



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:02 AM UTC

PDB ID : 9VVR / pdb_00009vvr
EMDB ID : EMD-65388
Title : Structure of the bacteriophage E1004 tail
Authors : Sun, B.N.; Liu, H.R.
Deposited on : 2025-07-16
Resolution : 3.11 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

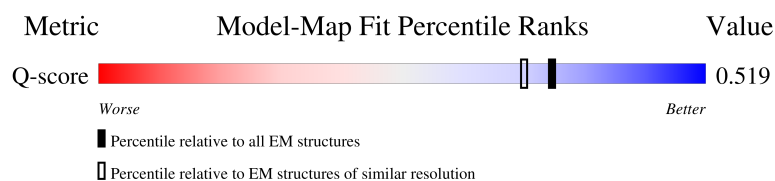
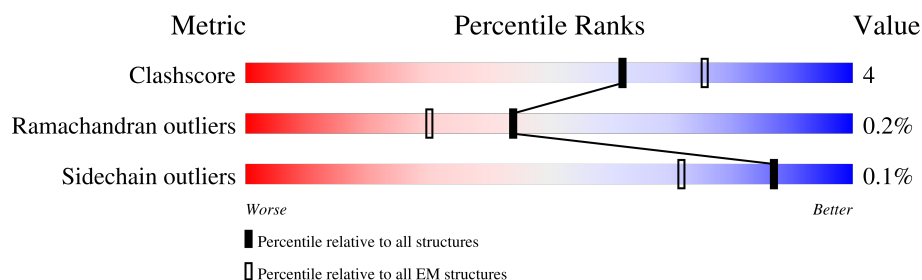
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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.



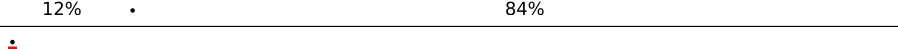
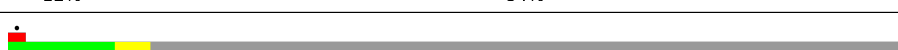
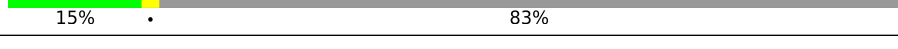
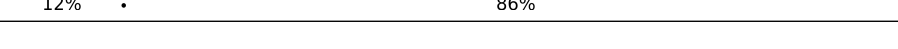
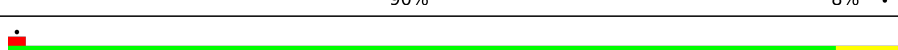
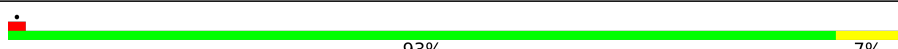
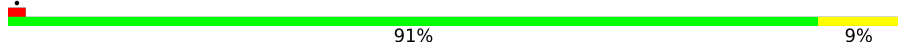
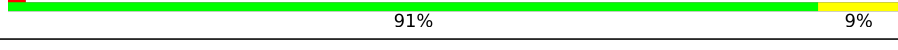
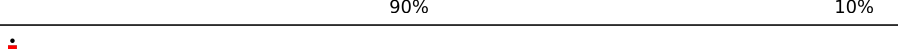
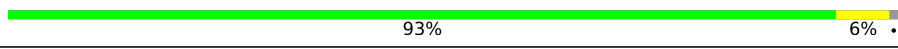
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14465 (2.61 - 3.61)

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	843	 12% 15% 12% 84% 84%
1	B	843	 12% 15% 12% 83% 83%
1	C	843	 12% 15% 12% 86% 86%
1	D	843	 12% 15% 12% 84% 84%

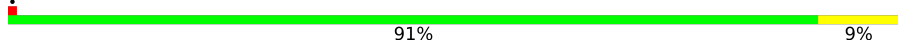
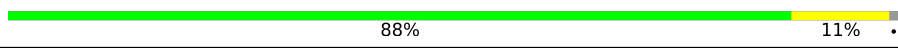
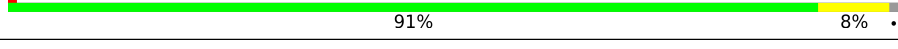
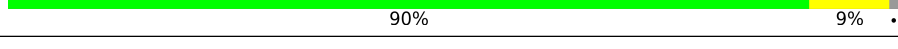
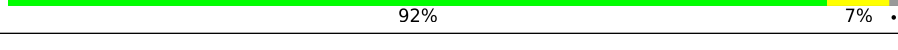
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Mol	Chain	Length	Quality of chain
1	E	843	
1	F	843	
1	G	843	
1	H	843	
1	I	843	
1	J	843	
1	K	843	
1	L	843	
1	M	843	
1	N	843	
1	O	843	
1	P	843	
1	Q	843	
1	R	843	
2	S	785	
2	V	785	
2	X	785	
2	Z	785	
2	b	785	
2	d	785	
3	T	188	
3	U	188	
3	W	188	
3	Y	188	
3	a	188	

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Mol	Chain	Length	Quality of chain
3	c	188	 91%9%
3	e	188	 91%9%
3	f	188	 88%11%.
3	g	188	 89%11%
3	h	188	 91%8%.
3	i	188	 90%9%.
3	j	188	 92%7%.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 72911 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	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	B	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	C	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	D	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	E	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	F	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	G	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	H	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	I	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	J	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	K	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	L	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		
1	M	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	N	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	O	121	Total	C	N	O	S	0	0
			956	596	166	192	2		
1	P	131	Total	C	N	O	S	0	0
			1017	629	178	208	2		
1	Q	140	Total	C	N	O	S	0	0
			1092	672	193	225	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	121	Total	C	N	O	S	0	0
			956	596	166	192	2		

- Molecule 2 is a protein called Nozzle protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	776	Total	C	N	O	S	0	0
			6048	3831	1027	1177	13		
2	V	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	X	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	Z	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	b	784	Total	C	N	O	S	0	0
			6101	3862	1036	1190	13		
2	d	780	Total	C	N	O	S	0	0
			6069	3842	1031	1183	13		

- Molecule 3 is a protein called Adaptor protein.

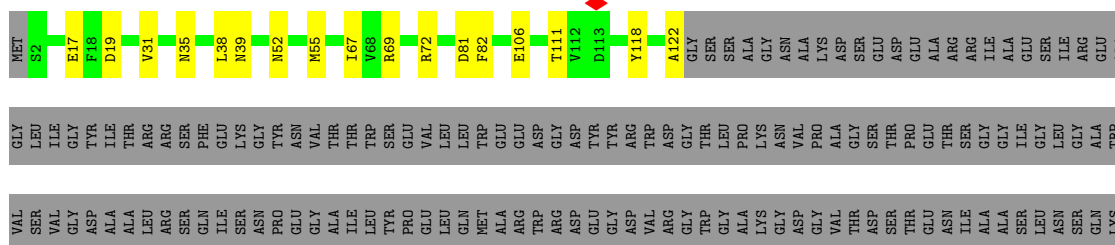
Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	U	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	W	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	Y	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	a	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	c	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	e	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	f	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	g	188	Total	C	N	O	S	0	0
			1504	944	251	299	10		
3	h	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	i	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		
3	j	187	Total	C	N	O	S	0	0
			1496	939	250	298	9		

Chain B: 15% 83%

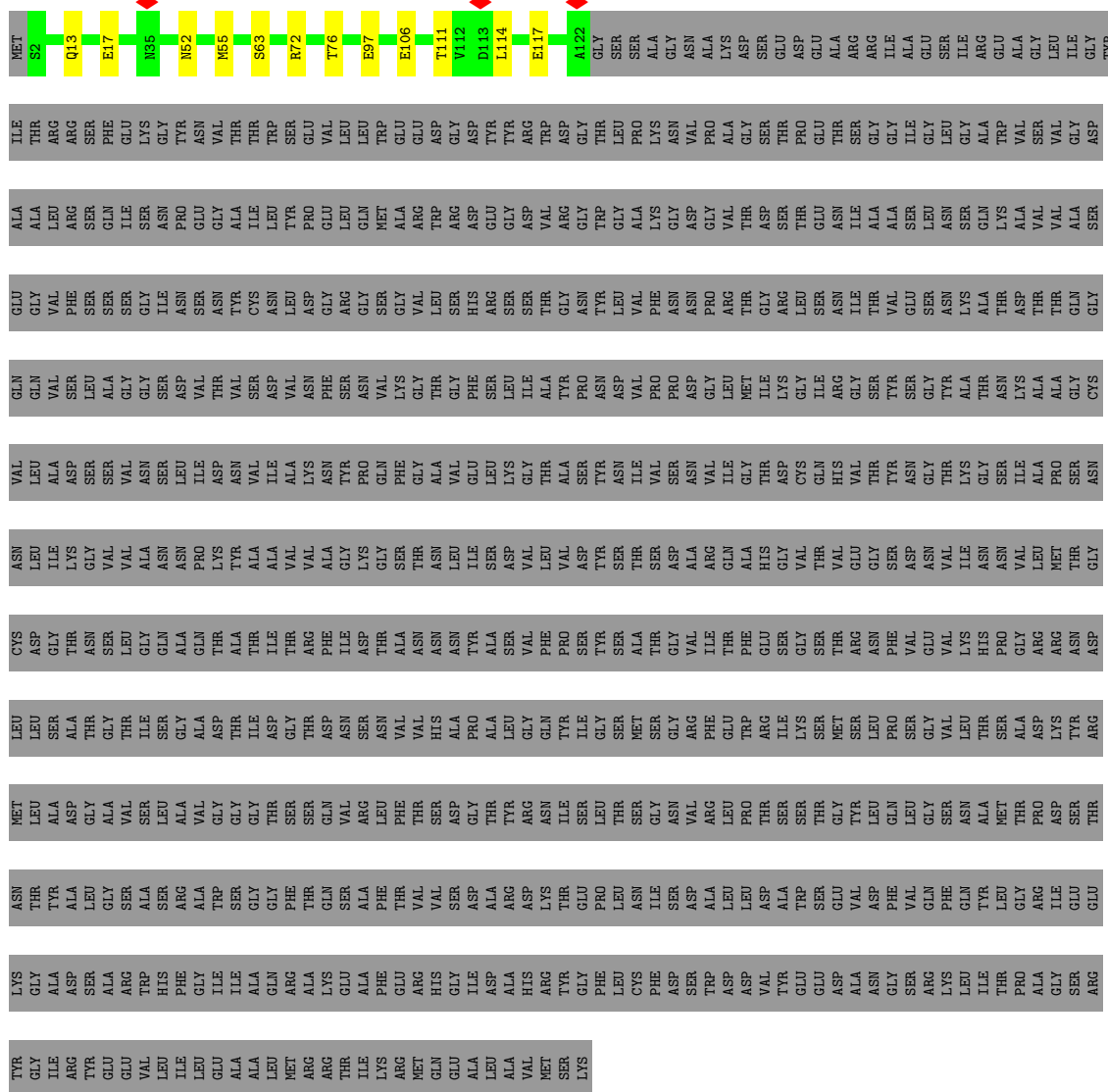


- Molecule 1: Tail spike protein

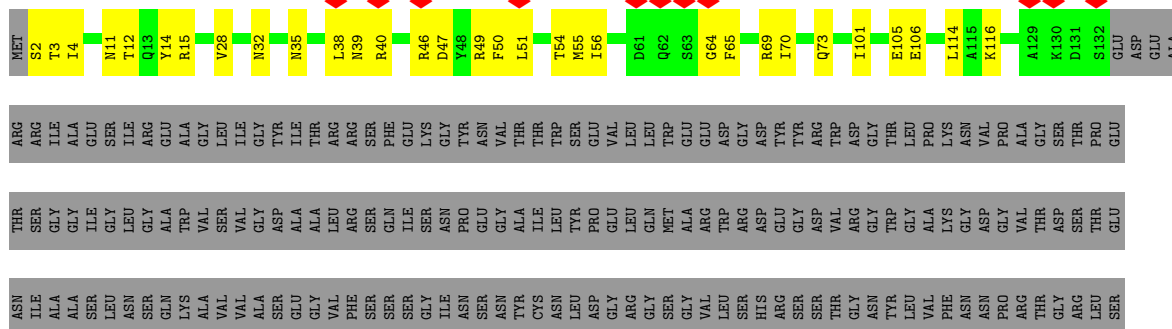
[illegible]

- Molecule 1: Tail spike protein

13% 86%

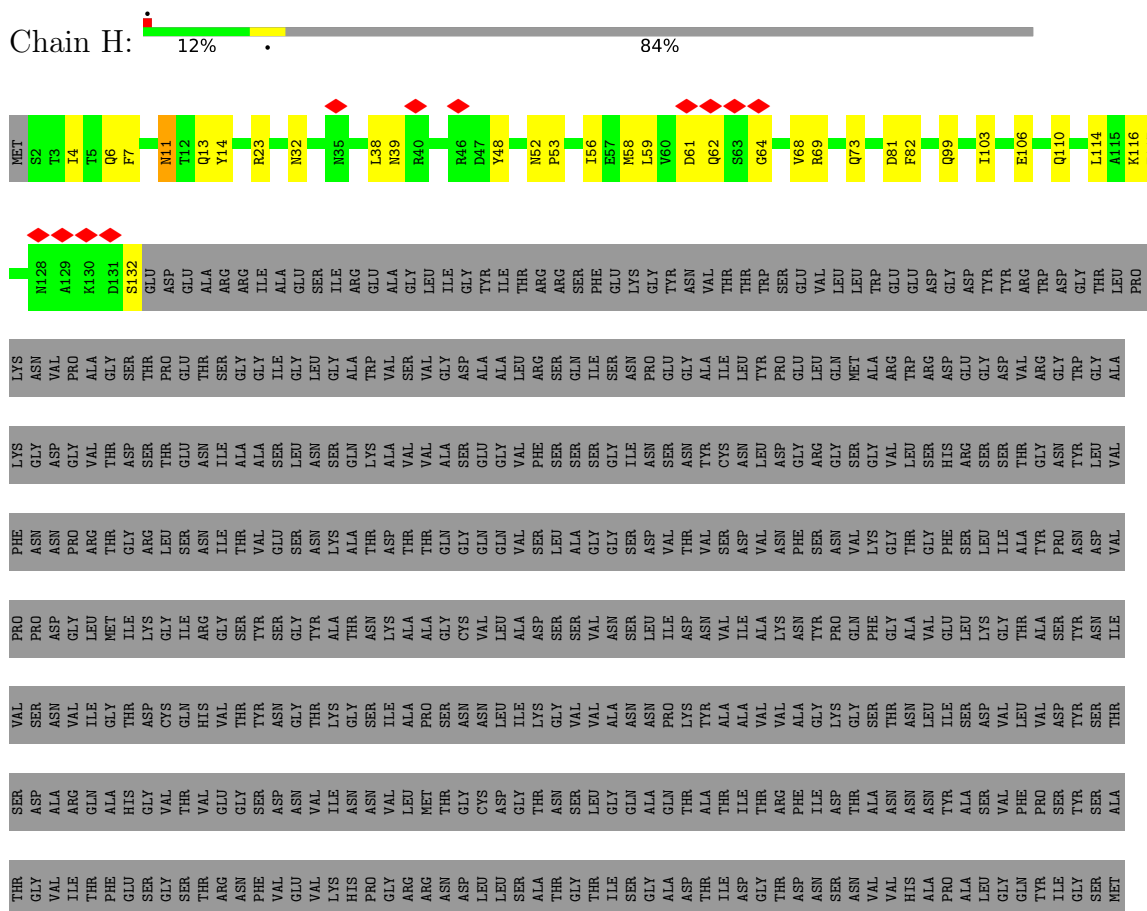


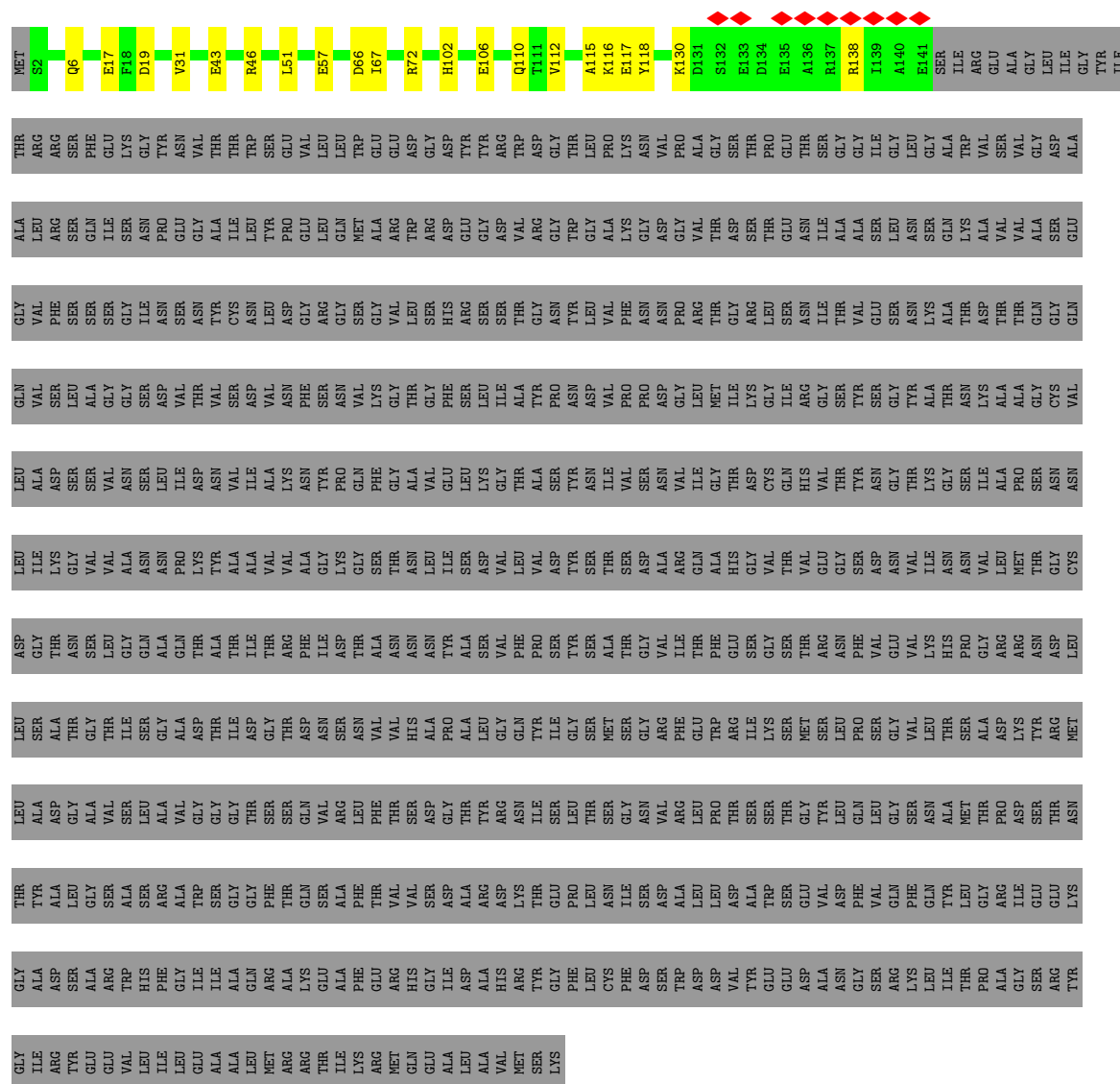
Chain G: 12% 84%



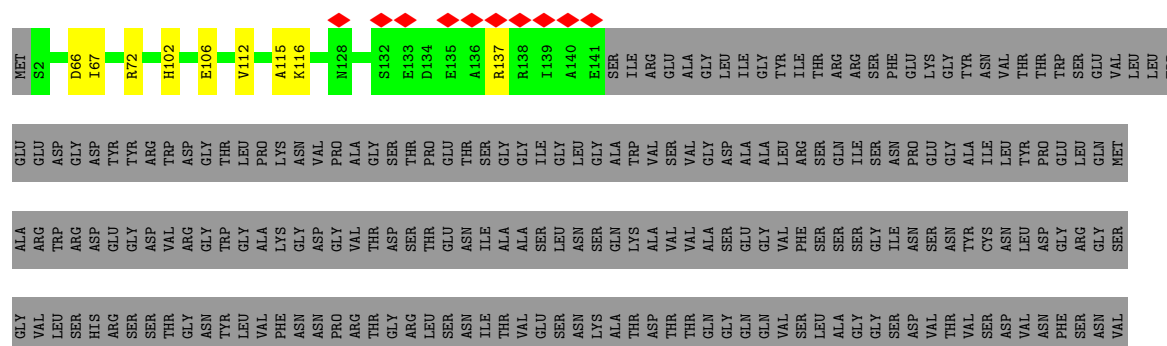
[illegible]

