



Full wwPDB EM Validation Report ⓘ

Nov 5, 2025 – 12:57 PM JST

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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

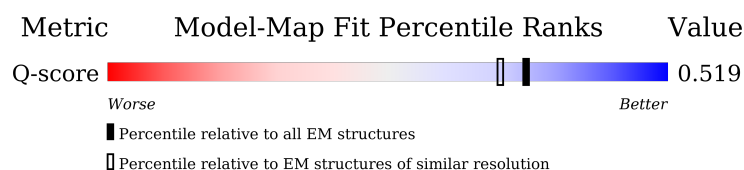
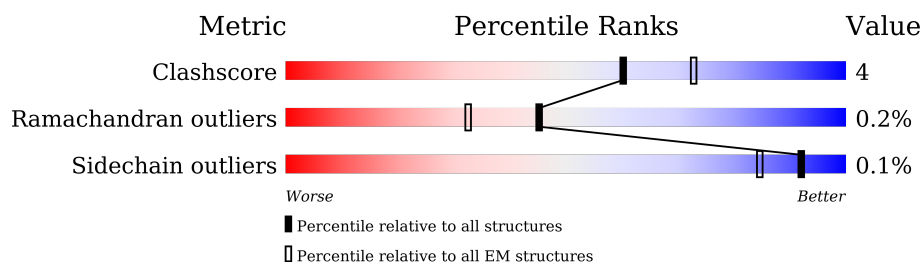
1 Overall quality at a glance

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.





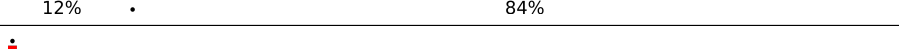
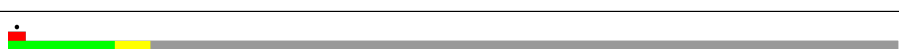


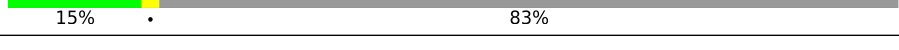
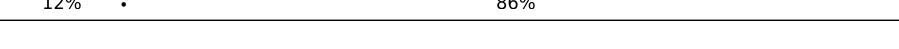



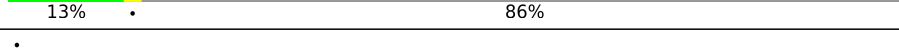
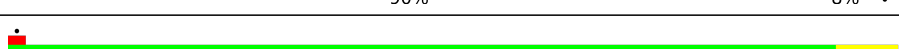
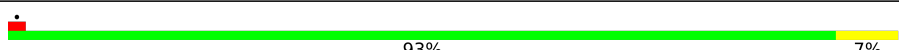
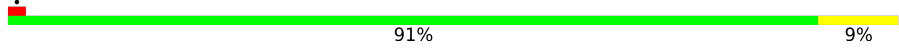
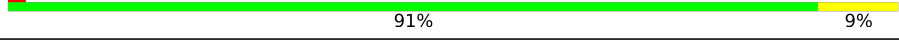
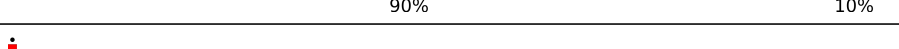


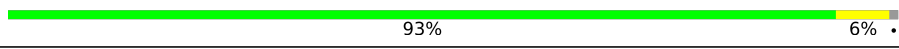




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14465 (2.61 - 3.61)

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	
1	B	843	
1	C	843	
1	D	843	

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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

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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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%





86%

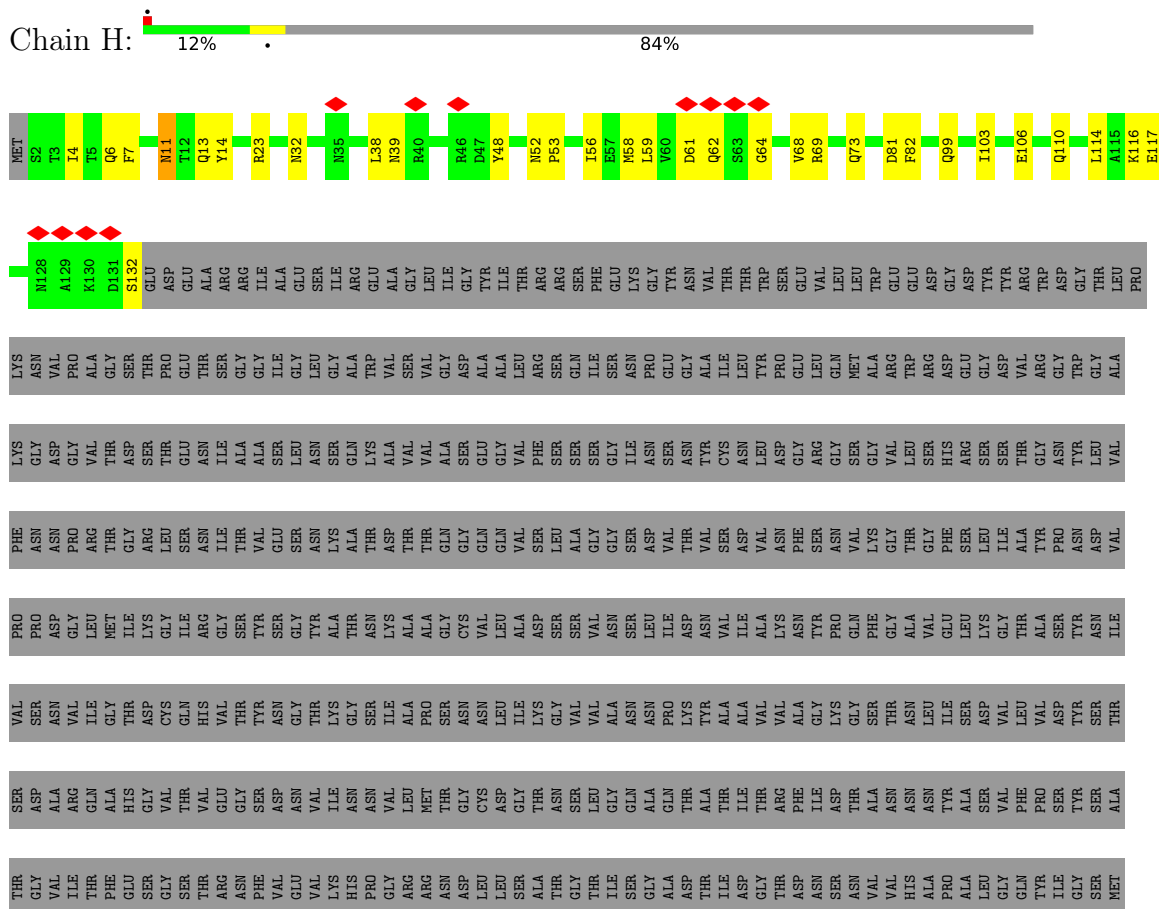


84%



[illegible]

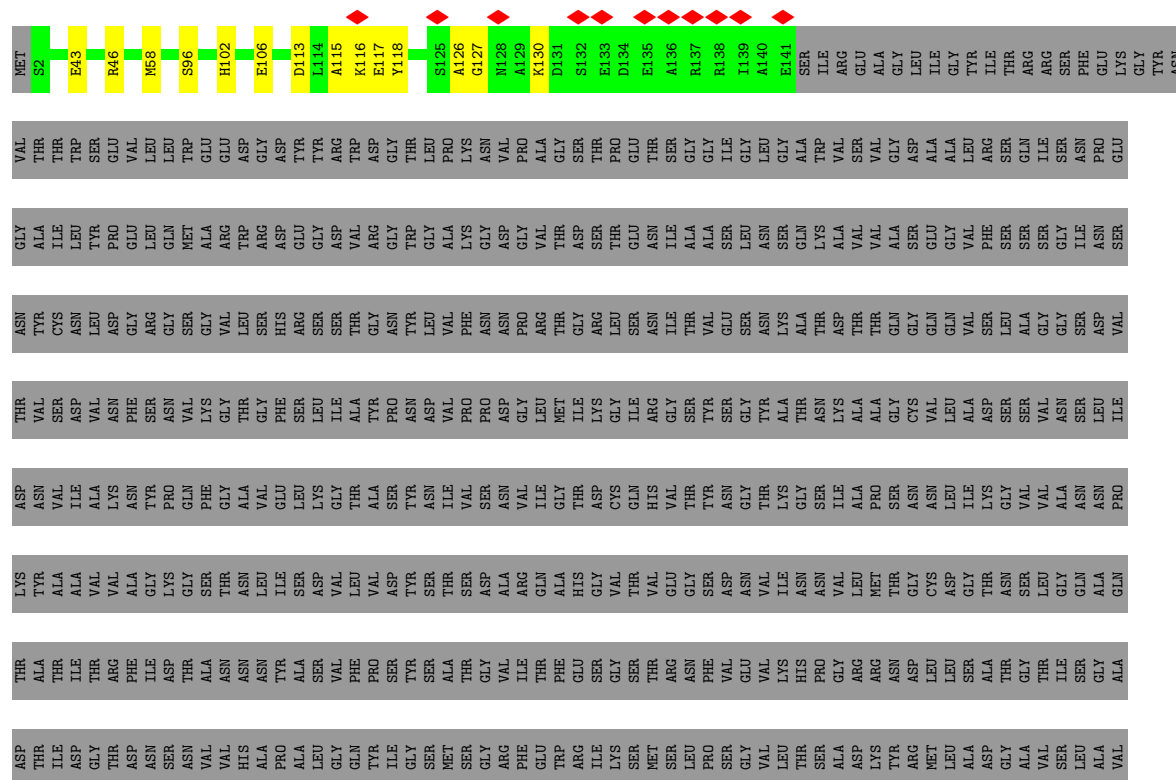
- Molecule 1: Tail spike protein



- Molecule 1: Tail spike protein

[illegible]

