



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 09:43 PM EDT

PDB ID : 8UFB
EMDB ID : EMD-42190
Title : Eastern equine encephalitis virus (PE-6) VLP in complex with full-length VLDLR (asymmetric unit)
Authors : Adams, L.J.; Fremont, D.H.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2023-10-04
Resolution : 3.89 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

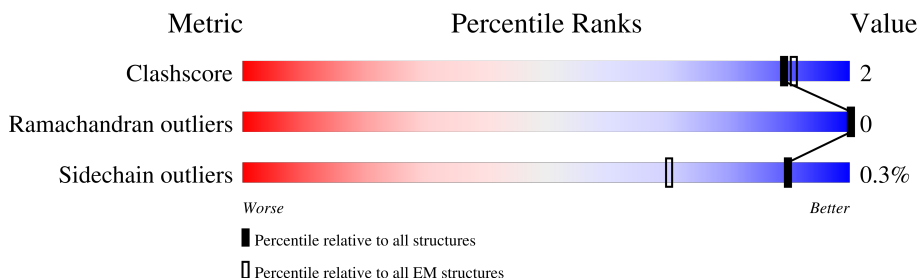
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.89 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	441	
1	D	441	
1	G	441	
1	J	441	
2	B	414	
2	E	414	
2	H	414	
2	K	414	

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Mol	Chain	Length	Quality of chain
3	C	151	
3	F	151	
3	I	151	
3	L	151	
4	R	748	
4	S	748	
4	T	748	
4	U	748	
4	V	748	
4	W	748	
4	X	748	
4	Y	748	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 34656 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 E1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		
1	D	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		
1	G	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		
1	J	441	Total	C	N	O	S	0	0
			3370	2151	559	640	20		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	TYR	TRP	conflict	UNP Q88678
A	392	ALA	PRO	conflict	UNP Q88678
D	89	TYR	TRP	conflict	UNP Q88678
D	392	ALA	PRO	conflict	UNP Q88678
G	89	TYR	TRP	conflict	UNP Q88678
G	392	ALA	PRO	conflict	UNP Q88678
J	89	TYR	TRP	conflict	UNP Q88678
J	392	ALA	PRO	conflict	UNP Q88678

- Molecule 2 is a protein called E2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	E	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	H	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		
2	K	414	Total	C	N	O	S	0	0
			3253	2058	589	582	24		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		
3	F	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		
3	I	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		
3	L	151	Total	C	N	O	S	0	0
			1164	734	207	219	4		

- Molecule 4 is a protein called Isoform Short of Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	W	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	X	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	Y	78	Total	C	N	O	S	0	0
			588	345	100	131	12		
4	R	35	Total	C	N	O	S	0	0
			258	150	46	56	6		
4	S	35	Total	C	N	O	S	0	0
			258	150	46	56	6		
4	T	35	Total	C	N	O	S	0	0
			258	150	46	56	6		
4	U	35	Total	C	N	O	S	0	0
			258	150	46	56	6		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	770	HIS	-	expression tag	UNP P98155
V	771	HIS	-	expression tag	UNP P98155
V	772	HIS	-	expression tag	UNP P98155
V	773	HIS	-	expression tag	UNP P98155
V	774	HIS	-	expression tag	UNP P98155
V	775	HIS	-	expression tag	UNP P98155
W	770	HIS	-	expression tag	UNP P98155
W	771	HIS	-	expression tag	UNP P98155
W	772	HIS	-	expression tag	UNP P98155
W	773	HIS	-	expression tag	UNP P98155
W	774	HIS	-	expression tag	UNP P98155

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Chain	Residue	Modelled	Actual	Comment	Reference
W	775	HIS	-	expression tag	UNP P98155
X	770	HIS	-	expression tag	UNP P98155
X	771	HIS	-	expression tag	UNP P98155
X	772	HIS	-	expression tag	UNP P98155
X	773	HIS	-	expression tag	UNP P98155
X	774	HIS	-	expression tag	UNP P98155
X	775	HIS	-	expression tag	UNP P98155
Y	770	HIS	-	expression tag	UNP P98155
Y	771	HIS	-	expression tag	UNP P98155
Y	772	HIS	-	expression tag	UNP P98155
Y	773	HIS	-	expression tag	UNP P98155
Y	774	HIS	-	expression tag	UNP P98155
Y	775	HIS	-	expression tag	UNP P98155
R	770	HIS	-	expression tag	UNP P98155
R	771	HIS	-	expression tag	UNP P98155
R	772	HIS	-	expression tag	UNP P98155
R	773	HIS	-	expression tag	UNP P98155
R	774	HIS	-	expression tag	UNP P98155
R	775	HIS	-	expression tag	UNP P98155
S	770	HIS	-	expression tag	UNP P98155
S	771	HIS	-	expression tag	UNP P98155
S	772	HIS	-	expression tag	UNP P98155
S	773	HIS	-	expression tag	UNP P98155
S	774	HIS	-	expression tag	UNP P98155
S	775	HIS	-	expression tag	UNP P98155
T	770	HIS	-	expression tag	UNP P98155
T	771	HIS	-	expression tag	UNP P98155
T	772	HIS	-	expression tag	UNP P98155
T	773	HIS	-	expression tag	UNP P98155
T	774	HIS	-	expression tag	UNP P98155
T	775	HIS	-	expression tag	UNP P98155
U	770	HIS	-	expression tag	UNP P98155
U	771	HIS	-	expression tag	UNP P98155
U	772	HIS	-	expression tag	UNP P98155
U	773	HIS	-	expression tag	UNP P98155
U	774	HIS	-	expression tag	UNP P98155
U	775	HIS	-	expression tag	UNP P98155

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	K	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	V	2	Total	Ca	0
			2	2	
6	W	2	Total	Ca	0
			2	2	
6	X	2	Total	Ca	0
			2	2	
6	Y	2	Total	Ca	0
			2	2	

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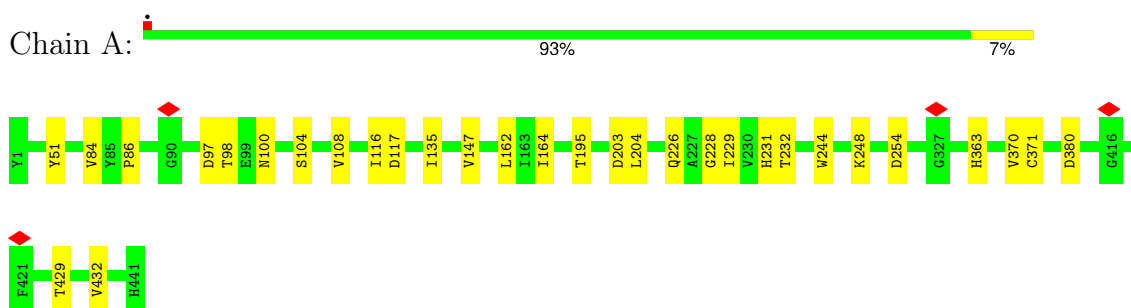
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Mol	Chain	Residues	Atoms		AltConf
6	R	1	Total 1	Ca 1	0
6	S	1	Total 1	Ca 1	0
6	T	1	Total 1	Ca 1	0
6	U	1	Total 1	Ca 1	0

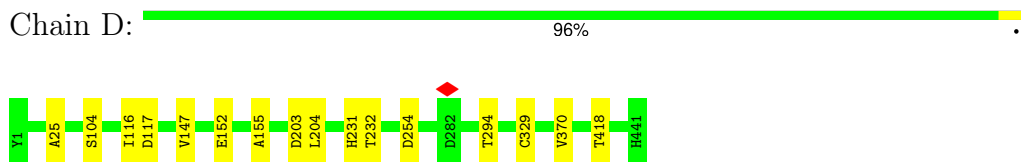
3 Residue-property plots

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.

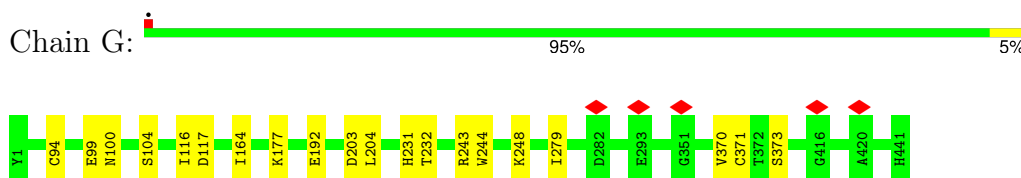
- Molecule 1: E1 protein



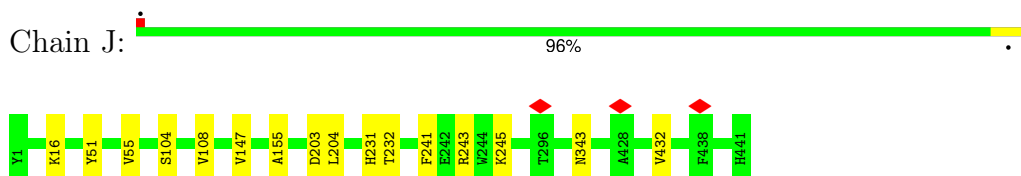
- Molecule 1: E1 protein



- Molecule 1: E1 protein

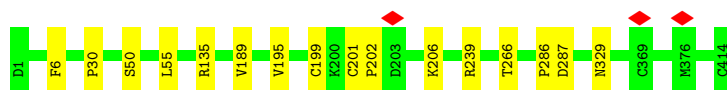


- Molecule 1: E1 protein



- Molecule 2: E2 protein





- Molecule 2: E2 protein



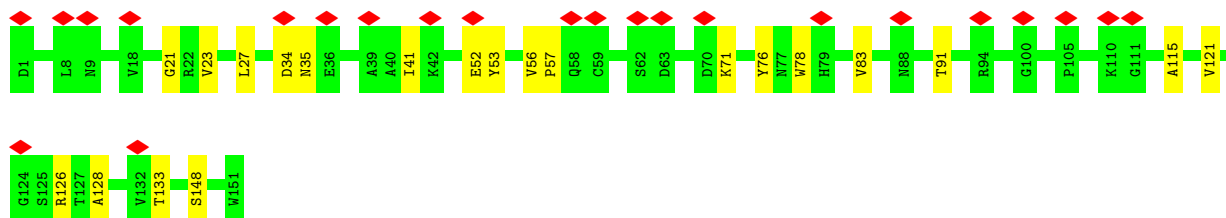
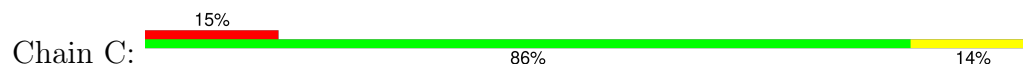
- Molecule 2: E2 protein



