



Full wwPDB EM Validation Report ⓘ

Mar 18, 2024 – 03:01 PM JST

PDB ID : 8K42
EMDB ID : EMD-36870
Title : Structure of full Banna virus
Authors : Li, Z.; Cao, S.
Deposited on : 2023-07-17
Resolution : 2.64 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:

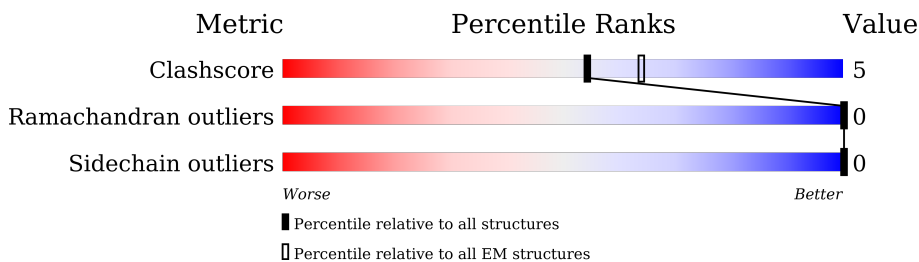
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.64 Å.

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


















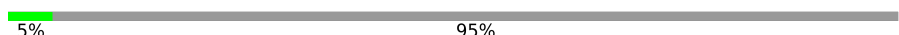
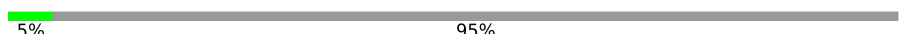
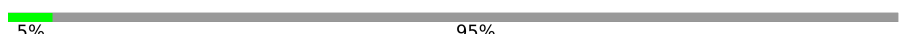
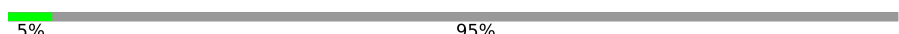
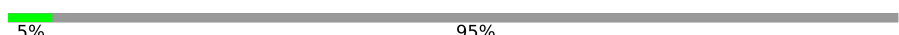
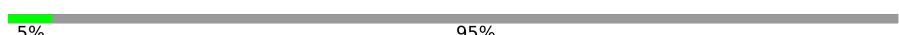
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	955	
1	B	955	
2	C	302	
2	D	302	
2	E	302	
2	F	302	
2	G	302	
2	H	302	

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Mol	Chain	Length	Quality of chain
2	I	302	 85% 14%
2	J	302	 88% 11%
2	K	302	 89% 9%
2	L	302	 85% 14%
2	M	302	 86% 13%
2	N	302	 86% 12%
2	O	302	 92% 6%
3	P	249	 86% 14%
3	Q	249	 85% 9% 6%
4	R	628	 85% 11%
4	S	628	 89% 10%
4	T	628	 83% 15%
4	U	628	 84% 12%
4	V	628	 86% 13%
4	W	628	 82% 15%
5	r	283	 5% 95%
5	s	283	 5% 95%
5	t	283	 5% 95%
5	u	283	 5% 95%
5	v	283	 5% 95%
5	w	283	 5% 95%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 76359 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 VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	774	6204	3941	1058	1178	27	0	0
1	B	904	7224	4587	1223	1387	27	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	LYS	ARG	conflict	UNP Q9INH3
B	97	LYS	ARG	conflict	UNP Q9INH3

- Molecule 2 is a protein called VP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	298	2277	1443	393	434	7	0	0
2	D	298	2277	1443	393	434	7	0	0
2	E	298	2277	1443	393	434	7	0	0
2	F	298	2277	1443	393	434	7	0	0
2	G	298	2277	1443	393	434	7	0	0
2	H	299	2288	1449	397	435	7	0	0
2	I	298	2277	1443	393	434	7	0	0
2	J	299	2288	1449	397	435	7	0	0
2	K	298	2277	1443	393	434	7	0	0
2	L	298	2277	1443	393	434	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	N	298	Total	C	N	O	S	0	0
			2277	1443	393	434	7		
2	O	297	Total	C	N	O	S	0	0
			2270	1438	392	433	7		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	136	ARG	GLN	conflict	UNP W0G587
C	185	LEU	MET	conflict	UNP W0G587
C	266	SER	ALA	conflict	UNP W0G587
D	136	ARG	GLN	conflict	UNP W0G587
D	185	LEU	MET	conflict	UNP W0G587
D	266	SER	ALA	conflict	UNP W0G587
E	136	ARG	GLN	conflict	UNP W0G587
E	185	LEU	MET	conflict	UNP W0G587
E	266	SER	ALA	conflict	UNP W0G587
F	136	ARG	GLN	conflict	UNP W0G587
F	185	LEU	MET	conflict	UNP W0G587
F	266	SER	ALA	conflict	UNP W0G587
G	136	ARG	GLN	conflict	UNP W0G587
G	185	LEU	MET	conflict	UNP W0G587
G	266	SER	ALA	conflict	UNP W0G587
H	136	ARG	GLN	conflict	UNP W0G587
H	185	LEU	MET	conflict	UNP W0G587
H	266	SER	ALA	conflict	UNP W0G587
I	136	ARG	GLN	conflict	UNP W0G587
I	185	LEU	MET	conflict	UNP W0G587
I	266	SER	ALA	conflict	UNP W0G587
J	136	ARG	GLN	conflict	UNP W0G587
J	185	LEU	MET	conflict	UNP W0G587
J	266	SER	ALA	conflict	UNP W0G587
K	136	ARG	GLN	conflict	UNP W0G587
K	185	LEU	MET	conflict	UNP W0G587
K	266	SER	ALA	conflict	UNP W0G587
L	136	ARG	GLN	conflict	UNP W0G587
L	185	LEU	MET	conflict	UNP W0G587
L	266	SER	ALA	conflict	UNP W0G587
M	136	ARG	GLN	conflict	UNP W0G587
M	185	LEU	MET	conflict	UNP W0G587

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Chain	Residue	Modelled	Actual	Comment	Reference
M	266	SER	ALA	conflict	UNP W0G587
N	136	ARG	GLN	conflict	UNP W0G587
N	185	LEU	MET	conflict	UNP W0G587
N	266	SER	ALA	conflict	UNP W0G587
O	136	ARG	GLN	conflict	UNP W0G587
O	185	LEU	MET	conflict	UNP W0G587
O	266	SER	ALA	conflict	UNP W0G587

- Molecule 3 is a protein called VP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	P	249	Total	C	N	O	S	0	0
			2014	1276	353	377	8		
3	Q	233	Total	C	N	O	S	0	0
			1876	1188	326	354	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	79	VAL	ILE	conflict	UNP A0A2H4QDD3
Q	79	VAL	ILE	conflict	UNP A0A2H4QDD3

- Molecule 4 is a protein called VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	602	Total	C	N	O	S	0	0
			4713	2973	815	909	16		
4	S	622	Total	C	N	O	S	0	0
			4860	3060	842	942	16		
4	T	616	Total	C	N	O	S	0	0
			4817	3034	835	932	16		
4	U	604	Total	C	N	O	S	0	0
			4731	2984	820	911	16		
4	V	622	Total	C	N	O	S	0	0
			4858	3060	841	941	16		
4	W	612	Total	C	N	O	S	0	0
			4786	3015	829	926	16		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	15	ASN	SER	conflict	UNP B4Y048

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Chain	Residue	Modelled	Actual	Comment	Reference
R	61	LEU	ILE	conflict	UNP B4Y048
R	62	ASN	ILE	conflict	UNP B4Y048
R	65	ALA	THR	conflict	UNP B4Y048
R	80	ASN	LYS	conflict	UNP B4Y048
R	94	ILE	VAL	conflict	UNP B4Y048
R	130	VAL	ILE	conflict	UNP B4Y048
R	154	VAL	ILE	conflict	UNP B4Y048
R	235	ALA	SER	conflict	UNP B4Y048
R	271	VAL	THR	conflict	UNP B4Y048
R	278	ILE	VAL	conflict	UNP B4Y048
R	307	LEU	MET	conflict	UNP B4Y048
R	322	ASN	THR	conflict	UNP B4Y048
R	369	ALA	VAL	conflict	UNP B4Y048
R	436	ASP	GLU	conflict	UNP B4Y048
R	439	GLN	LYS	conflict	UNP B4Y048
R	444	THR	ALA	conflict	UNP B4Y048
R	470	LYS	ARG	conflict	UNP B4Y048
R	500	THR	ALA	conflict	UNP B4Y048
R	524	VAL	ILE	conflict	UNP B4Y048
R	537	ASN	ASP	conflict	UNP B4Y048
R	539	SER	ASP	conflict	UNP B4Y048
R	543	SER	LEU	conflict	UNP B4Y048
R	545	ASN	LYS	conflict	UNP B4Y048
R	547	ARG	LYS	conflict	UNP B4Y048
R	575	ALA	THR	conflict	UNP B4Y048
R	628	PRO	SER	conflict	UNP B4Y048
S	15	ASN	SER	conflict	UNP B4Y048
S	61	LEU	ILE	conflict	UNP B4Y048
S	62	ASN	ILE	conflict	UNP B4Y048
S	65	ALA	THR	conflict	UNP B4Y048
S	80	ASN	LYS	conflict	UNP B4Y048
S	94	ILE	VAL	conflict	UNP B4Y048
S	130	VAL	ILE	conflict	UNP B4Y048
S	154	VAL	ILE	conflict	UNP B4Y048
S	235	ALA	SER	conflict	UNP B4Y048
S	271	VAL	THR	conflict	UNP B4Y048
S	278	ILE	VAL	conflict	UNP B4Y048
S	307	LEU	MET	conflict	UNP B4Y048
S	322	ASN	THR	conflict	UNP B4Y048
S	369	ALA	VAL	conflict	UNP B4Y048
S	436	ASP	GLU	conflict	UNP B4Y048
S	439	GLN	LYS	conflict	UNP B4Y048