GLY	VAL	ARG	ALA	GLU	MET
LEU	LEU	TRP	ARG	GLU	S2
SER	SER	ASP	ASP	GLY	D66
HIS	ARG	ASP	GLU	TYR	I67
ARG	SER	GLY	GLY	TYR	R72
SER	SER	ASP	ASP	TYR	
THR	THR	VAL	ARG	TRP	H102
GLY	GLY	ARG	GLY	GLY	E106
ASN	ASN	GLY	TRP	THR	
TYR	TYR	TRP	GLY	LEU	V112
LEU	LEU	ALA	GLY	PRO	
VAL	PHE	LYS	LYS	LYS	A115
ASN	ASN	ASN	ASN	ASN	K116
ASN	ASN	ASP	ASP	VAL	
PRO	PRO	GLY	GLY	PRO	N128
ARG	ARG	VAL	VAL	ALA	
THR	THR	THR	THR	GLY	S132
GLY	GLY	ASP	ASP	SER	E133
ARG	ARG	SER	SER	THR	D134
LEU	LEU	THR	THR	PRO	E135
SER	SER	GLU	GLU	GLU	A136
ILE	ILE	ASN	ASN	THR	
THR	THR	ALA	ALA	SER	R137
VAL	VAL	ALA	ALA	GLY	
GLU	GLU	SER	SER	GLY	I138
SER	SER	LEU	LEU	ILE	I139
ASN	ASN	ASN	ASN	GLY	A140
LYS	LYS	ASN	ASN	LEU	E141
ALA	ALA	GLN	GLN	GLY	SER
THR	THR	LYS	LYS	ALA	ILE
ASP	ASP	ALA	ALA	TRP	ARG
THR	THR	VAL	VAL	VAL	GLU
THR	THR	VAL	VAL	VAL	ALA
GLN	GLN	SER	SER	GLY	GLY
GLY	GLY	ASP	ASP	ASP	LEU
GLN	GLN	GLU	GLU	ALA	ILE
VAL	VAL	GLY	GLY	ALA	GLY
SER	SER	VAL	VAL	LEU	TYR
GLN	GLN	PHE	PHE	ARG	ILE
VAL	VAL	SER	SER	SER	THR
ALA	ALA	SER	SER	GLN	ARG
GLY	GLY	SER	SER	ILE	SER
SER	SER	ILE	ILE	SER	SER
ASP	ASP	ASN	ASN	ASN	PHE
VAL	VAL	SER	SER	PRO	GLY
THR	THR	ASN	ASN	GLU	LYS
VAL	VAL	TYR	TYR	GLY	GLY
SER	SER	CYS	CYS	ALA	TYR
VAL	VAL	ASN	ASN	LEU	ASN
PHE	PHE	LEU	LEU	LEU	VAL
ASN	ASN	ASP	ASP	TYR	THR
ASN	ASN	GLY	GLY	PRO	THR
VAL	VAL	ARG	ARG	GLU	TRP
		GLY	GLY	LEU	SER
		SER	SER	GLN	GLU
		VAL	VAL	MET	LEU
		SER	SER		LEU



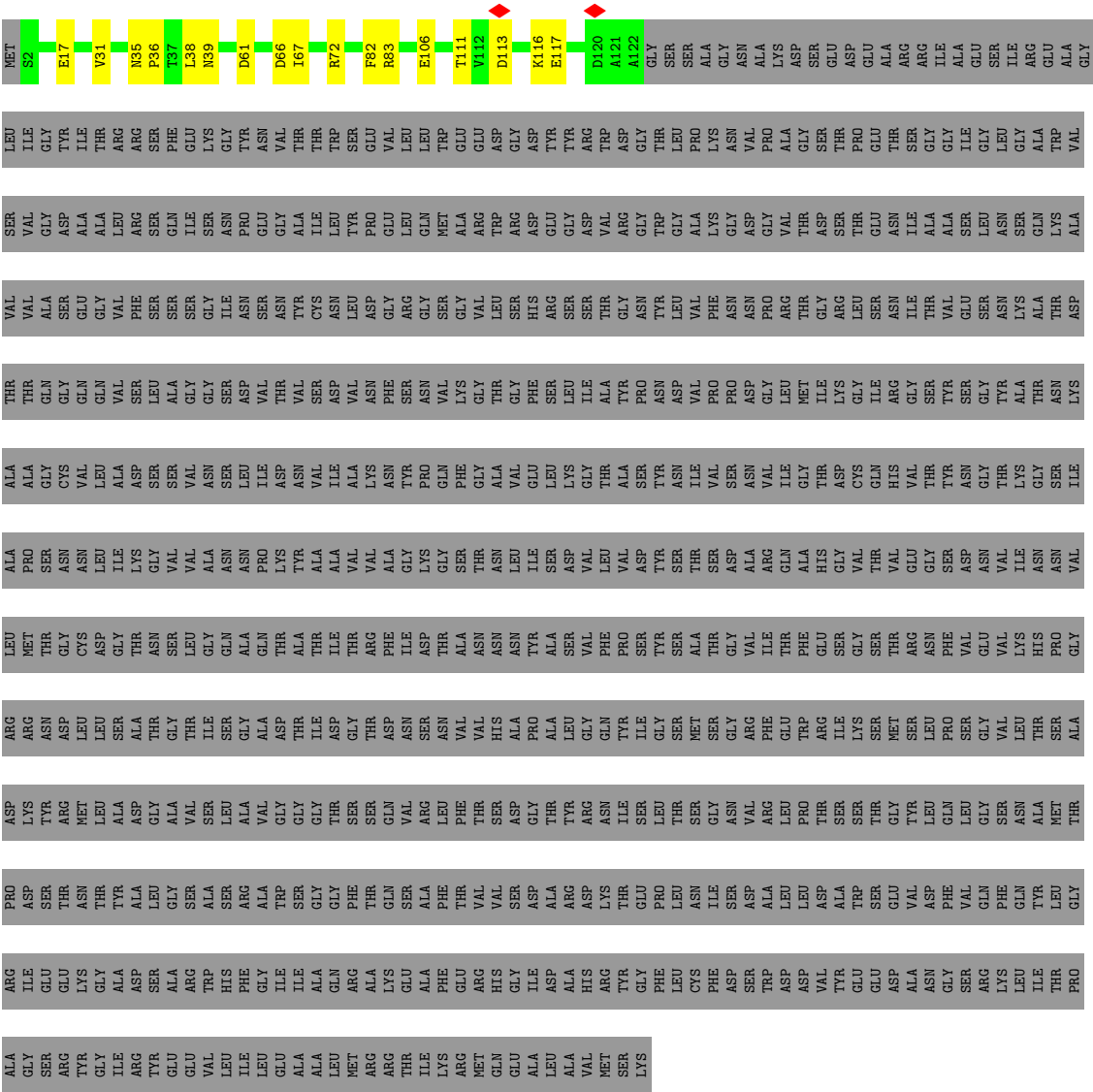
GLU	ALA	ALA	ILE	ILE	GLY	TRP	GLY
ALA	LEU	ALA	GLN	GLN	GLY	SER	GLY
MET	MET	LEU	ARG	ARG	PHE	THR	THR
ARG	ARG	ALA	ALA	ALA	THR	THR	SER
ARG	ARG	LYS	LYS	LYS	GLN	GLN	GLN
THR	THR	THR	GLU	GLU	SER	VAL	VAL
ILE	ILE	ALA	ALA	ALA	ALA	ALA	ARG
LYS	LYS	PHE	PHE	PHE	PHE	THR	PHE
ARG	ARG	GLU	GLU	GLU	THR	THR	THR
MET	MET	ARG	ARG	VAL	VAL	SER	SER
GLN	GLN	HIS	HIS	VAL	VAL	ASP	ASP
GLU	GLU	GLY	GLY	SER	SER	SER	GLY
ALA	ALA	ILE	ILE	ASP	ALA	THR	THR
LEU	LEU	ALA	ALA	ALA	ARG	TYR	TYR
ALA	ALA	HIS	HIS	ASP	ASP	ARG	ARG
VAL	VAL	ARG	ARG	LYS	LYS	ASN	ASN
MET	MET	TYR	TYR	ASP	ASP	VAL	VAL
SER	SER	GLY	GLY	TRP	TRP	ALA	ALA
LYS	LYS	PHE	PHE	ASP	ASP	LEU	LEU
		LEU	LEU	ASP	LEU	LEU	LEU
		LEU	LEU	ASP	LEU	PRO	PRO
		CYS	CYS	VAL	ASP	THR	THR
		PHE	PHE	TYR	ALA	SER	SER
		ASP	ASP	GLU	GLU	THR	THR
		ASP	ASP	GLU	GLU	GLY	GLY
		ALA	ALA	ASP	VAL	TYR	TYR
		ASN	ASN	ASP	ASP	LEU	LEU
		GLY	GLY	PHE	PHE	GLN	GLN
		SER	SER	VAL	VAL	LEU	LEU
		ARG	ARG	GLN	GLN	GLY	GLY
		LYS	LYS	PHE	PHE	SER	SER
		LEU	LEU	GLN	GLN	ASN	ASN
		ILE	ILE	TYR	TYR	ALA	ALA
		THR	THR	LYS	LYS	MET	MET
		PRO	PRO	ALA	ALA	THR	THR
		ALA	ALA	ARG	ARG	PRO	PRO
		GLY	GLY	ILE	ILE	ASP	ASP
		SER	SER	GLU	GLU	SER	SER
		ARG	ARG	GLU	GLU	THR	THR
		TYR	TYR	LYS	LYS	ASN	ASN
		ILE	ILE	ALA	ALA	TYR	TYR
		ARG	ARG	ASP	ASP	ALA	ALA
		TYR	TYR	SER	SER	LEU	LEU
		GLU	GLU	ALA	ALA	GLY	GLY
		VAL	VAL	TRP	TRP	SER	SER
		LEU	LEU	THR	THR	ALA	ALA
		ILE	ILE	PHE	PHE	ARG	ARG
		THR	THR	GLY	GLY	ALA	ALA

- Molecule 1: Tail spike protein

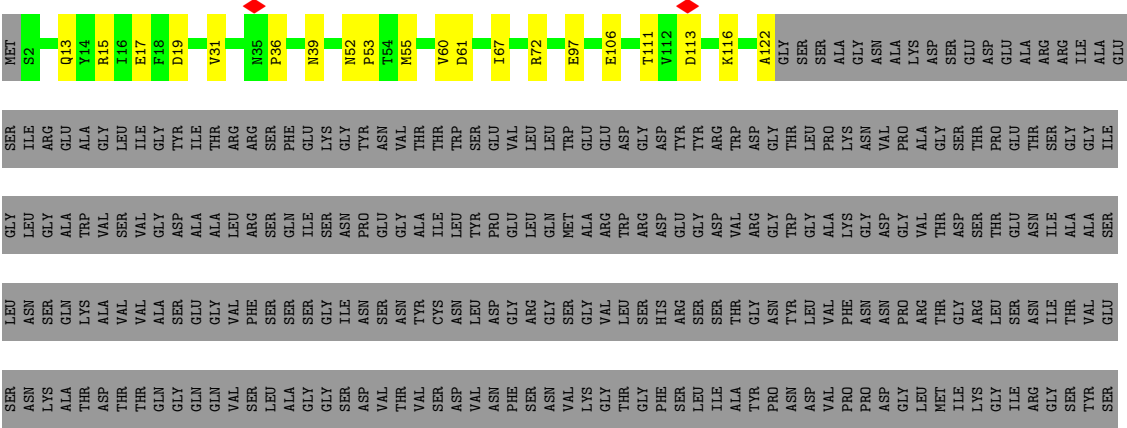
[illegible]

- Molecule 1: Tail spike protein





● Molecule 1: Tail spike protein



MET	ARG	LYS	ASN
SER	TYR	THR	ILE
LYS	GLY	GLU	SER
	PHE	PRO	LEU
	LEU	LEU	THR
	CYS	ASN	SER
	PHE	ILE	GLY
	ASP	SER	ASN
	ASP	ASP	VAL
	TRP	ALA	ARG
	ASP	LEU	LEU
	ASP	LEU	PRO
	VAL	ASP	THR
	TYR	ALA	SER
	GLU	TRP	SER
	GLU	THR	THR
	ASP	GLY	GLY
	ALA	VAL	LEU
	ASN	ASP	LEU
	GLY	PHE	GLN
	SER	VAL	GLY
	ARG	GLN	GLY
	LYS	PHE	SER
	LEU	GLN	ASN
	ILE	THR	ALA
	THR	LEU	ALA
	PRO	GLY	THR
	ALA	ARG	PRO
	GLY	ILE	ASP
	SER	GLU	SER
	ARG	GLU	THR
	TYR	LYS	ASN
	ILE	GLY	THR
	ARG	ALA	TYR
	TYR	ASP	ALA
	GLU	SER	LEU
	GLU	ALA	GLY
	VAL	ARG	SER
	LEU	HIS	SER
	ILE	PHE	ARG
	LEU	GLY	ALA
	GLU	ILE	TRP
	ALA	ILE	SER
	ALA	GLY	GLY
	LEU	GLN	GLY
	MET	ARG	PHE
	ARG	ALA	THR
	ARG	LYS	GLN
	ARG	GLU	SER
	ILE	ALA	ALA
	ILE	PHE	PHE
	ARG	GLU	THR
	MET	ARG	VAL
	GLN	HIS	VAL
	GLU	GLY	SER
	ALA	ILE	ASP
	LEU	ASP	ALA
	ALA	THR	ARG
	VAL	HIS	ASN

