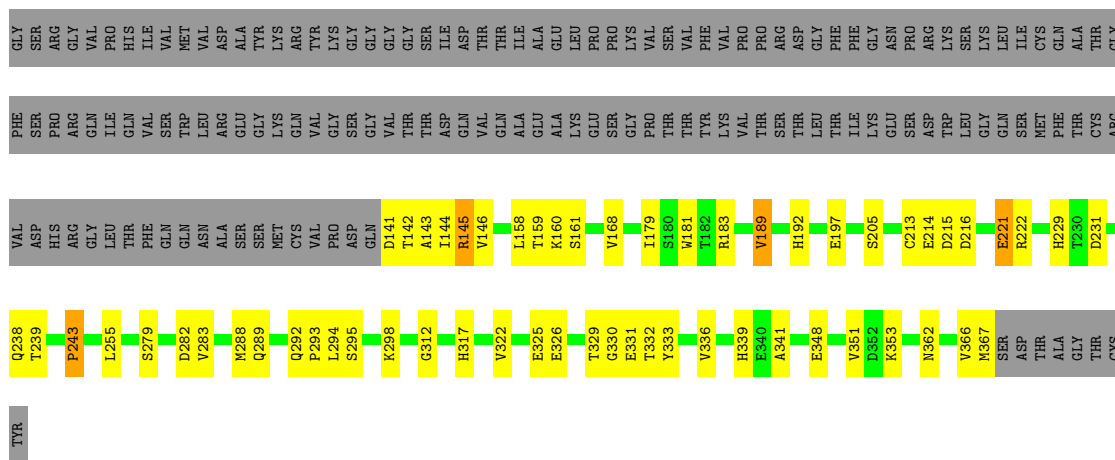


• Molecule 1: Isoform 1 of Immunoglobulin heavy constant mu

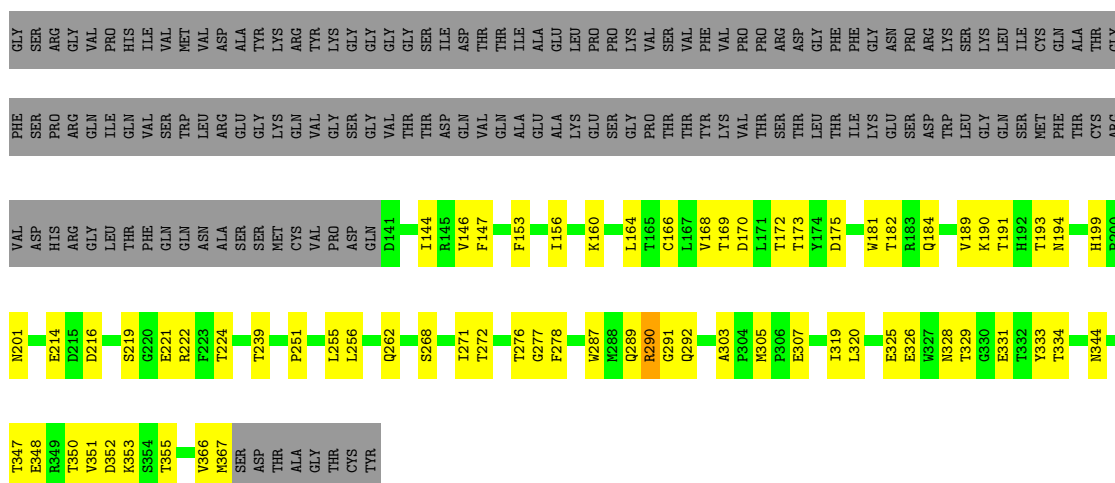
Chain L: 44% 15% 41%



- Molecule 1: Isoform 1 of Immunoglobulin heavy constant mu



- Molecule 1: Isoform 1 of Immunoglobulin heavy constant mu



- Molecule 1: Isoform 1 of Immunoglobulin heavy constant mu

Q289	Q290	Q291	Q292	V300	A303	P304	M305	F315	V322	S323	E324	E331	T332	Y333	V346	T350	V351	D352	T355	M362	M367	S368	ASP	THR	ALA	THR	GLY	THR	CYS	TYR																							
VAL	HIS	ARG	GLY	LEU	THR	PHE	GLN	ASN	ALA	SER	SER	MET	CYS	VAL	PRO	ASP	GLN	D141	I149	P150	P151	K163	L164	R183	T193	M194	D216	W217	N218	S219	R222	S241	R242	P243	K244	L248	L255	E267	S268	T272	L274	V275	T276										
GLY	SER	ARG	GLY	VAL	PRO	HIS	ILE	VAL	LEU	VAL	GLY	SER	GLY	THR	SER	ASP	GLN	D141	I149	P150	P151	K163	L164	R183	T193	M194	D216	W217	N218	S219	R222	S241	R242	P243	K244	L248	L255	E267	S268	T272	L274	V275	T276										
GLY	SER	ARG	GLN	ILE	GLM	VAL	SER	TRP	LEU	ARG	GLU	GLY	LYS	GLM	VAL	GLY	SER	GLY	THR	THR	ASP	GLM	VAL	GLM	ALA	GLU	ALA	LYS	GLU	SER	PRO	THR	THR	THR	LEU	LYS	ILE	GLY	ASN	PRO	ARG	LYS	SER	LEU	GLN	SER	ILE	CYS	GLN	ALA	THR	CYS	GLY

[illegible]

Met	Lys	Asn	His	Leu	Phe	Gly	Val	Leu	Ala	Val	Phe	Ile	Lys	Ala	Val	His	Lys	Gln	Glu	Asp	Glu	Arg	I28	V31	C37	I40	T41	S42	Arg	Ile	Ile	Arg	Ser	Ser	Glu	Asp	Pro	Asn	Glu	Asp	Ile	Arg	N59	I60	R61	I62	I63	V64	I67																											
L90	C91	K92	Lys	Cys	Asp	Pro	Thr	Glu	Val	Glu	Leu	Asp	Asn	Gln	Ile	Val	Thr	Thr	Ala	Ala	Gln	Ser	Asn	Ile	Cys	Asp	Glu	T122	T125	I126	D127	K130	P137	E143	E148	T157	Pro	Asp	His	H164	H165	H166	H167	H168	H169	H170	H171	H172	H173	H174	H175	H176	H177	H178	H179	H180	H181	H182	H183	H184	H185	H186	H187	H188	H189	H190	H191	H192	H193	H194	H195	H196	H197	H198	H199	H200

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	233181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.163	Depositor
Minimum map value	-0.428	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	480.96, 480.96, 480.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.336, 1.336, 1.336	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/1865	0.29	0/2554
1	B	0.15	0/1829	0.32	0/2506
1	C	0.16	0/1814	0.33	0/2485
1	D	0.16	0/1822	0.34	0/2496
1	E	0.15	0/1814	0.34	0/2485
1	L	0.15	0/1780	0.35	0/2439
1	M	0.18	0/1808	0.41	1/2477 (0.0%)
1	N	0.16	0/1808	0.37	0/2477
1	O	0.14	0/1814	0.32	0/2485
1	P	0.13	0/1865	0.30	0/2554
2	J	0.14	0/693	0.30	0/939
All	All	0.15	0/18912	0.34	1/25897 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	243	PRO	CA-N-CD	-8.27	100.43	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1819	1770	1769	28	0
1	B	1784	1741	1740	46	0
1	C	1769	1730	1729	29	0
1	D	1777	1734	1733	29	0
1	E	1769	1730	1729	47	0
1	L	1735	1701	1700	45	0
1	M	1763	1726	1725	40	0
1	N	1763	1725	1724	53	0
1	O	1769	1730	1729	35	0
1	P	1819	1771	1770	27	0
2	J	683	687	683	12	0
3	C	14	13	13	1	0
3	D	14	13	13	2	0
3	M	14	13	13	1	0
3	N	14	13	13	0	0
3	O	14	13	13	1	0
All	All	18520	18110	18096	362	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 10.

