



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:46 AM UTC

PDB ID : 8TVR / pdb_00008tvr
EMDB ID : EMD-41649
Title : In situ cryo-EM structure of bacteriophage P22 tail hub protein: tailspike protein complex at 2.8Å resolution
Authors : Iglesias, S.; Cingolani, G.; Feng-Hou, C.
Deposited on : 2023-08-18
Resolution : 2.80 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:

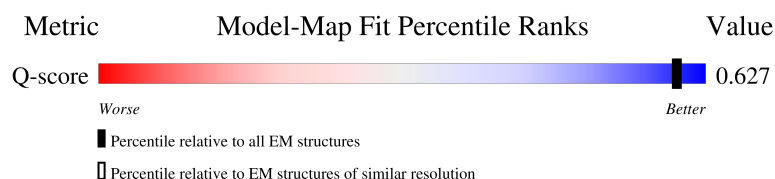
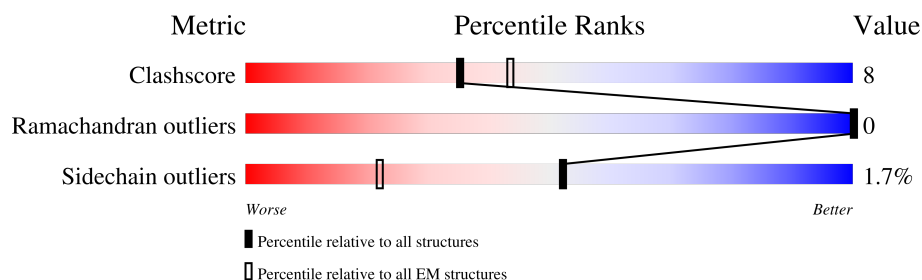
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.80 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.



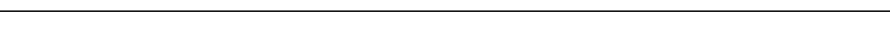
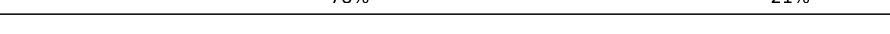
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	667	
1	B	667	
1	C	667	
1	D	667	

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Mol	Chain	Length	Quality of chain
1	E	667	 14% 82%
1	F	667	 15% 82%
1	H	667	 15% 82%
1	I	667	 13% 5% 82%
1	J	667	 15% 82%
1	L	667	 14% 82%
1	M	667	 13% 82%
1	N	667	 15% 82%
1	P	667	 15% 82%
1	Q	667	 14% 82%
1	R	667	 15% 82%
1	V	667	 15% 82%
1	W	667	 14% 82%
1	X	667	 15% 82%
2	G	472	 78% 21%
2	K	472	 74% 25%
2	O	472	 74% 25%
2	S	472	 76% 23%
2	T	472	 79% 20%
2	Y	472	 77% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38532 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 Tail spike protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	B	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	C	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	D	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	E	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	F	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	H	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	I	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	J	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	L	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	M	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	N	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	P	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	Q	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	R	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	V	118	Total 913	C 580	N 153	O 179	S 1	0	0
1	W	118	Total 913	C 580	N 153	O 179	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	X	118	Total	C	N	O	S	0	0
			913	580	153	179	1		

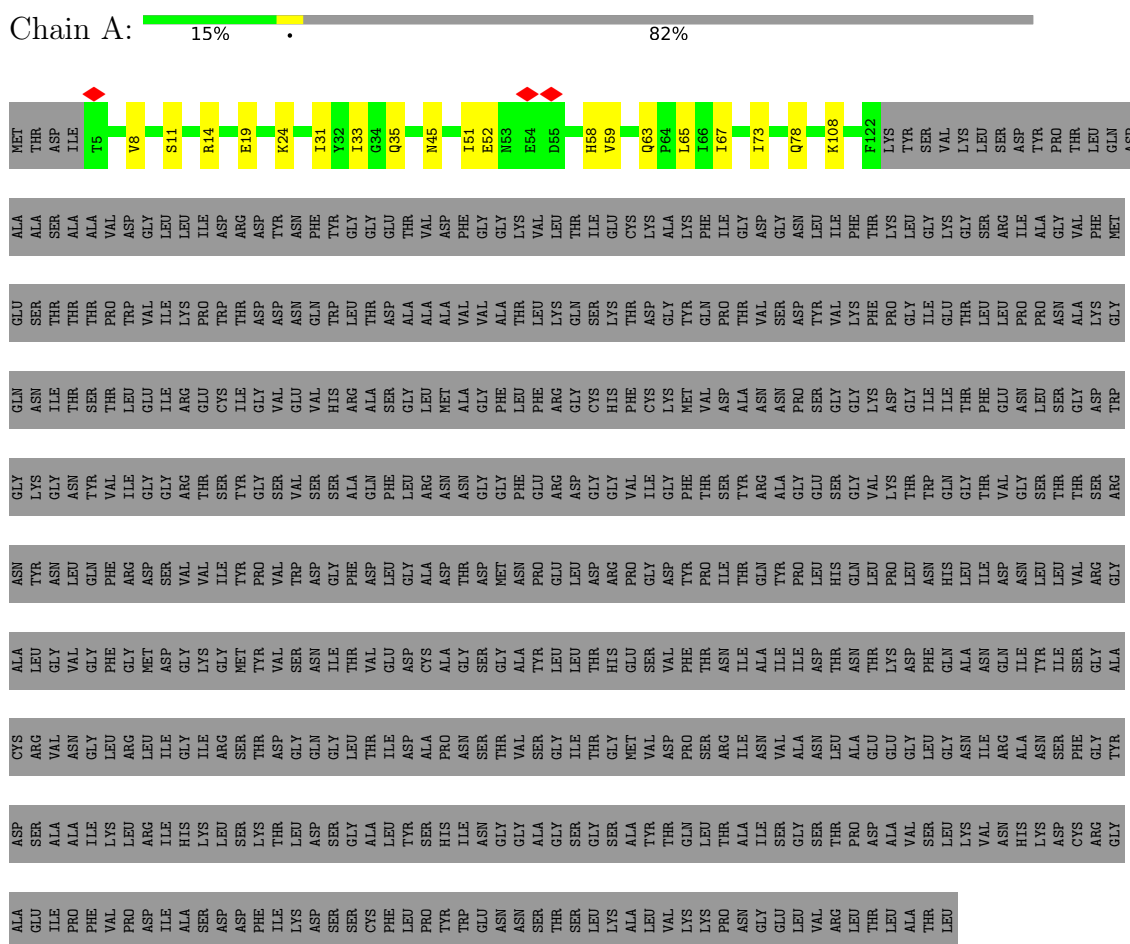
- Molecule 2 is a protein called Packaged DNA stabilization protein gp10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	G	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	K	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	O	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	T	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		
2	Y	471	Total	C	N	O	S	0	0
			3683	2325	631	709	18		

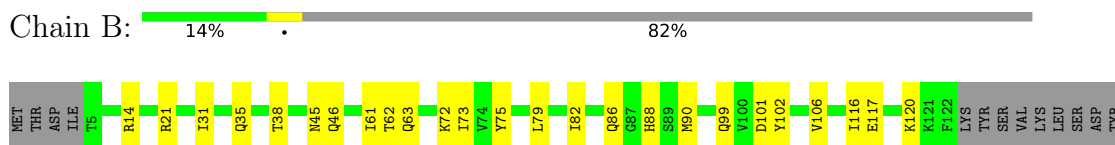
3 Residue-property plots

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: Tail spike protein



• Molecule 1: Tail spike protein



[illegible]

- Molecule 1: Tail spike protein

Chain C: 15% 2% 82%

[illegible]

● Molecule 1: Tail spike protein



MET	THR	ASP	ILE	T5	A6	N7	V8	R14	T18	A25	I31	T32	I33	Q34	Q35	N45	E54	D55	Q63	I73	G77	N90	I103	A118	D119	K120	K121	F122	LYS	TYR	SER	VAL	LYS	GLY	LEU	THR	ASP	PRO	THR	LEU	GLN	ASP	ALA	ALA	SER	THR	THR	ALA						
VAL	ASP	GLY	LEU	ILE	LEU	ILE	ASP	TYR	ASN	PHE	TYR	GLY	THR	VAL	PHE	GLY	LYS	VAL	THR	GLY	LYS	VAL	ILE	ASP	GLY	ASN	LEU	ILE	PHE	THR	LYS	PRO	GLY	ILE	GLY	LYS	THR	VAL	GLY	THR	LEU	VAL	PHE	GLN	ASP	GLY	ALA	ALA	SER	THR	THR			
PRO	TRP	VAL	ILE	LYS	PRO	TRP	THR	ASP	ASN	GLN	THR	ALA	ALA	ALA	VAL	ALA	THR	GLN	LYS	LYS	GLY	GLN	PRO	THR	VAL	THR	VAL	VAL	PHE	PRO	GLY	ILE	GLY	LYS	THR	THR	ALA	ALA	ASN	PRO	PRO	ASN	GLY	ALA	LYS	PHE	GLY	GLN	ASP	GLY	THR			
THR	LEU	GLY	ILE	ARG	GLY	CYS	GLY	VAL	GLU	VAL	ALA	GLY	LEU	MET	ALA	PHE	LEU	ARG	GLY	CYS	HIS	PHE	CYS	ALA	ASN	PRO	SER	GLY	GLY	LYS	ASP	GLY	ILE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
VAL	ILE	GLY	GLY	ARG	THR	SER	TYR	SER	VAL	SER	LEU	PHE	VAL	ASN	GLY	PHE	THR	ARG	GLY	GLY	ILE	VAL	VAL	ARG	ASN	GLY	GLY	SER	VAL	LYS	ASP	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
PHE	ARG	ASP	SER	VAL	VAL	ILE	THR	PRO	THR	ASP	LEU	GLY	ALA	ASN	THR	MET	ASP	GLY	ASP	PRO	GLY	ILE	THR	ARG	GLN	THR	PRO	GLY	GLN	VAL	LYS	PRO	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
PHE	GLY	MET	ASP	GLY	VAL	GLY	THR	VAL	ASN	THR	ASP	GLY	ALA	ALA	GLY	GLY	ALA	ALA	THR	HIS	GLY	THR	ILE	THR	GLN	THR	THR	THR	THR	THR	LYS	ASP	PHE	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
LEU	ARG	ILE	ILE	GLY	ILE	ARG	SER	THR	VAL	THR	ASP	ILE	ALA	PRO	SER	VAL	SER	GLY	THR	GLU	THR	ARG	ILE	ASN	VAL	VAL	ASN	ALA	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	
LYS	LEU	ARG	ILE	HIS	LEU	ARG	SER	THR	THR	ASP	THR	ASP	SER	HIS	TRP	ILE	ASN	GLY	THR	GLY	THR	THR	ILE	ALA	ILE	THR	SER	THR	THR	PRO	ASP	GLY	VAL	SER	SER	GLY	LEU	LYS	VAL	ASN	HIS	LYS	ASP	CYS	ARG	GLY	ALA	GLU	ILE	PRO	PHE	ILE		
VAL	PRO	ASP	ILE	ALA	SER	ASP	PHE	ILE	LYS	LEU	LEU	LEU	PHE	TRP	GLU	ASN	GLY	ASN	GLY	GLY	ALA	ALA	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY

● Molecule 1: Tail spike protein



THR	ASP	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	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: Tail spike protein



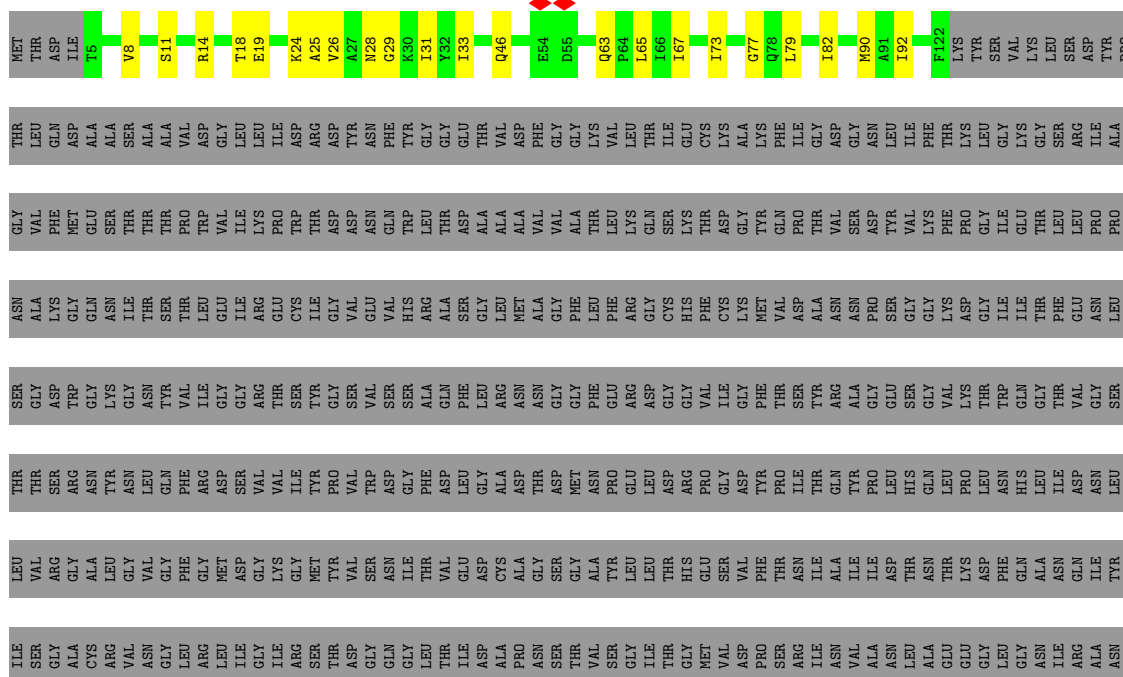
GLY	ILE	ASN	ALA	GLN	ARG	ASN	VAL	ASP	MET
GLU	SER	VAL	ILE	TYR	ALA	TYR	SER	GLY	THR
LEU	GLY	ALA	ILE	PRO	GLY	PRO	ASP	ASN	ASP
VAL	SER	ASN	ASP	LEU	GLU	SER	TYR	ILE	ILE
ARG	THR	LEU	THR	HIS	SER	GLY	VAL	ILE	T5
LEU	PRO	ALA	ASN	GLN	GLY	GLY	LYS	PHE	V10
THR	ASP	GLU	THR	LEU	VAL	LYS	PHE	THR	
LEU	ALA	GLU	LYS	PRO	LYS	ASP	PRO	LYS	R14
ALA	VAL	GLY	ASP	LEU	THR	LEU	GLY	SER	P15
THR	SER	LEU	PHE	ASN	TRP	ILE	ILE	VAL	
LEU	LEU	GLY	GLN	HIS	GLN	ILE	GLU	LYS	S20
	LYS	ASN	ALA	LEU	GLY	THR	THR	GLY	R21
	VAL	ILE	ASN	ILE	THR	PHE	LEU	SER	
	ASN	ALA	GLN	ASP	VAL	GLU	LEU	ARG	I31
	HIS	ALA	ILE	ASN	GLY	ASN	PRO	ASP	
	LYS	ASN	TYR	LEU	SER	LEU	PRO	ALA	Q35
	ASP	SER	ILE	LEU	THR	SER	ASN	GLY	
	CYS	PHE	SER	VAL	THR	GLY	ALA	VAL	T38
	ARG	GLY	GLY	ARG	SER	ASP	LYS	PHE	
	GLY	TYR	ALA	GLY	ARG	TRP	GLY	MET	Q46
	ALA	ASP	CYS	ALA	ASN	GLY	GLN	GLU	
	GLU	SER	ARG	LEU	TYR	LYS	ASN	SER	D55
	ILE	ALA	VAL	VAL	LEU	GLY	ILE	THR	G56
	PRO	ALA	ASN	GLY	ASN	ASN	THR	ALA	S57
	PHE	ILE	GLY	GLY	GLN	TYR	SER	THR	
	VAL	LYS	LEU	PHE	PHE	VAL	THR	PRO	I61
	PRO	LEU	ARG	GLY	ARG	ILE	LEU	ASP	T62
	ASP	ILE	LEU	ASP	MET	GLY	GLU	VAL	Q63
	ILE	ILE	ILE	ASP	SER	GLY	ILE	ILE	
	ALA	HIS	GLY	GLY	VAL	ARG	ARG	LYS	I67
	SER	LYS	ILE	LYS	VAL	THR	GLU	PRO	
	ASP	LEU	ARG	GLY	ILE	SER	CYS	TRP	
	ASP	SER	ILE	GLY	THR	TYR	ILE	ASP	K72
	PHE	SER	SER	THR	PHE	GLY	GLY	THR	I73
	ILE	THR	THR	VAL	PRO	VAL	VAL	TYR	V74
	LYS	LEU	GLY	ASP	TRP	SER	GLU	ASN	Y75
	ASP	ASP	GLN	SER	ASP	VAL	GLY	ASN	
	SER	SER	GLY	LEU	GLY	SER	VAL	GLN	L79
	SER	GLY	ILE	THR	PHE	ALA	HIS	THR	
	CYS	ALA	THR	VAL	ASP	PHE	GLN	ASP	I82
	PHE	LEU	ILE	GLU	LEU	PHE	SER	THR	V83
	LEU	TYR	ASP	ASP	GLY	LEU	GLY	ALA	T84
	PRO	SER	ILE	CYS	THR	ARG	GLY	VAL	V85
	TYR	HIS	PRO	ALA	ASP	ASN	LEU	ALA	Q86
	TRP	ILE	ASN	GLY	THR	ASN	ALA	PHE	G87
	GLU	ASN	ASN	SER	ASP	GLY	GLY	VAL	H88
	ASN	GLY	THR	GLY	MET	GLY	PHE	ALA	S89
	ASN	GLY	VAL	ASP	ASN	PHE	LEU	THR	M90
	SER	ALA	SER	TYR	PRO	PHE	LEU	VAL	
	SER	GLY	GLY	LEU	LEU	GLU	PHE	VAL	D94
	SER	SER	ILE	LEU	LEU	ARG	GLY	LYS	A95
	LEU	GLY	THR	THR	THR	ASP	CYS	SER	N96
	LYS	SER	GLY	HIS	ARG	GLY	HIS	LYS	
	ALA	ALA	MET	GLU	PRO	VAL	PHE	THR	D101
	LEU	TYR	VAL	SER	ASP	ILE	CYS	LYS	Y102
	VAL	THR	ASP	VAL	GLY	GLY	LYS	ASP	
	LYS	GLN	PRO	PHE	TYR	PHE	GLY	GLY	N105
	LYS	LEU	PRO	THR	PRO	THR	VAL	GLN	V106
	ASN	THR	SER	ILE	ASN	THR	ASP	THR	I107
	PRO	ALA	ILE	THR	THR	SER	ASP	PRO	K108
	ASN	ALA	THR	ILE	THR	TYR	ALA	THR	