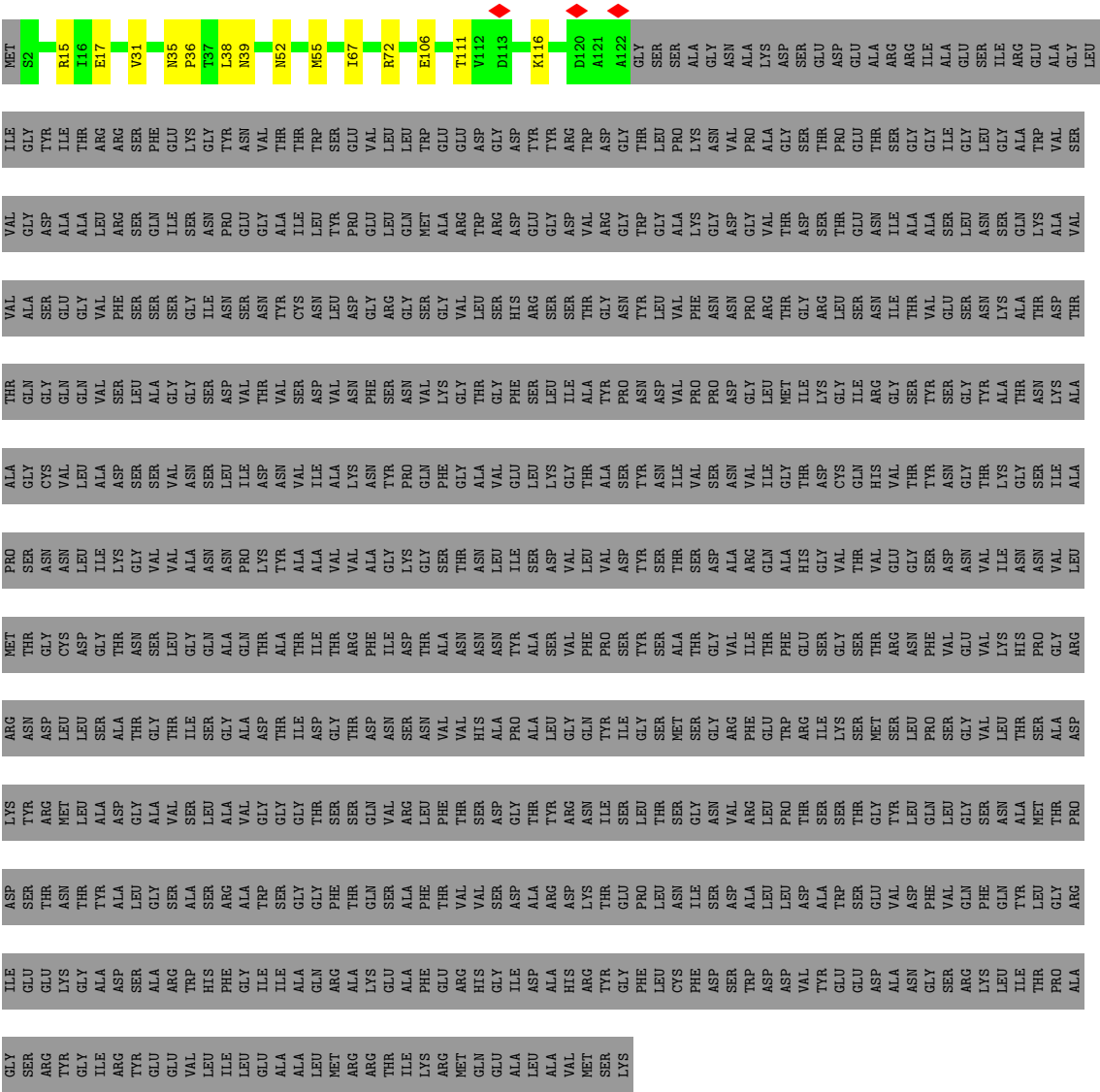
- Molecule 1: Tail spike protein



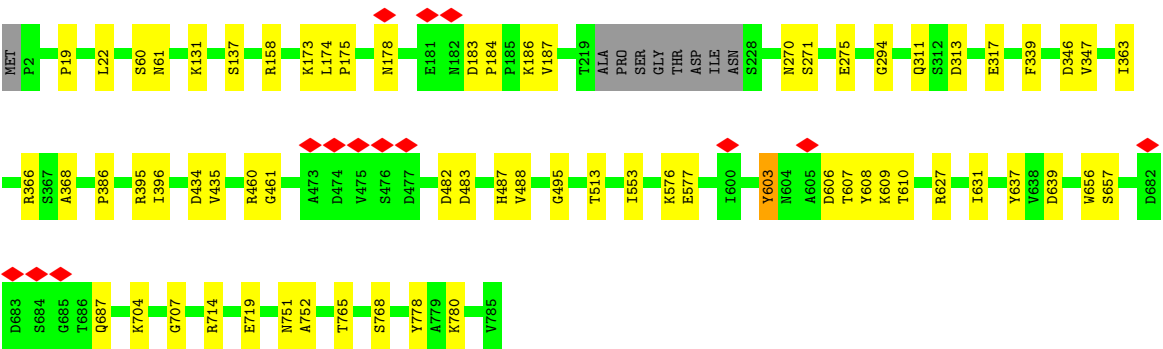
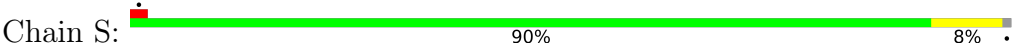
LEU	GLY	ALA	VAL	ALA	GLN	PRO	ILE	VAL	SER	GLU	ASN	ASN	MET
GLU	ILE	TRP	GLY	ASP	THR	LYS	ASP	THR	ASN	GLY	VAL	ILE	S2
ALA	ILE	SER	GLY	ILE	ALA	TYR	ASN	VAL	TYR	ALA	THR	ALA	Y14
LEU	GLN	GLY	THR	ASP	ILE	ALA	ILE	ASP	CYS	LEU	TRP	LEU	E17
MET	ARG	PHE	SER	SER	THR	VAL	LYS	VAL	LEU	TYR	SER	GLU	E43
ARG	ALA	THR	SER	GLN	ARG	ALA	ASN	PHE	ASP	GLU	VAL	VAL	R46
GLU	LYS	PHE	LEU	ASN	THR	GLY	GLN	VAL	SER	MET	TRP	LEU	M65
ARG	GLU	THR	PHE	VAL	ALA	SER	PHE	LYS	GLY	ALA	GLU	GLU	M68
MET	ARG	VAL	THR	VAL	ASN	THR	GLY	GLY	VAL	ARG	GLU	GLU	H102
GLN	HIS	VAL	SER	HIS	ASN	ASN	ALA	THR	LEU	TRP	ASP	GLY	E106
GLU	ILE	SER	GLY	PRO	TYR	ILE	GLU	PHE	HIS	ASP	ASP	GLY	V112
ALA	ASP	ALA	THR	ALA	ALA	SER	GLU	SER	ARG	GLU	TYR	ARG	L114
LEU	ASP	ASP	GLY	ILE	THR	ASP	ASN	PRO	ASN	GLY	GLY	GLY	A115
LEU	LEU	THR	THR	GLY	TYR	TYR	ASN	ASN	TYR	TRP	THR	GLY	K116
ALA	ALA	ARG	TYR	LEU	ALA	THR	ASN	ASP	LEU	ALA	PRO	PRO	
VAL	HIS	ASP	ARG	GLY	VAL	VAL	ILE	VAL	VAL	ALA	GLY	GLY	D120
MET	ARG	LYS	ASN	GLN	PHE	LEU	THR	ALA	THR	VAL	VAL	VAL	N128
SER	ASP	ASP	VAL	GLY	THR	ASP	SER	ASN	ASN	ASP	VAL	ALA	A129
LYS	GLY	GLU	ILE	ILE	PRO	VAL	GLY	VAL	PHE	GLY	GLY	GLY	
	PHE	ASP	THR	THR	TYR	THR	GLN	ILE	THR	THR	THR	THR	S132
	ASP	THR	THR	ILE	SER	GLY	ASP	LYS	ARG	SER	SER	SER	E133
	TYR	TRP	SER	ILE	GLY	VAL	CYS	GLY	GLY	THR	PRO	PRO	D134
	GLU	SER	THR	SER	SER	THR	GLN	ILE	SER	GLU	GLU	THR	E135
	ASP	GLU	GLY	MET	THR	VAL	HIS	ARG	ASN	ASN	THR	GLU	A136
	ALA	VAL	TYR	SER	ARG	GLU	VAL	GLY	ILE	ILE	SER	SER	R137
	GLY	PHE	ASN	PRO	PHE	GLY	THR	TYR	THR	ALA	GLY	ALA	I138
	SER	VAL	LEU	SER	VAL	ASN	ASN	SER	GLU	SER	ILE	GLY	I139
	ARG	GLN	GLY	GLY	GLU	ASN	GLY	GLY	SER	LEU	GLY	LEU	A140
	LYS	PHE	SER	VAL	VAL	VAL	THR	TYR	ASN	ASN	SER	GLY	E141
	LEU	GLN	ASN	LEU	LYS	ILE	THR	ALA	LYS	SER	GLY	GLY	SER
	ILE	ALA	ALA	HIS	THR	ASN	GLY	THR	ALA	GLN	ALA	ALA	ILE
	THR	LEU	ALA	PRO	PRO	ASN	SER	ASN	THR	LYS	TRP	TRP	ARG
	PRO	GLY	THR	ALA	GLY	VAL	ILE	LYS	ASP	ALA	VAL	VAL	GLU
	ALA	ARG	PRO	ASP	ARG	LEU	ALA	ALA	THR	VAL	VAL	VAL	ALA
	GLY	ILE	ASP	LYS	ASN	MET	SER	GLY	GLN	ALA	GLY	GLY	GLY
	SER	GLU	SER	THR	ASN	THR	SER	THR	GLN	ALA	GLY	GLY	LEU
	ARG	GLU	THR	THR	ASP	CYS	ASN	CYS	SER	SER	ASP	ASP	GLY
	TYR	GLY	THR	ALA	LEU	THR	ILE	VAL	LEU	PHE	ARG	TYR	TYR
	ILE	ALA	ALA	ASP	SER	GLY	GLY	ASP	LEU	SER	ARG	ILE	ILE
	ARG	ASP	ALA	THR	ALA	THR	LYS	ASP	SER	PHE	THR	THR	THR
	TYR	SER	LEU	GLY	THR	ASN	GLY	SER	LEU	SER	SER	THR	THR
	GLU	ALA	GLY	ALA	GLY	ASN	VAL	THR	GLN	SER	GLN	GLN	GLY
	GLU	ALA	THR	VAL	THR	THR	THR	THR	GLY	THR	GLN	GLN	GLY
	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