All (362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:GLU:O	1:D:329:THR:OG1	1.93	0.86
1:M:183:ARG:NH1	1:M:221:GLU:OE1	2.09	0.85
1:A:363:VAL:HG11	1:P:367:MET:HE1	1.59	0.85
1:D:185:ASN:ND2	1:D:187:GLU:OE2	2.10	0.84
1:N:325:GLU:OE2	1:N:325:GLU:N	2.10	0.84
1:L:333:TYR:O	1:L:350:THR:OG1	1.97	0.83
1:L:246:VAL:O	1:L:248:LEU:N	2.13	0.82
1:O:216:ASP:O	1:O:219:SER:OG	1.96	0.82
1:A:355:THR:O	1:B:260:ARG:NH2	2.13	0.82
1:B:190:LYS:NZ	1:B:193:THR:OG1	2.13	0.82
1:E:328:ASN:O	1:E:353:LYS:NZ	2.12	0.81
1:N:182:THR:OG1	1:N:224:THR:OG1	1.99	0.81
1:O:290:ARG:NH1	1:O:331:GLU:OE1	2.14	0.81
1:M:330:GLY:O	1:M:332:THR:N	2.14	0.80
1:B:183:ARG:NH1	1:B:188:ALA:O	2.14	0.80
1:O:352:ASP:O	1:O:355:THR:OG1	1.97	0.80
1:M:362:ASN:OD1	3:M:401:NAG:O3	1.98	0.80
1:O:242:ARG:NH2	1:O:282:ASP:OD1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLU:OE2	1:B:218:ASN:ND2	2.15	0.80
1:E:173:THR:OG1	1:E:202:ALA:O	2.01	0.79
1:A:220:GLY:O	1:A:241:SER:OG	1.97	0.79
1:N:214:GLU:OE1	1:N:214:GLU:N	2.15	0.79
1:M:295:SER:OG	1:M:298:LYS:NZ	2.15	0.79
1:D:328:ASN:O	1:D:353:LYS:NZ	2.15	0.79
1:M:179:ILE:O	1:M:192:HIS:NE2	2.15	0.78
1:D:362:ASN:OD1	3:D:401:NAG:O3	1.99	0.78
1:L:250:ARG:NH1	1:L:251:PRO:O	2.16	0.78
1:L:279:SER:OG	1:L:312:GLY:O	2.02	0.77
1:B:261:GLU:N	1:B:261:GLU:OE1	2.18	0.76
1:C:179:ILE:HD11	1:C:225:CYS:SG	2.25	0.76
1:L:214:GLU:OE1	1:L:214:GLU:N	2.18	0.76
1:L:326:GLU:OE2	1:L:333:TYR:OH	2.02	0.76
1:D:216:ASP:O	1:D:219:SER:OG	2.04	0.76
1:O:267:GLU:N	1:O:267:GLU:OE1	2.19	0.76
1:B:286:GLN:OE1	1:B:299:TYR:OH	2.06	0.73
1:C:362:ASN:ND2	3:C:401:NAG:O7	2.21	0.73
1:E:165:THR:OG1	1:E:209:GLU:OE2	2.05	0.73
1:P:261:GLU:N	1:P:261:GLU:OE1	2.21	0.72
1:D:305:MET:N	1:D:305:MET:HE2	2.04	0.72
1:B:290:ARG:O	1:B:292:GLN:NE2	2.23	0.71
1:B:326:GLU:OE1	1:B:333:TYR:OH	2.08	0.71
1:M:289:GLN:NE2	1:M:292:GLN:OE1	2.23	0.71
1:N:216:ASP:O	1:N:219:SER:OG	2.08	0.71
1:L:289:GLN:N	1:L:289:GLN:OE1	2.22	0.71
1:N:199:HIS:ND1	1:N:201:ASN:OD1	2.22	0.71
1:B:300:VAL:O	1:B:318:SER:OG	2.09	0.71
1:M:222:ARG:NH1	1:M:239:THR:OG1	2.24	0.70
1:L:190:LYS:NZ	1:L:209:GLU:OE1	2.24	0.70
1:C:262:GLN:NE2	1:C:268:SER:O	2.24	0.70
1:C:183:ARG:NH1	1:C:187:GLU:OE1	2.25	0.70
1:L:242:ARG:NH2	1:L:340:GLU:OE1	2.24	0.69
1:E:262:GLN:OE1	1:E:270:THR:OG1	2.10	0.69
1:E:317:HIS:HE2	1:L:319:ILE:HD11	1.57	0.69
1:B:266:ARG:O	1:B:266:ARG:NH1	2.26	0.69
1:A:309:GLN:N	1:A:309:GLN:OE1	2.26	0.68
1:P:155:SER:O	1:P:160:LYS:N	2.26	0.68
1:D:197:GLU:N	1:D:197:GLU:OE1	2.27	0.67
1:N:290:ARG:NH2	1:N:331:GLU:OE1	2.28	0.66
1:O:141:ASP:O	1:P:145:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:192:HIS:ND1	1:P:209:GLU:O	2.28	0.66
1:E:334:THR:OG1	1:E:348:GLU:OE1	2.13	0.66
1:P:182:THR:O	1:P:224:THR:OG1	2.13	0.65
1:B:295:SER:OG	1:B:297:GLU:OE2	2.14	0.65
1:D:229:HIS:NE2	1:D:231:ASP:OD2	2.30	0.64
1:B:326:GLU:O	1:B:329:THR:OG1	2.14	0.64
1:B:171:LEU:HD13	1:B:172:THR:O	1.97	0.64
1:E:317:HIS:NE2	1:L:319:ILE:HD11	2.11	0.64
1:A:325:GLU:O	1:A:329:THR:OG1	2.09	0.64
1:P:305:MET:SD	1:P:305:MET:N	2.71	0.64
1:N:184:GLN:OE1	1:N:222:ARG:NE	2.31	0.63
1:M:197:GLU:O	1:M:205:SER:OG	2.16	0.63
1:O:368:SER:OG	1:P:369:ASP:OD1	2.04	0.63
1:N:219:SER:OG	1:N:221:GLU:OE2	2.14	0.63
1:O:241:SER:OG	1:O:244:LYS:NZ	2.20	0.63
1:N:262:GLN:NE2	1:N:268:SER:O	2.32	0.63
1:B:305:MET:SD	1:B:305:MET:N	2.71	0.63
1:N:352:ASP:O	1:N:355:THR:OG1	2.12	0.63
1:D:201:ASN:OD1	1:D:203:THR:OG1	2.12	0.62
1:P:318:SER:C	1:P:319:ILE:HD13	2.24	0.62
1:O:267:GLU:N	1:O:324:GLU:OE2	2.31	0.62
1:P:267:GLU:OE1	1:P:267:GLU:N	2.32	0.62
1:D:255:LEU:HD21	1:D:271:ILE:CG2	2.30	0.62
1:M:326:GLU:O	1:M:329:THR:OG1	2.15	0.61
1:A:288:MET:HE1	2:J:137:PRO:HD2	1.82	0.61
1:E:189:VAL:HG21	1:E:210:ALA:HB1	1.81	0.61
1:D:305:MET:HE2	1:D:305:MET:H	1.65	0.60
1:B:145:ARG:O	1:B:169:THR:OG1	2.18	0.60
1:N:329:THR:OG1	1:N:331:GLU:OE2	2.11	0.60
1:O:362:ASN:ND2	3:O:401:NAG:O3	2.33	0.60
1:E:179:ILE:HD12	1:E:227:VAL:HG12	1.83	0.60
1:E:339:HIS:ND1	1:E:340:GLU:O	2.35	0.60
1:M:367:MET:HA	1:M:367:MET:HE2	1.85	0.59
1:E:315:PHE:CE1	1:L:319:ILE:HD12	2.37	0.59
1:N:326:GLU:OE2	1:N:333:TYR:OH	2.20	0.59
1:C:160:LYS:N	1:C:160:LYS:HD3	2.18	0.59
1:P:231:ASP:OD1	1:P:232:LEU:N	2.35	0.59
1:C:181:TRP:O	1:C:189:VAL:N	2.36	0.59
1:E:292:GLN:N	1:E:292:GLN:OE1	2.35	0.58
1:B:289:GLN:NE2	1:B:331:GLU:OE1	2.36	0.58
1:C:260:ARG:NH2	1:D:355:THR:OG1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:328:ASN:O	1:N:353:LYS:NZ	2.37	0.58
1:E:279:SER:O	1:E:339:HIS:NE2	2.33	0.58
1:M:243:PRO:HD2	1:M:243:PRO:O	2.02	0.58
1:E:352:ASP:O	1:E:355:THR:OG1	2.16	0.57
1:C:149:ILE:HD12	1:C:149:ILE:H	1.68	0.57
1:O:274:LEU:HD11	1:O:276:THR:OG1	2.04	0.57
1:B:294:LEU:HD12	1:B:294:LEU:O	2.04	0.57
1:E:197:GLU:OE1	1:E:197:GLU:N	2.37	0.57
1:P:187:GLU:N	1:P:187:GLU:OE1	2.38	0.57
1:N:255:LEU:HD11	1:N:271:ILE:HG22	1.87	0.57
1:A:305:MET:SD	1:A:305:MET:N	2.78	0.57
1:B:215:ASP:O	1:B:219:SER:N	2.34	0.56
1:M:325:GLU:N	1:M:325:GLU:OE1	2.38	0.56
1:B:255:LEU:CD2	1:B:351:VAL:HG22	2.35	0.56
2:J:127:ASP:OD2	2:J:130:LYS:N	2.38	0.56
1:C:145:ARG:NE	1:C:170:ASP:OD1	2.38	0.56
1:P:370:THR:HG23	1:P:370:THR:O	2.06	0.56
1:B:255:LEU:HD23	1:B:351:VAL:HG22	1.86	0.56
1:M:326:GLU:OE1	1:M:326:GLU:N	2.39	0.56
1:M:146:VAL:O	1:M:238:GLN:NE2	2.38	0.56
1:O:289:GLN:O	1:O:292:GLN:NE2	2.37	0.56
1:A:375:TYR:CE2	2:J:60:ILE:HD11	2.40	0.56
1:M:159:THR:O	1:M:161:SER:N	2.39	0.56
1:C:229:HIS:NE2	1:C:231:ASP:OD2	2.39	0.56
1:N:287:TRP:CG	1:N:320:LEU:HD12	2.41	0.55
1:O:268:SER:N	1:O:324:GLU:OE2	2.39	0.55
1:B:282:ASP:OD2	1:B:282:ASP:N	2.39	0.55
1:E:184:GLN:OE1	1:E:222:ARG:NE	2.39	0.55
1:A:155:SER:O	1:A:159:THR:OG1	2.18	0.55
1:D:361:TYR:OH	1:M:367:MET:HE1	2.07	0.55
1:C:351:VAL:HG13	1:C:355:THR:HG21	1.89	0.54
1:A:359:THR:O	1:B:359:THR:OG1	2.10	0.54
1:L:155:SER:HA	1:L:158:LEU:HD12	1.89	0.54
1:M:229:HIS:NE2	1:M:231:ASP:OD2	2.40	0.54
1:E:253:VAL:HG21	1:E:337:VAL:HG21	1.89	0.54
1:A:307:GLU:OE1	1:A:309:GLN:NE2	2.38	0.54
1:M:181:TRP:HB2	1:M:189:VAL:HG22	1.90	0.54
1:O:242:ARG:O	1:O:244:LYS:NZ	2.40	0.54
1:M:255:LEU:HD23	1:M:351:VAL:HG23	1.89	0.54
1:N:347:THR:OG1	1:N:348:GLU:N	2.41	0.54
1:M:279:SER:OG	1:M:312:GLY:O	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:ASN:OD1	1:E:329:THR:N	2.41	0.53
1:L:326:GLU:O	1:L:329:THR:OG1	2.25	0.53
1:C:262:GLN:O	1:C:268:SER:OG	2.25	0.53
1:N:289:GLN:NE2	1:N:292:GLN:OE1	2.42	0.53
1:D:303:ALA:O	1:D:305:MET:SD	2.67	0.53
1:L:337:VAL:HG13	1:L:337:VAL:O	2.08	0.53
1:E:309:GLN:OE1	1:L:298:LYS:NZ	2.36	0.52
1:O:274:LEU:HD12	1:O:275:VAL:N	2.24	0.52
1:M:317:HIS:HE2	1:N:319:ILE:CD1	2.23	0.52
1:N:224:THR:HG22	1:N:239:THR:HG23	1.92	0.51
1:C:316:ALA:O	1:C:317:HIS:ND1	2.43	0.51
1:E:282:ASP:OD1	1:E:282:ASP:N	2.42	0.51
1:L:150:PRO:O	1:L:152:SER:N	2.44	0.51
1:P:162:THR:OG1	1:P:212:ILE:O	2.29	0.51
1:A:372:GLY:O	1:A:374:CYS:N	2.43	0.51
1:A:287:TRP:NE1	1:A:318:SER:OG	2.43	0.51
1:A:363:VAL:HG11	1:P:367:MET:CE	2.37	0.50
1:L:267:GLU:N	1:L:267:GLU:OE1	2.43	0.50
1:A:372:GLY:N	1:A:375:TYR:OXT	2.44	0.50
1:E:152:SER:O	1:E:155:SER:OG	2.17	0.50
1:L:154:ALA:O	1:L:158:LEU:HG	2.11	0.50
1:N:334:THR:HG22	1:N:350:THR:OG1	2.11	0.50
1:A:339:HIS:CD2	1:A:341:ALA:HB3	2.46	0.50
1:D:182:THR:OG1	1:D:224:THR:OG1	2.05	0.50
1:N:222:ARG:CD	1:N:222:ARG:O	2.60	0.50
1:L:352:ASP:C	1:L:352:ASP:OD1	2.55	0.50
1:M:288:MET:HA	1:M:294:LEU:HD23	1.93	0.50
1:O:305:MET:SD	1:O:305:MET:N	2.85	0.50
1:M:141:ASP:OD1	1:M:142:THR:N	2.45	0.50
1:D:162:THR:OG1	1:D:212:ILE:O	2.30	0.49
1:M:143:ALA:O	1:M:145:ARG:N	2.44	0.49
1:N:201:ASN:O	1:N:201:ASN:ND2	2.45	0.49
1:O:216:ASP:OD1	1:O:217:TRP:N	2.44	0.49
1:D:255:LEU:HD21	1:D:271:ILE:HG22	1.94	0.49
1:C:179:ILE:O	1:C:192:HIS:NE2	2.46	0.49
2:J:59:ASN:OD1	2:J:60:ILE:N	2.45	0.49
1:N:367:MET:SD	1:N:367:MET:N	2.85	0.49
1:C:282:ASP:OD1	1:C:282:ASP:N	2.46	0.49
1:D:181:TRP:O	1:D:192:HIS:NE2	2.41	0.49
1:C:352:ASP:O	1:C:355:THR:OG1	2.21	0.49
1:N:169:THR:OG1	1:N:170:ASP:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:286:GLN:NE2	1:L:294:LEU:O	2.45	0.48
1:D:288:MET:HE1	1:D:336:VAL:CG1	2.43	0.48
1:E:278:PHE:CE2	1:E:283:VAL:HG23	2.49	0.48
1:B:266:ARG:O	1:B:266:ARG:HG2	2.14	0.48
2:J:31:VAL:HG11	2:J:90:LEU:HD23	1.96	0.48
1:N:287:TRP:CB	1:N:320:LEU:HD12	2.43	0.48
1:A:262:GLN:NE2	1:A:268:SER:O	2.47	0.48
1:C:272:THR:HG21	1:D:256:LEU:CD1	2.44	0.47
1:E:305:MET:SD	1:E:305:MET:N	2.87	0.47
1:N:193:THR:HG22	1:N:194:ASN:H	1.79	0.47
1:N:193:THR:HG22	1:N:194:ASN:N	2.28	0.47
1:O:193:THR:OG1	1:O:194:ASN:N	2.47	0.47
1:B:290:ARG:O	1:B:290:ARG:HG3	2.14	0.47
1:C:290:ARG:NH2	1:C:331:GLU:OE2	2.44	0.47
1:E:248:LEU:HB3	1:E:341:ALA:HB2	1.96	0.47
1:O:248:LEU:C	1:O:248:LEU:HD12	2.39	0.47
1:O:305:MET:HE2	1:O:315:PHE:CZ	2.50	0.47
1:B:142:THR:OG1	1:B:143:ALA:N	2.47	0.47
