



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:07 AM UTC

PDB ID : 8HQQ / pdb_00008hqq
EMDB ID : EMD-34949
Title : Capsid of DT57C bacteriophage in the empty state
Authors : Ayala, R.; Moiseenko, A.V.; Kulikov, E.E.; Golomidova, A.K.; Orekhov, P.S.;
Street, M.A.; Sokolova, O.S.; Letarov, A.V.; Wolf, M.
Deposited on : 2022-12-13
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
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

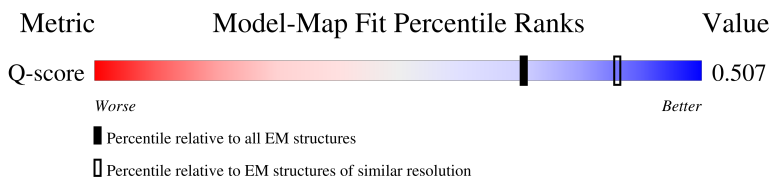
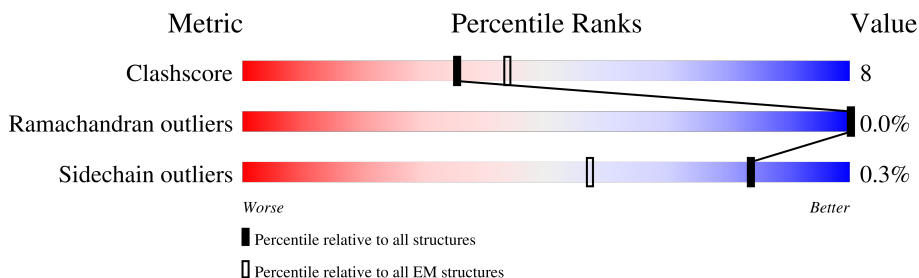
1 Overall quality at a glance

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	458	 51% 14% 35%
1	B	458	 55% 10% 35%
1	C	458	 53% 11% 35%
1	D	458	 51% 13% 35%

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Mol	Chain	Length	Quality of chain
1	E	458	 50% 14% 35%
1	F	458	 51% 14% 35%
1	G	458	 53% 11% 35%
1	H	458	 51% 13% 35%
1	I	458	 51% 14% 35%
1	J	458	 52% 12% 35%
1	K	458	 52% 13% 35%
1	L	458	 52% 12% 35%
1	M	458	 54% 9% 37%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 29730 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.

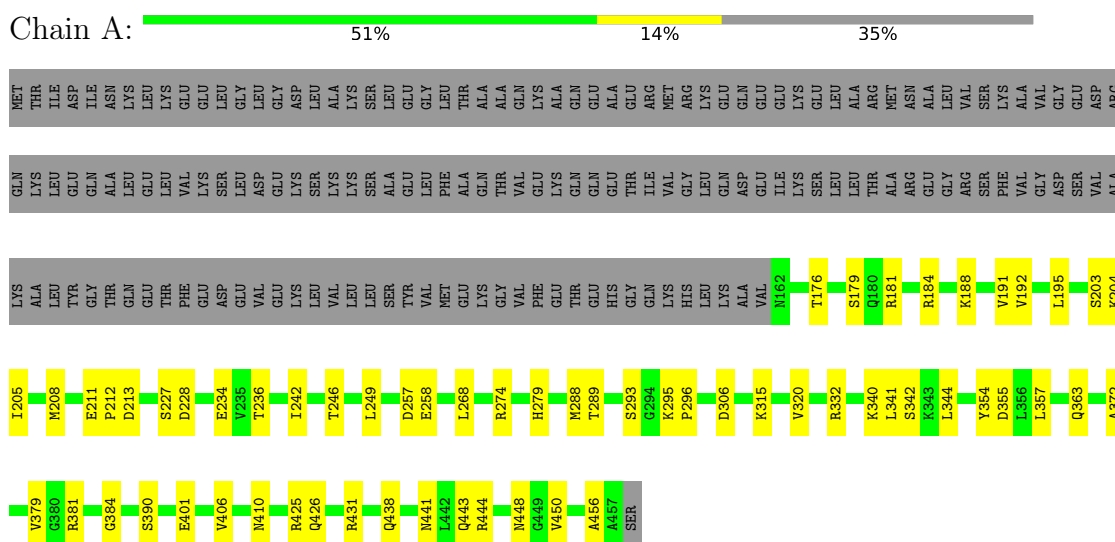
- Molecule 1 is a protein called Major head protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	B	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	C	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	D	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	E	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	F	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	G	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	H	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	I	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	J	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	K	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	L	296	Total 2291	C 1448	N 389	O 449	S 5	0	0
1	M	288	Total 2238	C 1417	N 379	O 437	S 5	0	0

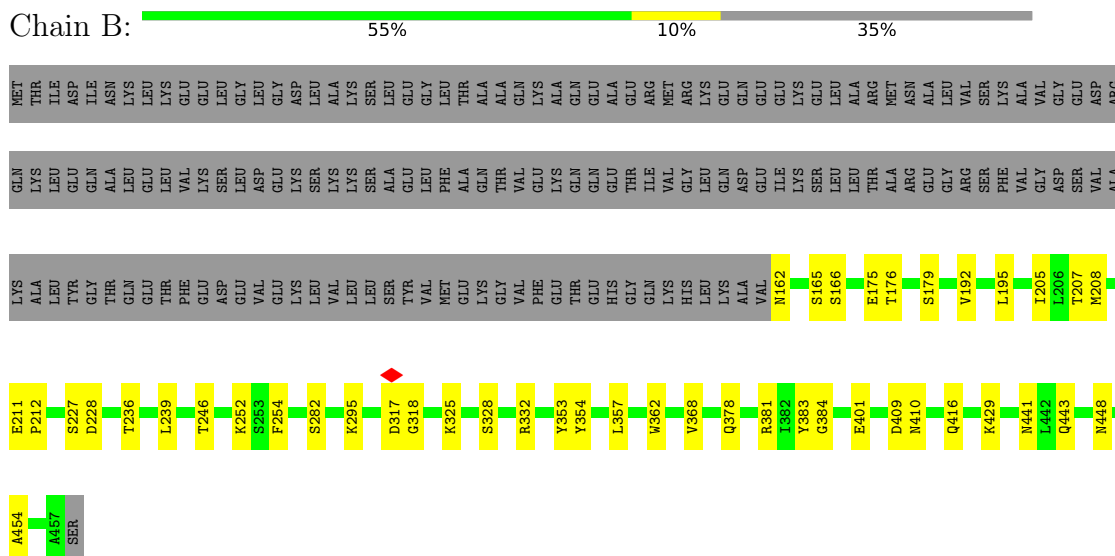
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Major head protein



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Q416	R423	K429	D432	N441	R444	N448	G449	V450	A457	SER	T207	V210	E211	P212	A217	E234	T240	T246	L249	R274	T289	G290	D291	G292	D306	K325	K329	L330	R331	R332	G338	L341	S342	K343	L357	E360	Q363	K372	K374	Q378	V379	S390	V406	Y407	N410	P414	R415															
LYS	ALA	TYR	GLY	THR	GLN	GLU	THR	PHE	GLU	ASP	GLU	VAL	GLY	LYS	LEU	VAL	LYS	LEU	LEU	SER	TYR	VAL	MET	GLU	LYS	GLY	GLN	GLN	GLY	HIS	LEU	LYS	ALA	VAL	N162	E172	E175	T176	S179	Q180	R181	I182	V191	V192	L195	L205	L206															
THR	MET	ILE	ASP	ILE	ASN	LYS	LEU	LYS	GLY	ASP	LEU	GLY	LEU	GLY	LEU	VAL	LYS	SER	LEU	ALA	LYS	SER	LEU	GLY	THR	ALA	GLN	ALA	GLY	THR	LEU	LYS	GLN	GLU	GLU	THR	ILE	VAL	GLY	LEU	GLN	ASP	GLU	ILE	LYS	SER	LEU	LEU	ALA	THR	ARG	ALA	ASN	ALA	GLY	VAL	GLY	ASP	GLY	ASP	VAL	ARG

• Molecule 1: Major head protein



MET	THR	ILE	ASP	ILE	ASN	LYS	LEU	LEU	LYS	GLU	GLU	LEU	GLY	LEU	GLY	ASP	LEU	LYS	ALA	LYS	SER	SER	LEU	GLY	THR	ALA	GLN	LYS	ALA	GLU	GLN	GLU	ALA	GLU	THR	GLN	ILE	ARG	MET	ARG	LYS	GLU	GLN	GLU	ILE	LYS	GLU	LYS	LEU	ALA	ASN	ALA	LEU	VAL	SER	LYS	ALA	VAL	GLY	ASP	SER	GLU	ASP	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
GLN	LYS	LEU	GLU	GLN	ALA	LEU	GLU	THR	PHE	GLU	VAL	LYS	ASP	GLY	LEU	LYS	SER	LYS	LYS	SER	ALA	GLU	PHE	ALA	GLN	THR	VAL	GLU	LYS	GLN	GLN	GLU	ALA	GLU	THR	GLN	ILE	ARG	VAL	GLY	LEU	GLN	ASP	GLU	ILE	LYS	SER	LEU	LEU	ALA	THR	ARG	GLY	VAL	SER	LYS	ALA	VAL	GLY	ASP	SER	VAL	ALA	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
L205	LYS	LEU	TYR	GLY	THR	GLN	GLU	THR	PHE	GLU	ASP	GLU	VAL	GLY	LYS	LEU	VAL	LYS	LEU	SER	TYR	VAL	MET	GLU	LYS	GLY	THR	VAL	PHE	GLU	THR	GLU	GLU	HIS	GLY	GLN	LYS	VAL	HIS	LEU	LYS	ALA	LYS	VAL	N162	V169	S170	E175	T176	S179	V191	V192	L195	E198	S203	K204																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
L206	L206	T207	M208	E211	P212		T236		E258	E261	L268		K273	R274	H279	A280	T283		F287	G290	D291	G292		G298		L302	A303	S304	E305	A316	D317	R332	L341	D355	L356	L357	V362	Q363	V368	A372	S390	P394	A395	K396																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										

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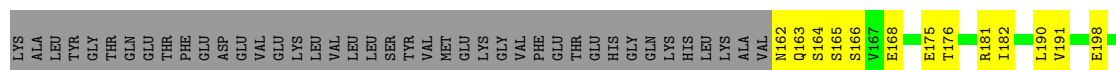
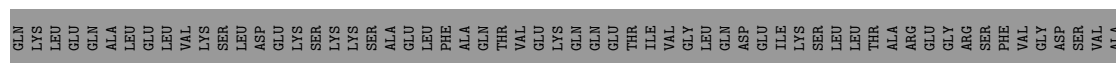
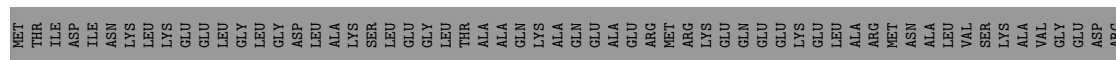


THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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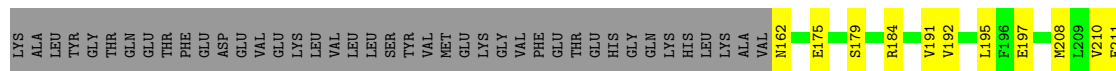
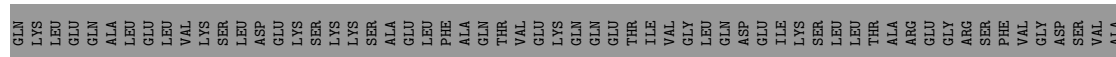
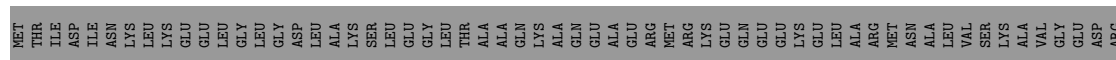
- Molecule 1: Major head protein

Chain F: 51% 14% 35%



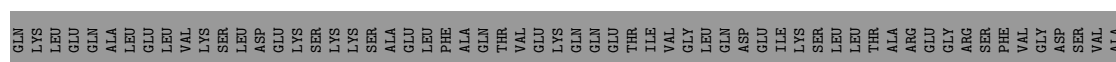
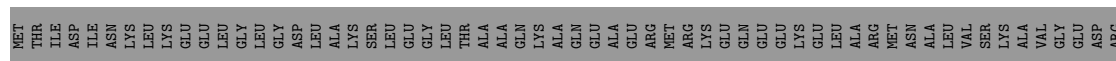
- Molecule 1: Major head protein