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Chain	Residue	Modelled	Actual	Comment	Reference
S	444	THR	ALA	conflict	UNP B4Y048
S	470	LYS	ARG	conflict	UNP B4Y048
S	500	THR	ALA	conflict	UNP B4Y048
S	524	VAL	ILE	conflict	UNP B4Y048
S	537	ASN	ASP	conflict	UNP B4Y048
S	539	SER	ASP	conflict	UNP B4Y048
S	543	SER	LEU	conflict	UNP B4Y048
S	545	ASN	LYS	conflict	UNP B4Y048
S	547	ARG	LYS	conflict	UNP B4Y048
S	575	ALA	THR	conflict	UNP B4Y048
S	628	PRO	SER	conflict	UNP B4Y048
T	15	ASN	SER	conflict	UNP B4Y048
T	61	LEU	ILE	conflict	UNP B4Y048
T	62	ASN	ILE	conflict	UNP B4Y048
T	65	ALA	THR	conflict	UNP B4Y048
T	80	ASN	LYS	conflict	UNP B4Y048
T	94	ILE	VAL	conflict	UNP B4Y048
T	130	VAL	ILE	conflict	UNP B4Y048
T	154	VAL	ILE	conflict	UNP B4Y048
T	235	ALA	SER	conflict	UNP B4Y048
T	271	VAL	THR	conflict	UNP B4Y048
T	278	ILE	VAL	conflict	UNP B4Y048
T	307	LEU	MET	conflict	UNP B4Y048
T	322	ASN	THR	conflict	UNP B4Y048
T	369	ALA	VAL	conflict	UNP B4Y048
T	436	ASP	GLU	conflict	UNP B4Y048
T	439	GLN	LYS	conflict	UNP B4Y048
T	444	THR	ALA	conflict	UNP B4Y048
T	470	LYS	ARG	conflict	UNP B4Y048
T	500	THR	ALA	conflict	UNP B4Y048
T	524	VAL	ILE	conflict	UNP B4Y048
T	537	ASN	ASP	conflict	UNP B4Y048
T	539	SER	ASP	conflict	UNP B4Y048
T	543	SER	LEU	conflict	UNP B4Y048
T	545	ASN	LYS	conflict	UNP B4Y048
T	547	ARG	LYS	conflict	UNP B4Y048
T	575	ALA	THR	conflict	UNP B4Y048
T	628	PRO	SER	conflict	UNP B4Y048
U	15	ASN	SER	conflict	UNP B4Y048
U	61	LEU	ILE	conflict	UNP B4Y048
U	62	ASN	ILE	conflict	UNP B4Y048
U	65	ALA	THR	conflict	UNP B4Y048

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Chain	Residue	Modelled	Actual	Comment	Reference
U	80	ASN	LYS	conflict	UNP B4Y048
U	94	ILE	VAL	conflict	UNP B4Y048
U	130	VAL	ILE	conflict	UNP B4Y048
U	154	VAL	ILE	conflict	UNP B4Y048
U	235	ALA	SER	conflict	UNP B4Y048
U	271	VAL	THR	conflict	UNP B4Y048
U	278	ILE	VAL	conflict	UNP B4Y048
U	307	LEU	MET	conflict	UNP B4Y048
U	322	ASN	THR	conflict	UNP B4Y048
U	369	ALA	VAL	conflict	UNP B4Y048
U	436	ASP	GLU	conflict	UNP B4Y048
U	439	GLN	LYS	conflict	UNP B4Y048
U	444	THR	ALA	conflict	UNP B4Y048
U	470	LYS	ARG	conflict	UNP B4Y048
U	500	THR	ALA	conflict	UNP B4Y048
U	524	VAL	ILE	conflict	UNP B4Y048
U	537	ASN	ASP	conflict	UNP B4Y048
U	539	SER	ASP	conflict	UNP B4Y048
U	543	SER	LEU	conflict	UNP B4Y048
U	545	ASN	LYS	conflict	UNP B4Y048
U	547	ARG	LYS	conflict	UNP B4Y048
U	575	ALA	THR	conflict	UNP B4Y048
U	628	PRO	SER	conflict	UNP B4Y048
V	15	ASN	SER	conflict	UNP B4Y048
V	61	LEU	ILE	conflict	UNP B4Y048
V	62	ASN	ILE	conflict	UNP B4Y048
V	65	ALA	THR	conflict	UNP B4Y048
V	80	ASN	LYS	conflict	UNP B4Y048
V	94	ILE	VAL	conflict	UNP B4Y048
V	130	VAL	ILE	conflict	UNP B4Y048
V	154	VAL	ILE	conflict	UNP B4Y048
V	235	ALA	SER	conflict	UNP B4Y048
V	271	VAL	THR	conflict	UNP B4Y048
V	278	ILE	VAL	conflict	UNP B4Y048
V	307	LEU	MET	conflict	UNP B4Y048
V	322	ASN	THR	conflict	UNP B4Y048
V	369	ALA	VAL	conflict	UNP B4Y048
V	436	ASP	GLU	conflict	UNP B4Y048
V	439	GLN	LYS	conflict	UNP B4Y048
V	444	THR	ALA	conflict	UNP B4Y048
V	470	LYS	ARG	conflict	UNP B4Y048
V	500	THR	ALA	conflict	UNP B4Y048

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Chain	Residue	Modelled	Actual	Comment	Reference
V	524	VAL	ILE	conflict	UNP B4Y048
V	537	ASN	ASP	conflict	UNP B4Y048
V	539	SER	ASP	conflict	UNP B4Y048
V	543	SER	LEU	conflict	UNP B4Y048
V	545	ASN	LYS	conflict	UNP B4Y048
V	547	ARG	LYS	conflict	UNP B4Y048
V	575	ALA	THR	conflict	UNP B4Y048
V	628	PRO	SER	conflict	UNP B4Y048
W	15	ASN	SER	conflict	UNP B4Y048
W	61	LEU	ILE	conflict	UNP B4Y048
W	62	ASN	ILE	conflict	UNP B4Y048
W	65	ALA	THR	conflict	UNP B4Y048
W	80	ASN	LYS	conflict	UNP B4Y048
W	94	ILE	VAL	conflict	UNP B4Y048
W	130	VAL	ILE	conflict	UNP B4Y048
W	154	VAL	ILE	conflict	UNP B4Y048
W	235	ALA	SER	conflict	UNP B4Y048
W	271	VAL	THR	conflict	UNP B4Y048
W	278	ILE	VAL	conflict	UNP B4Y048
W	307	LEU	MET	conflict	UNP B4Y048
W	322	ASN	THR	conflict	UNP B4Y048
W	369	ALA	VAL	conflict	UNP B4Y048
W	436	ASP	GLU	conflict	UNP B4Y048
W	439	GLN	LYS	conflict	UNP B4Y048
W	444	THR	ALA	conflict	UNP B4Y048
W	470	LYS	ARG	conflict	UNP B4Y048
W	500	THR	ALA	conflict	UNP B4Y048
W	524	VAL	ILE	conflict	UNP B4Y048
W	537	ASN	ASP	conflict	UNP B4Y048
W	539	SER	ASP	conflict	UNP B4Y048
W	543	SER	LEU	conflict	UNP B4Y048
W	545	ASN	LYS	conflict	UNP B4Y048
W	547	ARG	LYS	conflict	UNP B4Y048
W	575	ALA	THR	conflict	UNP B4Y048
W	628	PRO	SER	conflict	UNP B4Y048

- Molecule 5 is a protein called VP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	r	14	Total	C	N	O	0	0
			110	69	19	22		
5	s	14	Total	C	N	O	0	0
			110	69	19	22		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	t	14	110	69	19	22	0	0
5	u	14	110	69	19	22	0	0
5	v	14	110	69	19	22	0	0
5	w	14	110	69	19	22	0	0


There are 24 discrepancies between the modelled and reference sequences:

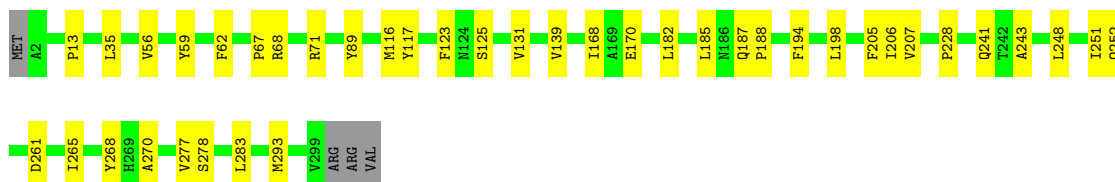
Chain	Residue	Modelled	Actual	Comment	Reference
r	150	TYR	HIS	conflict	UNP Q9YWN5
r	156	LEU	GLN	conflict	UNP Q9YWN5
r	184	THR	ALA	conflict	UNP Q9YWN5
r	191	ASN	ASP	conflict	UNP Q9YWN5
s	150	TYR	HIS	conflict	UNP Q9YWN5
s	156	LEU	GLN	conflict	UNP Q9YWN5
s	184	THR	ALA	conflict	UNP Q9YWN5
s	191	ASN	ASP	conflict	UNP Q9YWN5
t	150	TYR	HIS	conflict	UNP Q9YWN5
t	156	LEU	GLN	conflict	UNP Q9YWN5
t	184	THR	ALA	conflict	UNP Q9YWN5
t	191	ASN	ASP	conflict	UNP Q9YWN5
u	150	TYR	HIS	conflict	UNP Q9YWN5
u	156	LEU	GLN	conflict	UNP Q9YWN5
u	184	THR	ALA	conflict	UNP Q9YWN5
u	191	ASN	ASP	conflict	UNP Q9YWN5
v	150	TYR	HIS	conflict	UNP Q9YWN5
v	156	LEU	GLN	conflict	UNP Q9YWN5
v	184	THR	ALA	conflict	UNP Q9YWN5
v	191	ASN	ASP	conflict	UNP Q9YWN5
w	150	TYR	HIS	conflict	UNP Q9YWN5
w	156	LEU	GLN	conflict	UNP Q9YWN5
w	184	THR	ALA	conflict	UNP Q9YWN5
w	191	ASN	ASP	conflict	UNP Q9YWN5