2:J:143:GLU:N	2:J:143:GLU:OE1	2.48	0.47
1:M:213:CYS:N	1:M:216:ASP:OD1	2.40	0.47
1:M:367:MET:HE2	1:M:367:MET:CA	2.45	0.47
1:P:289:GLN:OE1	1:P:290:ARG:NH2	2.47	0.47
1:C:214:GLU:OE1	1:C:217:TRP:NE1	2.45	0.47
1:E:247:ALA:HB1	1:E:249:HIS:HE1	1.79	0.47
1:L:255:LEU:HD22	1:L:351:VAL:HG21	1.96	0.47
1:N:181:TRP:HB2	1:N:189:VAL:HG22	1.96	0.47
1:L:194:ASN:O	1:L:194:ASN:ND2	2.48	0.47
1:M:215:ASP:OD2	1:M:216:ASP:N	2.48	0.47
1:E:334:THR:OG1	1:E:349:ARG:O	2.33	0.46
1:O:303:ALA:O	1:O:305:MET:SD	2.74	0.46
1:L:181:TRP:HB3	1:L:189:VAL:HG11	1.97	0.46
1:B:290:ARG:O	1:B:290:ARG:CG	2.63	0.46
1:N:255:LEU:HD11	1:N:271:ILE:CG2	2.45	0.46
1:A:196:SER:OG	1:A:207:VAL:HG22	2.16	0.46
1:N:175:ASP:N	1:N:175:ASP:OD1	2.48	0.46
1:E:272:THR:HG21	1:L:256:LEU:CD1	2.46	0.45
1:L:279:SER:HB2	1:L:280:PRO:HD3	1.98	0.45
1:P:141:ASP:OD1	1:P:141:ASP:N	2.47	0.45
1:E:281:ALA:HB2	1:E:314:TYR:CE2	2.52	0.45
1:A:162:THR:HB	1:A:212:ILE:HG23	1.98	0.45
1:B:150:PRO:HB2	1:B:217:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:LEU:HD21	1:E:276:THR:OG1	2.16	0.45
1:M:282:ASP:O	1:M:283:VAL:HG13	2.17	0.45
1:M:317:HIS:HE2	1:N:319:ILE:HD12	1.80	0.45
1:O:324:GLU:OE1	1:O:324:GLU:N	2.45	0.45
1:B:215:ASP:OD2	1:B:215:ASP:C	2.59	0.45
1:L:361:TYR:CD1	1:L:361:TYR:O	2.70	0.45
1:L:283:VAL:HG23	1:L:283:VAL:O	2.16	0.45
1:M:336:VAL:HG12	1:M:348:GLU:HB3	1.99	0.45
1:P:368:SER:O	1:P:369:ASP:C	2.60	0.45
1:E:319:ILE:HD11	1:L:317:HIS:CE1	2.52	0.45
1:N:156:ILE:O	1:N:160:LYS:N	2.49	0.45
1:A:195:ILE:CG2	1:A:207:VAL:HG23	2.47	0.44
1:D:290:ARG:HB2	1:D:290:ARG:NH1	2.32	0.44
1:E:192:HIS:HB3	1:E:208:GLY:HA2	1.99	0.44
1:C:260:ARG:NH2	1:D:355:THR:O	2.50	0.44
1:N:172:THR:HG22	1:N:173:THR:N	2.31	0.44
1:L:274:LEU:C	1:L:274:LEU:HD12	2.43	0.44
1:L:283:VAL:HA	1:L:338:ALA:O	2.18	0.44
1:L:358:PRO:C	1:L:359:THR:HG23	2.43	0.44
1:N:190:LYS:O	1:N:191:THR:OG1	2.28	0.44
1:N:251:PRO:HA	1:N:278:PHE:HB3	1.99	0.44
1:C:287:TRP:CE3	1:C:320:LEU:HD13	2.53	0.44
1:E:319:ILE:HD11	1:L:317:HIS:HE1	1.82	0.44
1:C:189:VAL:HG11	1:C:192:HIS:CD2	2.53	0.43
1:M:213:CYS:SG	1:M:214:GLU:N	2.91	0.43
1:L:170:ASP:O	1:L:170:ASP:OD2	2.35	0.43
1:N:173:THR:HG23	1:N:173:THR:O	2.18	0.43
1:N:289:GLN:O	1:N:291:GLY:N	2.51	0.43
1:B:209:GLU:N	1:B:209:GLU:OE1	2.52	0.43
1:C:300:VAL:HG12	1:C:301:THR:N	2.34	0.43
1:N:146:VAL:CG1	1:N:168:VAL:HG12	2.49	0.43
1:N:276:THR:OG1	1:N:307:GLU:OE2	2.36	0.43
1:B:303:ALA:O	1:B:305:MET:SD	2.77	0.43
1:A:165:THR:HG23	1:A:192:HIS:NE2	2.34	0.43
1:B:301:THR:HG23	1:B:318:SER:HB2	2.00	0.43
1:C:307:GLU:HB2	1:C:310:ALA:HB3	2.01	0.43
1:E:331:GLU:OE1	1:E:333:TYR:OH	2.35	0.43
1:L:352:ASP:OD1	1:L:354:SER:N	2.52	0.43
1:O:149:ILE:O	1:O:151:PRO:HD3	2.19	0.43
1:B:155:SER:O	1:B:159:THR:OG1	2.20	0.43
1:L:316:ALA:O	1:L:317:HIS:ND1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:LEU:HD22	1:D:351:VAL:HB	2.00	0.43
1:D:279:SER:C	1:D:339:HIS:HE2	2.25	0.43
1:E:358:PRO:C	1:E:359:THR:HG23	2.43	0.43
2:J:31:VAL:HG11	2:J:90:LEU:CD2	2.49	0.43
1:N:168:VAL:HG23	1:N:168:VAL:O	2.18	0.43
1:M:339:HIS:CE1	1:M:341:ALA:HB3	2.54	0.43
1:B:146:VAL:O	1:B:238:GLN:NE2	2.52	0.42
1:D:180:SER:OG	1:D:226:THR:OG1	2.32	0.42
1:P:261:GLU:HA	1:P:264:ASN:OD1	2.18	0.42
1:P:276:THR:OG1	1:P:307:GLU:OE2	2.33	0.42
1:E:179:ILE:CD1	1:E:227:VAL:HG12	2.46	0.42
1:E:279:SER:C	1:E:339:HIS:HE2	2.24	0.42
1:P:303:ALA:O	1:P:305:MET:SD	2.77	0.42
1:B:177:VAL:O	1:B:177:VAL:HG23	2.18	0.42
1:N:146:VAL:HG13	1:N:168:VAL:HG12	2.01	0.42
1:B:280:PRO:O	1:B:339:HIS:NE2	2.47	0.42
1:B:301:THR:HG1	1:B:318:SER:CB	2.31	0.42
1:C:317:HIS:CE1	1:D:319:ILE:HG21	2.54	0.42
1:O:350:THR:HG22	1:O:351:VAL:N	2.35	0.42
1:P:217:TRP:O	1:P:242:ARG:NE	2.52	0.42
1:P:319:ILE:HD13	1:P:319:ILE:N	2.34	0.42
1:L:366:VAL:HB	1:M:366:VAL:HG23	2.01	0.42
1:N:272:THR:O	1:N:272:THR:HG23	2.20	0.42
1:O:282:ASP:O	1:O:282:ASP:CG	2.62	0.42
1:P:267:GLU:O	1:P:268:SER:OG	2.32	0.42
1:B:164:LEU:HD22	1:B:223:PHE:CG	2.54	0.42
1:B:212:ILE:HG12	1:B:216:ASP:HB3	2.00	0.42
1:E:339:HIS:CG	1:E:340:GLU:N	2.87	0.42
1:L:336:VAL:HG12	1:L:348:GLU:HG3	2.02	0.42
1:A:191:THR:HG22	1:A:192:HIS:N	2.34	0.42
3:D:401:NAG:O3	3:D:401:NAG:O7	2.38	0.42
1:M:282:ASP:OD1	1:M:282:ASP:N	2.52	0.42
1:P:205:SER:OG	1:P:206:ALA:N	2.52	0.42
1:E:176:SER:O	1:E:229:HIS:ND1	2.53	0.42
1:O:300:VAL:HG11	1:P:315:PHE:CZ	2.54	0.42
1:A:153:PHE:HA	1:A:156:ILE:HG22	2.02	0.42
2:J:60:ILE:HG22	2:J:62:ILE:CD1	2.50	0.42
1:L:166:CYS:SG	1:L:181:TRP:NE1	2.91	0.42
1:B:361:TYR:CE2	1:O:367:MET:HE3	2.54	0.42
1:E:156:ILE:O	1:E:160:LYS:N	2.50	0.42
1:E:311:PRO:O	1:E:313:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:330:GLY:HA2	1:M:353:LYS:HG3	2.02	0.42
1:N:276:THR:OG1	1:N:277:GLY:N	2.53	0.41
1:N:256:LEU:HB2	1:N:272:THR:HG23	2.02	0.41
1:C:180:SER:OG	1:C:189:VAL:HG12	2.21	0.41
1:M:293:PRO:O	1:M:294:LEU:HD22	2.20	0.41
1:M:317:HIS:NE2	1:N:319:ILE:HD11	2.36	0.41
1:N:164:LEU:HD12	1:N:181:TRP:CZ3	2.55	0.41
1:N:351:VAL:HA	1:N:355:THR:HG21	2.02	0.41
1:C:168:VAL:CG1	1:C:171:LEU:HD11	2.51	0.41
1:E:249:HIS:CE1	1:E:313:ARG:NH1	2.88	0.41
1:M:146:VAL:HG23	1:M:168:VAL:HG22	2.00	0.41
1:O:149:ILE:O	1:O:151:PRO:CD	2.68	0.41
1:A:261:GLU:OE1	1:A:261:GLU:N	2.41	0.41
1:A:302:SER:N	1:A:317:HIS:O	2.41	0.41
1:B:267:GLU:O	1:B:268:SER:OG	2.33	0.41
1:D:279:SER:O	1:D:339:HIS:NE2	2.49	0.41
1:E:300:VAL:HG22	1:E:301:THR:N	2.36	0.41
1:M:158:LEU:C	1:M:158:LEU:HD23	2.45	0.41
1:N:222:ARG:O	1:N:222:ARG:HD2	2.19	0.41
1:N:303:ALA:O	1:N:305:MET:SD	2.78	0.41
1:B:162:THR:OG1	1:B:212:ILE:HG22	2.21	0.41
1:L:303:ALA:O	1:L:305:MET:SD	2.79	0.41
1:N:153:PHE:HA	1:N:156:ILE:HG22	2.03	0.41
1:N:366:VAL:O	1:O:367:MET:HB2	2.20	0.41
1:A:365:LEU:HD11	1:B:365:LEU:HD12	2.02	0.41
1:E:307:GLU:HG3	1:E:313:ARG:O	2.21	0.41
1:A:344:ASN:ND2	2:J:148:GLU:OE1	2.54	0.41
1:B:171:LEU:HD12	1:B:204:PHE:HB2	2.03	0.41
1:B:324:GLU:O	1:B:328:ASN:OD1	2.38	0.41
1:B:336:VAL:HG23	1:B:348:GLU:OE1	2.20	0.41
1:D:164:LEU:HD11	1:D:240:ILE:CG2	2.51	0.41
1:L:170:ASP:O	1:L:170:ASP:CG	2.64	0.41
1:P:331:GLU:HB2	1:P:333:TYR:CE1	2.55	0.41
1:E:255:LEU:HD22	1:E:351:VAL:HG22	2.02	0.41
1:L:361:TYR:O	1:L:361:TYR:HD1	2.03	0.41
1:O:163:LYS:O	1:O:164:LEU:HD22	2.21	0.41
1:B:174:TYR:OH	1:B:230:THR:HG23	2.20	0.40
1:D:305:MET:HE2	1:D:315:PHE:O	2.22	0.40
1:E:246:VAL:HG21	1:E:280:PRO:HB3	2.04	0.40
1:E:313:ARG:HG3	1:E:313:ARG:HH11	1.86	0.40
1:C:166:CYS:SG	1:C:181:TRP:NE1	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASP:OD1	1:C:217:TRP:N	2.52	0.40
1:E:303:ALA:O	1:E:305:MET:HE1	2.22	0.40
1:O:322:VAL:HG21	1:O:333:TYR:OH	2.21	0.40
2:J:37:CYS:SG	2:J:125:THR:HG21	2.61	0.40
2:J:40:ILE:HD11	2:J:87:LEU:HD11	2.03	0.40
1:L:327:TRP:O	1:L:353:LYS:NZ	2.48	0.40
1:N:344:ASN:HD22	1:O:346:VAL:HG21	1.87	0.40
1:O:183:ARG:NH1	1:O:216:ASP:OD2	2.55	0.40
2:J:64:VAL:O	2:J:64:VAL:HG22	2.20	0.40
1:O:222:ARG:NH1	1:O:244:LYS:O	2.55	0.40
1:A:276:THR:HG22	1:A:277:GLY:N	2.36	0.40
1:L:149:ILE:O	1:L:151:PRO:HD3	2.22	0.40
1:L:339:HIS:CG	1:L:340:GLU:N	2.89	0.40
1:M:322:VAL:HG21	1:M:333:TYR:OH	2.21	0.40
1:N:166:CYS:HB2	1:N:181:TRP:CH2	2.56	0.40
1:O:255:LEU:HD12	1:O:272:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/375 (62%)	211 (91%)	22 (9%)	0	100	100
1	B	228/375 (61%)	208 (91%)	18 (8%)	2 (1%)	14	46
1	C	226/375 (60%)	208 (92%)	18 (8%)	0	100	100
1	D	227/375 (60%)	208 (92%)	18 (8%)	1 (0%)	30	61
1	E	226/375 (60%)	206 (91%)	19 (8%)	1 (0%)	30	61
1	L	221/375 (59%)	200 (90%)	20 (9%)	1 (0%)	24	57
1	M	225/375 (60%)	205 (91%)	17 (8%)	3 (1%)	9	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	225/375 (60%)	210 (93%)	13 (6%)	2 (1%)	14	46
1	O	226/375 (60%)	203 (90%)	23 (10%)	0	100	100
1	P	233/375 (62%)	212 (91%)	20 (9%)	1 (0%)	30	61
2	J	79/167 (47%)	72 (91%)	7 (9%)	0	100	100
All	All	2349/3917 (60%)	2143 (91%)	195 (8%)	11 (0%)	26	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	247	ALA
1	M	331	GLU
1	D	189	VAL
1	N	290	ARG
1	B	144	ILE
1	B	213	CYS
1	M	160	LYS
1	N	144	ILE
1	P	144	ILE
1	E	144	ILE
1	M	144	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/327 (64%)	208 (100%)	0	100	100
1	B	205/327 (63%)	204 (100%)	1 (0%)	81	80
1	C	203/327 (62%)	203 (100%)	0	100	100
1	D	204/327 (62%)	204 (100%)	0	100	100
1	E	203/327 (62%)	202 (100%)	1 (0%)	81	80
1	L	199/327 (61%)	199 (100%)	0	100	100
1	M	202/327 (62%)	199 (98%)	3 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	202/327 (62%)	201 (100%)	1 (0%)	81	80
1	O	203/327 (62%)	202 (100%)	1 (0%)	81	80
1	P	208/327 (64%)	208 (100%)	0	100	100
2	J	80/155 (52%)	79 (99%)	1 (1%)	61	72
All	All	2117/3425 (62%)	2109 (100%)	8 (0%)	81	81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	216	ASP
1	E	288	MET
2	J	31	VAL
1	M	145	ARG
1	M	189	VAL
1	M	221	GLU
1	N	147	PHE
1	O	305	MET