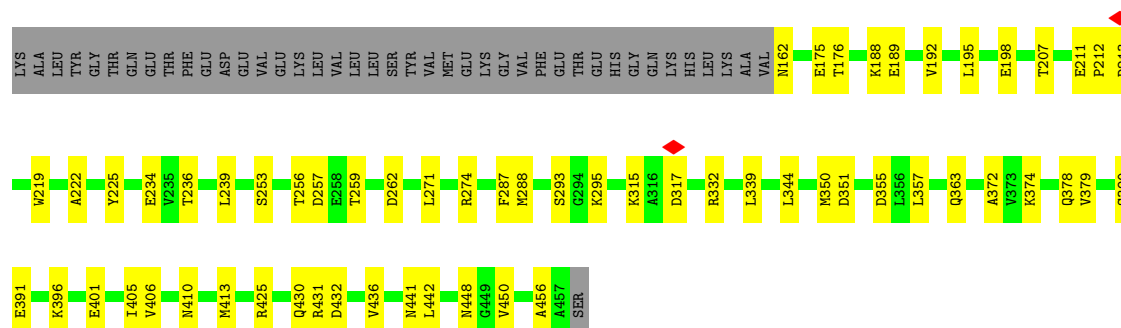
Chain G: 53% 11% 35%



- Molecule 1: Major head protein

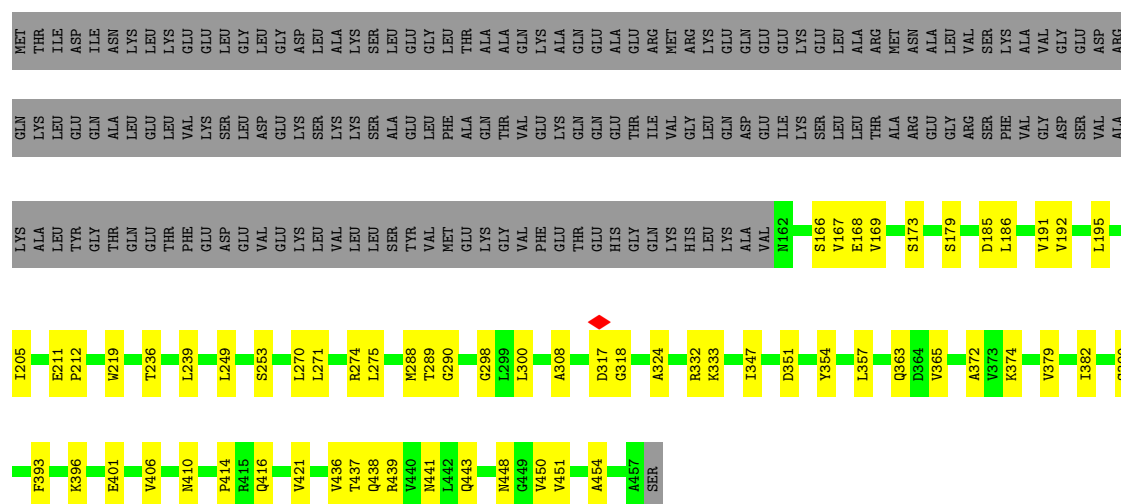
Chain H: 51% 13% 35%





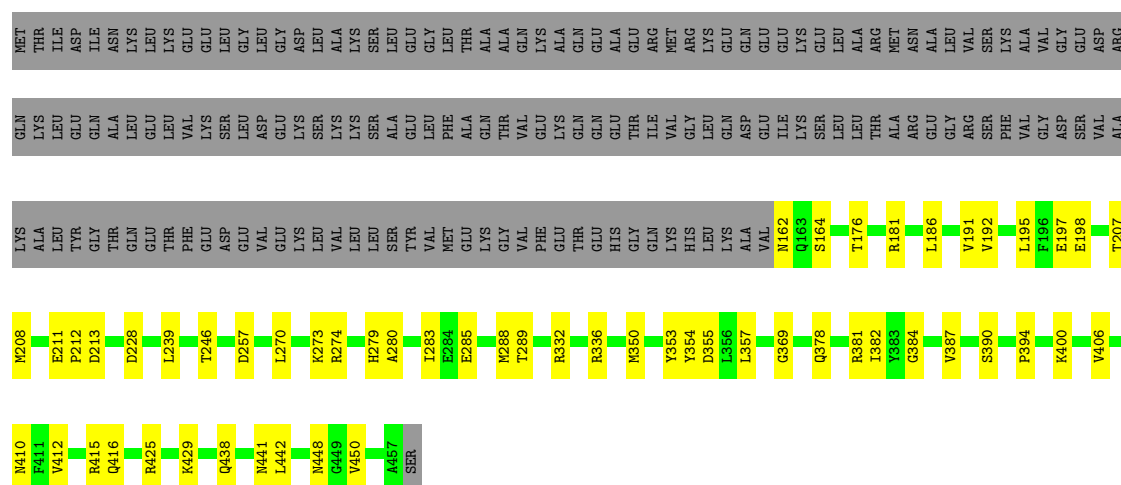
• Molecule 1: Major head protein

Chain I: 51% 14% 35%



• Molecule 1: Major head protein

Chain J: 52% 12% 35%



• Molecule 1: Major head protein

Chain K: 52% 13% 35%

D432				
N441				
L442				
Q443				
N448				
A457				
SER				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	27507	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	19.346	Depositor
Minimum map value	-5.025	Depositor
Average map value	0.003	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.4	Depositor
Map size (Å)	1248.2999, 1248.2999, 1248.2999	wwPDB
Map dimensions	900, 900, 900	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.387, 1.387, 1.387	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/2326	0.37	0/3144
1	B	0.26	0/2326	0.34	0/3144
1	C	0.27	0/2326	0.36	0/3144
1	D	0.25	0/2326	0.34	0/3144
1	E	0.26	0/2326	0.35	0/3144
1	F	0.27	0/2326	0.37	0/3144
1	G	0.26	0/2326	0.35	0/3144
1	H	0.26	0/2326	0.37	0/3144
1	I	0.26	0/2326	0.37	0/3144
1	J	0.25	0/2326	0.34	0/3144
1	K	0.26	0/2326	0.36	0/3144
1	L	0.25	0/2326	0.36	0/3144
1	M	0.15	0/2272	0.30	0/3068
All	All	0.25	0/30184	0.35	0/40796