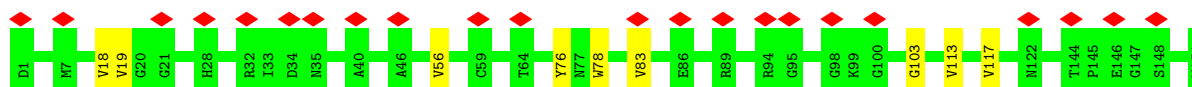
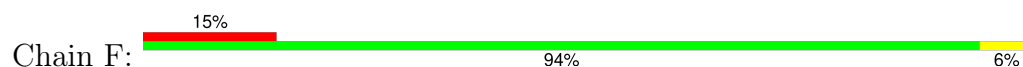
- Molecule 2: E2 protein



- Molecule 3: Capsid protein

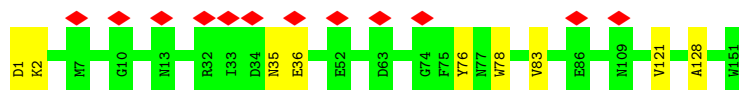


- Molecule 3: Capsid protein

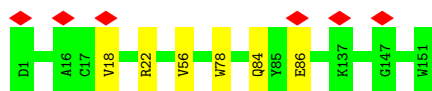


- Molecule 3: Capsid protein

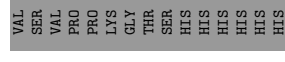
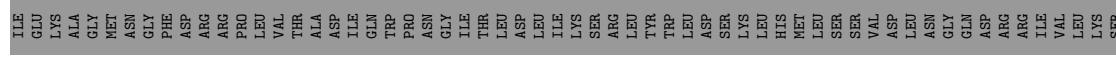
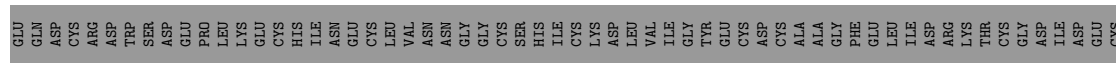
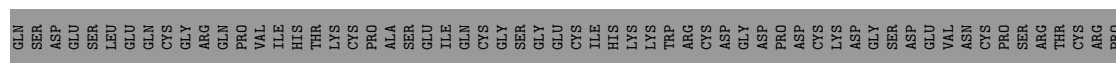
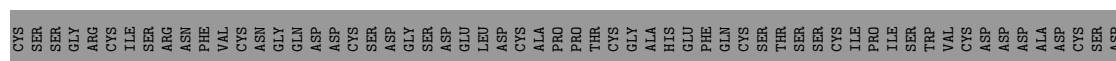
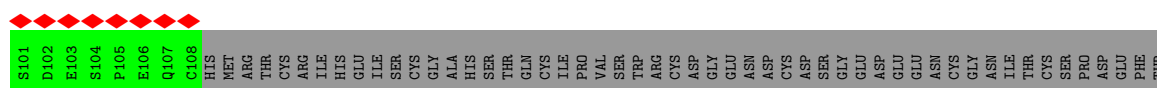
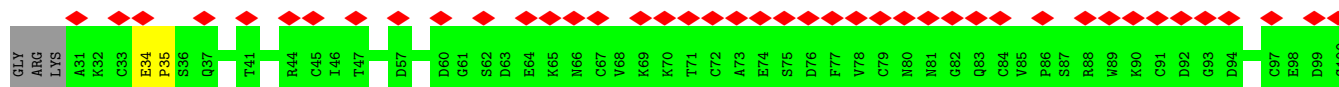




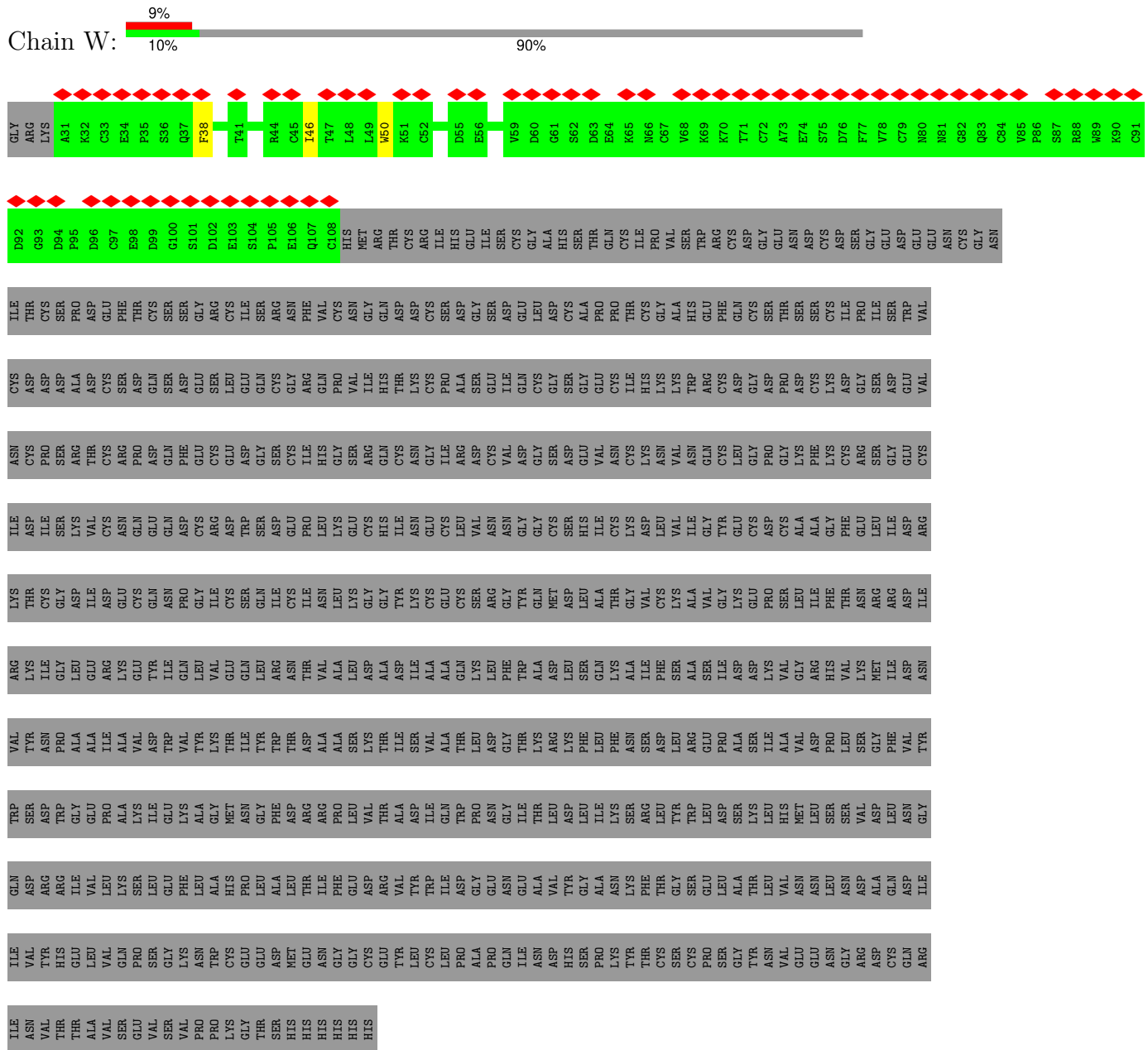
• Molecule 3: Capsid protein



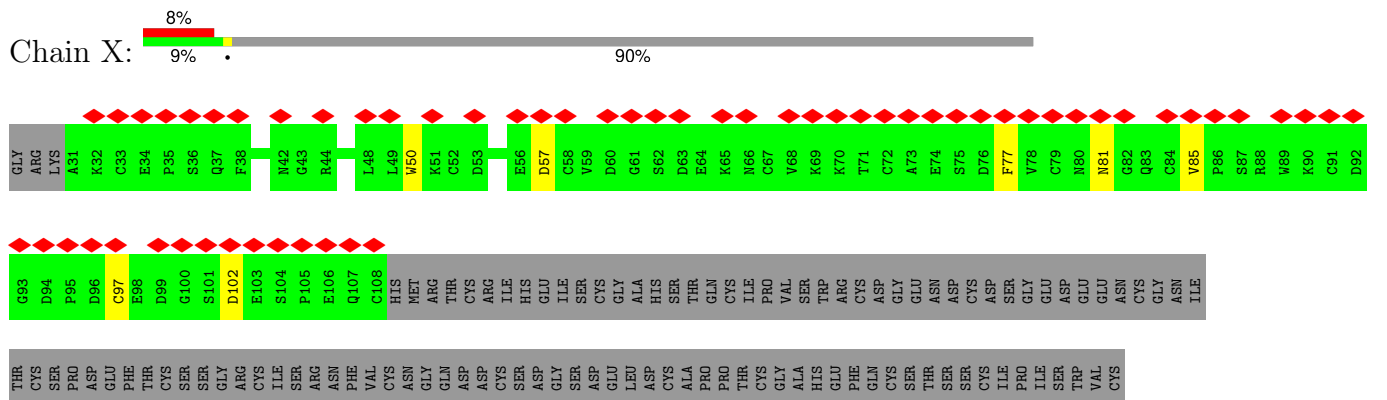
• Molecule 4: Isoform Short of Very low-density lipoprotein receptor