- Molecule 1: Tail spike protein





- Molecule 1: Tail spike protein





- Molecule 1: Tail spike protein

[illegible]

- Molecule 1: Tail spike protein

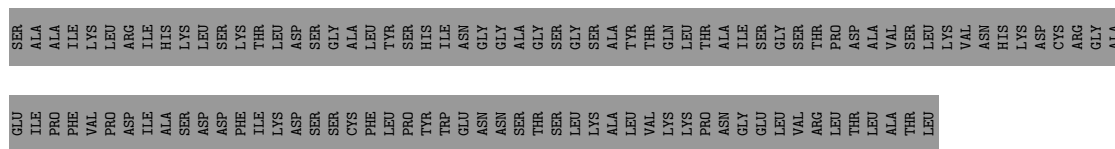


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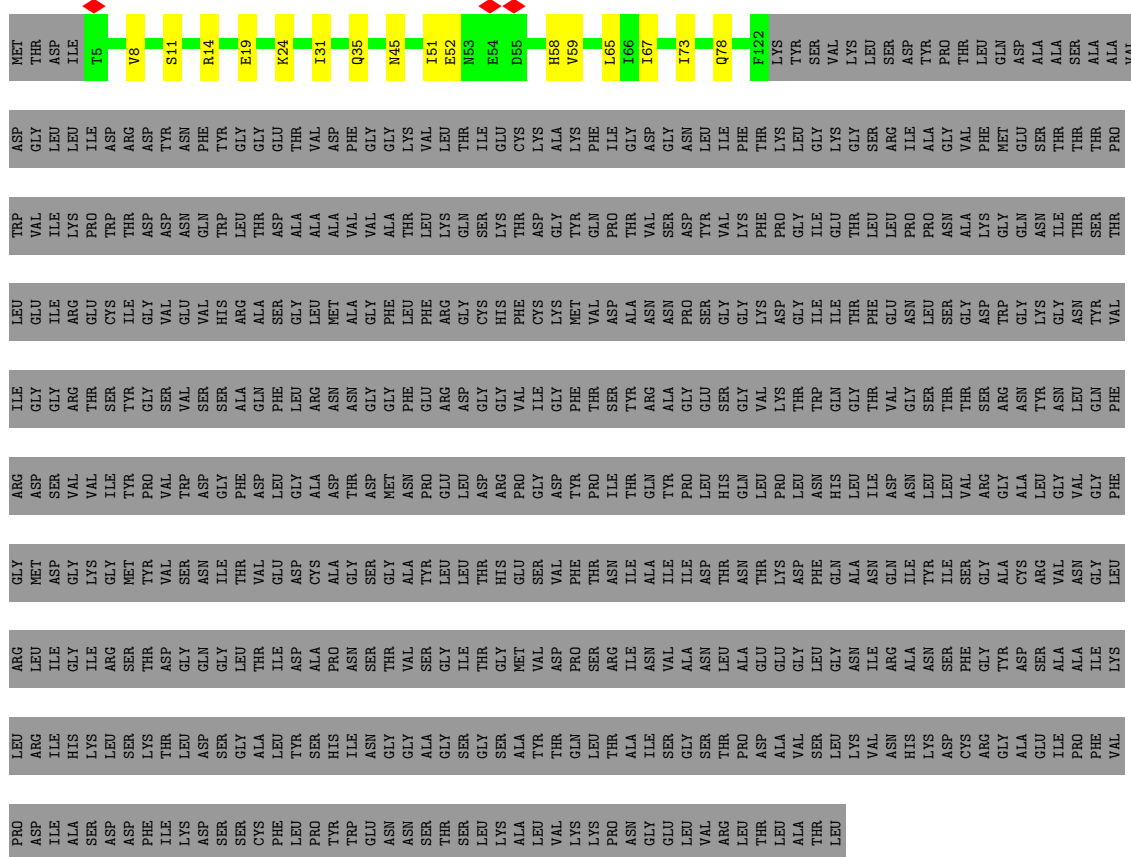
● Molecule 1: Tail spike protein



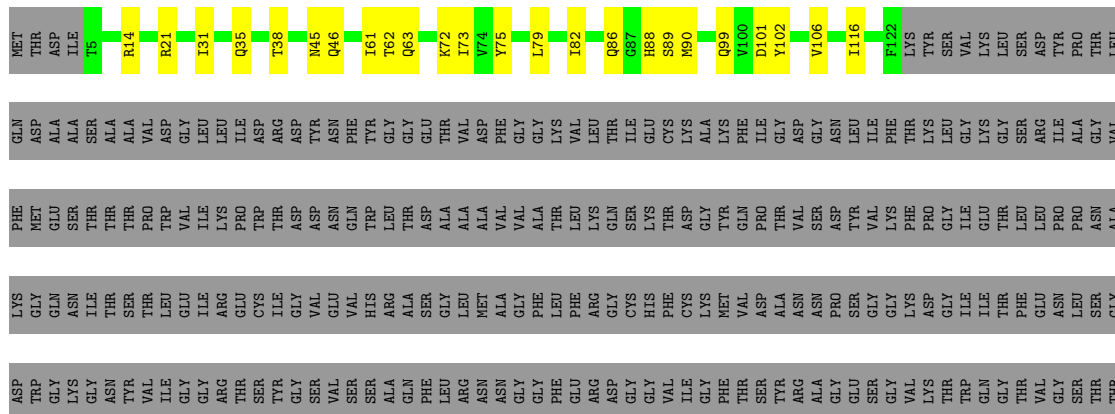
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- Molecule 1: Tail spike protein



- Molecule 1: Tail spike protein



[illegible]

- Molecule 1: Tail spike protein

Chain X: 15% 82%

[illegible]

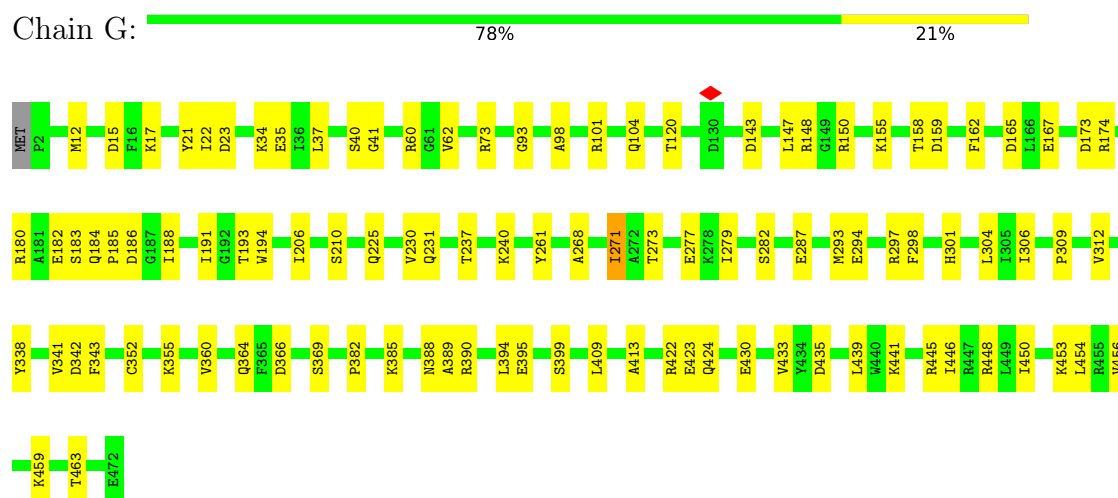
- Molecule 2: Packaged DNA stabilization protein gp10

Chain S: 76% 23%

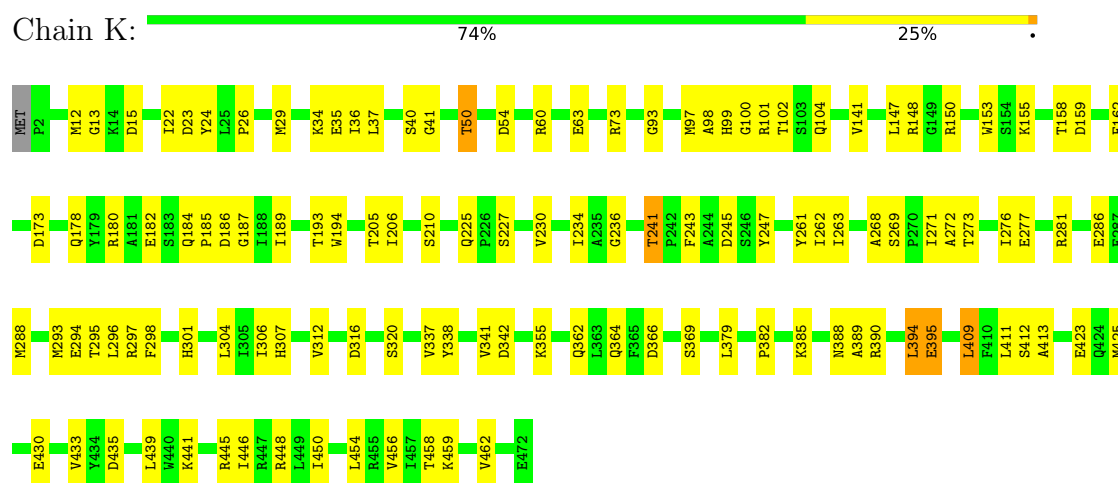
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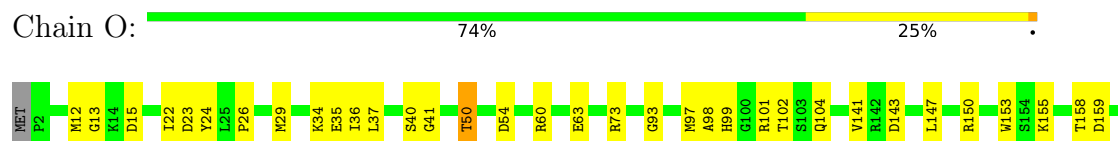
- Molecule 2: Packaged DNA stabilization protein gp10

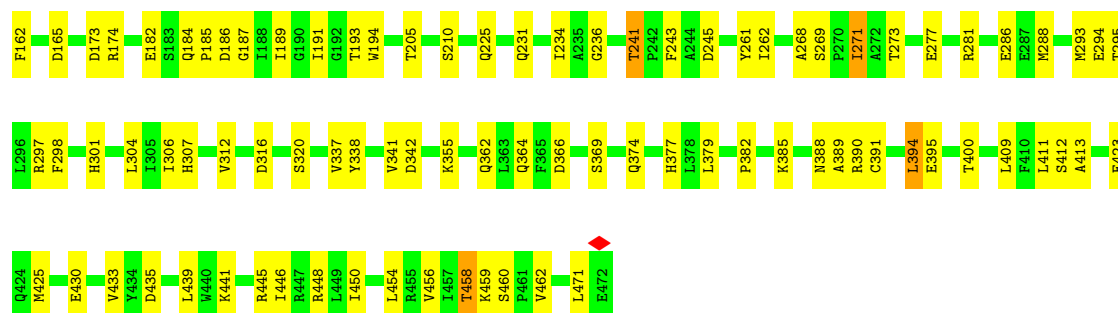


- Molecule 2: Packaged DNA stabilization protein gp10

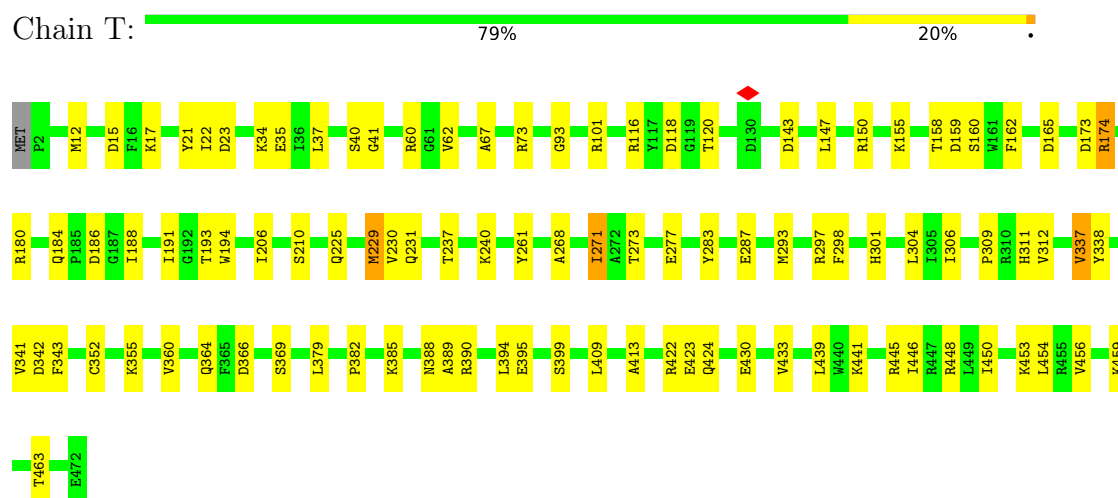


- Molecule 2: Packaged DNA stabilization protein gp10

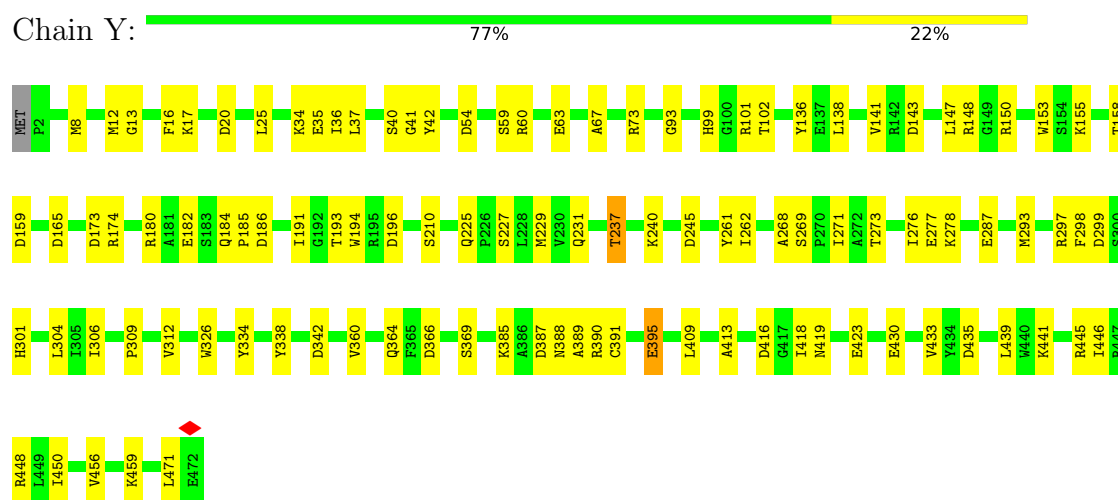




• Molecule 2: Packaged DNA stabilization protein gp10



• Molecule 2: Packaged DNA stabilization protein gp10



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	38155	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.08	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	35.452	Depositor
Minimum map value	-27.985	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.5	Depositor
Map size ($\text{\AA}$)	512.9599, 512.9599, 512.9599	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.165818, 1.165818, 1.165818	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/931	0.29	0/1270
1	B	0.15	0/931	0.33	0/1270
1	C	0.15	0/931	0.31	0/1270
1	D	0.11	0/931	0.29	0/1270
1	E	0.13	0/931	0.29	0/1270
1	F	0.12	0/931	0.30	0/1270
1	H	0.10	0/931	0.28	0/1270
1	I	0.12	0/931	0.29	0/1270
1	J	0.14	0/931	0.30	0/1270
1	L	0.10	0/931	0.29	0/1270
1	M	0.13	0/931	0.28	0/1270
1	N	0.14	0/931	0.30	0/1270
1	P	0.11	0/931	0.29	0/1270
1	Q	0.15	0/931	0.30	0/1270
1	R	0.12	0/931	0.29	0/1270
1	V	0.10	0/931	0.29	0/1270
1	W	0.13	0/931	0.29	0/1270
1	X	0.15	0/931	0.33	0/1270
2	G	0.13	0/3764	0.34	0/5097
2	K	0.12	0/3764	0.33	0/5097
2	O	0.12	0/3764	0.32	0/5097
2	S	0.12	0/3764	0.34	0/5097
2	T	0.12	0/3764	0.32	0/5097
2	Y	0.12	0/3764	0.34	0/5097
All	All	0.12	0/39342	0.32	0/53442