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

Mol	Chain	Res	Type
1	A	262	GLN
1	B	218	ASN
1	C	344	ASN
1	D	185	ASN
1	E	201	ASN
1	E	249	HIS
1	L	185	ASN
1	L	249	HIS
1	L	317	HIS
1	M	249	HIS
1	M	339	HIS

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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	O	401	-	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	C	401	-	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	D	401	-	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	M	401	-	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	N	401	-	14,14,15	0.21	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	O	401	-	-	4/6/23/26	0/1/1/1
3	NAG	C	401	-	-	3/6/23/26	0/1/1/1
3	NAG	D	401	-	-	1/6/23/26	0/1/1/1
3	NAG	M	401	-	-	2/6/23/26	0/1/1/1
3	NAG	N	401	-	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	401	NAG	C1-C2-N2-C7
3	O	401	NAG	C1-C2-N2-C7
3	M	401	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
3	C	401	NAG	C4-C5-C6-O6
3	M	401	NAG	C4-C5-C6-O6
3	O	401	NAG	O5-C5-C6-O6
3	O	401	NAG	C4-C5-C6-O6
3	N	401	NAG	O5-C5-C6-O6
3	O	401	NAG	C3-C2-N2-C7
3	D	401	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	401	NAG	1	0
3	C	401	NAG	1	0
3	D	401	NAG	2	0
3	M	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

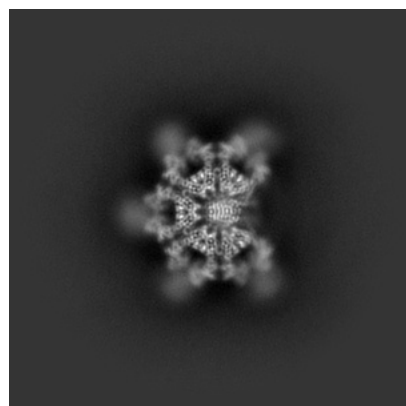
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43795. These allow visual inspection of the internal detail of the map and identification of artifacts.