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2291	0	2307	49	0
1	B	2291	0	2307	36	0
1	C	2291	0	2307	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2291	0	2307	44	0
1	E	2291	0	2307	56	0
1	F	2291	0	2307	54	0
1	G	2291	0	2307	40	0
1	H	2291	0	2307	49	0
1	I	2291	0	2307	43	0
1	J	2291	0	2307	39	0
1	K	2291	0	2307	45	0
1	L	2291	0	2307	45	0
1	M	2238	0	2257	26	0
All	All	29730	0	29941	471	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (471) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:HA	1:A:195:LEU:HD22	1.67	0.76
1:D:274:ARG:NH2	1:E:236:THR:O	2.20	0.75
1:K:426:GLN:OE1	1:K:431:ARG:NH2	2.22	0.72
1:K:331:ARG:NH1	1:K:338:GLY:O	2.24	0.71
1:C:331:ARG:NH1	1:C:338:GLY:O	2.24	0.70
1:C:176:THR:HG23	1:D:205:ILE:HB	1.72	0.70
1:G:410:ASN:ND2	1:G:448:ASN:O	2.24	0.70
1:H:344:LEU:HB3	1:H:405:ILE:HD11	1.71	0.70
1:I:410:ASN:ND2	1:I:448:ASN:O	2.24	0.70
1:G:423:ARG:NH2	1:G:432:ASP:OD2	2.25	0.69
1:E:192:VAL:HG21	1:E:288:MET:HE1	1.73	0.68
1:A:340:LYS:HZ2	1:A:342:SER:H	1.40	0.68
1:J:198:GLU:OE2	1:J:415:ARG:NH1	2.26	0.68
1:M:410:ASN:ND2	1:M:448:ASN:O	2.27	0.68
1:E:274:ARG:NH2	1:F:236:THR:O	2.26	0.68
1:I:274:ARG:NH1	1:J:213:ASP:O	2.27	0.68
1:I:211:GLU:HG3	1:I:212:PRO:HD2	1.75	0.68
1:D:203:SER:OG	1:D:204:LYS:N	2.27	0.67
1:C:274:ARG:NH2	1:D:236:THR:O	2.28	0.67
1:K:444:ARG:NH2	1:K:447:GLU:OE2	2.27	0.67
1:L:191:VAL:HG13	1:L:192:VAL:HG23	1.74	0.67
1:B:176:THR:HG23	1:C:205:ILE:HB	1.75	0.67
1:D:176:THR:HG23	1:E:205:ILE:HB	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:OD2	1:A:425:ARG:NH2	2.27	0.67
1:A:426:GLN:OE1	1:A:431:ARG:NH1	2.28	0.67
1:L:198:GLU:OE1	1:L:415:ARG:NH1	2.27	0.66
1:D:355:ASP:OD1	1:E:332:ARG:NH2	2.20	0.66
1:H:192:VAL:HA	1:H:195:LEU:HD22	1.78	0.66
1:I:354:TYR:HB3	1:J:332:ARG:HH21	1.61	0.66
1:H:274:ARG:NH2	1:I:236:THR:O	2.30	0.65
1:D:305:GLU:OE2	1:D:444:ARG:NH2	2.30	0.65
1:G:421:VAL:HG12	1:G:436:VAL:HG22	1.77	0.65
1:L:254:PHE:HB3	1:L:431:ARG:HD3	1.78	0.65
1:E:354:TYR:HB3	1:F:332:ARG:HH21	1.62	0.65
1:A:410:ASN:ND2	1:A:448:ASN:O	2.30	0.64
1:D:316:ALA:O	1:D:396:LYS:NZ	2.24	0.64
1:F:191:VAL:HG11	1:F:390:SER:HB2	1.80	0.63
1:F:211:GLU:HG3	1:F:212:PRO:HD2	1.80	0.63
1:K:354:TYR:HB3	1:L:332:ARG:HH21	1.63	0.63
1:G:332:ARG:NH2	1:L:355:ASP:OD1	2.28	0.63
1:A:236:THR:O	1:F:274:ARG:NH2	2.31	0.63
1:D:274:ARG:NH1	1:E:213:ASP:O	2.31	0.63
1:D:423:ARG:NH1	1:D:432:ASP:OD2	2.30	0.63
1:J:406:VAL:HG12	1:J:450:VAL:HG23	1.79	0.63
1:D:439:ARG:NH1	1:E:225:TYR:OH	2.32	0.63
1:A:213:ASP:O	1:F:274:ARG:NH1	2.32	0.63
1:A:203:SER:OG	1:A:204:LYS:N	2.31	0.62
1:H:176:THR:HG23	1:I:205:ILE:HB	1.80	0.62
1:G:192:VAL:HA	1:G:195:LEU:HD22	1.80	0.62
1:K:355:ASP:OD1	1:L:332:ARG:NH2	2.28	0.62
1:L:264:ILE:HD12	1:L:264:ILE:H	1.64	0.62
1:A:227:SER:OG	1:A:228:ASP:N	2.32	0.61
1:M:211:GLU:N	1:M:211:GLU:OE2	2.34	0.61
1:A:406:VAL:HG12	1:A:450:VAL:HG23	1.82	0.60
1:F:162:ASN:N	1:F:175:GLU:OE2	2.35	0.60
1:E:211:GLU:HG3	1:E:212:PRO:HD2	1.84	0.60
1:G:274:ARG:NH2	1:H:236:THR:O	2.32	0.60
1:L:190:LEU:HD11	1:L:280:ALA:HB1	1.83	0.60
1:C:410:ASN:ND2	1:C:448:ASN:O	2.34	0.60
1:E:176:THR:HG23	1:F:205:ILE:HB	1.84	0.60
1:E:444:ARG:HH21	1:E:447:GLU:HA	1.67	0.60
1:H:406:VAL:HG12	1:H:450:VAL:HG23	1.84	0.60
1:D:291:ASP:OD1	1:D:292:GLY:N	2.30	0.60
1:D:414:PRO:HG2	1:D:441:ASN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LEU:HD23	1:A:438:GLN:HE21	1.67	0.59
1:A:203:SER:OG	1:F:175:GLU:O	2.21	0.59
1:G:274:ARG:NH1	1:H:213:ASP:O	2.36	0.59
1:K:406:VAL:HG12	1:K:450:VAL:HG23	1.83	0.59
1:C:191:VAL:HG11	1:C:390:SER:HB2	1.85	0.59
1:E:162:ASN:ND2	1:H:259:THR:OG1	2.36	0.59
1:F:306:ASP:OD2	1:F:444:ARG:NH1	2.31	0.59
1:C:406:VAL:HG12	1:C:450:VAL:HG23	1.84	0.58
1:I:212:PRO:HD3	1:I:239:LEU:HD23	1.84	0.58
1:M:290:GLY:O	1:M:298:GLY:N	2.32	0.58
1:C:423:ARG:NH1	1:C:432:ASP:OD2	2.36	0.58
1:E:430:GLN:HE22	1:I:437:THR:HG21	1.68	0.58
1:G:355:ASP:OD1	1:H:332:ARG:NH2	2.36	0.58
1:F:258:GLU:HG3	1:F:259:THR:N	2.19	0.58
1:I:192:VAL:HA	1:I:195:LEU:HD22	1.86	0.58
1:A:381:ARG:NH2	1:A:384:GLY:O	2.36	0.58
1:J:270:LEU:HD23	1:J:274:ARG:HG3	1.85	0.58
1:E:426:GLN:OE1	1:E:431:ARG:NH2	2.36	0.58
1:C:306:ASP:OD2	1:C:444:ARG:NH1	2.27	0.57
1:J:246:THR:HG21	1:J:416:GLN:HG3	1.86	0.57
1:A:191:VAL:HG21	1:A:390:SER:HB2	1.85	0.57
1:K:293:SER:O	1:K:295:LYS:NZ	2.37	0.57
1:H:293:SER:O	1:H:295:LYS:NZ	2.37	0.57
1:M:245:SER:H	1:M:443:GLN:HE22	1.53	0.56
1:J:192:VAL:HA	1:J:195:LEU:HD22	1.87	0.56
1:D:211:GLU:HG3	1:D:212:PRO:HD2	1.85	0.56
1:F:406:VAL:HG12	1:F:450:VAL:HG22	1.88	0.56
1:A:211:GLU:HG3	1:A:212:PRO:HD2	1.88	0.56
1:B:192:VAL:HA	1:B:195:LEU:HD22	1.87	0.56
1:E:172:GLU:O	1:E:176:THR:OG1	2.20	0.56
1:B:165:SER:OG	1:B:166:SER:N	2.38	0.56
1:I:406:VAL:HG12	1:I:450:VAL:HG23	1.87	0.56
1:C:175:GLU:O	1:D:203:SER:OG	2.23	0.56
1:C:357:LEU:HD23	1:C:379:VAL:HG23	1.87	0.56
1:E:363:GLN:HB3	1:E:374:LYS:HE3	1.87	0.55
1:E:406:VAL:HG12	1:E:450:VAL:HG23	1.87	0.55
1:G:184:ARG:HD2	1:H:211:GLU:HB3	1.88	0.55
1:E:410:ASN:ND2	1:E:448:ASN:O	2.39	0.55
1:K:287:PHE:CE2	1:K:413:MET:HE1	2.41	0.55
1:D:290:GLY:O	1:D:298:GLY:N	2.39	0.55
1:L:192:VAL:HG21	1:L:288:MET:SD	2.47	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:363:GLN:HB3	1:L:374:LYS:HE3	1.89	0.55
1:I:401:GLU:HA	1:I:454:ALA:HA	1.89	0.55
1:M:423:ARG:NH2	1:M:432:ASP:OD2	2.40	0.55
1:J:176:THR:HG23	1:K:205:ILE:HB	1.89	0.55
1:H:355:ASP:OD1	1:I:332:ARG:NH2	2.32	0.55
1:M:256:THR:HA	1:M:431:ARG:HA	1.89	0.55
1:H:425:ARG:NH1	1:H:432:ASP:OD1	2.40	0.55
1:L:191:VAL:HG11	1:L:390:SER:HB2	1.87	0.55
1:D:410:ASN:ND2	1:D:448:ASN:O	2.39	0.55
1:G:162:ASN:N	1:G:175:GLU:OE2	2.40	0.55
1:H:390:SER:OG	1:H:391:GLU:N	2.36	0.55
1:K:162:ASN:N	1:K:163:GLN:OE1	2.40	0.55
1:L:421:VAL:HG22	1:L:436:VAL:HG22	1.89	0.55
1:H:441:ASN:OD1	1:H:442:LEU:N	2.38	0.54
1:H:198:GLU:HA	1:H:413:MET:HB3	1.89	0.54
1:I:192:VAL:HG11	1:I:288:MET:HE2	1.90	0.54
1:G:191:VAL:HG21	1:G:390:SER:HB2	1.88	0.54
1:G:179:SER:OG	1:H:207:THR:O	2.23	0.54
1:M:397:ALA:HB3	1:M:400:LYS:HG2	1.90	0.54
1:F:357:LEU:HD21	1:F:378:GLN:HA	1.90	0.54
1:D:279:HIS:CE1	1:D:436:VAL:HG12	2.42	0.53
1:F:165:SER:OG	1:F:166:SER:N	2.41	0.53
1:I:363:GLN:O	1:I:372:ALA:HB1	2.08	0.53
1:C:414:PRO:HG2	1:C:441:ASN:HB3	1.89	0.53
1:I:179:SER:OG	1:J:207:THR:O	2.25	0.53
1:A:176:THR:HG23	1:B:205:ILE:HB	1.91	0.53
1:E:179:SER:OG	1:F:207:THR:O	2.23	0.53
1:A:184:ARG:HD2	1:B:211:GLU:HB3	1.91	0.53
1:J:441:ASN:OD1	1:J:442:LEU:N	2.42	0.53
1:G:246:THR:HB	1:G:416:GLN:HE21	1.74	0.52
1:G:358:GLU:OE2	1:H:332:ARG:NH1	2.41	0.52
1:I:317:ASP:OD1	1:I:318:GLY:N	2.42	0.52
1:J:274:ARG:NH1	1:K:213:ASP:O	2.43	0.52
1:L:211:GLU:HG3	1:L:212:PRO:HD2	1.90	0.52
1:G:211:GLU:HG3	1:G:212:PRO:HD2	1.92	0.52
1:H:192:VAL:HG11	1:H:288:MET:HE2	1.91	0.52
1:A:357:LEU:HD23	1:A:379:VAL:HG23	1.90	0.52
1:E:429:LYS:HG2	1:J:228:ASP:HA	1.91	0.52
1:E:317:ASP:OD1	1:E:319:SER:OG	2.24	0.52
1:F:203:SER:OG	1:F:204:LYS:N	2.40	0.52
1:I:168:GLU:HG2	1:I:169:VAL:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:GLU:HA	1:B:454:ALA:HA	1.91	0.52
1:D:198:GLU:OE2	1:D:413:MET:HG2	2.10	0.52
1:F:162:ASN:HD22	1:F:164:SER:HB3	1.74	0.52
1:G:353:TYR:OH	1:G:378:GLN:OE1	2.28	0.52
1:M:374:LYS:HG3	1:M:378:GLN:HG2	1.92	0.52
1:K:439:ARG:NH1	1:L:225:TYR:OH	2.42	0.52
1:A:246:THR:HA	1:A:441:ASN:HB2	1.92	0.52
1:D:162:ASN:N	1:D:175:GLU:OE2	2.43	0.51
1:F:401:GLU:OE1	1:F:401:GLU:N	2.43	0.51
1:H:401:GLU:OE1	1:H:401:GLU:N	2.42	0.51
1:M:441:ASN:OD1	1:M:442:LEU:N	2.36	0.51
1:A:355:ASP:OD1	1:B:332:ARG:NH2	2.27	0.51
1:E:181:ARG:NE	1:F:208:MET:HE1	2.24	0.51
1:I:191:VAL:HG11	1:I:390:SER:HB2	1.91	0.51
1:J:410:ASN:ND2	1:J:448:ASN:O	2.43	0.51
1:D:179:SER:OG	1:E:207:THR:O	2.22	0.51
1:I:365:VAL:HG21	1:J:369:GLY:H	1.76	0.51
1:A:179:SER:OG	1:B:207:THR:O	2.29	0.51
1:G:295:LYS:HG2	1:H:219:TRP:CD1	2.45	0.51
1:G:391:GLU:N	1:G:391:GLU:OE1	2.44	0.51
1:K:421:VAL:HG23	1:K:436:VAL:HG22	1.93	0.51
1:J:211:GLU:HG3	1:J:212:PRO:HD2	1.92	0.51
1:E:355:ASP:OD1	1:F:332:ARG:NH2	2.38	0.51
1:K:256:THR:HG22	1:K:431:ARG:HG2	1.91	0.51
1:A:274:ARG:NH2	1:B:236:THR:O	2.44	0.50
1:I:290:GLY:O	1:I:298:GLY:N	2.39	0.50
1:K:273:LYS:NZ	1:L:211:GLU:OE2	2.38	0.50
1:K:192:VAL:HA	1:K:195:LEU:HD22	1.93	0.50
1:K:363:GLN:O	1:K:372:ALA:HB1	2.11	0.50
1:K:401:GLU:HA	1:K:454:ALA:HA	1.93	0.50
1:L:315:LYS:HD2	1:L:456:ALA:HB3	1.94	0.50
1:D:412:VAL:HG23	1:D:414:PRO:HD3	1.93	0.50
1:G:429:LYS:HB2	1:G:431:ARG:HG2	1.94	0.50
1:D:287:PHE:HE2	1:D:413:MET:HE1	1.76	0.49
1:B:162:ASN:ND2	1:B:175:GLU:OE2	2.42	0.49
1:B:227:SER:OG	1:B:228:ASP:N	2.45	0.49
1:I:347:ILE:HG22	1:I:393:PHE:HE1	1.77	0.49
1:J:279:HIS:CE1	1:J:438:GLN:HE21	2.30	0.49
1:J:354:TYR:HB3	1:K:332:ARG:HE	1.77	0.49
1:A:363:GLN:O	1:A:372:ALA:HB1	2.13	0.49
1:C:343:LYS:NZ	1:C:407:TYR:OH	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:272:ARG:HH12	1:L:421:VAL:HG11	1.76	0.49
1:M:315:LYS:O	1:M:317:ASP:N	2.46	0.49
1:B:252:LYS:HE3	1:B:254:PHE:HZ	1.78	0.49
1:F:305:GLU:OE2	1:F:444:ARG:NH2	2.45	0.49
1:H:287:PHE:HE2	1:H:413:MET:HE2	1.78	0.49
1:K:198:GLU:HA	1:K:413:MET:HB2	1.94	0.49
1:M:289:THR:O	1:M:289:THR:OG1	2.28	0.49
1:K:198:GLU:HA	1:K:413:MET:CB	2.43	0.49
1:B:212:PRO:HD3	1:B:239:LEU:HD23	1.94	0.49
1:G:211:GLU:HA	1:G:239:LEU:HD23	1.93	0.49
1:A:341:LEU:HD12	1:A:344:LEU:HD12	1.93	0.49
1:A:363:GLN:OE1	1:B:325:LYS:NZ	2.32	0.49
1:B:179:SER:OG	1:C:207:THR:O	2.31	0.49
1:E:246:THR:HG21	1:E:416:GLN:HG3	1.95	0.49
1:B:354:TYR:HB3	1:C:332:ARG:HH21	1.77	0.48
1:F:163:GLN:HA	1:F:168:GLU:HG2	1.94	0.48
1:G:336:ARG:HA	1:L:350:MET:HE1	1.95	0.48
1:J:353:TYR:OH	1:J:378:GLN:OE1	2.22	0.48
1:L:363:GLN:O	1:L:372:ALA:HB1	2.13	0.48
1:B:401:GLU:HG3	1:B:454:ALA:HB2	1.95	0.48
1:G:414:PRO:HG2	1:G:441:ASN:HB3	1.95	0.48
1:I:414:PRO:HG2	1:I:441:ASN:HB3	1.95	0.48
1:D:192:VAL:HA	1:D:195:LEU:HD22	1.94	0.48
1:E:421:VAL:HG22	1:E:436:VAL:HG22	1.96	0.48
1:G:279:HIS:HE1	1:G:438:GLN:HG2	1.79	0.48
1:L:441:ASN:OD1	1:L:442:LEU:N	2.41	0.48
1:C:182:ILE:HD11	1:D:211:GLU:HB2	1.94	0.48
1:E:289:THR:O	1:E:289:THR:OG1	2.30	0.48
1:K:254:PHE:HB3	1:K:431:ARG:HD2	1.95	0.48
1:B:353:TYR:OH	1:B:378:GLN:OE1	2.30	0.48
1:D:191:VAL:HG11	1:D:390:SER:HB2	1.94	0.48
1:E:212:PRO:HD3	1:E:239:LEU:HD23	1.95	0.48
1:K:414:PRO:HG2	1:K:441:ASN:HB3	1.94	0.48
1:H:222:ALA:HA	1:H:225:TYR:CE1	2.48	0.48
1:B:410:ASN:ND2	1:B:448:ASN:O	2.46	0.48
1:E:259:THR:HG22	1:H:162:ASN:HD22	1.77	0.48
1:E:306:ASP:OD2	1:E:444:ARG:NH2	2.35	0.48
1:G:401:GLU:N	1:G:401:GLU:OE1	2.44	0.48
1:M:165:SER:OG	1:M:166:SER:N	2.45	0.48
1:D:169:VAL:HG12	1:D:170:SER:H	1.79	0.48
1:D:258:GLU:HA	1:D:261:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:SER:OG	1:E:166:SER:N	2.46	0.48
1:C:211:GLU:HG3	1:C:212:PRO:HD2	1.96	0.47
1:I:333:LYS:HB3	1:I:451:VAL:HG21	1.97	0.47
1:E:381:ARG:NH2	1:E:384:GLY:O	2.47	0.47
1:E:414:PRO:HG3	1:E:443:GLN:HG3	1.96	0.47
1:L:407:TYR:HD2	1:L:410:ASN:HB2	1.78	0.47
1:D:363:GLN:O	1:D:372:ALA:HB1	2.13	0.47
1:E:290:GLY:O	1:E:298:GLY:N	2.33	0.47
1:G:381:ARG:NH2	1:G:384:GLY:O	2.47	0.47
1:H:357:LEU:HD23	1:H:379:VAL:HG23	1.95	0.47
1:J:192:VAL:HG11	1:J:288:MET:HE2	1.95	0.47
1:F:198:GLU:OE1	1:F:415:ARG:NH1	2.47	0.47
1:H:212:PRO:HD3	1:H:239:LEU:HD23	1.96	0.47
1:K:282:SER:OG	1:L:217:ALA:N	2.43	0.47
1:C:289:THR:O	1:C:289:THR:OG1	2.26	0.47
1:J:285:GLU:OE1	1:K:216:ARG:NH1	2.47	0.47
1:C:192:VAL:HA	1:C:195:LEU:HD22	1.96	0.47
1:C:360:GLU:N	1:C:360:GLU:OE1	2.47	0.47
1:E:274:ARG:NH1	1:F:213:ASP:O	2.47	0.47
1:G:357:LEU:HD23	1:G:357:LEU:HA	1.75	0.47
1:H:315:LYS:HD2	1:H:456:ALA:HB3	1.96	0.47
1:I:363:GLN:HB3	1:I:374:LYS:HE3	1.95	0.47
1:J:181:ARG:CZ	1:K:208:MET:HE1	2.45	0.47
1:H:363:GLN:O	1:H:372:ALA:HB1	2.15	0.47
1:A:315:LYS:HD2	1:A:456:ALA:HB3	1.96	0.47
1:K:285:GLU:OE1	1:L:216:ARG:NH1	2.48	0.47
1:A:205:ILE:HB	1:F:176:THR:HG23	1.95	0.47
1:F:222:ALA:HA	1:F:225:TYR:CE1	2.49	0.47
1:M:189:GLU:H	1:M:189:GLU:CD	2.23	0.47
1:C:246:THR:HG1	1:C:416:GLN:HE21	1.57	0.46
1:B:357:LEU:HD23	1:B:357:LEU:HA	1.80	0.46
1:G:197:GLU:OE2	1:G:412:VAL:HG12	2.16	0.46
1:G:210:VAL:HG22	1:L:183:ILE:HD11	1.97	0.46
1:I:351:ASP:OD2	1:I:396:LYS:NZ	2.31	0.46
1:K:357:LEU:HA	1:K:357:LEU:HD23	1.78	0.46
1:A:306:ASP:OD2	1:A:444:ARG:NH1	2.41	0.46
1:F:363:GLN:HB3	1:F:374:LYS:HE3	1.97	0.46
1:H:287:PHE:HE2	1:H:413:MET:CE	2.28	0.46
1:J:355:ASP:OD1	1:K:332:ARG:NH2	2.48	0.46
1:K:401:GLU:OE1	1:K:401:GLU:N	2.48	0.46
1:L:249:LEU:HD23	1:L:438:GLN:HE21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LYS:HG2	1:A:320:VAL:HB	1.98	0.46
1:C:325:LYS:HG3	1:C:329:LYS:HE3	1.97	0.46
1:D:394:PRO:HB2	1:D:400:LYS:NZ	2.31	0.46
1:G:288:MET:HA	1:G:288:MET:HE2	1.98	0.46
1:H:357:LEU:HD21	1:H:378:GLN:HA	1.98	0.46
1:M:414:PRO:HG2	1:M:441:ASN:HB3	1.98	0.46
1:E:181:ARG:HE	1:F:208:MET:HE1	1.81	0.46
1:F:357:LEU:HD23	1:F:379:VAL:HG23	1.98	0.46
1:I:166:SER:OG	1:I:167:VAL:N	2.48	0.46
1:M:338:GLY:HA2	1:M:344:LEU:HD11	1.98	0.45
1:E:175:GLU:O	1:F:203:SER:OG	2.34	0.45
1:H:410:ASN:ND2	1:H:448:ASN:O	2.49	0.45
1:M:346:LEU:HD13	1:M:405:ILE:HG12	1.98	0.45
1:H:211:GLU:HG3	1:H:212:PRO:HD2	1.98	0.45
1:J:212:PRO:HD3	1:J:239:LEU:HD23	1.98	0.45
1:L:216:ARG:HD3	1:L:216:ARG:HA	1.78	0.45
1:F:204:LYS:HB2	1:H:262:ASP:OD1	2.17	0.45
1:B:246:THR:HG21	1:B:416:GLN:HG3	1.99	0.45
1:L:306:ASP:CG	1:L:444:ARG:HH22	2.25	0.45
1:I:173:SER:O	1:I:173:SER:OG	2.35	0.45
1:L:306:ASP:OD2	1:L:444:ARG:NH1	2.47	0.45
1:E:191:VAL:HG11	1:E:390:SER:HB2	1.98	0.45
1:D:362:TRP:CZ3	1:D:368:VAL:HG11	2.52	0.45
1:F:401:GLU:HA	1:F:454:ALA:HA	1.98	0.45
1:G:208:MET:HE1	1:L:181:ARG:NE	2.32	0.45
1:J:162:ASN:ND2	1:J:164:SER:OG	2.46	0.45
1:C:172:GLU:CD	1:C:172:GLU:H	2.25	0.45
1:E:192:VAL:HA	1:E:195:LEU:CD2	2.47	0.45
1:G:343:LYS:HE2	1:G:343:LYS:HB3	1.72	0.45
1:G:350:MET:HE1	1:H:339:LEU:HD11	1.99	0.45
1:A:441:ASN:ND2	1:A:443:GLN:HE21	2.15	0.45
1:I:308:ALA:HB1	1:I:451:VAL:HG22	1.99	0.45
1:J:429:LYS:HE3	1:J:429:LYS:O	2.17	0.44
1:D:423:ARG:HG3	1:D:434:TYR:CE2	2.52	0.44
1:E:363:GLN:O	1:E:372:ALA:HB1	2.17	0.44
1:E:414:PRO:HG2	1:E:441:ASN:HB3	1.99	0.44
1:H:295:LYS:HG2	1:I:219:TRP:CG	2.53	0.44
1:A:208:MET:HB2	1:A:242:ILE:HG13	1.99	0.44
1:C:181:ARG:NH2	1:D:208:MET:HE1	2.33	0.44
1:G:216:ARG:NH1	1:L:285:GLU:OE1	2.50	0.44
1:H:257:ASP:HB2	1:H:430:GLN:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:401:GLU:OE1	1:L:401:GLU:N	2.49	0.44
1:M:382:ILE:HG23	1:M:383:TYR:H	1.83	0.44
1:B:295:LYS:HE2	1:B:295:LYS:HB2	1.80	0.44
1:E:268:LEU:HD12	1:E:268:LEU:HA	1.84	0.44
1:H:189:GLU:OE1	1:H:189:GLU:N	2.40	0.44
1:J:280:ALA:HA	1:J:283:ILE:HG22	2.00	0.44
1:M:190:LEU:HA	1:M:284:GLU:CD	2.43	0.44
1:M:218:THR:HG21	1:M:233:SER:H	1.83	0.44
1:E:302:LEU:HD13	1:E:444:ARG:HH11	1.82	0.44
1:F:333:LYS:HE3	1:F:333:LYS:HB3	1.86	0.44
1:K:373:VAL:O	1:K:377:GLY:N	2.49	0.44
1:L:340:LYS:HE3	1:L:340:LYS:HB2	1.76	0.44
1:L:420:THR:O	1:L:436:VAL:HA	2.18	0.44
1:A:332:ARG:HH21	1:F:354:TYR:HB3	1.82	0.44
1:H:351:ASP:OD2	1:H:396:LYS:NZ	2.39	0.44
1:A:181:ARG:NE	1:B:208:MET:HE1	2.33	0.44
1:A:208:MET:HE1	1:F:181:ARG:NE	2.32	0.44
1:K:415:ARG:HB2	1:K:440:VAL:HG12	2.00	0.44
1:L:415:ARG:HB2	1:L:440:VAL:HG12	2.00	0.44
1:F:210:VAL:N	1:F:240:THR:O	2.41	0.44
1:B:409:ASP:OD1	1:B:409:ASP:N	2.38	0.44
1:A:289:THR:O	1:A:289:THR:OG1	2.31	0.43
1:G:354:TYR:HD1	1:G:354:TYR:HA	1.70	0.43
1:H:363:GLN:HB3	1:H:374:LYS:HE3	1.99	0.43
1:M:375:LEU:H	1:M:378:GLN:HB2	1.82	0.43
1:A:332:ARG:HA	1:F:354:TYR:CE2	2.53	0.43
1:C:210:VAL:N	1:C:240:THR:O	2.28	0.43
1:K:211:GLU:HG3	1:K:212:PRO:HD2	2.00	0.43
1:B:441:ASN:ND2	1:B:443:GLN:HE21	2.16	0.43
1:I:324:ALA:HB1	1:I:382:ILE:HD11	2.00	0.43
1:K:186:LEU:HD23	1:K:186:LEU:HA	1.85	0.43
1:B:362:TRP:CZ3	1:B:368:VAL:HG11	2.53	0.43
1:C:363:GLN:HB3	1:C:374:LYS:HE3	2.00	0.43
1:F:381:ARG:NH2	1:F:384:GLY:O	2.51	0.43
1:A:191:VAL:HG23	1:A:192:VAL:HG13	1.99	0.43
1:B:246:THR:HA	1:B:441:ASN:HB2	2.00	0.43
1:D:268:LEU:HD12	1:D:268:LEU:HA	1.83	0.43
1:F:279:HIS:CE1	1:F:438:GLN:HE21	2.37	0.43
1:L:381:ARG:NH2	1:L:384:GLY:O	2.52	0.43
1:H:256:THR:HA	1:H:431:ARG:HA	1.99	0.43
1:I:416:GLN:HB2	1:I:439:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:164:SER:OG	1:K:165:SER:N	2.52	0.43
1:L:394:PRO:HB2	1:L:400:LYS:NZ	2.34	0.43
1:M:400:LYS:HA	1:M:400:LYS:HD2	1.72	0.43
1:A:211:GLU:N	1:F:182:ILE:HD11	2.34	0.43
1:D:273:LYS:HE2	1:D:273:LYS:HB3	1.64	0.43
1:D:357:LEU:HD23	1:D:357:LEU:HA	1.82	0.43
1:E:208:MET:HE3	1:E:208:MET:HB2	1.78	0.43
1:L:246:THR:HA	1:L:441:ASN:HB2	2.01	0.43
1:C:341:LEU:HD12	1:C:341:LEU:HA	1.79	0.43
1:F:357:LEU:HD23	1:F:357:LEU:HA	1.74	0.43
1:I:249:LEU:HD23	1:I:438:GLN:HE21	1.84	0.43
1:K:381:ARG:H	1:K:381:ARG:HG2	1.63	0.43
1:L:423:ARG:NH1	1:L:432:ASP:OD2	2.51	0.43
1:C:429:LYS:HB3	1:C:429:LYS:HE3	1.70	0.42
1:F:334:LEU:HD23	1:F:334:LEU:HA	1.83	0.42
1:I:357:LEU:HD23	1:I:379:VAL:HG23	2.00	0.42
1:M:341:LEU:HD11	1:M:385:LEU:HB2	2.02	0.42
1:M:408:LYS:HB2	1:M:408:LYS:HE3	1.73	0.42
1:B:282:SER:HB2	1:C:217:ALA:H	1.84	0.42
1:E:259:THR:HG22	1:H:162:ASN:ND2	2.33	0.42
1:D:287:PHE:HE2	1:D:413:MET:CE	2.31	0.42
1:F:190:LEU:HD13	1:F:284:GLU:CD	2.44	0.42
1:I:421:VAL:HG23	1:I:436:VAL:HG22	2.01	0.42
1:J:257:ASP:OD2	1:J:425:ARG:NH2	2.52	0.42
1:A:332:ARG:NH2	1:F:355:ASP:OD1	2.40	0.42
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.76	0.42
1:C:249:LEU:HD12	1:C:249:LEU:HA	1.87	0.42
1:J:288:MET:HG3	1:J:289:THR:HG23	2.01	0.42
1:J:394:PRO:HB2	1:J:400:LYS:NZ	2.35	0.42
1:H:198:GLU:OE1	1:H:413:MET:HG2	2.20	0.42
1:E:182:ILE:HD11	1:F:211:GLU:N	2.34	0.42
1:B:401:GLU:N	1:B:401:GLU:OE1	2.53	0.42
1:E:382:ILE:HD13	1:E:382:ILE:HA	1.80	0.42
1:F:246:THR:HA	1:F:441:ASN:HB2	2.01	0.42
1:I:185:ASP:OD1	1:I:186:LEU:N	2.46	0.42
1:J:273:LYS:NZ	1:K:211:GLU:OE2	2.45	0.42
1:L:280:ALA:O	1:L:283:ILE:HG22	2.19	0.42
1:D:280:ALA:O	1:D:283:ILE:HG13	2.20	0.42
1:L:299:LEU:HD23	1:L:299:LEU:HA	1.87	0.42
1:C:179:SER:OG	1:D:207:THR:O	2.38	0.41
1:E:216:ARG:HD3	1:E:216:ARG:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:LEU:HD23	1:I:274:ARG:HG3	2.01	0.41
1:J:197:GLU:OE2	1:J:412:VAL:HG12	2.20	0.41
1:M:378:GLN:HE22	1:M:386:PRO:HB3	1.85	0.41
1:B:162:ASN:N	1:B:162:ASN:OD1	2.53	0.41
1:E:249:LEU:HD13	1:F:219:TRP:CE2	2.55	0.41
1:E:441:ASN:OD1	1:E:442:LEU:N	2.52	0.41
1:K:414:PRO:HD2	1:K:441:ASN:O	2.20	0.41
1:A:258:GLU:C	1:A:258:GLU:CD	2.88	0.41
1:C:291:ASP:OD1	1:C:292:GLY:N	2.49	0.41
1:D:258:GLU:H	1:D:258:GLU:CD	2.28	0.41
1:E:191:VAL:HG13	1:E:192:VAL:HG23	2.02	0.41
1:G:341:LEU:HA	1:G:341:LEU:HD23	1.83	0.41
1:I:441:ASN:ND2	1:I:443:GLN:HE21	2.18	0.41
1:K:351:ASP:OD2	1:K:396:LYS:NZ	2.34	0.41
1:B:381:ARG:NH2	1:B:384:GLY:O	2.53	0.41
1:D:302:LEU:O	1:D:305:GLU:HG3	2.20	0.41
1:I:275:LEU:HD23	1:I:275:LEU:HA	1.93	0.41
1:L:177:ILE:HG13	1:L:177:ILE:O	2.21	0.41
1:M:315:LYS:HD2	1:M:315:LYS:HA	1.63	0.41
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.76	0.41
1:D:303:ALA:HB2	1:D:450:VAL:HG22	2.03	0.41
1:G:246:THR:HG21	1:G:416:GLN:HG3	2.03	0.41
1:G:332:ARG:HH21	1:L:354:TYR:CB	2.33	0.41
1:J:382:ILE:HG22	1:J:387:VAL:HG23	2.03	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.89	0.41
1:E:288:MET:HA	1:E:288:MET:HE2	2.02	0.41
1:G:324:ALA:HB1	1:G:382:ILE:HG23	2.03	0.41
1:I:186:LEU:O	1:J:336:ARG:NH1	2.53	0.41
1:K:268:LEU:HD11	1:K:434:TYR:OH	2.21	0.41
1:K:364:ASP:HB2	1:K:367:GLN:HG3	2.02	0.41
1:L:165:SER:OG	1:L:166:SER:N	2.52	0.41
1:C:357:LEU:HD23	1:C:357:LEU:HA	1.73	0.41
1:G:299:LEU:HD23	1:G:299:LEU:HA	1.86	0.41
1:H:253:SER:OG	1:H:271:LEU:HD11	2.21	0.41
1:J:381:ARG:HH11	1:J:384:GLY:HA2	1.85	0.41
1:B:429:LYS:HD2	1:B:429:LYS:HA	1.88	0.41
1:F:201:MET:HE3	1:F:201:MET:HB2	1.78	0.41
1:F:254:PHE:HB3	1:F:431:ARG:HD2	2.03	0.41
1:H:188:LYS:HE2	1:H:391:GLU:HB3	2.03	0.41
1:J:357:LEU:HA	1:J:357:LEU:HD23	1.80	0.41
1:L:332:ARG:HE	1:L:332:ARG:HB2	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:SER:O	1:A:295:LYS:NZ	2.54	0.41
1:A:296:PRO:HB3	1:A:441:ASN:OD1	2.21	0.41
1:D:341:LEU:HA	1:D:341:LEU:HD12	1.83	0.41
1:E:165:SER:HB2	1:H:256:THR:HG23	2.03	0.41
1:E:224:ALA:O	1:E:230:THR:OG1	2.27	0.41
1:I:253:SER:OG	1:I:271:LEU:HD11	2.21	0.41
1:J:186:LEU:HD23	1:J:186:LEU:HA	1.84	0.41
1:J:191:VAL:HG11	1:J:390:SER:HB2	2.03	0.41
1:J:354:TYR:CB	1:K:332:ARG:HE	2.34	0.41
1:K:203:SER:OG	1:K:204:LYS:N	2.54	0.41
1:K:416:GLN:NE2	1:K:439:ARG:HH21	2.19	0.41
1:M:347:ILE:HA	1:M:388:VAL:O	2.21	0.41
1:A:234:GLU:HG3	1:F:253:SER:HA	2.02	0.41
1:A:401:GLU:OE1	1:A:401:GLU:N	2.54	0.41
1:F:363:GLN:O	1:F:372:ALA:HB1	2.21	0.41
1:H:315:LYS:NZ	1:H:317:ASP:OD2	2.50	0.41
1:A:354:TYR:HD1	1:A:354:TYR:HA	1.78	0.40
1:B:317:ASP:OD1	1:B:318:GLY:N	2.54	0.40
1:E:256:THR:OG1	1:E:259:THR:HG23	2.21	0.40
1:F:211:GLU:HA	1:F:239:LEU:HD23	2.02	0.40
1:F:354:TYR:HD1	1:F:354:TYR:HA	1.73	0.40
1:H:288:MET:HE2	1:H:288:MET:HB2	1.91	0.40
1:C:363:GLN:O	1:C:372:ALA:HB1	2.20	0.40
1:E:296:PRO:HB3	1:E:441:ASN:OD1	2.21	0.40
1:A:288:MET:HE2	1:A:288:MET:HA	2.03	0.40
1:B:328:SER:HB2	1:B:383:TYR:CD2	2.56	0.40
1:C:357:LEU:HD21	1:C:378:GLN:HA	2.04	0.40
1:G:252:LYS:O	1:H:234:GLU:HA	2.22	0.40
1:H:162:ASN:N	1:H:175:GLU:OE2	2.54	0.40
1:I:186:LEU:HD23	1:I:186:LEU:HA	1.95	0.40
1:K:374:LYS:NZ	1:L:361:GLU:HB3	2.36	0.40
1:B:252:LYS:O	1:C:234:GLU:HA	2.21	0.40
1:D:332:ARG:HE	1:D:332:ARG:HB2	1.74	0.40
1:F:296:PRO:HB3	1:F:441:ASN:OD1	2.20	0.40
1:B:429:LYS:HB3	1:B:429:LYS:HE3	1.88	0.40
1:I:289:THR:HB	1:I:300:LEU:HD23	2.04	0.40
1:I:289:THR:O	1:I:289:THR:OG1	2.28	0.40
1:J:429:LYS:HD2	1:J:429:LYS:HA	1.84	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	294/458 (64%)	276 (94%)	18 (6%)	0	100	100
1	B	294/458 (64%)	277 (94%)	17 (6%)	0	100	100
1	C	294/458 (64%)	276 (94%)	18 (6%)	0	100	100
1	D	294/458 (64%)	276 (94%)	18 (6%)	0	100	100
1	E	294/458 (64%)	279 (95%)	15 (5%)	0	100	100
1	F	294/458 (64%)	276 (94%)	18 (6%)	0	100	100
1	G	294/458 (64%)	278 (95%)	16 (5%)	0	100	100
1	H	294/458 (64%)	275 (94%)	19 (6%)	0	100	100
1	I	294/458 (64%)	277 (94%)	17 (6%)	0	100	100
1	J	294/458 (64%)	277 (94%)	17 (6%)	0	100	100
1	K	294/458 (64%)	275 (94%)	19 (6%)	0	100	100
1	L	294/458 (64%)	275 (94%)	19 (6%)	0	100	100
1	M	284/458 (62%)	267 (94%)	16 (6%)	1 (0%)	30	61
All	All	3812/5954 (64%)	3584 (94%)	227 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	316	ALA