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 ⓘ

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	913	0	903	13	0
1	B	913	0	903	18	0
1	C	913	0	903	10	0
1	D	913	0	903	12	0
1	E	913	0	903	16	0
1	F	913	0	903	10	0
1	H	913	0	903	21	0
1	I	913	0	903	24	0
1	J	913	0	903	12	0
1	L	913	0	903	21	0
1	M	913	0	903	21	0
1	N	913	0	903	12	0
1	P	913	0	903	12	0
1	Q	913	0	903	16	0
1	R	913	0	903	11	0
1	V	913	0	903	11	0
1	W	913	0	903	18	0
1	X	913	0	903	10	0
2	G	3683	0	3590	68	0
2	K	3683	0	3590	82	0
2	O	3683	0	3590	80	0
2	S	3683	0	3590	71	0
2	T	3683	0	3590	66	0
2	Y	3683	0	3590	69	0
All	All	38532	0	37794	603	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 (603) 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:G:395:GLU:HG2	2:G:439:LEU:HD13	1.67	0.76
2:T:395:GLU:HG2	2:T:439:LEU:HD13	1.67	0.76
2:S:409:LEU:HD12	2:S:456:VAL:HG22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:262:ILE:HD12	2:S:271:ILE:HG13	1.68	0.76
2:K:395:GLU:HG2	2:K:439:LEU:HD13	1.68	0.75
2:O:395:GLU:HG2	2:O:439:LEU:HD13	1.68	0.75
2:O:73:ARG:NH2	2:O:342:ASP:O	2.20	0.75
2:K:73:ARG:NH2	2:K:342:ASP:O	2.20	0.75
1:W:31:ILE:HD12	1:W:73:ILE:HD11	1.69	0.75
2:K:158:THR:O	2:K:180:ARG:NH2	2.20	0.74
2:O:385:LYS:HB2	2:Y:37:LEU:HD13	1.69	0.73
2:Y:395:GLU:HG2	2:Y:439:LEU:HD13	1.71	0.73
1:B:31:ILE:HD12	1:B:73:ILE:HD11	1.69	0.73
2:Y:262:ILE:HD12	2:Y:271:ILE:HG13	1.70	0.72
2:S:298:PHE:O	2:S:301:HIS:HB2	1.89	0.72
2:G:422:ARG:NH2	2:G:424:GLN:OE1	2.23	0.72
2:T:422:ARG:NH2	2:T:424:GLN:OE1	2.23	0.72
2:S:165:ASP:OD2	2:S:174:ARG:NH1	2.23	0.72
2:O:165:ASP:OD2	2:O:174:ARG:NH1	2.24	0.71
2:Y:298:PHE:O	2:Y:301:HIS:HB2	1.89	0.71
2:O:409:LEU:HD12	2:O:456:VAL:HG22	1.71	0.71
2:O:231:GLN:NE2	2:Y:194:TRP:O	2.24	0.70
2:O:194:TRP:O	2:T:231:GLN:NE2	2.24	0.70
2:O:37:LEU:HD13	2:T:385:LYS:HB2	1.74	0.70
2:G:165:ASP:OD2	2:G:174:ARG:NH1	2.26	0.69
1:I:116:ILE:HD12	1:I:116:ILE:H	1.57	0.69
2:Y:165:ASP:OD2	2:Y:174:ARG:NH1	2.24	0.69
2:G:231:GLN:NE2	2:K:194:TRP:O	2.24	0.69
2:G:385:LYS:HB2	2:K:37:LEU:HD13	1.73	0.69
2:S:73:ARG:NH2	2:S:342:ASP:O	2.26	0.69
2:T:293:MET:HE3	2:T:304:LEU:HD11	1.76	0.68
2:Y:73:ARG:NH2	2:Y:342:ASP:O	2.26	0.68
2:K:409:LEU:HD12	2:K:456:VAL:HG22	1.75	0.68
2:G:293:MET:HE3	2:G:304:LEU:HD11	1.76	0.68
2:T:159:ASP:OD1	2:T:184:GLN:NE2	2.26	0.68
2:O:98:ALA:O	2:O:104:GLN:NE2	2.26	0.67
2:K:98:ALA:O	2:K:104:GLN:NE2	2.27	0.67
2:Y:439:LEU:HD21	2:Y:441:LYS:HE2	1.74	0.67
1:H:31:ILE:HG13	1:H:67:ILE:HD11	1.76	0.67
2:K:298:PHE:O	2:K:301:HIS:HB2	1.95	0.67
1:L:31:ILE:HG13	1:L:67:ILE:HD11	1.77	0.67
2:S:186:ASP:OD1	2:T:101:ARG:NH1	2.28	0.66
1:J:18:THR:HA	1:J:25:ALA:HA	1.77	0.66
2:S:159:ASP:OD1	2:S:184:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:ILE:HD12	1:E:73:ILE:HD11	1.77	0.66
1:Q:31:ILE:HD12	1:Q:73:ILE:HD11	1.77	0.66
2:S:231:GLN:NE2	2:T:194:TRP:O	2.29	0.66
1:N:18:THR:HA	1:N:25:ALA:HA	1.76	0.66
2:O:29:MET:HE1	2:O:462:VAL:HB	1.78	0.65
2:G:150:ARG:NH2	2:G:173:ASP:OD1	2.29	0.65
2:G:194:TRP:O	2:Y:231:GLN:NE2	2.29	0.65
2:G:297:ARG:NH2	2:Y:277:GLU:OE1	2.25	0.65
2:G:186:ASP:OD2	2:K:101:ARG:NH1	2.30	0.65
2:G:159:ASP:OD1	2:G:184:GLN:NE2	2.29	0.65
2:O:389:ALA:HB3	2:O:446:ILE:HD12	1.78	0.65
1:W:14:ARG:HB3	1:W:72:LYS:HD3	1.78	0.65
2:S:101:ARG:NH1	2:K:186:ASP:OD1	2.30	0.65
1:H:28:ASN:HA	1:H:67:ILE:O	1.97	0.65
2:O:298:PHE:O	2:O:301:HIS:HB2	1.95	0.65
2:Y:388:ASN:OD1	2:Y:445:ARG:NH2	2.30	0.65
2:K:159:ASP:OD1	2:K:184:GLN:NE2	2.29	0.64
2:O:159:ASP:OD1	2:O:184:GLN:NE2	2.30	0.64
2:G:23:ASP:OD1	2:K:34:LYS:NZ	2.29	0.64
2:O:34:LYS:NZ	2:T:23:ASP:OD1	2.29	0.64
1:L:28:ASN:HA	1:L:67:ILE:O	1.97	0.64
2:K:29:MET:HE1	2:K:462:VAL:HB	1.77	0.64
2:O:458:THR:HG22	2:O:460:SER:H	1.61	0.64
2:O:101:ARG:NH1	2:T:186:ASP:OD2	2.30	0.64
2:S:150:ARG:NH2	2:S:173:ASP:OD1	2.30	0.64
1:B:14:ARG:HB3	1:B:72:LYS:HD3	1.80	0.63
2:Y:150:ARG:NH2	2:Y:173:ASP:OD1	2.30	0.63
2:S:388:ASN:OD1	2:S:445:ARG:NH2	2.30	0.63
2:S:299:ASP:OD1	2:K:281:ARG:NH1	2.32	0.63
2:G:73:ARG:NH2	2:G:342:ASP:O	2.29	0.63
1:J:52:GLU:OE2	1:J:58:HIS:NE2	2.32	0.63
2:K:409:LEU:HD11	2:K:454:LEU:HG	1.79	0.63
2:T:409:LEU:HD12	2:T:456:VAL:HG22	1.81	0.63
2:O:281:ARG:NH1	2:Y:299:ASP:OD1	2.32	0.63
2:Y:20:ASP:OD2	2:Y:278:LYS:NZ	2.32	0.63
1:H:31:ILE:HD12	1:H:73:ILE:HD11	1.80	0.62
2:T:150:ARG:NH2	2:T:173:ASP:OD1	2.31	0.62
1:L:31:ILE:HD12	1:L:73:ILE:HD11	1.80	0.62
1:D:33:ILE:O	1:D:63:GLN:NE2	2.32	0.62
1:P:8:VAL:HG11	1:Q:86:GLN:HA	1.81	0.62
2:T:165:ASP:OD2	2:T:174:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:101:ARG:NH1	2:Y:186:ASP:OD1	2.31	0.62
2:S:20:ASP:OD2	2:S:278:LYS:NZ	2.32	0.62
2:S:37:LEU:HD13	2:K:385:LYS:HB2	1.81	0.62
1:D:8:VAL:HG11	1:E:86:GLN:HA	1.81	0.62
2:S:277:GLU:OE1	2:T:297:ARG:NH2	2.25	0.62
2:O:186:ASP:OD1	2:Y:101:ARG:NH1	2.31	0.61
2:G:409:LEU:HD12	2:G:456:VAL:HG22	1.82	0.61
2:O:150:ARG:NH2	2:O:173:ASP:OD1	2.34	0.61
1:V:19:GLU:HG3	1:V:24:LYS:HG3	1.82	0.61
1:F:18:THR:HA	1:F:25:ALA:HA	1.83	0.61
1:N:52:GLU:OE1	1:N:58:HIS:NE2	2.33	0.61
2:S:395:GLU:HB2	2:S:439:LEU:HD13	1.83	0.61
2:G:155:LYS:HE2	2:G:158:THR:HG21	1.81	0.61
2:G:180:ARG:NH2	2:G:182:GLU:OE2	2.33	0.61
2:O:241:THR:HG21	2:O:294:GLU:HA	1.82	0.61
1:H:19:GLU:HG3	1:H:24:LYS:HG3	1.82	0.61
1:A:8:VAL:HG11	1:B:86:GLN:HA	1.83	0.61
1:H:8:VAL:HG11	1:I:86:GLN:HA	1.82	0.60
1:V:8:VAL:HG11	1:W:86:GLN:HA	1.82	0.60
2:Y:364:GLN:NE2	2:Y:366:ASP:OD1	2.31	0.60
1:L:90:MET:HE2	1:N:10:VAL:HG13	1.82	0.60
1:L:8:VAL:HG11	1:M:86:GLN:HA	1.82	0.60
2:T:160:SER:OG	2:T:180:ARG:NH1	2.34	0.60
2:O:23:ASP:OD1	2:Y:34:LYS:NZ	2.35	0.59
2:T:155:LYS:HE2	2:T:158:THR:HG21	1.84	0.59
2:T:389:ALA:HB3	2:T:446:ILE:HD12	1.85	0.59
2:K:241:THR:HG21	2:K:294:GLU:HA	1.83	0.59
1:M:31:ILE:HD12	1:M:73:ILE:HD11	1.84	0.59
1:I:14:ARG:HG2	1:I:79:LEU:HD13	1.84	0.59
1:I:31:ILE:HD12	1:I:73:ILE:HD11	1.84	0.59
1:M:14:ARG:HG2	1:M:79:LEU:HD13	1.85	0.59
2:G:364:GLN:NE2	2:G:366:ASP:OD1	2.31	0.59
1:Q:54:GLU:OE1	2:T:453:LYS:NZ	2.26	0.59
1:E:112:ASP:OD2	1:E:115:SER:OG	2.20	0.59
2:O:293:MET:HG2	2:O:306:ILE:HG12	1.84	0.59
1:A:19:GLU:HG3	1:A:24:LYS:HG3	1.84	0.59
2:O:435:ASP:OD1	2:T:448:ARG:NH2	2.28	0.58
2:Y:159:ASP:OD1	2:Y:184:GLN:NE2	2.35	0.58
2:Y:389:ALA:HB3	2:Y:446:ILE:HD12	1.85	0.58
2:K:150:ARG:NH2	2:K:173:ASP:OD1	2.35	0.58
1:N:49:VAL:HG23	1:N:61:ILE:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:MET:HE2	1:J:10:VAL:HG13	1.85	0.58
2:S:293:MET:HE3	2:S:304:LEU:HD11	1.86	0.58
2:S:180:ARG:HG2	2:S:182:GLU:HG2	1.86	0.58
2:T:73:ARG:NH2	2:T:342:ASP:O	2.30	0.58
2:Y:143:ASP:HB3	2:Y:191:ILE:HG22	1.86	0.57
2:G:12:MET:HB3	2:G:382:PRO:HA	1.86	0.57
2:Y:430:GLU:HB3	2:Y:433:VAL:HB	1.86	0.57
2:S:143:ASP:HB3	2:S:191:ILE:HG22	1.86	0.57
2:K:293:MET:HG2	2:K:306:ILE:HG12	1.84	0.57
2:O:448:ARG:NH2	2:Y:435:ASP:OD1	2.25	0.57
2:T:12:MET:HB3	2:T:382:PRO:HA	1.86	0.57
2:S:389:ALA:HB3	2:S:446:ILE:HD12	1.87	0.57
1:B:116:ILE:HD12	1:B:116:ILE:H	1.69	0.57
2:O:388:ASN:OD1	2:O:445:ARG:NH2	2.34	0.57
1:R:16:ILE:HD11	1:R:72:LYS:HE2	1.87	0.57
1:L:33:ILE:O	1:L:63:GLN:NE2	2.38	0.57
1:R:99:GLN:NE2	2:T:423:GLU:O	2.37	0.57
1:M:116:ILE:H	1:M:116:ILE:HD12	1.69	0.57
1:F:99:GLN:NE2	2:G:423:GLU:O	2.38	0.57
2:G:159:ASP:HB2	2:K:101:ARG:HH12	1.69	0.57
2:K:389:ALA:HB3	2:K:446:ILE:HD12	1.87	0.57
2:S:287:GLU:HB3	2:S:309:PRO:HG3	1.86	0.57
2:S:430:GLU:HB3	2:S:433:VAL:HB	1.85	0.57
2:G:17:LYS:HA	2:G:17:LYS:HE2	1.87	0.57
2:O:430:GLU:HB3	2:O:433:VAL:HB	1.87	0.57
2:Y:158:THR:O	2:Y:180:ARG:NH2	2.38	0.57
2:O:101:ARG:HH12	2:T:159:ASP:HB2	1.70	0.56
2:K:430:GLU:HB3	2:K:433:VAL:HB	1.87	0.56
1:A:33:ILE:O	1:A:63:GLN:NE2	2.39	0.56
2:O:439:LEU:HD21	2:O:441:LYS:HE2	1.87	0.56
2:Y:293:MET:HE3	2:Y:304:LEU:HD11	1.86	0.56
2:G:389:ALA:HB3	2:G:446:ILE:HD12	1.86	0.56
1:H:33:ILE:O	1:H:63:GLN:NE2	2.38	0.56
2:O:36:ILE:HG23	2:T:12:MET:HE2	1.88	0.56
1:W:14:ARG:HG2	1:W:79:LEU:HD13	1.88	0.56
2:K:439:LEU:HD21	2:K:441:LYS:HE2	1.86	0.56
1:J:33:ILE:HG22	1:J:90:MET:HG3	1.87	0.56
1:F:55:ASP:OD1	1:F:55:ASP:N	2.39	0.56
2:K:34:LYS:H	2:K:41:GLY:HA2	1.71	0.56
1:F:16:ILE:HD11	1:F:72:LYS:HE2	1.87	0.55
2:G:12:MET:HE2	2:K:36:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:34:LYS:H	2:O:41:GLY:HA2	1.71	0.55
2:S:34:LYS:NZ	2:K:23:ASP:OD1	2.39	0.55
1:N:33:ILE:HG22	1:N:90:MET:HG3	1.87	0.55
2:O:413:ALA:HB1	2:O:450:ILE:HD11	1.88	0.55
1:P:118:ALA:HA	1:P:121:LYS:HG2	1.89	0.55
2:K:369:SER:HB3	2:K:459:LYS:HG2	1.89	0.55
2:T:17:LYS:HE2	2:T:17:LYS:HA	1.87	0.55
1:D:120:LYS:HD3	1:D:120:LYS:N	2.21	0.55
2:G:409:LEU:HD11	2:G:454:LEU:HG	1.89	0.55
2:T:293:MET:HG2	2:T:306:ILE:HG12	1.88	0.55
1:L:28:ASN:CA	1:L:67:ILE:O	2.55	0.55
1:H:28:ASN:CA	1:H:67:ILE:O	2.54	0.55
2:G:293:MET:HG2	2:G:306:ILE:HG12	1.88	0.54
2:K:388:ASN:OD1	2:K:445:ARG:NH2	2.35	0.54
1:P:120:LYS:HD3	1:P:120:LYS:N	2.22	0.54
2:K:390:ARG:HA	2:K:445:ARG:HA	1.88	0.54
1:B:73:ILE:HG21	1:B:82:ILE:HG13	1.88	0.54
1:D:118:ALA:HA	1:D:121:LYS:HG2	1.89	0.54
1:D:119:ASP:OD1	1:E:121:LYS:NZ	2.41	0.54
2:G:390:ARG:HA	2:G:445:ARG:HA	1.88	0.54
1:P:90:MET:HE3	1:P:103:ILE:HD13	1.89	0.54
1:W:116:ILE:H	1:W:116:ILE:HD12	1.71	0.54
2:O:50:THR:HG23	2:O:362:GLN:HG3	1.90	0.54
2:O:147:LEU:HB2	2:O:193:THR:HG21	1.89	0.54
2:S:147:LEU:HB2	2:S:193:THR:HG21	1.89	0.54
2:S:210:SER:OG	2:S:225:GLN:OE1	2.24	0.54
2:G:210:SER:OG	2:G:225:GLN:OE1	2.23	0.54
2:O:294:GLU:OE2	2:O:307:HIS:NE2	2.40	0.54
2:T:390:ARG:HA	2:T:445:ARG:HA	1.89	0.54
2:K:413:ALA:HB1	2:K:450:ILE:HD11	1.88	0.54
1:R:55:ASP:OD1	1:R:55:ASP:N	2.38	0.54
1:A:31:ILE:HB	1:A:65:LEU:HB2	1.89	0.54
1:D:90:MET:HE3	1:D:103:ILE:HD13	1.90	0.54
1:V:31:ILE:HB	1:V:65:LEU:HB2	1.89	0.54
2:Y:180:ARG:HG2	2:Y:182:GLU:HG2	1.90	0.54
2:O:369:SER:HB3	2:O:459:LYS:HG2	1.90	0.54
1:W:73:ILE:HG21	1:W:82:ILE:HG13	1.89	0.54
2:Y:147:LEU:HB2	2:Y:193:THR:HG21	1.89	0.54
1:R:18:THR:HA	1:R:25:ALA:HA	1.89	0.54
2:Y:369:SER:HB3	2:Y:459:LYS:HG2	1.91	0.53