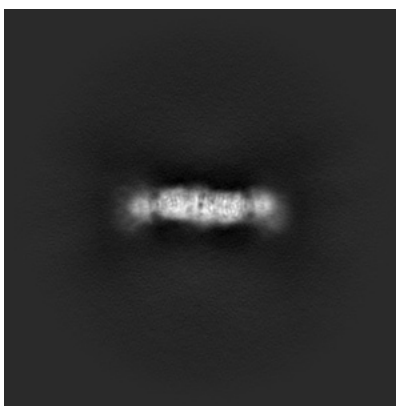
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

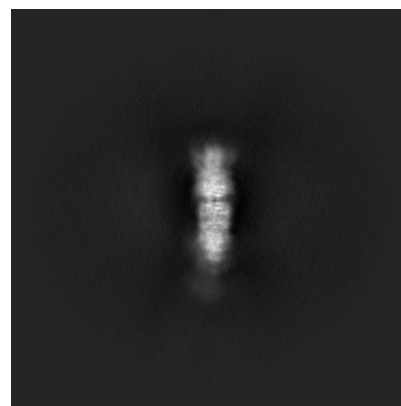
6.1.1 Primary map



X

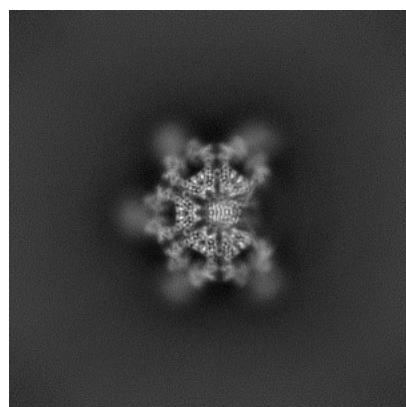


Y

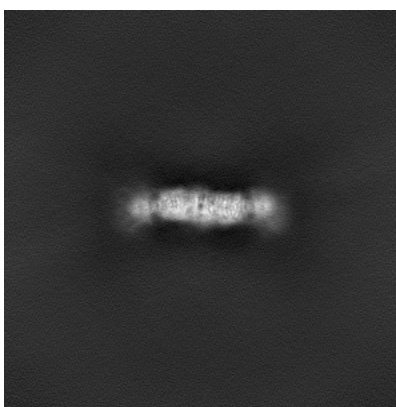


Z

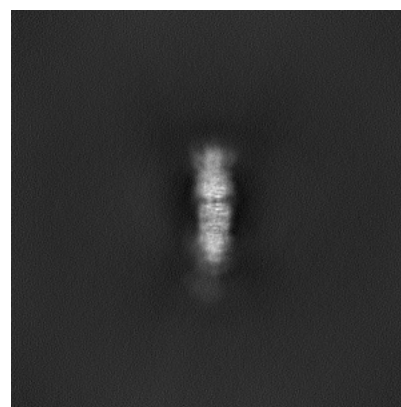
6.1.2 Raw map



X



Y

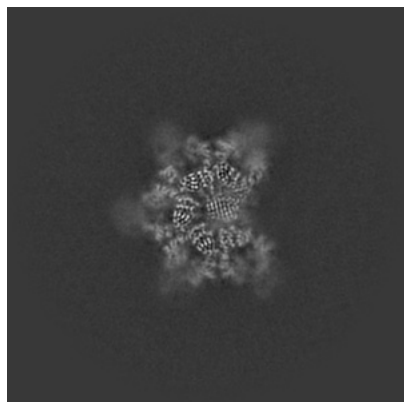


Z

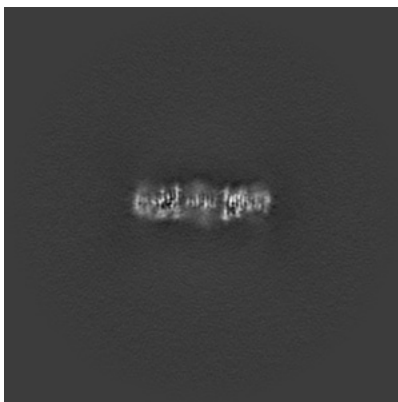
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

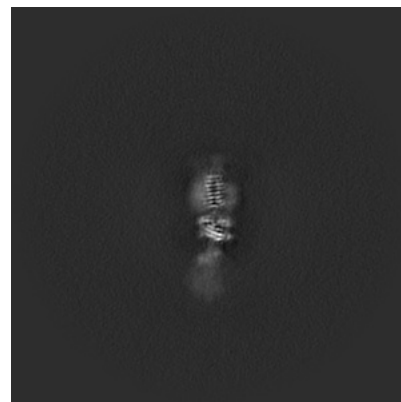
6.2.1 Primary map



X Index: 180

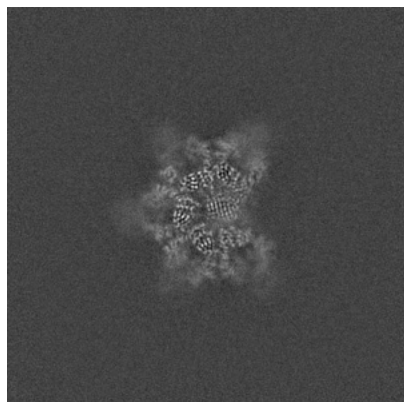


Y Index: 180

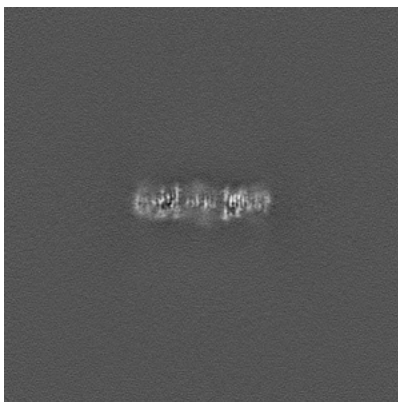


Z Index: 180

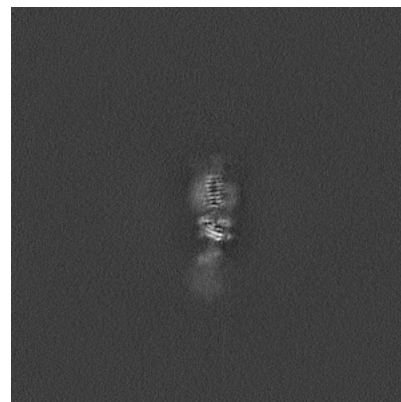
6.2.2 Raw map



X Index: 180



Y Index: 180

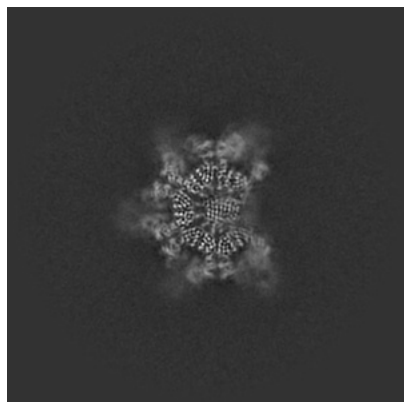


Z Index: 180

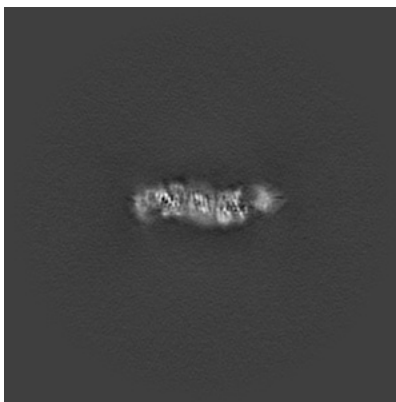
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