- Molecule 1: Tail spike protein



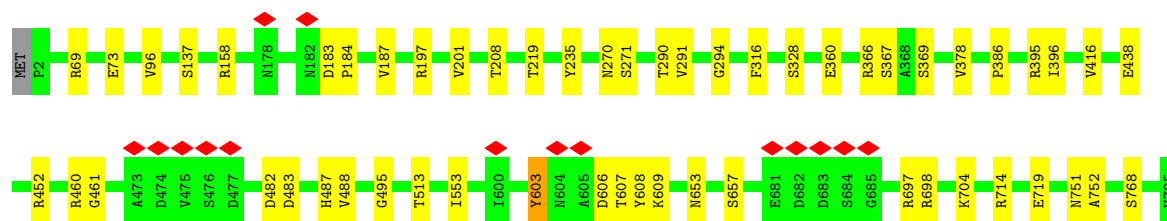


• Molecule 2: Nozzle protein



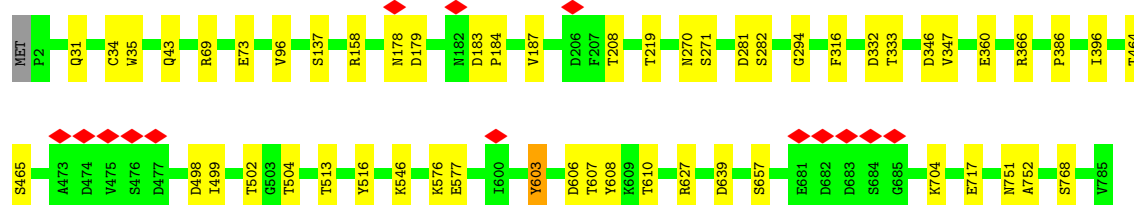
• Molecule 2: Nozzle protein

Chain V:  93% 7%




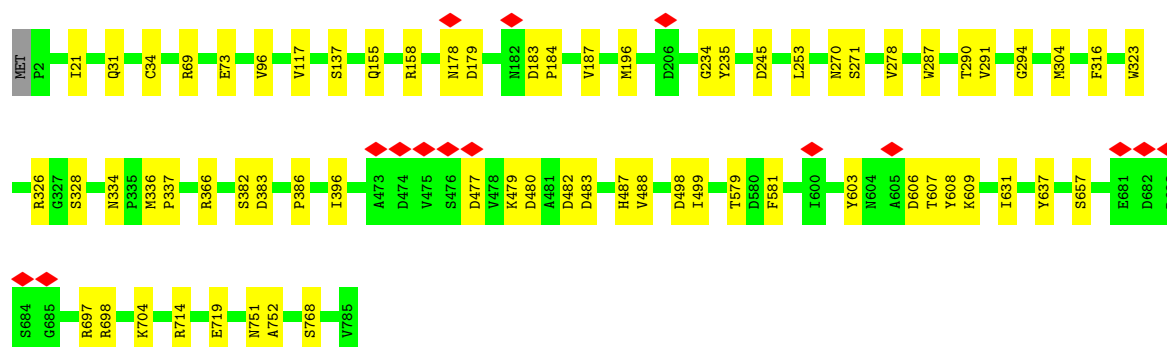
• Molecule 2: Nozzle protein

Chain X:  93% 7%




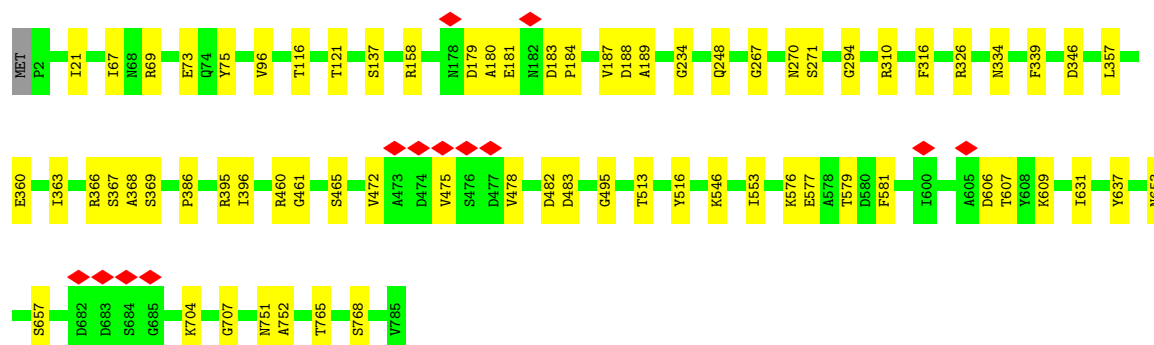
• Molecule 2: Nozzle protein

Chain Z:  91% 9%

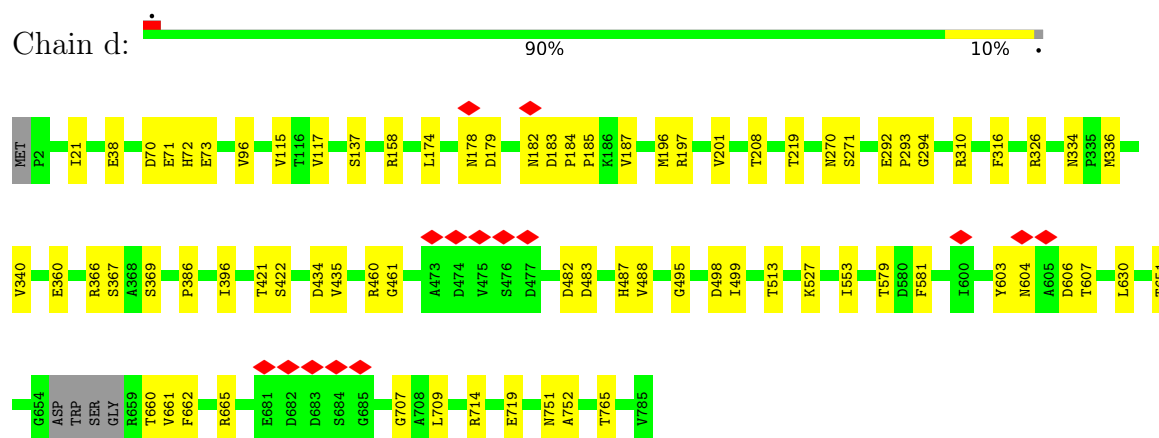


• Molecule 2: Nozzle protein

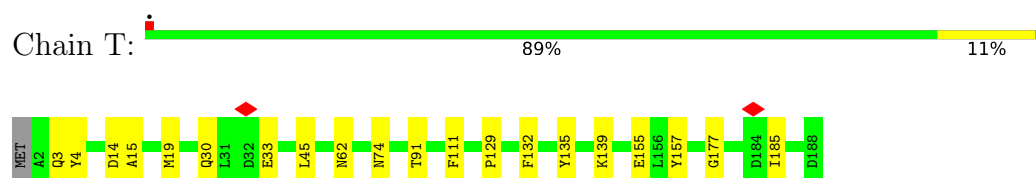
Chain b:  91% 9%



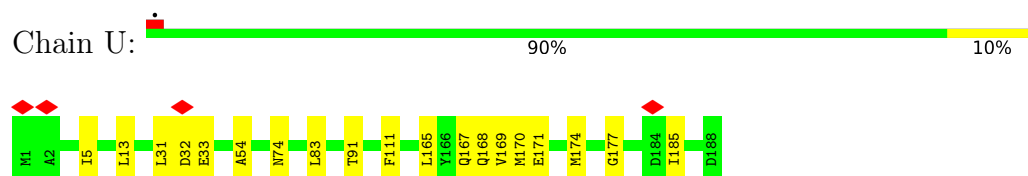
- Molecule 2: Nozzle protein



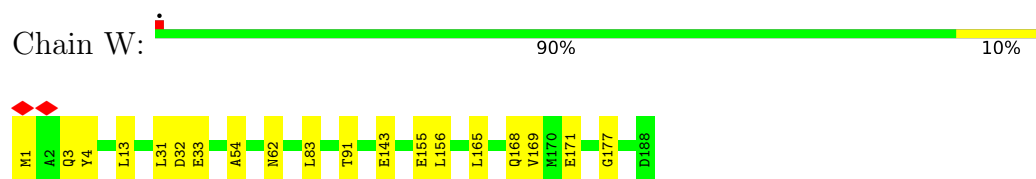
- Molecule 3: Adaptor protein



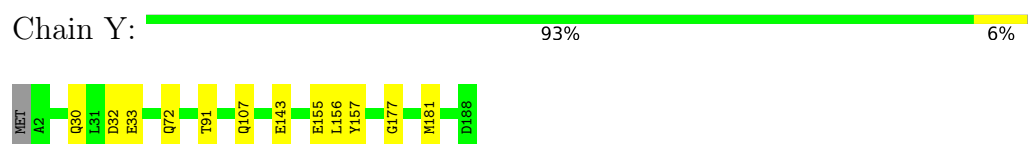
- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein

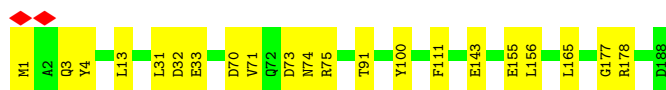


- Molecule 3: Adaptor protein

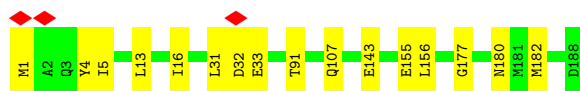
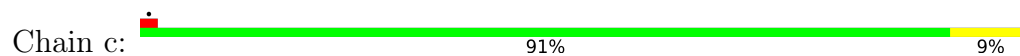


- Molecule 3: Adaptor protein





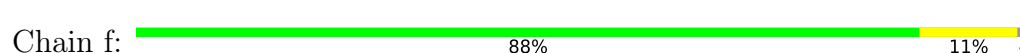
- Molecule 3: Adaptor protein



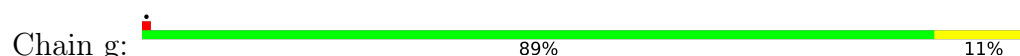
- Molecule 3: Adaptor protein



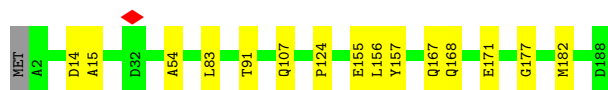
- Molecule 3: Adaptor protein



- Molecule 3: Adaptor protein



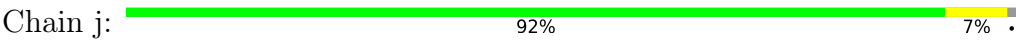
- Molecule 3: Adaptor protein



- 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.34	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	46
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	46
1	E	138/843 (16%)	130 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	119/843 (14%)	117 (98%)	1 (1%)	1 (1%)	16	46
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%)	25	56
2	V	782/785 (100%)	726 (93%)	53 (7%)	3 (0%)	30	61
2	X	782/785 (100%)	728 (93%)	51 (6%)	3 (0%)	30	61
2	Z	782/785 (100%)	726 (93%)	54 (7%)	2 (0%)	37	67
2	b	782/785 (100%)	725 (93%)	54 (7%)	3 (0%)	30	61
2	d	776/785 (99%)	716 (92%)	58 (8%)	2 (0%)	37	67
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9218/22140 (42%)	8666 (94%)	532 (6%)	20 (0%)	45	73

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%)	75	87
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	120/685 (18%)	119 (99%)	1 (1%)	79	89
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%)	75	87
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%)	92	97
2	b	669/670 (100%)	669 (100%)	0	100	100
2	d	666/670 (99%)	663 (100%)	3 (0%)	86	92
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

Continued on next page...