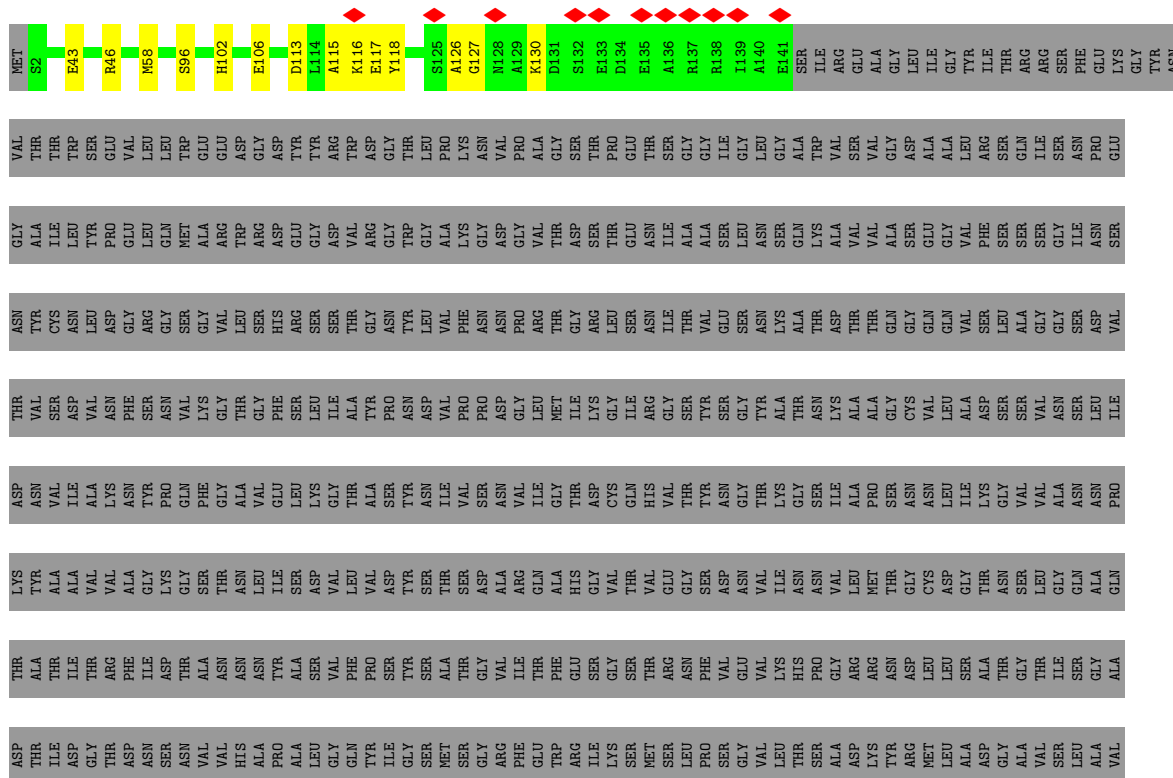
- Molecule 1: Tail spike protein





Chain K: 16% 83%





[illegible]

- Molecule 1: Tail spike protein

[illegible]

- Molecule 1: Tail spike protein







[illegible]

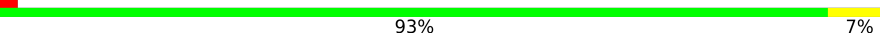
- Molecule 1: Tail spike protein

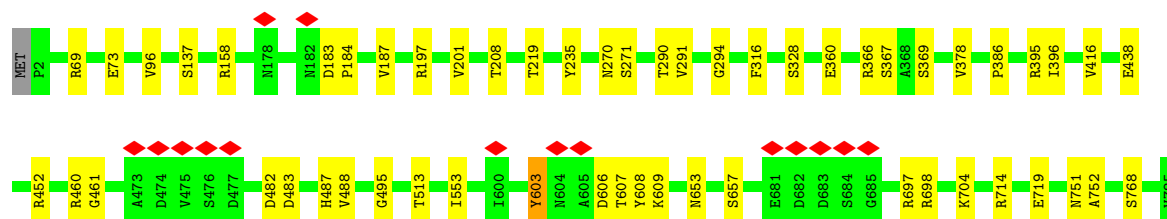


LEU	GLY	ALA	VAL	ALA	GLN	PRO	ILE	VAL	SER	GLU	ASN	ASN	MET
GLU	ILE	TRP	GLY	ASP	THR	LYS	ASP	THR	ASN	GLY	VAL	THR	S2
ALA	ILE	SER	GLY	ILE	ALA	TYR	ASN	VAL	TYR	ALA	THR	THR	Y14
LEU	GLN	GLY	THR	ASP	ILE	ALA	ILE	ASP	CYS	LEU	TRP	SER	E17
MET	ARG	PHE	SER	SER	THR	VAL	LYS	VAL	LEU	TYR	GLU	GLU	E43
ARG	ALA	THR	SER	GLN	ARG	ALA	ASN	ASN	ASP	PRO	VAL	VAL	E43
GLU	LYS	GLN	GLN	VAL	PHE	VAL	ASN	PHE	GLY	GLU	VAL	LEU	R46
ILE	ALA	ALA	ARG	ASN	ASP	LYS	PRO	ASN	GLY	GLN	LEU	LEU	R46
LYS	PHE	THR	LEU	ASN	THR	GLY	GLN	VAL	SER	MET	TRP	TRP	M65
ARG	GLU	THR	PHE	VAL	ALA	SER	PHE	LYS	GLY	ALA	GLU	GLU	M65
MET	ARG	VAL	THR	VAL	ASN	THR	GLY	GLY	VAL	ARG	GLU	GLU	M68
GLN	HIS	VAL	SER	HIS	ASN	ASN	ASN	ALA	LEU	TRP	ASP	ASP	M68
GLU	GLY	SER	ASP	ASP	ASN	LEU	VAL	GLY	SER	ARG	GLY	GLY	H102
ALA	ILE	ASP	GLY	PRO	TYR	ILE	GLU	PHE	HIS	ASP	ASP	ASP	H102
LEU	ASP	ALA	THR	ALA	ALA	SER	LEU	SER	ARG	GLU	TVR	TVR	E106
ALA	ALA	ARG	TVR	LEU	SER	ASP	GLY	ILE	SER	GLY	TVR	TVR	E106
VAL	HIS	ASP	ARG	GLY	VAL	VAL	GLY	ILE	SER	ASP	ARG	ARG	E106
VAL	ARG	LYS	ASN	GLN	PHE	LEU	THR	ALA	THR	VAL	TRP	TRP	V112
MET	ARG	THR	ILE	TYR	PRO	VAL	SER	TYR	GLY	ARG	ASP	ASP	D113
SER	LYS	THR	SER	ILE	SER	ASP	ALA	PRO	ASN	GLY	GLY	GLY	L114
GLY	GLY	GLU	SER	GLY	TYR	TYR	TYR	ASN	TYR	TRP	THR	THR	A115
PHE	LEU	PRO	LEU	GLY	THR	SER	ASN	ASP	LEU	GLY	LEU	LEU	K116
LEU	THR	LEU	THR	SER	ALA	THR	ILE	VAL	VAL	ALA	PRO	PRO	K116
CYS	SER	ASN	SER	MET	ALA	THR	ILE	VAL	VAL	ALA	PRO	PRO	K116
PHE	GLY	ILE	GLY	GLY	THR	SER	THR	VAL	PHE	LYS	LYS	LYS	D120
ASP	ASP	ASN	ASN	GLY	GLY	ASP	ASP	PRO	ASN	ASP	ASN	ASN	D120
ASP	SER	SER	VAL	ARG	VAL	ALA	VAL	GLY	PRO	GLY	VAL	VAL	A129
TRP	ALA	ALA	ARG	PHE	ILE	ARG	ASN	GLY	PRO	GLY	VAL	ALA	A129
LEU	LEU	GLU	LEU	GLU	THR	GLN	ILE	LEU	ARG	VAL	ALA	ALA	A129
ASP	ASP	PRO	PRO	TRP	PHE	GLU	GLY	MET	THR	THR	GLY	GLY	A129
VAL	VAL	THR	THR	ARG	GLU	HIS	THR	ILE	GLY	ASP	SER	SER	S132
TRP	ALA	SER	SER	ILE	SER	GLY	ASP	LYS	ARG	SER	THR	THR	E133
GLU	GLU	THR	THR	THR	SER	VAL	CYS	GLY	LEU	THR	PRO	PRO	D134
ASP	GLU	GLU	GLY	MET	THR	VAL	GLN	ILE	SER	GLU	GLU	GLU	E135
VAL	VAL	VAL	TYR	SER	ARG	GLU	VAL	GLY	ILE	ILE	SER	THR	E135
ASN	ASN	ASP	LEU	LEU	ASN	GLY	THR	THR	THR	ALA	SER	SER	A136
PHE	GLY	PHE	GLN	PRO	PHE	SER	TYR	TYR	VAL	ALA	GLY	GLY	R137
SER	SER	VAL	LEU	SER	VAL	ASN	ASN	ASN	GLU	SER	ILE	ILE	R138
ARG	ARG	GLN	GLY	GLY	GLU	ASN	GLY	GLY	SER	LEU	GLY	GLY	I139
LYS	LYS	PHE	SER	VAL	VAL	VAL	THR	TYR	SER	ASN	LEU	LEU	A140
ILE	ILE	GLN	ASN	LEU	LYS	ILE	THR	ALA	LYS	SER	GLY	GLY	E141
THR	THR	LEU	ALA	PRO	HIS	ASN	GLY	THR	ALA	GLN	ALA	ALA	SER
PRO	GLY	LEU	MET	VAL	PRO	ASN	SER	ASN	LYS	LYS	TRP	TRP	ILE
ALA	ALA	ARG	PRO	ALA	GLY	VAL	ILE	ASP	ALA	VAL	VAL	VAL	ARG
GLY	GLY	ILE	ASP	LYS	ARG	MET	ALA	THR	GLN	VAL	VAL	VAL	ALA
SER	SER	GLU	SER	THR	ASN	THR	SER	THR	GLN	ALA	GLY	GLY	ALA
ARG	ARG	GLU	THR	THR	ASP	CYS	ASN	ASP	SER	SER	ASP	ASP	LEU
TYR	TYR	GLY	THR	THR	LEU	GLY	ASN	GLY	GLY	GLY	GLY	GLY	LEU
ILE	ILE	ALA	TYR	ALA	SER	GLY	ILE	ALA	VAL	VAL	VAL	VAL	GLY
ARG	ARG	ASP	ALA	ASP	ALA	THR	LYS	ASP	SER	PHE	ARG	ARG	TYR
THR	THR	SER	LEU	GLY	THR	ASN	GLY	SER	LEU	SER	THR	THR	ILE
GLU	GLU	ALA	GLY	ALA	GLY	ASN	VAL	THR	SER	SER	SER	SER	THR
VAL	VAL	TRP	ALA	VAL	THR	LEU	VAL	VAL	GLY	GLY	ILE	ILE	GLY
ASN	ASN	HIS	SER	SER	ILE	GLN	ASN	SER	SER	ASN	ASN	ASN	TYR
PHE	ILE	PHE	SER	LEU	SER	ALA	ASN	SER	SER	ILE	ASN	ASN	ILE
GLY	GLY	THR	ARG	ALA	GLY	GLY	ASN	PRO	GLY	GLY	GLY	GLY	GLY
LYS	LYS	THR	ARG	VAL	THR	GLN	ASN	VAL	ASP	ASP	ASN	ASN	GLY
GLU	GLU	ALA	GLY	VAL	ALA	ALA	THR	VAL	GLY	VAL	VAL	VAL	GLY
ALA	ALA	ARG	TVR	LEU	SER	ASP	GLY	ILE	SER	GLY	TVR	TVR	GLY
VAL	VAL	ASP	ARG	GLY	VAL	VAL	GLY	ILE	SER	GLY	ARG	ARG	GLY
VAL	ARG	LYS	ASN	GLN	PHE	LEU	THR	ALA	THR	VAL	TRP	TRP	GLY
MET	MET	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY
SER	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
LYS	LYS	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
ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
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VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
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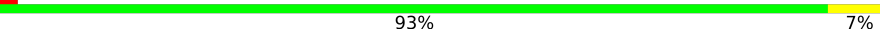
- Molecule 1: Tail spike protein