Chain C:  93% 6%




• Molecule 2: VP8

Chain D:  85% 13%




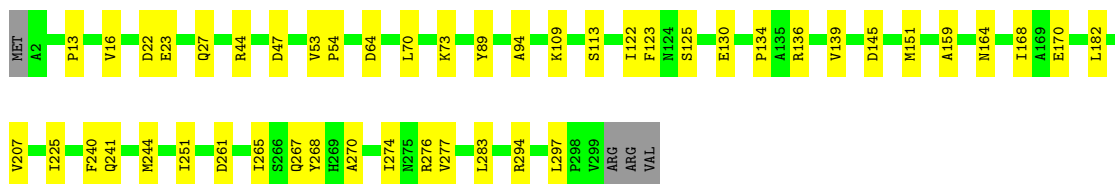
• Molecule 2: VP8

Chain E:  88% 10%




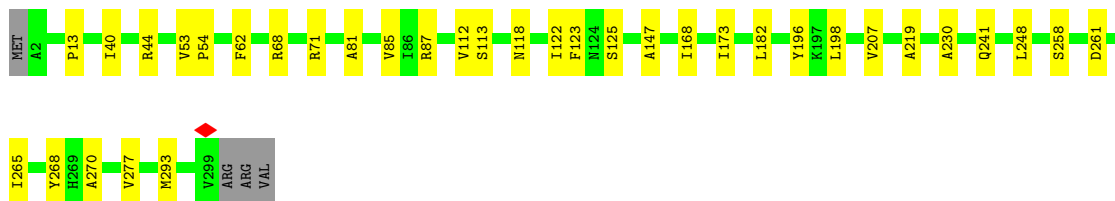
• Molecule 2: VP8

Chain F:  83% 16%




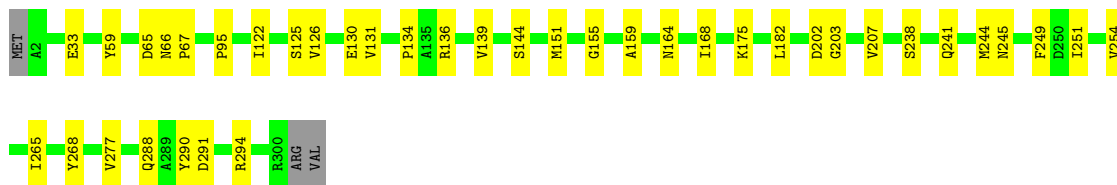
• Molecule 2: VP8

Chain G:  87% 12%

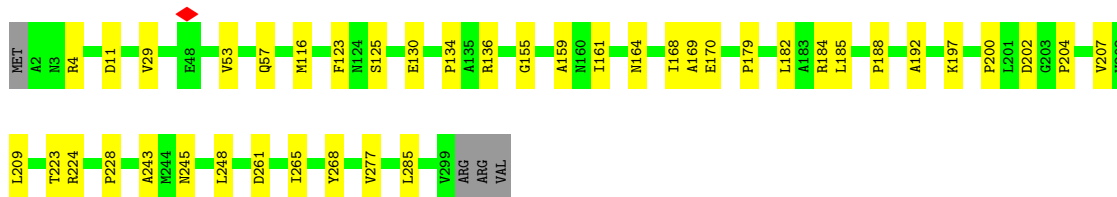
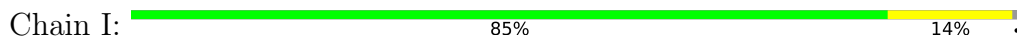


• Molecule 2: VP8

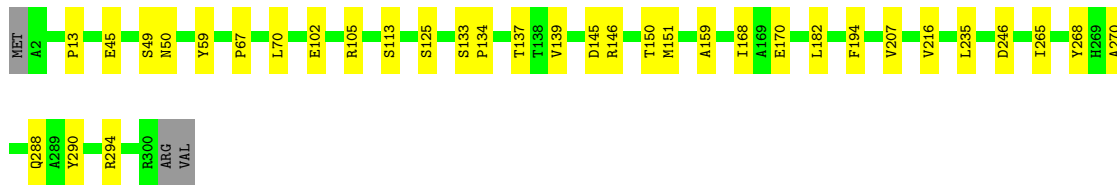
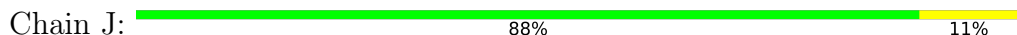
Chain H:  86% 13%



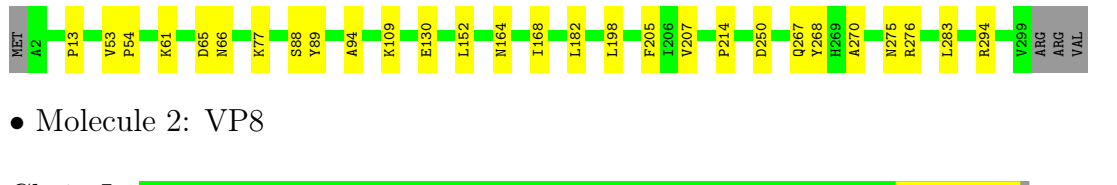
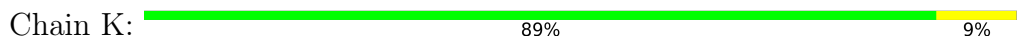
• Molecule 2: VP8



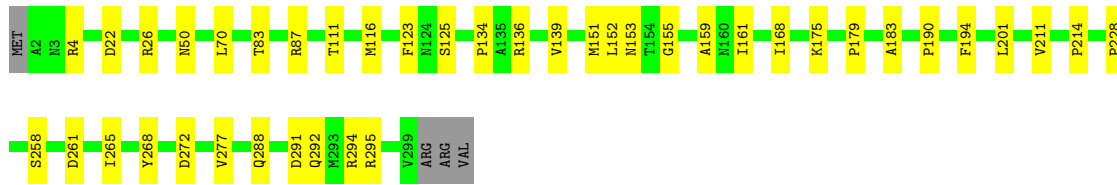
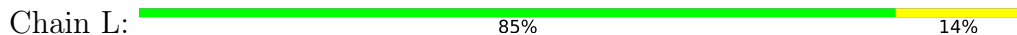
• Molecule 2: VP8



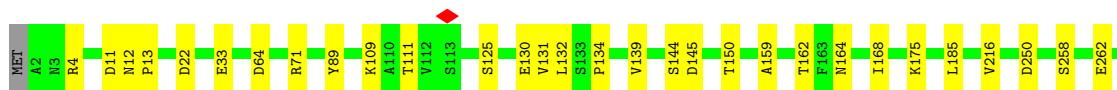
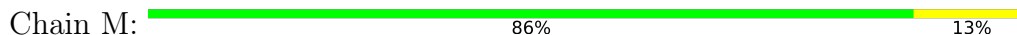
• Molecule 2: VP8



• Molecule 2: VP8

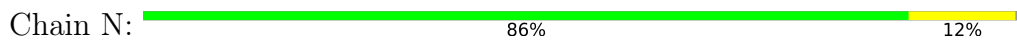


• Molecule 2: VP8





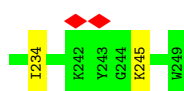
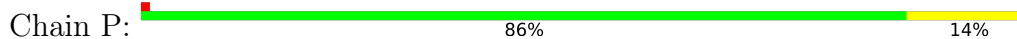
• Molecule 2: VP8



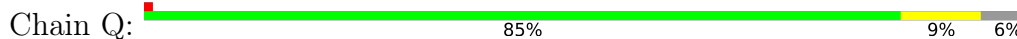
• Molecule 2: VP8



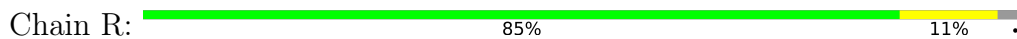
• Molecule 3: VP10



• Molecule 3: VP10

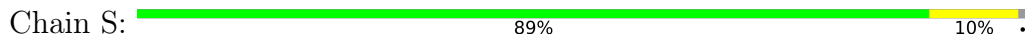


• Molecule 4: VP4

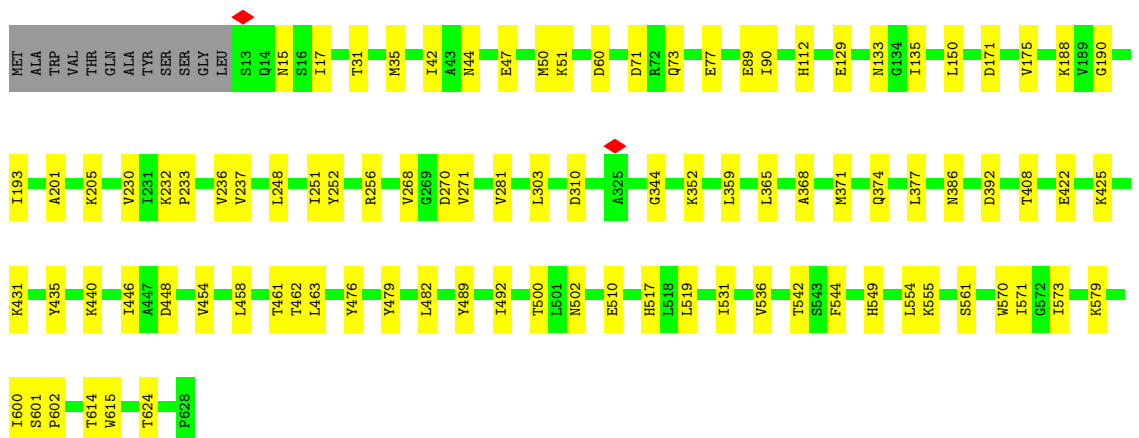
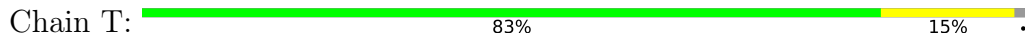