• Molecule 4: Isoform Short of Very low-density lipoprotein receptor

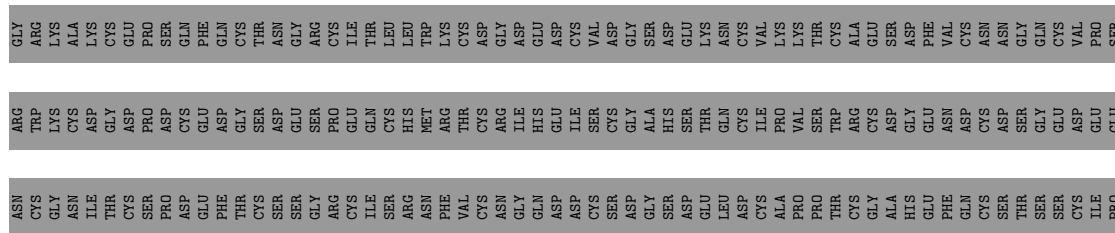


- Molecule 4: Isoform Short of Very low-density lipoprotein receptor





- Chain S:  95%



ILE	SER	TRP	VAL	CYS	ASP	ASP	ALA	ASP	CYS	SER	ASP	GLN	SER	ASP	GLU	SER	LEU	GLU	CYS	GLY	ARG	GLN	PRO	VAL	ILE	HIS	THR	LYS	C239	P240	A241	S242	E243	I244	Q245	C246	G247	S248	C249	E250	C251	I252	H253	K254	K255	I256	R257	C258	D261	K265	D266	G267	S268	D269	E270
V271	N272	C273	SER	SER	ARG	THR	CYS	THR	CYS	ASN	GLN	PRO	ASP	GLU	GLY	ASP	TRP	GLU	CYS	ASP	GLY	ARG	GLN	CYS	ILE	GLN	CYS	ILE	THR	ILE	ARG	ASN	GLY	THR	LYS	ASN	VAL	ASN	VAL	GLN	CYS	LEU	GLY	PRO	GLY	LYS	PHE	LYS	CYS	ARG	SER	GLY	GLU		
CYS	ILE	ASP	ILE	SER	VAL	CYS	GLN	ASP	GLN	ASP	GLN	ASP	TRP	GLU	GLY	SER	TRP	GLU	ASP	ASP	GLY	ARG	GLN	CYS	ILE	PRO	ASP	ILE	ASN	GLY	THR	LYS	ASN	VAL	ILE	GLY	VAL	TYR	GLN	CYS	LEU	CYS	ASP	CYS	ALA	GLY	PHE	LYS	CYS	ARG	GLY				
ARG	LYS	THR	CYS	GLY	ASP	ILE	ASP	CYS	GLU	PRO	GLY	ILE	ASP	GLU	ILE	GLN	SER	SER	CYS	ASP	GLY	THR	ILE	ILE	PRO	ASP	ILE	ASN	THR	ILE	ARG	ASN	THR	LYS	ASN	VAL	ILE	GLY	VAL	TYR	GLY	CYS	LEU	VAL	LYS	THR	ASN	ARG	ILE	ASP					
ILE	ARG	LYS	ILE	GLY	LEU	GLU	ARG	LYS	VAL	ILE	LEU	VAL	GLN	GLY	LEU	ARG	ASP	ASN	THR	ILE	VAL	ALA	GLY	LEU	ASP	ALA	GLN	LYS	THR	ILE	LEU	ASP	LYS	ASN	VAL	GLY	THR	LYS	ASN	VAL	ALA	GLY	VAL	LYS	THR	ASN	ARG	ILE	ASP						
ASN	VAL	TYR	ASN	PRO	ALA	ILE	ASP	VAL	TRP	VAL	TYR	TYR	LYS	THR	ILE	TRP	THR	ASP	THR	ASP	ALA	VAL	ILE	THR	ILE	VAL	ALA	GLN	THR	LEU	ASP	ASP	LYS	PHE	SER	LEU	ASP	LEU	VAL	ALA	ASP	PRO	ALA	GLY	THR	ASN	PHE	VAL							
TYR	TRP	SER	ASN	TRP	GLY	GLU	PRO	ALA	GLY	LYS	ALA	VAL	ASP	MET	ASN	PHE	GLY	THR	ASP	ASP	ARG	THR	ILE	ALA	VAL	ILE	GLN	TRP	PRO	ASN	GLY	LEU	ASP	ILE	LYS	PHE	THR	TRP	LEU	HIS	MET	ASN	VAL	SER	VAL	ASP	ASN								
GLY	GLN	ARG	ARG	ILE	VAL	LEU	LEU	SER	LEU	PHE	LEU	ALA	ASP	HIS	PRO	ALA	LEU	THR	ASP	ARG	VAL	THR	VAL	TYR	TRP	ILE	GLY	PRO	ASP	GLY	ALA	GLY	ASN	ALA	THR	TYR	GLY	ALA	ILE	LYS	ASN	THR	LEU	VAL	ASN	GLU	ASP								
ILE	ILE	VAL	TYR	HIS	THR	LEU	VAL	GLN	PRO	GLY	LYS	ASN	TRP	CYS	GLU	THR	ASP	MET	THR	ASP	HIS	THR	TYR	ILE	LEU	CYS	TRP	ILE	LEU	PRO	ALA	PRO	PRO	ILE	ASN	PRO	THR	CYS	PRO	GLY	TYR	ASN	VAL	GLU	ASN	GLY	ARG	CYS	GLN						
ARG	ILE	ASN	VAL	THR	ALA	VAL	SER	VAL	VAL	PRO	PRO	VAL	PRO	LYS	GLY	THR	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS					

● Molecule 4: Isoform Short of Very low-density lipoprotein receptor



ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	ARG	GLY	ASP	
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	391827	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 ($e^-/\text{\AA}^2$)	37.90	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.072	Depositor
Minimum map value	-0.915	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	281.06, 281.06, 281.06	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.081, 1.081, 1.081	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.26	0/3462	0.49	0/4724
1	D	0.26	0/3462	0.48	0/4724
1	G	0.26	0/3462	0.48	0/4724
1	J	0.26	0/3462	0.48	0/4724
2	B	0.25	0/3347	0.53	0/4565
2	E	0.25	0/3347	0.51	0/4565
2	H	0.25	0/3347	0.51	0/4565
2	K	0.25	0/3347	0.51	0/4565
3	C	0.24	0/1191	0.49	0/1615
3	F	0.24	0/1191	0.49	0/1615
3	I	0.25	0/1191	0.50	0/1615
3	L	0.25	0/1191	0.50	0/1615
4	R	0.22	0/262	0.46	0/351
4	S	0.22	0/262	0.47	0/351
4	T	0.22	0/262	0.47	0/351
4	U	0.24	0/262	0.55	0/351
4	V	0.24	0/597	0.45	0/805
4	W	0.24	0/597	0.45	0/805
4	X	0.23	0/597	0.46	0/805
4	Y	0.25	0/597	0.49	0/805
All	All	0.25	0/35436	0.50	0/48240

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	239	ARG	Sidechain

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	3370	0	3277	18	0
1	D	3370	0	3277	9	0
1	G	3370	0	3277	10	0
1	J	3370	0	3277	8	0
2	B	3253	0	3211	9	0
2	E	3253	0	3211	10	0
2	H	3253	0	3211	14	0
2	K	3253	0	3211	6	0
3	C	1164	0	1149	12	0
3	F	1164	0	1149	4	0
3	I	1164	0	1149	4	0
3	L	1164	0	1149	3	0
4	R	258	0	221	2	0
4	S	258	0	221	1	0
4	T	258	0	221	3	0
4	U	258	0	221	5	0
4	V	588	0	507	1	0
4	W	588	0	507	2	0
4	X	588	0	507	4	0
4	Y	588	0	507	3	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	G	14	0	13	0	0
5	H	14	0	13	0	0
5	J	14	0	13	0	0
5	K	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	U	1	0	0	0	0
6	V	2	0	0	0	0
6	W	2	0	0	0	0
6	X	2	0	0	0	0
6	Y	2	0	0	0	0
All	All	34656	0	33564	118	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 2.

