



## Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 10:50 PM EDT

PDB ID : 9YD0 / pdb\_00009yd0  
EMDB ID : EMD-72793  
Title : Structure of the Adenovirus-7 VLP, Class 1  
Authors : Khayat, R.; Madoo, K.  
Deposited on : 2025-09-20  
Resolution : 3.80 Å(reported)  
Based on initial model : .

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

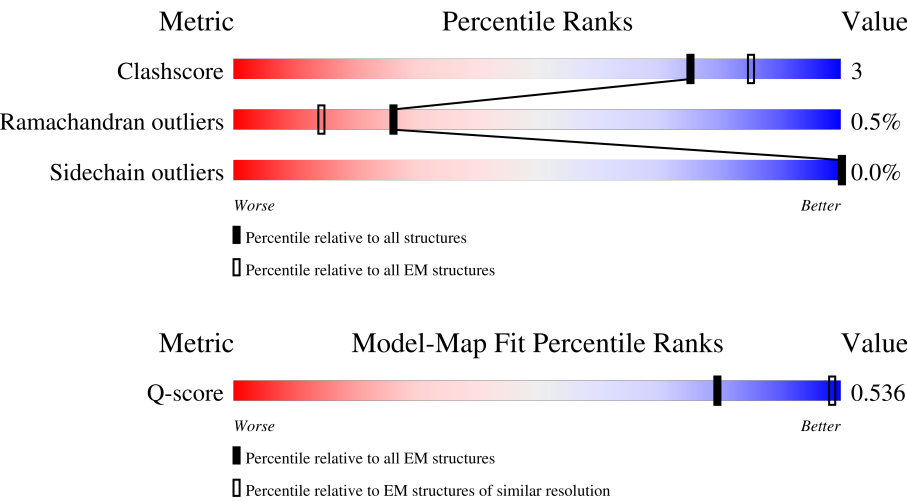
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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







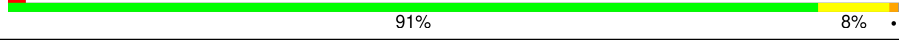
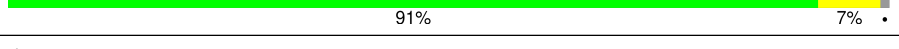
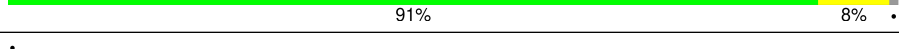
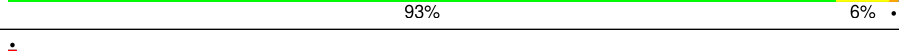
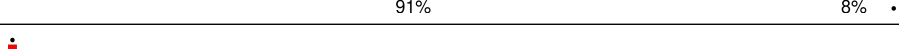
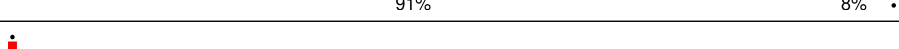
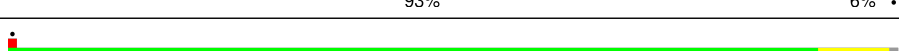
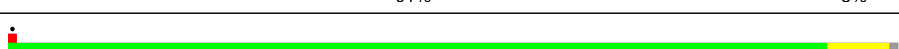


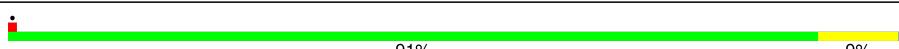








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 ( 3.30 - 4.30 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	0	250	
1	1	250	
1	2	250	
1	3	250	

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Mol	Chain	Length	Quality of chain
1	4	250	 7% 89%
1	W	250	 6% 90%
1	Y	250	 6% 90%
1	Z	250	 9% 89%
2	A	937	 91% 8%
2	B	937	 91% 7%
2	C	937	 91% 8%
2	D	937	 93% 6%
2	E	937	 91% 8%
2	F	937	 91% 8%
2	G	937	 93% 6%
2	H	937	 91% 8%
2	I	937	 92% 7%
2	J	937	 92% 7%
2	K	937	 90% 9%
2	L	937	 91% 9%
3	M	588	 7% 9% 87%
4	P	138	 33% 67% 28%
4	Q	138	 32% 62% 8% 30%
4	R	138	 22% 62% 5% 30%
4	S	138	 33% 68% 29%
5	U	227	 8% 31% 16% 52%
5	V	227	 42% 55%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 185977 atoms, of which 90839 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 Pre-protein VI.

Mol	Chain	Residues	Atoms					AltConf	Trace	
1	0	16	Total 227	C 71	H 109	N 24	O 23	0	0	
1	1	27	Total 405	C 130	H 195	N 39	O 40	S 1	0	0
1	2	27	Total 405	C 130	H 195	N 39	O 40	S 1	0	0
1	3	24	Total 350	C 110	H 171	N 35	O 33	S 1	0	0
1	4	27	Total 397	C 128	H 190	N 39	O 39	S 1	0	0
1	W	25	Total 378	C 119	H 185	N 36	O 37	S 1	0	0
1	Y	26	Total 385	C 121	H 188	N 37	O 38	S 1	0	0
1	Z	28	Total 402	C 126	H 196	N 39	O 40	S 1	0	0

- Molecule 2 is a protein called Hexon protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	932	Total 14510	C 4705	H 7092	N 1251	O 1425	S 37	0	0
2	B	927	Total 14454	C 4688	H 7065	N 1245	O 1419	S 37	0	0
2	C	929	Total 14465	C 4691	H 7069	N 1248	O 1422	S 35	0	0
2	D	932	Total 14507	C 4705	H 7089	N 1251	O 1425	S 37	0	0
2	E	929	Total 14475	C 4694	H 7075	N 1248	O 1421	S 37	0	0
2	F	931	Total 14496	C 4700	H 7085	N 1250	O 1424	S 37	0	0
2	G	932	Total 14509	C 4704	H 7091	N 1251	O 1426	S 37	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	931	Total	C	H	N	O	S	0	0
			14500	4702	7087	1250	1424	37		
2	I	930	Total	C	H	N	O	S	0	0
			14484	4697	7079	1249	1422	37		
2	J	931	Total	C	H	N	O	S	0	0
			14495	4700	7084	1250	1424	37		
2	K	932	Total	C	H	N	O	S	0	0
			14510	4704	7092	1251	1426	37		
2	L	932	Total	C	H	N	O	S	0	0
			14510	4705	7092	1251	1425	37		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	PHE	LEU	conflict	UNP P36851
A	61	SER	ARG	conflict	UNP P36851
A	76	ASN	HIS	conflict	UNP P36851
A	266	ALA	ARG	conflict	UNP P36851
A	592	THR	SER	conflict	UNP P36851
B	31	PHE	LEU	conflict	UNP P36851
B	61	SER	ARG	conflict	UNP P36851
B	76	ASN	HIS	conflict	UNP P36851
B	266	ALA	ARG	conflict	UNP P36851
B	592	THR	SER	conflict	UNP P36851
C	31	PHE	LEU	conflict	UNP P36851
C	61	SER	ARG	conflict	UNP P36851
C	76	ASN	HIS	conflict	UNP P36851
C	266	ALA	ARG	conflict	UNP P36851
C	592	THR	SER	conflict	UNP P36851
D	31	PHE	LEU	conflict	UNP P36851
D	61	SER	ARG	conflict	UNP P36851
D	76	ASN	HIS	conflict	UNP P36851
D	266	ALA	ARG	conflict	UNP P36851
D	592	THR	SER	conflict	UNP P36851
E	31	PHE	LEU	conflict	UNP P36851
E	61	SER	ARG	conflict	UNP P36851
E	76	ASN	HIS	conflict	UNP P36851
E	266	ALA	ARG	conflict	UNP P36851
E	592	THR	SER	conflict	UNP P36851
F	31	PHE	LEU	conflict	UNP P36851
F	61	SER	ARG	conflict	UNP P36851
F	76	ASN	HIS	conflict	UNP P36851
F	266	ALA	ARG	conflict	UNP P36851

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Chain	Residue	Modelled	Actual	Comment	Reference
F	592	THR	SER	conflict	UNP P36851
G	31	PHE	LEU	conflict	UNP P36851
G	61	SER	ARG	conflict	UNP P36851
G	76	ASN	HIS	conflict	UNP P36851
G	266	ALA	ARG	conflict	UNP P36851
G	592	THR	SER	conflict	UNP P36851
H	31	PHE	LEU	conflict	UNP P36851
H	61	SER	ARG	conflict	UNP P36851
H	76	ASN	HIS	conflict	UNP P36851
H	266	ALA	ARG	conflict	UNP P36851
H	592	THR	SER	conflict	UNP P36851
I	31	PHE	LEU	conflict	UNP P36851
I	61	SER	ARG	conflict	UNP P36851
I	76	ASN	HIS	conflict	UNP P36851
I	266	ALA	ARG	conflict	UNP P36851
I	592	THR	SER	conflict	UNP P36851
J	31	PHE	LEU	conflict	UNP P36851
J	61	SER	ARG	conflict	UNP P36851
J	76	ASN	HIS	conflict	UNP P36851
J	266	ALA	ARG	conflict	UNP P36851
J	592	THR	SER	conflict	UNP P36851
K	31	PHE	LEU	conflict	UNP P36851
K	61	SER	ARG	conflict	UNP P36851
K	76	ASN	HIS	conflict	UNP P36851
K	266	ALA	ARG	conflict	UNP P36851
K	592	THR	SER	conflict	UNP P36851
L	31	PHE	LEU	conflict	UNP P36851
L	61	SER	ARG	conflict	UNP P36851
L	76	ASN	HIS	conflict	UNP P36851
L	266	ALA	ARG	conflict	UNP P36851
L	592	THR	SER	conflict	UNP P36851

- Molecule 3 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	M	77	Total	C	H	N	O	S	0	0
			1224	377	621	114	110	2		

- Molecule 4 is a protein called Hexon-interlacing protein IX.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	P	99	Total	C	H	N	O	S	0	0
			1190	381	571	113	124	1		
4	Q	97	Total	C	H	N	O	S	0	0
			1172	375	563	111	122	1		
4	R	97	Total	C	H	N	O	S	0	0
			1171	375	562	111	122	1		
4	S	98	Total	C	H	N	O	S	0	0
			1170	378	556	112	123	1		

There are 172 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	92	UNK	PRO	conflict	UNP P68971
P	93	UNK	SER	conflict	UNP P68971
P	94	UNK	THR	conflict	UNP P68971
P	95	UNK	LEU	conflict	UNP P68971
P	96	UNK	ALA	conflict	UNP P68971
P	97	UNK	GLU	conflict	UNP P68971
P	98	UNK	ASP	conflict	UNP P68971
P	99	UNK	LYS	conflict	UNP P68971
P	100	UNK	LEU	conflict	UNP P68971
P	101	UNK	LEU	conflict	UNP P68971
P	102	UNK	VAL	conflict	UNP P68971
P	103	UNK	LEU	conflict	UNP P68971
P	104	UNK	LEU	conflict	UNP P68971
P	105	UNK	ALA	conflict	UNP P68971
P	106	UNK	GLN	conflict	UNP P68971
P	107	UNK	LEU	conflict	UNP P68971
P	108	UNK	GLU	conflict	UNP P68971
P	109	UNK	ALA	conflict	UNP P68971
P	110	UNK	LEU	conflict	UNP P68971
P	111	UNK	THR	conflict	UNP P68971
P	112	UNK	GLN	conflict	UNP P68971
P	113	UNK	ARG	conflict	UNP P68971
P	114	UNK	LEU	conflict	UNP P68971
P	115	UNK	GLY	conflict	UNP P68971
P	116	UNK	GLU	conflict	UNP P68971
P	117	UNK	LEU	conflict	UNP P68971
P	118	UNK	SER	conflict	UNP P68971
P	119	UNK	LYS	conflict	UNP P68971
P	120	UNK	GLN	conflict	UNP P68971
P	121	UNK	VAL	conflict	UNP P68971
P	122	UNK	ALA	conflict	UNP P68971

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Chain	Residue	Modelled	Actual	Comment	Reference
P	123	UNK	GLN	conflict	UNP P68971
P	124	UNK	LEU	conflict	UNP P68971
P	125	UNK	ARG	conflict	UNP P68971
P	126	UNK	GLU	conflict	UNP P68971
P	127	UNK	GLN	conflict	UNP P68971
P	128	UNK	THR	conflict	UNP P68971
P	129	UNK	GLU	conflict	UNP P68971
P	130	UNK	SER	conflict	UNP P68971
P	131	UNK	ALA	conflict	UNP P68971
P	132	UNK	VAL	conflict	UNP P68971
P	133	UNK	ALA	conflict	UNP P68971
P	134	UNK	THR	conflict	UNP P68971
Q	92	UNK	PRO	conflict	UNP P68971
Q	93	UNK	SER	conflict	UNP P68971
Q	94	UNK	THR	conflict	UNP P68971
Q	95	UNK	LEU	conflict	UNP P68971
Q	96	UNK	ALA	conflict	UNP P68971
Q	97	UNK	GLU	conflict	UNP P68971
Q	98	UNK	ASP	conflict	UNP P68971
Q	99	UNK	LYS	conflict	UNP P68971
Q	100	UNK	LEU	conflict	UNP P68971
Q	101	UNK	LEU	conflict	UNP P68971
Q	102	UNK	VAL	conflict	UNP P68971
Q	103	UNK	LEU	conflict	UNP P68971
Q	104	UNK	LEU	conflict	UNP P68971
Q	105	UNK	ALA	conflict	UNP P68971
Q	106	UNK	GLN	conflict	UNP P68971
Q	107	UNK	LEU	conflict	UNP P68971
Q	108	UNK	GLU	conflict	UNP P68971
Q	109	UNK	ALA	conflict	UNP P68971
Q	110	UNK	LEU	conflict	UNP P68971
Q	111	UNK	THR	conflict	UNP P68971
Q	112	UNK	GLN	conflict	UNP P68971
Q	113	UNK	ARG	conflict	UNP P68971
Q	114	UNK	LEU	conflict	UNP P68971
Q	115	UNK	GLY	conflict	UNP P68971
Q	116	UNK	GLU	conflict	UNP P68971
Q	117	UNK	LEU	conflict	UNP P68971
Q	118	UNK	SER	conflict	UNP P68971
Q	119	UNK	LYS	conflict	UNP P68971
Q	120	UNK	GLN	conflict	UNP P68971
Q	121	UNK	VAL	conflict	UNP P68971

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	122	UNK	ALA	conflict	UNP P68971
Q	123	UNK	GLN	conflict	UNP P68971
Q	124	UNK	LEU	conflict	UNP P68971
Q	125	UNK	ARG	conflict	UNP P68971
Q	126	UNK	GLU	conflict	UNP P68971
Q	127	UNK	GLN	conflict	UNP P68971
Q	128	UNK	THR	conflict	UNP P68971
Q	129	UNK	GLU	conflict	UNP P68971
Q	130	UNK	SER	conflict	UNP P68971
Q	131	UNK	ALA	conflict	UNP P68971
Q	132	UNK	VAL	conflict	UNP P68971
Q	133	UNK	ALA	conflict	UNP P68971
Q	134	UNK	THR	conflict	UNP P68971
R	92	UNK	PRO	conflict	UNP P68971
R	93	UNK	SER	conflict	UNP P68971
R	94	UNK	THR	conflict	UNP P68971
R	95	UNK	LEU	conflict	UNP P68971
R	96	UNK	ALA	conflict	UNP P68971
R	97	UNK	GLU	conflict	UNP P68971
R	98	UNK	ASP	conflict	UNP P68971
R	99	UNK	LYS	conflict	UNP P68971
R	100	UNK	LEU	conflict	UNP P68971
R	101	UNK	LEU	conflict	UNP P68971
R	102	UNK	VAL	conflict	UNP P68971
R	103	UNK	LEU	conflict	UNP P68971
R	104	UNK	LEU	conflict	UNP P68971
R	105	UNK	ALA	conflict	UNP P68971
R	106	UNK	GLN	conflict	UNP P68971
R	107	UNK	LEU	conflict	UNP P68971
R	108	UNK	GLU	conflict	UNP P68971
R	109	UNK	ALA	conflict	UNP P68971
R	110	UNK	LEU	conflict	UNP P68971
R	111	UNK	THR	conflict	UNP P68971
R	112	UNK	GLN	conflict	UNP P68971
R	113	UNK	ARG	conflict	UNP P68971
R	114	UNK	LEU	conflict	UNP P68971
R	115	UNK	GLY	conflict	UNP P68971
R	116	UNK	GLU	conflict	UNP P68971
R	117	UNK	LEU	conflict	UNP P68971
R	118	UNK	SER	conflict	UNP P68971
R	119	UNK	LYS	conflict	UNP P68971
R	120	UNK	GLN	conflict	UNP P68971

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Chain	Residue	Modelled	Actual	Comment	Reference
R	121	UNK	VAL	conflict	UNP P68971
R	122	UNK	ALA	conflict	UNP P68971
R	123	UNK	GLN	conflict	UNP P68971
R	124	UNK	LEU	conflict	UNP P68971
R	125	UNK	ARG	conflict	UNP P68971
R	126	UNK	GLU	conflict	UNP P68971
R	127	UNK	GLN	conflict	UNP P68971
R	128	UNK	THR	conflict	UNP P68971
R	129	UNK	GLU	conflict	UNP P68971
R	130	UNK	SER	conflict	UNP P68971
R	131	UNK	ALA	conflict	UNP P68971
R	132	UNK	VAL	conflict	UNP P68971
R	133	UNK	ALA	conflict	UNP P68971
R	134	UNK	THR	conflict	UNP P68971
S	92	UNK	PRO	conflict	UNP P68971
S	93	UNK	SER	conflict	UNP P68971
S	94	UNK	THR	conflict	UNP P68971
S	95	UNK	LEU	conflict	UNP P68971
S	96	UNK	ALA	conflict	UNP P68971
S	97	UNK	GLU	conflict	UNP P68971
S	98	UNK	ASP	conflict	UNP P68971
S	99	UNK	LYS	conflict	UNP P68971
S	100	UNK	LEU	conflict	UNP P68971
S	101	UNK	LEU	conflict	UNP P68971
S	102	UNK	VAL	conflict	UNP P68971
S	103	UNK	LEU	conflict	UNP P68971
S	104	UNK	LEU	conflict	UNP P68971
S	105	UNK	ALA	conflict	UNP P68971
S	106	UNK	GLN	conflict	UNP P68971
S	107	UNK	LEU	conflict	UNP P68971
S	108	UNK	GLU	conflict	UNP P68971
S	109	UNK	ALA	conflict	UNP P68971
S	110	UNK	LEU	conflict	UNP P68971
S	111	UNK	THR	conflict	UNP P68971
S	112	UNK	GLN	conflict	UNP P68971
S	113	UNK	ARG	conflict	UNP P68971
S	114	UNK	LEU	conflict	UNP P68971
S	115	UNK	GLY	conflict	UNP P68971
S	116	UNK	GLU	conflict	UNP P68971
S	117	UNK	LEU	conflict	UNP P68971
S	118	UNK	SER	conflict	UNP P68971
S	119	UNK	LYS	conflict	UNP P68971