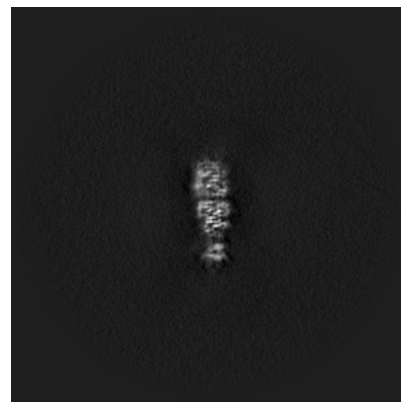
6.3.1 Primary map



X Index: 185

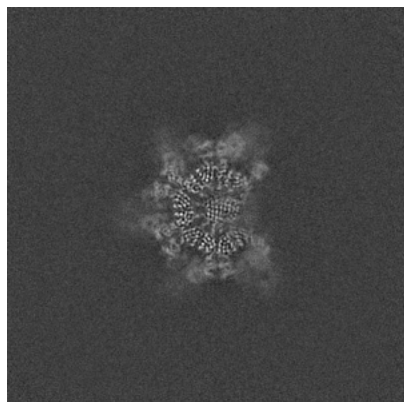


Y Index: 199

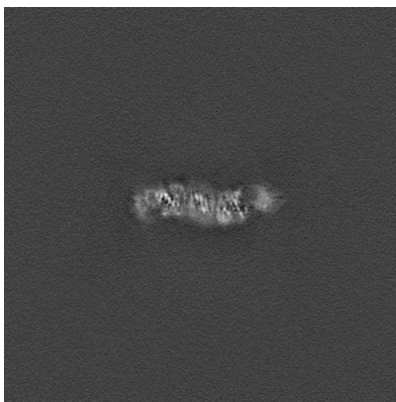


Z Index: 198

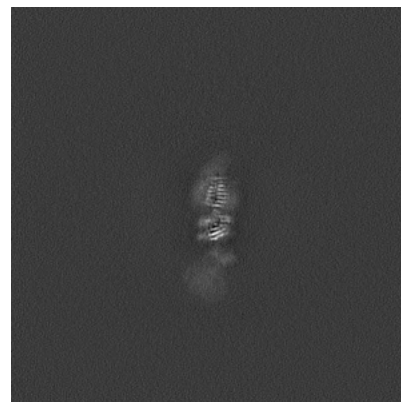
6.3.2 Raw map



X Index: 185



Y Index: 199

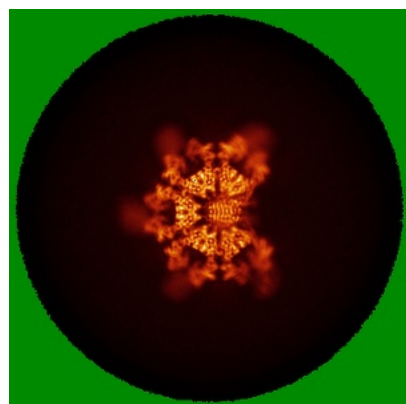


Z Index: 173

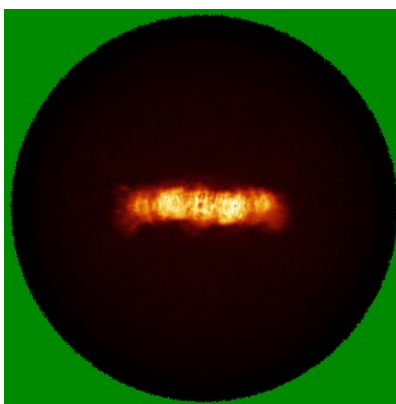
The images above show the largest variance slices of the map in three orthogonal directions.

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

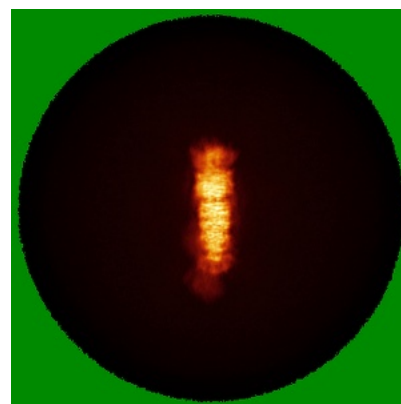
6.4.1 Primary map



X

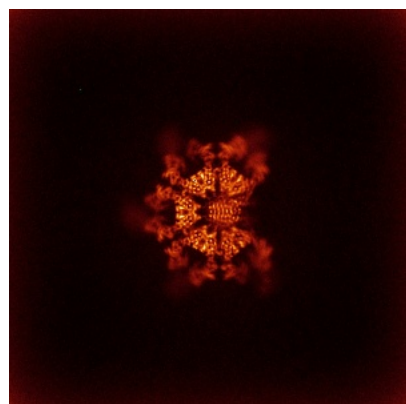


Y

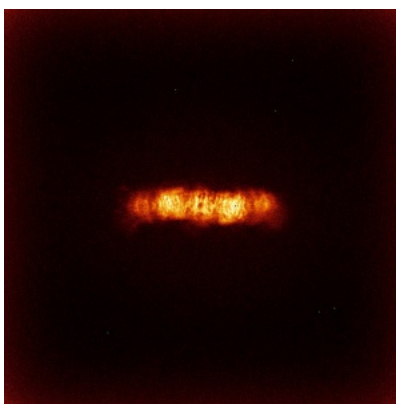


Z

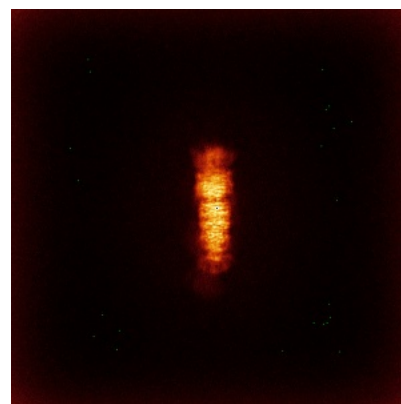
6.4.2 Raw map



X



Y

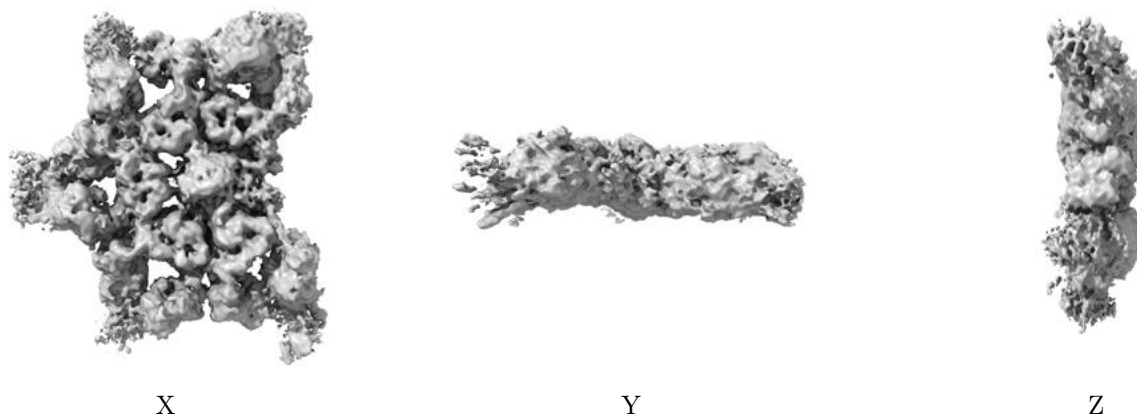


Z

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

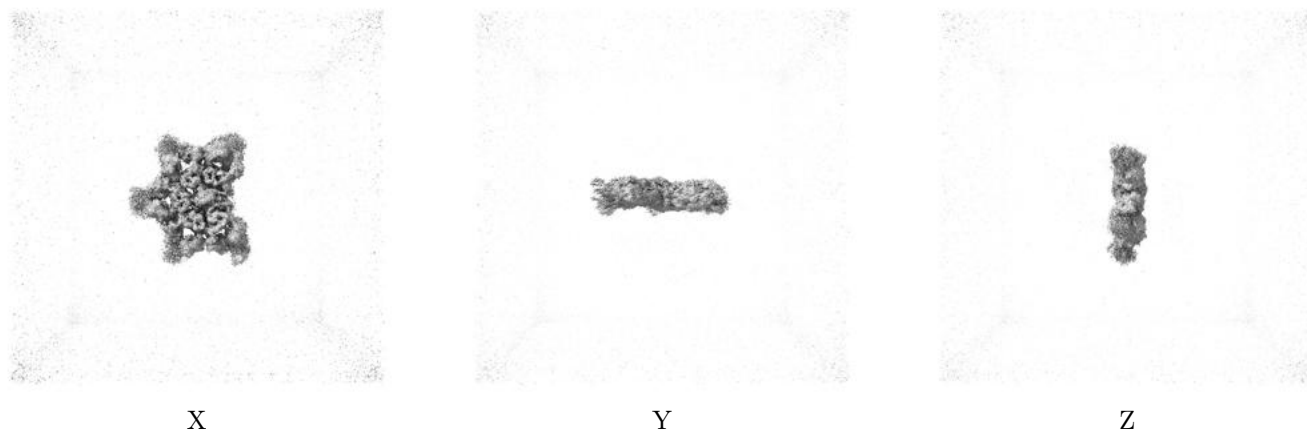
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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

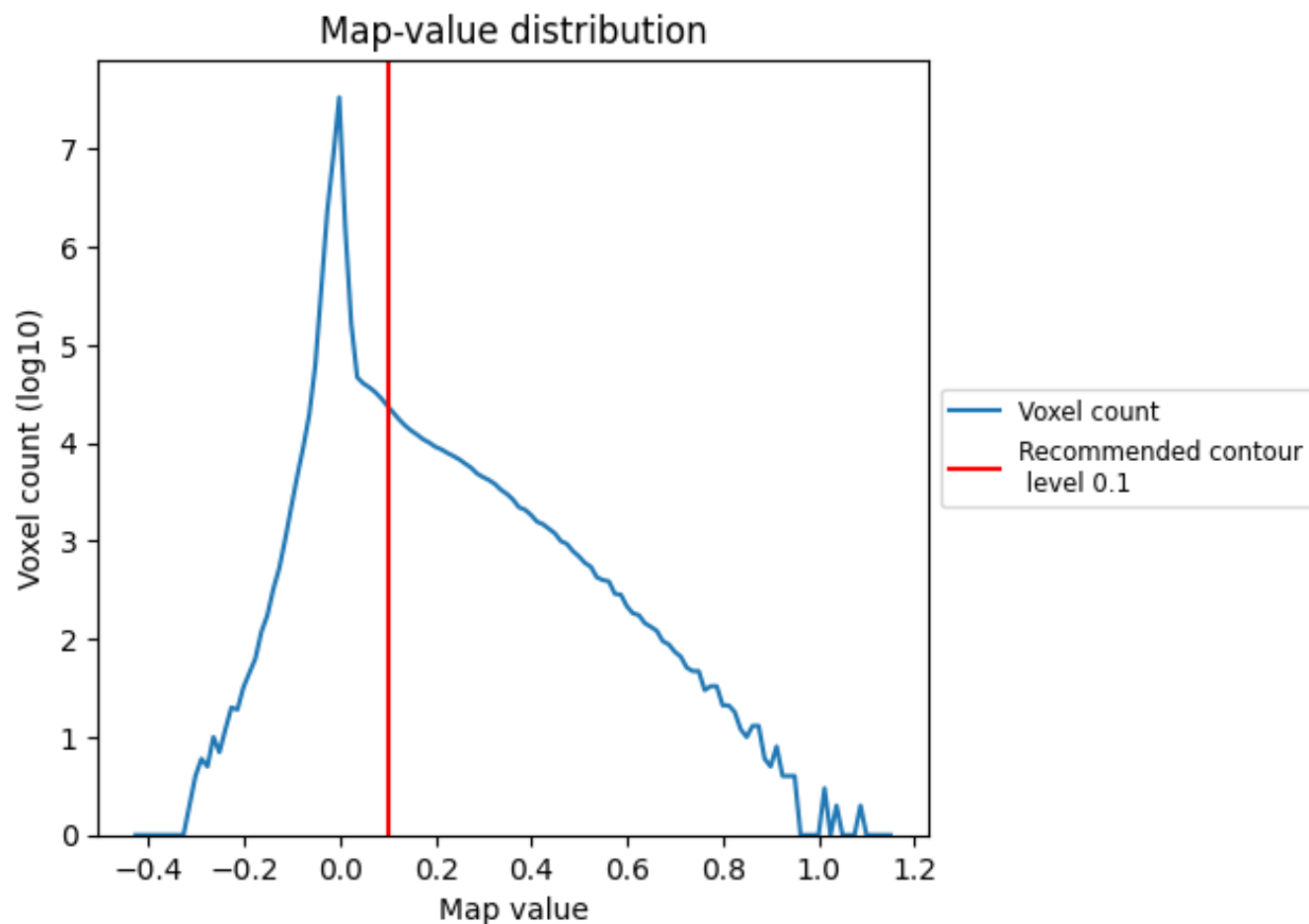
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