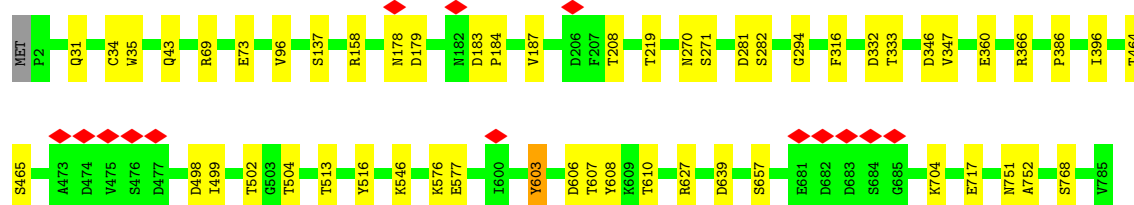


Chain V:  93% 7%



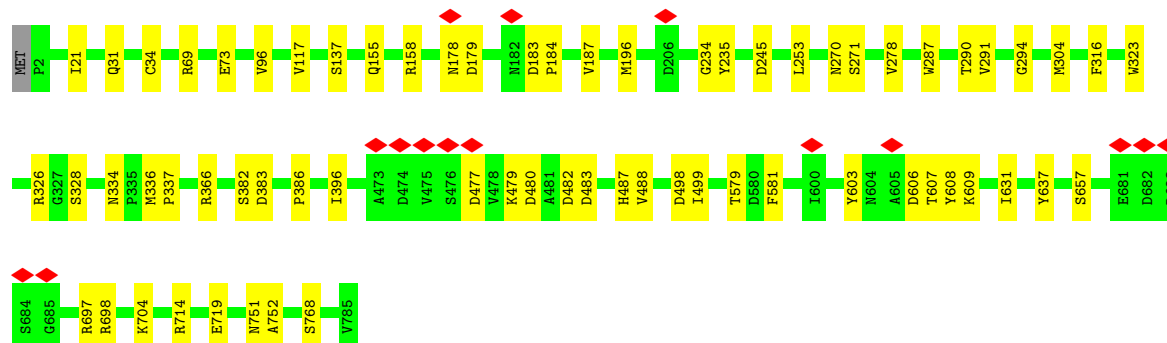
• Molecule 2: Nozzle protein

Chain X:  93% 7%



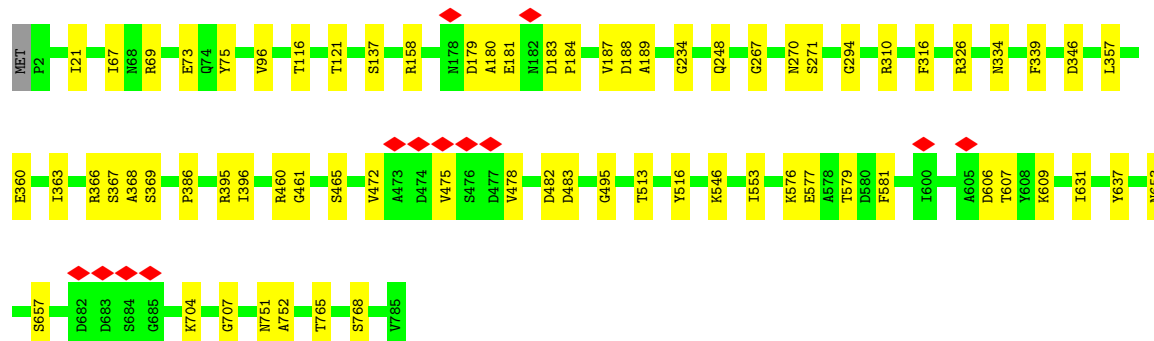
• Molecule 2: Nozzle protein

Chain Z:  91% 9%

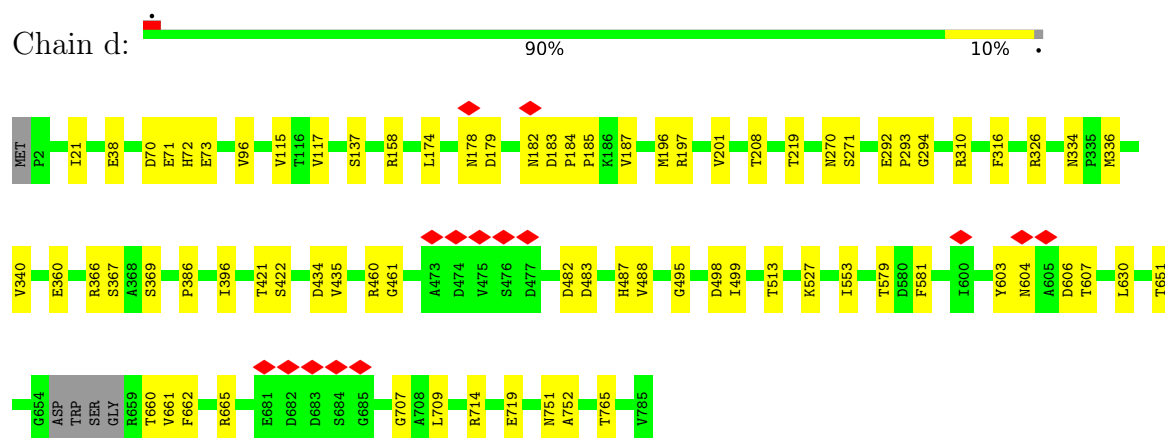


• Molecule 2: Nozzle protein

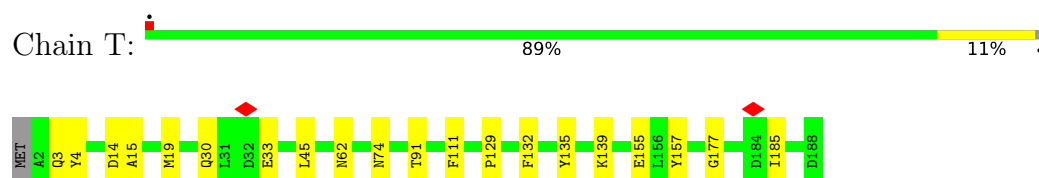
Chain b:  91% 9%



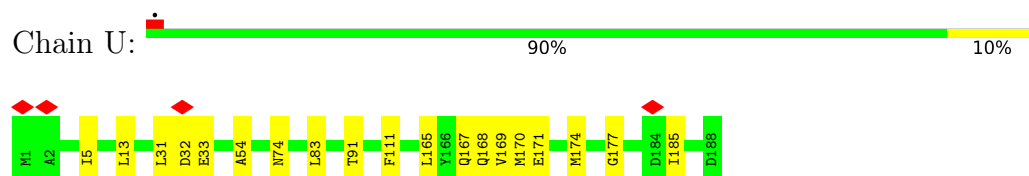
- Molecule 2: Nozzle protein



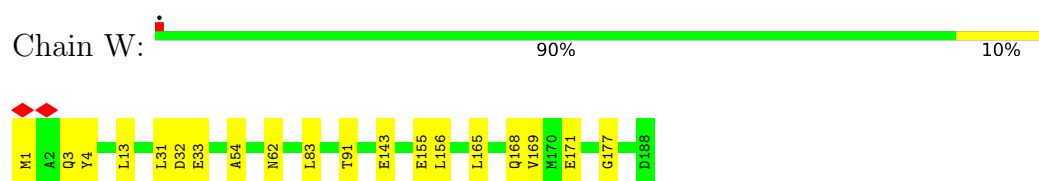
- Molecule 3: Adaptor protein



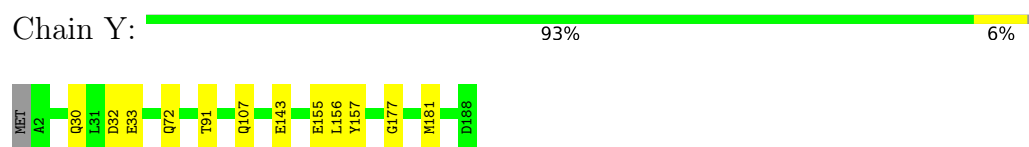
- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein

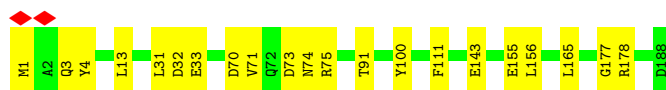


- Molecule 3: Adaptor protein

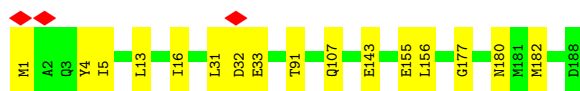
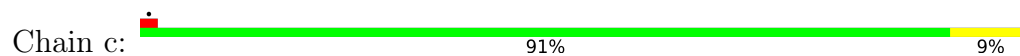


- Molecule 3: Adaptor protein





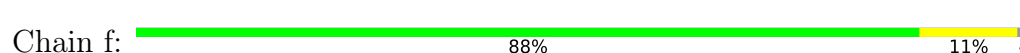
- Molecule 3: Adaptor protein



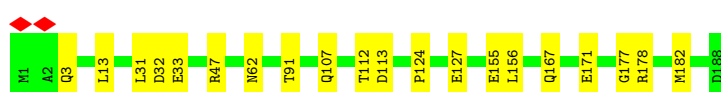
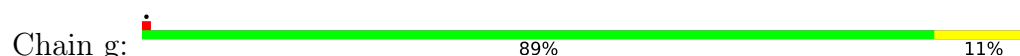
- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



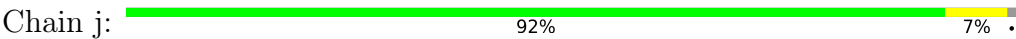
- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50105	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 ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.439	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.18	Depositor
Map size (Å)	484.0, 484.0, 484.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.34	0/1031	0.56	0/1400
1	B	0.18	0/1106	0.40	0/1500
1	C	0.14	0/970	0.31	0/1319
1	D	0.28	0/1031	0.51	0/1400
1	E	0.30	0/1106	0.53	0/1500
1	F	0.15	0/970	0.34	0/1319
1	G	0.19	0/1031	0.46	0/1400
1	H	0.35	0/1031	0.60	0/1400
1	I	0.19	0/1031	0.48	0/1400
1	J	0.17	0/1106	0.37	0/1500
1	K	0.16	0/1106	0.36	0/1500
1	L	0.16	0/1106	0.39	0/1500
1	M	0.15	0/970	0.36	0/1319
1	N	0.16	0/970	0.38	0/1319
1	O	0.17	0/970	0.42	0/1319
1	P	0.19	0/1031	0.46	0/1400
1	Q	0.17	0/1106	0.39	0/1500
1	R	0.15	0/970	0.35	0/1319
2	S	0.16	0/6184	0.37	0/8396
2	V	0.15	0/6239	0.36	0/8474
2	X	0.15	0/6239	0.36	0/8474
2	Z	0.19	0/6239	0.41	0/8474
2	b	0.15	0/6239	0.36	0/8474
2	d	0.18	0/6204	0.41	0/8424
3	T	0.14	0/1525	0.36	0/2069
3	U	0.15	0/1533	0.41	0/2079
3	W	0.15	0/1533	0.39	0/2079
3	Y	0.15	0/1525	0.35	0/2069
3	a	0.16	0/1533	0.39	0/2079
3	c	0.15	0/1533	0.40	0/2079
3	e	0.15	0/1533	0.38	0/2079
3	f	0.15	0/1525	0.36	0/2069
3	g	0.15	0/1533	0.38	0/2079
3	h	0.15	0/1525	0.37	0/2069

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	i	0.16	0/1525	0.37	0/2069
3	j	0.15	0/1525	0.37	0/2069
All	All	0.17	0/74334	0.39	0/100918

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	1017	0	986	23	0
1	B	1092	0	1055	11	0
1	C	956	0	932	11	0
1	D	1017	0	986	18	0
1	E	1092	0	1055	17	0
1	F	956	0	932	10	0
1	G	1017	0	986	20	0
1	H	1017	0	986	24	0
1	I	1017	0	986	26	0
1	J	1092	0	1055	14	0
1	K	1092	0	1055	6	0
1	L	1092	0	1055	10	0
1	M	956	0	932	13	0
1	N	956	0	932	11	0
1	O	956	0	932	15	0
1	P	1017	0	986	21	0
1	Q	1092	0	1055	11	0
1	R	956	0	932	10	0
2	S	6048	0	5900	41	0
2	V	6101	0	5949	32	0
2	X	6101	0	5949	31	0
2	Z	6101	0	5949	39	0
2	b	6101	0	5949	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	6069	0	5926	51	0
3	T	1496	0	1430	13	0
3	U	1504	0	1442	12	0
3	W	1504	0	1442	13	0
3	Y	1496	0	1430	15	0
3	a	1504	0	1442	15	0
3	c	1504	0	1442	12	0
3	e	1504	0	1442	12	0
3	f	1496	0	1430	19	0
3	g	1504	0	1442	15	0
3	h	1496	0	1430	12	0
3	i	1496	0	1430	11	0
3	j	1496	0	1430	10	0
All	All	72911	0	70692	613	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 4.