2:S:369:SER:HB3	2:S:459:LYS:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:409:LEU:HD11	2:T:454:LEU:HG	1.89	0.53
2:K:155:LYS:HE2	2:K:158:THR:HG21	1.91	0.53
2:O:155:LYS:HE2	2:O:158:THR:HG21	1.90	0.53
2:S:439:LEU:HD21	2:S:441:LYS:HE2	1.90	0.53
2:S:194:TRP:NE1	2:S:245:ASP:O	2.35	0.53
1:B:14:ARG:HG2	1:B:79:LEU:HD13	1.90	0.52
2:G:37:LEU:HD13	2:Y:385:LYS:HB2	1.90	0.52
2:G:148:ARG:HA	2:Y:182:GLU:O	2.08	0.52
2:K:50:THR:HG23	2:K:362:GLN:HG3	1.91	0.52
1:V:51:ILE:HG12	1:V:59:VAL:HB	1.91	0.52
2:T:210:SER:OG	2:T:225:GLN:OE1	2.24	0.52
2:T:364:GLN:NE2	2:T:366:ASP:OD1	2.31	0.52
1:X:33:ILE:HG22	1:X:90:MET:HG3	1.91	0.52
1:F:53:ASN:OD1	1:F:57:SER:OG	2.20	0.52
1:R:33:ILE:HG22	1:R:90:MET:HG3	1.90	0.52
2:S:385:LYS:HB2	2:T:37:LEU:HD13	1.91	0.52
1:F:33:ILE:HG22	1:F:90:MET:HG3	1.91	0.52
1:C:31:ILE:HB	1:C:65:LEU:HB2	1.92	0.52
1:J:49:VAL:HG23	1:J:61:ILE:HG13	1.92	0.52
1:A:31:ILE:HG13	1:A:67:ILE:HD11	1.92	0.52
1:A:51:ILE:HG12	1:A:59:VAL:HB	1.92	0.52
2:S:435:ASP:OD1	2:K:448:ARG:NH2	2.26	0.52
1:L:11:SER:O	1:M:90:MET:HE1	2.10	0.52
2:Y:210:SER:OG	2:Y:225:GLN:OE1	2.27	0.52
2:G:35:GLU:HA	2:G:40:SER:HA	1.93	0.51
2:S:404:GLN:OE1	2:S:460:SER:OG	2.26	0.51
1:X:31:ILE:HB	1:X:65:LEU:HB2	1.93	0.51
2:T:369:SER:HB3	2:T:459:LYS:HG2	1.93	0.51
1:D:31:ILE:HD12	1:D:73:ILE:HD11	1.93	0.51
2:K:294:GLU:OE2	2:K:307:HIS:NE2	2.40	0.51
1:P:31:ILE:HD12	1:P:73:ILE:HD11	1.92	0.51
1:M:14:ARG:HB3	1:M:72:LYS:HD3	1.92	0.51
2:K:147:LEU:HB2	2:K:193:THR:HG21	1.93	0.51
2:K:364:GLN:NE2	2:K:366:ASP:OD1	2.28	0.51
1:V:78:GLN:HA	1:W:21:ARG:HH22	1.76	0.51
2:G:101:ARG:NH2	2:Y:185:PRO:O	2.44	0.51
2:T:34:LYS:H	2:T:41:GLY:HA2	1.76	0.51
2:T:283:TYR:OH	2:T:311:HIS:ND1	2.33	0.51
2:S:390:ARG:HA	2:S:445:ARG:HA	1.92	0.51
2:O:262:ILE:HD12	2:O:271:ILE:HG13	1.93	0.51
2:O:390:ARG:HA	2:O:445:ARG:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLN:HA	1:B:21:ARG:HH22	1.76	0.51
2:G:369:SER:HB3	2:G:459:LYS:HG2	1.93	0.51
2:G:448:ARG:NH2	2:K:435:ASP:OD1	2.28	0.51
2:Y:63:GLU:OE1	2:Y:99:HIS:ND1	2.44	0.51
1:C:31:ILE:HG13	1:C:67:ILE:HD11	1.93	0.50
1:I:14:ARG:HB3	1:I:72:LYS:HD3	1.94	0.50
2:T:439:LEU:HD21	2:T:441:LYS:HE2	1.92	0.50
1:V:31:ILE:HG13	1:V:67:ILE:HD11	1.93	0.50
2:Y:390:ARG:HA	2:Y:445:ARG:HA	1.93	0.50
1:H:11:SER:O	1:I:90:MET:HE1	2.10	0.50
2:O:97:MET:HE2	2:O:104:GLN:NE2	2.27	0.50
2:S:237:THR:O	2:S:240:LYS:NZ	2.45	0.50
2:K:312:VAL:HG21	2:K:338:TYR:HB3	1.94	0.50
2:Y:194:TRP:NE1	2:Y:245:ASP:O	2.35	0.50
2:G:60:ARG:HD2	2:G:93:GLY:O	2.12	0.50
1:X:31:ILE:HG13	1:X:67:ILE:HD11	1.93	0.50
2:G:439:LEU:HD21	2:G:441:LYS:HE2	1.93	0.50
1:P:14:ARG:NH1	1:Q:101:ASP:OD1	2.44	0.50
2:T:60:ARG:HD2	2:T:93:GLY:O	2.12	0.50
2:G:183:SER:HB2	2:K:148:ARG:NH1	2.27	0.50
2:K:97:MET:HE2	2:K:104:GLN:NE2	2.27	0.49
1:D:14:ARG:NH1	1:E:101:ASP:OD1	2.45	0.49
1:J:47:ILE:HD11	1:J:88:HIS:HB3	1.94	0.49
1:N:47:ILE:HD11	1:N:88:HIS:HB3	1.94	0.49
2:G:34:LYS:H	2:G:41:GLY:HA2	1.76	0.49
1:P:19:GLU:HG3	1:P:24:LYS:HG3	1.94	0.49
2:Y:136:TYR:HB2	2:Y:138:LEU:HD13	1.93	0.49
1:I:73:ILE:HG21	1:I:82:ILE:HG13	1.94	0.49
2:K:316:ASP:O	2:K:320:SER:OG	2.30	0.49
2:O:194:TRP:NE1	2:O:245:ASP:O	2.39	0.49
2:Y:237:THR:O	2:Y:240:LYS:NZ	2.45	0.49
2:S:413:ALA:HB1	2:S:450:ILE:HD11	1.95	0.49
2:T:143:ASP:HB3	2:T:191:ILE:HG22	1.95	0.49
2:T:298:PHE:O	2:T:301:HIS:HB2	2.12	0.49
2:K:13:GLY:HA3	2:K:24:TYR:CZ	2.48	0.49
2:O:312:VAL:HG21	2:O:338:TYR:HB3	1.94	0.48
1:R:30:LYS:HB2	1:R:30:LYS:HE2	1.58	0.48
2:K:15:ASP:HB2	2:K:22:ILE:HD13	1.95	0.48
2:K:261:TYR:HB3	2:K:268:ALA:HB1	1.94	0.48
2:G:298:PHE:O	2:G:301:HIS:HB2	2.12	0.48
2:O:261:TYR:HB3	2:O:268:ALA:HB1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:THR:HA	1:L:25:ALA:HA	1.94	0.48
1:V:31:ILE:HD12	1:V:73:ILE:HD11	1.96	0.48
2:Y:12:MET:HG3	2:Y:13:GLY:N	2.28	0.48
2:Y:17:LYS:HE2	2:Y:17:LYS:HA	1.96	0.48
2:G:182:GLU:O	2:K:148:ARG:HA	2.14	0.48
1:I:117:GLU:O	1:I:121:LYS:HB2	2.14	0.48
2:T:62:VAL:HG23	2:T:73:ARG:HG2	1.96	0.48
2:S:63:GLU:OE2	2:S:99:HIS:ND1	2.46	0.48
2:O:13:GLY:HA3	2:O:24:TYR:CZ	2.48	0.48
2:S:17:LYS:HA	2:S:17:LYS:HE2	1.96	0.48
2:S:23:ASP:OD1	2:T:34:LYS:NZ	2.47	0.48
1:M:73:ILE:HG21	1:M:82:ILE:HG13	1.95	0.48
2:T:388:ASN:OD1	2:T:445:ARG:NH1	2.47	0.48
2:Y:413:ALA:HB1	2:Y:450:ILE:HD11	1.96	0.48
1:Q:38:THR:O	1:Q:102:TYR:OH	2.29	0.47
1:A:31:ILE:HD12	1:A:73:ILE:HD11	1.96	0.47
2:Y:261:TYR:HB3	2:Y:268:ALA:HB1	1.97	0.47
1:A:108:LYS:HD2	1:C:112:ASP:OD2	2.13	0.47
2:S:409:LEU:O	2:S:425:MET:HA	2.14	0.47
2:G:143:ASP:HB3	2:G:191:ILE:HG22	1.95	0.47
2:T:312:VAL:HG21	2:T:338:TYR:HB3	1.96	0.47
2:S:297:ARG:NH2	2:K:277:GLU:OE1	2.33	0.47
2:K:35:GLU:HA	2:K:40:SER:HA	1.97	0.47
1:M:117:GLU:O	1:M:121:LYS:HB2	2.15	0.47
2:O:15:ASP:HB2	2:O:22:ILE:HD13	1.95	0.47
2:S:293:MET:HG2	2:S:306:ILE:HG12	1.96	0.47
2:K:63:GLU:OE2	2:K:99:HIS:ND1	2.46	0.47
2:S:312:VAL:HG21	2:S:338:TYR:HB3	1.97	0.47
2:K:12:MET:HB3	2:K:382:PRO:HA	1.96	0.47
2:O:12:MET:HB3	2:O:382:PRO:HA	1.96	0.47
1:Q:35:GLN:O	1:Q:38:THR:HG22	2.15	0.47
2:T:261:TYR:HB3	2:T:268:ALA:HB1	1.96	0.47
2:Y:293:MET:HG2	2:Y:306:ILE:HG12	1.95	0.47
2:G:312:VAL:HG21	2:G:338:TYR:HB3	1.95	0.47
2:G:388:ASN:OD1	2:G:445:ARG:NH1	2.48	0.47
2:O:316:ASP:O	2:O:320:SER:OG	2.30	0.47
1:V:35:GLN:HG2	1:V:45:ASN:O	2.15	0.47
2:S:16:PHE:HB3	2:S:418:ILE:HD13	1.97	0.47
2:Y:391:CYS:HB3	2:Y:471:LEU:HD23	1.97	0.47
1:B:46:GLN:CD	1:B:63:GLN:HG2	2.40	0.47
1:D:18:THR:HA	1:D:25:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLN:O	1:E:89:SER:OG	2.24	0.47
2:G:341:VAL:HB	2:G:355:LYS:HE3	1.97	0.46
2:S:261:TYR:HB3	2:S:268:ALA:HB1	1.97	0.46
1:W:35:GLN:O	1:W:89:SER:OG	2.27	0.46
2:S:34:LYS:O	2:S:41:GLY:N	2.49	0.46
2:O:35:GLU:HA	2:O:40:SER:HA	1.97	0.46
2:Y:312:VAL:HG21	2:Y:338:TYR:HB3	1.97	0.46
2:G:62:VAL:HG23	2:G:73:ARG:HG2	1.97	0.46
2:K:194:TRP:NE1	2:K:245:ASP:O	2.39	0.46
1:W:46:GLN:CD	1:W:63:GLN:HG2	2.40	0.46
2:Y:155:LYS:HE2	2:Y:158:THR:HG21	1.98	0.46
2:Y:287:GLU:HB3	2:Y:309:PRO:HG3	1.97	0.46
2:G:185:PRO:HB3	2:K:100:GLY:HA2	1.97	0.46
1:R:53:ASN:OD1	1:R:57:SER:OG	2.20	0.46
2:G:12:MET:HE1	2:G:21:TYR:HB3	1.98	0.46
1:L:19:GLU:HG3	1:L:24:LYS:HG3	1.98	0.46
2:O:341:VAL:HB	2:O:355:LYS:HE3	1.97	0.46
2:Y:59:SER:OG	2:Y:342:ASP:OD2	2.26	0.46
1:A:11:SER:O	1:B:90:MET:HE1	2.16	0.46
2:K:341:VAL:HB	2:K:355:LYS:HE3	1.97	0.46
1:X:52:GLU:HG3	1:X:58:HIS:NE2	2.31	0.46
1:A:35:GLN:HG2	1:A:45:ASN:O	2.15	0.46
2:K:184:GLN:NE2	2:K:187:GLY:O	2.44	0.46
1:X:85:VAL:HG23	1:X:86:GLN:HG2	1.98	0.46
2:Y:35:GLU:HA	2:Y:40:SER:HA	1.98	0.46
1:A:52:GLU:OE2	1:A:58:HIS:NE2	2.50	0.45
2:G:261:TYR:HB3	2:G:268:ALA:HB1	1.96	0.45
1:J:22:SER:HB2	1:J:24:LYS:NZ	2.31	0.45
1:C:68:ASN:ND2	1:C:69:ALA:H	2.14	0.45
1:E:35:GLN:O	1:E:38:THR:HG22	2.17	0.45
1:J:99:GLN:NE2	2:K:423:GLU:O	2.46	0.45
1:W:35:GLN:O	1:W:38:THR:HG22	2.16	0.45
2:S:158:THR:O	2:S:180:ARG:NH2	2.49	0.45
1:I:55:ASP:OD1	1:I:57:SER:OG	2.23	0.45
2:O:63:GLU:OE2	2:O:99:HIS:ND1	2.47	0.45
1:V:11:SER:O	1:W:90:MET:HE1	2.16	0.45
2:G:399:SER:HB3	2:G:463:THR:HB	1.97	0.45
2:O:364:GLN:NE2	2:O:366:ASP:OD1	2.28	0.45
1:B:35:GLN:O	1:B:38:THR:HG22	2.17	0.45
1:C:85:VAL:HG23	1:C:86:GLN:HG2	1.98	0.45
2:S:185:PRO:O	2:T:101:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:THR:HA	1:H:25:ALA:HA	1.97	0.45
1:X:47:ILE:HD11	1:X:88:HIS:HB3	1.98	0.45
2:Y:16:PHE:HB3	2:Y:418:ILE:HD13	1.97	0.45
2:Y:34:LYS:O	2:Y:41:GLY:N	2.49	0.45
1:E:14:ARG:HD2	1:E:79:LEU:HD13	1.97	0.45
1:E:121:LYS:HB3	1:E:121:LYS:HE2	1.62	0.45
2:S:59:SER:OG	2:S:342:ASP:OD2	2.26	0.45
2:S:273:THR:O	2:S:277:GLU:HG3	2.16	0.45
2:S:391:CYS:HB3	2:S:471:LEU:HD23	1.99	0.45
2:K:456:VAL:HG12	2:K:458:THR:HG23	1.99	0.45
2:T:312:VAL:HG23	2:T:337:VAL:HG22	1.99	0.45
1:L:14:ARG:NH1	1:M:101:ASP:OD1	2.49	0.45
1:L:46:GLN:HB3	1:L:63:GLN:HE21	1.81	0.45
2:T:116:ARG:NH1	2:T:118:ASP:OD2	2.49	0.45
1:X:68:ASN:ND2	1:X:69:ALA:H	2.15	0.45
2:G:206:ILE:HB	2:G:230:VAL:HB	1.99	0.45
1:H:14:ARG:NH1	1:I:101:ASP:OD1	2.50	0.45
1:Q:14:ARG:HD2	1:Q:79:LEU:HD13	1.99	0.45
1:Q:46:GLN:CD	1:Q:63:GLN:HG2	2.42	0.45
1:Q:61:ILE:HD11	1:Q:75:TYR:CE1	2.52	0.45
2:T:15:ASP:HB2	2:T:22:ILE:HD13	1.99	0.45
1:C:52:GLU:HG3	1:C:58:HIS:NE2	2.32	0.44
1:E:46:GLN:CD	1:E:63:GLN:HG2	2.42	0.44
2:G:413:ALA:HB1	2:G:450:ILE:HD11	1.99	0.44
1:H:46:GLN:HB3	1:H:63:GLN:HE21	1.81	0.44
2:K:141:VAL:HG22	2:K:153:TRP:CD1	2.52	0.44
2:T:399:SER:HB3	2:T:463:THR:HB	1.98	0.44
2:K:262:ILE:HD12	2:K:271:ILE:HG13	1.99	0.44
1:M:46:GLN:CD	1:M:63:GLN:HG2	2.43	0.44
2:S:116:ARG:NH1	2:S:118:ASP:OD2	2.50	0.44
1:F:30:LYS:HE2	1:F:30:LYS:HB2	1.58	0.44
2:G:435:ASP:OD1	2:Y:448:ARG:NH2	2.44	0.44
1:H:28:ASN:N	1:H:67:ILE:O	2.51	0.44
1:H:77:GLY:O	1:I:21:ARG:NH2	2.51	0.44
1:M:61:ILE:HD11	1:M:75:TYR:CE1	2.52	0.44
1:W:21:ARG:HA	1:W:21:ARG:HD3	1.85	0.44
1:B:61:ILE:HD12	1:B:61:ILE:HA	1.87	0.44
1:L:28:ASN:N	1:L:67:ILE:O	2.50	0.44
1:L:77:GLY:O	1:M:21:ARG:NH2	2.51	0.44
1:N:22:SER:HB2	1:N:24:LYS:NZ	2.31	0.44
2:T:413:ALA:HB1	2:T:450:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ILE:HD11	1:B:75:TYR:CE1	2.53	0.44
2:S:155:LYS:HE2	2:S:158:THR:HG21	2.00	0.44
2:S:364:GLN:NE2	2:S:366:ASP:OD1	2.27	0.44
2:G:277:GLU:OE1	2:K:297:ARG:NH2	2.35	0.44
1:I:46:GLN:CD	1:I:63:GLN:HG2	2.43	0.44
1:I:61:ILE:HD11	1:I:75:TYR:CE1	2.52	0.44
2:O:184:GLN:NE2	2:O:187:GLY:O	2.44	0.44
2:T:12:MET:HE1	2:T:21:TYR:HB3	1.98	0.44
2:G:15:ASP:HB2	2:G:22:ILE:HD13	1.99	0.44
2:G:430:GLU:HB3	2:G:433:VAL:HB	1.99	0.44
1:I:35:GLN:O	1:I:38:THR:HG22	2.18	0.44
2:O:391:CYS:HB3	2:O:471:LEU:HD23	1.99	0.44
2:O:409:LEU:O	2:O:425:MET:HA	2.18	0.44
2:T:147:LEU:HB2	2:T:193:THR:HG21	2.00	0.44
1:W:61:ILE:HD11	1:W:75:TYR:CE1	2.53	0.44
2:Y:141:VAL:HG22	2:Y:153:TRP:CD1	2.53	0.44
1:C:99:GLN:NE2	2:S:423:GLU:O	2.51	0.44
2:S:148:ARG:HA	2:K:182:GLU:O	2.18	0.44
2:G:167:GLU:HG3	2:G:174:ARG:HH12	1.82	0.44
2:O:297:ARG:NH2	2:T:277:GLU:OE1	2.35	0.44
2:Y:60:ARG:HD2	2:Y:93:GLY:O	2.18	0.44
2:T:35:GLU:HA	2:T:40:SER:HA	2.00	0.44
2:T:341:VAL:HB	2:T:355:LYS:HE3	1.98	0.44