All (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:398:LYS:O	3:L:22:ARG:NH1	2.26	0.68
1:A:254:ASP:OD2	2:B:135:ARG:NH2	2.28	0.66
1:A:203:ASP:OD1	1:A:204:LEU:N	2.29	0.65
3:L:84:GLN:NE2	3:L:86:GLU:OE2	2.31	0.63
3:I:76:TYR:O	3:I:83:VAL:N	2.26	0.62
1:D:203:ASP:OD1	1:D:204:LEU:N	2.31	0.62
2:H:271:PRO:HB3	2:H:284:LEU:HD23	1.81	0.62
1:A:84:VAL:O	1:A:100:ASN:ND2	2.34	0.60
2:H:38:GLY:O	2:H:131:ARG:NH1	2.33	0.60
1:J:203:ASP:OD1	1:J:204:LEU:N	2.33	0.60
3:C:76:TYR:O	3:C:83:VAL:N	2.33	0.59
1:G:203:ASP:OD1	1:G:204:LEU:N	2.34	0.59
4:W:38:PHE:N	4:W:46:ILE:O	2.37	0.57
4:U:260:GLY:N	4:U:270:GLU:OE1	2.37	0.56
2:H:142:PRO:HG3	2:H:266:THR:HG23	1.88	0.55
1:G:244:TRP:O	1:G:248:LYS:N	2.40	0.55
1:G:104:SER:HB3	1:G:232:THR:HG23	1.90	0.53
3:F:76:TYR:O	3:F:83:VAL:N	2.36	0.52
1:D:329:CYS:SG	1:D:370:VAL:HG12	2.51	0.51
3:I:1:ASP:OD1	3:I:2:LYS:N	2.41	0.51
3:I:35:ASN:OD1	3:I:36:GLU:N	2.44	0.51
4:Y:38:PHE:N	4:Y:46:ILE:O	2.44	0.51
2:E:206:LYS:NZ	4:T:261:ASP:OD2	2.44	0.51
2:B:266:THR:O	2:B:329:ASN:ND2	2.37	0.50
1:G:370:VAL:O	1:G:373:SER:N	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:201:CYS:HB2	2:H:202:PRO:HD2	1.94	0.50
2:K:199:CYS:HB3	2:K:217:CYS:SG	2.51	0.50
1:G:99:GLU:OE1	1:G:99:GLU:N	2.38	0.50
3:C:27:LEU:HD23	3:C:52:GLU:HG3	1.94	0.49
3:L:18:VAL:HG13	3:L:56:VAL:HG11	1.94	0.49
1:D:418:THR:HG23	2:E:378:SER:CB	2.43	0.49
3:C:34:ASP:OD1	3:C:35:ASN:N	2.46	0.49
4:X:81:ASN:ND2	4:X:97:CYS:SG	2.83	0.48
1:G:177:LYS:NZ	1:G:192:GLU:OE2	2.33	0.48
1:A:162:LEU:HD21	1:A:164:ILE:HD11	1.96	0.48
3:I:121:VAL:O	3:I:128:ALA:N	2.47	0.48
2:B:201:CYS:HB3	2:B:202:PRO:HD2	1.96	0.47
2:K:1:ASP:OD1	2:K:2:LEU:N	2.47	0.47
3:F:18:VAL:HG13	3:F:56:VAL:HG11	1.96	0.47
2:B:30:PRO:O	2:B:50:SER:OG	2.32	0.47
4:T:252:ILE:HA	4:T:256:TRP:CZ3	2.50	0.47
2:B:6:PHE:CD1	2:B:55:LEU:HD21	2.49	0.47
1:J:16:LYS:NZ	1:J:343:ASN:OD1	2.39	0.47
1:A:226:GLN:CB	1:A:229:ILE:HD12	2.46	0.46
4:Y:33:CYS:SG	4:Y:34:GLU:N	2.89	0.46
2:B:199:CYS:SG	2:B:201:CYS:SG	3.13	0.46
2:B:206:LYS:NZ	4:U:259:ASP:OD2	2.49	0.46
2:K:203:ASP:HB3	2:K:216:THR:HG21	1.97	0.46
3:C:121:VAL:O	3:C:128:ALA:N	2.48	0.46
1:D:104:SER:HB3	1:D:232:THR:HG23	1.96	0.46
1:A:429:THR:O	1:A:432:VAL:HG12	2.16	0.46
1:G:116:ILE:HG13	1:G:117:ASP:N	2.31	0.45
2:E:6:PHE:CD2	2:E:55:LEU:HD21	2.51	0.45
3:C:21:GLY:O	3:C:56:VAL:HG23	2.17	0.45
2:K:156:LYS:HE3	4:W:50:TRP:CG	2.52	0.45
2:E:150:CYS:N	2:E:261:ALA:O	2.41	0.45
1:A:116:ILE:HG13	1:A:117:ASP:N	2.31	0.45
1:D:25:ALA:CB	1:D:294:THR:HG21	2.46	0.45
4:U:248:SER:OG	4:U:250:GLU:OE1	2.27	0.45
2:H:53:PHE:CZ	2:H:99:ILE:HD11	2.52	0.44
1:J:147:VAL:HG12	1:J:155:ALA:CB	2.48	0.44
3:C:115:ALA:HB2	3:C:133:THR:HG22	1.99	0.44
4:S:244:ILE:O	4:S:252:ILE:N	2.42	0.44
1:G:370:VAL:O	1:G:371:CYS:C	2.56	0.44
4:X:102:ASP:OD1	4:X:102:ASP:N	2.51	0.44
1:A:195:THR:HG21	1:D:152:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:PHE:CE2	1:J:245:LYS:HE3	2.52	0.43
1:A:147:VAL:HG21	1:A:164:ILE:HD12	1.99	0.43
3:F:103:GLY:N	3:F:117:VAL:O	2.37	0.43
4:T:269:ASP:N	4:T:269:ASP:OD1	2.47	0.43
1:D:116:ILE:HG13	1:D:117:ASP:N	2.34	0.43
1:A:135:ILE:HD11	1:A:162:LEU:HD22	1.99	0.43
3:C:41:ILE:HD11	3:C:57:PRO:HD3	2.00	0.42
3:C:71:LYS:HG3	3:C:71:LYS:O	2.19	0.42
1:G:94:CYS:SG	1:G:100:ASN:ND2	2.91	0.42
2:H:196:LYS:HB2	2:H:228:ILE:HD11	2.00	0.42
1:A:244:TRP:O	1:A:248:LYS:N	2.53	0.42
3:C:23:VAL:O	3:C:53:TYR:HA	2.19	0.42
2:B:189:VAL:HG13	2:B:195:VAL:HG23	2.01	0.42
2:H:9:TYR:HB3	2:H:55:LEU:HD11	2.01	0.42
4:R:269:ASP:OD1	4:R:269:ASP:N	2.47	0.42
1:A:86:PRO:HA	1:A:228:GLY:HA2	2.00	0.42
1:A:97:ASP:OD1	1:A:98:THR:N	2.52	0.42
1:A:363:HIS:ND1	1:A:380:ASP:OD1	2.47	0.42
1:J:432:VAL:HB	2:K:389:THR:HG23	2.02	0.42
4:X:50:TRP:HB3	4:X:57:ASP:OD2	2.20	0.42
2:E:201:CYS:HB2	2:E:202:PRO:HD2	2.02	0.42
3:C:91:THR:CG2	3:C:126:ARG:HB3	2.50	0.42
4:X:77:PHE:N	4:X:85:VAL:O	2.53	0.42
2:E:44:VAL:HG21	2:E:152:ARG:HE	1.84	0.42
1:A:226:GLN:HB2	1:A:229:ILE:HD12	2.02	0.41
1:A:370:VAL:O	1:A:371:CYS:C	2.59	0.41
1:D:147:VAL:HG12	1:D:155:ALA:CB	2.50	0.41
2:B:286:PRO:O	2:B:287:ASP:HB2	2.20	0.41
3:C:121:VAL:N	3:C:128:ALA:O	2.42	0.41
2:H:206:LYS:NZ	4:R:259:ASP:OD2	2.48	0.41
2:H:167:HIS:CD2	2:H:236:ASN:HB3	2.55	0.41
2:H:10:LYS:HE2	2:H:60:VAL:HG23	2.01	0.41
4:Y:38:PHE:O	4:Y:46:ILE:N	2.50	0.41
1:A:51:TYR:HB2	1:A:108:VAL:HG13	2.01	0.41
1:A:104:SER:HB3	1:A:232:THR:HG23	2.03	0.41
3:C:121:VAL:HG22	3:C:148:SER:HA	2.02	0.41
1:D:254:ASP:OD2	2:E:135:ARG:NH2	2.48	0.41
2:E:1:ASP:OD1	2:E:2:LEU:N	2.53	0.41
2:H:3:ASP:O	2:H:7:THR:HG23	2.21	0.41
1:J:55:VAL:HG11	1:J:232:THR:HB	2.03	0.41
2:E:33:ILE:HD11	2:E:111:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:19:VAL:HG11	3:F:113:VAL:HG11	2.03	0.40
1:J:51:TYR:HB2	1:J:108:VAL:HG13	2.03	0.40
4:U:269:ASP:OD1	4:U:269:ASP:N	2.54	0.40
2:H:141:PRO:HA	2:H:142:PRO:HD3	1.96	0.40
1:J:104:SER:HB3	1:J:232:THR:HG23	2.02	0.40
2:E:136:GLU:OE2	2:E:268:ALA:N	2.54	0.40
1:G:164:ILE:CD1	1:G:279:ILE:HG22	2.51	0.40
2:K:31:ILE:O	2:K:31:ILE:HG23	2.20	0.40
2:H:83:VAL:HG23	2:H:91:LEU:HD21	2.03	0.40
4:U:245:GLN:HA	4:U:251:CYS:HA	2.04	0.40
4:V:34:GLU:HB2	4:V:35:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/441 (100%)	430 (98%)	9 (2%)	0	100	100
1	D	439/441 (100%)	433 (99%)	6 (1%)	0	100	100
1	G	439/441 (100%)	434 (99%)	5 (1%)	0	100	100
1	J	439/441 (100%)	434 (99%)	5 (1%)	0	100	100
2	B	412/414 (100%)	397 (96%)	15 (4%)	0	100	100
2	E	412/414 (100%)	397 (96%)	15 (4%)	0	100	100
2	H	412/414 (100%)	392 (95%)	20 (5%)	0	100	100
2	K	412/414 (100%)	396 (96%)	16 (4%)	0	100	100
3	C	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
3	F	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
3	I	149/151 (99%)	147 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	149/151 (99%)	148 (99%)	1 (1%)	0	100	100
4	R	33/748 (4%)	30 (91%)	3 (9%)	0	100	100
4	S	33/748 (4%)	30 (91%)	3 (9%)	0	100	100
4	T	33/748 (4%)	31 (94%)	2 (6%)	0	100	100
4	U	33/748 (4%)	31 (94%)	2 (6%)	0	100	100
4	V	76/748 (10%)	73 (96%)	3 (4%)	0	100	100
4	W	76/748 (10%)	76 (100%)	0	0	100	100
4	X	76/748 (10%)	74 (97%)	2 (3%)	0	100	100
4	Y	76/748 (10%)	76 (100%)	0	0	100	100
All	All	4436/10008 (44%)	4323 (98%)	113 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	370/370 (100%)	369 (100%)	1 (0%)	91	92
1	D	370/370 (100%)	369 (100%)	1 (0%)	91	92
1	G	370/370 (100%)	368 (100%)	2 (0%)	86	90
1	J	370/370 (100%)	368 (100%)	2 (0%)	86	90
2	B	362/362 (100%)	362 (100%)	0	100	100
2	E	362/362 (100%)	361 (100%)	1 (0%)	91	92
2	H	362/362 (100%)	361 (100%)	1 (0%)	91	92
2	K	362/362 (100%)	361 (100%)	1 (0%)	91	92
3	C	125/125 (100%)	124 (99%)	1 (1%)	79	84
3	F	125/125 (100%)	124 (99%)	1 (1%)	79	84
3	I	125/125 (100%)	124 (99%)	1 (1%)	79	84
3	L	125/125 (100%)	124 (99%)	1 (1%)	79	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	R	30/655 (5%)	30 (100%)	0	100	100
4	S	30/655 (5%)	30 (100%)	0	100	100
4	T	30/655 (5%)	30 (100%)	0	100	100
4	U	30/655 (5%)	30 (100%)	0	100	100
4	V	70/655 (11%)	70 (100%)	0	100	100
4	W	70/655 (11%)	70 (100%)	0	100	100
4	X	70/655 (11%)	70 (100%)	0	100	100
4	Y	70/655 (11%)	70 (100%)	0	100	100
All	All	3828/8668 (44%)	3815 (100%)	13 (0%)	90	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
3	C	78	TRP
1	D	231	HIS
2	E	27	CYS
3	F	78	TRP
1	G	231	HIS
1	G	243	ARG
2	H	27	CYS
3	I	78	TRP
1	J	231	HIS
1	J	243	ARG
2	K	22	CYS
3	L	78	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
2	B	162	HIS
1	D	73	HIS
2	E	160	GLN
3	F	37	GLN
1	G	73	HIS
2	H	114	HIS
2	H	160	GLN

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Mol	Chain	Res	Type
2	H	162	HIS
3	I	11	GLN
1	J	73	HIS
2	K	114	HIS
2	K	160	GLN
2	K	230	ASN
4	Y	83	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](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
5	NAG	D	501	1	14,14,15	0.32	0	17,19,21	0.59	0
5	NAG	J	501	1	14,14,15	0.28	0	17,19,21	0.82	1 (5%)
5	NAG	B	501	2	14,14,15	0.16	0	17,19,21	0.44	0
5	NAG	E	501	2	14,14,15	0.18	0	17,19,21	0.57	0
5	NAG	H	501	2	14,14,15	0.37	0	17,19,21	1.28	1 (5%)
5	NAG	G	501	1	14,14,15	0.24	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	501	2	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	A	501	1	14,14,15	0.22	0	17,19,21	0.67	1 (5%)

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
5	NAG	D	501	1	-	2/6/23/26	0/1/1/1
5	NAG	J	501	1	-	1/6/23/26	0/1/1/1
5	NAG	B	501	2	-	0/6/23/26	0/1/1/1
5	NAG	E	501	2	-	0/6/23/26	0/1/1/1
5	NAG	H	501	2	-	1/6/23/26	0/1/1/1
5	NAG	G	501	1	-	1/6/23/26	0/1/1/1
5	NAG	K	501	2	-	4/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	NAG	C1-O5-C5	4.77	118.57	112.19
5	J	501	NAG	C1-O5-C5	2.71	115.82	112.19
5	A	501	NAG	C1-O5-C5	2.14	115.06	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	501	NAG	O5-C5-C6-O6
5	K	501	NAG	C4-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	J	501	NAG	O5-C5-C6-O6
5	G	501	NAG	O5-C5-C6-O6
5	K	501	NAG	C3-C2-N2-C7
5	K	501	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	H	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

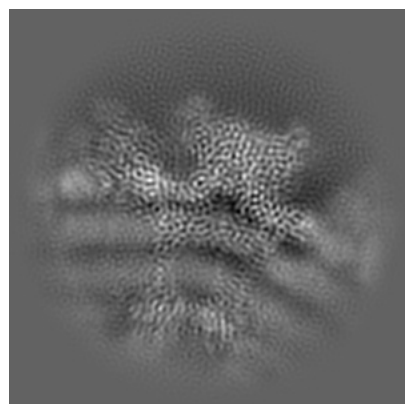
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42190. These allow visual inspection of the internal detail of the map and identification of artifacts.