Continued from previous page...

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%)	92	97

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

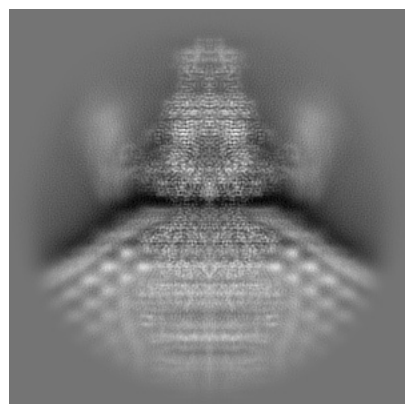
6 Map visualisation [i](#)

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.

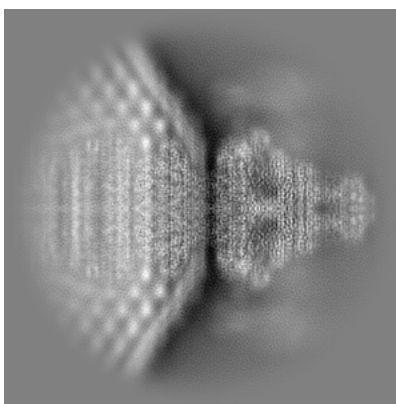
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

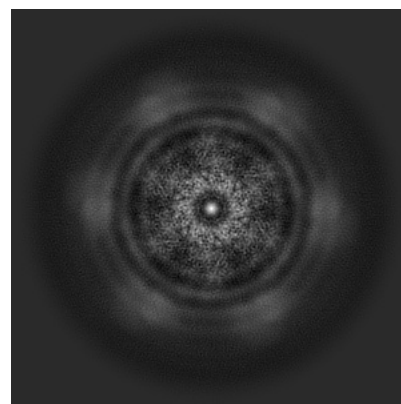
6.1.1 Primary map



X

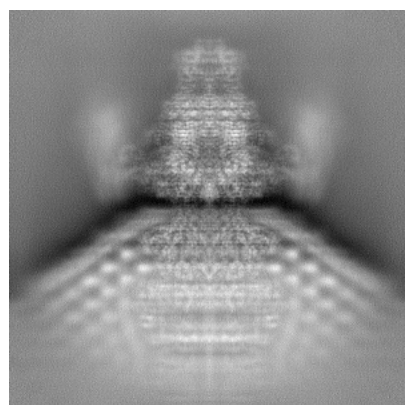


Y

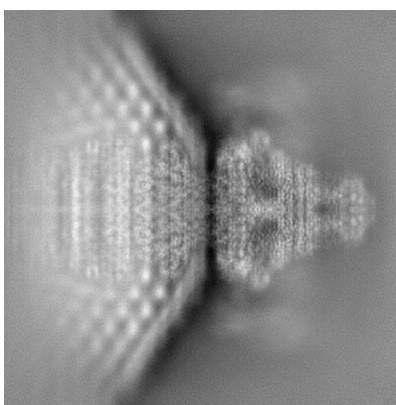


Z

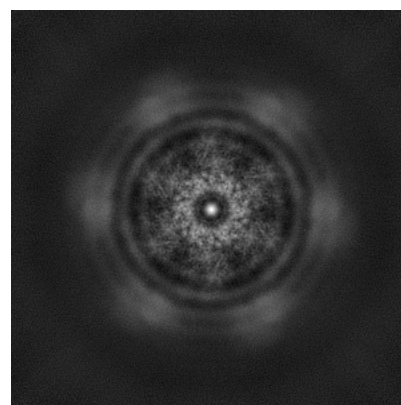
6.1.2 Raw map



X



Y

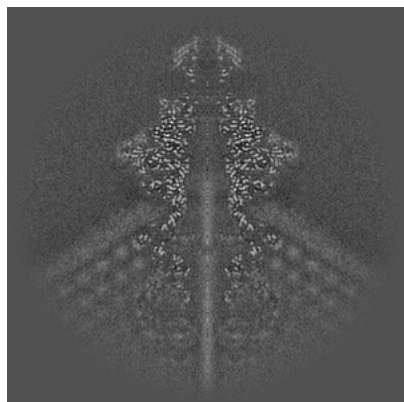


Z

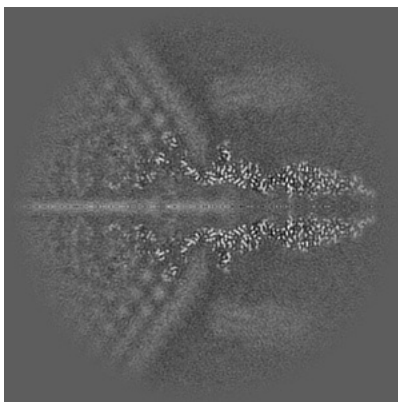
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

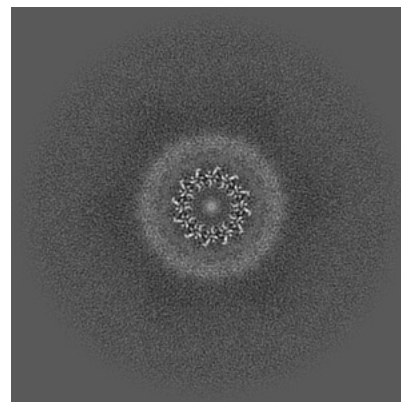
6.2.1 Primary map



X Index: 220

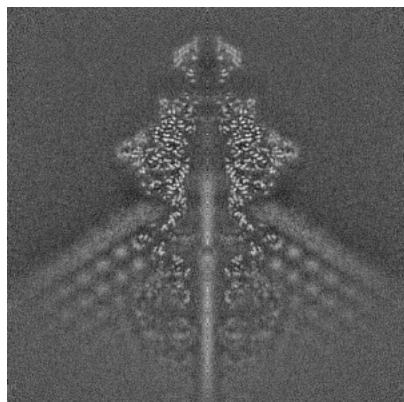


Y Index: 220

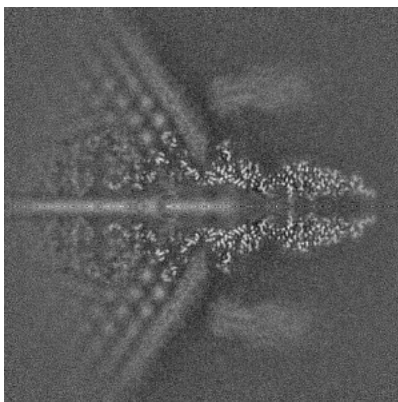


Z Index: 220

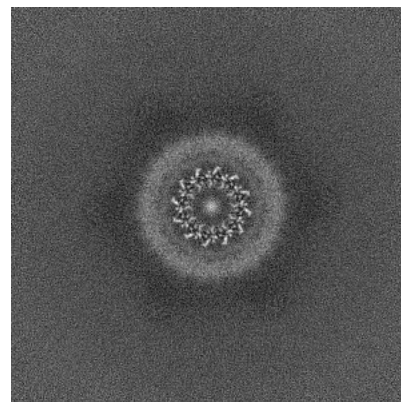
6.2.2 Raw map



X Index: 220



Y Index: 220

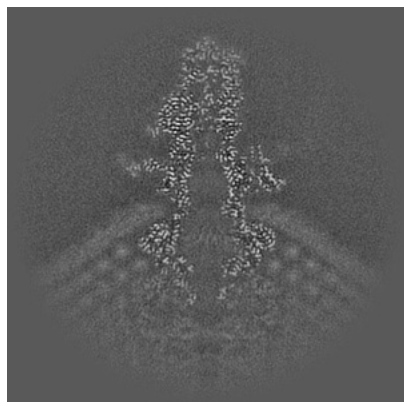


Z Index: 220

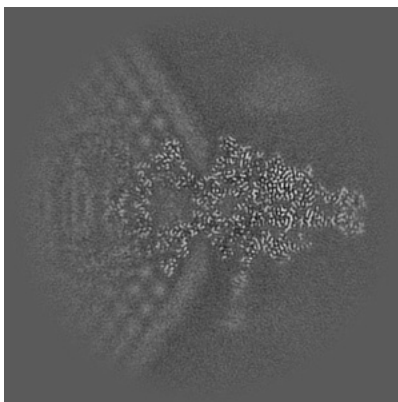
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

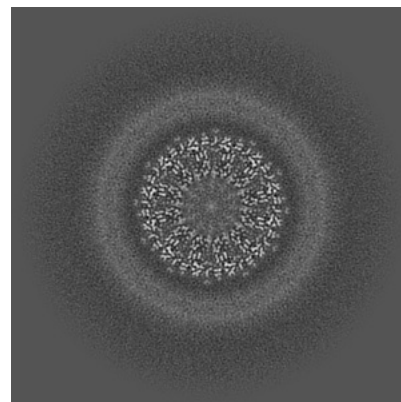
6.3.1 Primary map



X Index: 206

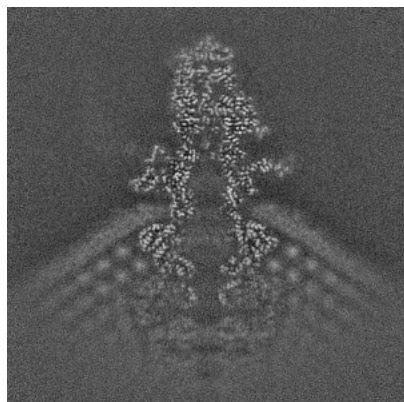


Y Index: 196

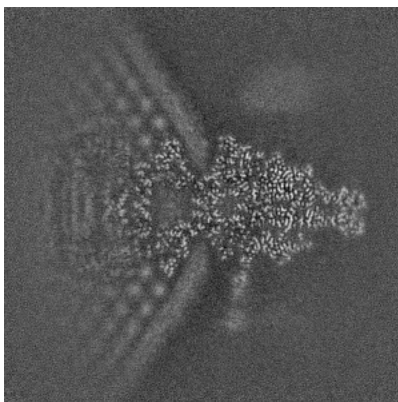


Z Index: 184

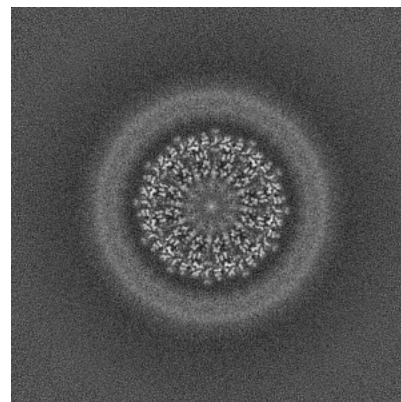
6.3.2 Raw map



X Index: 235



Y Index: 196

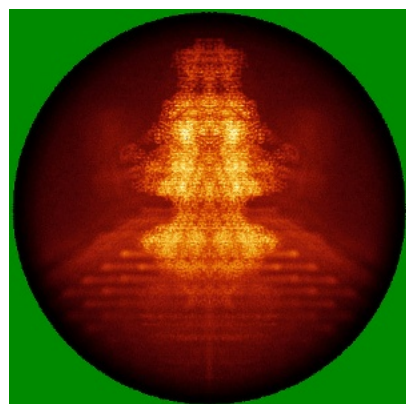


Z Index: 184

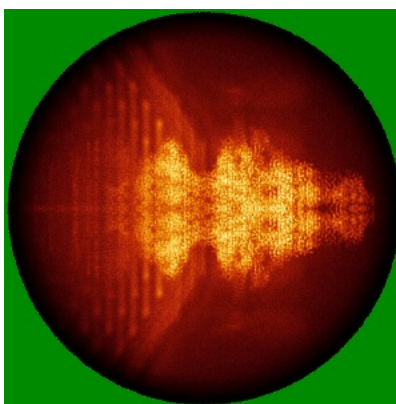
The images above show the largest variance slices of the map in three orthogonal directions.