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	245/382 (64%)	243 (99%)	2 (1%)	73	77
1	B	245/382 (64%)	245 (100%)	0	100	100
1	C	245/382 (64%)	245 (100%)	0	100	100
1	D	245/382 (64%)	244 (100%)	1 (0%)	84	81
1	E	245/382 (64%)	245 (100%)	0	100	100
1	F	245/382 (64%)	244 (100%)	1 (0%)	84	81
1	G	245/382 (64%)	245 (100%)	0	100	100
1	H	245/382 (64%)	243 (99%)	2 (1%)	73	77
1	I	245/382 (64%)	245 (100%)	0	100	100
1	J	245/382 (64%)	243 (99%)	2 (1%)	73	77
1	K	245/382 (64%)	244 (100%)	1 (0%)	84	81
1	L	245/382 (64%)	245 (100%)	0	100	100
1	M	240/382 (63%)	240 (100%)	0	100	100
All	All	3180/4966 (64%)	3171 (100%)	9 (0%)	84	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	279	HIS
1	D	442	LEU
1	F	382	ILE
1	H	350	MET
1	H	436	VAL
1	J	208	MET
1	J	350	MET
1	K	334	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	367	GLN
1	A	410	ASN
1	A	438	GLN
1	A	443	GLN
1	B	163	GLN