1:H:31:ILE:HB	1:H:65:LEU:HB2	2.00	0.43
1:H:79:LEU:HD11	1:I:20:SER:HB2	2.00	0.43
2:S:60:ARG:HD2	2:S:93:GLY:O	2.18	0.43
1:F:36:ILE:HA	1:F:89:SER:HB3	1.99	0.43
2:G:271:ILE:HD13	2:G:271:ILE:HA	1.75	0.43
2:O:143:ASP:HB3	2:O:191:ILE:HG22	1.99	0.43
1:Q:35:GLN:O	1:Q:89:SER:OG	2.24	0.43
2:T:343:PHE:CD1	2:T:352:CYS:HB3	2.53	0.43
2:T:430:GLU:HB3	2:T:433:VAL:HB	1.99	0.43
1:X:18:THR:HA	1:X:25:ALA:HA	1.99	0.43
1:E:61:ILE:HD11	1:E:75:TYR:CE1	2.54	0.43
2:G:287:GLU:HB3	2:G:309:PRO:HG3	2.00	0.43
1:L:11:SER:HA	1:M:15:PRO:HG2	2.00	0.43
1:X:36:ILE:HD12	2:Y:334:TYR:CE2	2.53	0.43
1:I:31:ILE:HG13	1:I:67:ILE:HD11	2.01	0.43
2:O:141:VAL:HG22	2:O:153:TRP:CD1	2.52	0.43
2:O:243:PHE:HA	2:O:295:THR:HG21	2.00	0.43
2:S:141:VAL:HG22	2:S:153:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:186:ASP:HB3	2:T:67:ALA:HA	2.00	0.43
1:F:74:VAL:HG12	1:F:79:LEU:HD23	2.00	0.43
1:L:79:LEU:HD11	1:M:20:SER:HB2	2.00	0.43
1:R:36:ILE:HA	1:R:89:SER:HB3	2.00	0.43
2:T:155:LYS:HB2	2:T:162:PHE:HE1	1.84	0.43
2:S:67:ALA:HA	2:K:186:ASP:HB3	2.01	0.43
2:G:273:THR:O	2:G:277:GLU:HG3	2.19	0.43
1:P:6:ALA:HB1	1:Q:84:THR:O	2.19	0.43
2:Y:271:ILE:HG22	2:Y:326:TRP:HZ2	1.84	0.43
1:B:99:GLN:NE2	1:B:102:TYR:HB2	2.34	0.43
1:J:30:LYS:HB2	1:J:30:LYS:HE2	1.52	0.43
2:O:182:GLU:O	2:Y:148:ARG:HA	2.19	0.43
1:H:11:SER:HA	1:I:15:PRO:HG2	2.00	0.43
2:K:234:ILE:HD12	2:K:236:GLY:O	2.18	0.43
1:N:99:GLN:NE2	2:O:423:GLU:O	2.46	0.43
2:O:394:LEU:HD13	2:O:411:LEU:HD21	2.00	0.43
1:Q:61:ILE:HD12	1:Q:61:ILE:HA	1.91	0.43
1:R:74:VAL:HG12	1:R:79:LEU:HD23	2.01	0.43
1:X:99:GLN:NE2	2:Y:423:GLU:O	2.50	0.43
1:C:52:GLU:HG3	1:C:58:HIS:CD2	2.54	0.43
2:S:35:GLU:HA	2:S:40:SER:HA	2.01	0.43
2:G:343:PHE:CD1	2:G:352:CYS:HB3	2.53	0.43
1:I:61:ILE:HD12	1:I:61:ILE:HA	1.89	0.43
2:K:26:PRO:HB2	2:K:29:MET:HB2	2.00	0.43
2:K:155:LYS:HB2	2:K:162:PHE:HE1	1.84	0.43
2:O:234:ILE:HD12	2:O:236:GLY:O	2.18	0.43
2:Y:416:ASP:OD2	2:Y:419:ASN:ND2	2.51	0.43
1:E:54:GLU:OE1	2:G:453:LYS:NZ	2.30	0.43
2:G:155:LYS:HB2	2:G:162:PHE:HE1	1.84	0.43
2:K:243:PHE:HA	2:K:295:THR:HG21	2.01	0.43
1:L:31:ILE:HB	1:L:65:LEU:HB2	2.00	0.43
2:O:409:LEU:HD21	2:O:454:LEU:HD12	2.00	0.43
2:T:287:GLU:HB3	2:T:309:PRO:HG3	1.99	0.43
1:W:99:GLN:NE2	1:W:102:TYR:HB2	2.34	0.43
2:G:159:ASP:HA	2:G:188:ILE:HB	2.00	0.42
2:K:162:PHE:CE2	2:K:178:GLN:HG3	2.54	0.42
1:M:35:GLN:O	1:M:38:THR:HG22	2.18	0.42
2:Y:229:MET:HE3	2:Y:231:GLN:HG2	2.01	0.42
1:M:31:ILE:HG13	1:M:67:ILE:HD11	2.00	0.42
2:O:26:PRO:HB2	2:O:29:MET:HB2	2.01	0.42
2:O:155:LYS:HB2	2:O:162:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:237:THR:O	2:T:240:LYS:NZ	2.53	0.42
2:T:271:ILE:HD13	2:T:271:ILE:HA	1.75	0.42
2:S:271:ILE:HG22	2:S:326:TRP:HZ2	1.84	0.42
2:S:416:ASP:OD2	2:S:419:ASN:ND2	2.52	0.42
2:O:400:THR:OG1	2:O:433:VAL:O	2.26	0.42
2:S:25:LEU:HD11	2:S:276:ILE:HD11	2.01	0.42
2:O:293:MET:HE3	2:O:304:LEU:HD11	2.02	0.42
2:T:273:THR:O	2:T:277:GLU:HG3	2.19	0.42
2:Y:409:LEU:HD13	2:Y:456:VAL:HG22	2.00	0.42
2:K:26:PRO:HB3	2:K:379:LEU:HD23	2.02	0.42
2:K:394:LEU:HD13	2:K:411:LEU:HD21	2.01	0.42
2:Y:273:THR:O	2:Y:277:GLU:HG3	2.18	0.42
2:G:185:PRO:O	2:G:186:ASP:HB2	2.19	0.42
1:H:46:GLN:CD	1:H:63:GLN:HG2	2.44	0.42
2:K:286:GLU:C	2:K:288:MET:H	2.27	0.42
2:O:412:SER:HB3	2:O:423:GLU:HG3	2.02	0.42
1:V:14:ARG:NH1	1:W:101:ASP:OD1	2.52	0.42
2:K:206:ILE:HB	2:K:230:VAL:HB	2.02	0.42
2:T:159:ASP:HA	2:T:188:ILE:HB	2.02	0.42
2:G:147:LEU:HB2	2:G:193:THR:HG21	2.01	0.42
2:O:60:ARG:HD2	2:O:93:GLY:O	2.19	0.42
2:O:273:THR:O	2:O:277:GLU:HG3	2.20	0.42
1:B:88:HIS:CE1	1:B:106:VAL:HG21	2.55	0.42
1:C:18:THR:HA	1:C:25:ALA:HA	2.00	0.42
2:S:387:ASP:OD1	2:S:448:ARG:HA	2.20	0.42
1:I:88:HIS:CE1	1:I:106:VAL:HG21	2.55	0.42
2:K:296:LEU:HD23	2:K:296:LEU:HA	1.90	0.42
2:O:185:PRO:O	2:Y:101:ARG:NH2	2.53	0.42
1:V:52:GLU:OE2	1:V:58:HIS:NE2	2.52	0.42
2:S:101:ARG:NH2	2:K:185:PRO:O	2.52	0.42
1:D:6:ALA:HB1	1:E:84:THR:O	2.19	0.42
1:I:38:THR:O	1:I:102:TYR:OH	2.27	0.42
2:K:273:THR:O	2:K:277:GLU:HG3	2.20	0.42
2:K:293:MET:HE3	2:K:304:LEU:HD11	2.02	0.42
1:M:10:VAL:HB	1:N:82:ILE:HB	2.02	0.42
1:M:35:GLN:O	1:M:89:SER:OG	2.28	0.42
2:O:210:SER:OG	2:O:225:GLN:OE1	2.37	0.42
1:W:88:HIS:CE1	1:W:106:VAL:HG21	2.54	0.42
1:E:94:ASP:HB3	1:E:96:ASN:OD1	2.20	0.41
2:K:189:ILE:H	2:K:189:ILE:HG12	1.68	0.41
1:P:77:GLY:O	1:Q:21:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HG22	1:C:90:MET:HG3	2.02	0.41
2:S:409:LEU:HD11	2:S:454:LEU:HG	2.01	0.41
2:G:237:THR:O	2:G:240:LYS:NZ	2.53	0.41
2:K:210:SER:OG	2:K:225:GLN:OE1	2.34	0.41
1:M:88:HIS:CE1	1:M:106:VAL:HG21	2.55	0.41
1:W:38:THR:O	1:W:102:TYR:OH	2.32	0.41
2:G:98:ALA:O	2:G:104:GLN:NE2	2.53	0.41
2:K:409:LEU:O	2:K:425:MET:HA	2.21	0.41
1:Q:94:ASP:HB3	1:Q:96:ASN:OD1	2.20	0.41
2:Y:25:LEU:HD11	2:Y:276:ILE:HD11	2.02	0.41
1:H:6:ALA:HB1	1:I:84:THR:O	2.20	0.41
2:K:60:ARG:HD2	2:K:93:GLY:O	2.20	0.41
1:L:46:GLN:CD	1:L:63:GLN:HG2	2.44	0.41
2:T:229:MET:HE2	2:T:229:MET:HB3	1.79	0.41
1:A:14:ARG:NH1	1:B:101:ASP:OD1	2.53	0.41
2:S:34:LYS:H	2:S:41:GLY:HA2	1.85	0.41
1:N:61:ILE:HD11	1:N:82:ILE:HD12	2.02	0.41
2:O:277:GLU:OE1	2:Y:297:ARG:NH2	2.33	0.41
2:O:286:GLU:C	2:O:288:MET:H	2.27	0.41
2:T:379:LEU:HD23	2:T:379:LEU:HA	1.92	0.41
1:W:38:THR:HG21	1:W:45:ASN:HB3	2.01	0.41
1:D:77:GLY:O	1:E:21:ARG:NH2	2.54	0.41
2:G:279:ILE:O	2:G:282:SER:OG	2.30	0.41
1:L:82:ILE:HB	1:N:10:VAL:HB	2.02	0.41
1:I:10:VAL:HB	1:J:82:ILE:HB	2.02	0.41
2:K:412:SER:HB3	2:K:423:GLU:HG3	2.02	0.41
1:L:26:VAL:HG12	1:L:29:GLY:HA3	2.02	0.41
2:O:186:ASP:HB3	2:Y:67:ALA:HA	2.02	0.41
2:O:189:ILE:H	2:O:189:ILE:HG12	1.68	0.41
2:T:206:ILE:HB	2:T:230:VAL:HB	2.03	0.41
1:B:38:THR:HG21	1:B:45:ASN:HB3	2.02	0.41
2:S:29:MET:HE2	2:S:379:LEU:HD11	2.02	0.41
2:S:229:MET:HE3	2:S:231:GLN:HG2	2.03	0.41
1:F:49:VAL:HG23	1:F:61:ILE:HG13	2.03	0.41
1:J:61:ILE:HD11	1:J:82:ILE:HD12	2.02	0.41
2:K:272:ALA:HB1	2:K:276:ILE:HB	2.03	0.41
1:L:90:MET:SD	1:L:92:ILE:HD11	2.61	0.41
1:M:105:ASN:ND2	1:M:108:LYS:HE3	2.36	0.41
1:N:30:LYS:HE2	1:N:30:LYS:HB2	1.52	0.41
1:P:25:ALA:HB2	1:Q:23:PHE:CD1	2.56	0.41
1:P:78:GLN:HA	1:Q:21:ARG:HH22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:49:VAL:HG23	1:R:61:ILE:HG13	2.03	0.41
2:S:364:GLN:HB3	2:S:367:ILE:HG12	2.02	0.41
2:O:374:GLN:HB3	2:O:459:LYS:HG3	2.03	0.41
2:Y:36:ILE:HD11	2:Y:42:TYR:CD1	2.56	0.41
1:B:116:ILE:HG22	1:B:120:LYS:HE3	2.02	0.40
2:S:257:ALA:HA	2:S:258:PRO:HD3	1.95	0.40
1:D:35:GLN:HG2	1:D:45:ASN:O	2.21	0.40
2:O:101:ARG:HE	2:O:101:ARG:HB2	1.59	0.40
1:R:31:ILE:HB	1:R:65:LEU:HB2	2.04	0.40
2:S:99:HIS:NE2	2:K:185:PRO:HG2	2.36	0.40
1:E:84:THR:OG1	1:E:85:VAL:N	2.55	0.40
1:H:82:ILE:HB	1:J:10:VAL:HB	2.02	0.40
1:H:90:MET:SD	1:H:92:ILE:HD11	2.61	0.40
1:I:94:ASP:HB3	1:I:96:ASN:OD1	2.21	0.40
2:K:271:ILE:HD13	2:K:271:ILE:HA	1.93	0.40
1:M:94:ASP:HB3	1:M:96:ASN:OD1	2.21	0.40
1:P:35:GLN:HG2	1:P:45:ASN:O	2.20	0.40
2:Y:387:ASP:OD1	2:Y:448:ARG:HA	2.20	0.40
1:I:105:ASN:ND2	1:I:108:LYS:HE3	2.36	0.40
2:O:409:LEU:HD11	2:O:454:LEU:HG	2.03	0.40
2:Y:8:MET:HE3	2:Y:8:MET:HB2	1.91	0.40
1:B:21:ARG:HD3	1:B:21:ARG:HA	1.85	0.40
2:Y:34:LYS:H	2:Y:41:GLY:HA2	1.86	0.40
2:K:247:TYR:HB2	2:K:263:ILE:HD12	2.04	0.40
2:O:26:PRO:HB3	2:O:379:LEU:HD23	2.02	0.40
2:O:29:MET:HE3	2:O:377:HIS:HB3	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	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	B	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	C	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	D	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	E	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	F	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	H	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	I	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	J	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	L	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	M	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	N	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	P	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	Q	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	R	116/667 (17%)	112 (97%)	4 (3%)	0	100	100
1	V	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	W	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
1	X	116/667 (17%)	113 (97%)	3 (3%)	0	100	100
2	G	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
2	K	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
2	O	469/472 (99%)	439 (94%)	30 (6%)	0	100	100
2	S	469/472 (99%)	437 (93%)	32 (7%)	0	100	100
2	T	469/472 (99%)	439 (94%)	30 (6%)	0	100	100
2	Y	469/472 (99%)	440 (94%)	29 (6%)	0	100	100
All	All	4902/14838 (33%)	4662 (95%)	240 (5%)	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	101/548 (18%)	101 (100%)	0	100	100
1	B	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	C	101/548 (18%)	97 (96%)	4 (4%)	28	63
1	D	101/548 (18%)	101 (100%)	0	100	100
1	E	101/548 (18%)	100 (99%)	1 (1%)	68	88
1	F	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	H	101/548 (18%)	101 (100%)	0	100	100
1	I	101/548 (18%)	101 (100%)	0	100	100
1	J	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	L	101/548 (18%)	101 (100%)	0	100	100
1	M	101/548 (18%)	101 (100%)	0	100	100
1	N	101/548 (18%)	100 (99%)	1 (1%)	68	88
1	P	101/548 (18%)	101 (100%)	0	100	100
1	Q	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	R	101/548 (18%)	99 (98%)	2 (2%)	48	80
1	V	101/548 (18%)	101 (100%)	0	100	100
1	W	101/548 (18%)	100 (99%)	1 (1%)	68	88
1	X	101/548 (18%)	96 (95%)	5 (5%)	22	54
2	G	394/395 (100%)	389 (99%)	5 (1%)	61	86
2	K	394/395 (100%)	383 (97%)	11 (3%)	38	73
2	O	394/395 (100%)	384 (98%)	10 (2%)	42	76
2	S	394/395 (100%)	386 (98%)	8 (2%)	48	80
2	T	394/395 (100%)	387 (98%)	7 (2%)	51	82
2	Y	394/395 (100%)	386 (98%)	8 (2%)	48	80
All	All	4182/12234 (34%)	4111 (98%)	71 (2%)	52	83