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

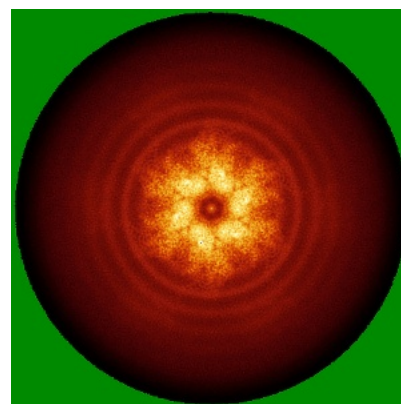
6.4.1 Primary map



X

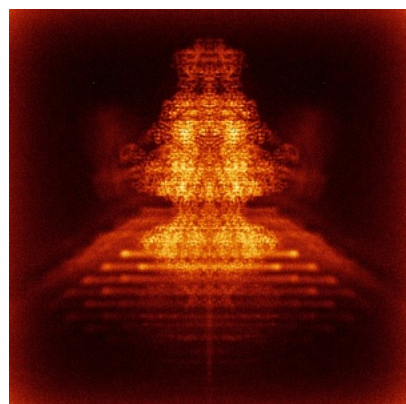


Y

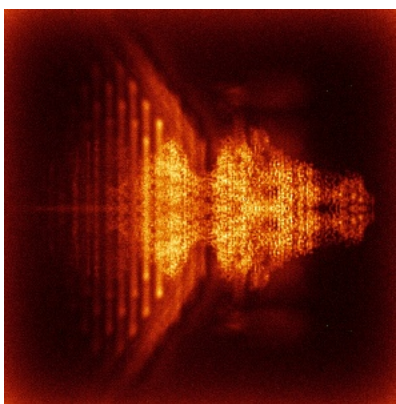


Z

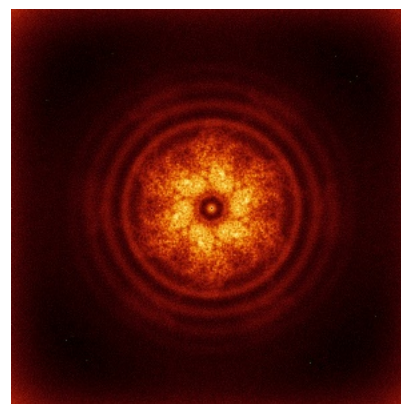
6.4.2 Raw map



X



Y

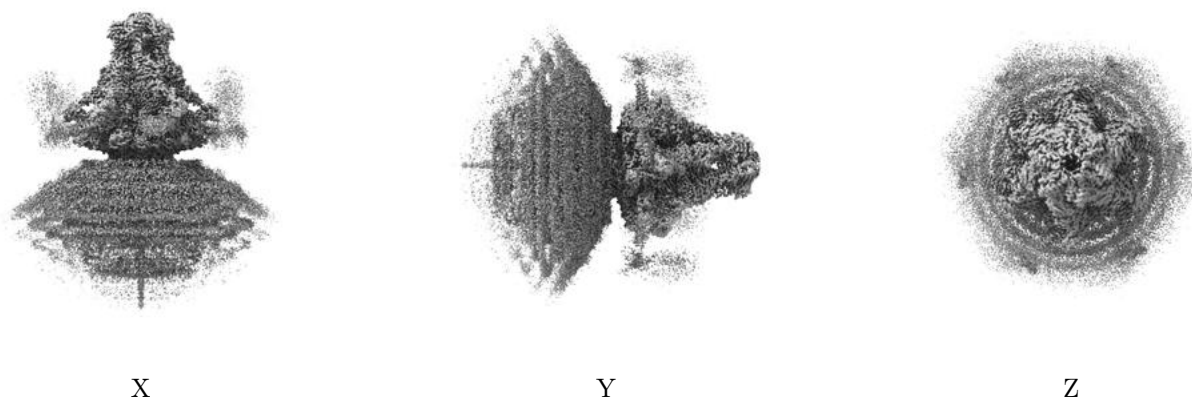


Z

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.

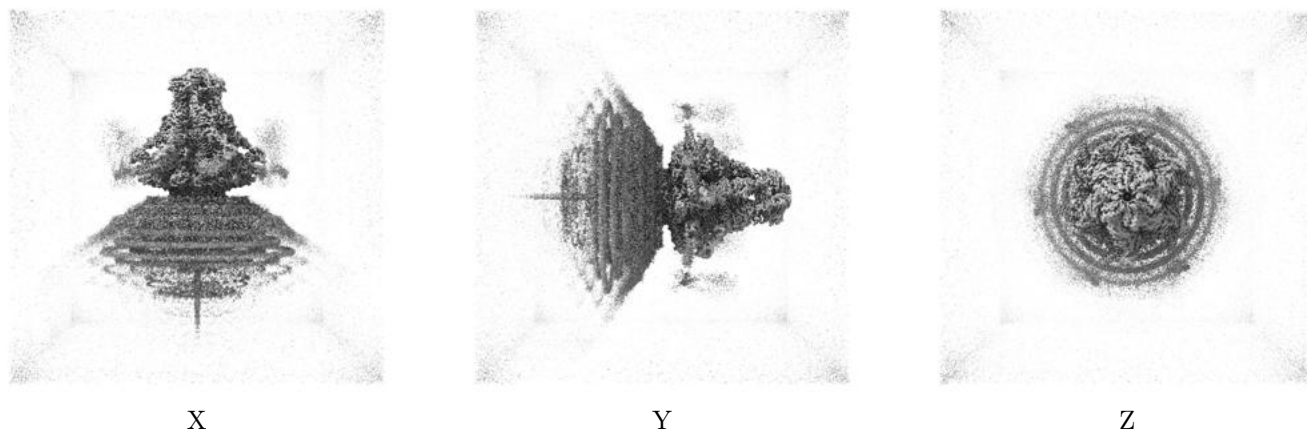
6.5 Orthogonal surface views [i](#)

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.

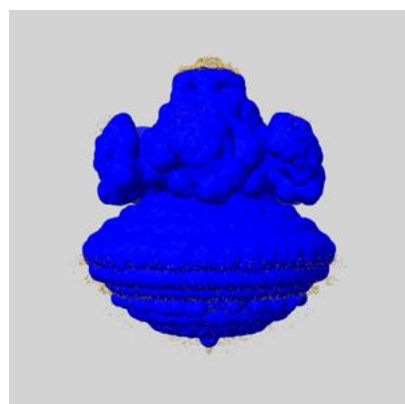
6.6 Mask visualisation [i](#)

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

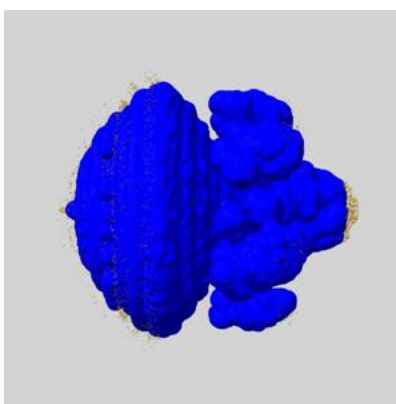
A mask typically either:

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

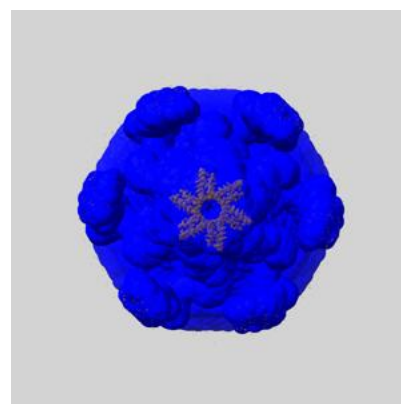
6.6.1 emd_65388_msk_1.map [i](#)