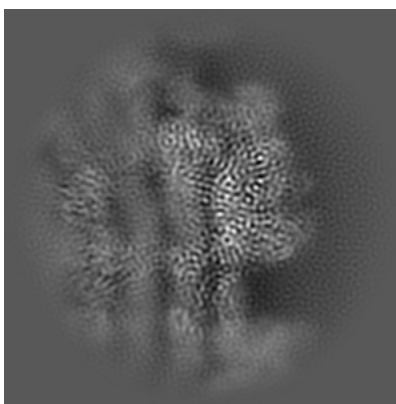
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

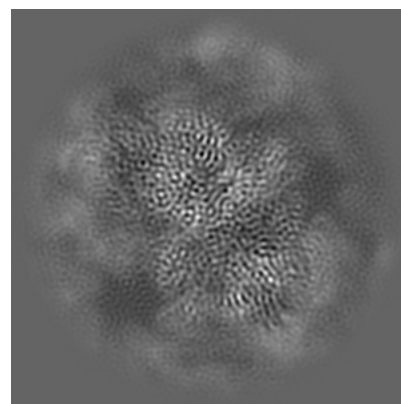
6.1.1 Primary map



X

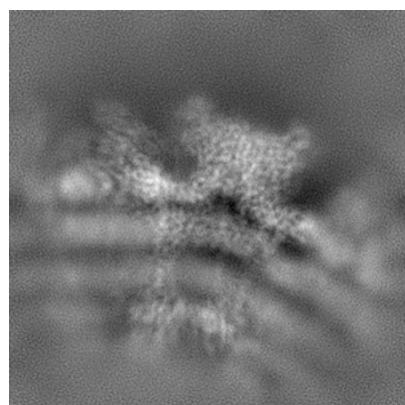


Y

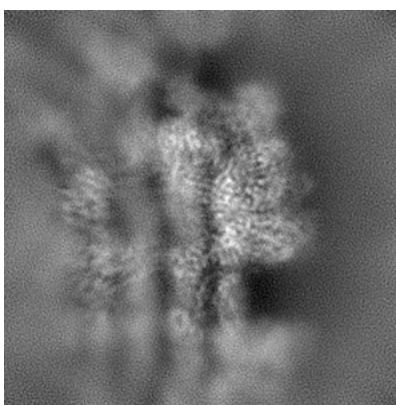


Z

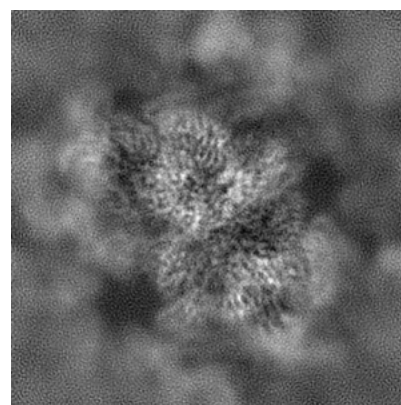
6.1.2 Raw map



X



Y

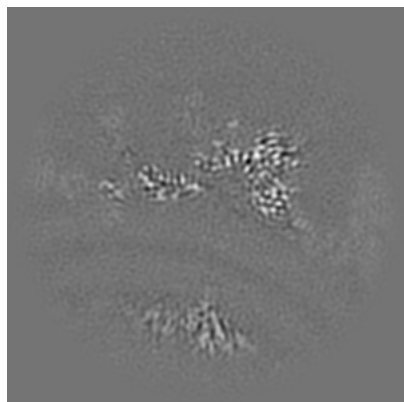


Z

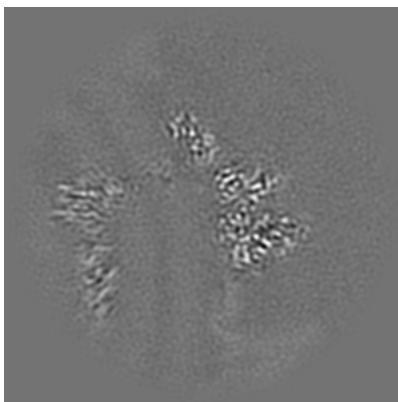
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

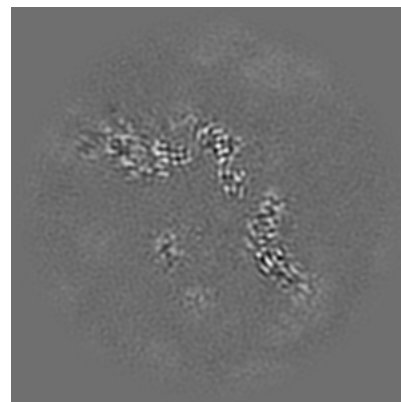
6.2.1 Primary map



X Index: 130

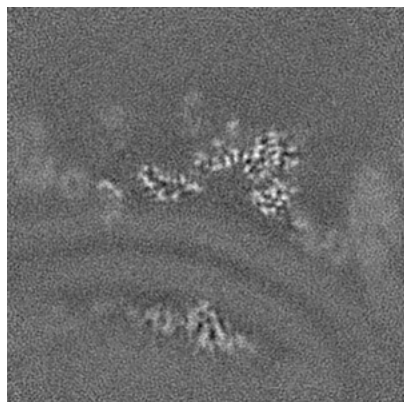


Y Index: 130

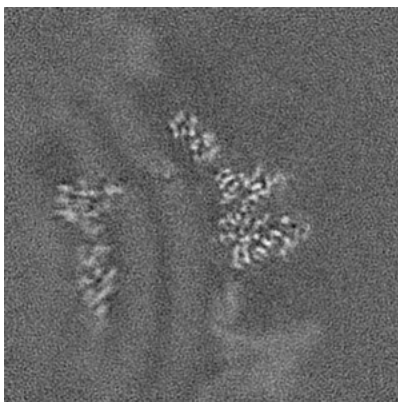


Z Index: 130

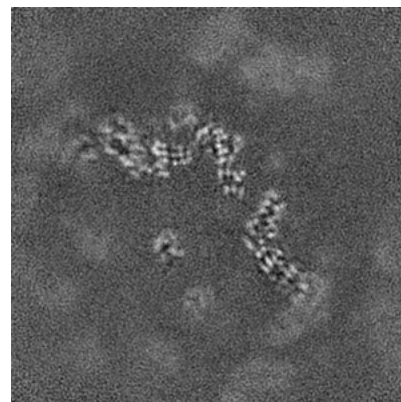
6.2.2 Raw map



X Index: 130



Y Index: 130

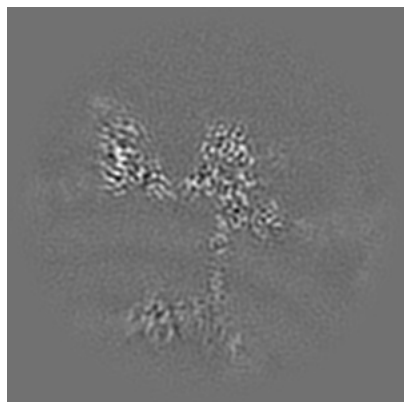


Z Index: 130

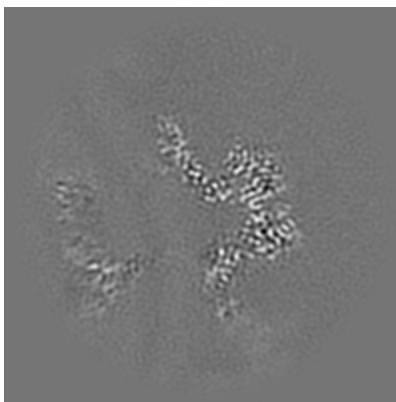
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

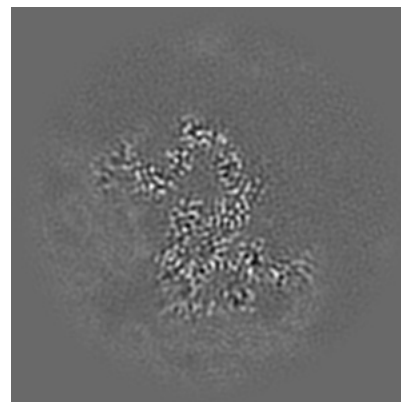
6.3.1 Primary map



X Index: 148

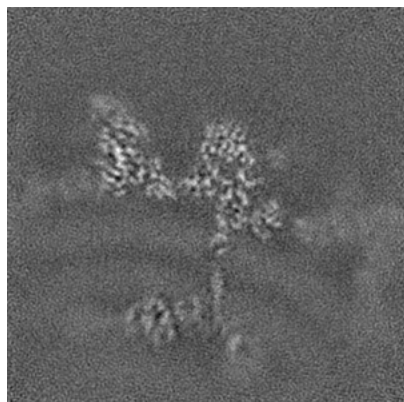


Y Index: 148

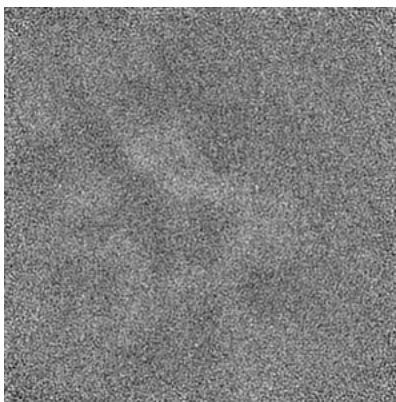


Z Index: 144

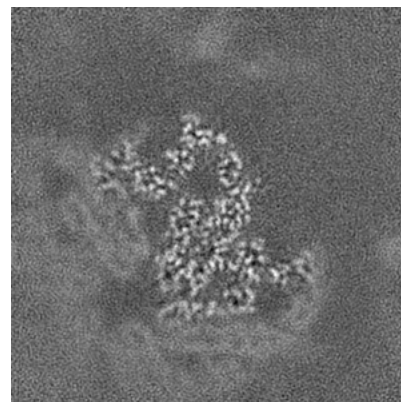
6.3.2 Raw map



X Index: 148



Y Index: 0

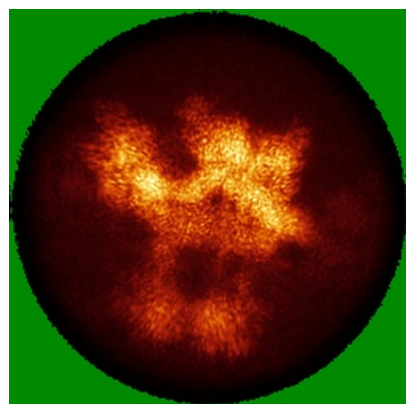


Z Index: 144

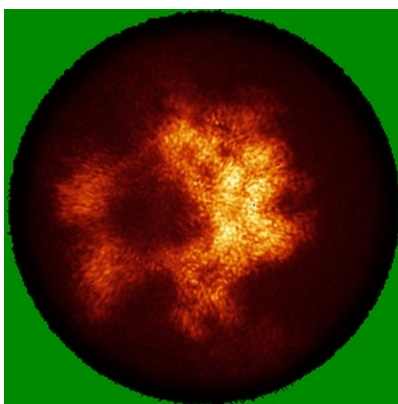
The images above show the largest variance slices of the map in three orthogonal directions.