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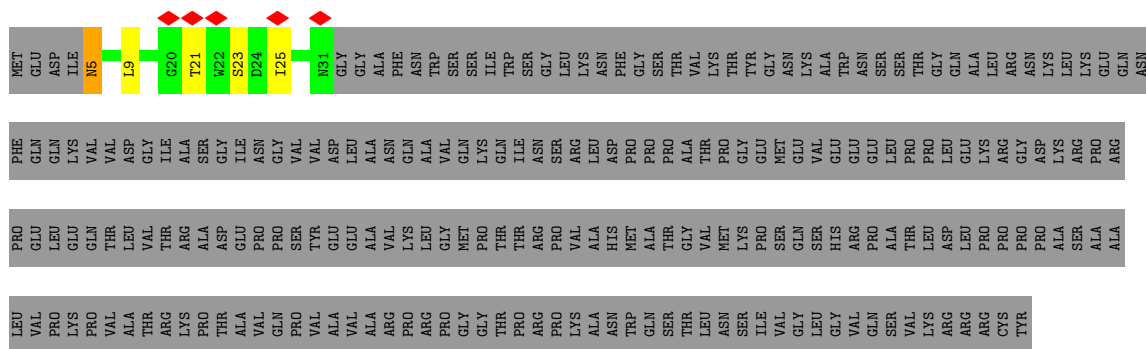
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Chain	Residue	Modelled	Actual	Comment	Reference
S	120	UNK	GLN	conflict	UNP P68971
S	121	UNK	VAL	conflict	UNP P68971
S	122	UNK	ALA	conflict	UNP P68971
S	123	UNK	GLN	conflict	UNP P68971
S	124	UNK	LEU	conflict	UNP P68971
S	125	UNK	ARG	conflict	UNP P68971
S	126	UNK	GLU	conflict	UNP P68971
S	127	UNK	GLN	conflict	UNP P68971
S	128	UNK	THR	conflict	UNP P68971
S	129	UNK	GLU	conflict	UNP P68971
S	130	UNK	SER	conflict	UNP P68971
S	131	UNK	ALA	conflict	UNP P68971
S	132	UNK	VAL	conflict	UNP P68971
S	133	UNK	ALA	conflict	UNP P68971
S	134	UNK	THR	conflict	UNP P68971

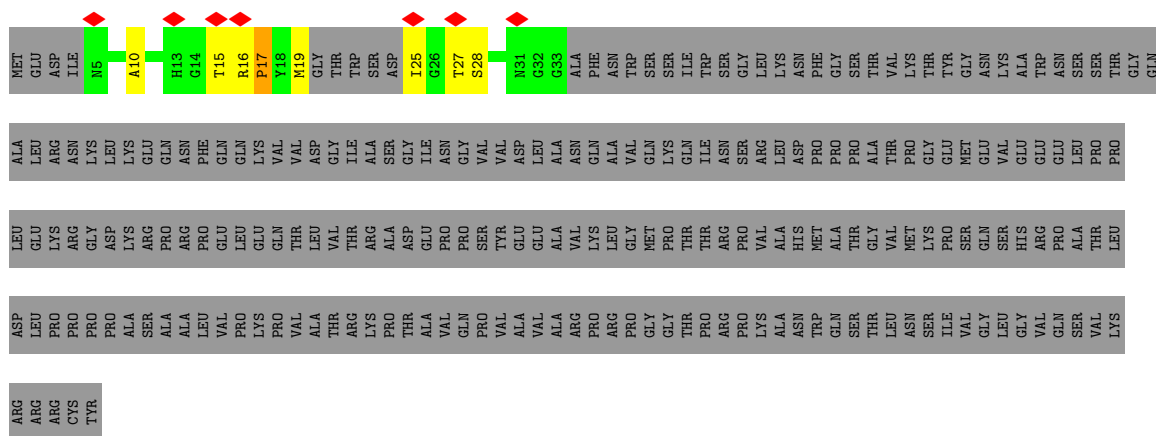
- Molecule 5 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	U	108	Total	C	H	N	O	S	0	0
			1635	539	789	135	168	4		
5	V	102	Total	C	H	N	O	S	0	0
			1551	512	748	129	158	4		