All (613) 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:d:630:LEU:HD11	2:d:661:VAL:HG11	1.16	1.09
2:d:630:LEU:CD1	2:d:661:VAL:HG11	1.85	1.05
2:d:661:VAL:HG12	2:d:662:PHE:N	1.87	0.87
2:d:661:VAL:HG12	2:d:662:PHE:H	1.42	0.83
1:A:32:ASN:HD22	1:A:38:LEU:HD23	1.44	0.81
2:d:630:LEU:CD1	2:d:661:VAL:CG1	2.61	0.77
3:a:70:ASP:OD1	3:a:71:VAL:N	2.18	0.77
1:B:115:ALA:HB1	1:C:111:THR:HG21	1.65	0.76
2:d:661:VAL:CG1	2:d:662:PHE:H	1.99	0.75
1:J:115:ALA:HB1	1:M:111:THR:HG21	1.69	0.74
1:J:130:LYS:HD2	1:M:122:ALA:HA	1.71	0.73
1:Q:115:ALA:HB1	1:R:111:THR:HG21	1.71	0.72
3:i:30:GLN:NE2	3:i:33:GLU:OE1	2.23	0.72
1:H:116:LYS:HE3	1:H:116:LYS:HA	1.72	0.72
1:H:38:LEU:HG	1:H:39:ASN:H	1.55	0.71
1:K:115:ALA:HB1	1:N:111:THR:HG21	1.72	0.71
2:V:290:THR:HG22	2:V:291:VAL:H	1.55	0.71
2:X:346:ASP:OD1	2:X:347:VAL:N	2.24	0.71
2:d:661:VAL:CG1	2:d:662:PHE:N	2.53	0.70
3:e:155:GLU:HG3	3:e:156:LEU:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:460:ARG:HG2	2:V:461:GLY:H	1.57	0.70
2:Z:290:THR:HG22	2:Z:291:VAL:H	1.55	0.70
2:V:607:THR:HG22	2:V:609:LYS:HD3	1.72	0.70
1:B:126:ALA:HB1	1:C:122:ALA:HB2	1.74	0.69
1:E:115:ALA:HB1	1:F:111:THR:HG21	1.74	0.69
1:I:32:ASN:ND2	1:I:64:GLY:O	2.25	0.69
3:W:143:GLU:OE2	3:i:161:GLN:NE2	2.26	0.69
1:Q:43:GLU:OE2	1:Q:46:ARG:NH2	2.26	0.68
1:L:43:GLU:OE2	1:L:46:ARG:NH2	2.27	0.67
2:S:346:ASP:OD2	2:S:347:VAL:N	2.28	0.67
2:X:516:TYR:HB3	2:X:546:LYS:HA	1.76	0.67
1:D:42:LEU:HD23	1:D:47:ASP:HB3	1.77	0.67
2:X:576:LYS:HG2	2:X:577:GLU:OE1	1.94	0.66
1:I:32:ASN:HD22	1:I:65:PHE:HA	1.60	0.66
1:L:115:ALA:HB1	1:O:111:THR:HG21	1.77	0.66
2:V:137:SER:OG	2:V:294:GLY:N	2.29	0.66
2:Z:137:SER:OG	2:Z:294:GLY:N	2.28	0.66
1:O:36:PRO:O	1:O:39:ASN:ND2	2.25	0.66
2:S:137:SER:OG	2:S:294:GLY:N	2.29	0.65
2:b:707:GLY:HA3	2:b:765:THR:HG21	1.77	0.65
2:V:328:SER:HB2	2:V:378:VAL:HG23	1.79	0.65
1:H:58:MET:HE1	1:H:61:ASP:HB2	1.76	0.65
2:X:137:SER:OG	2:X:294:GLY:N	2.30	0.65
3:c:13:LEU:HD13	3:c:31:LEU:HB2	1.79	0.65
3:U:170:MET:HG3	3:U:174:MET:HE3	1.79	0.65
3:W:155:GLU:HG3	3:W:156:LEU:H	1.63	0.64
2:Z:477:ASP:OD1	2:Z:479:LYS:NZ	2.30	0.64
1:H:32:ASN:N	1:H:39:ASN:OD1	2.24	0.64
1:H:32:ASN:ND2	1:H:64:GLY:O	2.29	0.64
2:X:627:ARG:NH2	2:X:639:ASP:OD2	2.31	0.63
2:d:707:GLY:HA3	2:d:765:THR:HG21	1.81	0.63
2:d:71:GLU:OE2	2:d:72:HIS:NE2	2.32	0.63
2:b:137:SER:OG	2:b:294:GLY:N	2.31	0.63
2:b:576:LYS:HG2	2:b:577:GLU:HG2	1.81	0.63
1:G:46:ARG:NH1	1:G:47:ASP:OD1	2.32	0.63
1:C:72:ARG:NE	1:C:106:GLU:OE2	2.31	0.62
1:I:4:ILE:HD11	1:I:69:ARG:HD2	1.80	0.62
2:S:19:PRO:HG2	2:S:22:LEU:HD12	1.82	0.62
3:h:155:GLU:HG3	3:h:156:LEU:H	1.65	0.62
1:I:6:GLN:HE22	1:I:69:ARG:HH21	1.48	0.61
1:P:116:LYS:HE3	1:P:116:LYS:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:606:ASP:OD1	2:d:607:THR:N	2.34	0.61
3:c:155:GLU:HG3	3:c:156:LEU:H	1.65	0.61
2:b:607:THR:HG22	2:b:609:LYS:HG2	1.83	0.61
3:f:88:ALA:O	3:g:178:ARG:NH2	2.33	0.61
1:P:12:THR:HA	1:P:58:MET:HE2	1.83	0.60
3:c:177:GLY:HA2	3:j:91:THR:HG22	1.83	0.60
3:T:30:GLN:NE2	3:T:33:GLU:OE1	2.30	0.60
2:X:606:ASP:OD1	2:X:607:THR:N	2.34	0.60
1:B:36:PRO:O	1:B:39:ASN:ND2	2.35	0.60
1:H:6:GLN:HB2	1:H:69:ARG:HH12	1.67	0.60
1:N:72:ARG:NE	1:N:106:GLU:OE1	2.34	0.60
2:S:173:LYS:NZ	2:S:174:LEU:O	2.34	0.60
2:b:366:ARG:HG2	2:b:386:PRO:HD3	1.83	0.59
2:b:482:ASP:OD1	2:b:483:ASP:N	2.35	0.59
2:d:178:ASN:OD1	2:d:179:ASP:N	2.35	0.59
1:A:39:ASN:HD22	1:A:40:ARG:H	1.51	0.59
2:S:137:SER:HG	2:S:294:GLY:H	1.50	0.59
2:S:60:SER:OG	2:S:61:ASN:N	2.35	0.59
2:Z:606:ASP:OD1	2:Z:607:THR:N	2.36	0.59
3:T:177:GLY:HA2	3:g:91:THR:HG22	1.84	0.59
1:J:43:GLU:OE2	1:J:46:ARG:NH2	2.36	0.58
2:X:137:SER:HG	2:X:294:GLY:H	1.50	0.58
3:Y:157:TYR:HE2	3:a:143:GLU:HG3	1.67	0.58
1:G:116:LYS:HE3	1:G:116:LYS:HA	1.86	0.58
2:X:366:ARG:HG2	2:X:386:PRO:HD3	1.86	0.58
3:U:91:THR:HG22	3:h:177:GLY:HA2	1.86	0.58
3:a:32:ASP:OD1	3:a:33:GLU:N	2.36	0.58
2:b:179:ASP:OD1	2:b:180:ALA:N	2.36	0.58
2:d:714:ARG:HG2	2:d:719:GLU:HG2	1.84	0.58
1:G:32:ASN:N	1:G:39:ASN:OD1	2.25	0.58
3:T:91:THR:HG22	3:U:177:GLY:HA2	1.85	0.58
1:D:31:VAL:HB	1:D:67:ILE:HG13	1.86	0.58
1:M:72:ARG:NE	1:M:106:GLU:OE2	2.36	0.58
1:R:36:PRO:O	1:R:39:ASN:ND2	2.37	0.58
2:S:606:ASP:OD1	2:S:607:THR:N	2.37	0.58
3:g:32:ASP:OD1	3:g:33:GLU:N	2.37	0.57
1:C:69:ARG:NH2	1:C:118:TYR:OH	2.29	0.57
3:c:143:GLU:HG3	3:f:157:TYR:HE2	1.69	0.57
1:P:36:PRO:O	1:P:39:ASN:ND2	2.36	0.57
3:T:3:GLN:CD	3:T:4:TYR:H	2.13	0.57
3:a:13:LEU:HD13	3:a:31:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:GLN:O	1:J:110:GLN:NE2	2.36	0.57
2:b:606:ASP:OD1	2:b:607:THR:N	2.37	0.57
3:c:107:GLN:OE1	3:f:62:ASN:ND2	2.36	0.57
1:A:32:ASN:HB3	1:A:38:LEU:HB3	1.87	0.57
3:W:32:ASP:OD1	3:W:33:GLU:N	2.34	0.57
3:h:14:ASP:OD1	3:h:15:ALA:N	2.38	0.56
1:I:38:LEU:HG	1:I:39:ASN:H	1.69	0.56
2:V:606:ASP:OD1	2:V:607:THR:N	2.38	0.56
1:D:92:ASP:OD1	1:D:93:LEU:N	2.38	0.56
3:W:13:LEU:HD13	3:W:31:LEU:HB2	1.87	0.56
3:a:178:ARG:NH2	3:i:88:ALA:O	2.39	0.56
3:f:14:ASP:OD1	3:f:15:ALA:N	2.39	0.56
1:D:6:GLN:HE22	1:D:69:ARG:HH21	1.53	0.56
1:E:43:GLU:OE1	1:E:46:ARG:NH2	2.38	0.56
1:N:35:ASN:HB3	1:N:38:LEU:HD13	1.87	0.56
1:E:58:MET:HE2	1:E:62:GLN:HE21	1.70	0.56
1:I:42:LEU:HD23	1:I:47:ASP:HB3	1.88	0.56
3:U:13:LEU:HD13	3:U:31:LEU:HB2	1.88	0.56
1:O:19:ASP:O	1:O:72:ARG:NH1	2.35	0.56
2:X:502:THR:HG22	2:X:504:THR:H	1.71	0.56
2:d:137:SER:OG	2:d:294:GLY:N	2.24	0.56
3:a:177:GLY:HA2	3:i:91:THR:HG22	1.88	0.56
1:M:15:ARG:HD2	1:M:55:MET:HE3	1.88	0.56
1:M:52:ASN:HD21	1:M:55:MET:HG3	1.71	0.55
1:D:52:ASN:HB3	1:D:55:MET:HB2	1.88	0.55
2:V:137:SER:HG	2:V:294:GLY:H	1.54	0.55
3:Y:91:THR:HG22	3:e:177:GLY:HA2	1.88	0.55
1:C:19:ASP:O	1:C:72:ARG:NH1	2.34	0.55
2:d:366:ARG:HG2	2:d:386:PRO:HD3	1.88	0.55
3:U:32:ASP:OD1	3:U:33:GLU:N	2.34	0.55
1:E:80:VAL:HG11	1:E:92:ASP:HB3	1.88	0.55
3:e:32:ASP:OD1	3:e:33:GLU:N	2.40	0.55
3:g:155:GLU:HG3	3:g:156:LEU:H	1.71	0.55
1:I:116:LYS:HE3	1:I:116:LYS:HA	1.89	0.55
1:R:72:ARG:NE	1:R:106:GLU:OE1	2.39	0.55
3:f:91:THR:HG22	3:g:177:GLY:HA2	1.88	0.55
3:W:177:GLY:HA2	3:h:91:THR:HG22	1.89	0.54
2:V:69:ARG:HB2	2:V:73:GLU:HB2	1.88	0.54
2:d:434:ASP:OD1	2:d:435:VAL:N	2.40	0.54
3:a:1:MET:HG2	3:a:3:GLN:H	1.72	0.54
1:R:31:VAL:HB	1:R:67:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:69:ARG:HB2	2:Z:73:GLU:HB2	1.90	0.54
3:c:91:THR:HG22	3:f:177:GLY:HA2	1.89	0.54
1:P:128:ASN:HA	1:P:131:ASP:OD2	2.08	0.54
2:V:197:ARG:O	2:V:201:VAL:HG23	2.07	0.54
2:X:513:THR:HA	2:X:516:TYR:HE1	1.72	0.54
2:b:69:ARG:HB2	2:b:73:GLU:HB2	1.88	0.54
1:J:112:VAL:O	1:J:116:LYS:HG2	2.08	0.54
1:O:113:ASP:O	1:O:116:LYS:HB2	2.08	0.54
2:d:158:ARG:HB2	2:d:174:LEU:HD12	1.89	0.53
3:f:70:ASP:OD1	3:f:71:VAL:N	2.38	0.53
1:M:42:LEU:HD23	1:M:47:ASP:HB3	1.91	0.53
1:A:42:LEU:HD23	1:A:47:ASP:HB3	1.90	0.53
2:Z:366:ARG:HG2	2:Z:386:PRO:HD3	1.90	0.53
3:T:14:ASP:OD1	3:T:15:ALA:N	2.42	0.53
3:f:107:GLN:OE1	3:g:62:ASN:ND2	2.38	0.53
2:b:73:GLU:OE1	2:b:310:ARG:NH1	2.41	0.53
2:Z:487:HIS:CD2	2:Z:488:VAL:HG13	2.44	0.53
3:W:54:ALA:HB2	3:W:83:LEU:HD13	1.91	0.52
1:E:131:ASP:OD1	1:E:132:SER:N	2.43	0.52
2:S:434:ASP:OD1	2:S:435:VAL:N	2.37	0.52
2:Z:751:ASN:OD1	2:Z:752:ALA:N	2.42	0.52
1:G:50:PHE:HE1	1:G:56:ILE:HD13	1.74	0.52
1:E:134:ASP:O	1:E:138:ARG:HG2	2.08	0.52
1:I:97:GLU:OE2	1:L:96:SER:HB2	2.10	0.52
2:S:366:ARG:HG2	2:S:386:PRO:HD3	1.89	0.52
2:X:69:ARG:HB2	2:X:73:GLU:HB2	1.91	0.52
1:C:81:ASP:OD1	1:C:82:PHE:N	2.43	0.52
1:M:31:VAL:HB	1:M:67:ILE:HB	1.92	0.52
2:Z:270:ASN:OD1	2:Z:271:SER:N	2.43	0.52
3:W:91:THR:HG22	3:i:177:GLY:HA2	1.92	0.52
2:b:475:VAL:HB	2:b:478:VAL:HG21	1.92	0.52
2:X:603:TYR:HD2	2:X:608:TYR:HA	1.74	0.52
2:Z:187:VAL:HG13	2:d:158:ARG:HH12	1.75	0.52
1:B:112:VAL:O	1:B:116:LYS:HE2	2.10	0.51
1:D:54:THR:O	1:D:55:MET:HE2	2.10	0.51
1:H:13:GLN:HA	1:H:13:GLN:HE21	1.75	0.51
1:P:49:ARG:HG3	1:P:57:GLU:OE2	2.09	0.51
1:G:32:ASN:ND2	1:G:64:GLY:O	2.34	0.51
3:a:155:GLU:HG3	3:a:156:LEU:H	1.75	0.51
2:S:395:ARG:HH11	2:S:395:ARG:HG3	1.76	0.51
2:S:495:GLY:HA3	2:S:513:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:630:LEU:HD12	2:d:661:VAL:CG1	2.38	0.51
3:i:124:PRO:HG2	3:i:127:GLU:HG3	1.92	0.51
1:B:72:ARG:NE	1:B:106:GLU:OE2	2.44	0.51
3:g:124:PRO:HG2	3:g:127:GLU:HG3	1.93	0.51
1:G:73:GLN:HA	1:G:106:GLU:OE2	2.11	0.51
1:H:48:TYR:HA	1:H:59:LEU:HD23	1.91	0.51
1:O:52:ASN:HB2	1:O:53:PRO:HD2	1.93	0.51
3:T:33:GLU:OE1	3:T:33:GLU:N	2.42	0.51
3:W:155:GLU:HG3	3:W:156:LEU:N	2.26	0.51
2:S:576:LYS:HG2	2:S:577:GLU:HG2	1.93	0.51
3:T:185:ILE:HG13	3:T:185:ILE:O	2.10	0.51
1:O:72:ARG:NE	1:O:106:GLU:OE2	2.44	0.51
1:K:112:VAL:O	1:K:116:LYS:HG2	2.10	0.51
2:S:460:ARG:HG2	2:S:461:GLY:H	1.76	0.50
3:U:54:ALA:HB2	3:U:83:LEU:HD13	1.93	0.50
3:i:166:TYR:CZ	3:i:170:MET:HE1	2.47	0.50
1:F:72:ARG:NE	1:F:106:GLU:OE1	2.44	0.50
1:I:29:THR:OG1	1:I:40:ARG:O	2.29	0.50
1:P:4:ILE:HD11	1:P:69:ARG:HD3	1.93	0.50
3:Y:177:GLY:HA2	3:a:91:THR:HG22	1.93	0.50
1:B:134:ASP:OD1	1:B:135:GLU:N	2.45	0.50
2:V:270:ASN:OD1	2:V:271:SER:N	2.44	0.50
2:V:751:ASN:OD1	2:V:752:ALA:N	2.45	0.50
2:Z:326:ARG:NH2	2:Z:334:ASN:O	2.43	0.50
2:b:495:GLY:HA3	2:b:513:THR:HG22	1.93	0.50
1:G:32:ASN:HD22	1:G:38:LEU:HD13	1.75	0.50
2:S:158:ARG:HB2	2:S:174:LEU:HD12	1.93	0.50
2:V:366:ARG:HG2	2:V:386:PRO:HD3	1.93	0.50
1:H:114:LEU:HD13	1:H:117:GLU:OE2	2.12	0.50
1:P:73:GLN:HA	1:P:106:GLU:OE2	2.11	0.50
3:f:124:PRO:HG2	3:f:127:GLU:OE1	2.12	0.50
1:A:69:ARG:HG3	1:A:69:ARG:HH11	1.76	0.50
3:e:103:ASP:OD2	3:e:105:SER:OG	2.26	0.50
2:b:631:ILE:HG13	2:b:637:TYR:HB3	1.94	0.49
3:Y:155:GLU:HG3	3:Y:156:LEU:H	1.76	0.49
1:G:4:ILE:HD11	1:G:69:ARG:HD3	1.93	0.49
1:I:32:ASN:N	1:I:39:ASN:OD1	2.28	0.49
1:O:31:VAL:HB	1:O:67:ILE:HB	1.94	0.49
2:V:96:VAL:HG22	2:V:316:PHE:HB2	1.93	0.49
3:W:168:GLN:HA	3:W:171:GLU:OE2	2.12	0.49
1:F:13:GLN:HB3	1:F:55:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:LEU:O	1:F:117:GLU:HG3	2.11	0.49
1:M:30:LEU:HG	1:M:42:LEU:HD11	1.94	0.49
2:S:707:GLY:HA3	2:S:765:THR:HG21	1.94	0.49
2:Z:697:ARG:O	2:Z:698:ARG:HD2	2.13	0.49
1:A:55:MET:HE3	1:A:55:MET:HA	1.95	0.49
1:E:31:VAL:HB	1:E:67:ILE:HB	1.95	0.49
1:P:29:THR:OG1	1:P:40:ARG:O	2.28	0.49
2:Z:137:SER:HG	2:Z:294:GLY:H	1.59	0.49
1:N:36:PRO:O	1:N:39:ASN:ND2	2.44	0.49
1:L:127:GLY:O	1:L:130:LYS:HG3	2.12	0.49
1:P:6:GLN:HE21	1:P:67:ILE:HB	1.77	0.49
2:Z:482:ASP:OD1	2:Z:483:ASP:N	2.46	0.49
2:b:609:LYS:HD3	2:b:653:ASN:HA	1.93	0.49
2:b:751:ASN:OD1	2:b:752:ALA:N	2.45	0.49
2:S:178:ASN:ND2	2:b:181:GLU:OE1	2.44	0.48
2:X:751:ASN:OD1	2:X:752:ALA:N	2.45	0.48
3:Y:143:GLU:HG2	3:e:157:TYR:CE2	2.48	0.48
3:f:30:GLN:NE2	3:f:33:GLU:O	2.44	0.48
3:f:168:GLN:HA	3:f:171:GLU:HG2	1.93	0.48
1:E:105:GLU:OE2	1:F:76:THR:HG23	2.13	0.48
2:V:609:LYS:HG3	2:V:653:ASN:HA	1.96	0.48
3:U:185:ILE:HG13	3:U:185:ILE:O	2.13	0.48
3:c:32:ASP:OD1	3:c:33:GLU:N	2.37	0.48
1:H:52:ASN:OD1	1:H:53:PRO:HD2	2.12	0.48
3:c:143:GLU:HG3	3:f:157:TYR:CE2	2.48	0.48
1:J:31:VAL:HB	1:J:67:ILE:HB	1.94	0.48
3:h:54:ALA:HB2	3:h:83:LEU:HD13	1.95	0.48
1:H:23:ARG:HH21	2:S:608:TYR:HD1	1.60	0.48
3:g:112:THR:HG23	3:g:113:ASP:OD1	2.13	0.48
1:K:72:ARG:NE	1:K:106:GLU:OE2	2.45	0.48
2:S:339:PHE:HD1	2:S:363:ILE:HD13	1.79	0.48
2:d:196:MET:HA	2:d:196:MET:HE2	1.95	0.48
1:D:23:ARG:HD2	1:D:50:PHE:HD2	1.79	0.48
1:H:99:GLN:O	1:H:103:ILE:HG13	2.13	0.48
2:V:697:ARG:O	2:V:698:ARG:HD2	2.13	0.48
1:G:32:ASN:OD1	1:G:65:PHE:HA	2.14	0.48
2:b:516:TYR:HD2	2:b:546:LYS:HB3	1.79	0.48
2:d:751:ASN:OD1	2:d:752:ALA:N	2.46	0.48
1:E:17:GLU:N	1:E:17:GLU:OE2	2.47	0.47
1:G:49:ARG:NH2	1:G:51:LEU:HD11	2.29	0.47
1:I:96:SER:HB2	1:O:97:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:135:TYR:CZ	3:T:139:LYS:HD2	2.49	0.47
3:T:74:ASN:HB3	3:T:111:PHE:O	2.14	0.47
1:A:131:ASP:OD1	1:A:132:SER:N	2.47	0.47
1:E:66:ASP:O	1:E:67:ILE:HD13	2.15	0.47
1:H:114:LEU:HA	1:H:117:GLU:OE2	2.14	0.47
1:K:66:ASP:OD2	1:K:67:ILE:HG13	2.14	0.47
1:P:110:GLN:O	1:P:114:LEU:HD23	2.14	0.47
1:R:17:GLU:N	1:R:17:GLU:OE2	2.47	0.47
2:X:96:VAL:HG22	2:X:316:PHE:HB2	1.96	0.47
1:H:7:PHE:O	1:H:68:VAL:N	2.39	0.47
1:D:81:ASP:OD1	1:D:82:PHE:N	2.48	0.47
1:I:99:GLN:O	1:I:103:ILE:HG13	2.14	0.47
1:J:19:ASP:O	1:J:72:ARG:NH1	2.46	0.47
2:S:275:GLU:OE1	2:S:275:GLU:N	2.47	0.47
2:S:311:GLN:NE2	2:S:317:GLU:OE2	2.47	0.47
2:X:332:ASP:OD1	2:X:333:THR:N	2.47	0.47
2:X:603:TYR:HB3	2:X:610:THR:HB	1.95	0.47
3:Y:157:TYR:CE2	3:a:143:GLU:HG3	2.47	0.47
1:A:30:LEU:HD22	1:A:68:VAL:HG12	1.97	0.47
1:A:52:ASN:OD1	1:A:53:PRO:HD2	2.15	0.47
2:Z:158:ARG:HD2	2:Z:234:GLY:HA3	1.96	0.47
1:C:31:VAL:HB	1:C:67:ILE:HB	1.97	0.47
1:D:80:VAL:HG11	1:D:92:ASP:HB2	1.96	0.47
1:Q:120:ASP:N	1:Q:120:ASP:OD1	2.47	0.47
1:Q:129:ALA:O	1:Q:133:GLU:HG3	2.15	0.47
2:d:460:ARG:HG2	2:d:461:GLY:H	1.79	0.47
2:S:631:ILE:HG13	2:S:637:TYR:HB3	1.97	0.47
2:b:248:GLN:NE2	2:b:267:GLY:O	2.47	0.47
2:b:360:GLU:OE1	2:b:360:GLU:N	2.48	0.47
3:g:13:LEU:HD13	3:g:31:LEU:HB2	1.96	0.47
1:E:66:ASP:OD1	1:E:67:ILE:HG12	2.15	0.46
1:H:11:ASN:HB2	1:H:14:TYR:HE2	1.80	0.46
2:S:751:ASN:OD1	2:S:752:ALA:N	2.48	0.46
2:b:346:ASP:HB3	2:b:357:LEU:HD12	1.96	0.46
1:G:54:THR:O	1:G:55:MET:HE2	2.15	0.46
1:G:101:ILE:O	1:G:105:GLU:OE1	2.33	0.46
1:H:73:GLN:HA	1:H:106:GLU:OE2	2.15	0.46
1:I:54:THR:O	1:I:55:MET:HE2	2.14	0.46
1:R:31:VAL:HA	1:R:39:ASN:OD1	2.14	0.46
2:X:704:LYS:O	2:X:768:SER:HB2	2.15	0.46
2:Z:196:MET:HE2	2:Z:196:MET:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:96:VAL:HG22	2:d:316:PHE:HB2	1.98	0.46
2:d:336:MET:HB3	2:d:340:VAL:HG21	1.97	0.46
2:Z:96:VAL:HG22	2:Z:316:PHE:HB2	1.98	0.46
2:d:197:ARG:O	2:d:201:VAL:HG23	2.15	0.46
1:P:54:THR:O	1:P:55:MET:HE2	2.15	0.46
2:V:495:GLY:HA3	2:V:513:THR:HG22	1.97	0.46
2:X:158:ARG:HH12	2:d:187:VAL:HG13	1.81	0.46
2:Z:382:SER:OG	2:Z:383:ASP:N	2.49	0.46
2:b:367:SER:O	2:b:369:SER:N	2.48	0.46
3:h:156:LEU:O	3:h:156:LEU:HD23	2.15	0.46
1:E:92:ASP:N	1:E:92:ASP:OD1	2.46	0.46
1:L:113:ASP:HA	1:L:116:LYS:NZ	2.30	0.46
1:M:52:ASN:OD1	1:M:55:MET:N	2.49	0.46
1:Q:14:TYR:O	1:Q:55:MET:HG3	2.16	0.46
2:Z:714:ARG:HG2	2:Z:719:GLU:HG2	1.96	0.46
2:b:472:VAL:HB	2:b:478:VAL:HG23	1.96	0.46
1:Q:58:MET:HE3	1:Q:58:MET:HB3	1.81	0.46
2:Z:336:MET:SD	2:Z:337:PRO:HD2	2.55	0.46
2:b:137:SER:HG	2:b:294:GLY:N	2.13	0.46
3:a:1:MET:N	3:a:4:TYR:O	2.43	0.46
3:i:61:ILE:HG23	3:i:118:GLU:OE2	2.16	0.46