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

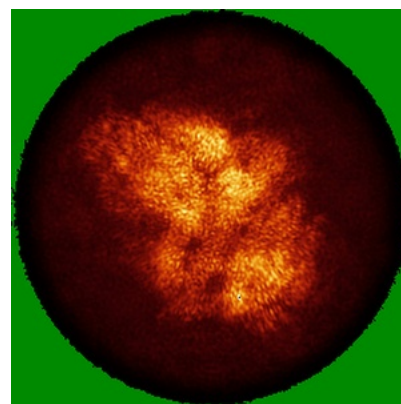
6.4.1 Primary map



X

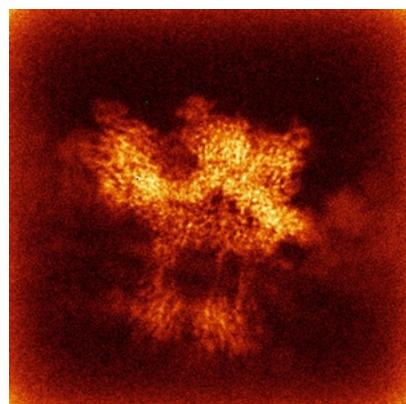


Y

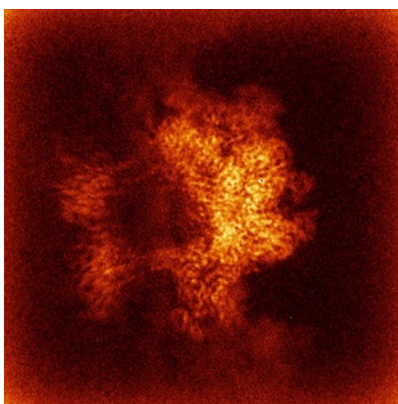


Z

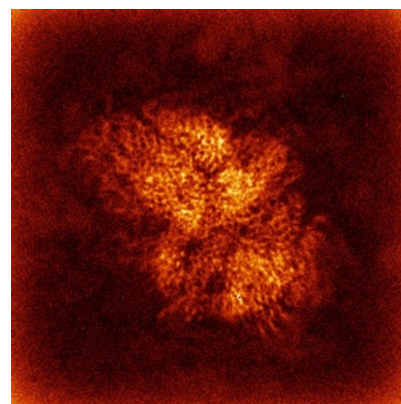
6.4.2 Raw map



X



Y

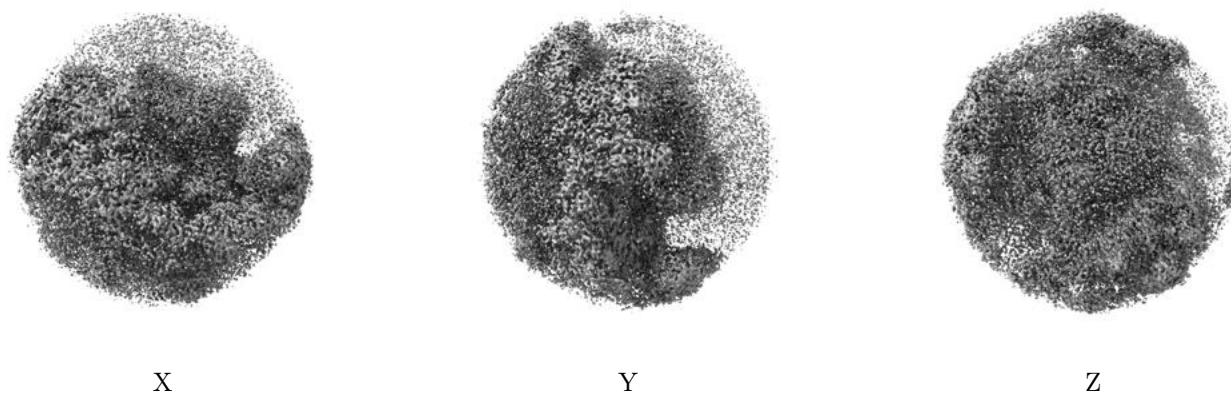


Z

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.

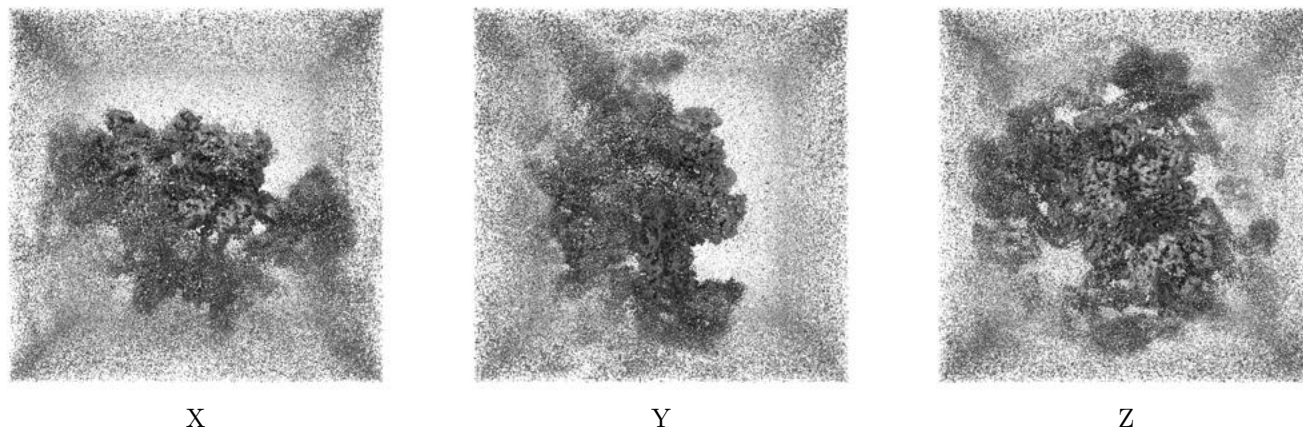
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

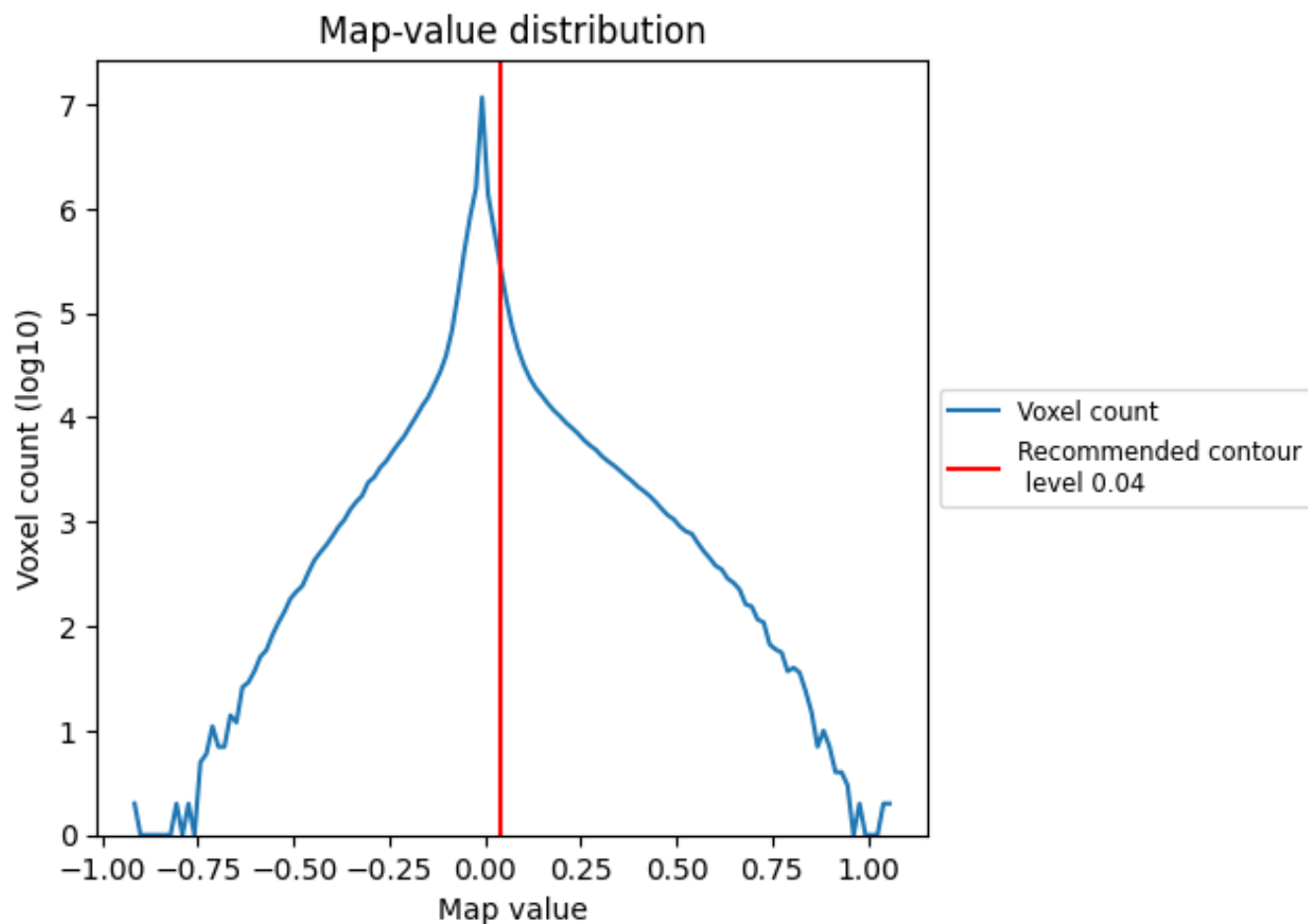
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