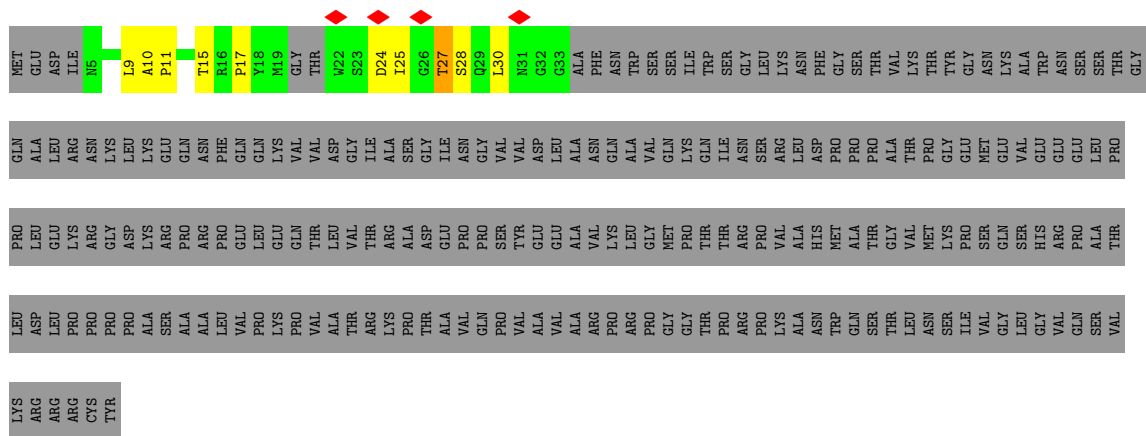




- Molecule 1: Pre-protein VI



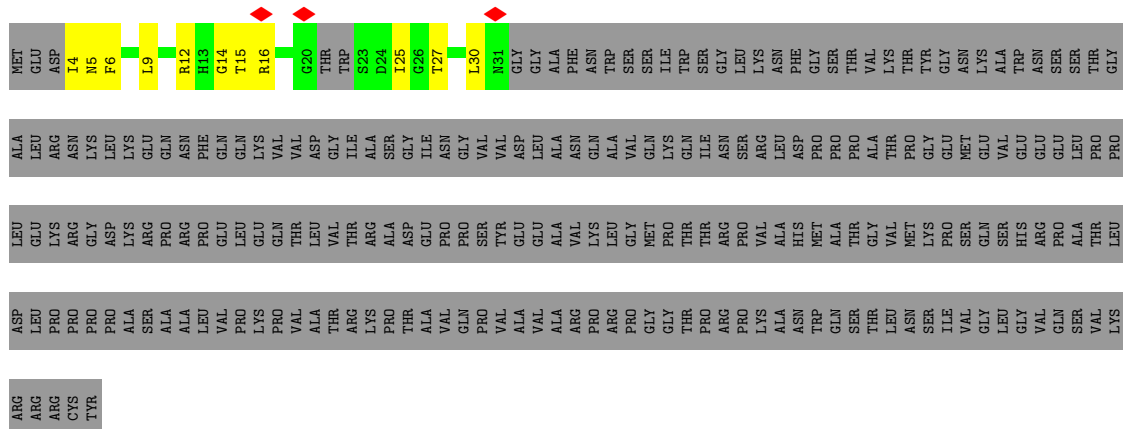
- Molecule 1: Pre-protein VI



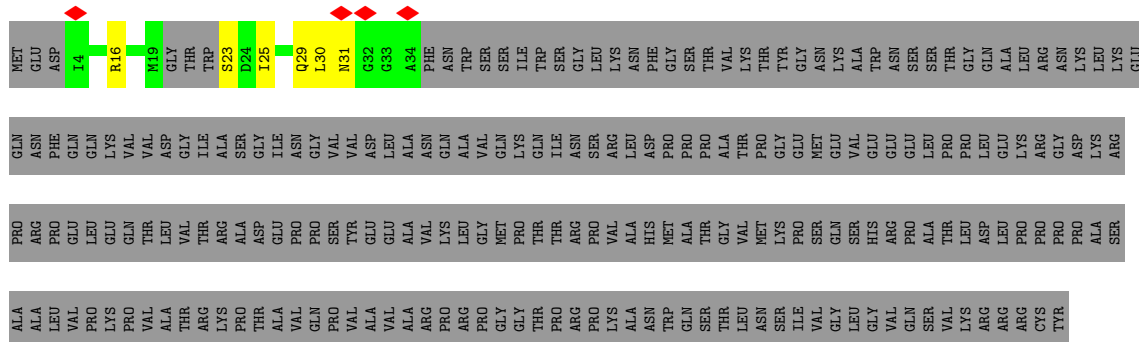
- Molecule 1: Pre-protein VI



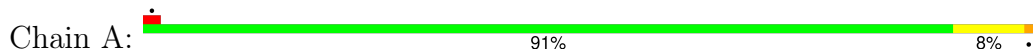
- Molecule 1: Pre-protein VI

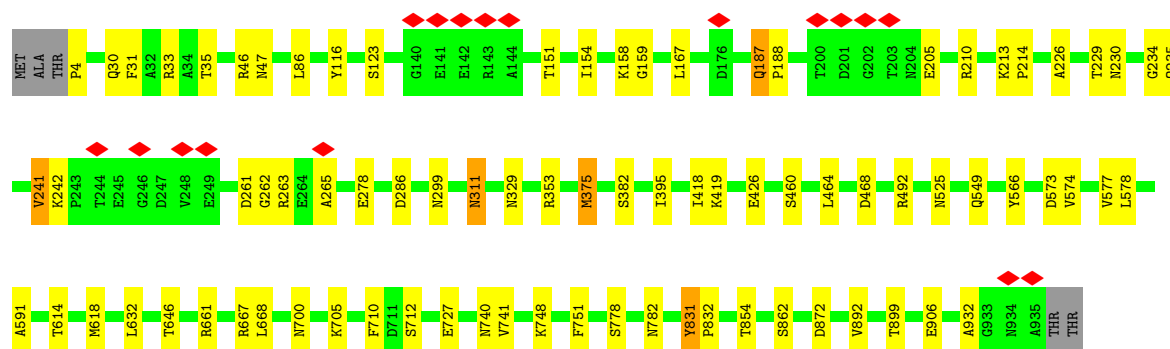


- Molecule 1: Pre-protein VI

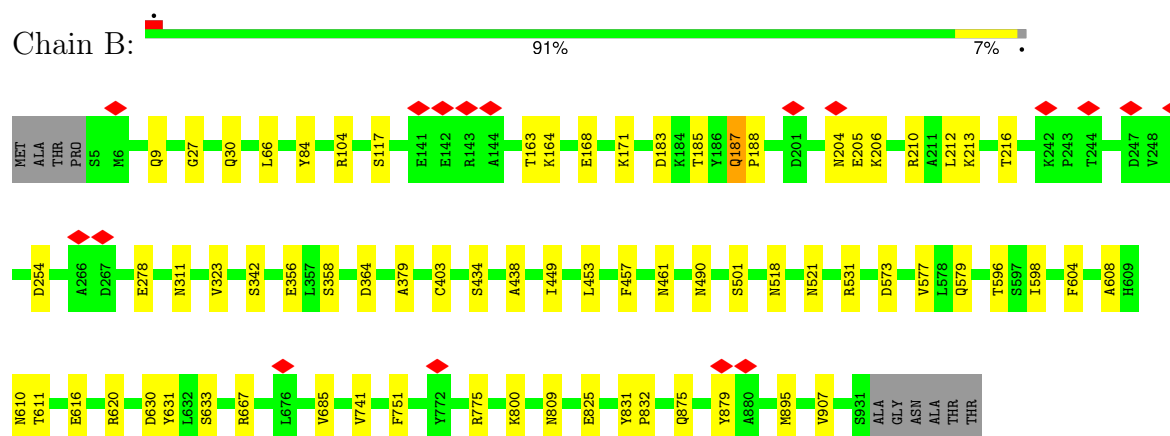


- Molecule 2: Hexon protein

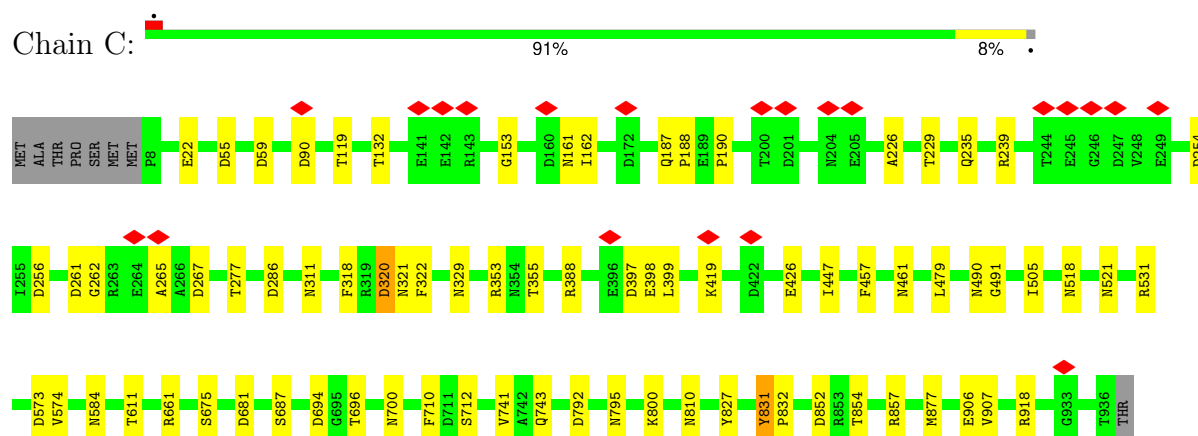


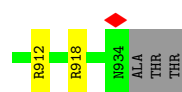


• Molecule 2: Hexon protein



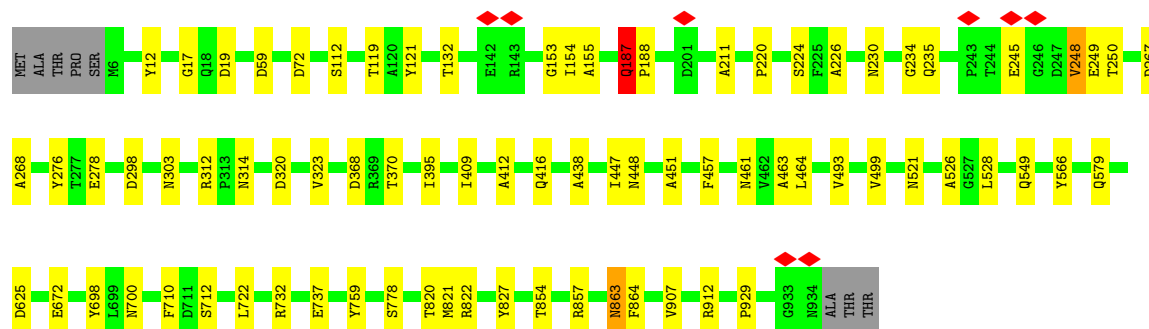
• Molecule 2: Hexon protein





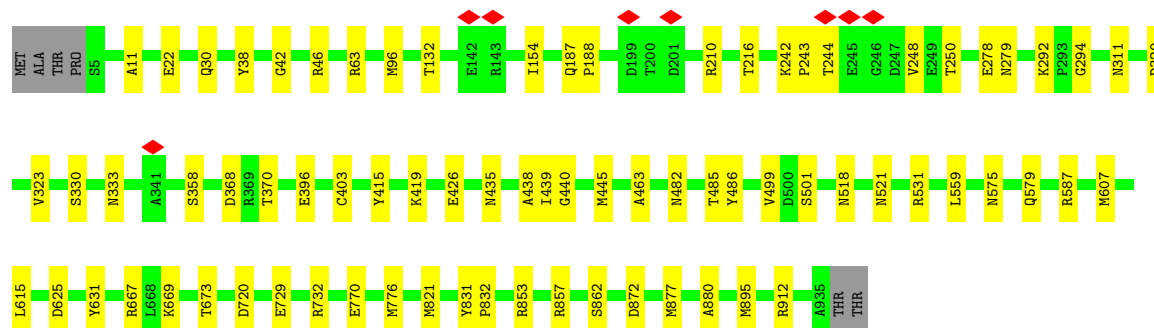
• Molecule 2: Hexon protein

Chain E: 91% 8%



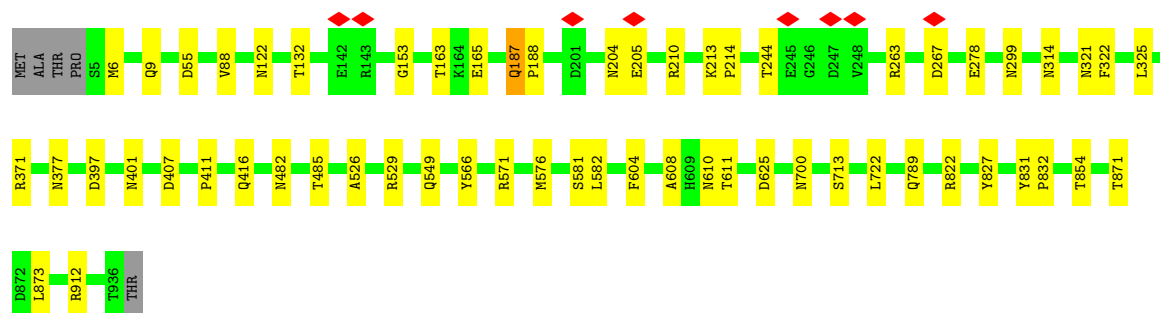
• Molecule 2: Hexon protein

Chain F: 91% 8%



• Molecule 2: Hexon protein

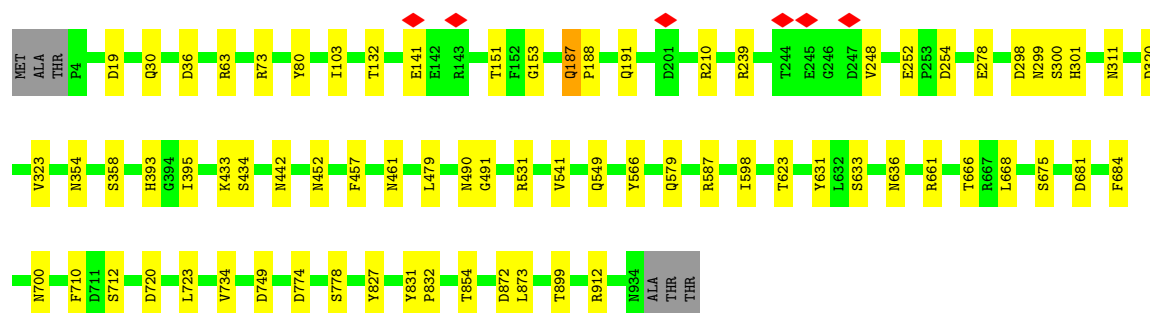
Chain G: 93% 6%



• Molecule 2: Hexon protein

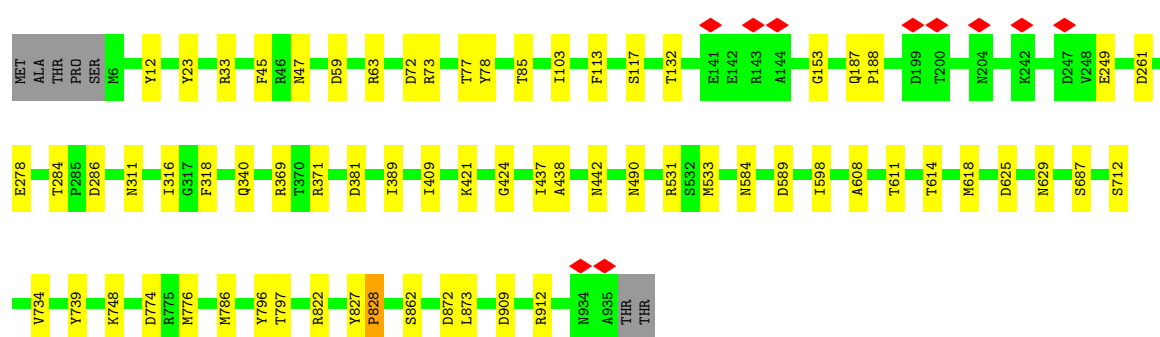
Chain H: 91% 8%





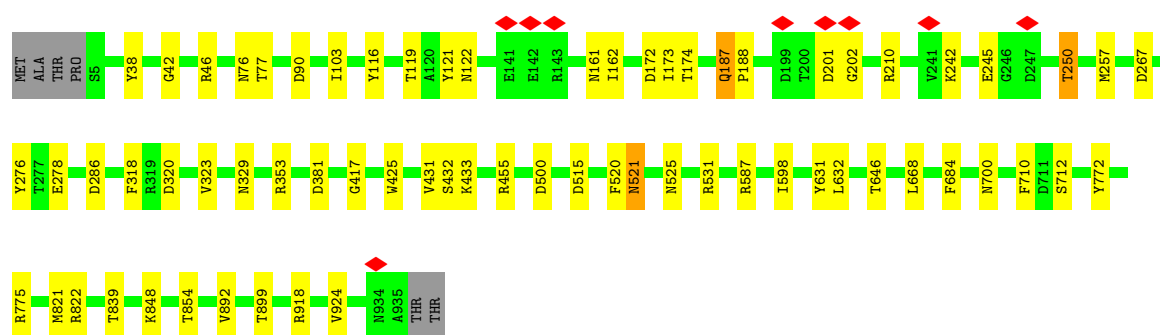
• Molecule 2: Hexon protein

Chain I: 92% 7%



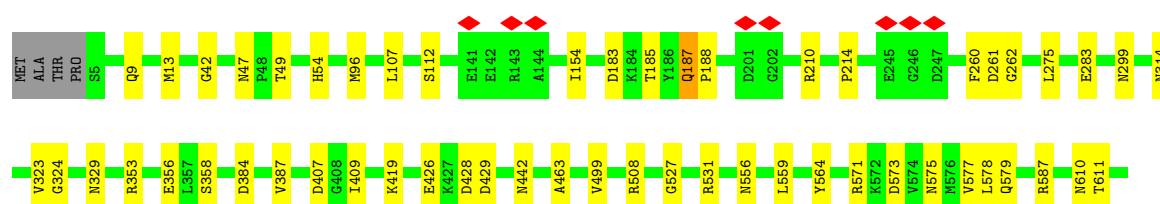
• Molecule 2: Hexon protein

Chain J: 92% 7%



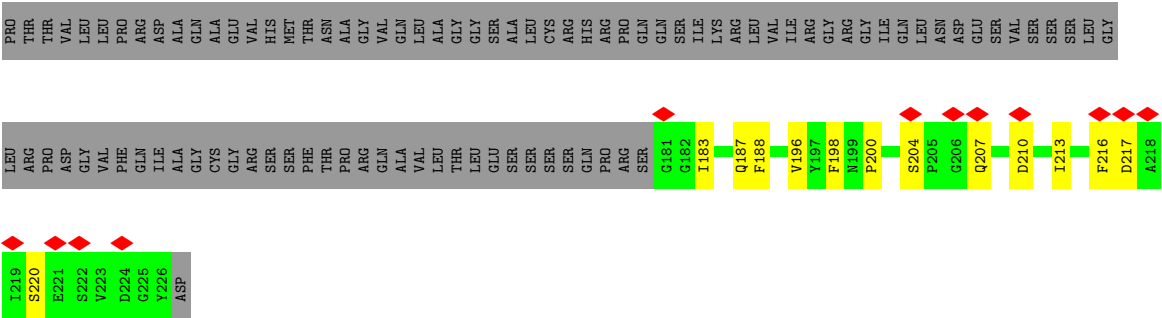
• Molecule 2: Hexon protein

Chain K: 90% 9%

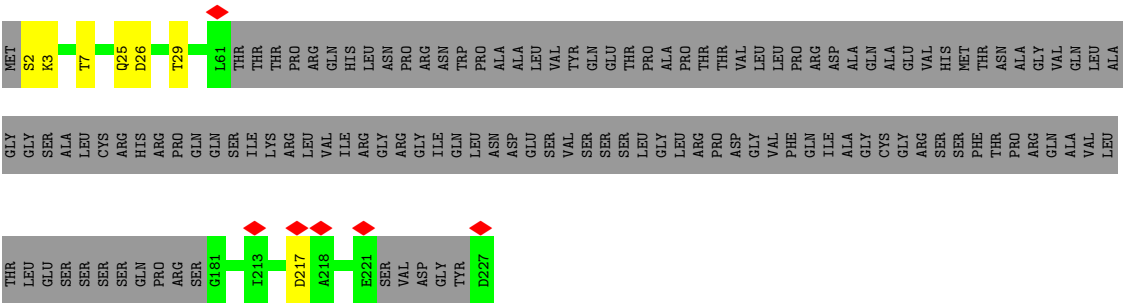








● Molecule 5: Pre-hexon-linking protein VIII



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	360841	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 ( $e^-/\text{\AA}^2$ )	53.35	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	11.273	Depositor
Minimum map value	-7.855	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1	Depositor
Map size (Å)	295.659, 475.43698, 252.33899	wwPDB
Map dimensions	233, 439, 273	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	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	0	0.13	0/119	0.31	0/158
1	1	0.17	0/216	0.60	0/293
1	2	0.16	0/216	0.45	0/293
1	3	0.24	0/182	0.63	1/243 (0.4%)
1	4	0.14	0/212	0.42	0/285
1	W	0.19	0/196	0.38	0/263
1	Y	0.13	0/200	0.50	0/268
1	Z	0.16	0/209	0.44	0/280
2	A	0.24	0/7619	0.54	2/10369 (0.0%)
2	B	0.24	0/7589	0.54	0/10328
2	C	0.25	0/7596	0.54	1/10339 (0.0%)
2	D	0.25	0/7619	0.54	1/10370 (0.0%)
2	E	0.24	0/7600	0.53	1/10343 (0.0%)
2	F	0.26	0/7611	0.60	7/10358 (0.1%)
2	G	0.26	0/7618	0.55	2/10368 (0.0%)
2	H	0.24	0/7614	0.51	0/10362
2	I	0.24	0/7605	0.52	0/10350
2	J	0.23	0/7611	0.52	2/10358 (0.0%)
2	K	0.24	0/7618	0.53	0/10368
2	L	0.25	0/7619	0.56	6/10369 (0.1%)
3	M	0.15	0/612	0.45	0/833
4	P	0.26	0/449	0.59	0/618
4	Q	0.23	0/449	0.52	0/618
4	R	0.52	0/443	1.16	2/607 (0.3%)
4	S	0.25	0/444	0.59	0/611
5	U	0.18	0/870	0.44	0/1184
5	V	0.23	0/825	0.52	0/1120
All	All	0.25	0/96961	0.54	25/131956 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	4
2	B	0	2
2	C	0	2
2	D	0	2
2	E	0	4
2	F	0	2
2	G	0	3
2	H	0	2
2	I	0	1
2	J	0	1
2	K	0	1
2	L	0	3
All	All	0	27

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	57	PRO	N-CA-C	18.08	136.53	111.22
4	R	57	PRO	N-CA-CB	-12.29	87.19	103.42
2	F	243	PRO	CA-C-N	11.36	142.78	123.91
2	F	243	PRO	C-N-CA	11.36	142.78	123.91
2	L	243	PRO	CA-C-N	8.88	133.38	120.95
2	L	243	PRO	C-N-CA	8.88	133.38	120.95
2	L	246	GLY	CA-C-N	8.81	134.59	122.34
2	L	246	GLY	C-N-CA	8.81	134.59	122.34
2	F	242	LYS	N-CA-C	7.70	120.77	109.30
2	E	187	GLN	C-N-CD	-7.21	95.43	125.00
2	G	244	THR	CA-CB-CG2	6.48	121.52	110.50
2	F	250	THR	OG1-CB-CG2	6.29	121.87	109.30
2	F	244	THR	OG1-CB-CG2	6.26	121.82	109.30
2	C	831	TYR	C-N-CD	-6.08	100.07	125.00
1	3	17	PRO	CA-N-CD	-5.94	103.68	112.00
2	G	244	THR	OG1-CB-CG2	5.80	120.89	109.30
2	A	151	THR	OG1-CB-CG2	5.69	120.69	109.30
2	L	434	SER	N-CA-C	5.69	118.59	110.68
2	D	154	ILE	CG1-CB-CG2	5.67	127.72	110.70
2	J	250	THR	OG1-CB-CG2	5.62	120.54	109.30
2	L	831	TYR	C-N-CD	-5.62	101.97	125.00
2	J	250	THR	CA-CB-CG2	5.36	119.61	110.50
2	A	831	TYR	C-N-CD	-5.03	104.38	125.00
2	F	250	THR	CA-CB-CG2	5.01	119.02	110.50
2	F	244	THR	CA-CB-CG2	5.00	119.00	110.50

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	187	GLN	Peptide
2	A	311	ASN	Peptide
2	A	831	TYR	Peptide
2	A	932	ALA	Peptide
2	B	187	GLN	Peptide
2	B	831	TYR	Peptide
2	C	187	GLN	Peptide
2	C	831	TYR	Peptide
2	D	187	GLN	Peptide
2	D	321	ASN	Peptide
2	E	187	GLN	Peptide
2	E	526	ALA	Peptide
2	E	863	ASN	Peptide
2	E	864	PHE	Peptide
2	F	187	GLN	Peptide
2	F	831	TYR	Peptide
2	G	187	GLN	Peptide
2	G	407	ASP	Peptide
2	G	831	TYR	Peptide
2	H	187	GLN	Peptide
2	H	831	TYR	Peptide
2	I	187	GLN	Peptide
2	J	187	GLN	Peptide
2	K	187	GLN	Peptide
2	L	187	GLN	Peptide
2	L	46	ARG	Sidechain
2	L	831	TYR	Peptide

## 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	0	118	109	109	1	0
1	1	210	195	195	7	0
1	2	210	195	195	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	179	171	171	9	0
1	4	207	190	190	8	0
1	W	193	185	185	13	0
1	Y	197	188	188	11	0
1	Z	206	196	196	6	0
2	A	7418	7092	7092	48	0
2	B	7389	7065	7065	41	0
2	C	7396	7069	7069	43	0
2	D	7418	7089	7088	40	0
2	E	7400	7075	7074	47	0
2	F	7411	7085	7084	44	0
2	G	7418	7091	7091	34	0
2	H	7413	7087	7087	49	0
2	I	7405	7079	7079	46	0
2	J	7411	7084	7084	39	0
2	K	7418	7092	7091	54	0
2	L	7418	7092	7092	52	0
3	M	603	621	621	27	0
4	P	619	571	466	7	0
4	Q	609	563	464	7	0
4	R	609	562	460	13	0
4	S	614	556	461	2	0
5	U	846	789	789	26	0
5	V	803	748	748	4	0
All	All	95138	90839	90434	578	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 3.