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	62	THR
1	B	117	GLU
1	C	24	LYS
1	C	57	SER

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Mol	Chain	Res	Type
1	C	86	GLN
1	C	106	VAL
2	S	54	ASP
2	S	196	ASP
2	S	227	SER
2	S	237	THR
2	S	269	SER
2	S	357	GLU
2	S	360	VAL
2	S	435	ASP
1	E	116	ILE
1	F	84	THR
1	F	106	VAL
2	G	120	THR
2	G	271	ILE
2	G	294	GLU
2	G	360	VAL
2	G	394	LEU
1	J	16	ILE
1	J	84	THR
2	K	50	THR
2	K	54	ASP
2	K	102	THR
2	K	205	THR
2	K	227	SER
2	K	241	THR
2	K	269	SER
2	K	337	VAL
2	K	394	LEU
2	K	395	GLU
2	K	409	LEU
1	N	84	THR
2	O	50	THR
2	O	54	ASP
2	O	102	THR
2	O	205	THR
2	O	241	THR
2	O	269	SER
2	O	271	ILE
2	O	337	VAL
2	O	394	LEU
2	O	458	THR

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Mol	Chain	Res	Type
1	Q	36	ILE
1	Q	116	ILE
1	R	55	ASP
1	R	84	THR
2	T	120	THR
2	T	174	ARG
2	T	229	MET
2	T	271	ILE
2	T	337	VAL
2	T	360	VAL
2	T	394	LEU
1	W	62	THR
1	X	24	LYS
1	X	57	SER
1	X	84	THR
1	X	86	GLN
1	X	106	VAL
2	Y	54	ASP
2	Y	102	THR
2	Y	196	ASP
2	Y	227	SER
2	Y	237	THR
2	Y	269	SER
2	Y	360	VAL
2	Y	395	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	53	ASN
1	B	99	GLN
1	C	68	ASN
1	C	88	HIS
1	C	113	GLN
1	D	53	ASN
1	D	113	GLN
1	E	53	ASN
2	G	267	GLN
2	G	377	HIS
2	G	404	GLN
2	G	419	ASN

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Mol	Chain	Res	Type
1	I	53	ASN
1	I	105	ASN
2	K	404	GLN
2	K	419	ASN
1	L	46	GLN
1	M	53	ASN
1	M	105	ASN
1	N	12	ASN
1	N	78	GLN
2	O	267	GLN
2	O	404	GLN
2	O	419	ASN
1	P	53	ASN
1	P	113	GLN
1	Q	53	ASN
1	R	86	GLN
2	T	377	HIS
2	T	404	GLN
2	T	419	ASN
1	V	46	GLN
1	W	99	GLN
1	X	53	ASN
1	X	68	ASN
2	Y	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

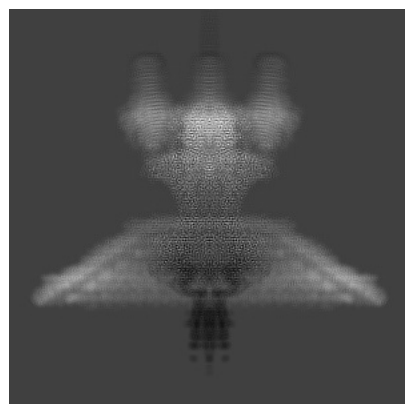
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41649. These allow visual inspection of the internal detail of the map and identification of artifacts.

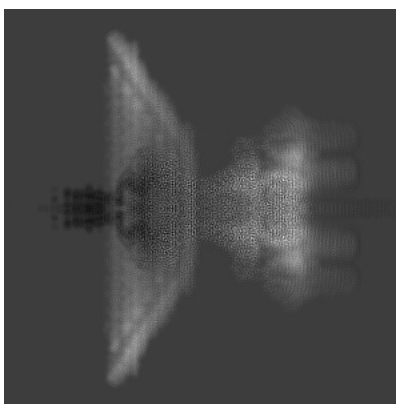
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

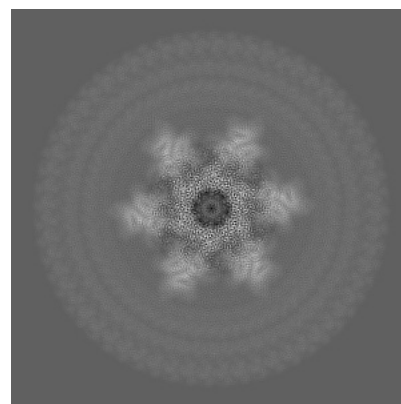
6.1.1 Primary map



X

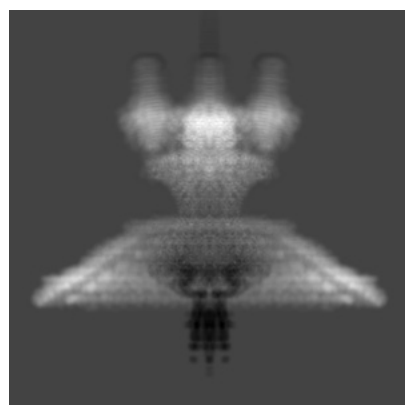


Y

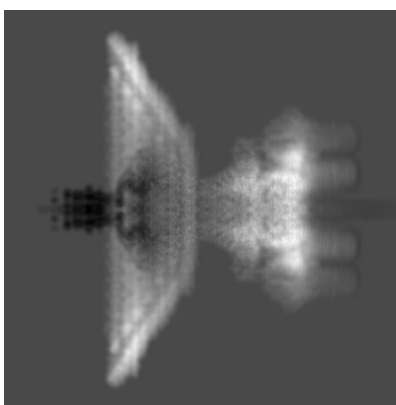


Z

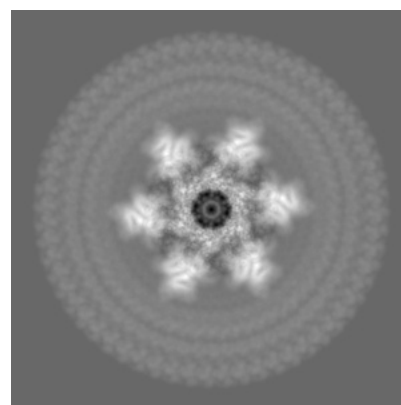
6.1.2 Raw map



X



Y



Z

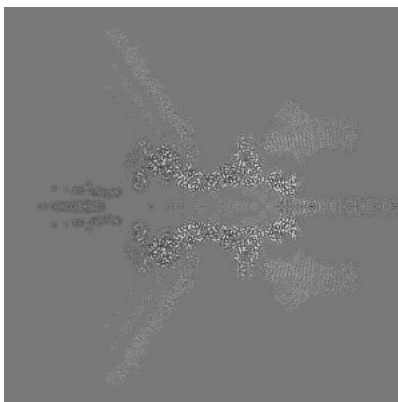
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

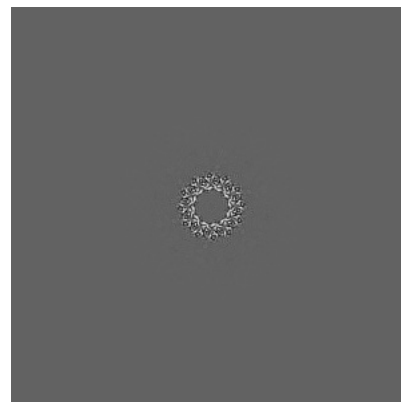
6.2.1 Primary map



X Index: 220

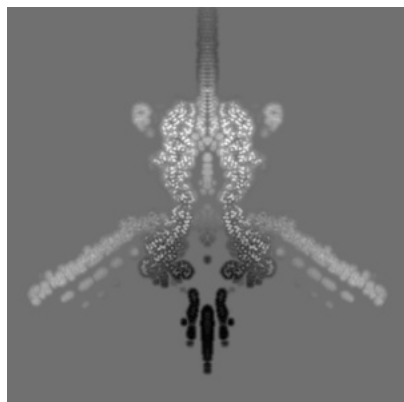


Y Index: 220

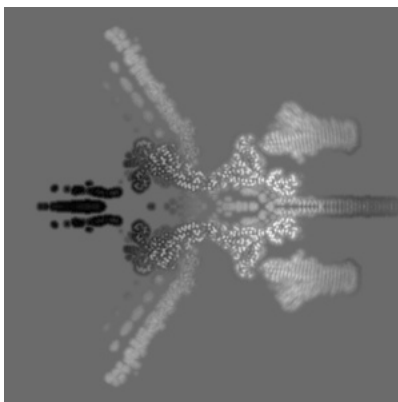


Z Index: 220

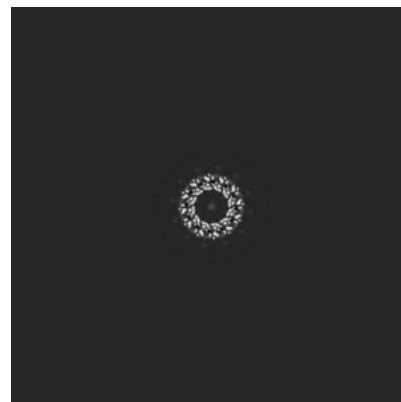
6.2.2 Raw map



X Index: 220



Y Index: 220

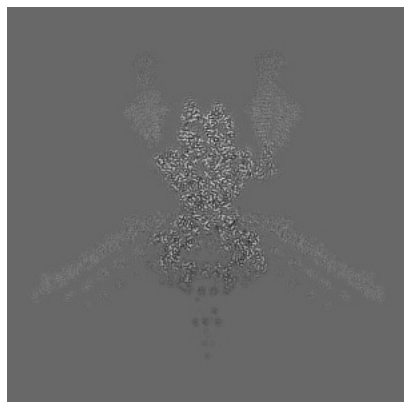


Z Index: 220

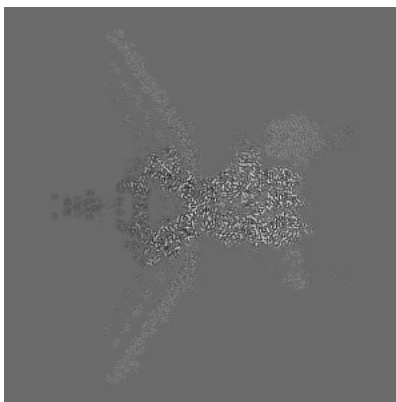
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

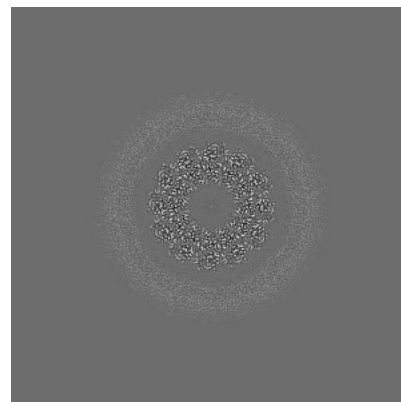
6.3.1 Primary map



X Index: 244



Y Index: 241

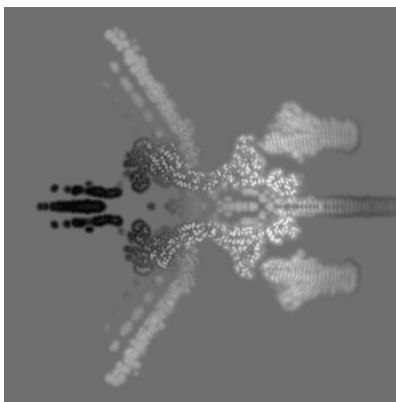


Z Index: 182

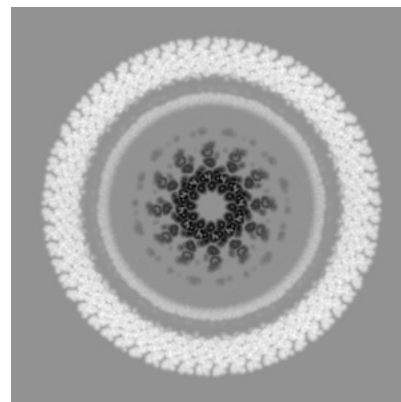
6.3.2 Raw map



X Index: 236



Y Index: 221

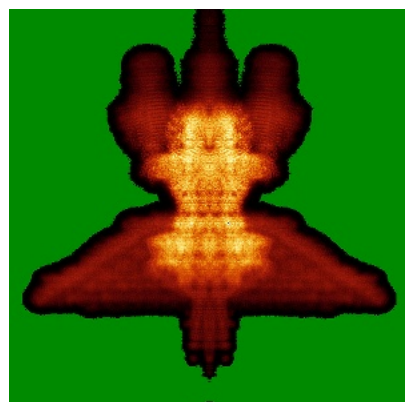


Z Index: 143

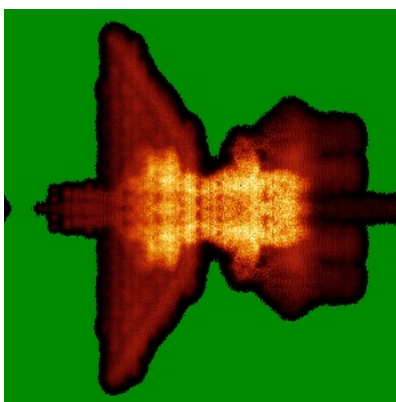
The images above show the largest variance slices of the map in three orthogonal directions.