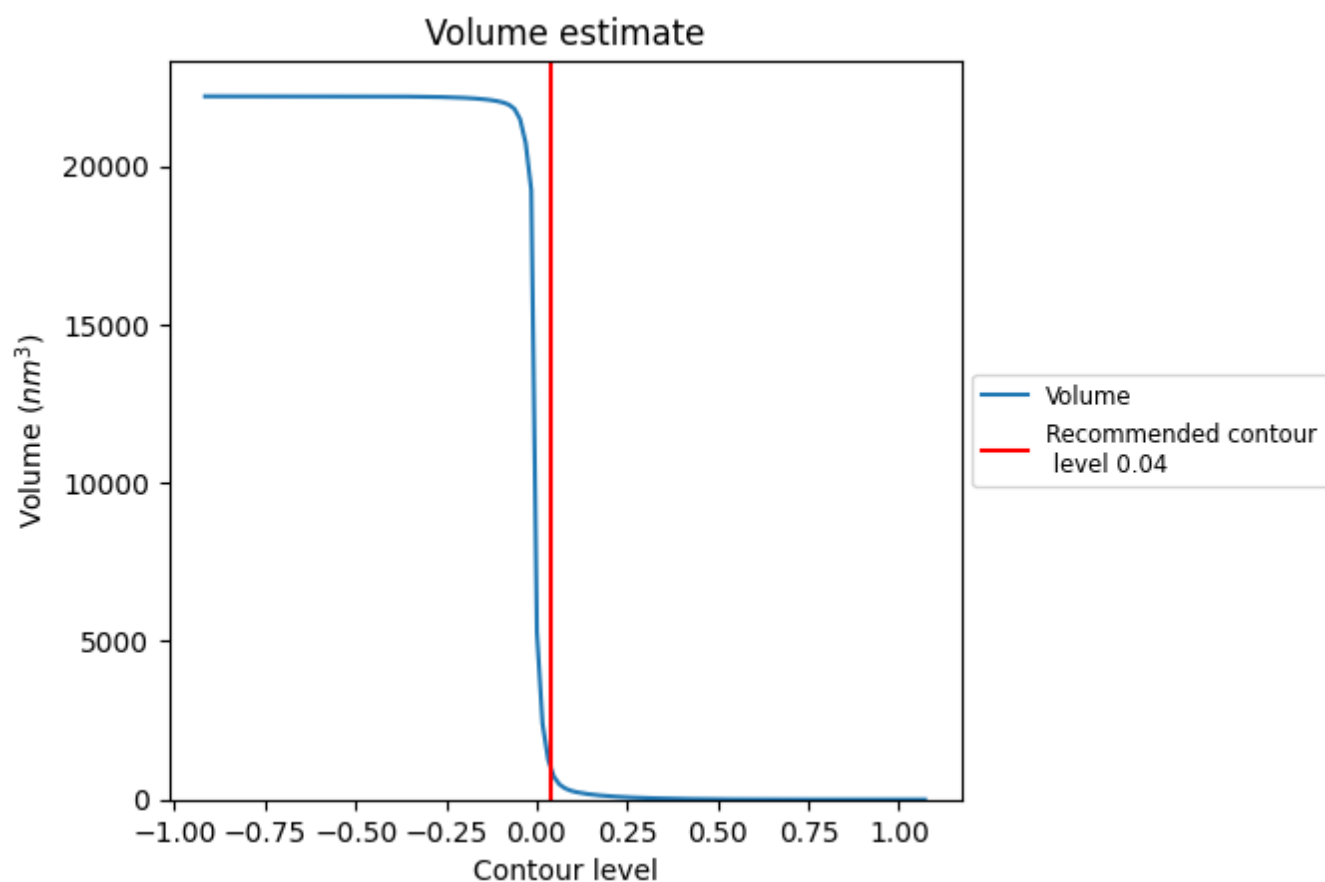
This section contains the results of statistical analysis of the map.

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.

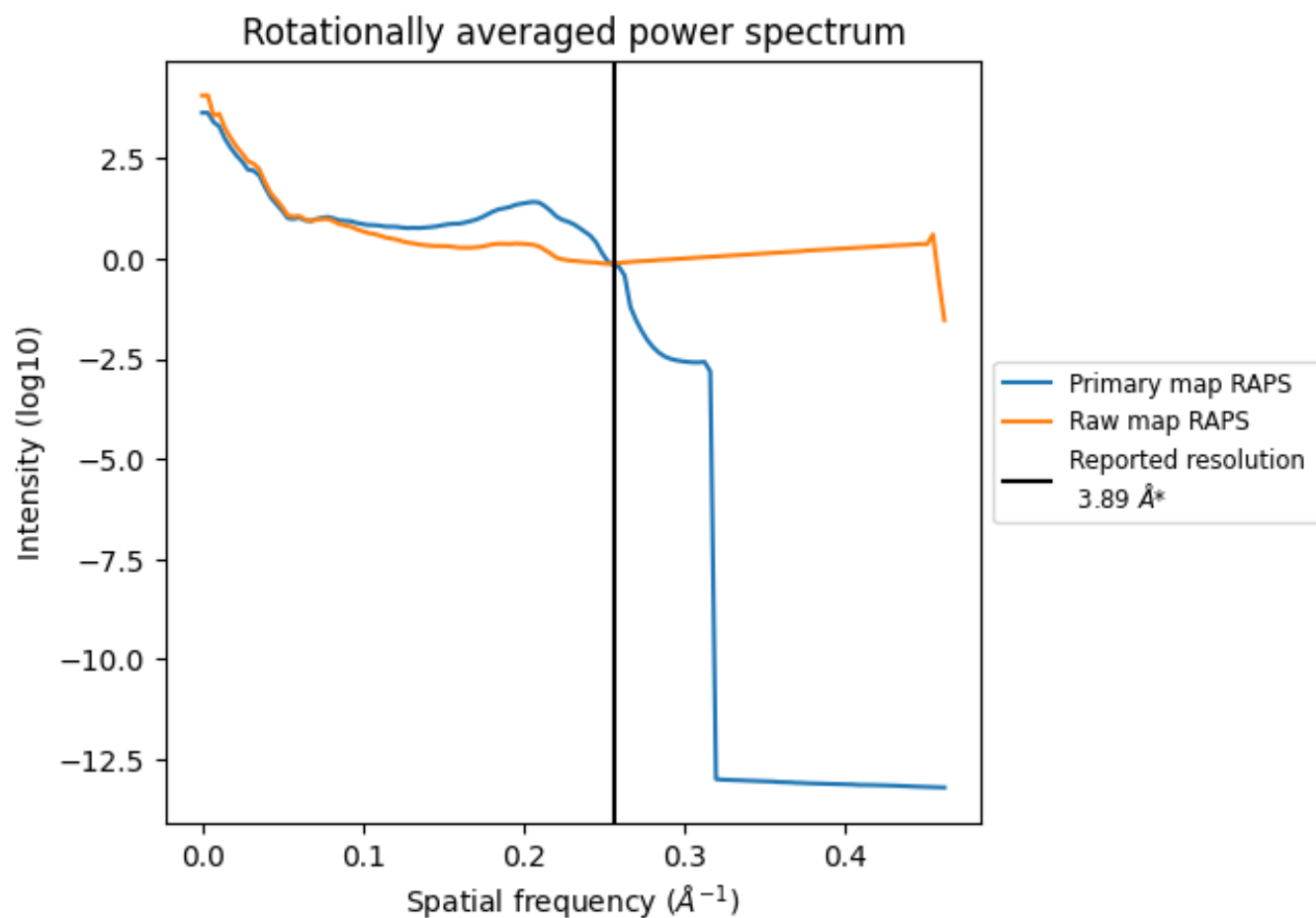
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 978 nm³; this corresponds to an approximate mass of 883 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 ⓘ