All (578) 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)
4:R:56:SER:C	4:R:57:PRO:N	2.06	1.13
3:M:34:ARG:HG3	3:M:38:LEU:HD23	1.48	0.96
2:D:409:ILE:HD13	2:F:154:ILE:HD12	1.52	0.89
3:M:32:MET:HE3	3:M:62:VAL:HG23	1.57	0.86
2:L:549:GLN:HE22	2:L:554:VAL:HG23	1.49	0.78
2:D:154:ILE:HB	2:E:409:ILE:HD13	1.66	0.77
1:2:5:ASN:N	2:H:30:GLN:HE22	1.83	0.77
5:U:59:SER:HA	5:U:63:THR:HB	1.66	0.76
2:I:286:ASP:O	2:I:311:ASN:ND2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:549:GLN:NE2	2:L:554:VAL:HG23	2.03	0.72
2:D:827:TYR:OH	2:E:278:GLU:OE1	2.07	0.72
2:A:668:LEU:O	2:A:899:THR:OG1	2.08	0.71
2:F:877:MET:O	2:F:880:ALA:O	2.09	0.71
2:L:729:GLU:O	2:L:747:THR:OG1	2.10	0.70
2:A:30:GLN:OE1	2:A:33:ARG:NH2	2.25	0.70
2:E:827:TYR:OH	2:F:278:GLU:OE2	2.10	0.69
3:M:32:MET:HE1	3:M:61:ALA:HB3	1.74	0.69
2:L:571:ARG:NH1	2:L:576:MET:SD	2.65	0.69
2:A:263:ARG:NH2	2:B:434:SER:OG	2.26	0.69
2:H:700:ASN:ND2	2:H:854:THR:O	2.25	0.69
2:H:187:GLN:O	2:H:210:ARG:NH1	2.26	0.68
2:G:187:GLN:O	2:G:210:ARG:NH1	2.27	0.68
2:K:668:LEU:O	2:K:899:THR:OG1	2.10	0.68
2:B:616:GLU:OE2	2:B:620:ARG:NH1	2.26	0.68
2:G:549:GLN:OE1	2:G:566:TYR:OH	2.10	0.68
2:E:298:ASP:O	2:E:303:ASN:ND2	2.27	0.68
2:H:549:GLN:OE1	2:H:566:TYR:OH	2.12	0.68
3:M:74:VAL:HG21	3:M:100:LEU:HD23	1.76	0.68
2:K:527:GLY:O	2:K:531:ARG:NH1	2.27	0.67
2:A:286:ASP:O	2:A:311:ASN:ND2	2.28	0.67
2:A:705:LYS:NZ	2:A:727:GLU:OE1	2.27	0.67
2:G:625:ASP:OD2	2:G:912:ARG:NH1	2.27	0.67
2:H:778:SER:O	2:H:854:THR:OG1	2.11	0.67
2:F:518:ASN:ND2	2:F:521:ASN:OD1	2.28	0.67
2:A:187:GLN:O	2:A:210:ARG:NH1	2.27	0.67
2:F:216:THR:OG1	2:F:279:ASN:OD1	2.12	0.67
2:I:625:ASP:OD2	2:I:912:ARG:NH1	2.28	0.67
2:J:381:ASP:OD1	2:J:531:ARG:NH2	2.28	0.67
2:K:556:ASN:OD1	2:L:43:ASN:ND2	2.27	0.67
5:V:7:THR:OG1	5:V:25:GLN:OE1	2.14	0.66
2:B:187:GLN:O	2:B:210:ARG:NH1	2.29	0.66
2:I:584:ASN:ND2	2:I:589:ASP:OD2	2.27	0.66
2:G:571:ARG:NH1	2:G:576:MET:SD	2.68	0.66
2:J:668:LEU:O	2:J:899:THR:OG1	2.13	0.66
2:G:214:PRO:O	2:G:299:ASN:ND2	2.28	0.66
2:A:329:ASN:ND2	2:A:353:ARG:O	2.28	0.66
2:F:368:ASP:OD2	2:F:370:THR:OG1	2.14	0.66
2:F:625:ASP:OD2	2:F:912:ARG:NH1	2.28	0.66
2:C:675:SER:OG	2:C:681:ASP:OD2	2.13	0.66
2:H:675:SER:OG	2:H:681:ASP:OD2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:90:ASP:OD1	2:J:918:ARG:NH1	2.29	0.65
2:K:183:ASP:OD1	2:K:185:THR:OG1	2.11	0.65
2:C:329:ASN:ND2	2:C:353:ARG:O	2.28	0.65
1:2:23:SER:O	1:2:25:ILE:HG23	1.96	0.65
1:4:9:LEU:O	2:J:38:TYR:OH	2.10	0.65
2:F:776:MET:SD	2:F:853:ARG:NH1	2.69	0.65
2:E:625:ASP:OD2	2:E:912:ARG:NH1	2.30	0.65
3:M:48:GLN:O	1:W:12:ARG:NH2	2.29	0.65
2:H:827:TYR:OH	2:I:278:GLU:OE2	2.14	0.65
2:B:741:VAL:HG21	2:B:751:PHE:HB2	1.79	0.65
2:K:625:ASP:OD2	2:K:912:ARG:NH1	2.30	0.65
1:2:5:ASN:N	1:2:5:ASN:HD22	1.94	0.64
1:1:25:ILE:O	2:I:47:ASN:ND2	2.30	0.64
2:K:531:ARG:NH2	2:K:579:GLN:OE1	2.30	0.64
2:K:214:PRO:O	2:K:299:ASN:ND2	2.30	0.64
2:A:214:PRO:O	2:A:299:ASN:ND2	2.31	0.64
2:H:531:ARG:NH2	2:H:579:GLN:OE1	2.30	0.64
2:B:379:ALA:O	2:B:531:ARG:NH1	2.31	0.64
2:J:116:TYR:OH	2:J:286:ASP:OD2	2.16	0.64
2:C:694:ASP:OD1	2:C:696:THR:OG1	2.11	0.63
1:2:5:ASN:N	2:H:30:GLN:NE2	2.45	0.63
2:D:625:ASP:OD2	2:D:912:ARG:NH1	2.30	0.63
2:K:154:ILE:HG22	2:L:438:ALA:HB3	1.80	0.63
2:A:740:ASN:O	2:A:748:LYS:NZ	2.30	0.63
2:J:329:ASN:ND2	2:J:353:ARG:O	2.31	0.63
2:E:457:PHE:O	2:E:461:ASN:ND2	2.31	0.63
2:G:700:ASN:ND2	2:G:854:THR:O	2.31	0.63
2:B:311:ASN:OD1	2:B:490:ASN:ND2	2.30	0.63
2:F:292:LYS:NZ	2:F:294:GLY:O	2.32	0.63
2:A:226:ALA:O	2:A:235:GLN:NE2	2.32	0.63
2:C:857:ARG:NH1	1:W:31:ASN:OD1	2.32	0.63
2:F:419:LYS:O	2:F:426:GLU:N	2.32	0.63
2:G:416:GLN:N	2:I:261:ASP:O	2.31	0.63
2:A:278:GLU:OE2	2:C:827:TYR:OH	2.16	0.62
2:C:320:ASP:O	2:C:322:PHE:N	2.32	0.62
2:L:19:ASP:OD1	2:L:47:ASN:ND2	2.32	0.62
1:4:25:ILE:HG22	1:4:27:THR:H	1.65	0.62
2:J:318:PHE:O	2:J:531:ARG:NH1	2.33	0.62
4:R:56:SER:CA	4:R:57:PRO:N	2.62	0.62
2:L:116:TYR:OH	2:L:286:ASP:OD2	2.10	0.62
2:E:409:ILE:HD11	2:E:438:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:329:ASN:ND2	2:K:353:ARG:O	2.32	0.62
2:B:633:SER:OG	2:B:907:VAL:O	2.18	0.61
2:D:500:ASP:OD1	2:D:501:SER:N	2.33	0.61
2:L:661:ARG:NH2	2:L:906:GLU:OE1	2.33	0.61
2:F:857:ARG:NH1	1:Z:31:ASN:OD1	2.33	0.61
2:A:468:ASP:O	2:A:492:ARG:NH2	2.34	0.61
2:C:320:ASP:OD1	2:C:321:ASN:ND2	2.33	0.61
2:F:30:GLN:NE2	1:Y:5:ASN:O	2.34	0.61
2:G:6:MET:SD	2:G:9:GLN:NE2	2.74	0.61
2:K:759:TYR:OH	2:K:774:ASP:OD1	2.19	0.61
2:D:442:ASN:O	2:E:822:ARG:NH1	2.34	0.61
4:R:67:THR:O	4:R:68:ALA:HB2	2.00	0.61
2:C:256:ASP:O	2:C:277:THR:OG1	2.15	0.60
2:D:321:ASN:O	2:D:550:LYS:NZ	2.27	0.60
2:L:776:MET:O	2:L:782:ASN:ND2	2.34	0.60
1:O:31:ASN:OD1	2:D:857:ARG:NH1	2.34	0.60
2:B:358:SER:OG	2:B:631:TYR:O	2.17	0.60
2:J:278:GLU:OE1	2:L:827:TYR:OH	2.17	0.60
2:A:154:ILE:HG22	2:B:438:ALA:HB3	1.83	0.60
2:C:239:ARG:NH1	2:C:254:ASP:OD1	2.35	0.60
2:D:577:VAL:HG23	2:D:578:LEU:HD12	1.83	0.60
2:D:700:ASN:ND2	2:D:854:THR:O	2.35	0.60
2:G:371:ARG:NH2	2:I:774:ASP:OD2	2.35	0.60
2:J:839:THR:OG1	2:K:283:GLU:OE2	2.12	0.60
2:K:620:ARG:NH1	2:K:917:HIS:O	2.35	0.60
4:R:62:ALA:O	4:R:63:ALA:HB2	2.02	0.60
4:S:130:UNK:O	4:S:134:UNK:N	2.35	0.60
2:K:323:VAL:HG23	2:K:356:GLU:OE1	2.01	0.59
1:4:10:ALA:HB3	1:4:17:PRO:HB2	1.84	0.59
2:K:442:ASN:O	2:L:822:ARG:NH1	2.36	0.59
2:C:792:ASP:OD2	2:C:795:ASN:ND2	2.35	0.59
5:U:10:MET:HG2	5:U:26:ASP:HB3	1.85	0.59
2:F:669:LYS:O	2:F:673:THR:OG1	2.17	0.59
2:H:457:PHE:O	2:H:461:ASN:ND2	2.36	0.59
2:J:187:GLN:O	2:J:210:ARG:NH1	2.35	0.59
2:K:187:GLN:O	2:K:210:ARG:NH1	2.36	0.59
2:K:618:MET:O	2:K:624:ASN:ND2	2.36	0.58
2:F:531:ARG:NH2	2:F:579:GLN:OE1	2.37	0.58
2:C:311:ASN:OD1	2:C:490:ASN:ND2	2.37	0.58
2:I:318:PHE:O	2:I:531:ARG:NH1	2.37	0.58
2:D:524:ARG:NH1	2:F:396:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:183:ILE:HG23	5:U:187:GLN:HB2	1.84	0.58
2:E:700:ASN:ND2	2:E:854:THR:O	2.37	0.58
1:2:21:THR:HG21	2:H:36:ASP:OD2	2.04	0.58
2:B:667:ARG:NH2	2:B:895:MET:SD	2.77	0.57
2:J:924:VAL:HG23	2:K:13:MET:HE1	1.86	0.57
2:A:549:GLN:OE1	2:A:566:TYR:OH	2.22	0.57
2:F:463:ALA:HB2	2:F:499:VAL:CG1	2.35	0.57
2:L:256:ASP:O	2:L:277:THR:OG1	2.23	0.57
2:A:700:ASN:ND2	2:A:854:THR:O	2.39	0.56
3:M:32:MET:HE3	3:M:62:VAL:CG2	2.34	0.56
2:A:419:LYS:N	2:A:426:GLU:O	2.38	0.56
2:H:239:ARG:NH2	2:H:254:ASP:OD1	2.39	0.56
2:D:187:GLN:O	2:D:210:ARG:NH1	2.38	0.56
2:D:63:ARG:NH1	2:F:720:ASP:OD1	2.39	0.56
2:C:132:THR:HG23	2:C:153:GLY:HA3	1.86	0.56
2:F:42:GLY:HA3	1:Y:25:ILE:HG22	1.88	0.56
2:K:508:ARG:NH2	2:K:784:GLN:OE1	2.38	0.56
5:U:6:PRO:HG2	5:U:196:VAL:HG13	1.88	0.56
2:H:141:GLU:N	2:H:141:GLU:OE1	2.39	0.56
2:J:700:ASN:ND2	2:J:854:THR:O	2.39	0.56
2:H:633:SER:OG	2:H:661:ARG:NH2	2.39	0.56
1:I:14:GLY:HA3	2:H:19:ASP:OD1	2.06	0.55
2:F:729:GLU:OE1	2:F:732:ARG:NH1	2.39	0.55
2:K:463:ALA:HB2	2:K:499:VAL:CG1	2.36	0.55
2:B:457:PHE:O	2:B:461:ASN:ND2	2.39	0.55
2:F:38:TYR:OH	1:Y:9:LEU:O	2.21	0.55
2:F:358:SER:OG	2:F:631:TYR:O	2.19	0.55
2:G:322:PHE:HB3	2:G:325:LEU:HD12	1.89	0.55
2:H:668:LEU:O	2:H:899:THR:OG1	2.24	0.55
2:F:311:ASN:O	2:F:486:TYR:OH	2.23	0.55
2:F:330:SER:OG	2:F:333:ASN:O	2.25	0.55
1:I:26:GLY:HA3	2:I:47:ASN:ND2	2.22	0.55
2:H:587:ARG:NH2	2:H:684:PHE:O	2.40	0.55
2:F:320:ASP:OD1	2:F:531:ARG:NH1	2.40	0.55
2:H:132:THR:HG23	2:H:153:GLY:HA3	1.89	0.55
2:J:455:ARG:NH1	2:J:500:ASP:OD1	2.40	0.55
2:L:862:SER:OG	2:L:872:ASP:OD2	2.22	0.55
2:L:419:LYS:N	2:L:426:GLU:O	2.41	0.54
2:A:574:VAL:HG21	2:A:591:ALA:HB1	1.89	0.54
2:J:103:ILE:HG12	2:J:598:ILE:HD12	1.89	0.54
1:W:4:ILE:N	1:W:7:SER:HG	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:SER:O	2:B:501:SER:OG	2.25	0.54
2:J:515:ASP:OD2	2:J:848:LYS:NZ	2.39	0.54
5:U:13:TYR:HB2	5:U:188:PHE:CZ	2.42	0.54
2:A:86:LEU:HD13	2:A:566:TYR:HB2	1.89	0.54
2:A:646:THR:HG23	2:A:892:VAL:O	2.07	0.54
2:K:770:GLU:N	2:K:770:GLU:OE1	2.41	0.54
2:K:871:THR:OG1	2:K:873:LEU:O	2.23	0.54
3:M:68:ASN:HD21	3:M:70:THR:HB	1.73	0.54
2:F:210:ARG:NH2	2:F:278:GLU:OE1	2.40	0.54
2:I:381:ASP:OD1	2:I:531:ARG:NH2	2.40	0.54
2:A:31:PHE:O	2:A:35:THR:OG1	2.19	0.54
2:H:311:ASN:OD1	2:H:490:ASN:ND2	2.41	0.54
2:D:709:MET:O	2:D:887:ASP:N	2.41	0.53
2:L:72:ASP:OD1	2:L:73:ARG:N	2.41	0.53
2:L:616:GLU:OE2	2:L:620:ARG:NH1	2.41	0.53
3:M:68:ASN:HB3	3:M:71:HIS:CE1	2.43	0.53
2:B:183:ASP:OD2	2:B:185:THR:OG1	2.27	0.53
2:I:113:PHE:HB2	2:I:316:ILE:HD12	1.89	0.53
3:M:34:ARG:O	3:M:38:LEU:HB3	2.08	0.53
5:U:41:ILE:O	5:U:45:ASN:N	2.35	0.53
2:F:770:GLU:N	2:F:770:GLU:OE1	2.40	0.53
2:H:434:SER:O	2:H:434:SER:OG	2.25	0.53
3:M:70:THR:O	3:M:74:VAL:HG23	2.09	0.53
2:K:54:HIS:NE2	5:V:217:ASP:OD2	2.27	0.53
2:D:778:SER:O	2:D:782:ASN:ND2	2.41	0.53
2:G:213:LYS:N	2:G:278:GLU:O	2.41	0.53
2:I:739:TYR:O	2:I:748:LYS:N	2.41	0.53
2:B:84:TYR:OH	2:B:598:ILE:O	2.18	0.53
2:F:501:SER:O	2:F:501:SER:OG	2.26	0.53
2:H:354:ASN:H	2:H:636:ASN:ND2	2.06	0.53
2:L:380:VAL:HG21	2:L:776:MET:HE1	1.89	0.53
4:Q:93:UNK:HA	4:S:102:UNK:CB	2.39	0.53
5:U:31:MET:H	5:U:48:ARG:HH22	1.57	0.53
2:D:47:ASN:HD21	1:Z:25:ILE:HA	1.74	0.53
2:K:96:MET:HE1	2:K:559:LEU:HD22	1.90	0.53
2:L:239:ARG:HB3	2:L:241:VAL:HG12	1.91	0.53
3:M:50:PRO:CG	1:W:12:ARG:HG3	2.39	0.53
1:4:24:ASP:HA	2:J:42:GLY:O	2.08	0.53
2:E:710:PHE:O	2:E:712:SER:N	2.42	0.53
2:E:412:ALA:HB2	2:E:438:ALA:HB2	1.91	0.53
2:L:213:LYS:N	2:L:278:GLU:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:442:ASN:O	2:I:822:ARG:NH1	2.42	0.52
4:P:57:PRO:CB	4:P:60:ALA:HB3	2.39	0.52
2:B:875:GLN:HG3	3:M:52:ALA:HB2	1.90	0.52
2:D:647:ASN:O	4:R:13:SER:OG	2.20	0.52
1:W:7:SER:HA	1:W:19:MET:HE1	1.91	0.52
2:K:827:TYR:OH	2:L:278:GLU:OE2	2.27	0.52
2:E:312:ARG:NH1	2:E:464:LEU:O	2.43	0.52
2:A:862:SER:OG	2:A:872:ASP:OD2	2.21	0.52
2:B:825:GLU:N	2:C:190:PRO:O	2.42	0.52
2:C:584:ASN:O	2:C:687:SER:OG	2.24	0.52
2:H:239:ARG:NH1	2:H:252:GLU:OE2	2.42	0.52
5:U:198:PHE:O	5:U:200:PRO:HD3	2.10	0.52
2:K:575:ASN:OD1	2:K:587:ARG:NE	2.43	0.52
1:Z:23:SER:O	1:Z:25:ILE:HG23	2.10	0.52
4:Q:55:SER:O	4:Q:58:LEU:HG	2.10	0.51
2:A:230:ASN:OD1	2:A:234:GLY:N	2.43	0.51
2:I:862:SER:OG	2:I:872:ASP:OD2	2.20	0.51
3:M:68:ASN:HB3	3:M:71:HIS:ND1	2.25	0.51
2:J:646:THR:OG1	2:J:892:VAL:O	2.11	0.51
2:H:191:GLN:N	2:H:191:GLN:OE1	2.43	0.51
2:H:210:ARG:NE	2:H:278:GLU:OE2	2.36	0.51
2:L:573:ASP:OD2	2:L:587:ARG:NH2	2.42	0.51
3:M:68:ASN:ND2	3:M:70:THR:HB	2.25	0.51
1:3:27:THR:HG23	2:K:49:THR:HG21	1.91	0.51
2:E:17:GLY:O	1:Y:15:THR:HG23	2.10	0.51
2:E:463:ALA:HB2	2:E:499:VAL:CG1	2.40	0.51
2:J:710:PHE:O	2:J:712:SER:N	2.43	0.51
2:L:737:GLU:OE1	2:L:737:GLU:N	2.42	0.51
4:R:66:ALA:C	4:R:68:ALA:H	2.17	0.51
2:E:119:THR:HG22	2:E:121:TYR:H	1.76	0.51
2:H:912:ARG:NH1	2:I:12:TYR:O	2.43	0.51
2:L:770:GLU:N	2:L:770:GLU:OE1	2.43	0.51
5:U:57:GLU:O	5:U:61:LEU:HG	2.10	0.51
1:3:25:ILE:HA	2:K:42:GLY:O	2.10	0.51
2:H:395:ILE:O	2:I:117:SER:OG	2.24	0.51
2:I:103:ILE:HG12	2:I:598:ILE:HD12	1.93	0.51
1:I:26:GLY:HA2	2:I:45:PHE:O	2.09	0.51
2:D:47:ASN:ND2	1:Z:25:ILE:HA	2.25	0.51
2:G:210:ARG:O	2:I:827:TYR:OH	2.27	0.51
2:I:389:ILE:HG12	2:I:786:MET:HE1	1.93	0.51
5:U:204:SER:OG	5:U:207:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:463:ALA:HB2	2:K:499:VAL:HG12	1.93	0.51
2:C:226:ALA:HB3	2:C:235:GLN:OE1	2.10	0.51
2:J:320:ASP:O	2:J:323:VAL:HG23	2.11	0.51
3:M:60:GLU:O	3:M:64:PRO:HA	2.11	0.51
4:P:57:PRO:HB3	4:P:60:ALA:HB3	1.92	0.51
1:W:6:PHE:HB3	1:W:9:LEU:HD12	1.92	0.51
2:E:230:ASN:OD1	2:E:234:GLY:N	2.43	0.50
2:E:112:SER:O	2:E:314:ASN:ND2	2.44	0.50
2:K:729:GLU:O	2:K:747:THR:OG1	2.23	0.50
2:L:577:VAL:HG23	2:L:578:LEU:HD12	1.91	0.50
5:U:58:GLN:O	5:U:62:THR:HB	2.11	0.50
2:D:295:THR:OG1	2:D:296:SER:N	2.44	0.50
2:E:154:ILE:HD13	2:F:438:ALA:HB3	1.92	0.50
2:B:518:ASN:ND2	2:B:521:ASN:OD1	2.43	0.50
2:E:248:VAL:HG13	2:E:249:GLU:H	1.77	0.50
2:D:28:LEU:HD23	2:D:28:LEU:O	2.12	0.50
2:K:929:PRO:O	5:U:28:SER:HB2	2.10	0.50
1:Y:4:ILE:HG22	1:Y:6:PHE:H	1.76	0.50
2:F:96:MET:HE1	2:F:559:LEU:HD22	1.94	0.50
2:L:655:ARG:NH2	2:L:929:PRO:O	2.45	0.50
2:A:460:SER:HA	2:A:464:LEU:HD12	1.94	0.50
2:E:759:TYR:OH	2:E:778:SER:OG	2.28	0.50
2:C:661:ARG:NH1	2:C:907:VAL:O	2.45	0.49
2:D:861:SER:OG	2:D:863:ASN:O	2.15	0.49
2:D:449:ILE:HD11	2:E:447:ILE:HD11	1.94	0.49
3:M:96:TYR:O	3:M:100:LEU:HG	2.11	0.49
5:U:12:SER:HB2	5:U:21:ALA:O	2.12	0.49
2:J:432:SER:OG	2:J:433:LYS:N	2.44	0.49
3:M:28:TRP:HB2	3:M:62:VAL:HA	1.94	0.49
4:R:56:SER:C	4:R:57:PRO:CD	2.84	0.49
2:K:154:ILE:HG23	2:L:409:ILE:HG22	1.94	0.49
4:R:56:SER:HB2	4:R:57:PRO:HD3	1.94	0.49
2:A:661:ARG:NH2	2:A:906:GLU:OE1	2.46	0.49
2:A:710:PHE:O	2:A:712:SER:N	2.44	0.49
2:C:59:ASP:N	2:C:59:ASP:OD1	2.45	0.49
2:C:90:ASP:OD1	2:C:918:ARG:NH1	2.46	0.49
2:H:479:LEU:HD21	2:H:491:GLY:HA3	1.94	0.49
2:B:403:CYS:SG	2:C:447:ILE:HD12	2.53	0.49
2:K:419:LYS:NZ	2:K:426:GLU:OE1	2.42	0.49
1:I:11:PRO:O	1:I:18:TYR:N	2.42	0.49
2:B:449:ILE:O	2:B:453:LEU:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:358:SER:OG	2:H:631:TYR:O	2.24	0.49
2:I:584:ASN:O	2:I:687:SER:OG	2.21	0.49
2:J:76:ASN:OD1	2:J:77:THR:N	2.44	0.49
2:A:46:ARG:HD2	1:W:27:THR:HG22	1.94	0.49
2:A:741:VAL:HG11	2:A:751:PHE:HB2	1.94	0.49
2:G:122:ASN:ND2	2:I:828:PRO:O	2.45	0.49
2:H:103:ILE:HG12	2:H:598:ILE:HD12	1.95	0.49
1:3:16:ARG:CZ	1:3:17:PRO:HD3	2.43	0.49
1:4:15:THR:HG23	2:L:18:GLN:HA	1.95	0.49