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

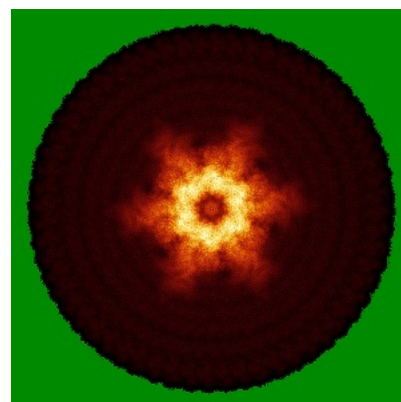
6.4.1 Primary map



X

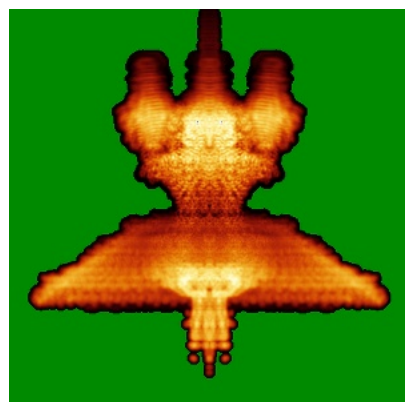


Y

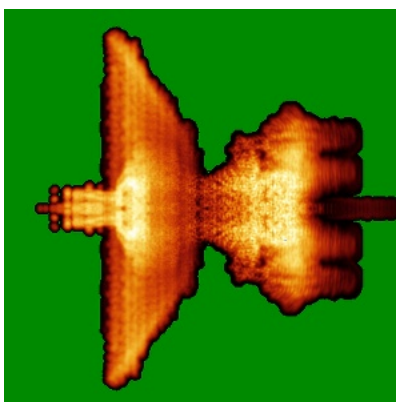


Z

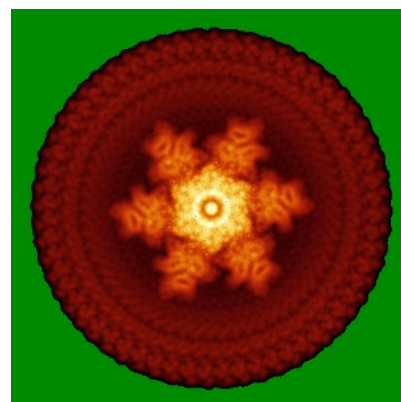
6.4.2 Raw map



X



Y

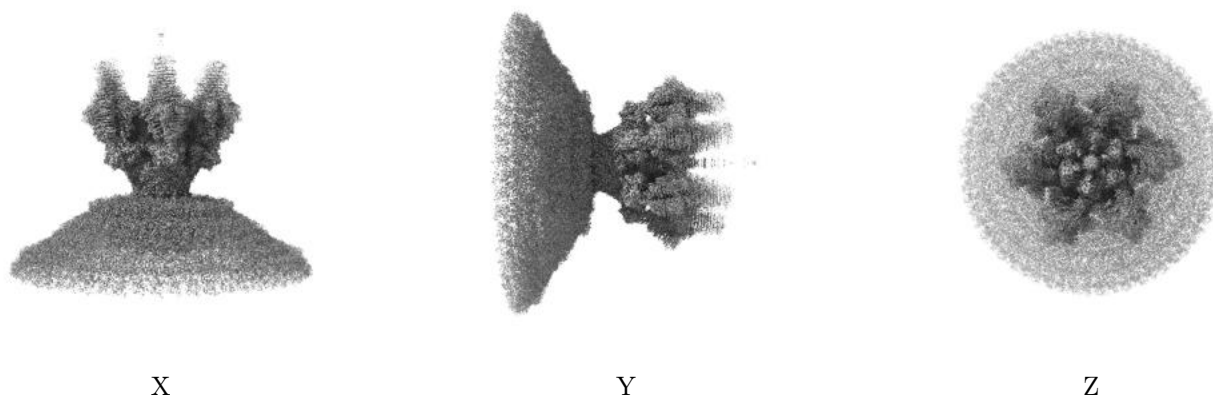


Z

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.

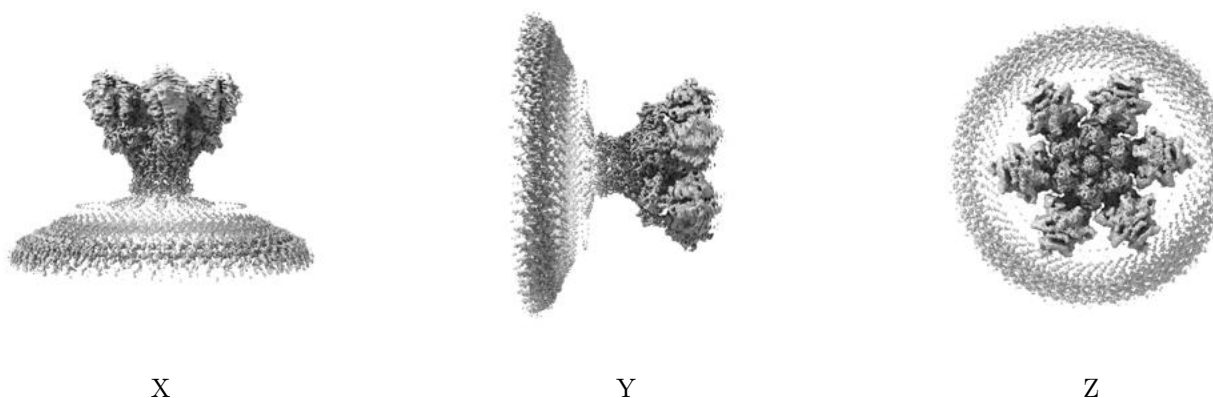
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. 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.

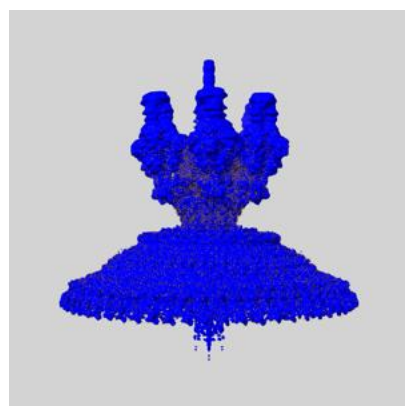
6.6 Mask visualisation [i](#)

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

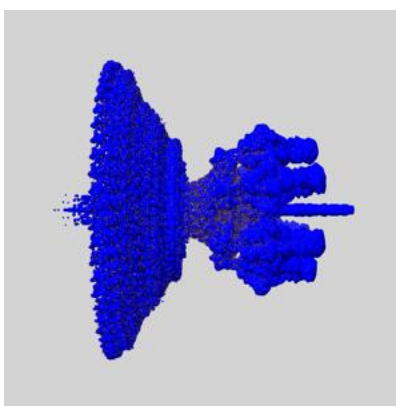
A mask typically either:

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

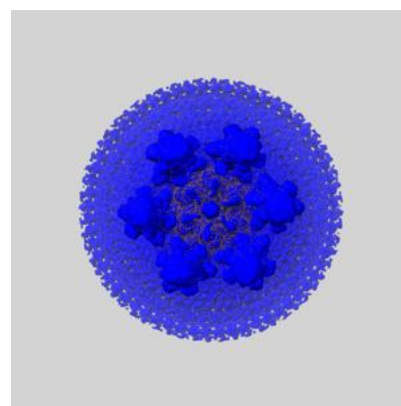
6.6.1 emd_41649_msk_1.map [i](#)



X



Y

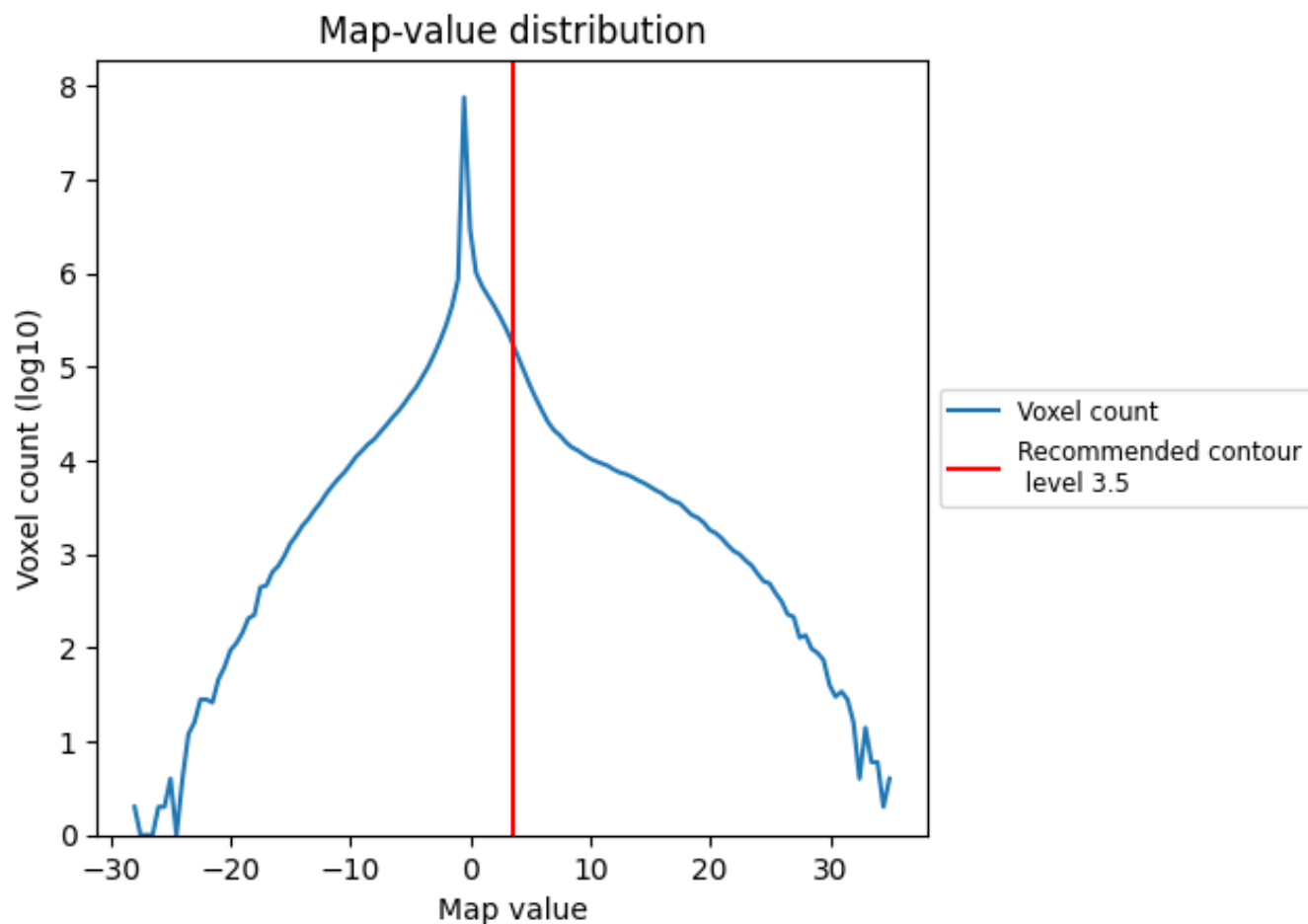


Z

7 Map analysis [i](#)

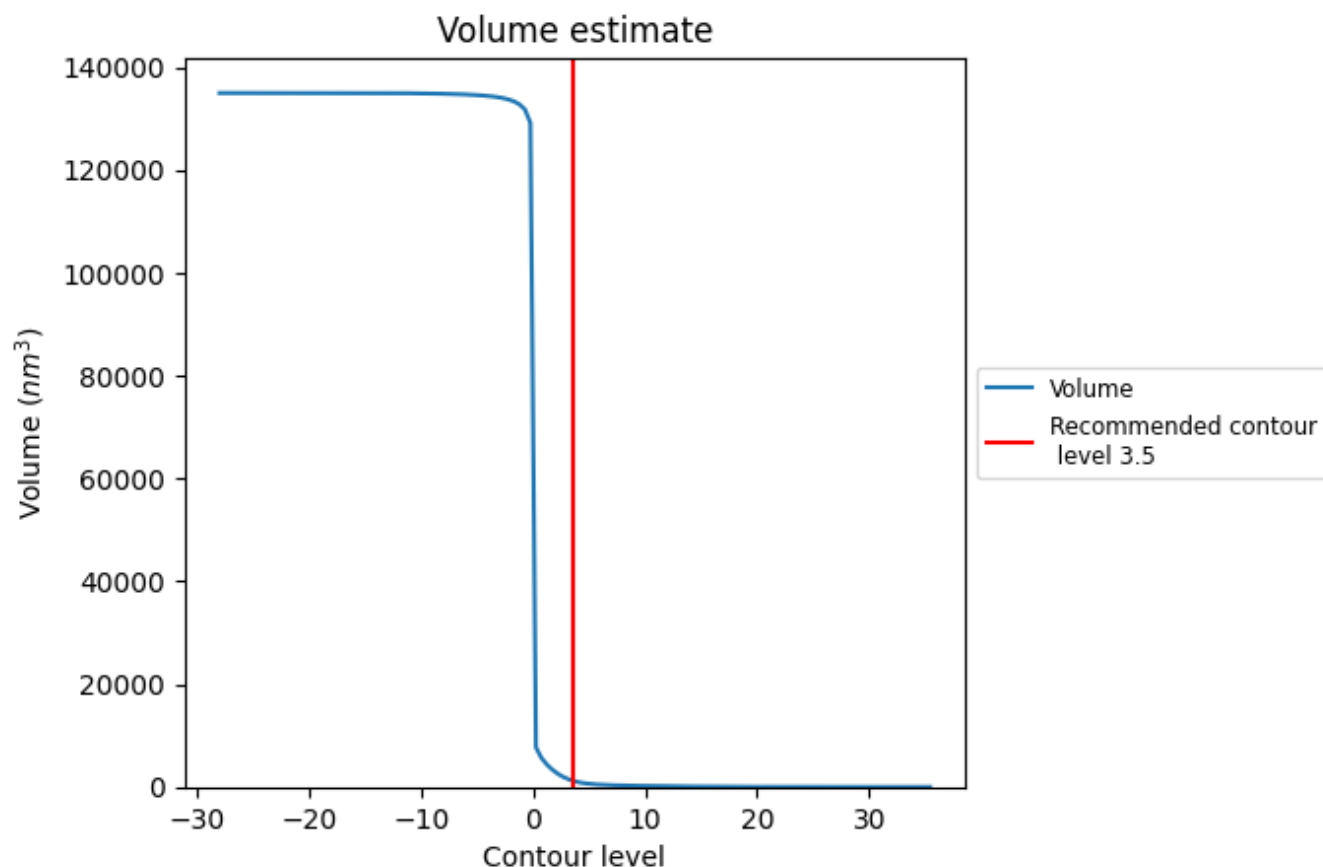
This section contains the results of statistical analysis of the map.

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.