1:J:6:GLN:OE1	3:Y:72:GLN:NE2	2.49	0.46
3:f:30:GLN:OE1	3:f:32:ASP:N	2.49	0.46
1:I:6:GLN:HE22	1:I:69:ARG:NH2	2.13	0.46
1:Q:112:VAL:O	1:Q:116:LYS:HG3	2.16	0.46
3:e:91:THR:HG22	3:j:177:GLY:HA2	1.98	0.46
1:D:102:HIS:O	1:D:104:ALA:N	2.49	0.45
1:G:2:SER:OG	1:G:3:THR:N	2.48	0.45
1:G:40:ARG:HA	1:G:40:ARG:NE	2.31	0.45
1:H:4:ILE:HD11	1:H:69:ARG:HD3	1.98	0.45
1:I:114:LEU:HD12	1:I:118:TYR:HE2	1.81	0.45
1:A:40:ARG:HD3	1:A:65:PHE:CZ	2.51	0.45
1:H:81:ASP:OD1	1:H:82:PHE:N	2.50	0.45
2:S:607:THR:O	2:S:609:LYS:HG2	2.16	0.45
2:b:339:PHE:HD1	2:b:363:ILE:HD13	1.81	0.45
2:d:73:GLU:OE1	2:d:310:ARG:NH1	2.50	0.45
3:Y:30:GLN:OE1	3:Y:32:ASP:N	2.48	0.45
1:A:13:GLN:HE22	1:A:57:GLU:HG3	1.81	0.45
1:A:73:GLN:HA	1:A:106:GLU:OE2	2.16	0.45
1:R:35:ASN:HB3	1:R:38:LEU:HD23	1.98	0.45
2:V:487:HIS:ND1	2:V:488:VAL:HG13	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:482:ASP:OD1	2:d:483:ASP:N	2.49	0.45
3:Y:155:GLU:HG3	3:Y:156:LEU:N	2.31	0.45
1:J:51:LEU:HD12	1:J:57:GLU:OE2	2.16	0.45
1:O:17:GLU:N	1:O:17:GLU:OE2	2.49	0.45
3:T:62:ASN:ND2	3:g:107:GLN:OE1	2.42	0.45
3:g:47:ARG:HG2	3:g:47:ARG:HH11	1.81	0.45
1:E:113:ASP:HA	1:E:116:LYS:NZ	2.31	0.45
1:M:31:VAL:HA	1:M:39:ASN:OD1	2.16	0.45
2:S:778:TYR:OH	2:S:780:LYS:NZ	2.50	0.45
2:V:360:GLU:OE1	2:V:360:GLU:N	2.50	0.45
2:b:326:ARG:NH2	2:b:334:ASN:O	2.50	0.45
2:d:208:THR:HB	2:d:219:THR:HB	1.98	0.45
3:W:4:TYR:HD2	3:h:124:PRO:HG3	1.81	0.45
1:A:13:GLN:HE21	1:A:55:MET:HE2	1.81	0.45
1:G:35:ASN:HB3	1:G:38:LEU:HD12	1.98	0.45
1:I:38:LEU:HA	1:I:40:ARG:HH12	1.82	0.45
1:O:60:VAL:HG22	1:O:61:ASP:H	1.82	0.45
2:S:175:PRO:HG3	2:S:186:LYS:HD2	1.98	0.45
2:d:487:HIS:CD2	2:d:488:VAL:HG13	2.51	0.45
1:B:137:ARG:HD2	1:B:137:ARG:HA	1.79	0.45
1:L:102:HIS:O	1:L:106:GLU:OE1	2.35	0.45
2:b:183:ASP:HB2	2:b:184:PRO:HD3	1.99	0.45
2:d:270:ASN:OD1	2:d:271:SER:N	2.50	0.45
1:G:11:ASN:HB3	1:G:14:TYR:CE1	2.51	0.45
2:d:70:ASP:OD1	2:d:71:GLU:N	2.45	0.45
2:d:184:PRO:O	2:d:187:VAL:HG12	2.16	0.45
2:S:482:ASP:OD1	2:S:483:ASP:N	2.49	0.45
1:H:69:ARG:HG3	1:H:69:ARG:HH11	1.82	0.45
1:O:52:ASN:OD1	1:O:55:MET:HB2	2.17	0.45
2:d:498:ASP:OD1	2:d:499:ILE:N	2.50	0.45
1:C:17:GLU:N	1:C:17:GLU:OE2	2.50	0.44
1:F:17:GLU:N	1:F:17:GLU:OE1	2.50	0.44
1:C:52:ASN:OD1	1:C:55:MET:N	2.48	0.44
1:F:13:GLN:HB3	1:F:55:MET:CE	2.48	0.44
1:E:51:LEU:HG	1:E:57:GLU:OE2	2.18	0.44
1:O:31:VAL:HA	1:O:39:ASN:OD1	2.17	0.44
3:h:168:GLN:HA	3:h:171:GLU:CD	2.42	0.44
1:C:31:VAL:HA	1:C:39:ASN:OD1	2.18	0.44
1:G:11:ASN:OD1	1:G:12:THR:N	2.50	0.44
1:I:31:VAL:HA	1:I:39:ASN:OD1	2.18	0.44
1:J:66:ASP:OD1	1:J:67:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:GLU:HG2	1:L:118:TYR:N	2.32	0.44
1:N:17:GLU:OE2	1:N:17:GLU:N	2.51	0.44
2:Z:704:LYS:O	2:Z:768:SER:HB2	2.17	0.44
2:b:704:LYS:O	2:b:768:SER:HB2	2.18	0.44
1:A:23:ARG:HD2	1:A:50:PHE:HD2	1.81	0.44
2:d:183:ASP:HB2	2:d:184:PRO:HD3	2.00	0.44
3:j:73:ASP:OD2	3:j:73:ASP:N	2.49	0.44
1:A:23:ARG:HH21	2:Z:608:TYR:HD1	1.66	0.44
2:V:184:PRO:O	2:V:187:VAL:HG12	2.18	0.44
2:Z:184:PRO:O	2:Z:187:VAL:HG12	2.17	0.44
3:W:165:LEU:O	3:W:169:VAL:HG23	2.18	0.44
3:e:165:LEU:O	3:e:169:VAL:HG23	2.18	0.44
1:D:28:VAL:HG13	1:D:70:ILE:HG13	1.99	0.44
1:M:17:GLU:N	1:M:17:GLU:OE2	2.51	0.44
1:Q:102:HIS:O	1:Q:106:GLU:OE1	2.35	0.44
2:V:367:SER:O	2:V:369:SER:N	2.49	0.44
2:Z:328:SER:HB2	2:Z:334:ASN:HD22	1.83	0.44
1:D:35:ASN:OD1	1:D:37:THR:OG1	2.29	0.44
1:D:102:HIS:O	1:D:103:ILE:C	2.61	0.44
1:J:102:HIS:O	1:J:106:GLU:OE1	2.35	0.44
1:N:61:ASP:OD1	1:N:61:ASP:N	2.42	0.44
1:N:66:ASP:OD1	1:N:67:ILE:N	2.51	0.44
3:Y:156:LEU:HD23	3:Y:156:LEU:O	2.17	0.44
3:h:182:MET:HE3	3:h:182:MET:HB3	1.80	0.44
3:j:30:GLN:HE22	3:j:33:GLU:HB2	1.83	0.44
1:D:102:HIS:C	1:D:104:ALA:N	2.76	0.44
2:V:603:TYR:HD2	2:V:608:TYR:HA	1.82	0.44
2:d:367:SER:O	2:d:369:SER:N	2.47	0.44
2:d:495:GLY:HA3	2:d:513:THR:HG22	1.99	0.44
1:E:117:GLU:HG2	1:E:118:TYR:N	2.32	0.43
1:O:15:ARG:HG3	1:O:15:ARG:HH11	1.82	0.43
1:P:80:VAL:HG11	1:P:92:ASP:HB3	1.99	0.43
1:Q:113:ASP:HA	1:Q:116:LYS:NZ	2.33	0.43
2:V:704:LYS:O	2:V:768:SER:HB2	2.18	0.43
2:X:717:GLU:N	2:X:717:GLU:OE1	2.51	0.43
3:U:165:LEU:O	3:U:169:VAL:HG23	2.18	0.43
1:A:94:THR:O	1:A:98:LEU:HD23	2.19	0.43
1:H:61:ASP:OD1	1:H:62:GLN:N	2.51	0.43
1:P:94:THR:O	1:P:98:LEU:HD23	2.18	0.43
1:P:117:GLU:HA	1:P:120:ASP:OD2	2.18	0.43
2:d:421:THR:OG1	2:d:422:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASP:O	1:A:59:LEU:N	2.50	0.43
1:N:82:PHE:O	1:N:83:ARG:HD3	2.18	0.43
2:X:208:THR:HB	2:X:219:THR:HB	1.99	0.43
2:d:714:ARG:NE	2:d:719:GLU:OE2	2.40	0.43
3:h:167:GLN:O	3:h:171:GLU:OE1	2.37	0.43
2:S:183:ASP:HB2	2:S:184:PRO:HD3	2.01	0.43
2:X:498:ASP:OD1	2:X:499:ILE:N	2.51	0.43
3:f:155:GLU:HG3	3:f:156:LEU:N	2.34	0.43
3:g:47:ARG:HG2	3:g:47:ARG:NH1	2.32	0.43
1:I:114:LEU:HD12	1:I:118:TYR:CE2	2.54	0.43
2:V:452:ARG:NH1	2:Z:480:ASP:OD2	2.51	0.43
2:X:183:ASP:HB2	2:X:184:PRO:HD3	2.01	0.43
2:Z:278:VAL:HG12	2:Z:287:TRP:HE3	1.83	0.43
2:b:395:ARG:HG3	2:b:395:ARG:HH11	1.83	0.43
3:U:167:GLN:O	3:U:171:GLU:OE1	2.36	0.43
3:Y:107:GLN:OE1	3:e:62:ASN:ND2	2.47	0.43
1:A:32:ASN:ND2	1:A:38:LEU:HD23	2.23	0.43
1:D:96:SER:HB2	1:F:97:GLU:OE1	2.18	0.43
1:E:30:LEU:HD23	1:E:65:PHE:CD2	2.53	0.43
2:V:208:THR:HB	2:V:219:THR:HB	2.01	0.43
2:V:553:ILE:HG23	2:V:553:ILE:O	2.19	0.43
1:H:14:TYR:O	1:H:56:ILE:HG22	2.17	0.43
1:I:52:ASN:OD1	1:I:53:PRO:HD2	2.19	0.43
1:N:113:ASP:O	1:N:116:LYS:HB3	2.19	0.43
1:R:15:ARG:HH11	1:R:15:ARG:HG3	1.83	0.43
2:S:714:ARG:HG2	2:S:719:GLU:HG2	2.01	0.43
2:d:487:HIS:HD2	2:d:488:VAL:HG13	1.83	0.43
3:c:4:TYR:CE2	3:c:5:ILE:HG12	2.54	0.43
3:e:13:LEU:HD13	3:e:31:LEU:HB2	2.00	0.43
3:h:155:GLU:C	3:h:157:TYR:H	2.26	0.43
1:G:114:LEU:HD23	1:G:114:LEU:HA	1.85	0.43
1:M:19:ASP:O	1:M:72:ARG:NH1	2.44	0.43
2:S:553:ILE:HG23	2:S:553:ILE:O	2.19	0.43
3:Y:143:GLU:HG2	3:e:157:TYR:HE2	1.82	0.43
1:J:117:GLU:HG2	1:J:118:TYR:N	2.33	0.43
2:Z:245:ASP:N	2:Z:245:ASP:OD1	2.51	0.43
2:Z:498:ASP:OD2	2:Z:499:ILE:N	2.52	0.43
1:B:80:VAL:HG11	1:B:92:ASP:HB3	2.00	0.42
1:F:52:ASN:OD1	1:F:55:MET:N	2.52	0.42
2:S:395:ARG:HG3	2:S:395:ARG:NH1	2.34	0.42
2:X:184:PRO:O	2:X:187:VAL:HG12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:HB2	1:A:56:ILE:HD11	2.02	0.42
1:K:102:HIS:O	1:K:106:GLU:OE1	2.37	0.42
2:X:360:GLU:OE1	2:X:360:GLU:N	2.52	0.42
2:Z:155:GLN:HG3	2:Z:235:TYR:CE2	2.54	0.42
3:i:155:GLU:C	3:i:157:TYR:H	2.26	0.42
1:N:31:VAL:HA	1:N:39:ASN:OD1	2.19	0.42
2:Z:603:TYR:CD2	2:Z:608:TYR:HA	2.54	0.42
2:b:184:PRO:O	2:b:187:VAL:HG12	2.19	0.42
3:g:167:GLN:O	3:g:171:GLU:OE1	2.37	0.42
1:A:110:GLN:O	1:A:114:LEU:HD23	2.19	0.42
1:P:15:ARG:HG3	1:P:17:GLU:OE2	2.19	0.42
1:H:38:LEU:CG	1:H:39:ASN:H	2.30	0.42
1:I:46:ARG:CZ	1:I:46:ARG:HB3	2.49	0.42
2:b:270:ASN:OD1	2:b:271:SER:N	2.53	0.42
3:T:155:GLU:C	3:T:157:TYR:H	2.26	0.42
1:B:102:HIS:O	1:B:106:GLU:OE1	2.38	0.42
1:N:113:ASP:O	1:N:117:GLU:OE1	2.36	0.42
2:S:184:PRO:O	2:S:187:VAL:HG12	2.19	0.42
2:V:416:VAL:HG12	2:V:438:GLU:OE1	2.18	0.42
2:d:21:ILE:H	2:d:21:ILE:HD12	1.84	0.42
3:f:155:GLU:HG3	3:f:156:LEU:H	1.84	0.42
3:g:182:MET:O	3:g:182:MET:HG2	2.20	0.42
2:V:714:ARG:NH1	2:V:719:GLU:OE1	2.49	0.42
3:c:1:MET:HB3	3:c:4:TYR:O	2.19	0.42
1:L:126:ALA:HB1	1:O:122:ALA:HB2	2.02	0.42
2:b:579:THR:OG1	2:b:581:PHE:O	2.37	0.42
3:e:155:GLU:HG3	3:e:156:LEU:N	2.29	0.42
3:f:124:PRO:HB3	3:g:3:GLN:O	2.19	0.42
3:j:155:GLU:C	3:j:157:TYR:H	2.27	0.42
1:I:38:LEU:O	1:I:39:ASN:HB2	2.20	0.42
2:S:158:ARG:HH12	2:b:187:VAL:HG13	1.85	0.42
2:V:158:ARG:HH21	2:V:235:TYR:HE1	1.67	0.42
2:V:183:ASP:HB2	2:V:184:PRO:HD3	2.02	0.42
3:i:167:GLN:O	3:i:171:GLU:OE1	2.37	0.42
1:A:38:LEU:HD12	1:A:38:LEU:HA	1.90	0.42
2:Z:178:ASN:OD1	2:Z:179:ASP:N	2.52	0.42
3:U:168:GLN:HA	3:U:171:GLU:CD	2.45	0.42
1:I:32:ASN:ND2	1:I:65:PHE:HA	2.30	0.41
1:I:80:VAL:HG11	1:I:92:ASP:HB3	2.01	0.41
1:P:118:TYR:CE2	1:R:116:LYS:HD3	2.55	0.41
1:Q:17:GLU:OE1	1:Q:17:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:187:VAL:HG13	2:b:158:ARG:HH12	1.85	0.41
3:f:129:PRO:HG2	3:f:132:PHE:CD1	2.55	0.41
1:H:106:GLU:O	1:H:110:GLN:HG3	2.20	0.41
1:I:43:GLU:O	1:I:47:ASP:HB2	2.19	0.41
1:P:114:LEU:HD13	1:P:117:GLU:OE2	2.19	0.41
2:S:270:ASN:OD1	2:S:271:SER:N	2.53	0.41
2:X:31:GLN:HE21	2:X:34:CYS:HB2	1.86	0.41
2:X:35:TRP:HD1	2:X:43:GLN:HE21	1.68	0.41
2:Z:21:ILE:H	2:Z:21:ILE:HD12	1.85	0.41
2:Z:304:MET:HE3	2:Z:323:TRP:CE2	2.55	0.41
2:d:38:GLU:N	2:d:38:GLU:OE1	2.53	0.41
3:a:75:ARG:HD3	3:a:100:TYR:CE2	2.55	0.41
3:i:168:GLN:HA	3:i:171:GLU:CD	2.44	0.41
3:j:30:GLN:OE1	3:j:32:ASP:N	2.54	0.41
1:G:15:ARG:NE	1:G:55:MET:HE1	2.35	0.41
1:M:23:ARG:HH12	3:j:7:LEU:HB2	1.85	0.41
1:O:13:GLN:HB3	1:O:55:MET:HE1	2.01	0.41
2:V:482:ASP:OD1	2:V:483:ASP:N	2.54	0.41
2:Z:607:THR:O	2:Z:609:LYS:HG2	2.20	0.41
2:b:96:VAL:HG22	2:b:316:PHE:HB2	2.01	0.41
1:H:132:SER:O	1:K:137:ARG:NH1	2.54	0.41
1:J:17:GLU:N	1:J:17:GLU:OE2	2.54	0.41
2:V:438:GLU:OE1	2:V:438:GLU:HA	2.21	0.41
2:d:115:VAL:HG12	2:d:117:VAL:HG23	2.03	0.41
2:d:527:LYS:HE2	2:d:527:LYS:HB2	1.96	0.41
2:d:579:THR:OG1	2:d:581:PHE:O	2.35	0.41
3:W:1:MET:HG3	3:W:3:GLN:H	1.85	0.41
1:A:80:VAL:HG11	1:A:92:ASP:HB3	2.03	0.41
1:B:135:GLU:O	1:B:139:ILE:HG12	2.21	0.41
1:I:81:ASP:OD2	1:I:82:PHE:N	2.54	0.41
1:L:58:MET:HE3	1:L:58:MET:HB3	1.94	0.41
1:P:57:GLU:N	1:P:57:GLU:OE1	2.53	0.41
2:X:281:ASP:OD1	2:X:282:SER:N	2.53	0.41
1:D:48:TYR:HB2	1:D:56:ILE:HD11	2.03	0.41
1:D:116:LYS:HE3	1:D:116:LYS:HA	2.02	0.41
1:E:72:ARG:NE	1:E:106:GLU:OE2	2.51	0.41
1:I:40:ARG:HA	1:I:40:ARG:NE	2.35	0.41
1:L:113:ASP:HA	1:L:116:LYS:HZ2	1.85	0.41
2:S:603:TYR:HB3	2:S:610:THR:HB	2.01	0.41
2:S:610:THR:HG21	2:S:656:TRP:HB2	2.02	0.41
3:f:156:LEU:O	3:f:156:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.85	0.41
1:R:52:ASN:OD1	1:R:55:MET:N	2.54	0.41
2:b:460:ARG:NH2	2:b:465:SER:HB2	2.35	0.41
2:d:604:ASN:OD1	2:d:604:ASN:N	2.54	0.41
3:U:74:ASN:HB3	3:U:111:PHE:O	2.20	0.41
3:a:74:ASN:HB3	3:a:111:PHE:O	2.21	0.41
1:D:6:GLN:HE22	1:D:69:ARG:NH2	2.17	0.41
1:F:52:ASN:OD1	1:F:55:MET:HB2	2.21	0.41
1:G:28:VAL:HG22	1:G:70:ILE:HD12	2.02	0.41
1:P:105:GLU:HA	1:P:108:ARG:HH11	1.86	0.41
1:P:105:GLU:OE1	1:P:105:GLU:N	2.52	0.41
2:S:131:LYS:HD3	2:S:131:LYS:HA	1.90	0.41
2:Z:31:GLN:HE21	2:Z:34:CYS:HB2	1.86	0.41
2:Z:183:ASP:HB2	2:Z:184:PRO:HD3	2.03	0.41
2:b:67:ILE:HD12	2:b:75:TYR:HE1	1.85	0.41
2:b:553:ILE:HG23	2:b:553:ILE:O	2.21	0.41
2:d:182:ASN:C	2:d:185:PRO:HD2	2.46	0.41
2:d:292:GLU:HA	2:d:293:PRO:HD3	1.94	0.41
3:j:74:ASN:HB3	3:j:111:PHE:O	2.21	0.41
1:C:35:ASN:HB3	1:C:38:LEU:HG	2.02	0.41
1:P:99:GLN:O	1:P:103:ILE:HG13	2.21	0.41
2:S:487:HIS:HD2	2:S:488:VAL:HG13	1.85	0.41
2:S:687:GLN:N	2:S:687:GLN:OE1	2.54	0.41
2:b:460:ARG:HG2	2:b:461:GLY:H	1.85	0.41
2:d:326:ARG:NH2	2:d:334:ASN:O	2.52	0.41
3:T:129:PRO:HG2	3:T:132:PHE:CD1	2.56	0.41
3:Y:181:MET:HE2	3:Y:181:MET:HB3	1.92	0.41
3:e:124:PRO:HG2	3:e:127:GLU:HG3	2.02	0.41
1:A:99:GLN:O	1:A:103:ILE:HG13	2.21	0.40
2:S:313:ASP:N	2:S:313:ASP:OD1	2.54	0.40
2:V:395:ARG:NH1	2:V:438:GLU:OE2	2.54	0.40
3:T:19:MET:HE1	3:T:45:LEU:HB2	2.02	0.40
1:Q:138:ARG:HD3	1:Q:138:ARG:HA	1.93	0.40
2:S:704:LYS:O	2:S:768:SER:HB2	2.21	0.40
2:X:270:ASN:OD1	2:X:271:SER:N	2.54	0.40
2:Z:253:LEU:HD23	2:Z:253:LEU:HA	1.91	0.40
2:d:553:ILE:HG23	2:d:553:ILE:O	2.20	0.40
2:d:709:LEU:HD12	2:d:709:LEU:HA	1.90	0.40
3:a:165:LEU:HD23	3:a:165:LEU:HA	1.93	0.40
3:c:180:ASN:OD1	3:c:182:MET:HE3	2.20	0.40
2:S:627:ARG:NH2	2:S:639:ASP:OD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:178:ASN:OD1	2:X:179:ASP:N	2.54	0.40
2:Z:579:THR:OG1	2:Z:581:PHE:O	2.37	0.40
2:Z:631:ILE:HG13	2:Z:637:TYR:HB3	2.02	0.40
2:b:21:ILE:HD12	2:b:21:ILE:H	1.85	0.40
2:b:158:ARG:HD2	2:b:234:GLY:HA3	2.02	0.40
2:b:188:ASP:OD1	2:b:189:ALA:N	2.53	0.40
3:f:70:ASP:CG	3:f:71:VAL:H	2.28	0.40
1:J:138:ARG:HA	1:J:138:ARG:HD3	1.78	0.40
2:X:464:THR:HG22	2:X:465:SER:N	2.36	0.40
2:d:360:GLU:OE1	2:d:360:GLU:N	2.55	0.40
3:a:73:ASP:OD1	3:a:75:ARG:HD2	2.21	0.40
3:j:68:THR:HA	3:j:69:PRO:HD3	1.92	0.40
3:j:182:MET:HE2	3:j:182:MET:HB2	1.96	0.40
2:b:116:THR:HG22	2:b:121:THR:HG23	2.04	0.40
3:U:5:ILE:HD12	3:U:5:ILE:H	1.86	0.40
3:W:62:ASN:ND2	3:h:107:GLN:OE1	2.45	0.40
3:Y:30:GLN:NE2	3:Y:33:GLU:O	2.47	0.40
3:Y:72:GLN:HA	3:Y:72:GLN:OE1	2.22	0.40
3:c:16:ILE:HD13	3:c:16:ILE:HA	1.97	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	129/843 (15%)	123 (95%)	5 (4%)	1 (1%)	16	45
1	B	138/843 (16%)	135 (98%)	3 (2%)	0	100	100
1	C	119/843 (14%)	118 (99%)	1 (1%)	0	100	100
1	D	129/843 (15%)	120 (93%)	8 (6%)	1 (1%)	16	45
1	E	138/843 (16%)	130 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	119/843 (14%)	117 (98%)	1 (1%)	1 (1%)	16	45
1	G	129/843 (15%)	124 (96%)	5 (4%)	0	100	100
1	H	129/843 (15%)	120 (93%)	9 (7%)	0	100	100
1	I	129/843 (15%)	125 (97%)	4 (3%)	0	100	100
1	J	138/843 (16%)	137 (99%)	1 (1%)	0	100	100
1	K	138/843 (16%)	133 (96%)	5 (4%)	0	100	100
1	L	138/843 (16%)	137 (99%)	1 (1%)	0	100	100
1	M	119/843 (14%)	117 (98%)	2 (2%)	0	100	100
1	N	119/843 (14%)	117 (98%)	2 (2%)	0	100	100
1	O	119/843 (14%)	114 (96%)	5 (4%)	0	100	100
1	P	129/843 (15%)	125 (97%)	4 (3%)	0	100	100
1	Q	138/843 (16%)	136 (99%)	2 (1%)	0	100	100
1	R	119/843 (14%)	118 (99%)	1 (1%)	0	100	100
2	S	772/785 (98%)	717 (93%)	51 (7%)	4 (0%)	24	55
2	V	782/785 (100%)	726 (93%)	53 (7%)	3 (0%)	30	60
2	X	782/785 (100%)	728 (93%)	51 (6%)	3 (0%)	30	60
2	Z	782/785 (100%)	726 (93%)	54 (7%)	2 (0%)	36	65
2	b	782/785 (100%)	725 (93%)	54 (7%)	3 (0%)	30	60
2	d	776/785 (99%)	716 (92%)	58 (8%)	2 (0%)	36	65
3	T	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
3	U	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
3	W	186/188 (99%)	176 (95%)	10 (5%)	0	100	100
3	Y	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
3	a	186/188 (99%)	176 (95%)	10 (5%)	0	100	100
3	c	186/188 (99%)	170 (91%)	16 (9%)	0	100	100
3	e	186/188 (99%)	171 (92%)	15 (8%)	0	100	100
3	f	185/188 (98%)	170 (92%)	15 (8%)	0	100	100
3	g	186/188 (99%)	174 (94%)	12 (6%)	0	100	100
3	h	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
3	i	185/188 (98%)	174 (94%)	11 (6%)	0	100	100
3	j	185/188 (98%)	174 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9218/22140 (42%)	8666 (94%)	532 (6%)	20 (0%)	44	71