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Mol	Chain	Res	Type
1	B	180	GLN
1	B	243	HIS
1	B	410	ASN
1	B	426	GLN
1	B	438	GLN
1	B	443	GLN
1	C	279	HIS
1	C	376	GLN
1	C	443	GLN
1	D	180	GLN
1	D	337	HIS
1	D	370	ASN
1	D	410	ASN
1	E	162	ASN
1	E	180	GLN
1	E	187	GLN
1	E	229	ASN
1	E	243	HIS
1	E	279	HIS
1	E	363	GLN
1	E	430	GLN
1	E	443	GLN
1	F	162	ASN
1	F	363	GLN
1	F	438	GLN
1	G	162	ASN
1	G	279	HIS
1	G	367	GLN
1	G	370	ASN
1	G	416	GLN
1	G	443	GLN
1	H	162	ASN
1	H	337	HIS
1	H	430	GLN
1	I	410	ASN
1	I	438	GLN
1	I	443	GLN
1	J	162	ASN
1	J	279	HIS
1	J	438	GLN
1	J	443	GLN
1	K	162	ASN

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Mol	Chain	Res	Type
1	K	438	GLN
1	L	162	ASN
1	L	438	GLN
1	M	229	ASN
1	M	279	HIS
1	M	378	GLN
1	M	416	GLN
1	M	438	GLN
1	M	443	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

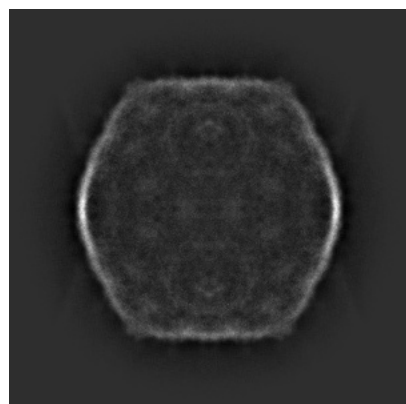
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34949. These allow visual inspection of the internal detail of the map and identification of artifacts.