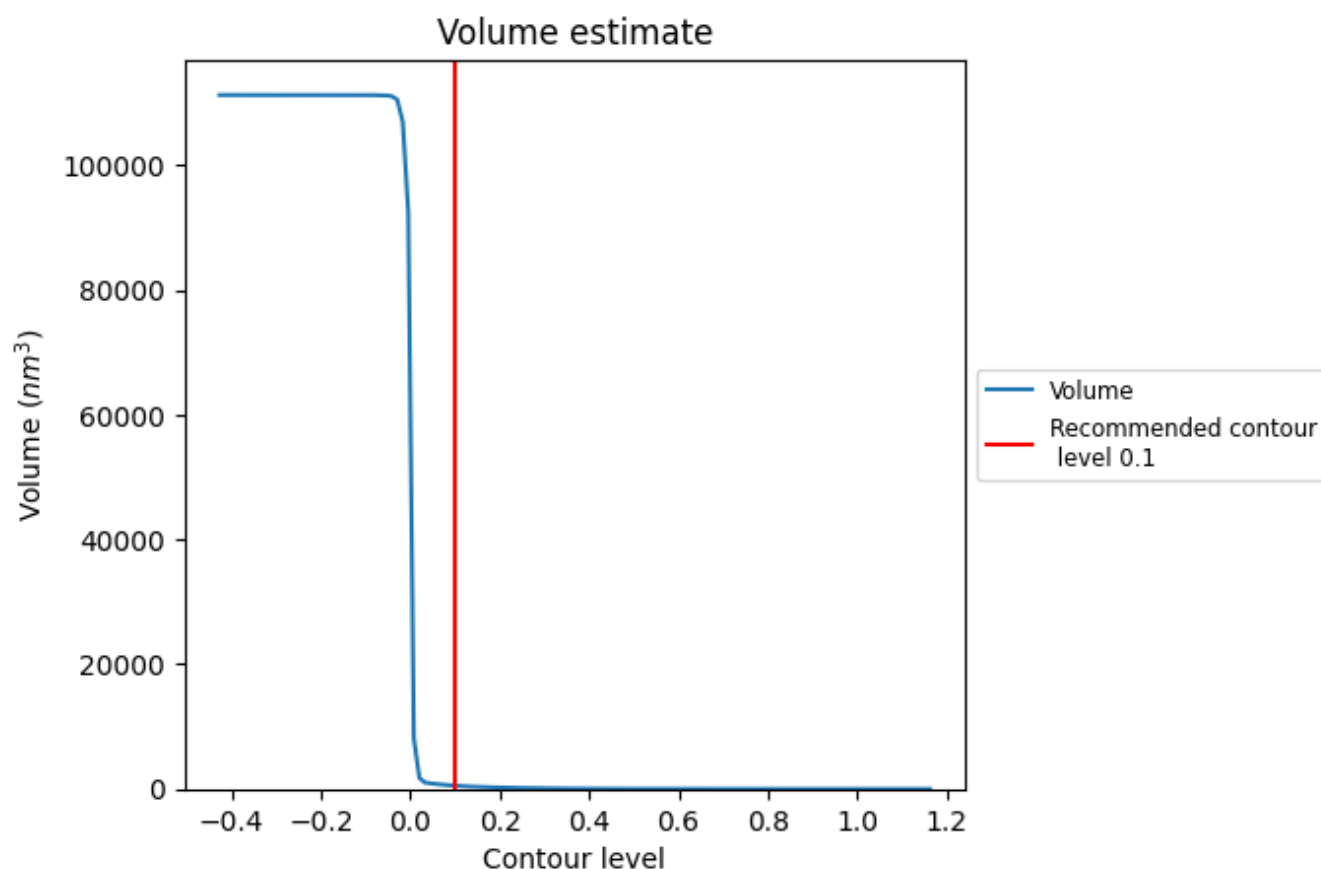
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

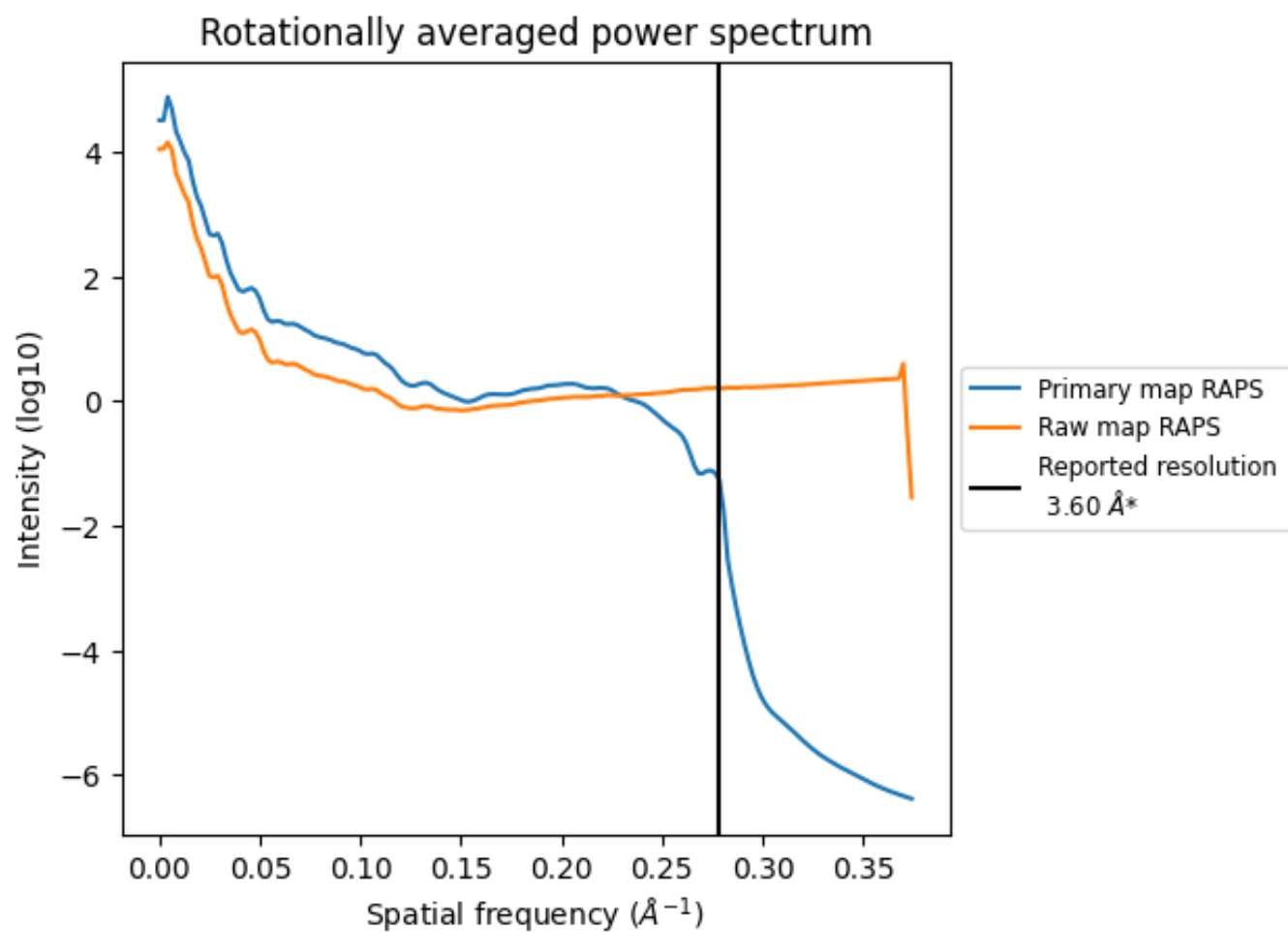
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 520 nm^3 ; this corresponds to an approximate mass of 470 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