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	603	TYR
2	d	603	TYR
1	A	40	ARG
1	D	103	ILE
1	F	63	SER
2	S	368	ALA
2	Z	396	ILE
2	b	368	ALA
2	S	396	ILE
2	V	396	ILE
2	X	396	ILE
2	b	396	ILE
2	d	396	ILE
2	S	603	TYR
2	V	657	SER
2	X	603	TYR
2	X	657	SER
2	Z	657	SER
2	b	657	SER
2	S	657	SER

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	113/685 (16%)	112 (99%)	1 (1%)	70	78
1	B	120/685 (18%)	120 (100%)	0	100	100
1	C	107/685 (16%)	107 (100%)	0	100	100
1	D	113/685 (16%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	120/685 (18%)	119 (99%)	1 (1%)	73	80
1	F	107/685 (16%)	107 (100%)	0	100	100
1	G	113/685 (16%)	113 (100%)	0	100	100
1	H	113/685 (16%)	112 (99%)	1 (1%)	70	78
1	I	113/685 (16%)	113 (100%)	0	100	100
1	J	120/685 (18%)	120 (100%)	0	100	100
1	K	120/685 (18%)	120 (100%)	0	100	100
1	L	120/685 (18%)	120 (100%)	0	100	100
1	M	107/685 (16%)	107 (100%)	0	100	100
1	N	107/685 (16%)	107 (100%)	0	100	100
1	O	107/685 (16%)	107 (100%)	0	100	100
1	P	113/685 (16%)	113 (100%)	0	100	100
1	Q	120/685 (18%)	120 (100%)	0	100	100
1	R	107/685 (16%)	107 (100%)	0	100	100
2	S	663/670 (99%)	663 (100%)	0	100	100
2	V	669/670 (100%)	669 (100%)	0	100	100
2	X	669/670 (100%)	669 (100%)	0	100	100
2	Z	669/670 (100%)	668 (100%)	1 (0%)	88	90
2	b	669/670 (100%)	669 (100%)	0	100	100
2	d	666/670 (99%)	663 (100%)	3 (0%)	81	83
3	T	162/163 (99%)	162 (100%)	0	100	100
3	U	163/163 (100%)	163 (100%)	0	100	100
3	W	163/163 (100%)	163 (100%)	0	100	100
3	Y	162/163 (99%)	162 (100%)	0	100	100
3	a	163/163 (100%)	163 (100%)	0	100	100
3	c	163/163 (100%)	163 (100%)	0	100	100
3	e	163/163 (100%)	163 (100%)	0	100	100
3	f	162/163 (99%)	162 (100%)	0	100	100
3	g	163/163 (100%)	163 (100%)	0	100	100
3	h	162/163 (99%)	162 (100%)	0	100	100
3	i	162/163 (99%)	162 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	j	162/163 (99%)	162 (100%)	0	100	100
All	All	7995/18306 (44%)	7988 (100%)	7 (0%)	87	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	E	92	ASP
1	H	11	ASN
2	Z	117	VAL
2	d	651	THR
2	d	660	THR
2	d	665	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	32	ASN
1	A	39	ASN
1	C	102	HIS
1	D	6	GLN
1	D	62	GLN
1	D	84	ASN
1	D	102	HIS
1	E	13	GLN
1	F	110	GLN
1	G	84	ASN
1	H	6	GLN
1	H	11	ASN
1	H	95	ASN
1	I	13	GLN
1	J	13	GLN
1	K	6	GLN
1	K	13	GLN
1	N	11	ASN
1	O	95	ASN
1	P	6	GLN
2	S	17	GLN
2	S	150	ASN
2	S	172	HIS

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Mol	Chain	Res	Type
2	S	311	GLN
2	V	6	GLN
2	V	72	HIS
2	V	93	GLN
2	V	172	HIS
2	V	393	HIS
2	V	634	GLN
2	V	738	ASN
2	X	93	GLN
2	X	172	HIS
2	X	266	GLN
2	X	334	ASN
2	X	722	ASN
2	X	738	ASN
2	Z	6	GLN
2	Z	93	GLN
2	Z	107	ASN
2	Z	172	HIS
2	Z	334	ASN
2	Z	393	HIS
2	Z	687	GLN
2	b	72	HIS
2	b	107	ASN
2	b	150	ASN
2	b	172	HIS
2	b	248	GLN
2	b	393	HIS
2	b	695	GLN
2	d	6	GLN
2	d	17	GLN
2	d	172	HIS
2	d	182	ASN
2	d	237	ASN
2	d	334	ASN
2	d	511	ASN
2	d	634	GLN
3	U	145	ASN
3	W	58	ASN
3	W	107	GLN
3	W	145	ASN
3	a	30	GLN
3	a	145	ASN

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Mol	Chain	Res	Type
3	c	60	ASN
3	c	145	ASN
3	e	145	ASN
3	g	145	ASN
3	i	42	GLN
3	i	60	ASN
3	i	62	ASN
3	i	96	ASN
3	j	58	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

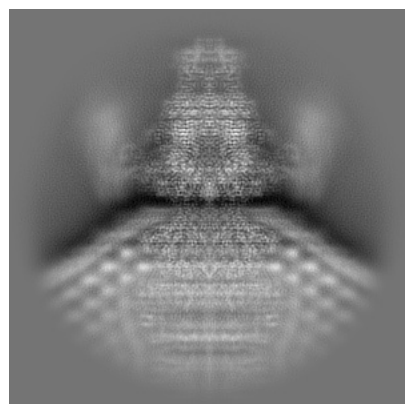
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65388. These allow visual inspection of the internal detail of the map and identification of artifacts.

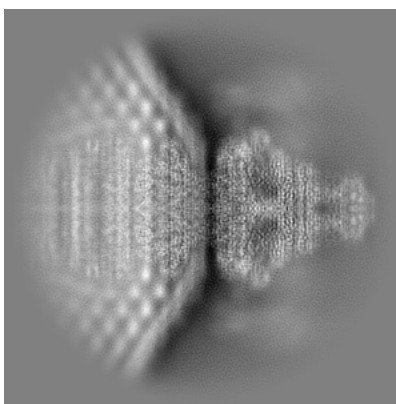
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

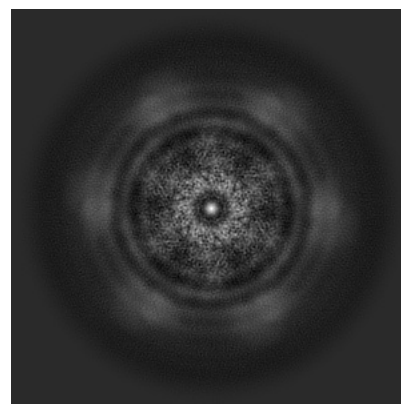
6.1.1 Primary map



X

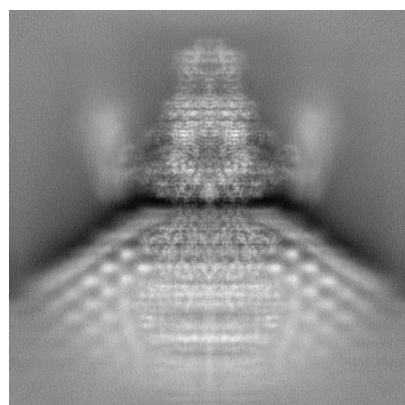


Y

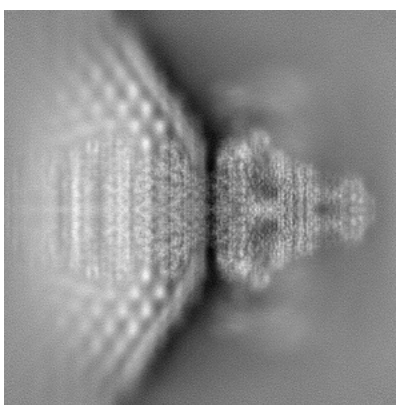


Z

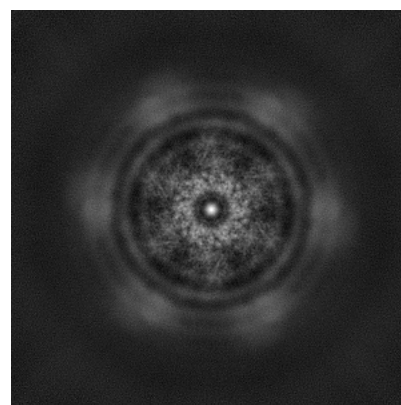
6.1.2 Raw map



X



Y

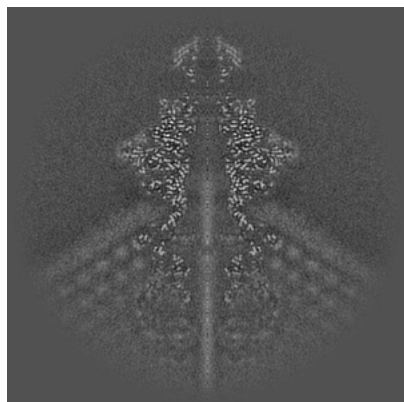


Z

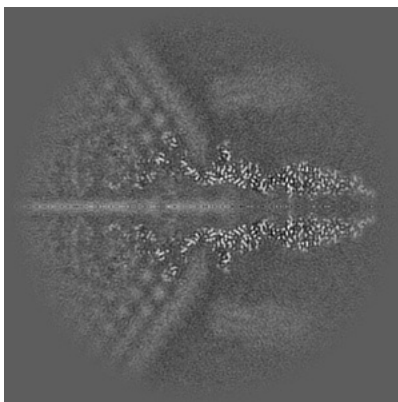
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

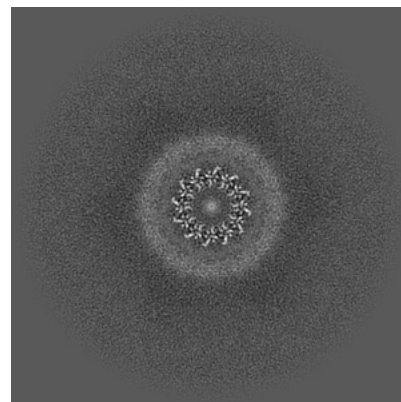
6.2.1 Primary map



X Index: 220

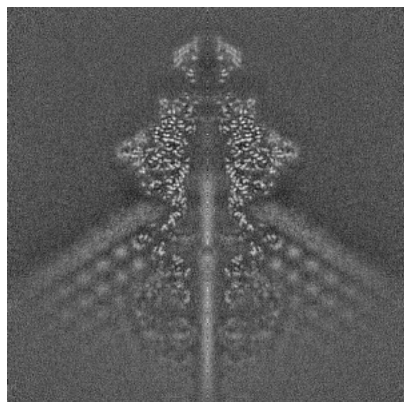


Y Index: 220

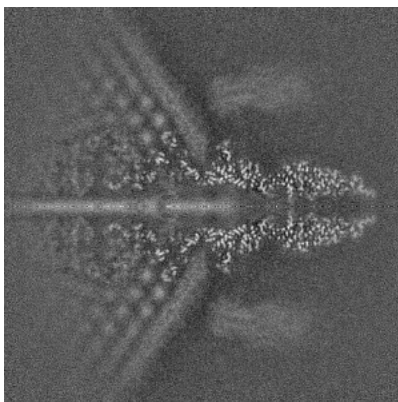


Z Index: 220

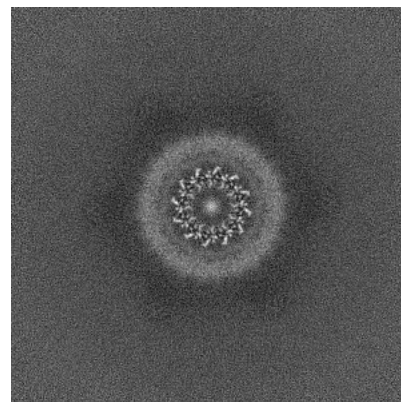
6.2.2 Raw map



X Index: 220



Y Index: 220

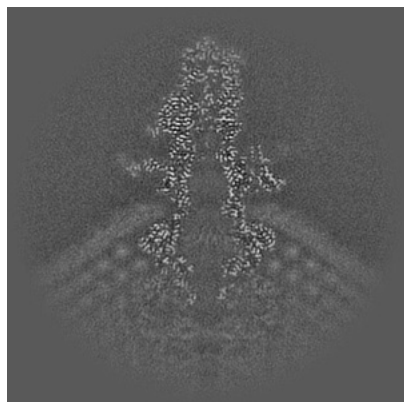


Z Index: 220

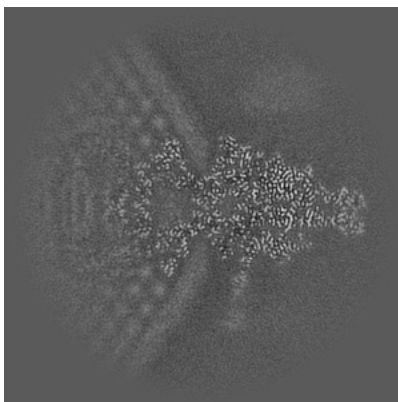
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