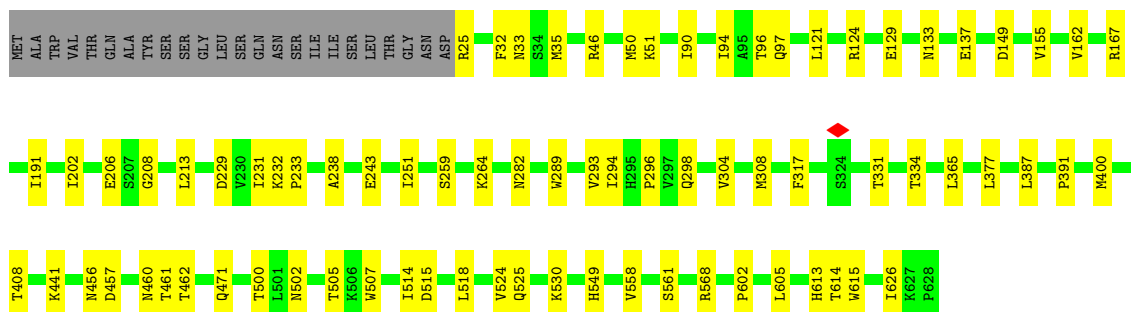
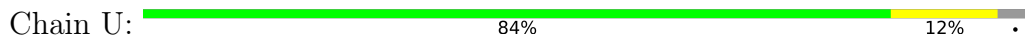
• Molecule 4: VP4



• Molecule 4: VP4



• Molecule 4: VP4



• Molecule 4: VP4

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293354	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.616	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.019	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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	0.26	0/6339	0.47	0/8607
1	B	0.26	0/7375	0.46	0/10006
2	C	0.27	0/2322	0.47	0/3165
2	D	0.26	0/2322	0.47	0/3165
2	E	0.27	0/2322	0.48	0/3165
2	F	0.27	0/2322	0.48	0/3165
2	G	0.27	0/2322	0.49	0/3165
2	H	0.26	0/2333	0.46	0/3179
2	I	0.26	0/2322	0.46	0/3165
2	J	0.26	0/2333	0.47	0/3179
2	K	0.29	0/2322	0.48	0/3165
2	L	0.27	0/2322	0.48	0/3165
2	M	0.26	0/2322	0.47	0/3165
2	N	0.27	0/2322	0.49	0/3165
2	O	0.29	0/2315	0.48	0/3155
3	P	0.26	0/2050	0.46	0/2772
3	Q	0.25	0/1909	0.46	0/2584
4	R	0.26	0/4806	0.44	0/6525
4	S	0.25	0/4954	0.44	0/6725
4	T	0.26	0/4911	0.45	0/6668
4	U	0.27	0/4825	0.46	0/6551
4	V	0.26	0/4953	0.45	0/6725
4	W	0.28	0/4879	0.46	0/6625
5	r	0.21	0/109	0.44	0/144
5	s	0.21	0/109	0.44	0/144
5	t	0.21	0/109	0.44	0/144
5	u	0.35	0/109	0.49	0/144
5	v	0.24	0/109	0.45	0/144
5	w	0.33	0/109	0.52	0/144
All	All	0.27	0/77856	0.46	0/105815

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	6204	0	6121	42	0
1	B	7224	0	7152	66	0
2	C	2277	0	2270	21	0
2	D	2277	0	2270	33	0
2	E	2277	0	2270	24	0
2	F	2277	0	2270	45	0
2	G	2277	0	2270	29	0
2	H	2288	0	2283	28	0
2	I	2277	0	2270	29	0
2	J	2288	0	2283	27	0
2	K	2277	0	2270	22	0
2	L	2277	0	2270	33	0
2	M	2277	0	2270	30	0
2	N	2277	0	2270	26	0
2	O	2270	0	2261	19	0
3	P	2014	0	2036	31	0
3	Q	1876	0	1892	18	0
4	R	4713	0	4656	45	0
4	S	4860	0	4797	45	0
4	T	4817	0	4758	65	0
4	U	4731	0	4676	57	0
4	V	4858	0	4796	65	0
4	W	4786	0	4725	71	0
5	r	110	0	123	0	0
5	s	110	0	123	0	0
5	t	110	0	123	0	0
5	u	110	0	123	0	0
5	v	110	0	123	0	0
5	w	110	0	123	0	0
All	All	76359	0	75874	810	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 5.