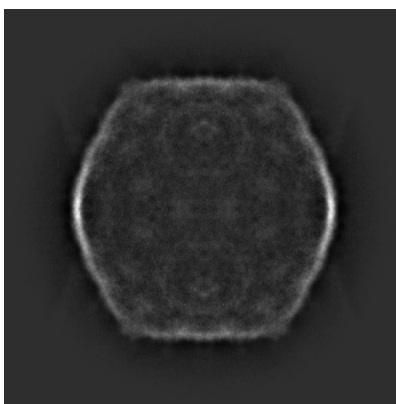
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

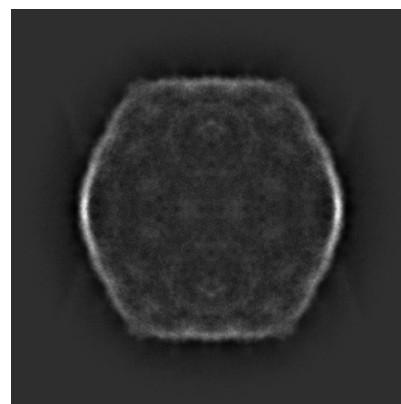
6.1.1 Primary map



X

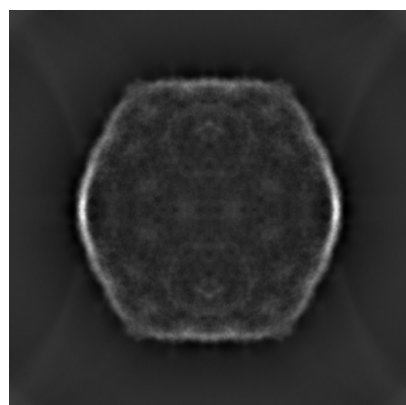


Y

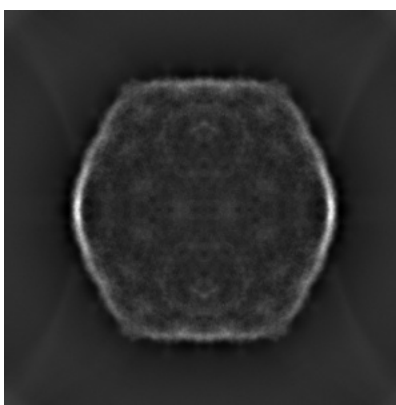


Z

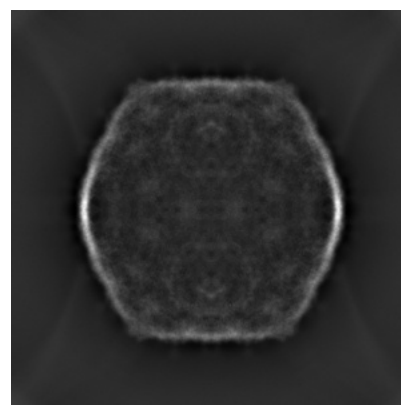
6.1.2 Raw map



X



Y

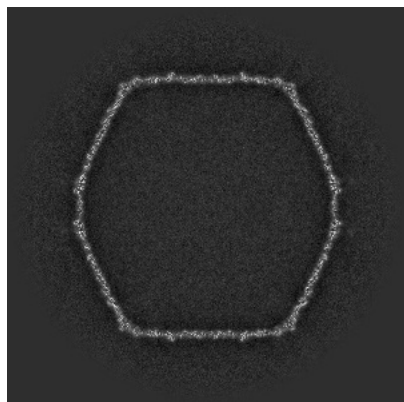


Z

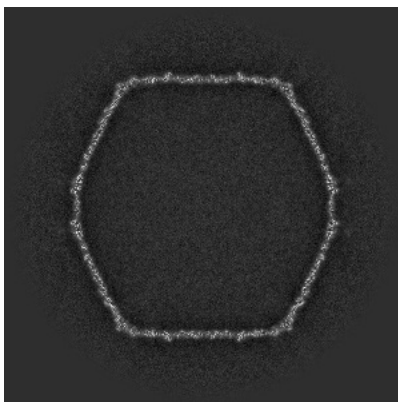
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

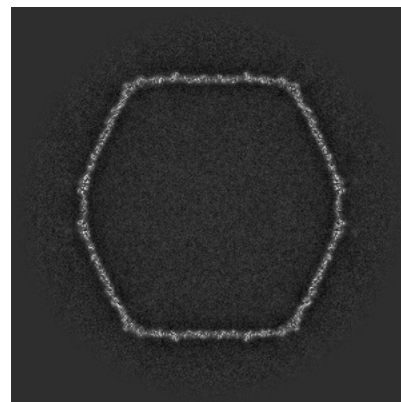
6.2.1 Primary map



X Index: 450

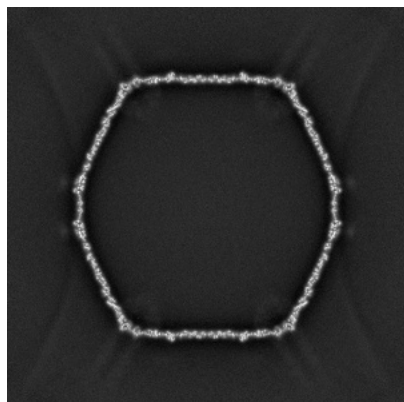


Y Index: 450

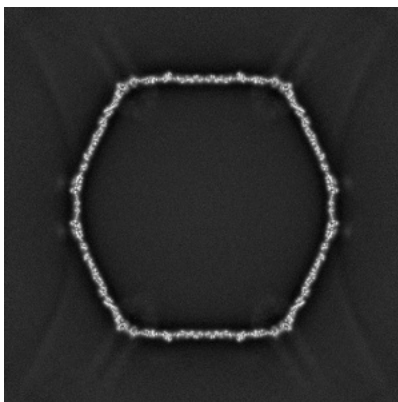


Z Index: 450

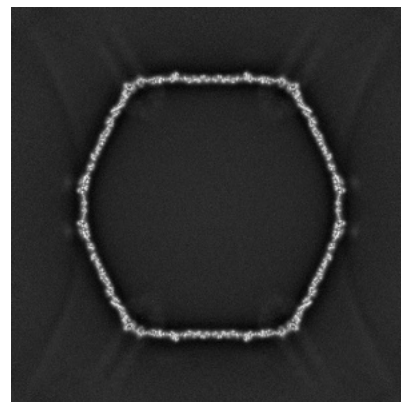
6.2.2 Raw map



X Index: 450



Y Index: 450

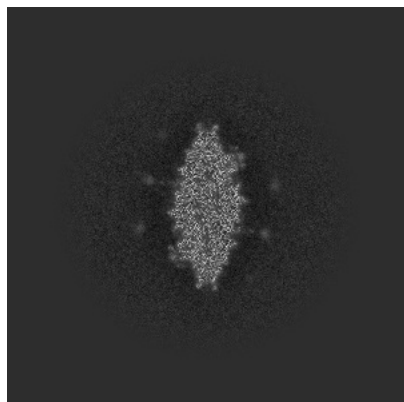


Z Index: 450

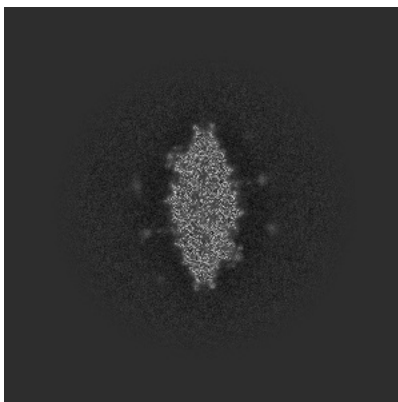
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