X



Y

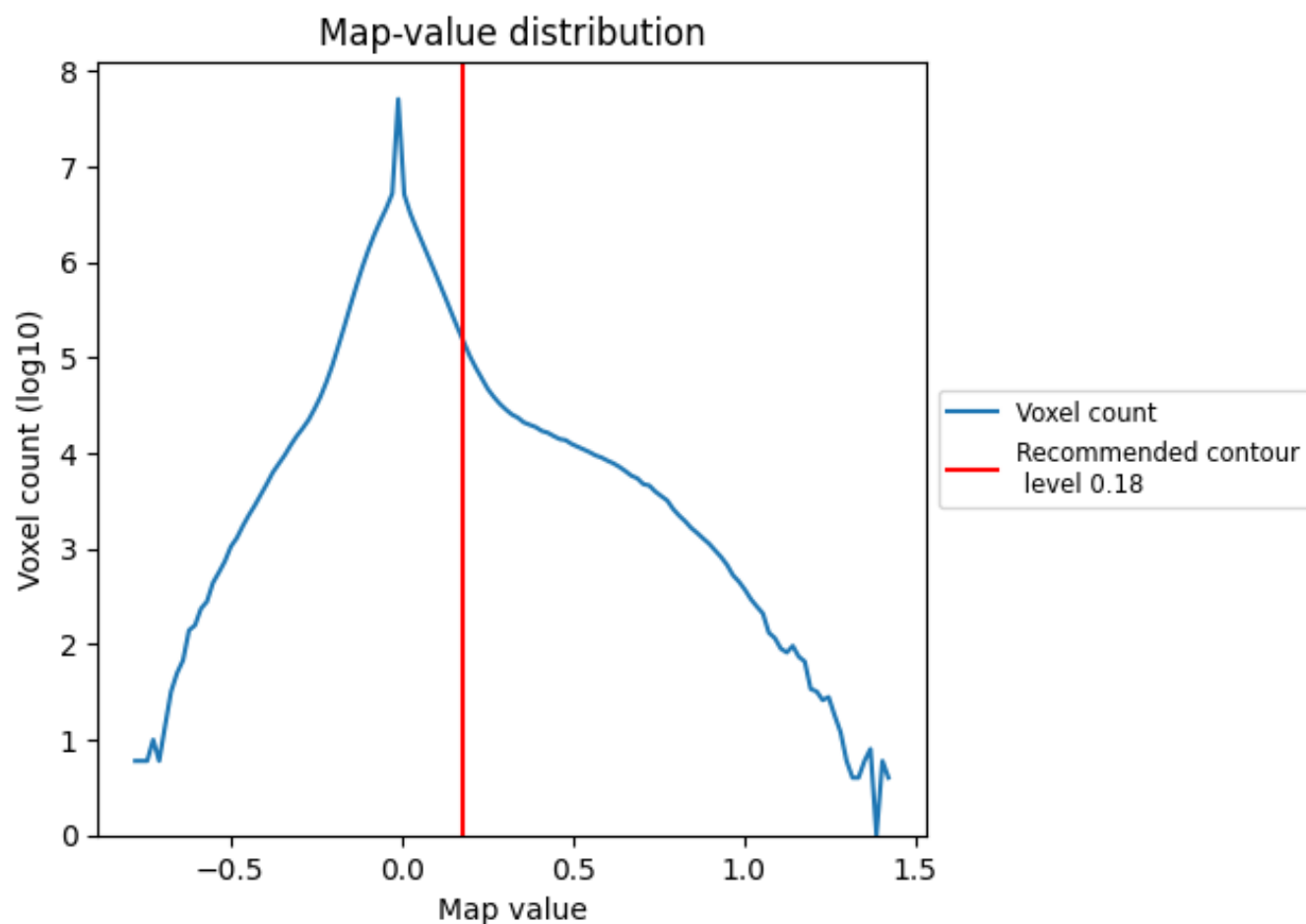


Z

7 Map analysis [i](#)

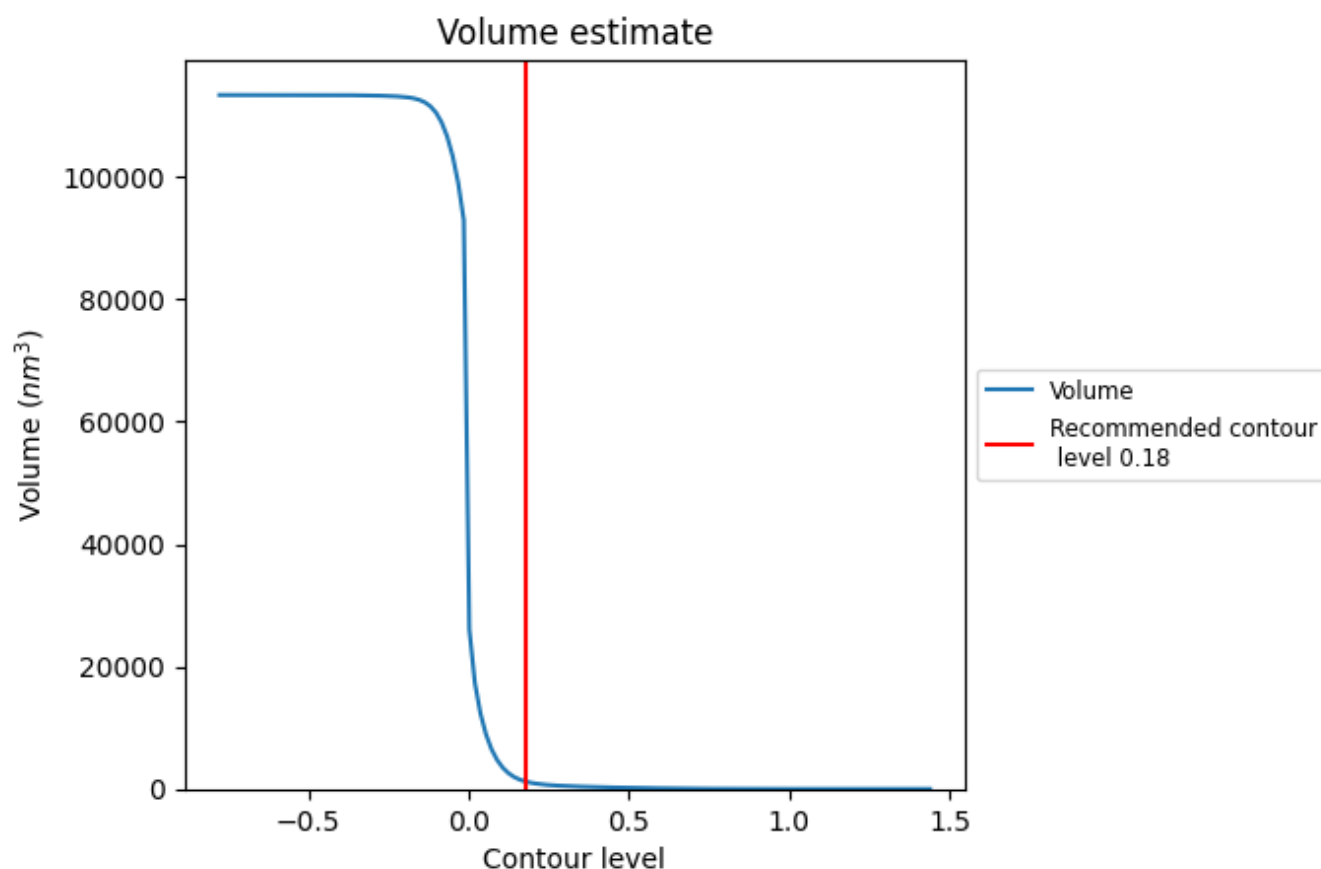
This section contains the results of statistical analysis of the map.

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.

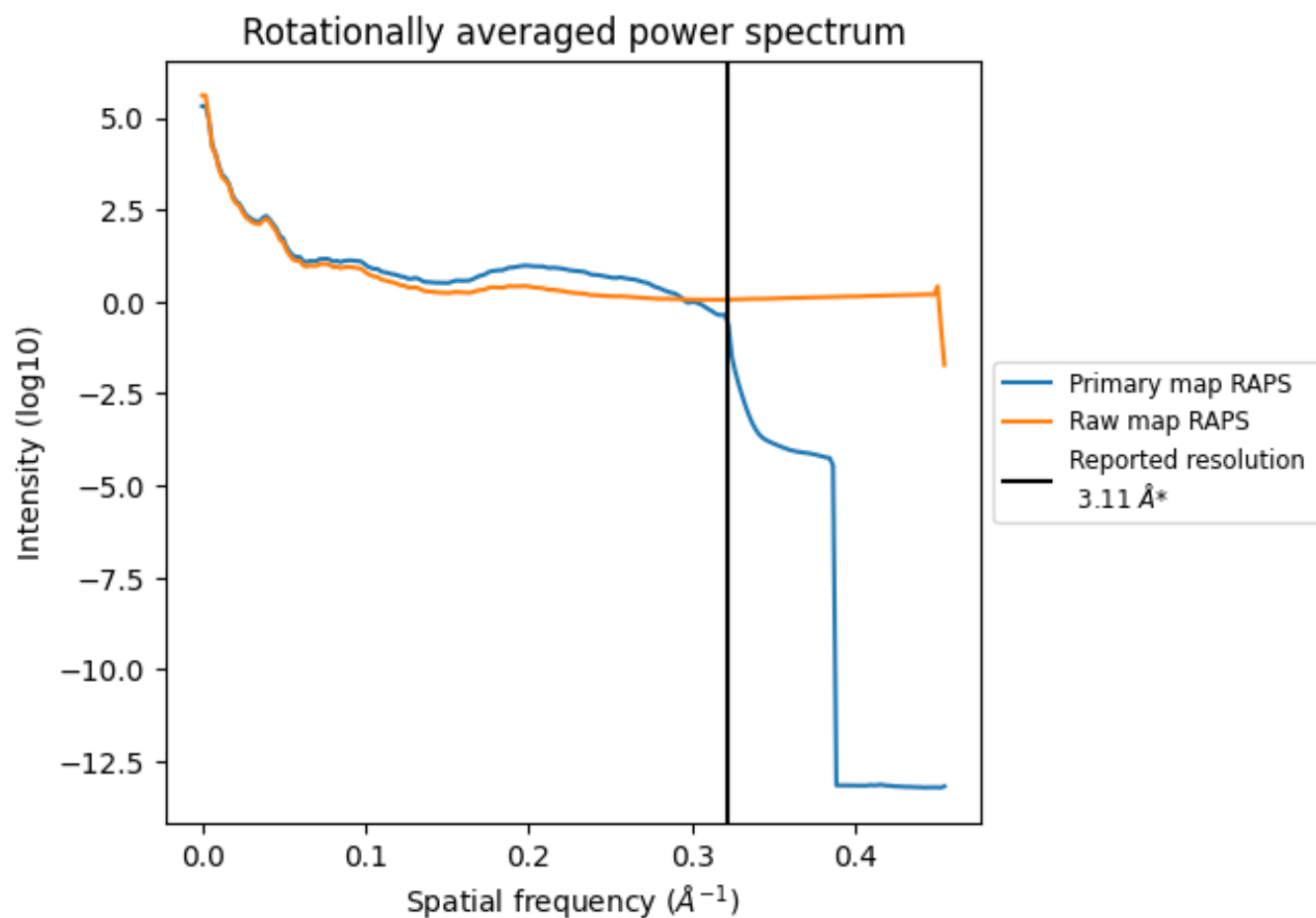
7.2 Volume estimate [i](#)