2:C:318:PHE:O	2:C:531:ARG:NH1	2.45	0.49
2:E:820:THR:HG22	2:E:821:MET:H	1.78	0.49
2:J:242:LYS:HD2	2:J:250:THR:HB	1.95	0.49
2:K:610:ASN:OD1	2:K:611:THR:N	2.45	0.49
4:Q:56:SER:OG	4:Q:57:PRO:HD3	2.13	0.48
2:H:710:PHE:O	2:H:712:SER:N	2.46	0.48
2:C:479:LEU:HD21	2:C:491:GLY:HA3	1.95	0.48
2:E:732:ARG:NH2	2:E:737:GLU:OE1	2.46	0.48
2:G:827:TYR:OH	2:H:278:GLU:OE1	2.27	0.48
3:M:88:ARG:HD2	3:M:90:ASP:HB2	1.95	0.48
5:U:40:MET:O	5:U:44:VAL:HG23	2.13	0.48
2:C:457:PHE:O	2:C:461:ASN:ND2	2.46	0.48
2:G:789:GLN:NE2	2:H:541:VAL:HG12	2.28	0.48
2:H:300:SER:OG	2:H:301:HIS:N	2.46	0.48
2:D:353:ARG:NH1	2:D:909:ASP:OD2	2.46	0.48
2:D:684:PHE:HZ	2:D:690:ILE:HD11	1.78	0.48
2:G:822:ARG:NH1	2:I:442:ASN:O	2.47	0.48
2:B:27:GLY:N	2:B:30:GLN:OE1	2.47	0.48
2:A:159:GLY:HA3	2:A:167:LEU:HD11	1.95	0.48
2:E:320:ASP:O	2:E:323:VAL:HG23	2.14	0.48
2:K:712:SER:O	5:U:16:GLN:NE2	2.46	0.48
2:L:775:ARG:O	2:L:778:SER:OG	2.30	0.48
3:M:28:TRP:CE3	3:M:62:VAL:HG22	2.49	0.48
2:A:4:PRO:HB3	2:C:877:MET:SD	2.54	0.47
2:F:862:SER:OG	2:F:872:ASP:OD2	2.25	0.47
2:G:401:ASN:ND2	2:H:452:ASN:OD1	2.46	0.47
2:B:210:ARG:NE	2:B:278:GLU:OE2	2.40	0.47
2:D:261:ASP:O	2:E:416:GLN:N	2.43	0.47
2:F:667:ARG:NH1	2:F:895:MET:SD	2.87	0.47
2:G:871:THR:OG1	2:G:873:LEU:O	2.16	0.47
4:Q:63:ALA:O	4:Q:67:THR:HG23	2.15	0.47
3:M:50:PRO:CD	1:W:12:ARG:HG3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:661:ARG:NH2	2:C:906:GLU:OE1	2.47	0.47
2:A:158:LYS:NZ	2:A:205:GLU:OE1	2.47	0.47
2:C:22:GLU:OE1	1:W:15:THR:OG1	2.32	0.47
2:D:608:ALA:HB3	2:D:611:THR:HG22	1.97	0.47
2:L:90:ASP:OD1	2:L:918:ARG:NH2	2.47	0.47
1:2:9:LEU:HD22	2:G:55:ASP:O	2.14	0.47
2:A:47:ASN:H	1:W:27:THR:HG23	1.78	0.47
2:F:42:GLY:CA	1:Y:25:ILE:HG22	2.45	0.47
2:G:204:ASN:OD1	2:G:205:GLU:N	2.44	0.47
2:I:614:THR:HG22	2:I:618:MET:HE3	1.97	0.47
5:U:6:PRO:HG3	5:U:198:PHE:HA	1.96	0.47
1:3:25:ILE:HB	2:K:47:ASN:HD21	1.80	0.47
2:A:778:SER:O	2:A:782:ASN:ND2	2.48	0.47
2:B:323:VAL:HG12	2:B:356:GLU:OE1	2.15	0.47
2:K:573:ASP:O	2:K:577:VAL:HG22	2.14	0.47
2:A:123:SER:N	2:C:810:ASN:OD1	2.48	0.47
2:B:168:GLU:OE2	2:B:171:LYS:NZ	2.48	0.47
2:C:397:ASP:O	2:C:399:LEU:N	2.48	0.47
2:I:59:ASP:OD1	2:I:59:ASP:N	2.46	0.47
2:A:395:ILE:N	2:B:117:SER:O	2.45	0.47
2:E:528:LEU:HD21	2:E:579:GLN:CD	2.39	0.47
2:F:46:ARG:NH1	1:Y:27:THR:OG1	2.48	0.46
2:I:311:ASN:OD1	2:I:490:ASN:ND2	2.43	0.46
2:I:872:ASP:OD1	2:I:873:LEU:N	2.47	0.46
2:D:610:ASN:OD1	2:D:611:THR:N	2.47	0.46
2:K:700:ASN:ND2	2:K:854:THR:O	2.48	0.46
2:L:618:MET:O	2:L:624:ASN:ND2	2.46	0.46
5:U:217:ASP:HB3	5:U:220:SER:OG	2.14	0.46
2:D:732:ARG:NE	2:D:735:ASP:OD1	2.42	0.46
2:J:172:ASP:O	2:J:174:THR:N	2.44	0.46
2:K:629:ASN:OD1	2:K:630:ASP:N	2.49	0.46
2:J:417:GLY:HA3	2:J:431:VAL:HG21	1.96	0.46
3:M:32:MET:CE	3:M:61:ALA:HB3	2.43	0.46
5:U:13:TYR:HB2	5:U:188:PHE:CE2	2.49	0.46
1:3:28:SER:HB2	2:J:631:TYR:OH	2.15	0.46
2:B:610:ASN:OD1	2:B:611:THR:N	2.49	0.46
2:C:55:ASP:O	2:C:611:THR:HG21	2.14	0.46
2:E:857:ARG:NH2	1:Y:30:LEU:HD21	2.30	0.46
2:G:314:ASN:OD1	2:G:582:LEU:HD13	2.15	0.46
2:C:743:GLN:OE1	2:C:743:GLN:N	2.49	0.46
2:E:395:ILE:CD1	2:E:451:ALA:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:132:THR:HG23	2:I:153:GLY:HA3	1.97	0.46
2:H:393:HIS:ND1	2:I:533:MET:HE1	2.31	0.46
2:K:778:SER:O	2:K:782:ASN:ND2	2.49	0.46
2:A:382:SER:N	2:A:525:ASN:OD1	2.46	0.46
2:E:211:ALA:N	2:E:276:TYR:O	2.48	0.46
2:I:608:ALA:HB3	2:I:611:THR:HG22	1.97	0.46
5:U:13:TYR:CE2	5:U:15:PRO:HA	2.51	0.46
2:E:132:THR:HG23	2:E:153:GLY:HA3	1.98	0.46
2:E:395:ILE:HD12	2:E:451:ALA:HB2	1.98	0.46
2:E:672:GLU:OE1	2:E:698:TYR:OH	2.31	0.46
2:J:821:MET:HE1	2:J:822:ARG:NH1	2.31	0.46
1:I:20:GLY:HA2	2:I:33:ARG:NH1	2.31	0.45
2:F:607:MET:HE1	2:F:615:LEU:HD22	1.98	0.45
2:H:774:ASP:OD2	2:I:371:ARG:NH2	2.49	0.45
2:L:608:ALA:O	2:L:612:ALA:N	2.46	0.45
2:B:104:ARG:O	2:B:596:THR:OG1	2.34	0.45
2:C:329:ASN:OD1	2:C:355:THR:HG22	2.16	0.45
5:U:41:ILE:HG22	5:U:45:ASN:OD1	2.16	0.45
1:Y:12:ARG:HA	1:Y:16:ARG:O	2.16	0.45
2:A:375:MET:HE3	2:C:741:VAL:HG13	1.98	0.45
2:B:213:LYS:NZ	2:B:254:ASP:OD1	2.34	0.45
2:F:403:CYS:N	2:F:445:MET:O	2.50	0.45
2:G:9:GLN:N	2:G:9:GLN:OE1	2.48	0.45
2:G:263:ARG:NH2	2:H:433:LYS:O	2.48	0.45
2:H:298:ASP:OD1	2:H:299:ASN:N	2.49	0.45
2:I:409:ILE:HG12	2:I:438:ALA:HB3	1.99	0.45
2:A:213:LYS:N	2:A:278:GLU:O	2.47	0.45
2:B:573:ASP:O	2:B:577:VAL:HG22	2.17	0.45
2:C:388:ARG:NH1	2:C:852:ASP:OD1	2.47	0.45
2:D:713:SER:OG	2:L:931:SER:O	2.26	0.45
2:L:573:ASP:O	2:L:577:VAL:HG22	2.17	0.45
2:I:77:THR:HG23	2:I:78:TYR:HD1	1.81	0.45
2:L:320:ASP:O	2:L:323:VAL:HG13	2.16	0.45
1:4:25:ILE:HG22	1:4:27:THR:N	2.30	0.45
2:E:154:ILE:HD11	2:F:440:GLY:O	2.17	0.45
2:J:521:ASN:O	2:J:521:ASN:ND2	2.41	0.45
5:U:2:SER:HB3	5:U:200:PRO:HD2	1.99	0.45
2:E:220:PRO:O	2:E:224:SER:OG	2.35	0.45
2:E:722:LEU:O	2:F:63:ARG:NH1	2.49	0.45
2:D:573:ASP:O	2:D:577:VAL:HG22	2.16	0.45
2:E:267:ASP:OD1	2:E:268:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:U:14:GLN:HG2	5:U:17:MET:SD	2.57	0.45
1:W:7:SER:HA	1:W:19:MET:CE	2.46	0.45
2:C:710:PHE:O	2:C:712:SER:N	2.48	0.45
2:C:261:ASP:OD1	2:C:262:GLY:N	2.50	0.45
2:D:577:VAL:O	2:D:578:LEU:HD12	2.17	0.45
2:E:59:ASP:OD1	2:E:59:ASP:N	2.49	0.44
2:E:249:GLU:O	2:E:250:THR:OG1	2.35	0.44
4:R:67:THR:O	4:R:68:ALA:CB	2.65	0.44
1:Z:29:GLN:HG2	1:Z:30:LEU:H	1.81	0.44
2:A:632:LEU:HD23	2:A:632:LEU:O	2.17	0.44
2:H:623:THR:OG1	2:I:23:TYR:O	2.35	0.44
2:J:257:MET:HE2	2:J:276:TYR:CE2	2.52	0.44
2:E:72:ASP:OD1	2:E:72:ASP:N	2.50	0.44
2:G:163:THR:OG1	2:G:165:GLU:OE1	2.30	0.44
2:L:549:GLN:OE1	2:L:566:TYR:OH	2.35	0.44
2:B:531:ARG:NH2	2:B:579:GLN:OE1	2.50	0.44
2:B:800:LYS:NZ	2:C:229:THR:O	2.51	0.44
1:3:17:PRO:O	1:3:19:MET:HG2	2.18	0.44
2:B:875:GLN:HE21	3:M:52:ALA:H	1.65	0.44
2:E:907:VAL:HG12	2:E:929:PRO:HG2	1.99	0.44
2:L:132:THR:HG23	2:L:153:GLY:HA3	1.98	0.44
4:P:55:SER:HB3	4:P:58:LEU:HD21	1.98	0.44
2:F:575:ASN:OD1	2:F:587:ARG:NE	2.50	0.44
5:U:210:ASP:HB3	5:U:216:PHE:CE2	2.53	0.44
1:W:12:ARG:NH1	1:W:17:PRO:HG3	2.33	0.44
2:A:577:VAL:HG23	2:A:578:LEU:CD1	2.48	0.44
2:C:119:THR:OG1	2:C:286:ASP:OD1	2.30	0.44
2:L:318:PHE:O	2:L:531:ARG:NH1	2.50	0.44
2:A:261:ASP:OD1	2:A:262:GLY:N	2.50	0.44
2:B:879:TYR:HB2	3:M:55:LEU:HD13	1.99	0.44
5:U:213:ILE:HG22	5:U:216:PHE:H	1.82	0.44
2:K:428:ASP:OD1	2:K:429:ASP:N	2.51	0.43
4:R:56:SER:HB2	4:R:57:PRO:CD	2.47	0.43
2:G:608:ALA:HB3	2:G:611:THR:HG22	1.99	0.43
2:K:924:VAL:HG23	5:U:40:MET:SD	2.59	0.43
2:H:73:ARG:NE	2:H:80:TYR:OH	2.51	0.43
2:I:421:LYS:O	2:I:424:GLY:N	2.50	0.43
2:L:629:ASN:OD1	2:L:630:ASP:N	2.51	0.43
4:R:56:SER:HA	4:R:57:PRO:N	2.32	0.43
2:F:415:TYR:N	2:F:435:ASN:O	2.49	0.43
2:B:204:ASN:O	2:B:206:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:722:LEU:O	2:H:63:ARG:NH1	2.51	0.43
2:K:559:LEU:HD21	2:K:564:TYR:CD2	2.53	0.43
2:K:732:ARG:NH1	2:K:735:ASP:OD1	2.52	0.43
1:3:15:THR:O	1:3:16:ARG:HD2	2.18	0.43
2:H:666:THR:OG1	2:H:700:ASN:OD1	2.14	0.43
2:J:119:THR:HG22	2:J:121:TYR:H	1.81	0.43
2:B:163:THR:OG1	2:B:164:LYS:N	2.52	0.43
2:C:161:ASN:OD1	2:C:162:ILE:N	2.51	0.43
2:E:154:ILE:HD12	2:E:155:ALA:H	1.82	0.43
2:F:132:THR:HG21	2:F:210:ARG:O	2.19	0.43
2:H:151:THR:HB	2:I:437:ILE:HD11	2.00	0.43
2:L:584:ASN:ND2	2:L:589:ASP:OD2	2.52	0.43
2:A:577:VAL:HG23	2:A:578:LEU:HD13	2.00	0.43
2:D:196:SER:HA	2:F:821:MET:SD	2.59	0.43
2:D:584:ASN:O	2:D:687:SER:OG	2.29	0.43
2:H:872:ASP:OD1	2:H:873:LEU:N	2.52	0.43
2:J:520:PHE:O	2:J:525:ASN:ND2	2.51	0.43
4:P:56:SER:HB2	4:P:57:PRO:HD2	2.01	0.43
2:B:608:ALA:HB3	2:B:611:THR:HG22	2.01	0.43
2:B:633:SER:OG	2:B:633:SER:O	2.36	0.43
2:D:618:MET:O	2:D:624:ASN:ND2	2.51	0.43
2:K:261:ASP:OD1	2:K:262:GLY:N	2.52	0.43
2:F:22:GLU:OE2	1:Z:16:ARG:NH1	2.52	0.42
2:L:796:TYR:O	2:L:797:THR:OG1	2.30	0.42
3:M:50:PRO:HG2	3:M:53:ASN:OD1	2.20	0.42
2:I:249:GLU:N	2:I:249:GLU:OE1	2.52	0.42
2:L:872:ASP:OD1	2:L:873:LEU:N	2.52	0.42
3:M:74:VAL:HG21	3:M:100:LEU:CD2	2.47	0.42
5:U:6:PRO:HG2	5:U:196:VAL:CG1	2.49	0.42
5:V:26:ASP:OD2	5:V:29:THR:OG1	2.37	0.42
2:D:577:VAL:C	2:D:578:LEU:HD12	2.45	0.42
2:J:632:LEU:O	2:J:632:LEU:HD23	2.20	0.42
2:K:324:GLY:O	2:K:571:ARG:NE	2.52	0.42
4:Q:34:THR:HG21	4:Q:38:ARG:NH2	2.35	0.42
1:2:23:SER:HB2	1:2:25:ILE:HG12	2.02	0.42
1:3:10:ALA:HB3	1:3:17:PRO:HB2	2.01	0.42
2:D:630:ASP:O	2:D:633:SER:OG	2.30	0.42
2:E:549:GLN:OE1	2:E:566:TYR:OH	2.37	0.42
2:L:449:ILE:HG22	2:L:453:LEU:HD23	2.01	0.42
2:A:229:THR:O	2:C:800:LYS:NZ	2.53	0.42
2:F:482:ASN:O	2:F:485:THR:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:796:TYR:O	2:I:797:THR:OG1	2.27	0.42
2:G:397:ASP:OD1	2:G:397:ASP:N	2.51	0.42
2:J:122:ASN:OD1	2:L:810:ASN:N	2.49	0.42
2:J:587:ARG:NH2	2:J:684:PHE:O	2.52	0.42
2:K:407:ASP:OD1	2:K:407:ASP:N	2.51	0.42
2:A:667:ARG:NH1	2:A:899:THR:HG21	2.34	0.42
2:D:531:ARG:NH2	2:D:579:GLN:OE1	2.52	0.42
2:I:712:SER:O	4:R:19:ARG:NH2	2.52	0.42
2:K:154:ILE:HG23	2:L:409:ILE:CG2	2.50	0.42
2:K:260:PHE:HE2	2:K:275:LEU:HD12	1.85	0.42
2:B:364:ASP:O	2:B:775:ARG:NH2	2.53	0.42
2:G:482:ASN:O	2:G:485:THR:HG22	2.20	0.42
2:H:723:LEU:N	2:H:749:ASP:OD1	2.52	0.42
2:I:284:THR:O	2:I:284:THR:OG1	2.31	0.42
2:I:369:ARG:HB2	2:I:776:MET:HE2	2.01	0.42
4:P:63:ALA:O	4:P:67:THR:HG23	2.20	0.42
2:D:726:ASN:ND2	2:L:351:GLN:OE1	2.53	0.42
2:H:720:ASP:OD1	2:I:63:ARG:NH2	2.48	0.42
2:C:419:LYS:N	2:C:426:GLU:O	2.53	0.42
1:4:28:SER:H	2:J:46:ARG:NH2	2.18	0.41
2:K:107:LEU:HD11	2:K:578:LEU:HD21	2.02	0.41
1:Y:15:THR:O	1:Y:16:ARG:HG3	2.20	0.41
2:A:241:VAL:HG23	2:A:242:LYS:H	1.85	0.41
2:A:573:ASP:O	2:A:577:VAL:HG22	2.20	0.41
2:L:713:SER:OG	2:L:714:VAL:N	2.53	0.41
3:M:74:VAL:HG11	3:M:100:LEU:CD2	2.50	0.41
2:B:685:VAL:HG23	2:B:685:VAL:O	2.20	0.41
2:F:320:ASP:O	2:F:323:VAL:HG23	2.20	0.41
2:I:85:THR:HG23	2:I:340:GLN:NE2	2.35	0.41
2:K:384:ASP:HB3	2:K:387:VAL:HG22	2.01	0.41
1:W:4:ILE:O	1:W:4:ILE:HG13	2.21	0.41
2:D:842:LYS:HD2	4:P:58:LEU:HD13	2.02	0.41
2:E:368:ASP:OD1	2:E:370:THR:HG22	2.20	0.41
2:E:448:ASN:O	2:E:451:ALA:N	2.52	0.41
2:I:72:ASP:OD1	2:I:73:ARG:N	2.53	0.41
5:V:2:SER:OG	5:V:3:LYS:N	2.52	0.41
1:2:5:ASN:N	1:2:5:ASN:ND2	2.65	0.41
2:C:573:ASP:OD1	2:C:574:VAL:N	2.53	0.41
2:G:581:SER:O	2:G:582:LEU:HD12	2.21	0.41
2:G:132:THR:HG23	2:G:153:GLY:HA3	2.01	0.41
2:H:320:ASP:O	2:H:323:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:629:ASN:ND2	2:I:909:ASP:O	2.54	0.41
1:3:27:THR:CG2	2:K:49:THR:HG21	2.51	0.41
1:4:11:PRO:HB3	2:K:867:MET:O	2.21	0.41
2:A:116:TYR:CD1	2:C:505:ILE:HG22	2.56	0.41
4:Q:57:PRO:CB	4:Q:60:ALA:HB3	2.51	0.41
2:A:614:THR:HG22	2:A:618:MET:HE3	2.02	0.41
2:B:358:SER:OG	2:B:630:ASP:OD1	2.37	0.41
2:D:912:ARG:NE	2:E:12:TYR:O	2.53	0.41
2:E:19:ASP:OD1	1:Y:14:GLY:HA3	2.21	0.41
2:E:226:ALA:HB3	2:E:235:GLN:OE1	2.21	0.41
2:G:88:VAL:HG23	2:G:604:PHE:HE2	1.85	0.41
2:G:526:ALA:HA	2:G:529:ARG:HB2	2.02	0.41
2:J:201:ASP:OD1	2:J:202:GLY:N	2.54	0.41
4:Q:57:PRO:HB2	4:Q:61:ALA:H	1.85	0.41
4:R:12:PHE:O	4:R:13:SER:OG	2.38	0.41
2:C:518:ASN:ND2	2:C:521:ASN:OD1	2.51	0.41
2:J:242:LYS:NZ	2:J:245:GLU:OE1	2.54	0.41
2:L:577:VAL:O	2:L:578:LEU:HD12	2.20	0.41
4:P:57:PRO:HB2	4:P:60:ALA:HB3	2.02	0.41
2:B:212:LEU:HD23	2:B:216:THR:HG21	2.02	0.40
2:J:161:ASN:OD1	2:J:162:ILE:N	2.54	0.40
2:C:700:ASN:ND2	2:C:854:THR:O	2.53	0.40
2:G:321:ASN:N	2:G:377:ASN:O	2.45	0.40
2:K:358:SER:OG	2:K:630:ASP:OD1	2.35	0.40
1:1:31:ASN:OD1	2:H:661:ARG:NH1	2.55	0.40
2:K:112:SER:O	2:K:314:ASN:ND2	2.55	0.40
2:L:666:THR:HG23	2:L:700:ASN:OD1	2.20	0.40
2:L:675:SER:O	2:L:675:SER:OG	2.38	0.40
2:A:574:VAL:HG21	2:A:591:ALA:CB	2.52	0.40
2:B:66:LEU:HD13	2:B:604:PHE:CE1	2.56	0.40
2:G:55:ASP:OD1	2:G:610:ASN:ND2	2.50	0.40
2:J:267:ASP:OD1	2:J:267:ASP:N	2.54	0.40
2:J:772:TYR:O	2:J:775:ARG:NH1	2.54	0.40
2:L:577:VAL:C	2:L:578:LEU:HD12	2.46	0.40
2:L:584:ASN:O	2:L:687:SER:OG	2.34	0.40
3:M:88:ARG:HG3	3:M:91:GLU:H	1.87	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	12/250 (5%)	11 (92%)	1 (8%)	0	100	100
1	1	25/250 (10%)	18 (72%)	7 (28%)	0	100	100
1	2	25/250 (10%)	20 (80%)	5 (20%)	0	100	100
1	3	20/250 (8%)	18 (90%)	2 (10%)	0	100	100
1	4	23/250 (9%)	19 (83%)	2 (9%)	2 (9%)	0	9
1	W	21/250 (8%)	19 (90%)	2 (10%)	0	100	100
1	Y	22/250 (9%)	19 (86%)	3 (14%)	0	100	100
1	Z	24/250 (10%)	18 (75%)	6 (25%)	0	100	100
2	A	930/937 (99%)	836 (90%)	88 (10%)	6 (1%)	21	54
2	B	925/937 (99%)	839 (91%)	80 (9%)	6 (1%)	21	54
2	C	927/937 (99%)	843 (91%)	78 (8%)	6 (1%)	21	54
2	D	930/937 (99%)	862 (93%)	63 (7%)	5 (0%)	24	57
2	E	927/937 (99%)	855 (92%)	66 (7%)	6 (1%)	21	54
2	F	929/937 (99%)	843 (91%)	81 (9%)	5 (0%)	24	57
2	G	930/937 (99%)	857 (92%)	68 (7%)	5 (0%)	24	57
2	H	929/937 (99%)	849 (91%)	76 (8%)	4 (0%)	30	62
2	I	928/937 (99%)	860 (93%)	65 (7%)	3 (0%)	36	67
2	J	929/937 (99%)	846 (91%)	80 (9%)	3 (0%)	36	67
2	K	930/937 (99%)	853 (92%)	73 (8%)	4 (0%)	30	62
2	L	930/937 (99%)	870 (94%)	56 (6%)	4 (0%)	30	62
3	M	75/588 (13%)	72 (96%)	3 (4%)	0	100	100
4	P	61/138 (44%)	56 (92%)	4 (7%)	1 (2%)	7	35
4	Q	61/138 (44%)	56 (92%)	5 (8%)	0	100	100
4	R	58/138 (42%)	51 (88%)	4 (7%)	3 (5%)	1	17
4	S	60/138 (44%)	57 (95%)	2 (3%)	1 (2%)	7	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	U	104/227 (46%)	97 (93%)	7 (7%)	0	100	100
5	V	97/227 (43%)	91 (94%)	6 (6%)	0	100	100
All	All	11832/14838 (80%)	10835 (92%)	933 (8%)	64 (0%)	26	57