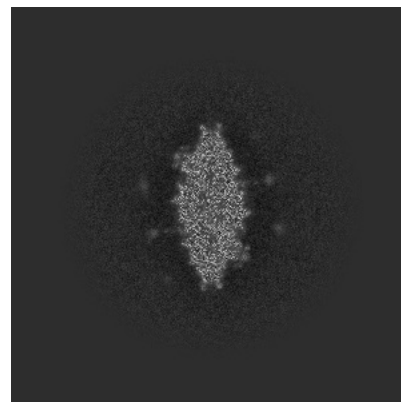
6.3.1 Primary map



X Index: 733

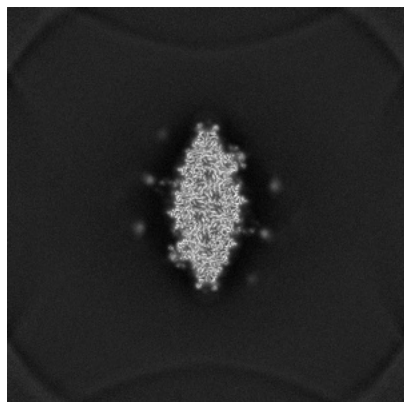


Y Index: 167

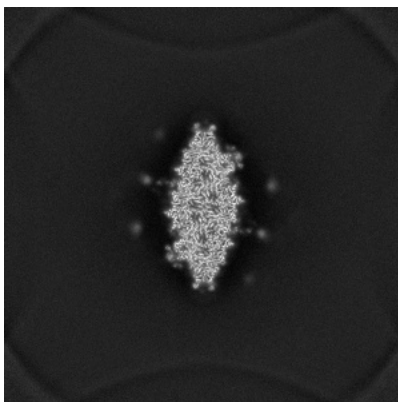


Z Index: 167

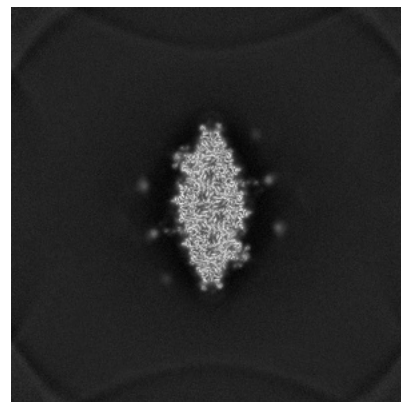
6.3.2 Raw map



X Index: 733



Y Index: 733

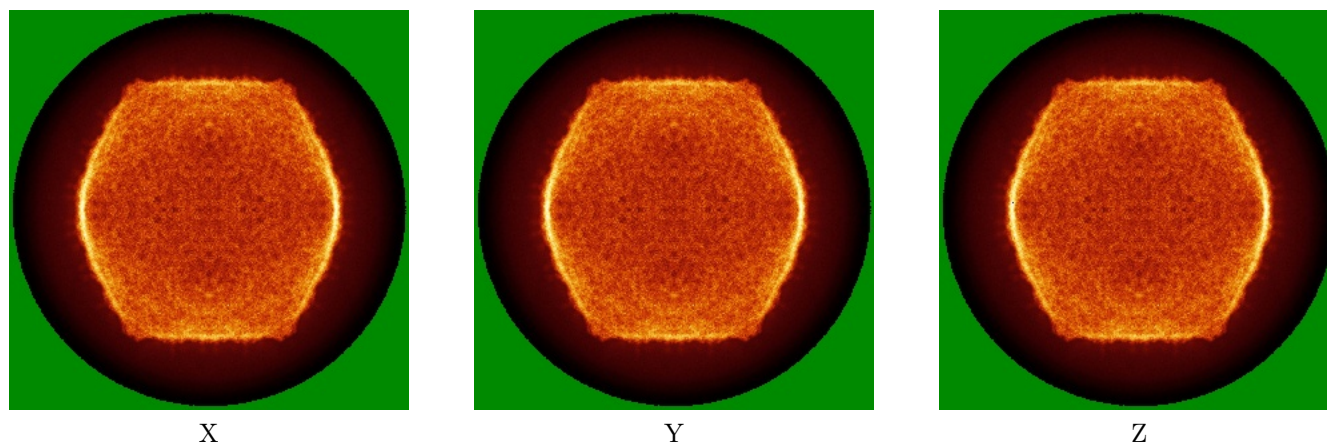


Z Index: 167

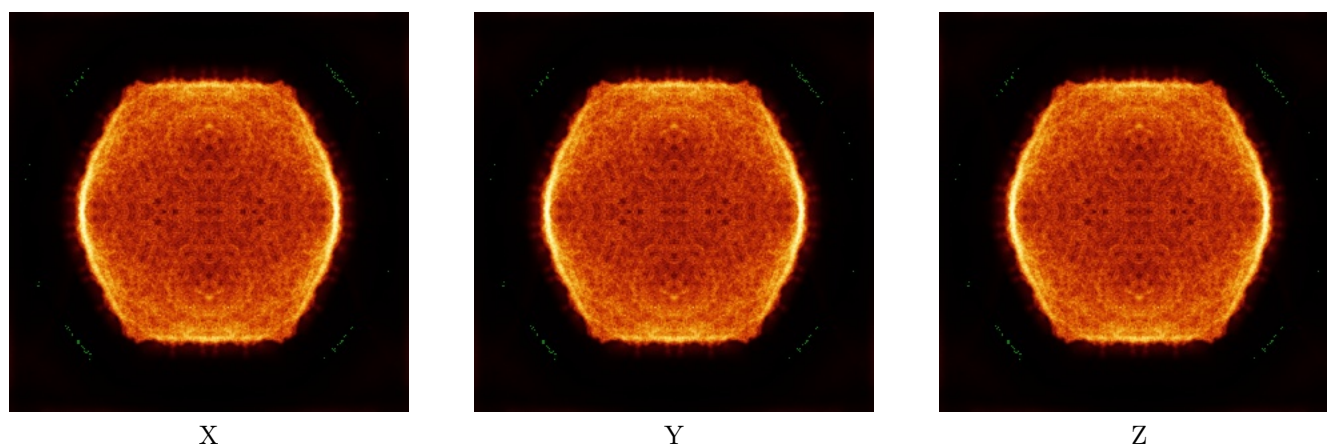
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

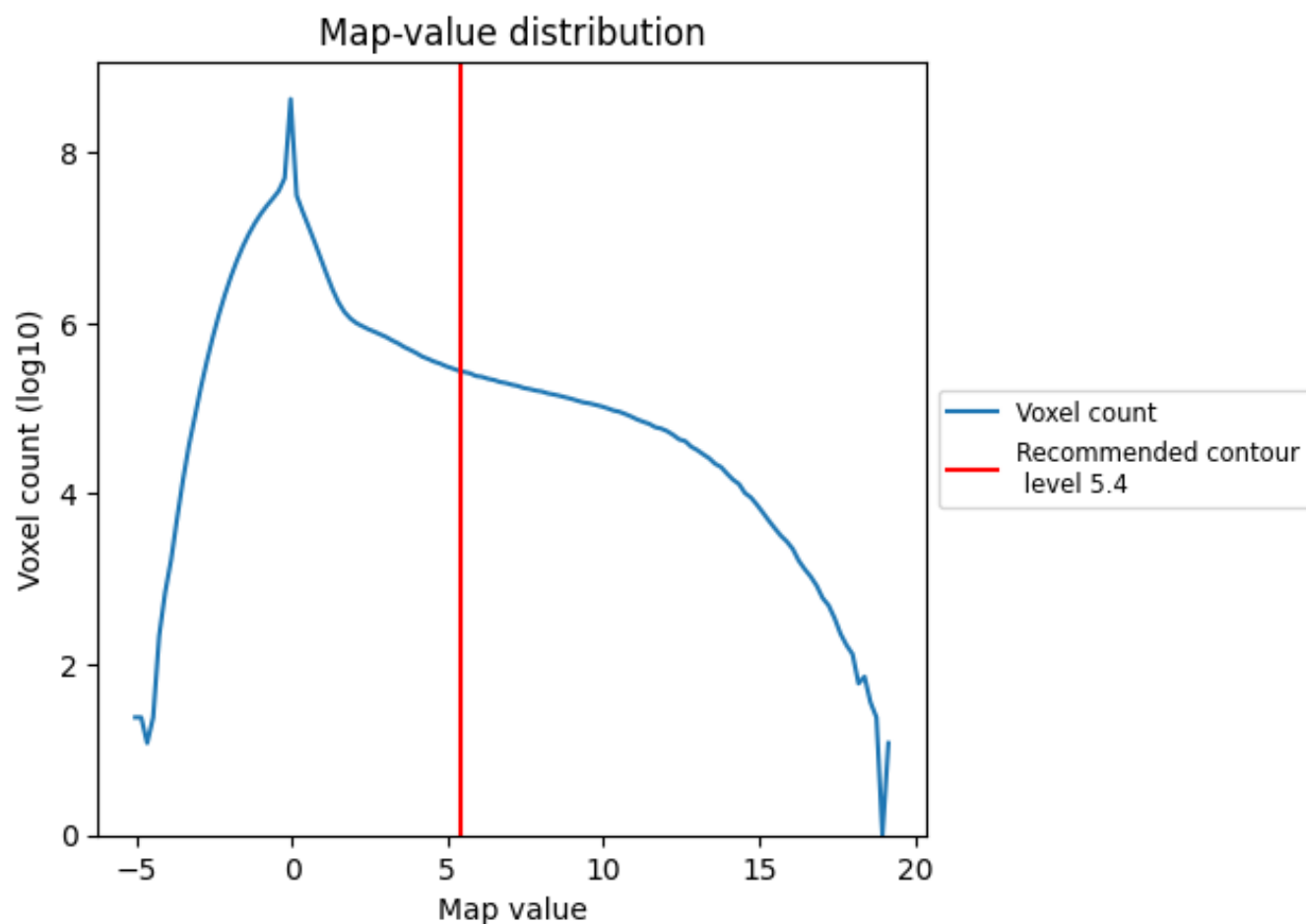
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

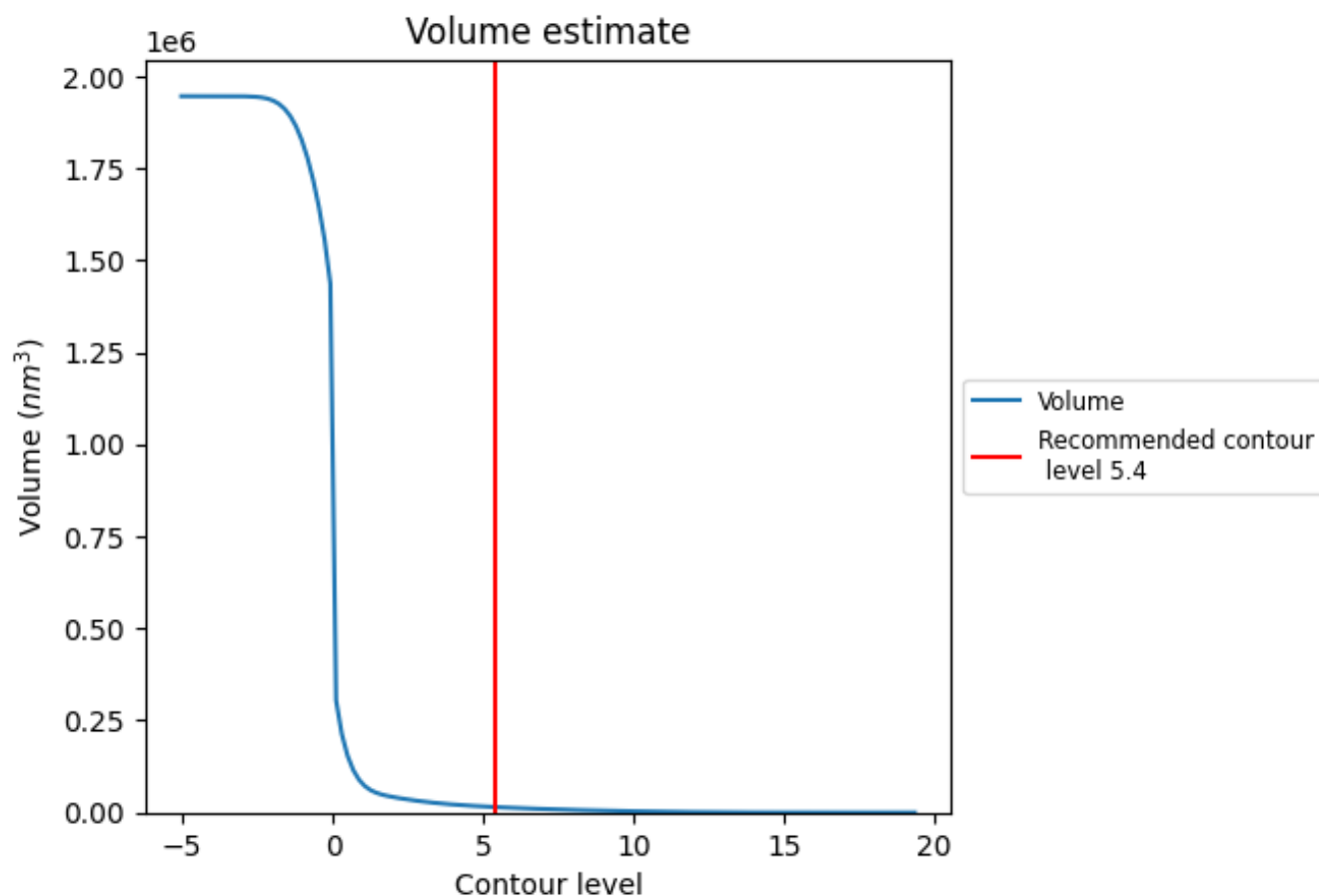
This section contains the results of statistical analysis of the map.

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.