All (810) 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:268:TYR:CD1	2:D:277:VAL:HG21	1.66	1.30
2:O:268:TYR:CD1	2:O:277:VAL:HG11	1.68	1.27
3:P:145:TYR:CZ	3:P:172:PRO:HD2	1.71	1.24
2:C:268:TYR:CD1	2:C:277:VAL:HG11	1.75	1.20
2:H:268:TYR:CD1	2:H:277:VAL:HG21	1.79	1.16
2:G:268:TYR:CD1	2:G:277:VAL:HG21	1.84	1.13
2:L:268:TYR:CD1	2:L:277:VAL:HG21	1.84	1.13
2:N:268:TYR:CD2	2:N:277:VAL:HG21	1.87	1.10
3:P:145:TYR:CD1	3:P:172:PRO:HG2	1.87	1.09
2:I:268:TYR:CD1	2:I:277:VAL:HG21	1.89	1.07
4:T:517:HIS:HD2	4:T:519:LEU:CD1	1.67	1.07
4:T:517:HIS:CD2	4:T:519:LEU:CD1	2.42	1.02
4:W:188:LYS:HG2	4:W:191:ILE:HD11	1.40	1.02
2:J:168:ILE:HG21	2:J:268:TYR:HD1	1.26	1.00
1:B:336:ILE:HD13	1:B:370:ARG:HE	1.26	0.99
2:D:268:TYR:HD1	2:D:277:VAL:HG21	1.25	0.96
3:P:145:TYR:CE2	3:P:172:PRO:HD2	2.02	0.95
4:T:517:HIS:CD2	4:T:519:LEU:HD11	2.03	0.94
2:C:268:TYR:HD1	2:C:277:VAL:HG11	1.19	0.93
4:V:497:VAL:CG2	4:V:565:LYS:HB2	1.98	0.93
2:J:168:ILE:HG21	2:J:268:TYR:CD1	2.05	0.92
1:B:336:ILE:CD1	1:B:370:ARG:HE	1.81	0.92
2:O:268:TYR:HD1	2:O:277:VAL:HG11	1.06	0.91
4:V:461:THR:HG23	4:V:463:LEU:HG	1.51	0.91
1:A:903:ARG:NH2	1:A:904:TYR:HE1	1.70	0.89
1:A:345:ILE:HG22	1:B:144:GLU:OE1	1.73	0.88
4:R:459:ARG:HA	4:R:568:ARG:NH2	1.89	0.88
4:V:532:LEU:HD11	4:V:534:LEU:HD21	1.58	0.85
2:I:170:GLU:OE2	2:I:224:ARG:HG2	1.77	0.85
3:P:145:TYR:CE1	3:P:172:PRO:HD2	2.12	0.85
2:D:117:TYR:OH	2:D:278:SER:HB2	1.78	0.84
4:V:459:ARG:HA	4:V:568:ARG:HH22	1.42	0.83
4:V:532:LEU:HD21	4:V:534:LEU:HD11	1.60	0.83
2:E:168:ILE:HG21	2:E:268:TYR:CD2	2.15	0.81
4:R:458:LEU:O	4:R:461:THR:HG22	1.80	0.81
4:U:289:TRP:HB3	4:U:308:MET:SD	2.20	0.81
4:S:51:LYS:HD2	4:S:387:LEU:HD23	1.63	0.81
4:T:517:HIS:CD2	4:T:519:LEU:HD13	2.15	0.80
3:P:145:TYR:CZ	3:P:172:PRO:CD	2.59	0.80
4:W:483:ILE:HD11	4:W:554:LEU:HB2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:268:TYR:CD1	2:D:277:VAL:CG2	2.61	0.78
4:U:289:TRP:CB	4:U:308:MET:SD	2.73	0.77
1:B:370:ARG:NH1	1:B:372:LEU:HD21	2.00	0.77
2:H:168:ILE:HG12	2:H:268:TYR:CD2	2.19	0.77
3:P:145:TYR:CE1	3:P:172:PRO:CD	2.67	0.77
2:O:268:TYR:CD1	2:O:277:VAL:CG1	2.62	0.76
4:T:236:VAL:HG13	4:T:237:VAL:HG13	1.68	0.75
4:U:51:LYS:HD3	4:U:387:LEU:HD11	1.68	0.75
2:L:136:ARG:HE	2:L:155:GLY:HA2	1.50	0.75
4:S:51:LYS:CD	4:S:387:LEU:HD23	2.16	0.74
4:U:51:LYS:HD3	4:U:387:LEU:CD1	2.18	0.74
2:M:168:ILE:HG21	2:M:268:TYR:CD2	2.22	0.74
2:O:268:TYR:HD1	2:O:277:VAL:CG1	1.95	0.73
2:J:102:GLU:OE2	2:J:105:ARG:NH2	2.21	0.73
4:T:171:ASP:OD2	4:T:175:VAL:HG23	1.89	0.72
2:H:268:TYR:CD1	2:H:277:VAL:CG2	2.67	0.72
4:W:483:ILE:HD11	4:W:554:LEU:CB	2.18	0.72
4:R:44:ASN:HD22	4:R:47:GLU:HG3	1.53	0.72
2:E:268:TYR:CD1	2:E:277:VAL:HG11	2.25	0.71
2:K:130:GLU:HG2	2:K:164:ASN:HB3	1.71	0.71
1:A:345:ILE:CG2	1:B:144:GLU:OE1	2.38	0.71
2:J:168:ILE:CG2	2:J:268:TYR:CD1	2.73	0.71
2:C:168:ILE:HG21	2:C:268:TYR:CD2	2.26	0.70
2:F:244:MET:CE	2:G:173:ILE:HD11	2.22	0.70
1:B:880:ASP:OD1	1:B:881:THR:N	2.25	0.70
4:U:294:ILE:HG22	4:U:296:PRO:HD3	1.73	0.69
2:F:168:ILE:HG12	2:F:268:TYR:CE2	2.25	0.69
4:V:82:LEU:HB3	4:V:84:LEU:HD21	1.73	0.69
2:K:168:ILE:HD13	2:K:268:TYR:HD2	1.57	0.69
4:V:461:THR:CG2	4:V:463:LEU:HG	2.23	0.69
4:W:68:GLU:OE1	4:W:102:ARG:NH2	2.25	0.69
4:T:270:ASP:OD1	4:T:271:VAL:N	2.26	0.69
2:F:139:VAL:HG22	2:F:151:MET:HG2	1.75	0.68
4:V:46:ARG:HG2	4:W:39:ARG:HH21	1.59	0.68
2:I:168:ILE:HG12	2:I:268:TYR:CD2	2.28	0.68
3:P:145:TYR:CD1	3:P:172:PRO:CG	2.73	0.68
1:A:702:LEU:HD12	1:B:568:LYS:HE2	1.75	0.68
1:B:370:ARG:HH12	1:B:372:LEU:CG	2.06	0.67
4:V:458:LEU:O	4:V:461:THR:HG22	1.94	0.67
4:R:410:GLN:HE21	4:R:582:MET:HB3	1.60	0.67
2:C:268:TYR:CD1	2:C:277:VAL:CG1	2.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:468:GLU:OE1	4:R:468:GLU:N	2.28	0.67
2:D:185:LEU:HD12	2:D:206:ILE:HD11	1.77	0.67
2:D:268:TYR:HD1	2:D:277:VAL:CG2	2.04	0.67
1:A:576:GLU:OE2	1:A:607:ARG:NH1	2.29	0.66
4:S:50:MET:SD	4:T:50:MET:SD	2.93	0.66
1:B:576:GLU:HG2	1:B:607:ARG:NH1	2.10	0.66
2:M:33:GLU:OE2	2:M:288:GLN:NE2	2.29	0.66
2:M:168:ILE:HG12	2:M:268:TYR:CD2	2.30	0.66
2:O:168:ILE:HG21	2:O:268:TYR:CD2	2.31	0.65
1:A:754:ASP:OD2	1:B:615:ARG:NH1	2.29	0.65
2:K:168:ILE:HD13	2:K:268:TYR:CD2	2.31	0.65
4:W:258:HIS:CD2	4:W:356:GLN:HE22	2.14	0.65
1:B:370:ARG:HH12	1:B:372:LEU:HD11	1.62	0.65
2:G:268:TYR:HD1	2:G:277:VAL:HG21	1.55	0.65
4:S:22:GLY:O	4:S:25:ARG:NH1	2.29	0.65
4:V:294:ILE:HG22	4:V:296:PRO:HD3	1.79	0.65
2:N:139:VAL:HG22	2:N:151:MET:HG2	1.78	0.64
1:A:791:GLU:OE2	1:A:829:ARG:NH2	2.27	0.64
1:B:576:GLU:HG2	1:B:607:ARG:HH12	1.61	0.64
4:U:32:PHE:HA	4:U:35:MET:HE2	1.78	0.64
3:Q:66:ASN:ND2	3:Q:68:ASN:HB2	2.13	0.64
4:U:46:ARG:HH22	4:V:50:MET:HE3	1.63	0.64
4:W:188:LYS:CG	4:W:191:ILE:HD11	2.23	0.64
2:L:179:PRO:HD3	2:L:194:PHE:CE1	2.32	0.64
4:W:520:ILE:HD11	4:W:531:ILE:HG22	1.80	0.64
4:T:489:TYR:HA	4:T:536:VAL:HG23	1.79	0.63
4:W:489:TYR:HA	4:W:536:VAL:HG23	1.79	0.63
1:B:542:ASP:OD1	1:B:556:ARG:HD3	1.99	0.63
2:J:168:ILE:HG23	2:J:268:TYR:CE1	2.34	0.63
4:S:51:LYS:HD3	4:S:387:LEU:CD2	2.29	0.63
2:G:241:GLN:HB2	2:H:122:ILE:HD13	1.80	0.63
4:W:454:VAL:HA	4:W:573:ILE:HD11	1.80	0.63
4:V:497:VAL:HG23	4:V:565:LYS:HB2	1.80	0.63
2:H:268:TYR:CE1	2:H:277:VAL:HG21	2.32	0.63
2:M:168:ILE:HG12	2:M:268:TYR:HD2	1.63	0.63
2:L:134:PRO:HG2	2:L:159:ALA:HB1	1.79	0.62
2:G:268:TYR:CD1	2:G:277:VAL:CG2	2.73	0.62
2:N:268:TYR:CD2	2:N:277:VAL:CG2	2.74	0.62
4:S:51:LYS:CD	4:S:387:LEU:CD2	2.77	0.62
2:E:168:ILE:HG21	2:E:268:TYR:HD2	1.65	0.62
2:F:168:ILE:HG21	2:F:268:TYR:CD2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:136:ARG:HE	2:L:155:GLY:CA	2.12	0.62
2:L:268:TYR:CD1	2:L:277:VAL:CG2	2.74	0.62
2:C:11:ASP:OD2	2:D:194:PHE:HD2	1.82	0.61
2:O:125:SER:HB2	2:O:265:ILE:HG13	1.82	0.61
2:F:244:MET:HE2	2:G:173:ILE:HD11	1.82	0.61
2:L:168:ILE:HD12	2:L:268:TYR:CE2	2.35	0.61
2:I:169:ALA:HA	2:I:223:THR:HG22	1.83	0.61
4:U:289:TRP:HB2	4:U:308:MET:SD	2.41	0.61
1:A:901:LYS:NZ	1:A:905:GLU:OE2	2.31	0.61
1:B:370:ARG:NH1	1:B:372:LEU:CD2	2.63	0.61
4:R:459:ARG:HA	4:R:568:ARG:HH21	1.65	0.61
2:L:123:PHE:HB3	2:L:261:ASP:OD1	2.01	0.61
2:H:65:ASP:OD1	2:H:66:ASN:N	2.34	0.61