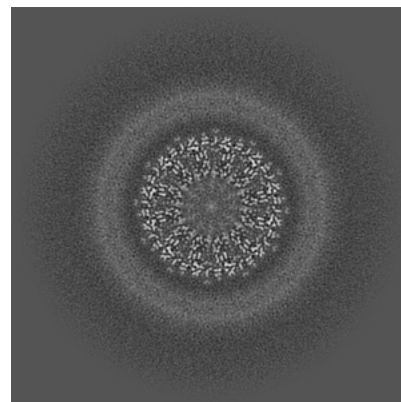
6.3.1 Primary map



X Index: 206

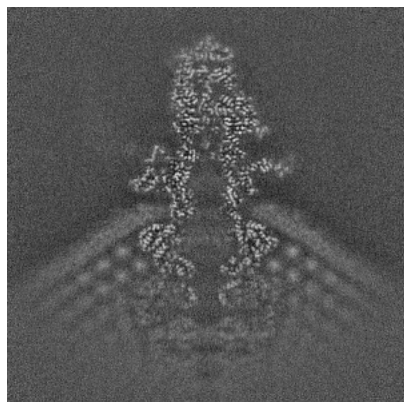


Y Index: 196

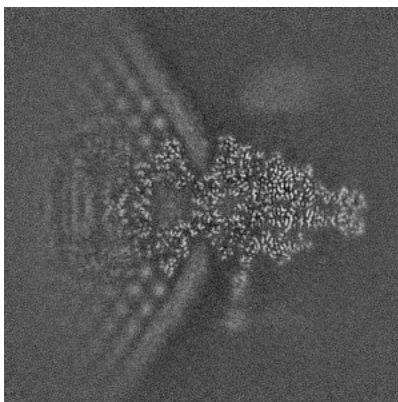


Z Index: 184

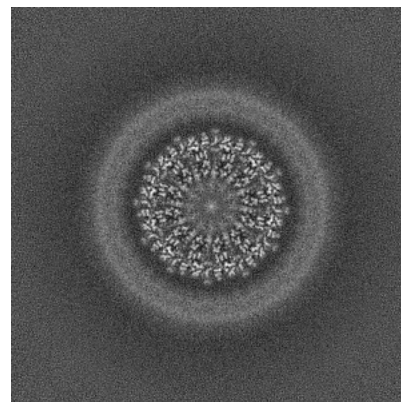
6.3.2 Raw map



X Index: 235



Y Index: 196

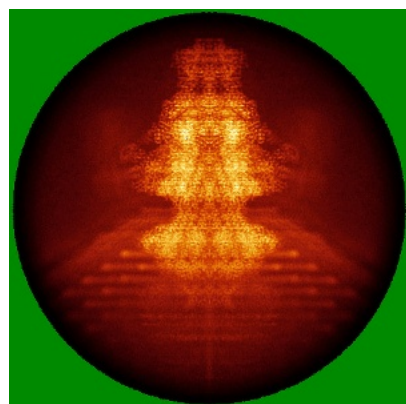


Z Index: 184

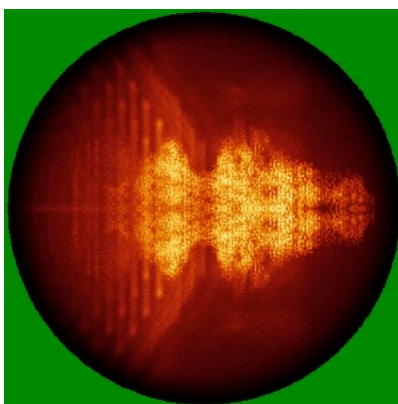
The images above show the largest variance slices of the map in three orthogonal directions.

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

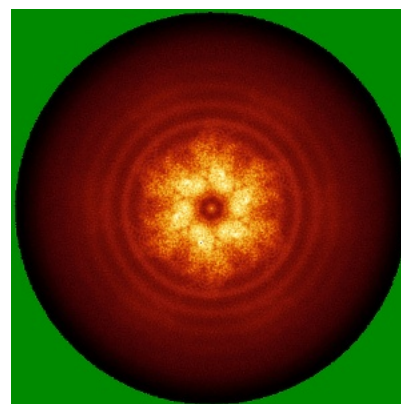
6.4.1 Primary map



X

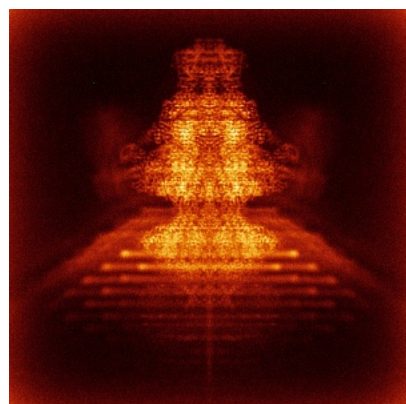


Y

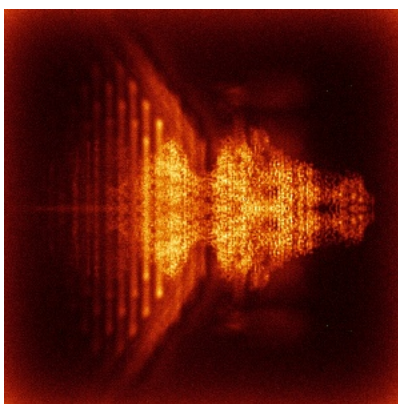


Z

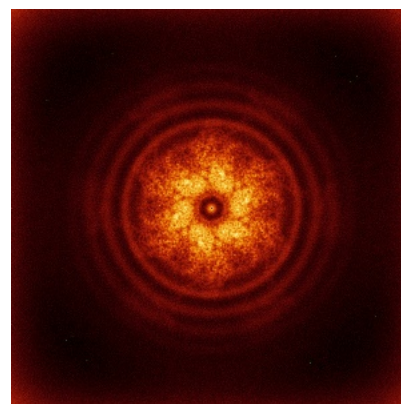
6.4.2 Raw map



X



Y

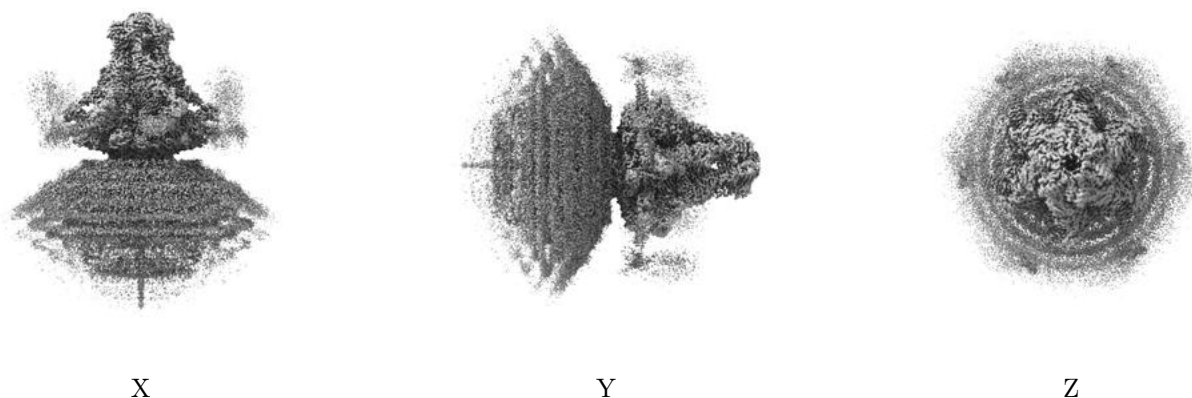


Z

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.

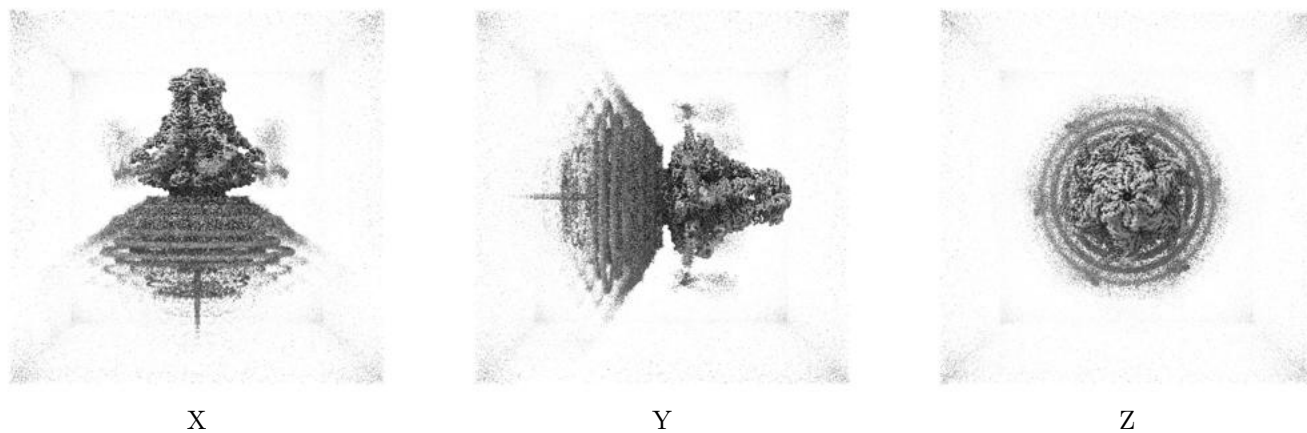
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.18. 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.

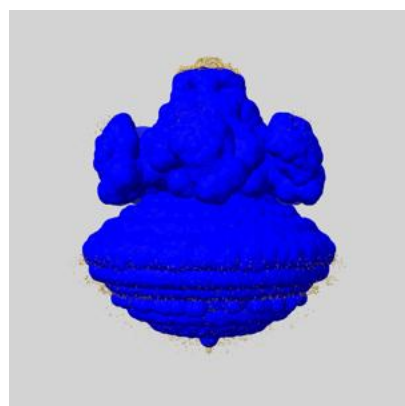
6.6 Mask visualisation [i](#)

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

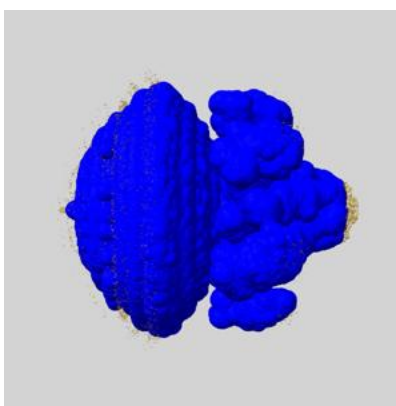
A mask typically either:

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

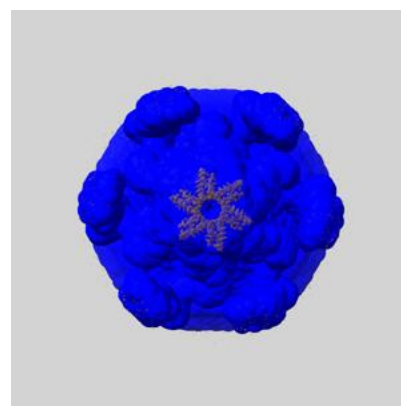
6.6.1 emd_65388_msk_1.map [i](#)



X



Y

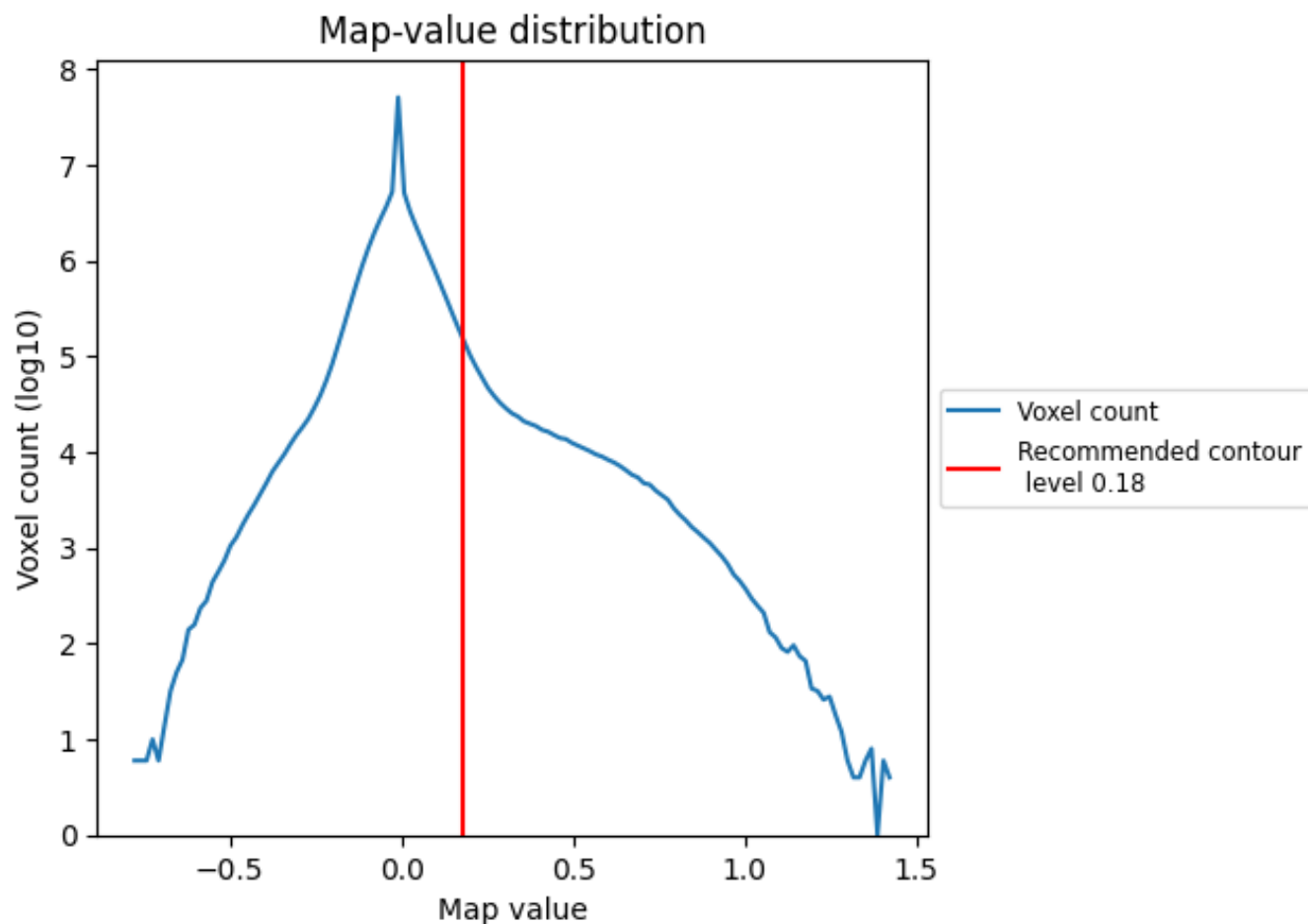


Z

7 Map analysis [i](#)

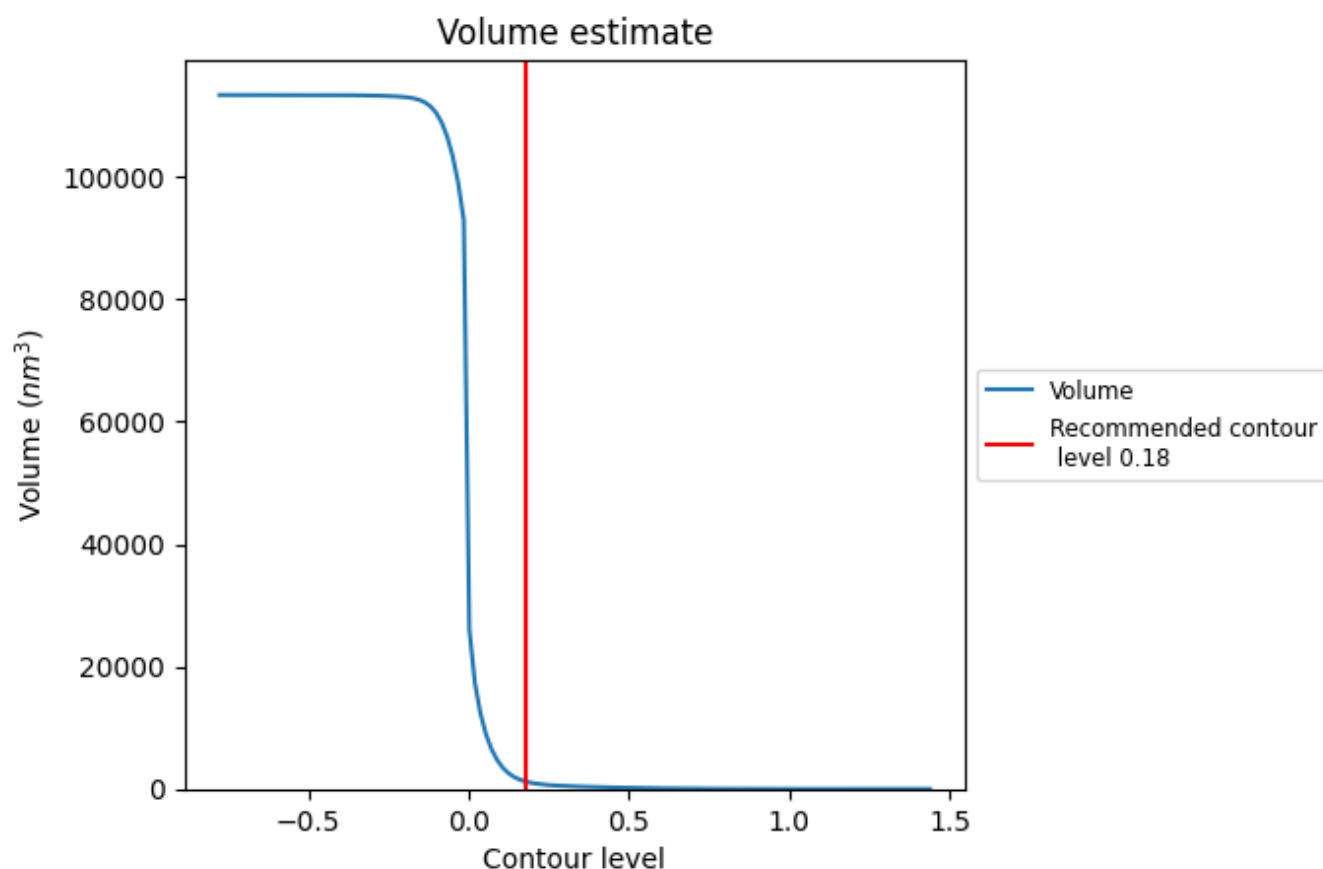
This section contains the results of statistical analysis of the map.