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	188	PRO
2	A	375	MET
2	A	832	PRO
2	B	188	PRO
2	B	342	SER
2	B	832	PRO
2	C	188	PRO
2	C	265	ALA
2	C	267	ASP
2	C	832	PRO
2	D	188	PRO
2	D	295	THR
2	D	713	SER
2	D	918	ARG
2	E	188	PRO
2	E	248	VAL
2	F	11	ALA
2	F	188	PRO
2	F	248	VAL
2	F	832	PRO
2	G	188	PRO
2	G	267	ASP
2	G	411	PRO
2	G	832	PRO
2	H	188	PRO
2	H	248	VAL
2	H	832	PRO
2	I	188	PRO
2	J	188	PRO
2	K	9	GLN
2	K	188	PRO
2	K	409	ILE
2	L	188	PRO
2	L	243	PRO

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Mol	Chain	Res	Type
2	L	832	PRO
4	P	57	PRO
4	R	63	ALA
4	R	68	ALA
4	S	57	PRO
2	A	241	VAL
2	A	418	ILE
2	B	9	GLN
2	E	245	GLU
2	E	493	VAL
2	G	713	SER
2	I	734	VAL
2	K	713	SER
2	L	713	SER
4	R	58	LEU
2	A	265	ALA
2	B	205	GLU
2	C	320	ASP
1	4	30	LEU
2	B	809	ASN
2	C	398	GLU
2	E	863	ASN
2	J	425	TRP
1	4	27	THR
2	D	320	ASP
2	H	734	VAL
2	J	173	ILE
2	I	828	PRO
2	E	187	GLN
2	F	439	ILE

### 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	0	13/209 (6%)	13 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	23/209 (11%)	23 (100%)	0	100	100
1	2	23/209 (11%)	22 (96%)	1 (4%)	26	50
1	3	19/209 (9%)	19 (100%)	0	100	100
1	4	22/209 (10%)	22 (100%)	0	100	100
1	W	22/209 (10%)	22 (100%)	0	100	100
1	Y	22/209 (10%)	22 (100%)	0	100	100
1	Z	22/209 (10%)	22 (100%)	0	100	100
2	A	807/811 (100%)	807 (100%)	0	100	100
2	B	805/811 (99%)	805 (100%)	0	100	100
2	C	804/811 (99%)	804 (100%)	0	100	100
2	D	807/811 (100%)	807 (100%)	0	100	100
2	E	805/811 (99%)	804 (100%)	1 (0%)	88	89
2	F	806/811 (99%)	806 (100%)	0	100	100
2	G	807/811 (100%)	807 (100%)	0	100	100
2	H	807/811 (100%)	807 (100%)	0	100	100
2	I	805/811 (99%)	805 (100%)	0	100	100
2	J	806/811 (99%)	805 (100%)	1 (0%)	88	89
2	K	807/811 (100%)	807 (100%)	0	100	100
2	L	807/811 (100%)	807 (100%)	0	100	100
3	M	64/504 (13%)	64 (100%)	0	100	100
4	P	44/69 (64%)	44 (100%)	0	100	100
4	Q	44/69 (64%)	44 (100%)	0	100	100
4	R	44/69 (64%)	42 (96%)	2 (4%)	24	48
4	S	44/69 (64%)	44 (100%)	0	100	100
5	U	92/192 (48%)	92 (100%)	0	100	100
5	V	87/192 (45%)	87 (100%)	0	100	100
All	All	10258/12568 (82%)	10253 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	5	ASN
2	E	521	ASN

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Mol	Chain	Res	Type
2	J	521	ASN
4	R	57	PRO
4	R	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	299	ASN
2	A	306	GLN
2	A	321	ASN
2	A	452	ASN
2	A	609	HIS
2	A	782	ASN
2	A	875	GLN
2	B	161	ASN
2	B	303	ASN
2	B	306	GLN
2	B	416	GLN
2	B	435	ASN
2	B	518	ASN
2	B	760	ASN
2	B	782	ASN
2	B	789	GLN
2	B	823	GLN
2	B	884	HIS
2	B	915	GLN
2	C	740	ASN
2	D	122	ASN
2	D	134	GLN
2	D	281	ASN
2	D	360	GLN
2	D	401	ASN
2	D	484	ASN
2	D	647	ASN
2	D	915	GLN
2	E	288	HIS
2	E	435	ASN
2	E	452	ASN
2	E	764	GLN
2	E	795	ASN
2	F	9	GLN
2	F	131	ASN

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Mol	Chain	Res	Type
2	F	281	ASN
2	F	288	HIS
2	F	333	ASN
2	F	435	ASN
2	F	518	ASN
2	F	521	ASN
2	F	624	ASN
2	F	917	HIS
2	G	303	ASN
2	G	360	GLN
2	G	452	ASN
2	G	846	GLN
2	H	9	GLN
2	H	43	ASN
2	H	47	ASN
2	H	54	HIS
2	H	321	ASN
2	H	476	ASN
2	H	516	ASN
2	H	621	ASN
2	H	629	ASN
2	H	823	GLN
2	H	875	GLN
2	H	914	HIS
2	I	131	ASN
2	I	150	ASN
2	I	177	ASN
2	I	288	HIS
2	I	629	ASN
2	I	743	GLN
2	I	863	ASN
2	I	914	HIS
2	J	14	HIS
2	J	54	HIS
2	J	288	HIS
2	J	301	HIS
2	J	314	ASN
2	J	378	GLN
2	J	401	ASN
2	J	482	ASN
2	J	575	ASN
2	J	917	HIS

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Mol	Chain	Res	Type
2	K	14	HIS
2	K	306	GLN
2	K	314	ASN
2	K	476	ASN
2	K	809	ASN
2	K	863	ASN
2	L	9	GLN
2	L	122	ASN
2	L	516	ASN
3	M	48	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	56:SER	C	57:PRO	N	2.06

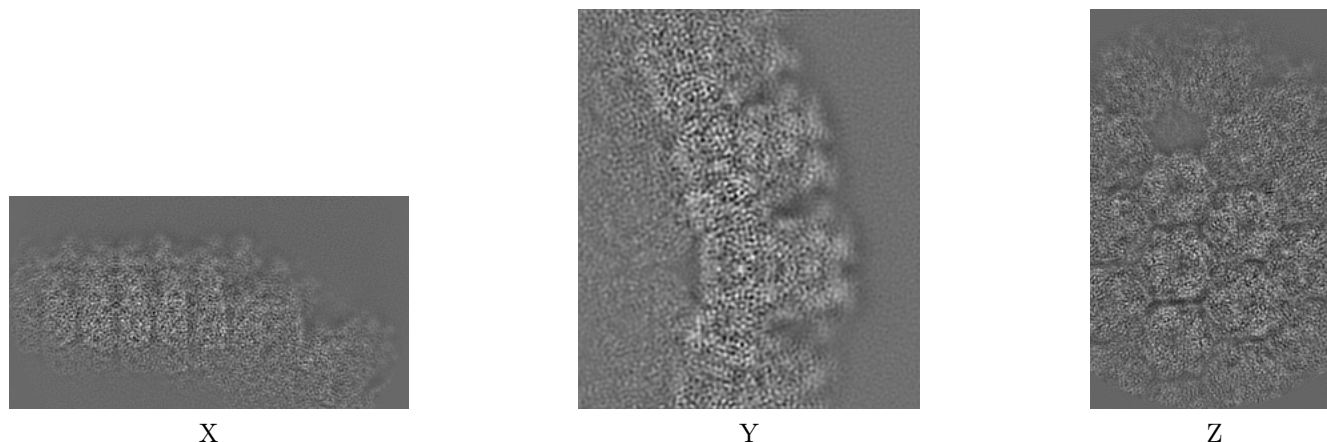
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72793. These allow visual inspection of the internal detail of the map and identification of artifacts.