2:J:145:ASP:OD1	2:J:146:ARG:N	2.34	0.61
2:M:258:SER:OG	2:N:175:LYS:NZ	2.33	0.61
4:R:454:VAL:HA	4:R:573:ILE:HD11	1.82	0.61
4:V:303:LEU:HD11	4:V:359:LEU:HD13	1.83	0.60
4:R:41:VAL:HG11	4:R:387:LEU:HD11	1.82	0.60
2:F:13:PRO:HB2	2:F:276:ARG:NH1	2.17	0.60
2:I:197:LYS:NZ	2:K:250:ASP:OD1	2.34	0.60
4:S:46:ARG:CZ	4:S:50:MET:HE2	2.31	0.60
2:L:175:LYS:NZ	2:N:262:GLU:OE2	2.32	0.60
1:B:542:ASP:OD1	1:B:556:ARG:CD	2.49	0.60
4:W:517:HIS:CD2	4:W:519:LEU:HD23	2.37	0.60
2:O:149:VAL:CG2	2:O:217:ILE:HB	2.32	0.60
4:V:532:LEU:HD11	4:V:534:LEU:CD2	2.30	0.60
1:B:370:ARG:HH12	1:B:372:LEU:CD1	2.15	0.60
4:T:461:THR:HG23	4:T:463:LEU:HG	1.82	0.59
2:I:134:PRO:HG2	2:I:159:ALA:HB1	1.83	0.59
4:U:457:ASP:O	4:U:461:THR:HG23	2.02	0.59
4:S:51:LYS:HD3	4:S:387:LEU:HD21	1.84	0.59
1:A:720:ILE:HG13	1:A:750:ARG:HG3	1.84	0.59
1:A:903:ARG:HH22	1:A:904:TYR:HE1	1.50	0.59
2:C:272:ASP:OD1	2:C:272:ASP:N	2.36	0.59
3:P:31:THR:OG1	3:P:61:ARG:NH1	2.35	0.59
4:U:602:PRO:HA	4:U:605:LEU:HD12	1.83	0.59
2:N:268:TYR:CE2	2:N:277:VAL:HG21	2.36	0.59
4:T:365:LEU:HD22	4:T:377:LEU:HD23	1.84	0.59
2:E:268:TYR:CE1	2:E:277:VAL:HG21	2.37	0.58
2:F:125:SER:HB2	2:F:265:ILE:HG13	1.84	0.58
4:U:514:ILE:H	4:U:549:HIS:CE1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:252:TYR:O	4:V:256:ARG:HG2	2.02	0.58
2:F:13:PRO:HB2	2:F:276:ARG:HH12	1.68	0.58
2:M:134:PRO:HG2	2:M:159:ALA:HB1	1.85	0.58
2:M:168:ILE:HG23	2:M:268:TYR:CE2	2.38	0.58
3:Q:8:SER:OG	3:Q:11:GLU:OE1	2.21	0.58
4:T:454:VAL:HA	4:T:573:ILE:HD11	1.84	0.58
2:C:245:ASN:ND2	2:D:170:GLU:OE1	2.35	0.58
2:J:139:VAL:HG22	2:J:151:MET:HG2	1.83	0.58
4:R:365:LEU:HD22	4:R:377:LEU:HD23	1.85	0.58
1:B:370:ARG:NH1	1:B:372:LEU:CG	2.67	0.58
1:A:355:PRO:HB2	1:A:357:ARG:HH12	1.69	0.58
1:B:791:GLU:OE2	1:B:829:ARG:NH2	2.36	0.58
2:H:238:SER:HB3	2:H:291:ASP:OD2	2.04	0.58
3:P:145:TYR:CG	3:P:172:PRO:HG2	2.38	0.58
4:R:143:THR:OG1	4:R:146:GLU:OE1	2.21	0.58
4:R:505:THR:HG22	4:R:525:GLN:HE21	1.69	0.58
2:G:53:VAL:HG13	2:G:54:PRO:HD3	1.85	0.58
2:M:13:PRO:HG2	2:M:270:ALA:HB2	1.85	0.58
2:I:168:ILE:HG12	2:I:268:TYR:HD2	1.69	0.57
2:K:61:LYS:O	2:K:109:LYS:NZ	2.36	0.57
2:I:268:TYR:HD1	2:I:277:VAL:HG21	1.65	0.57
2:M:130:GLU:HG2	2:M:164:ASN:HB3	1.86	0.57
2:I:125:SER:HB2	2:I:265:ILE:HG13	1.86	0.57
2:L:168:ILE:HD12	2:L:268:TYR:HE2	1.69	0.57
4:S:162:VAL:O	4:S:167:ARG:NH1	2.37	0.57
4:R:44:ASN:ND2	4:R:47:GLU:HG3	2.20	0.57
2:H:202:ASP:OD1	2:H:203:GLY:N	2.38	0.57
4:R:139:GLN:HB3	4:R:142:ILE:HD11	1.87	0.57
4:S:500:THR:HG22	4:S:502:ASN:H	1.70	0.57
2:C:268:TYR:HD1	2:C:277:VAL:CG1	2.07	0.56
4:W:240:THR:HG23	4:W:243:GLU:H	1.70	0.56
1:A:903:ARG:NH2	1:A:904:TYR:CE1	2.62	0.56
2:I:185:LEU:HD22	2:I:204:PRO:HG2	1.87	0.56
2:J:13:PRO:HG2	2:J:270:ALA:HB2	1.87	0.56
4:R:322:ASN:OD1	4:R:322:ASN:O	2.23	0.56
4:S:129:GLU:O	4:S:133:ASN:ND2	2.35	0.56
4:T:112:HIS:CE1	4:T:482:LEU:H	2.23	0.56
4:T:268:VAL:HG12	4:T:431:LYS:HB2	1.86	0.56
4:V:497:VAL:HG21	4:V:565:LYS:HE3	1.86	0.56
4:S:307:LEU:HD21	4:S:312:LEU:HD12	1.87	0.56
4:S:456:ASN:H	4:S:461:THR:HG22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:466:LYS:HE2	4:V:563:SER:HB2	1.88	0.56
1:B:810:ARG:HB2	1:B:895:GLU:HB2	1.87	0.56
4:W:115:GLU:OE1	4:W:482:LEU:HD23	2.06	0.56
4:U:46:ARG:NH2	4:V:50:MET:CE	2.69	0.56
2:I:188:PRO:HB2	4:U:334:THR:HB	1.88	0.56
4:S:278:ILE:HD12	4:S:291:LEU:HD23	1.88	0.56
4:T:188:LYS:HE2	4:T:190:GLY:O	2.06	0.56
4:V:135:ILE:HD13	4:V:150:LEU:HB3	1.87	0.56
4:V:204:VAL:O	4:V:207:SER:OG	2.23	0.56
4:W:496:VAL:HG22	4:W:566:VAL:HG22	1.87	0.56
2:M:168:ILE:CG2	2:M:268:TYR:CE2	2.89	0.56
2:K:65:ASP:OD1	2:K:66:ASN:N	2.38	0.55
4:S:259:SER:HA	4:S:298:GLN:HG2	1.88	0.55
4:W:115:GLU:OE1	4:W:482:LEU:CD2	2.54	0.55
1:B:197:GLN:HG3	1:B:204:ALA:HB2	1.87	0.55
4:W:51:LYS:HE2	4:W:386:ASN:CG	2.26	0.55
4:W:602:PRO:HA	4:W:605:LEU:HD12	1.87	0.55
2:J:168:ILE:HG23	2:J:268:TYR:HE1	1.70	0.55
2:O:23:GLU:OE1	2:O:26:ARG:NH1	2.40	0.55
1:A:793:MET:HE3	1:A:819:PRO:HD2	1.88	0.55
2:J:235:LEU:HB3	2:J:288:GLN:HG3	1.88	0.55
3:P:33:PRO:O	3:P:53:THR:OG1	2.21	0.55
1:A:725:ALA:O	1:B:156:LYS:NZ	2.31	0.55
2:G:168:ILE:HG21	2:G:268:TYR:CD2	2.42	0.55
4:T:171:ASP:OD2	4:T:175:VAL:CG2	2.54	0.55
4:V:82:LEU:HB3	4:V:84:LEU:CD2	2.37	0.55
4:U:505:THR:HG22	4:U:525:GLN:HE21	1.72	0.55
1:B:204:ALA:HB3	1:B:925:LEU:HD22	1.89	0.55
1:B:792:ILE:HG22	1:B:916:ILE:HG22	1.89	0.55
2:L:268:TYR:HD1	2:L:277:VAL:HG21	1.65	0.55
4:V:489:TYR:CE1	4:V:576:PRO:HB2	2.42	0.55
2:E:93:ASN:HB2	2:E:251:ILE:HD11	1.89	0.54
2:I:243:ALA:HB1	2:I:248:LEU:HD11	1.89	0.54
2:L:4:ARG:HG2	2:L:4:ARG:HH11	1.72	0.54
4:R:42:ILE:HD12	4:R:382:GLU:HG2	1.89	0.54
1:A:374:GLN:NE2	1:A:551:PRO:HD3	2.22	0.54
2:E:168:ILE:CG2	2:E:268:TYR:CE2	2.90	0.54
1:B:370:ARG:NH1	1:B:372:LEU:HG	2.22	0.54
2:D:241:GLN:HB2	2:E:122:ILE:HD13	1.89	0.54
2:H:139:VAL:HG22	2:H:151:MET:HG2	1.90	0.54
4:T:51:LYS:HE2	4:T:386:ASN:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASN:OD1	1:A:200:ASN:N	2.41	0.54
2:E:168:ILE:CG2	2:E:268:TYR:CD2	2.89	0.54
4:S:492:ILE:HD11	4:S:568:ARG:HG3	1.90	0.54
4:U:514:ILE:H	4:U:549:HIS:HE1	1.56	0.54
1:A:805:ASP:OD1	1:A:805:ASP:N	2.34	0.54
2:H:136:ARG:HH11	2:H:155:GLY:HA3	1.73	0.54
3:P:145:TYR:CE1	3:P:172:PRO:HG2	2.38	0.54
4:V:500:THR:HG22	4:V:561:SER:HA	1.89	0.54
4:U:507:TRP:HE1	4:U:524:VAL:H	1.56	0.54
4:V:497:VAL:HG22	4:V:565:LYS:HB2	1.88	0.54
3:P:71:ILE:HG13	3:P:114:LEU:HD21	1.91	0.53
4:T:129:GLU:O	4:T:133:ASN:ND2	2.31	0.53
4:T:193:ILE:HG12	4:T:205:LYS:HD3	1.89	0.53
4:U:457:ASP:HB2	4:U:460:ASN:HB2	1.90	0.53
4:U:456:ASN:H	4:U:461:THR:HG22	1.73	0.53
1:B:336:ILE:CD1	1:B:370:ARG:NE	2.64	0.53
4:S:365:LEU:HD22	4:S:377:LEU:HD23	1.90	0.53
1:B:945:ILE:HG22	1:B:947:ASP:H	1.73	0.53
2:J:134:PRO:HG2	2:J:159:ALA:HB1	1.89	0.53
4:T:112:HIS:HE1	4:T:482:LEU:H	1.56	0.53
4:W:259:SER:HA	4:W:298:GLN:HG2	1.89	0.53
1:B:542:ASP:OD1	1:B:556:ARG:CG	2.56	0.53
3:Q:15:HIS:O	3:Q:19:THR:OG1	2.26	0.53
4:T:251:ILE:HG13	4:T:408:THR:HG21	1.90	0.53
2:F:244:MET:HE1	2:G:173:ILE:HD11	1.88	0.53
4:V:510:GLU:HB2	4:V:519:LEU:HD12	1.90	0.53
1:B:492:GLU:OE1	1:B:492:GLU:N	2.42	0.53
4:R:139:GLN:O	4:R:147:ARG:NH1	2.36	0.53