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.

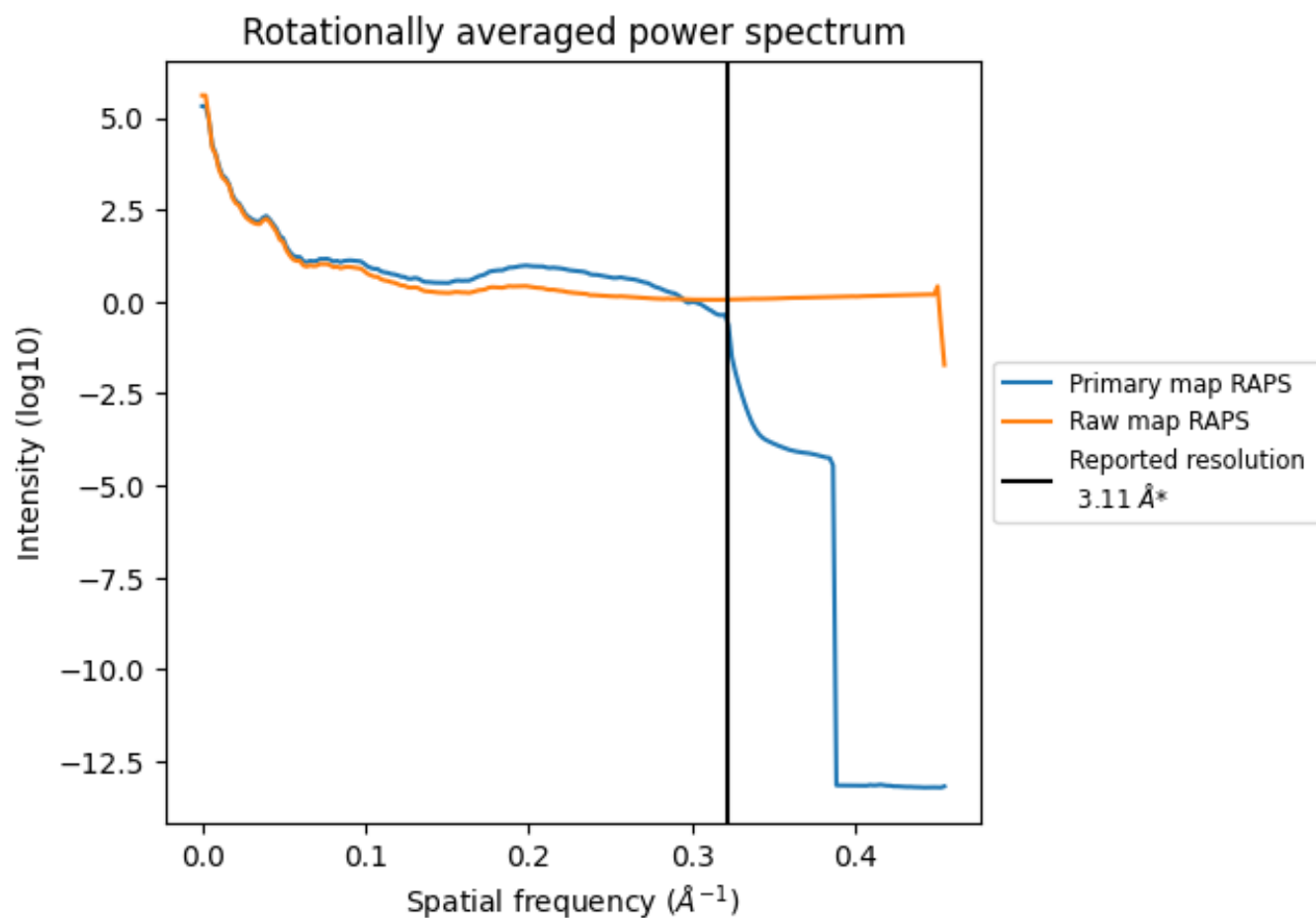
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1184 nm^3 ; this corresponds to an approximate mass of 1069 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 ⓘ

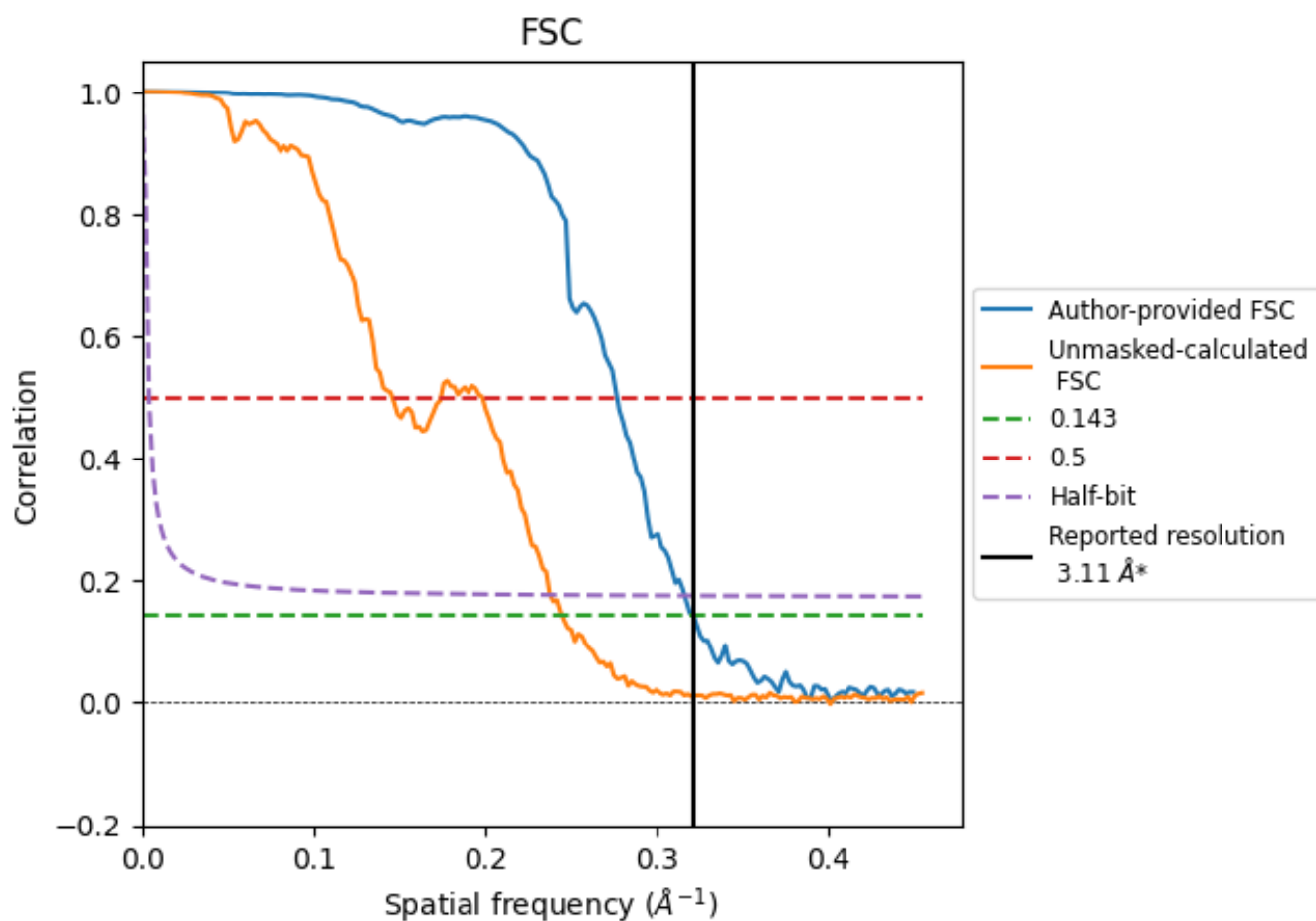


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

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 $0.322 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

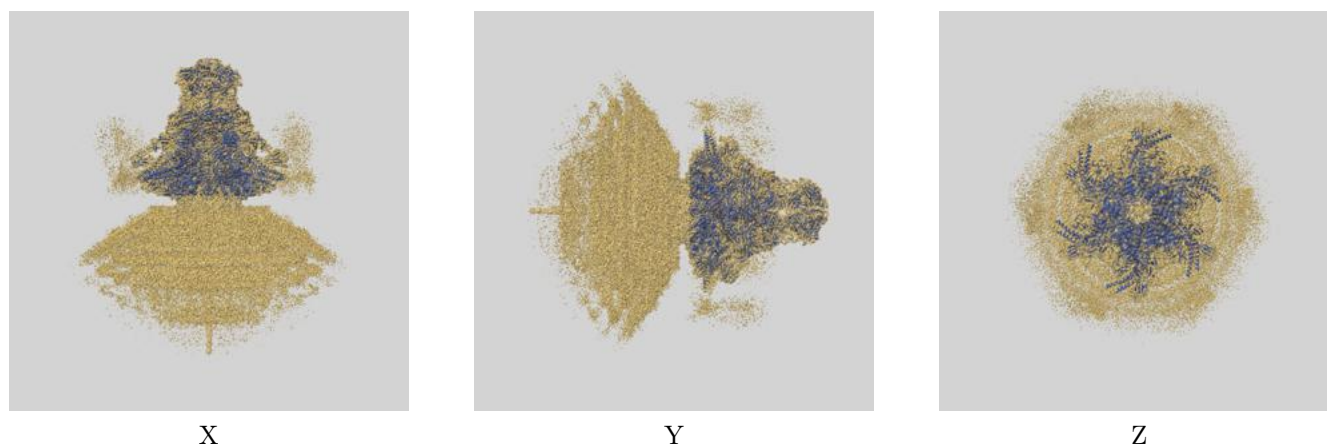
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.62	3.16
Unmasked-calculated*	4.09	6.87	4.21

*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 4.09 differs from the reported value 3.11 by more than 10 %

9 Map-model fit [i](#)

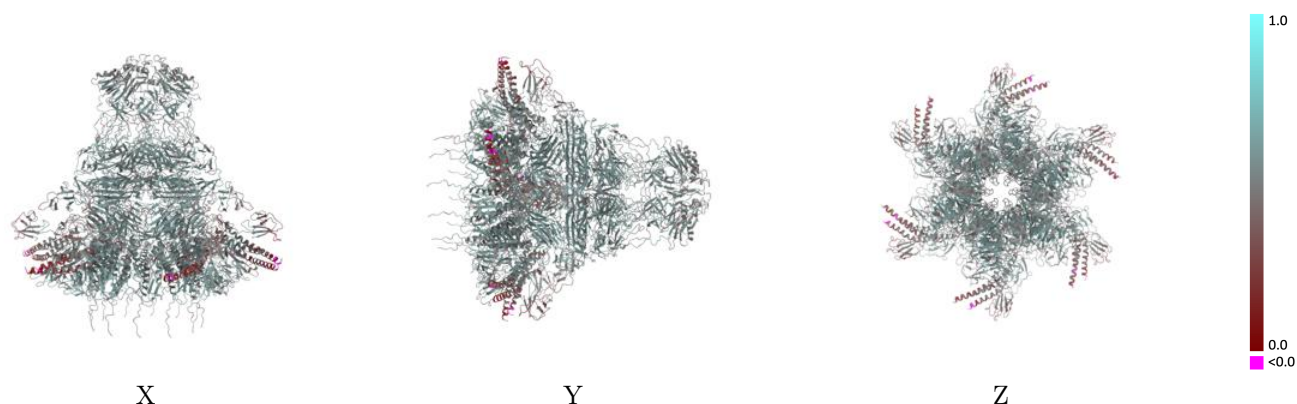
This section contains information regarding the fit between EMDB map EMD-65388 and PDB model 9VVR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



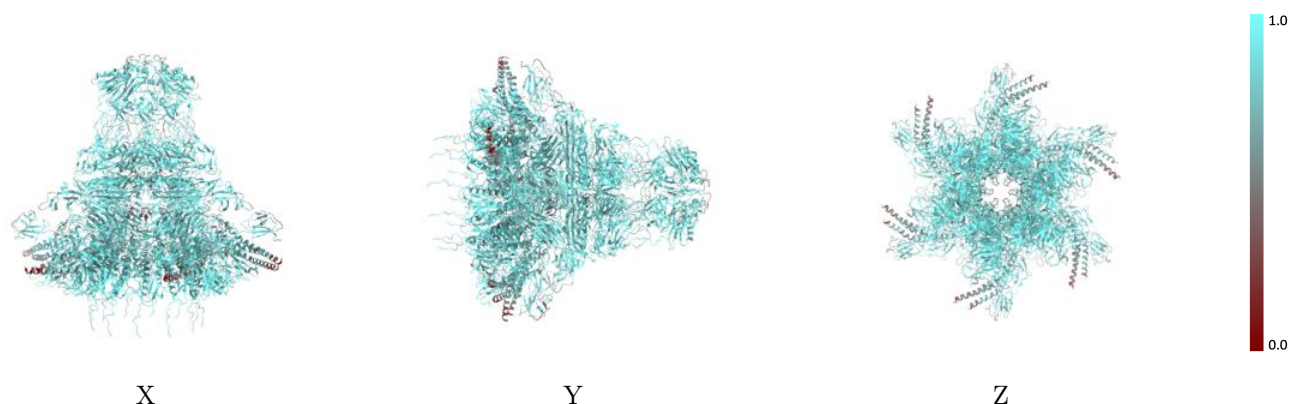
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



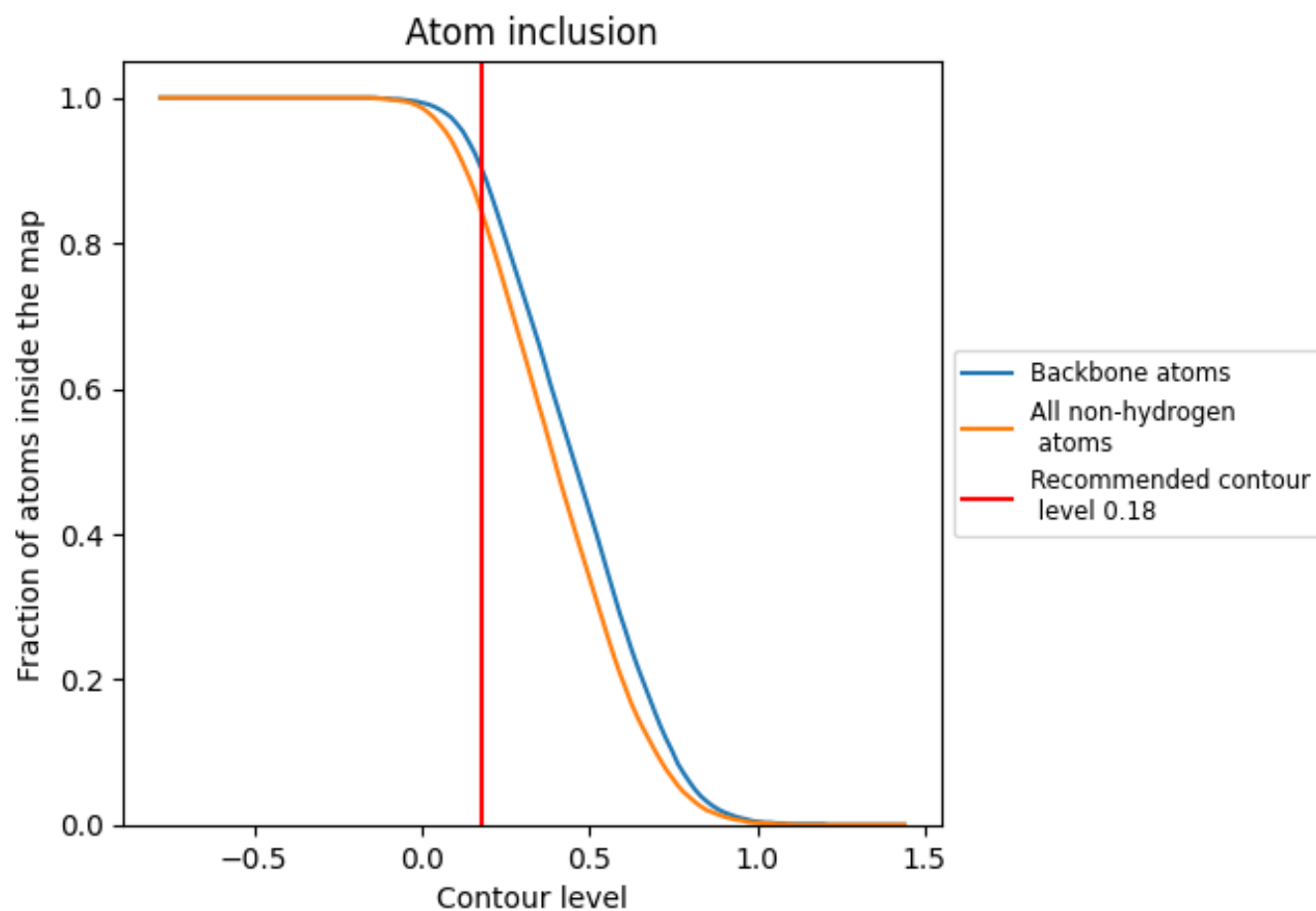
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.5190
A	 0.7240	 0.4060
B	 0.7920	 0.4770
C	 0.8190	 0.4950
D	 0.7340	 0.4020
E	 0.7870	 0.4870
F	 0.8260	 0.4940
G	 0.7290	 0.4070
H	 0.7240	 0.4100
I	 0.7110	 0.3940
J	 0.7940	 0.4820
K	 0.7920	 0.4840
L	 0.7840	 0.4820
M	 0.8230	 0.5020
N	 0.8190	 0.5010
O	 0.8260	 0.4940
P	 0.7270	 0.4100
Q	 0.7890	 0.4780
R	 0.8220	 0.4990
S	 0.8660	 0.5380
T	 0.8630	 0.5410
U	 0.8500	 0.5370
V	 0.8660	 0.5380
W	 0.8540	 0.5380
X	 0.8670	 0.5370
Y	 0.8640	 0.5420
Z	 0.8680	 0.5390
a	 0.8500	 0.5370
b	 0.8670	 0.5360
c	 0.8450	 0.5340
d	 0.8690	 0.5380
e	 0.8520	 0.5330
f	 0.8610	 0.5440
g	 0.8540	 0.5370
h	 0.8620	 0.5420



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Chain	Atom inclusion	Q-score
i	 0.8630	 0.5410
j	 0.8670	 0.5400