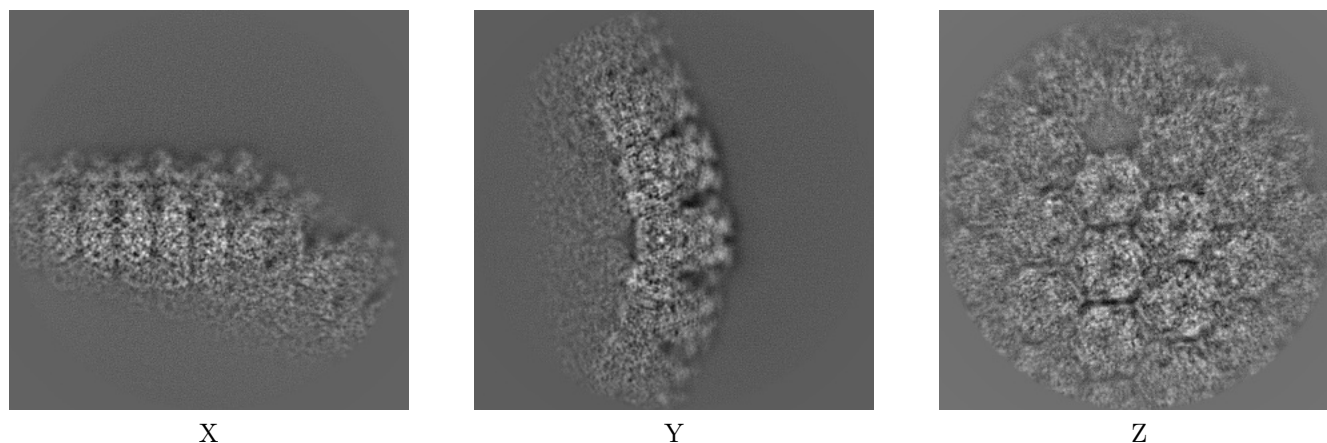
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



#### 6.1.2 Raw map

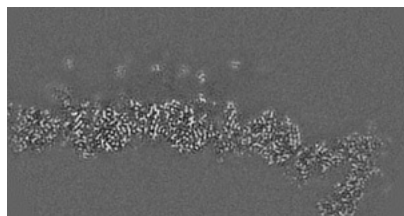


The images above show the map projected in three orthogonal directions.

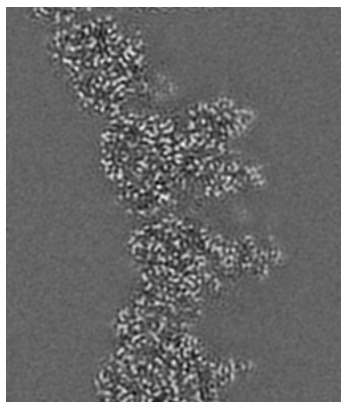


## 6.2 Central slices [i](#)

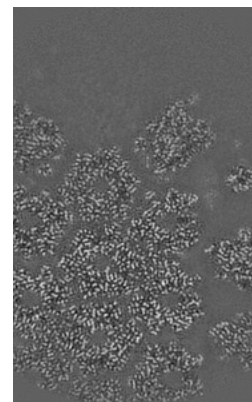
### 6.2.1 Primary map



X Index: 136

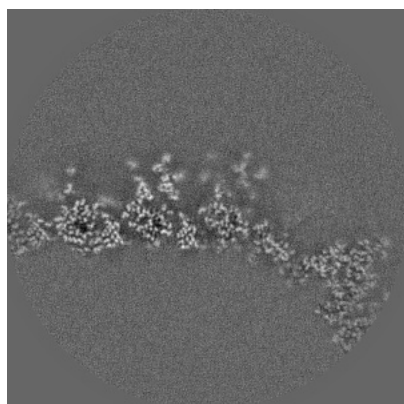


Y Index: 219

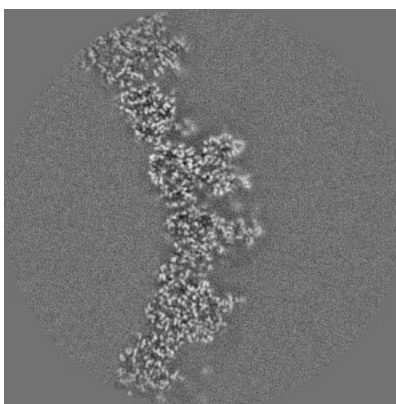


Z Index: 116

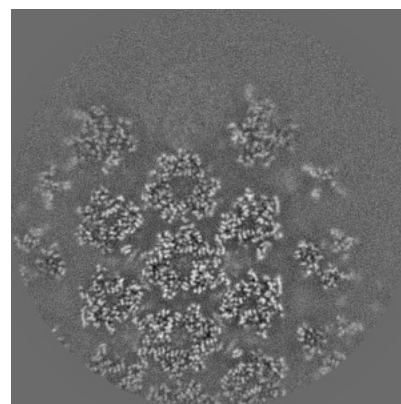
### 6.2.2 Raw map



X Index: 220



Y Index: 220

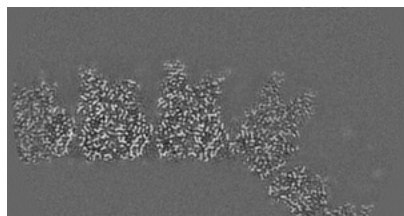


Z Index: 220

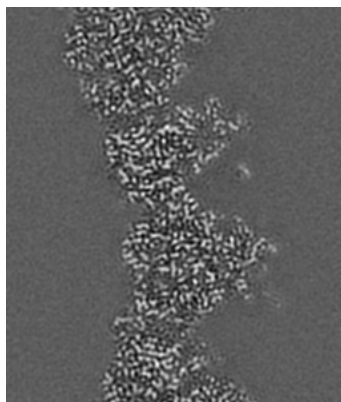
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

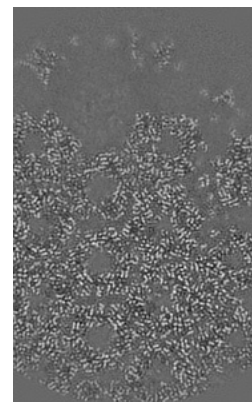
### 6.3.1 Primary map



X Index: 185

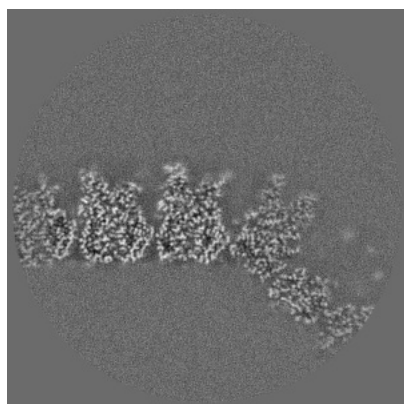


Y Index: 142

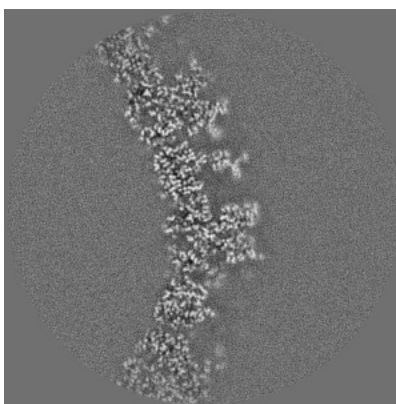


Z Index: 93

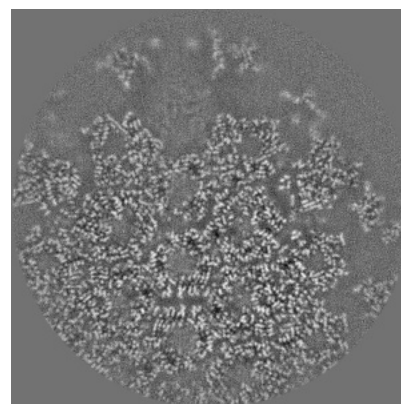
### 6.3.2 Raw map



X Index: 277



Y Index: 174

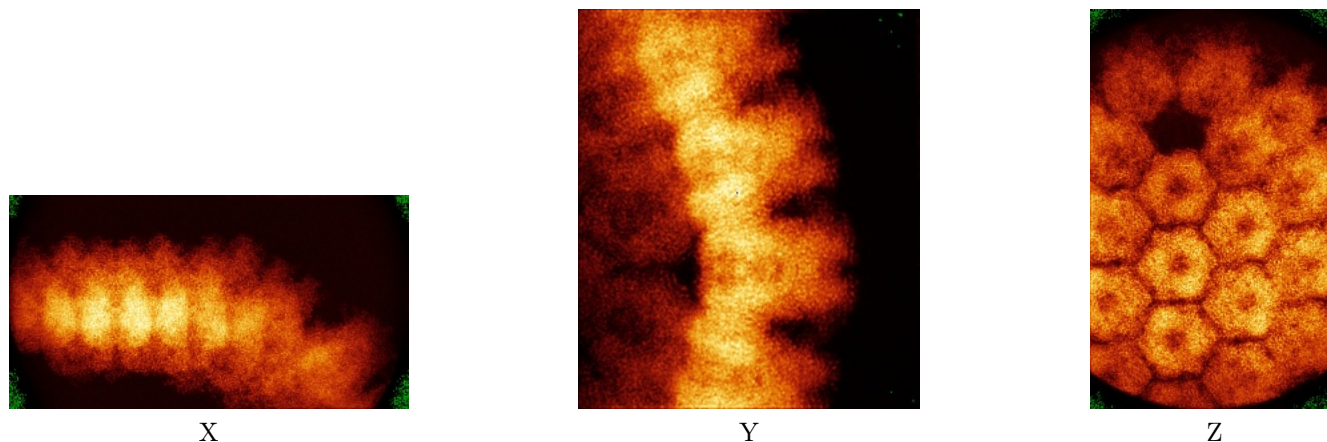


Z Index: 187

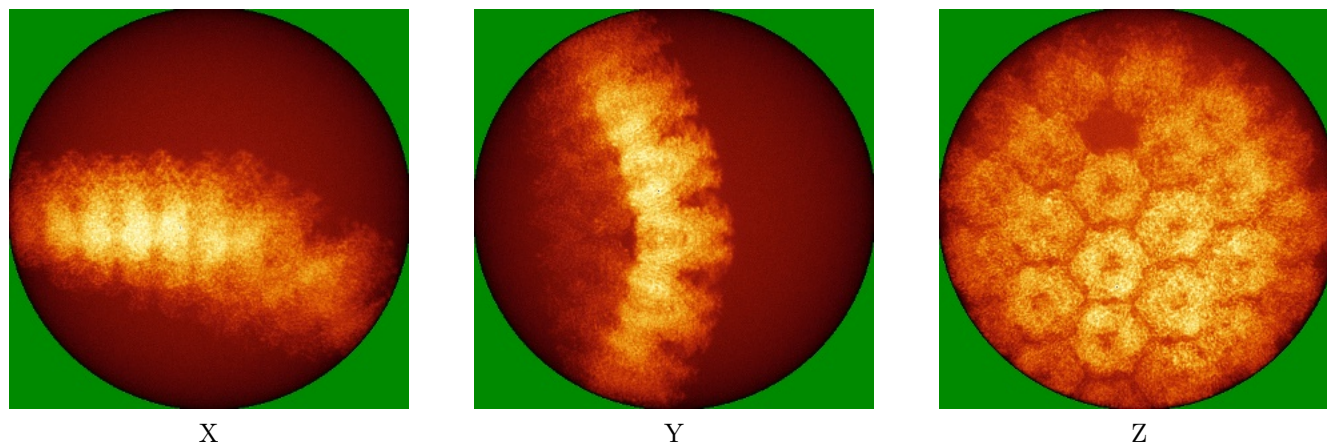
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



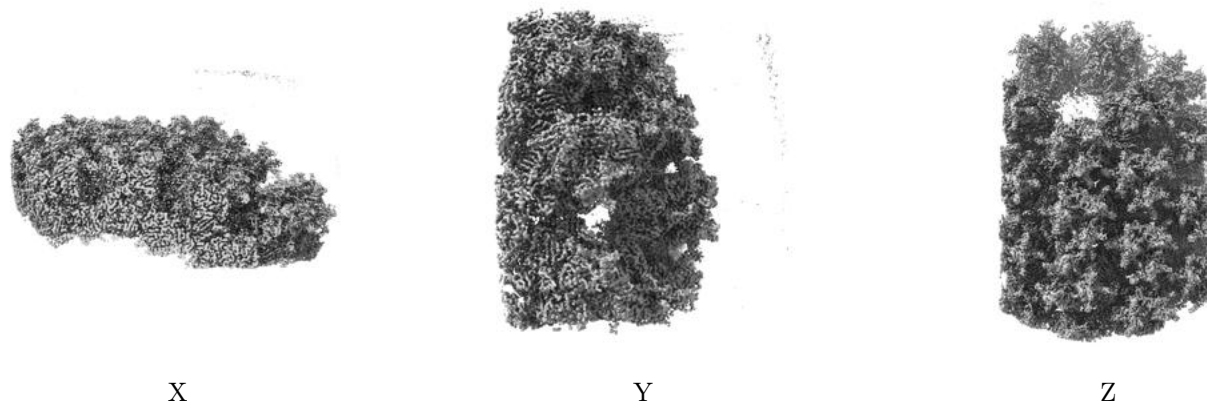
### 6.4.2 Raw map



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

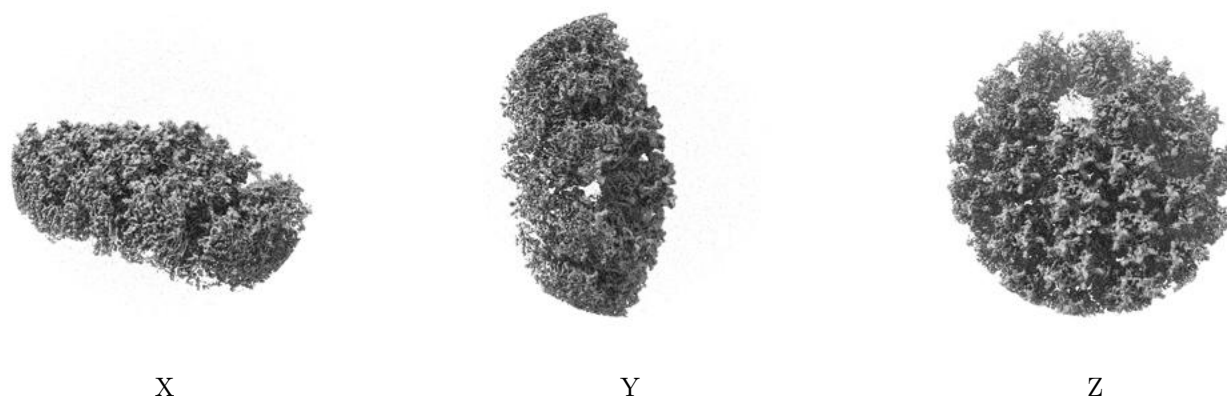
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

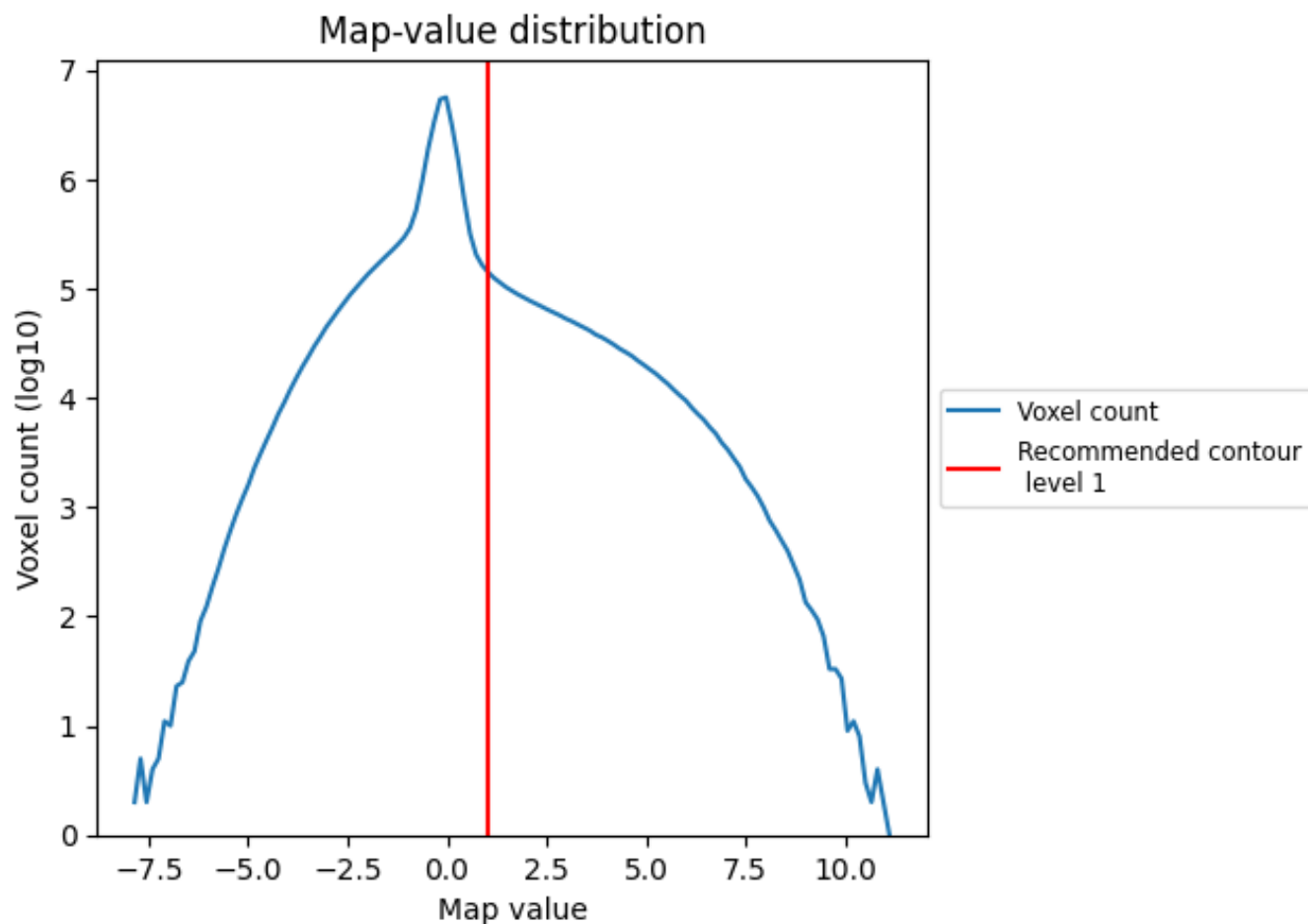
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