4:W:258:HIS:NE2	4:W:356:GLN:NE2	2.55	0.53
2:C:168:ILE:HD12	2:C:268:TYR:HE2	1.73	0.53
2:I:11:ASP:OD2	2:J:194:PHE:HD2	1.92	0.52
2:G:196:TYR:HB3	2:G:198:LEU:HD21	1.90	0.52
4:U:317:PHE:HA	4:U:331:THR:HA	1.90	0.52
1:B:880:ASP:OD1	1:B:881:THR:HG23	2.09	0.52
2:G:87:ARG:HG2	2:G:248:LEU:HB2	1.91	0.52
1:B:727:LYS:HE3	1:B:730:ILE:HD11	1.91	0.52
4:W:356:GLN:HG3	4:W:416:TRP:CZ2	2.45	0.52
2:C:168:ILE:HG23	2:C:268:TYR:CE2	2.44	0.52
2:H:125:SER:HB2	2:H:265:ILE:HG13	1.91	0.52
2:H:182:LEU:HD12	2:H:207:VAL:HG22	1.90	0.52
2:J:125:SER:HB2	2:J:265:ILE:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:THR:HG21	1:A:598:THR:HA	1.91	0.52
2:F:64:ASP:OD1	2:F:109:LYS:NZ	2.34	0.52
2:K:53:VAL:HG13	2:K:54:PRO:HD3	1.92	0.52
4:S:303:LEU:HD11	4:S:359:LEU:HD13	1.92	0.52
1:A:368:VAL:HG11	1:A:948:PRO:HB3	1.90	0.52
1:B:542:ASP:OD1	1:B:556:ARG:HG2	2.10	0.52
2:D:168:ILE:HG12	2:D:268:TYR:CD2	2.45	0.52
2:E:268:TYR:CD1	2:E:277:VAL:CG1	2.93	0.52
4:U:614:THR:HG22	4:U:615:TRP:N	2.25	0.52
4:W:51:LYS:HE2	4:W:386:ASN:ND2	2.25	0.52
2:F:268:TYR:CD1	2:F:277:VAL:HG21	2.44	0.52
2:K:130:GLU:HG2	2:K:164:ASN:CB	2.39	0.52
2:F:168:ILE:HG12	2:F:268:TYR:CD2	2.44	0.51
2:H:268:TYR:HD1	2:H:277:VAL:HG21	1.60	0.51
2:L:50:ASN:HB2	2:M:111:THR:HG21	1.91	0.51
2:M:250:ASP:OD1	2:N:197:LYS:NZ	2.39	0.51
4:T:17:ILE:HD13	4:T:368:ALA:HB2	1.91	0.51
4:T:31:THR:O	4:T:35:MET:HG3	2.10	0.51
2:J:150:THR:HG23	2:J:216:VAL:HG22	1.91	0.51
2:M:168:ILE:CG2	2:M:268:TYR:CD2	2.92	0.51
1:A:841:ILE:O	1:A:845:ILE:HG12	2.10	0.51
2:E:182:LEU:HD12	2:E:207:VAL:HG22	1.91	0.51
2:K:152:LEU:HD13	2:K:214:PRO:HB3	1.91	0.51
4:S:457:ASP:O	4:S:461:THR:HG23	2.10	0.51
4:S:493:ASP:HB3	4:S:530:LYS:NZ	2.25	0.51
4:T:51:LYS:HD2	4:T:386:ASN:O	2.11	0.51
2:I:169:ALA:HB3	2:I:200:PRO:HG2	1.92	0.51
2:J:168:ILE:CG2	2:J:268:TYR:CE1	2.93	0.51
3:P:93:LEU:HD11	3:P:109:LEU:HD13	1.93	0.51
4:U:191:ILE:HD12	4:U:208:GLY:HA3	1.93	0.51
2:F:53:VAL:HG12	2:F:54:PRO:HD3	1.93	0.51
2:M:168:ILE:HD13	2:M:269:HIS:CD2	2.45	0.51
4:R:459:ARG:HA	4:R:568:ARG:HH22	1.75	0.51
4:R:498:VAL:HG22	4:R:564:VAL:HG22	1.92	0.51
4:T:90:ILE:HD12	4:T:462:THR:HB	1.90	0.51
4:T:281:VAL:HG13	4:T:344:GLY:HA2	1.93	0.51
2:M:131:VAL:HG11	2:M:139:VAL:HG11	1.92	0.51
2:D:116:MET:HE3	2:D:228:PRO:HG3	1.91	0.51
2:F:168:ILE:HG12	2:F:268:TYR:HE2	1.71	0.51
2:G:13:PRO:HG2	2:G:270:ALA:HB2	1.93	0.51
4:R:317:PHE:HA	4:R:331:THR:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:238:ALA:HB1	4:U:243:GLU:HB3	1.92	0.51
2:K:275:ASN:HD21	3:Q:50:PRO:HB2	1.75	0.51
4:U:121:LEU:HD21	4:U:231:ILE:HD12	1.93	0.51
4:W:63:ARG:NH2	4:W:176:VAL:O	2.36	0.51
1:A:695:VAL:HG23	1:A:753:LEU:HD22	1.93	0.50
4:T:303:LEU:HD11	4:T:359:LEU:HD13	1.93	0.50
2:M:132:LEU:HB2	2:M:162:THR:HB	1.93	0.50
3:Q:10:LYS:HG3	3:Q:11:GLU:OE1	2.12	0.50
2:I:11:ASP:OD2	2:J:194:PHE:CD2	2.64	0.50
4:R:135:ILE:HD13	4:R:150:LEU:HB3	1.93	0.50
4:U:515:ASP:OD1	4:U:515:ASP:N	2.44	0.50
4:V:12:LEU:HD11	4:V:406:LEU:HD13	1.93	0.50
2:J:45:GLU:O	2:J:49:SER:OG	2.28	0.50
2:E:130:GLU:HG2	2:E:164:ASN:HB3	1.92	0.50
4:V:616:ASP:OD1	4:V:616:ASP:N	2.41	0.50
4:U:558:VAL:HG13	4:U:561:SER:HB2	1.92	0.50
1:A:784:SER:HB3	1:A:919:PRO:HA	1.94	0.50
4:U:50:MET:SD	4:W:50:MET:SD	3.10	0.50
2:G:147:ALA:HB3	2:G:219:ALA:HB3	1.92	0.50
4:S:517:HIS:ND1	4:S:615:TRP:CZ3	2.80	0.50
2:F:145:ASP:OD1	2:F:145:ASP:N	2.45	0.50
2:K:13:PRO:HG2	2:K:270:ALA:HB2	1.94	0.50
3:P:145:TYR:CE1	3:P:172:PRO:CG	2.93	0.50
2:F:94:ALA:HB2	2:F:251:ILE:HD13	1.94	0.49
2:F:182:LEU:HD12	2:F:207:VAL:HG22	1.92	0.49
4:S:616:ASP:OD1	4:S:616:ASP:N	2.43	0.49
4:T:422:GLU:OE2	4:T:425:LYS:NZ	2.45	0.49
2:D:131:VAL:HG11	2:D:139:VAL:HG11	1.94	0.49
4:S:602:PRO:HA	4:S:605:LEU:HD12	1.93	0.49
1:A:230:VAL:HG11	1:B:155:ALA:HB2	1.93	0.49
1:A:395:LYS:NZ	1:A:680:GLU:OE1	2.46	0.49
1:B:945:ILE:HD12	1:B:945:ILE:H	1.78	0.49
4:T:193:ILE:HD12	4:T:201:ALA:HB1	1.95	0.49
2:D:243:ALA:HB1	2:D:248:LEU:HD11	1.93	0.49
2:E:31:VAL:HG22	2:E:110:ALA:HB3	1.94	0.49
2:O:134:PRO:HG2	2:O:159:ALA:HB1	1.94	0.49
4:T:252:TYR:O	4:T:256:ARG:HG2	2.12	0.49
4:W:296:PRO:HG2	4:W:355:ALA:HB2	1.95	0.49
2:D:182:LEU:HD21	2:D:198:LEU:HD21	1.95	0.49
2:F:168:ILE:CG2	2:F:268:TYR:CE2	2.96	0.49
4:R:489:TYR:CE1	4:R:576:PRO:HB2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:268:VAL:HG12	4:W:431:LYS:HB2	1.94	0.49
2:I:182:LEU:HD12	2:I:207:VAL:HG22	1.94	0.49
4:U:25:ARG:HG3	4:W:308:MET:HB3	1.95	0.49
4:W:216:VAL:HG22	4:W:272:ILE:HG23	1.95	0.49
1:A:705:THR:HG1	1:A:708:SER:HG	1.61	0.49
1:A:792:ILE:HG22	1:A:916:ILE:HG22	1.94	0.49
2:D:125:SER:HB2	2:D:265:ILE:HG13	1.94	0.49
4:S:493:ASP:HB3	4:S:530:LYS:HZ2	1.77	0.49
4:U:46:ARG:HH22	4:V:50:MET:CE	2.26	0.49
4:R:613:HIS:CG	4:R:626:ILE:HD11	2.48	0.49
4:T:536:VAL:HG12	4:T:542:THR:HB	1.95	0.49
4:V:457:ASP:OD1	4:V:458:LEU:N	2.45	0.49
2:L:4:ARG:HG2	2:L:4:ARG:NH1	2.28	0.49
4:S:276:TYR:OH	4:S:327:GLU:OE2	2.29	0.49
1:B:796:PRO:HD2	1:B:799:ILE:HD12	1.95	0.48
2:J:290:TYR:O	2:J:294:ARG:HG2	2.13	0.48
4:T:15:ASN:HB3	4:T:371:MET:SD	2.53	0.48
2:F:136:ARG:HG3	2:F:136:ARG:HH11	1.78	0.48
2:H:290:TYR:O	2:H:294:ARG:HG2	2.14	0.48
3:Q:15:HIS:HA	3:Q:18:LYS:HE2	1.93	0.48
3:Q:63:GLY:HA2	4:W:286:TYR:OH	2.13	0.48
4:S:440:LYS:NZ	4:S:440:LYS:HB3	2.28	0.48
4:U:96:THR:HG23	4:U:213:LEU:HD22	1.95	0.48
4:U:251:ILE:HG12	4:U:408:THR:HG21	1.95	0.48
4:V:514:ILE:HG13	4:V:549:HIS:CD2	2.49	0.48
4:W:547:ARG:HB3	4:W:549:HIS:HE1	1.78	0.48
4:U:94:ILE:HB	4:U:97:GLN:HG3	1.95	0.48
2:E:46:SER:HB2	2:F:70:LEU:HD11	1.94	0.48
2:M:125:SER:HB2	2:M:265:ILE:HG13	1.95	0.48
2:C:152:LEU:HD13	2:C:214:PRO:HG3	1.95	0.48
2:D:62:PHE:CE2	2:D:293:MET:SD	3.07	0.48
2:G:123:PHE:HB3	2:G:261:ASP:OD1	2.13	0.48
2:I:136:ARG:HE	2:I:155:GLY:HA2	1.79	0.48
2:L:125:SER:HB2	2:L:265:ILE:HG13	1.94	0.48
2:O:44:ARG:HG3	2:O:44:ARG:HH11	1.79	0.48
3:P:24:ALA:O	3:P:83:GLY:HA3	2.13	0.48
2:L:183:ALA:HB2	2:L:190:PRO:HD3	1.95	0.48
4:R:496:VAL:HG22	4:R:566:VAL:HG22	1.94	0.48
4:S:232:LYS:HB2	4:S:233:PRO:HD3	1.95	0.48
1:B:576:GLU:CG	1:B:607:ARG:HH12	2.25	0.48
2:C:145:ASP:OD1	2:C:145:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:62:PHE:HE2	2:G:293:MET:SD	2.36	0.48