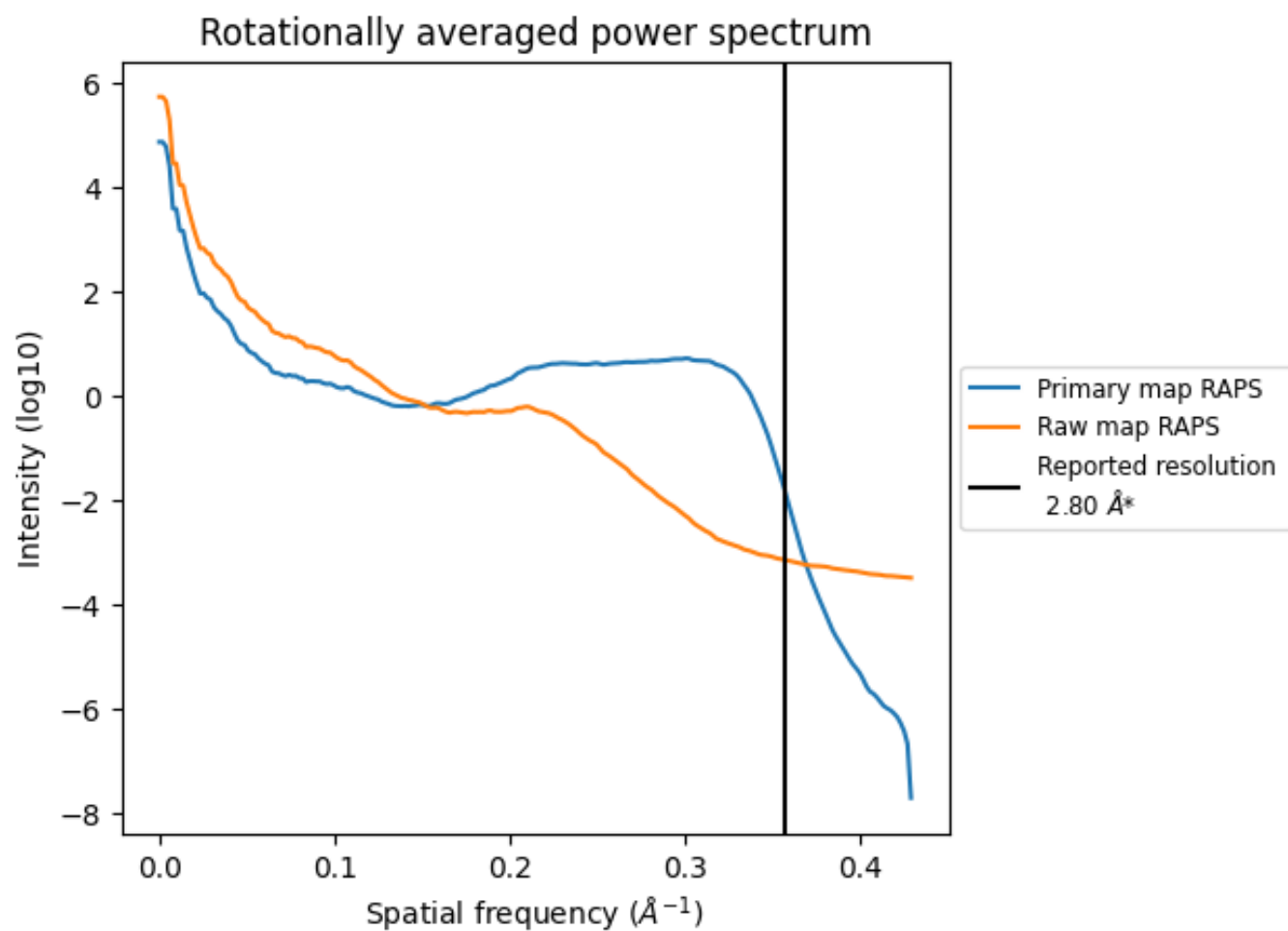
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1261 nm³; this corresponds to an approximate mass of 1139 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 ⓘ

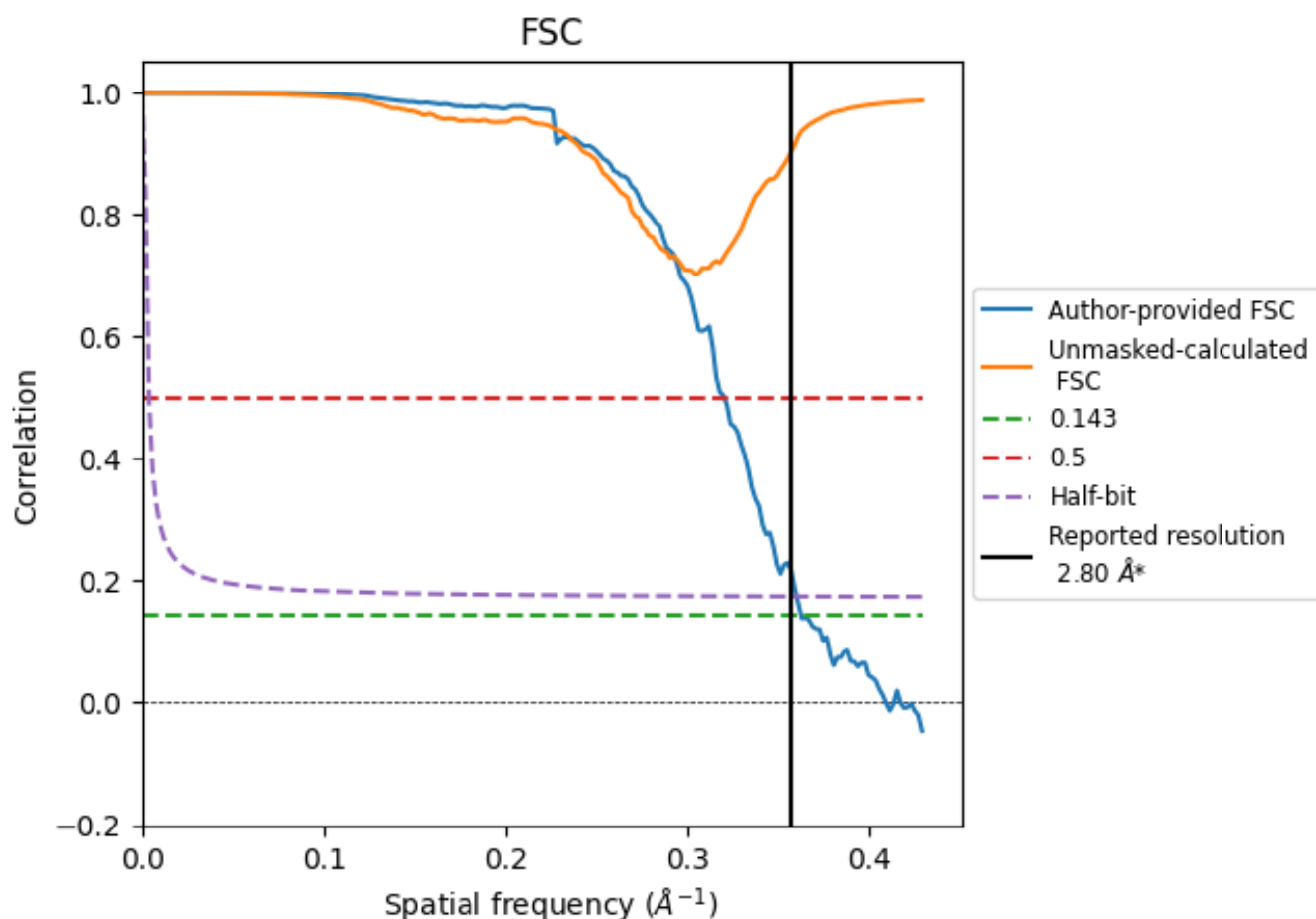


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

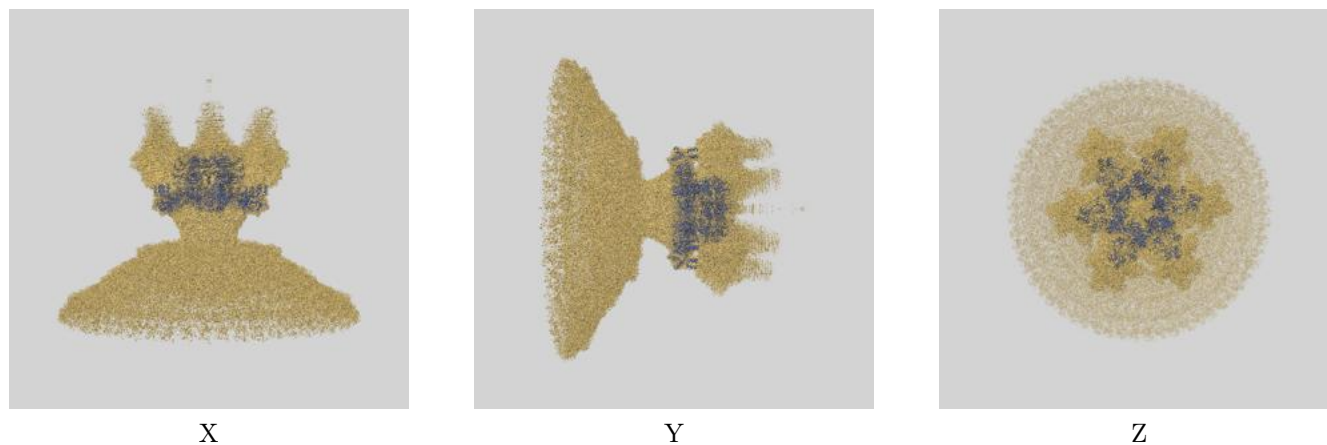
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.12	2.78
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

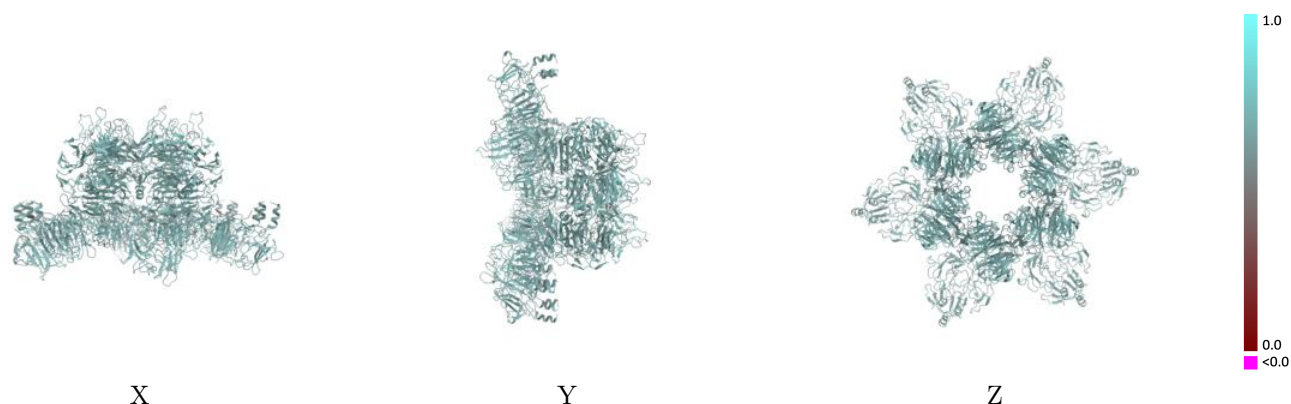
This section contains information regarding the fit between EMDB map EMD-41649 and PDB model 8TVR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



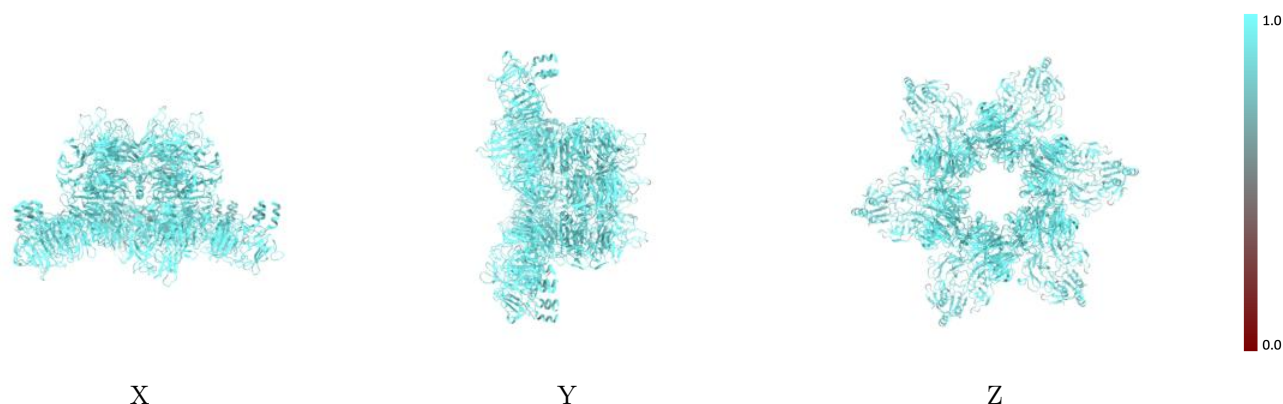
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



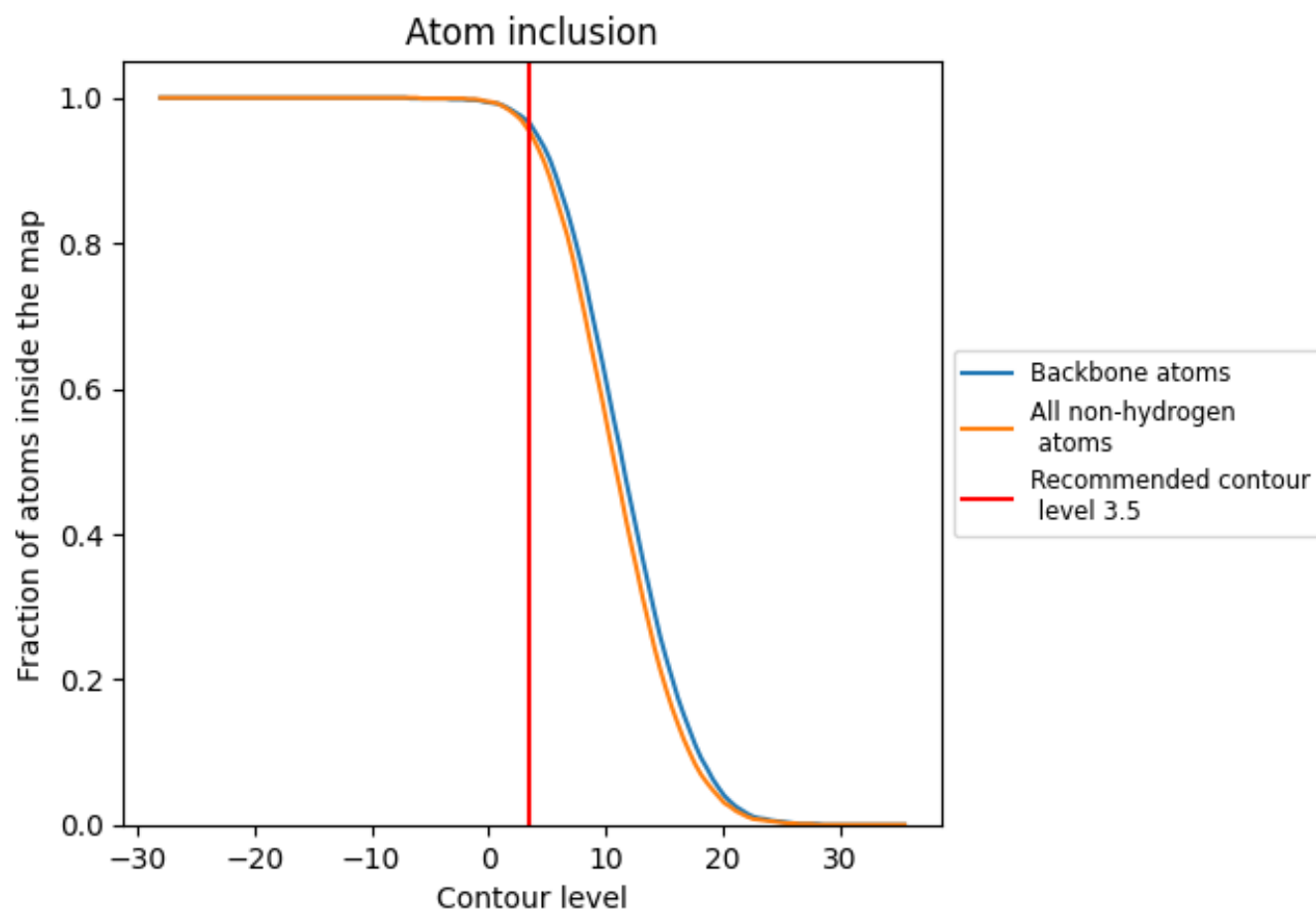
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.6270
A	 0.8980	 0.6060
B	 0.9520	 0.6230
C	 0.9510	 0.6290
D	 0.8940	 0.6060
E	 0.9520	 0.6250
F	 0.9530	 0.6280
G	 0.9680	 0.6320
H	 0.8990	 0.6080
I	 0.9470	 0.6270
J	 0.9530	 0.6280
K	 0.9690	 0.6340
L	 0.8990	 0.6070
M	 0.9490	 0.6260
N	 0.9520	 0.6300
O	 0.9670	 0.6340
P	 0.8910	 0.6080
Q	 0.9510	 0.6230
R	 0.9510	 0.6310
S	 0.9670	 0.6330
T	 0.9680	 0.6310
V	 0.8980	 0.6070
W	 0.9500	 0.6230
X	 0.9480	 0.6280
Y	 0.9680	 0.6330