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 ⓘ

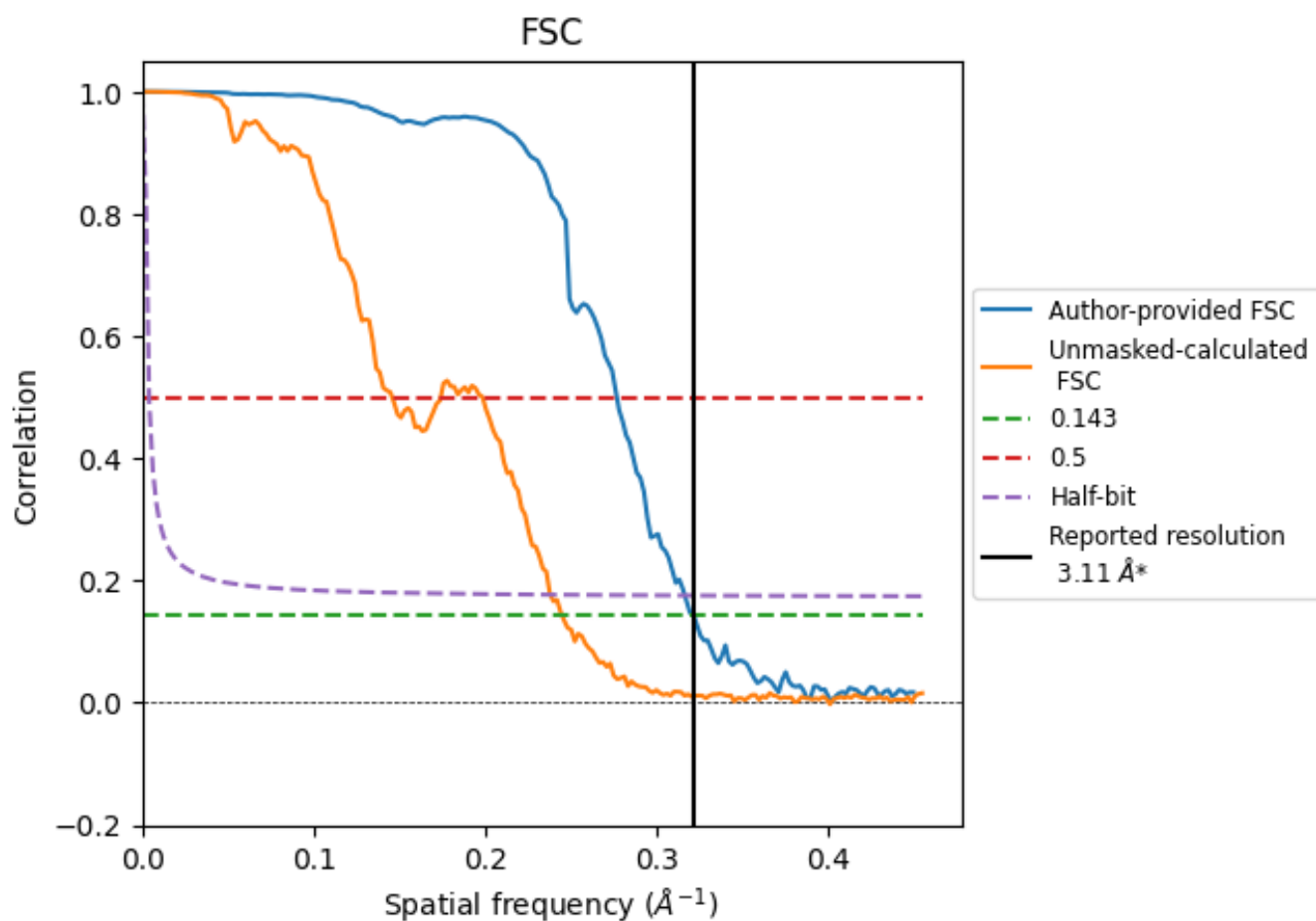


*Reported resolution corresponds to spatial frequency of 0.322 Å⁻¹

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 \AA^{-1}

8.2 Resolution estimates [i](#)

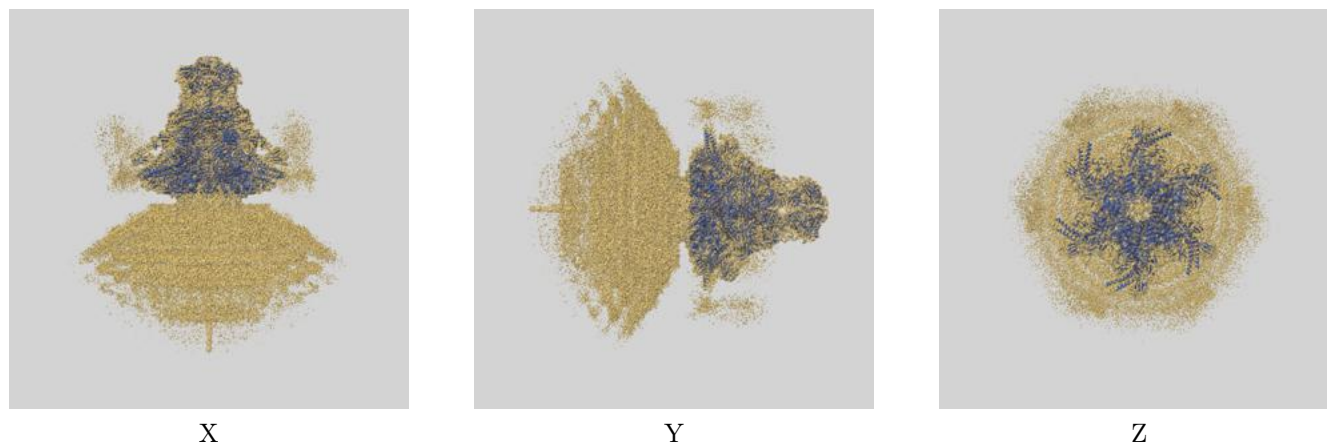
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.62	3.16
Unmasked-calculated*	4.09	6.87	4.21

*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](#)

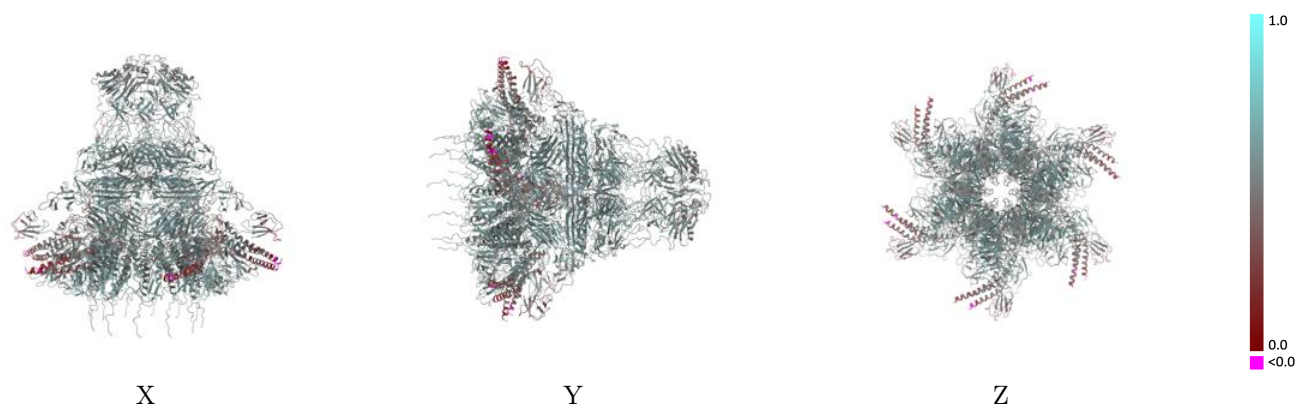
This section contains information regarding the fit between EMDB map EMD-65388 and PDB model 9VVR. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



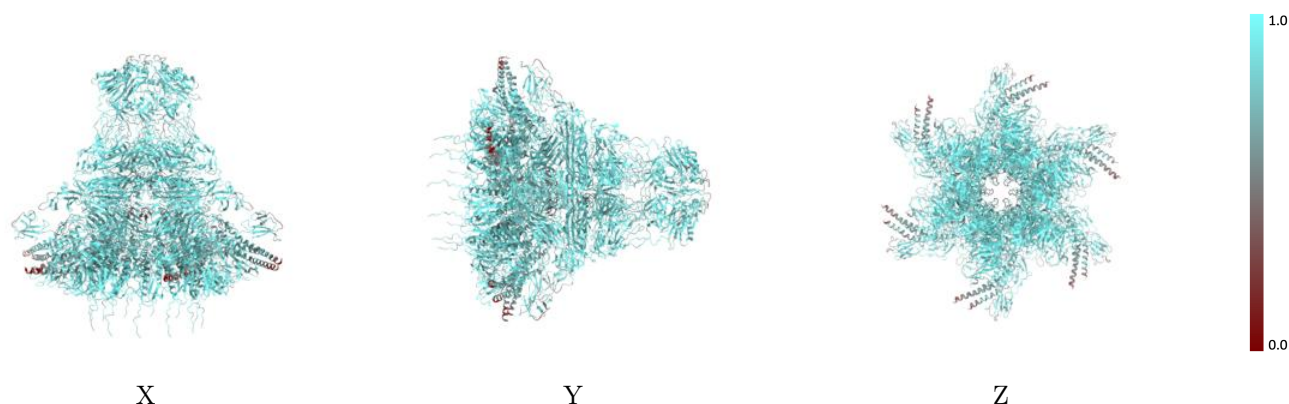
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



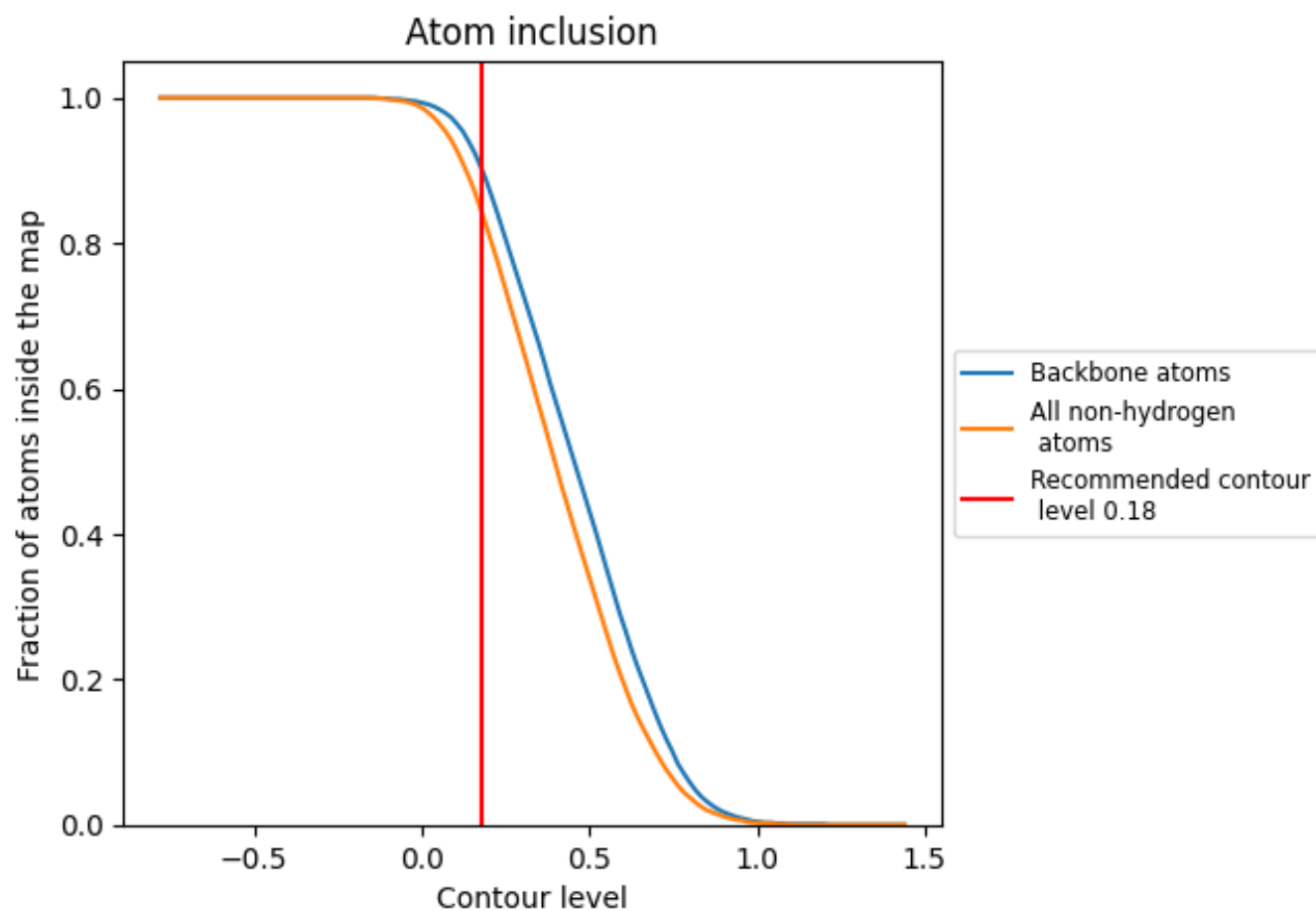
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



Continued on next page...

Continued from previous page...

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