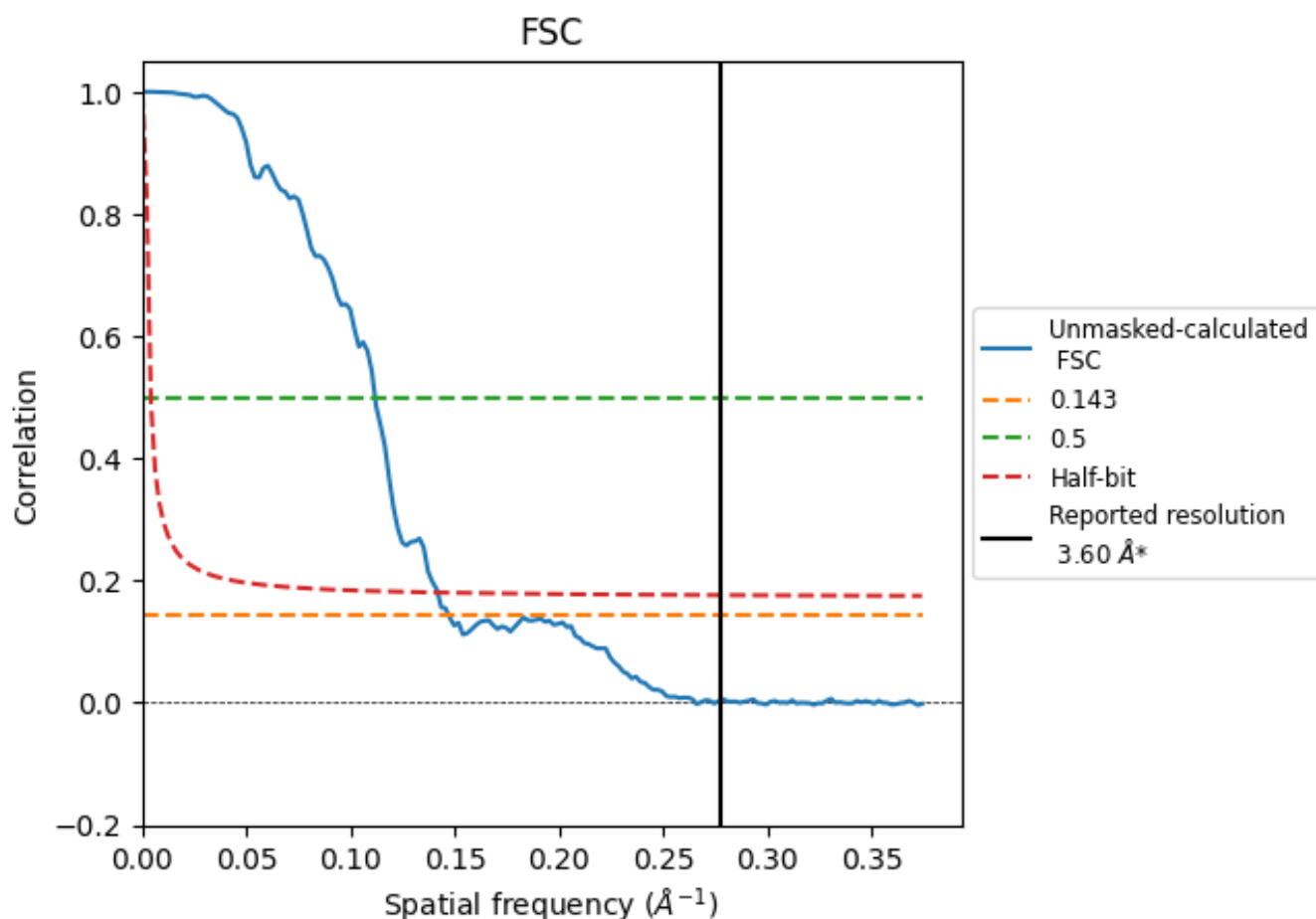


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

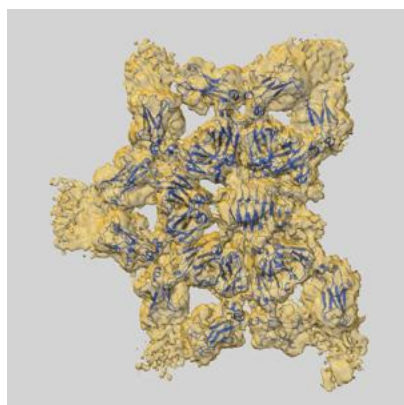
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.80	8.95	7.06

*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 6.80 differs from the reported value 3.6 by more than 10 %

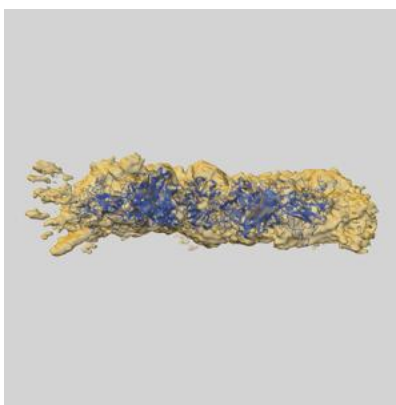
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43795 and PDB model 9ARV. Per-residue inclusion information can be found in section 3 on page 13.

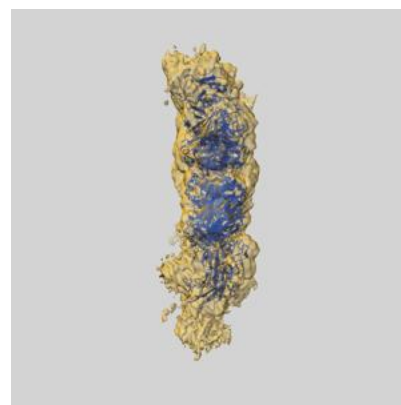
9.1 Map-model overlay [i](#)



X



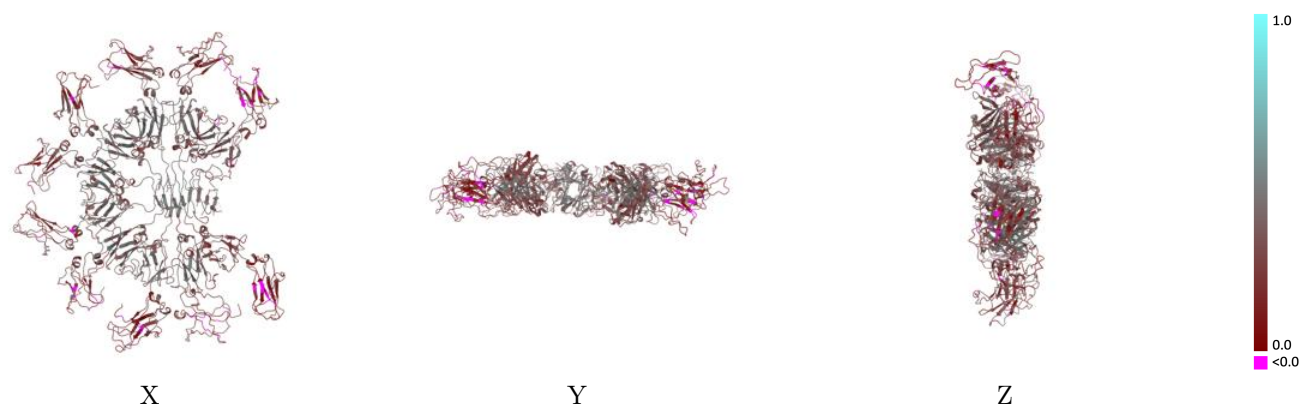
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)



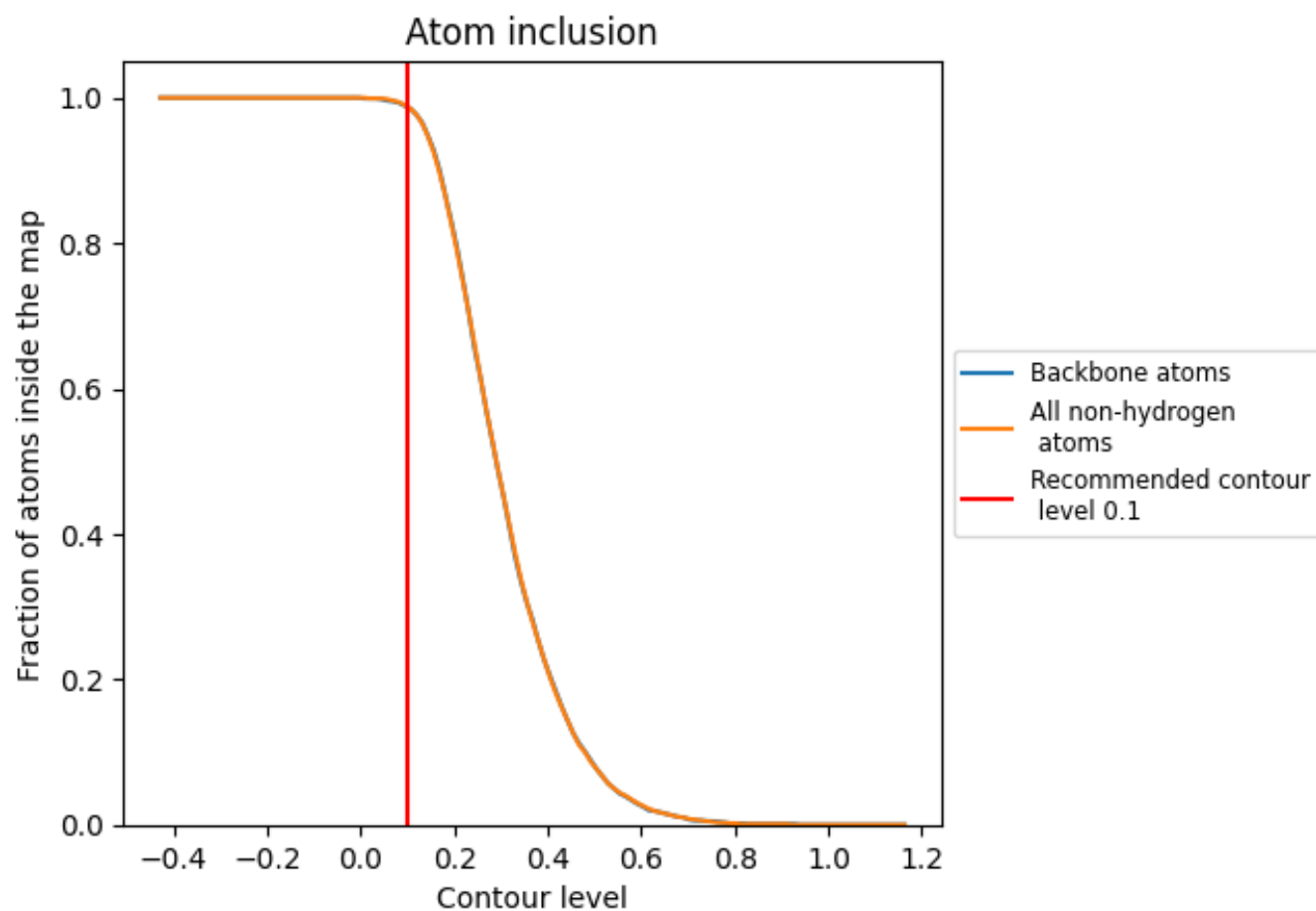
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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, 99% of all backbone atoms, 99% 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	0.9880	0.3110
A	0.9920	0.2750
B	0.9870	0.3040
C	0.9880	0.3310
D	0.9960	0.3330
E	0.9840	0.3400
J	0.9960	0.3660
L	0.9910	0.3290
M	0.9910	0.3070
N	0.9930	0.3150
O	0.9790	0.2950
P	0.9880	0.2580

1.0

0.0

<0.0