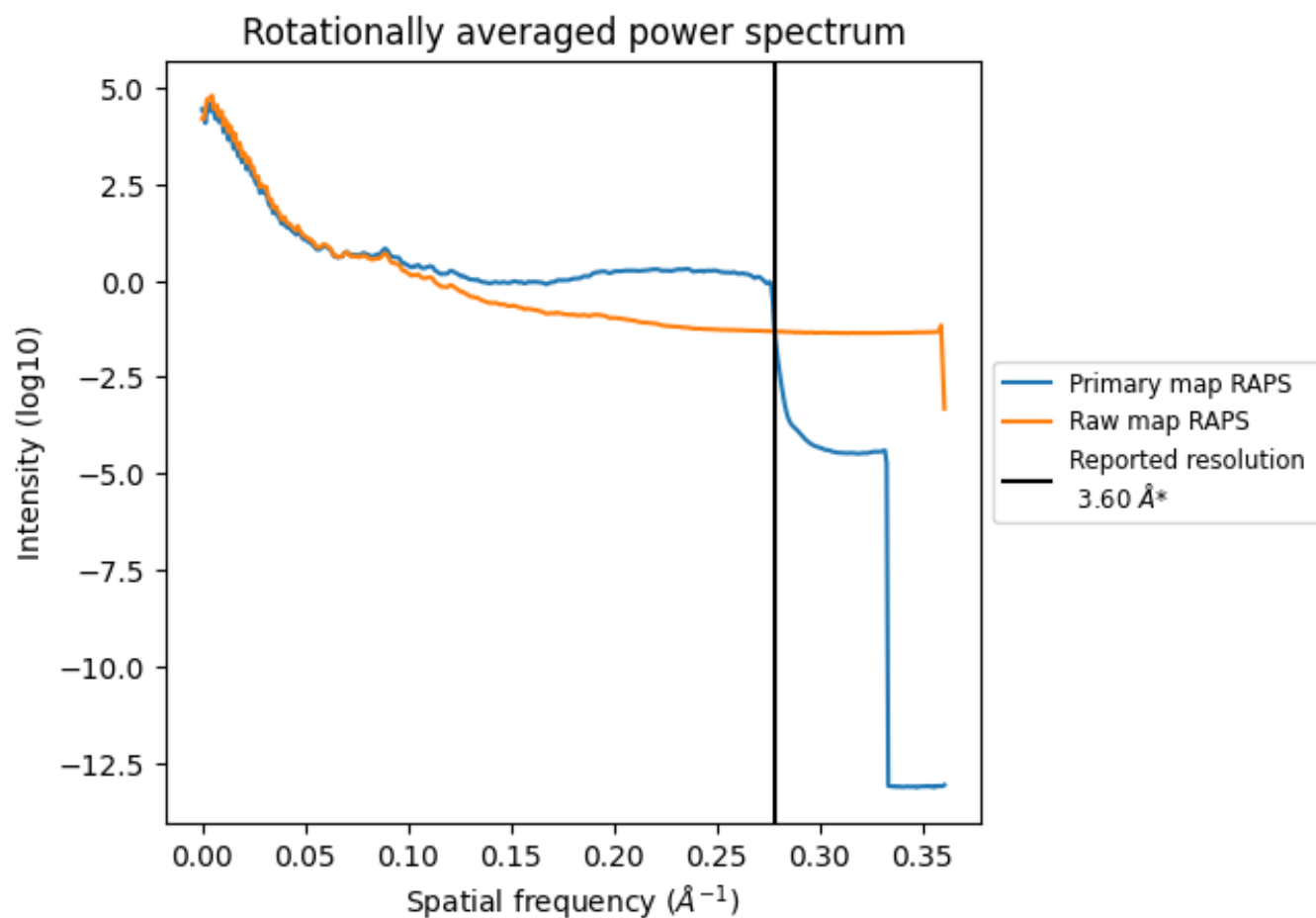
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14845 nm³; this corresponds to an approximate mass of 13410 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 ⓘ

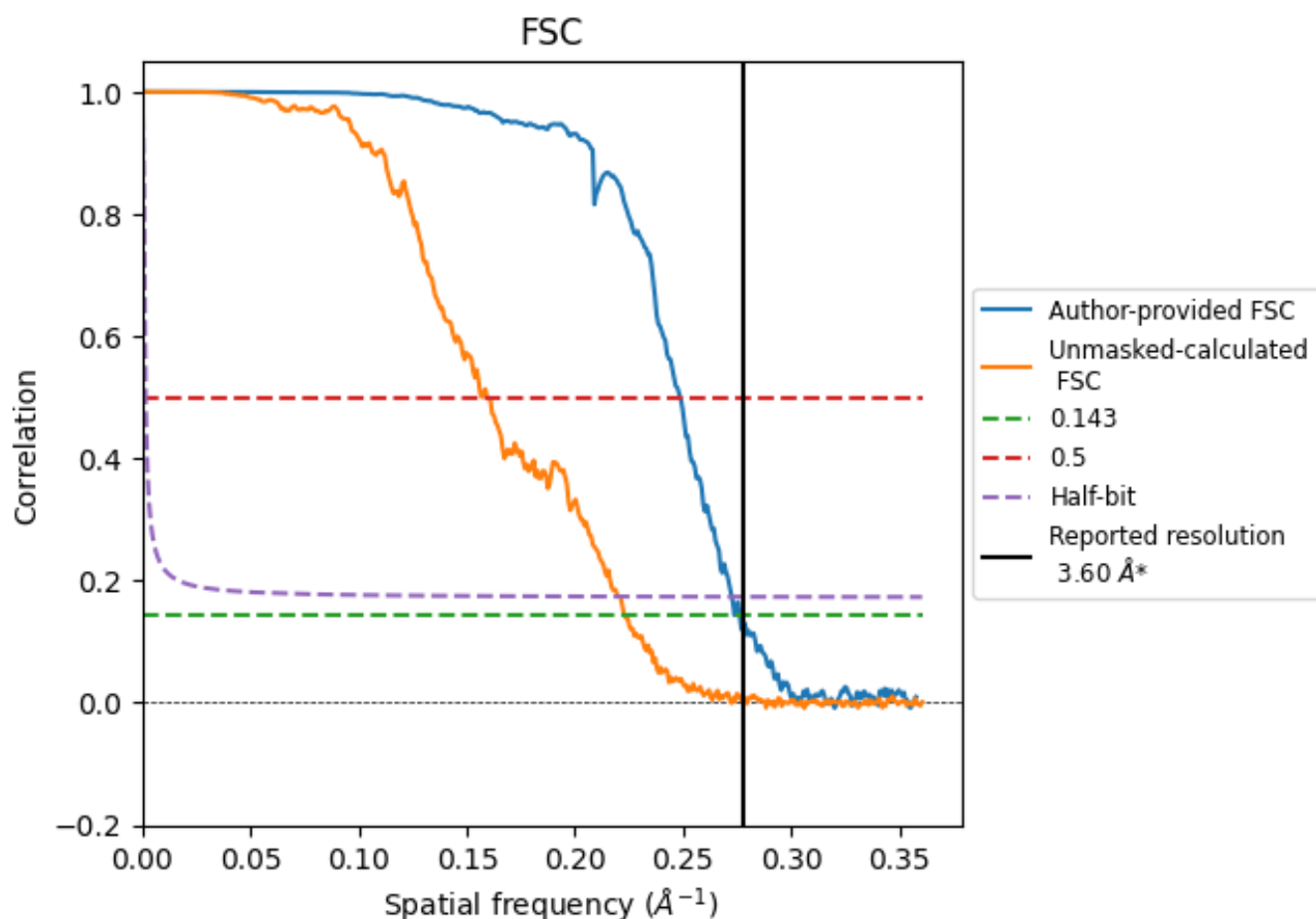


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

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	3.62	4.02	3.67
Unmasked-calculated*	4.48	6.27	4.53

*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 4.48 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-34949 and PDB model 8HQQ. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

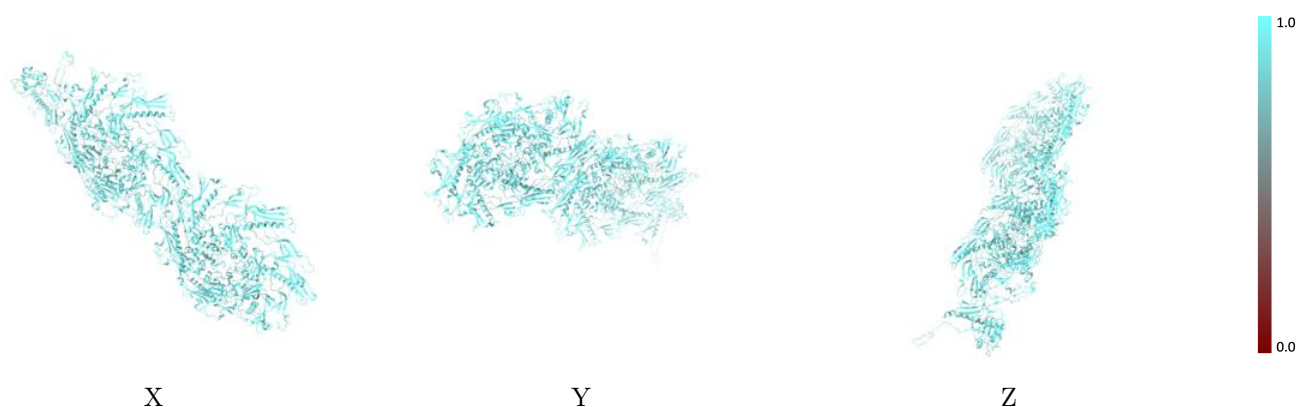
This section was not generated.

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



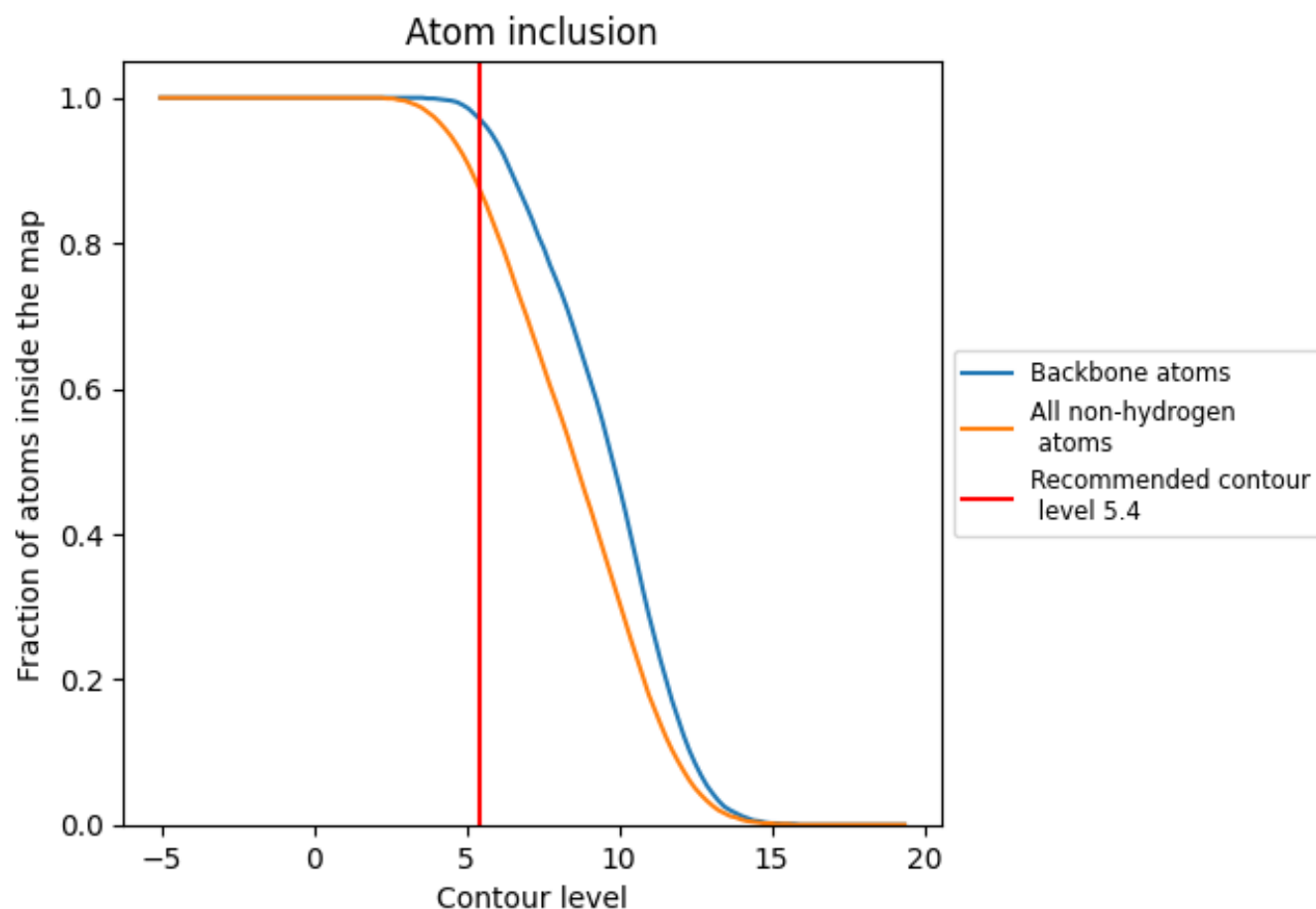
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 88% 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 (5.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.5070
A	 0.8850	 0.5110
B	 0.8860	 0.5110
C	 0.8830	 0.5100
D	 0.8810	 0.5060
E	 0.8880	 0.5110
F	 0.8800	 0.5090
G	 0.8780	 0.5090
H	 0.8830	 0.5110
I	 0.8850	 0.5100
J	 0.8790	 0.5080
K	 0.8700	 0.5040
L	 0.8700	 0.5030
M	 0.8270	 0.4850