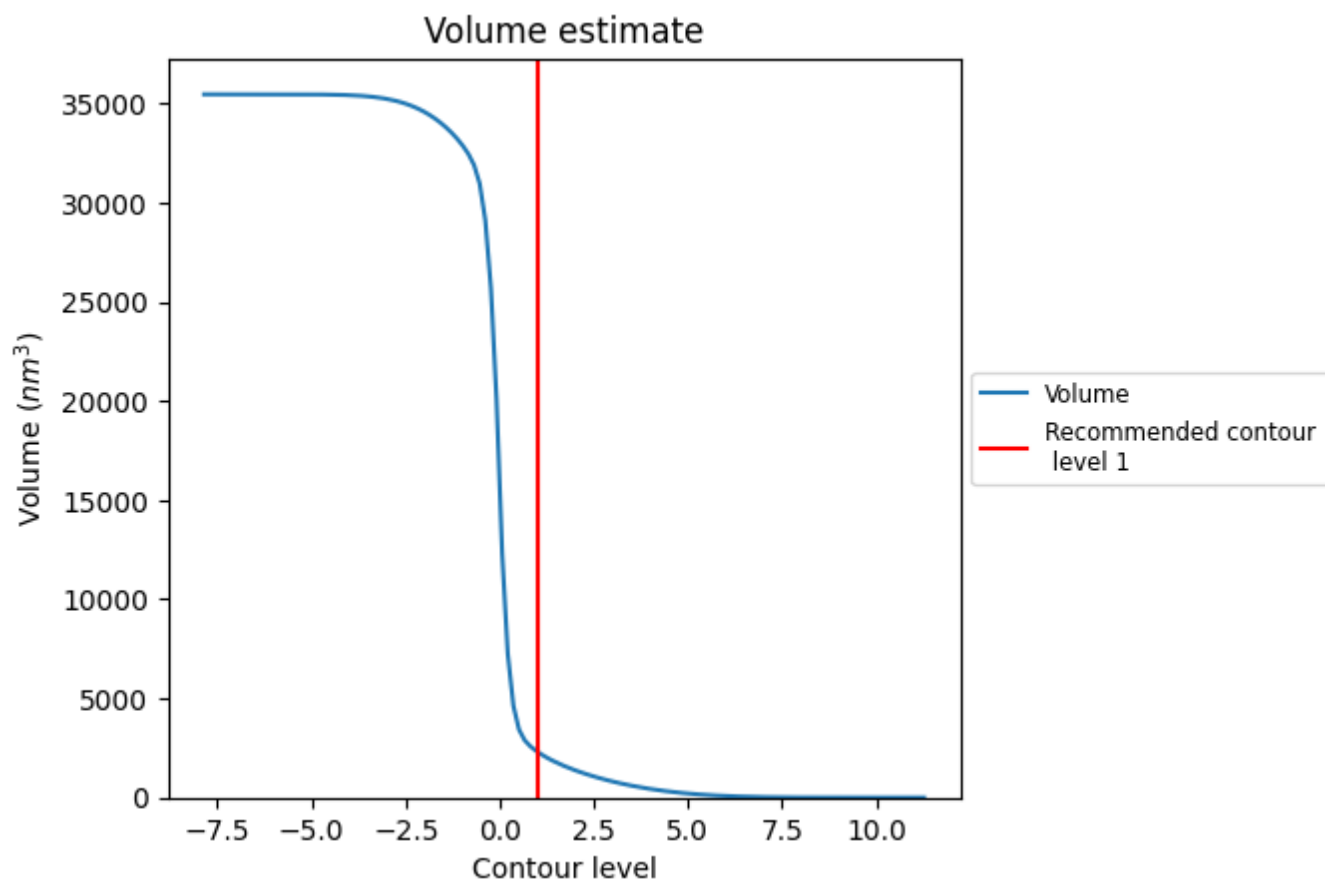
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2314 nm<sup>3</sup>; this corresponds to an approximate mass of 2090 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.

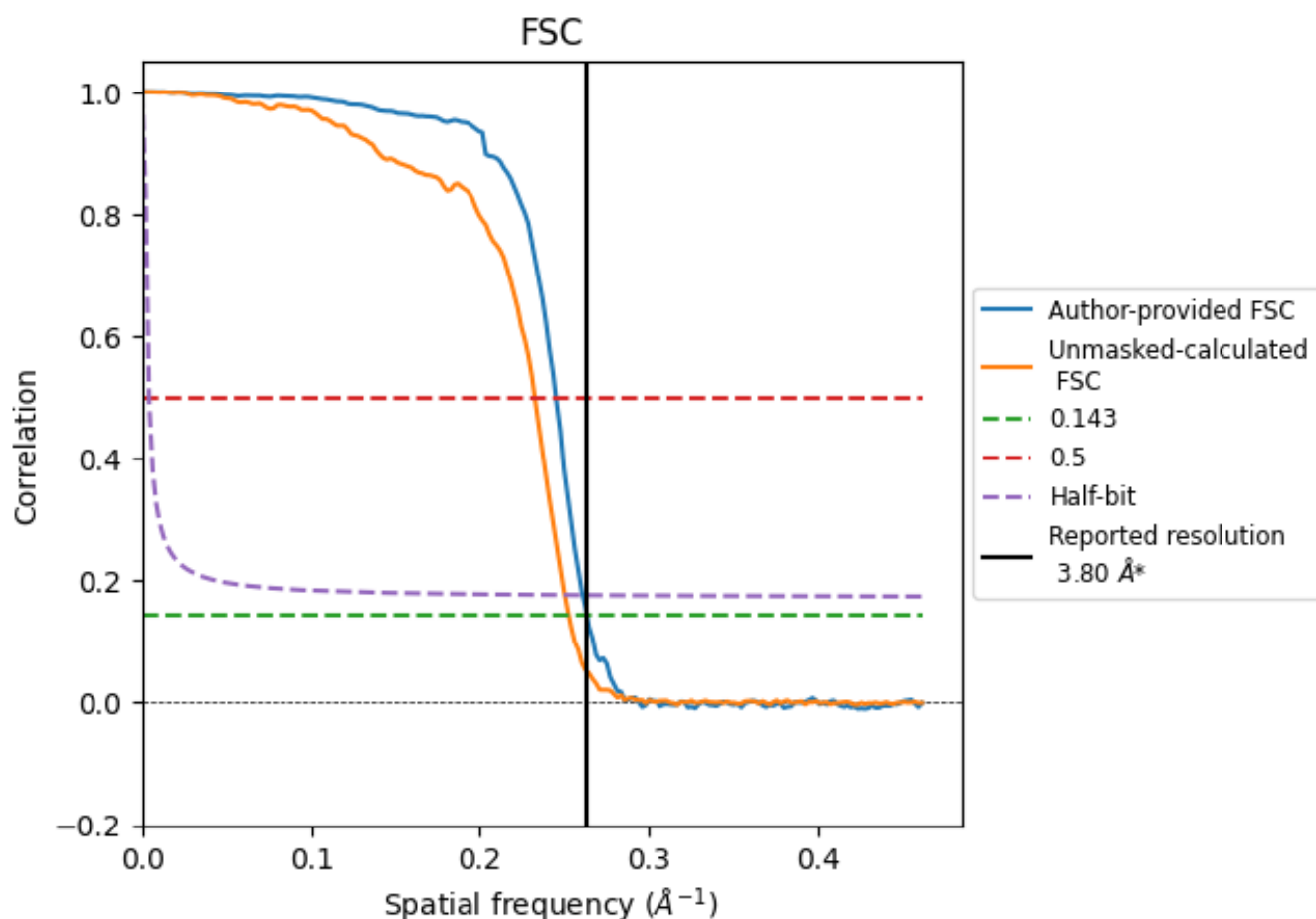
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.263  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.80	4.08	3.84
Unmasked-calculated*	3.96	4.30	4.00

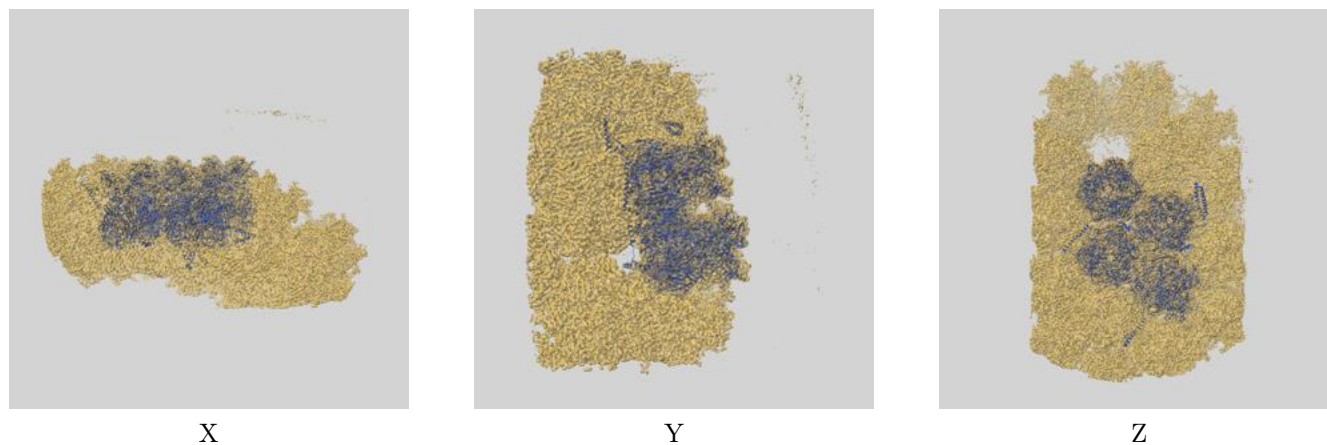
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

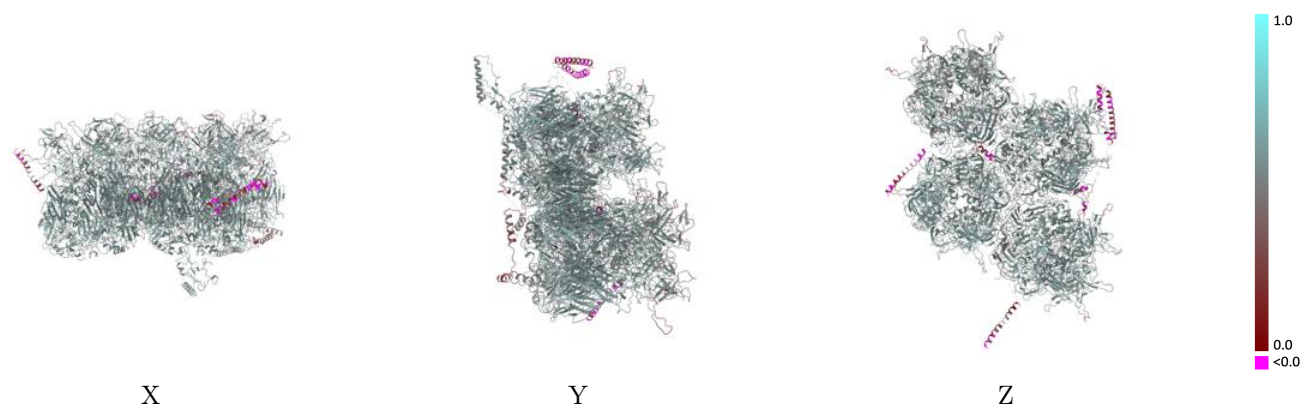
This section contains information regarding the fit between EMDB map EMD-72793 and PDB model 9YD0. Per-residue inclusion information can be found in section [3](#) on page [12](#).

### 9.1 Map-model overlay [i](#)



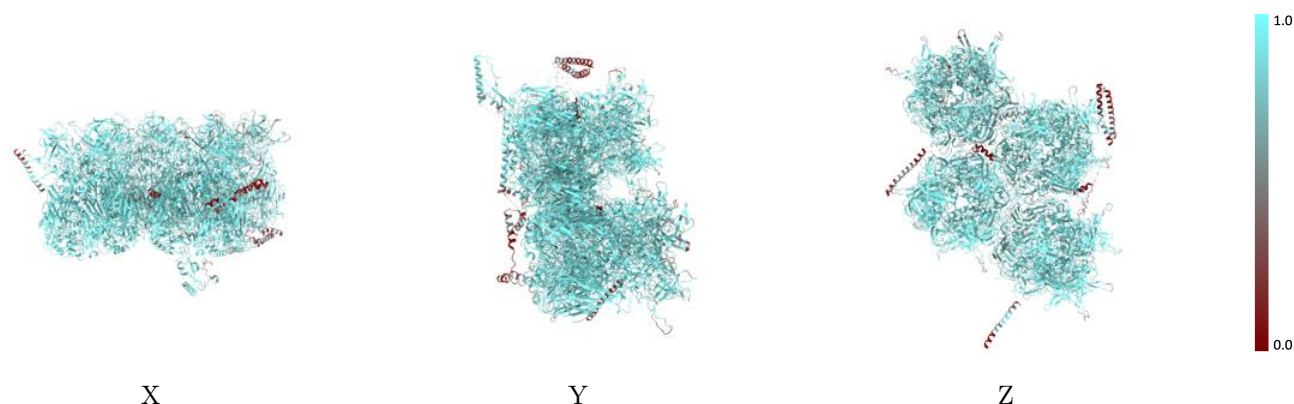
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



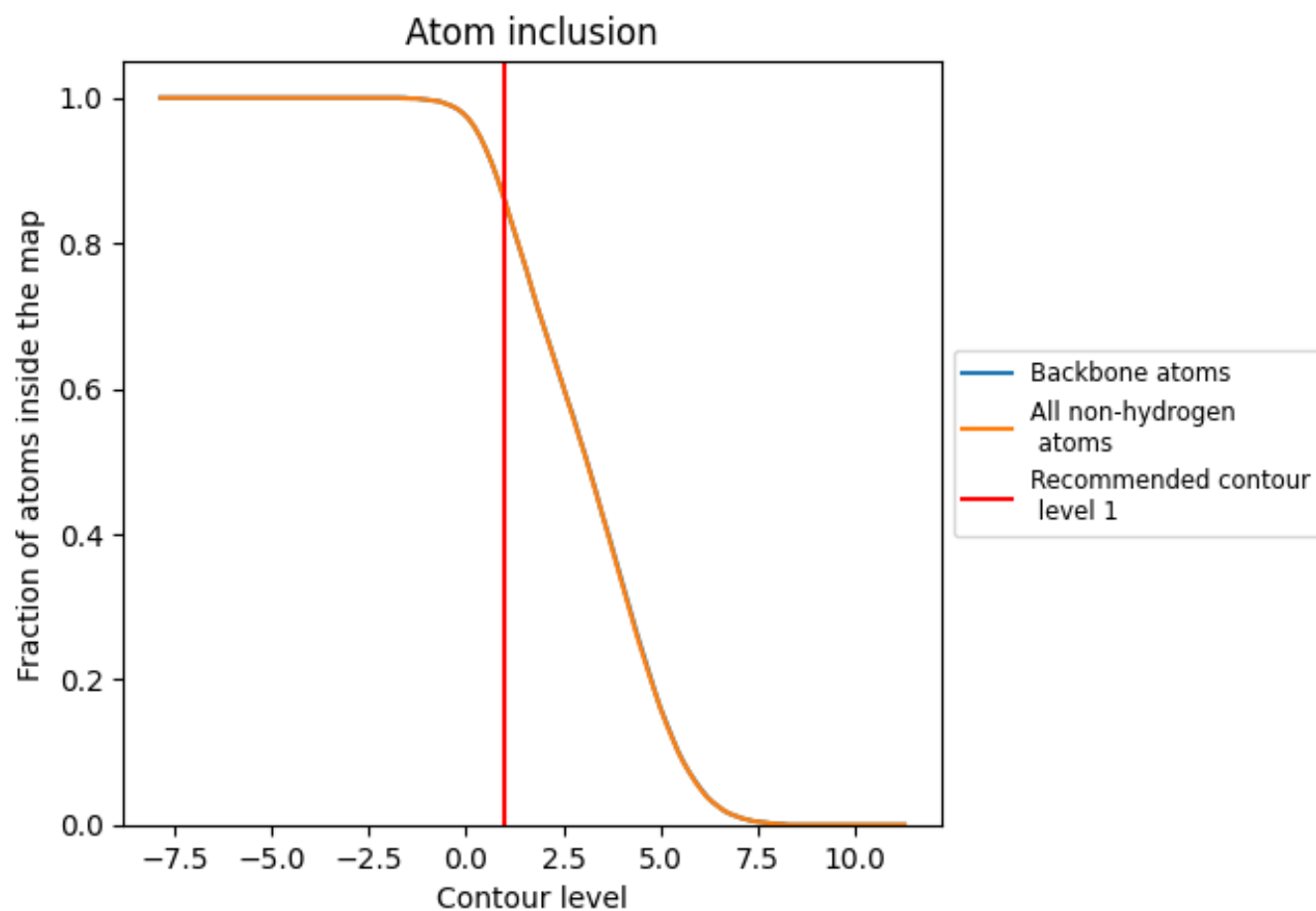
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.5360
0	 0.7410	 0.5280
1	 0.6910	 0.4890
2	 0.6180	 0.4720
3	 0.5400	 0.5090
4	 0.6170	 0.4450
A	 0.8480	 0.5350
B	 0.8230	 0.5260
C	 0.8370	 0.5290
D	 0.8930	 0.5490
E	 0.8920	 0.5490
F	 0.8890	 0.5460
G	 0.8950	 0.5480
H	 0.8970	 0.5490
I	 0.9000	 0.5490
J	 0.8900	 0.5460
K	 0.8870	 0.5480
L	 0.8950	 0.5510
M	 0.3240	 0.3360
P	 0.5590	 0.3260
Q	 0.5600	 0.3460
R	 0.6680	 0.3860
S	 0.5470	 0.3390
U	 0.6810	 0.4840
V	 0.7360	 0.5160
W	 0.6060	 0.4870
Y	 0.6980	 0.4970
Z	 0.7260	 0.4730