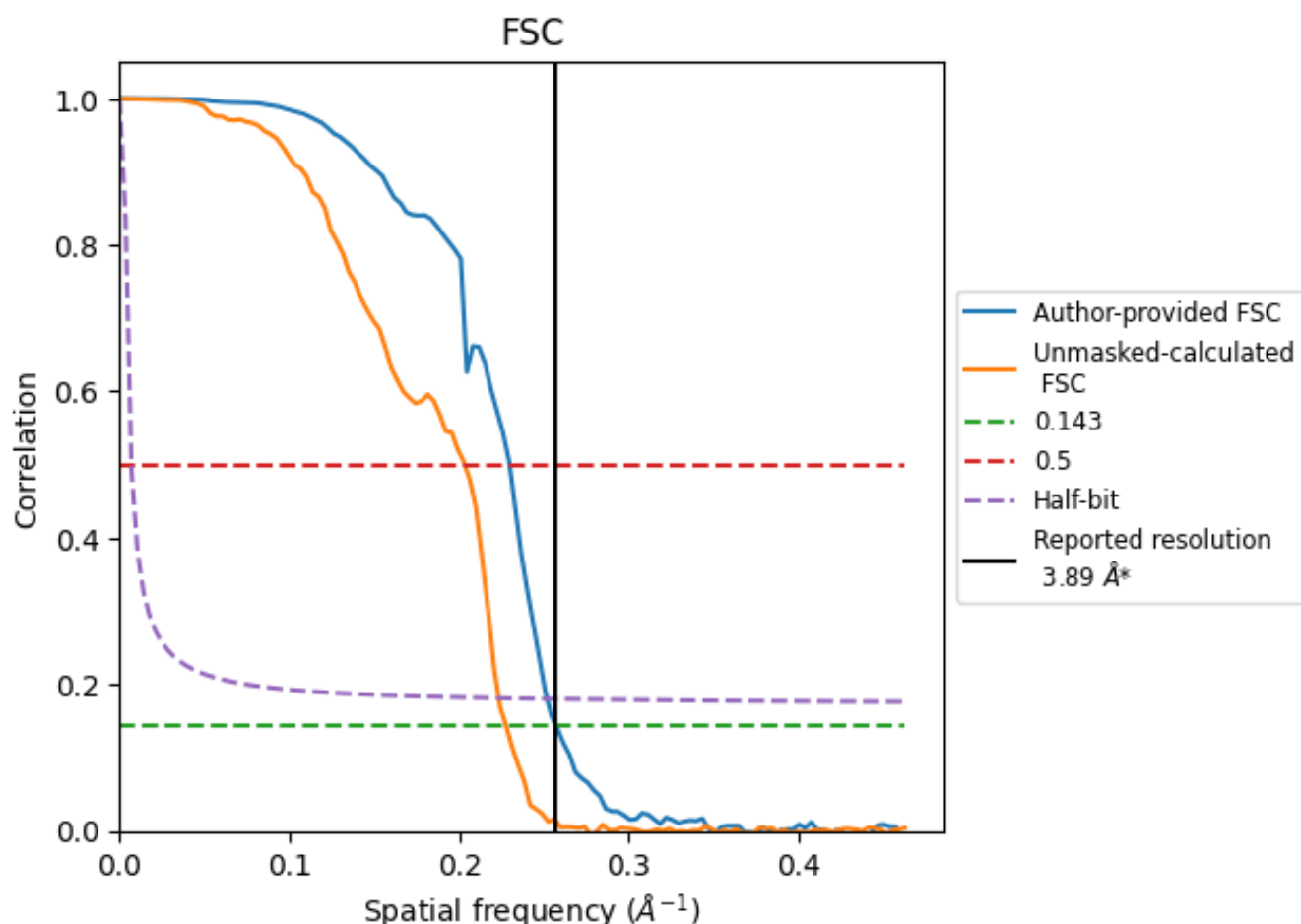


*Reported resolution corresponds to spatial frequency of 0.257 Å⁻¹

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 0.257 \AA^{-1}

8.2 Resolution estimates [i](#)

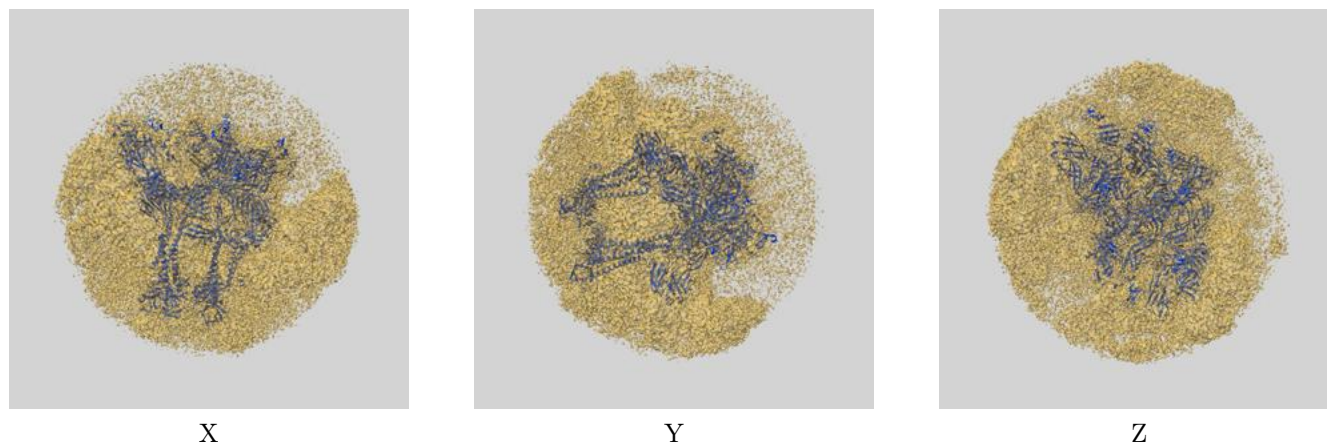
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.89	4.35	3.97
Unmasked-calculated*	4.39	4.92	4.48

*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 4.39 differs from the reported value 3.89 by more than 10 %

9 Map-model fit [i](#)

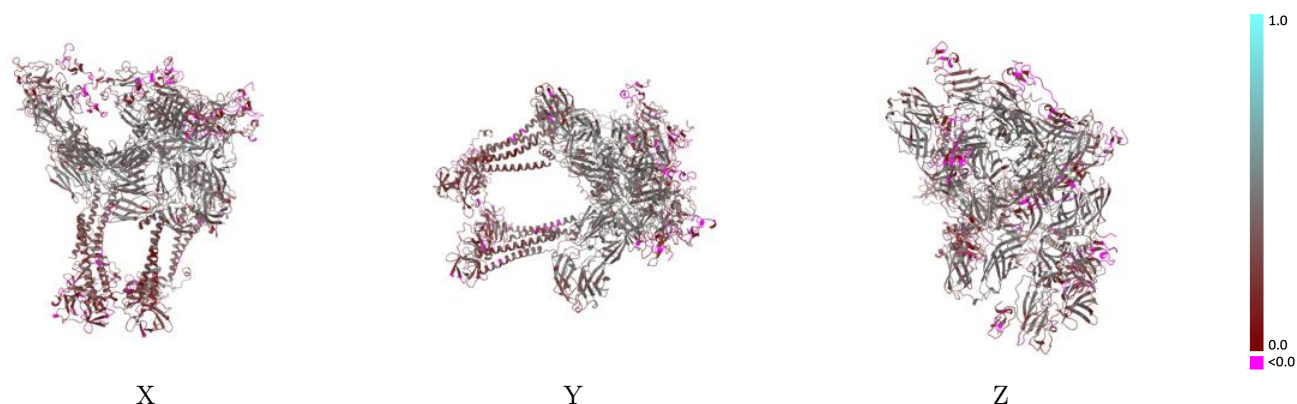
This section contains information regarding the fit between EMDB map EMD-42190 and PDB model 8UFB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



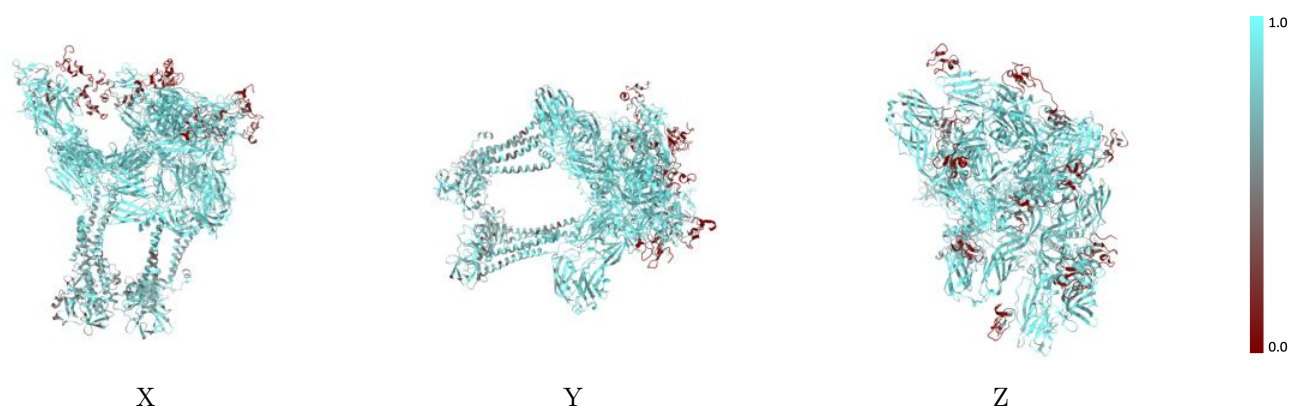
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



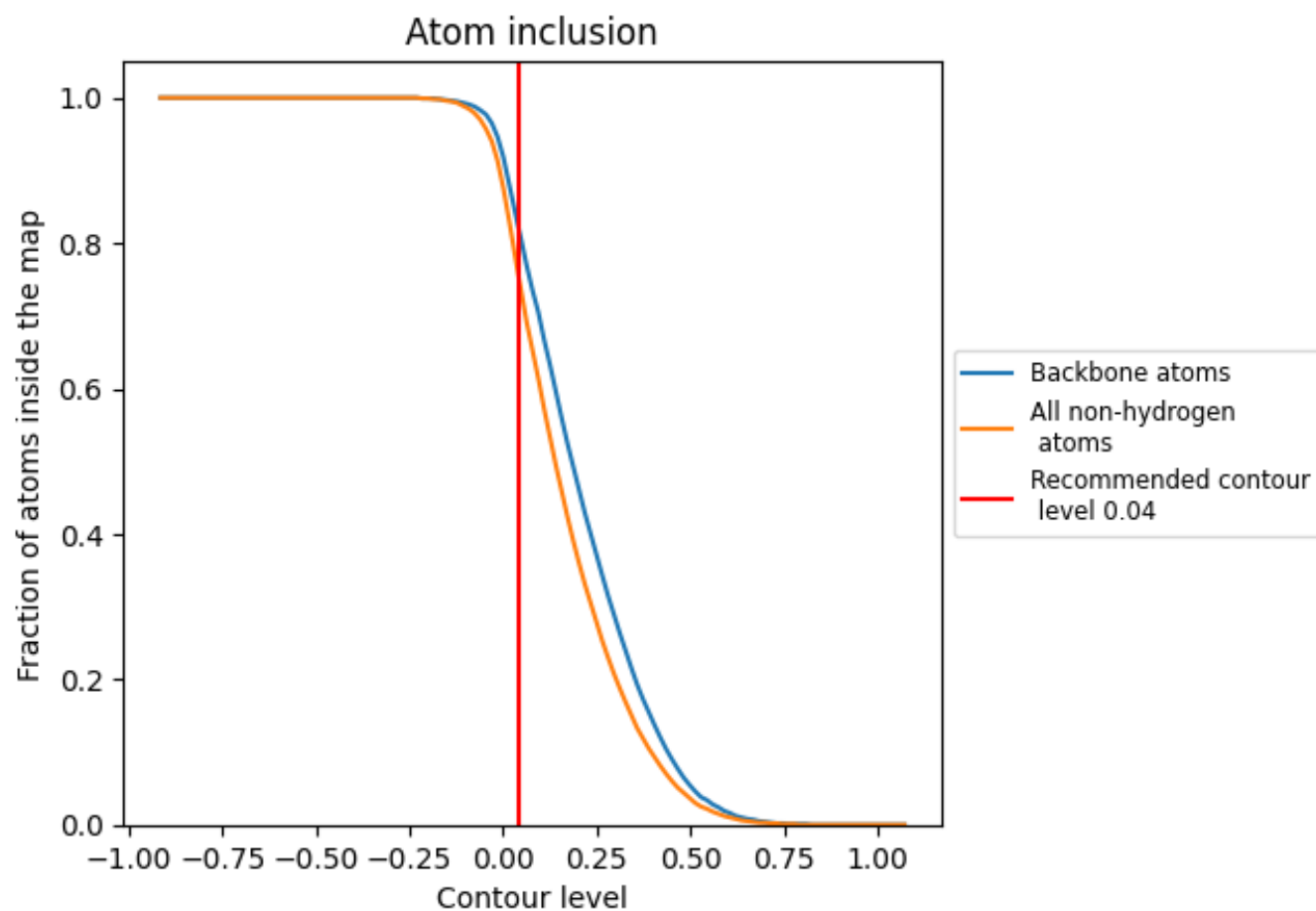
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 76% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7570	 0.3360
A	 0.8370	 0.3910
B	 0.8210	 0.3580
C	 0.6440	 0.1830
D	 0.8520	 0.4060
E	 0.8360	 0.3840
F	 0.6570	 0.2060
G	 0.8380	 0.3810
H	 0.8440	 0.3850
I	 0.7140	 0.2370
J	 0.8370	 0.3920
K	 0.8460	 0.3950
L	 0.7240	 0.2360
R	 0.1640	 0.1160
S	 0.2150	 0.1610
T	 0.2970	 0.1220
U	 0.2380	 0.1640
V	 0.3130	 0.1270
W	 0.2120	 0.0640
X	 0.1950	 0.1060
Y	 0.1300	 0.0630