2:I:123:PHE:HB3	2:I:261:ASP:OD1	2.14	0.48
2:L:116:MET:HA	2:L:228:PRO:HG3	1.96	0.48
1:B:793:MET:SD	1:B:795:MET:SD	3.11	0.48
2:D:68:ARG:HB2	2:D:71:ARG:HG3	1.96	0.48
2:E:59:TYR:CD1	2:E:67:PRO:HG3	2.49	0.48
2:M:145:ASP:OD1	2:M:145:ASP:N	2.46	0.48
4:S:122:ILE:HG23	4:S:245:ILE:HD13	1.95	0.48
1:B:795:MET:HG2	1:B:848:GLY:HA3	1.96	0.48
2:D:56:VAL:HA	2:D:67:PRO:HG2	1.95	0.48
2:D:89:TYR:HB2	2:D:283:LEU:HD13	1.94	0.48
2:D:168:ILE:HG21	2:D:268:TYR:CD2	2.49	0.48
2:F:123:PHE:HE2	2:F:225:ILE:HB	1.77	0.48
2:L:272:ASP:OD1	2:L:272:ASP:N	2.32	0.48
2:N:189:MET:HG3	2:N:190:PRO:HD2	1.96	0.48
1:B:330:GLN:HB3	1:B:767:PRO:HB3	1.96	0.47
2:F:13:PRO:HG2	2:F:270:ALA:HB2	1.96	0.47
2:F:134:PRO:HG2	2:F:159:ALA:HB1	1.96	0.47
2:N:134:PRO:HG2	2:N:159:ALA:HB1	1.95	0.47
4:R:46:ARG:HG2	4:R:46:ARG:HH11	1.79	0.47
4:T:392:ASP:OD1	4:T:392:ASP:O	2.32	0.47
4:U:613:HIS:HD2	4:U:626:ILE:HG21	1.77	0.47
4:T:614:THR:HG22	4:T:615:TRP:N	2.29	0.47
1:A:342:ILE:O	1:A:346:THR:HG23	2.13	0.47
2:D:182:LEU:HD12	2:D:207:VAL:HG22	1.95	0.47
2:L:268:TYR:CE1	2:L:277:VAL:HG21	2.44	0.47
2:M:150:THR:HG23	2:M:216:VAL:HG22	1.95	0.47
2:N:115:ASP:OD1	2:N:116:MET:N	2.48	0.47
4:S:410:GLN:HE21	4:S:584:ASN:H	1.62	0.47
4:V:502:ASN:HB2	4:V:505:THR:HG22	1.97	0.47
2:C:197:LYS:HD3	2:E:256:TYR:CD1	2.49	0.47
2:K:267:GLN:OE1	2:K:276:ARG:NH1	2.41	0.47
4:V:254:ARG:HD3	4:V:254:ARG:HA	1.61	0.47
2:C:35:LEU:HB3	2:C:62:PHE:HD1	1.79	0.47
2:D:268:TYR:CE1	2:D:277:VAL:HG21	2.36	0.47
2:N:125:SER:HB2	2:N:265:ILE:HG13	1.95	0.47
4:T:310:ASP:OD1	4:T:374:GLN:HG3	2.15	0.47
4:T:510:GLU:HG2	4:T:555:LYS:HB2	1.95	0.47
1:B:336:ILE:HD11	1:B:370:ARG:HE	1.73	0.47
2:C:168:ILE:CG2	2:C:268:TYR:CE2	2.98	0.47
2:D:123:PHE:HB3	2:D:261:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:601:SER:H	4:T:624:THR:CG2	2.27	0.47
4:U:94:ILE:HD12	4:U:206:GLU:OE1	2.15	0.47
1:A:451:VAL:HG12	1:A:455:MET:HE2	1.97	0.47
1:B:380:LEU:HD11	1:B:740:ILE:HD12	1.96	0.47
2:D:251:ILE:HG13	2:D:252:GLN:H	1.79	0.47
4:V:328:PHE:CE2	4:V:340:THR:HG21	2.50	0.47
4:W:230:VAL:HG12	4:W:248:LEU:HD23	1.97	0.47
1:B:351:LYS:HE2	2:J:50:ASN:HD21	1.80	0.47
2:F:241:GLN:HB2	2:G:122:ILE:HD13	1.97	0.47
2:I:245:ASN:ND2	2:J:170:GLU:OE1	2.48	0.47
2:L:83:THR:O	2:L:87:ARG:HG3	2.14	0.47
2:L:288:GLN:O	2:L:292:GLN:NE2	2.48	0.47
4:U:232:LYS:HB2	4:U:233:PRO:HD3	1.97	0.47
4:V:330:LYS:NZ	4:V:331:THR:H	2.13	0.47
4:W:232:LYS:HB2	4:W:233:PRO:HD3	1.97	0.47
4:W:307:LEU:HD23	4:W:378:ILE:HD11	1.97	0.47
2:F:73:LYS:HB3	2:F:297:LEU:HD22	1.96	0.47
2:I:184:ARG:NH1	2:I:202:ASP:O	2.47	0.47
4:V:482:LEU:HD21	4:V:551:ARG:HD3	1.97	0.47
4:V:598:LYS:HD3	4:V:623:TRP:CE2	2.51	0.47
4:W:115:GLU:OE2	4:W:551:ARG:NH1	2.48	0.47
1:A:801:VAL:HG12	1:A:822:ILE:HD12	1.97	0.46
2:C:101:VAL:HG21	3:P:180:HIS:O	2.14	0.46
2:G:81:ALA:O	2:G:85:VAL:HG23	2.16	0.46
2:H:131:VAL:HG11	2:H:139:VAL:HG11	1.97	0.46
3:P:8:SER:OG	3:P:11:GLU:HG3	2.15	0.46
4:R:66:LYS:HB3	4:R:66:LYS:HE2	1.60	0.46
2:H:168:ILE:HG12	2:H:268:TYR:HD2	1.76	0.46
4:R:124:ARG:NH2	4:R:127:GLU:OE2	2.46	0.46
4:R:268:VAL:HG23	4:R:270:ASP:H	1.79	0.46
4:V:508:TYR:CD1	4:V:602:PRO:HB3	2.50	0.46
1:A:663:ASP:OD1	1:A:664:ASP:N	2.48	0.46
2:E:136:ARG:NH1	2:E:155:GLY:HA3	2.31	0.46
2:M:144:SER:OG	2:M:262:GLU:HG2	2.15	0.46
2:F:123:PHE:HB3	2:F:261:ASP:OD1	2.16	0.46
2:I:161:ILE:HD11	2:I:209:LEU:HD22	1.98	0.46
4:T:232:LYS:HB2	4:T:233:PRO:HD3	1.98	0.46
2:E:139:VAL:HG22	2:E:151:MET:HG2	1.96	0.46
2:K:168:ILE:CD1	2:K:268:TYR:HD2	2.25	0.46
2:M:64:ASP:OD1	2:M:109:LYS:HE3	2.16	0.46
2:O:168:ILE:HG23	2:O:268:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:236:VAL:HG23	4:S:237:VAL:HG13	1.96	0.46
4:V:278:ILE:HD12	4:V:291:LEU:HD23	1.97	0.46
2:C:26:ARG:HD2	2:C:116:MET:HG3	1.98	0.46
2:G:62:PHE:CE2	2:G:293:MET:SD	3.08	0.46
4:R:440:LYS:NZ	4:R:440:LYS:HB3	2.31	0.46
4:V:93:ASP:OD1	4:V:94:ILE:N	2.48	0.46
2:C:11:ASP:OD1	2:C:12:ASN:HB2	2.16	0.46
2:C:168:ILE:CG2	2:C:268:TYR:CD2	2.98	0.46
2:L:152:LEU:HD12	2:L:214:PRO:HG3	1.98	0.46
4:U:530:LYS:HB2	4:U:530:LYS:NZ	2.30	0.46
1:A:386:LYS:HE3	1:A:386:LYS:HB3	1.73	0.46
2:H:134:PRO:HG2	2:H:159:ALA:HB1	1.98	0.46
4:U:441:LYS:HE2	4:U:441:LYS:HB2	1.67	0.46
4:V:112:HIS:CE1	4:V:482:LEU:H	2.33	0.46
4:W:328:PHE:CZ	4:W:340:THR:HG21	2.51	0.46
2:E:125:SER:HB2	2:E:265:ILE:HG13	1.98	0.46
2:F:170:GLU:OE1	2:H:245:ASN:ND2	2.49	0.46
2:G:268:TYR:CE1	2:G:277:VAL:HG21	2.46	0.46
2:L:134:PRO:HD2	2:L:161:ILE:HD13	1.97	0.46
4:T:42:ILE:HG12	4:T:386:ASN:ND2	2.31	0.46
4:T:479:TYR:OH	4:T:561:SER:OG	2.22	0.46
2:H:33:GLU:OE2	2:H:288:GLN:NE2	2.50	0.45
2:O:59:TYR:CD1	2:O:67:PRO:HG3	2.50	0.45
3:Q:29:ILE:HD12	3:Q:30:GLY:O	2.16	0.45
4:U:500:THR:HG22	4:U:502:ASN:H	1.82	0.45
4:S:489:TYR:CZ	4:S:576:PRO:HB2	2.51	0.45
4:V:375:GLY:HA3	4:W:30:GLY:O	2.16	0.45
4:W:489:TYR:CE1	4:W:576:PRO:HB2	2.51	0.45
2:M:130:GLU:OE2	2:M:164:ASN:ND2	2.46	0.45
3:Q:71:ILE:HG13	3:Q:114:LEU:HD11	1.98	0.45
4:R:459:ARG:CA	4:R:568:ARG:HH21	2.29	0.45
4:V:139:GLN:HB3	4:V:142:ILE:HD11	1.98	0.45
4:W:24:ASP:OD1	4:W:24:ASP:N	2.49	0.45
4:W:482:LEU:HD12	4:W:552:LEU:O	2.17	0.45
2:H:168:ILE:HG12	2:H:268:TYR:CE2	2.50	0.45
2:L:139:VAL:HG22	2:L:151:MET:HG2	1.97	0.45
2:L:258:SER:OG	2:M:175:LYS:NZ	2.49	0.45
4:V:520:ILE:HD11	4:V:531:ILE:HG23	1.97	0.45
4:V:532:LEU:CD2	4:V:534:LEU:HD11	2.38	0.45
2:K:53:VAL:CG1	2:K:54:PRO:HD3	2.47	0.45
2:O:149:VAL:HG23	2:O:149:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:41:VAL:HG11	4:S:387:LEU:HD11	1.98	0.45
4:T:544:PHE:HB3	4:T:549:HIS:ND1	2.32	0.45
4:T:600:ILE:HB	4:T:624:THR:HG22	1.97	0.45
4:W:188:LYS:HE2	4:W:191:ILE:CD1	2.46	0.45
2:N:150:THR:HG23	2:N:216:VAL:HG22	1.99	0.45
4:W:489:TYR:CZ	4:W:576:PRO:HB2	2.52	0.45
2:D:168:ILE:HG12	2:D:268:TYR:CE2	2.51	0.45
2:I:130:GLU:HG3	2:I:164:ASN:HB3	1.98	0.45
2:M:22:ASP:OD1	2:M:22:ASP:N	2.46	0.45
2:N:116:MET:SD	2:N:228:PRO:HG3	2.57	0.45
3:Q:194:ARG:HE	3:Q:194:ARG:HB2	1.52	0.45
4:T:44:ASN:HB3	4:T:47:GLU:HB2	1.98	0.45
4:T:230:VAL:HG21	4:T:252:TYR:CE1	2.51	0.45
4:W:410:GLN:HE21	4:W:584:ASN:H	1.65	0.45
4:V:497:VAL:CG2	4:V:565:LYS:CB	2.85	0.45
4:W:492:ILE:HD11	4:W:568:ARG:HG3	1.98	0.45
1:A:897:ARG:HA	1:A:897:ARG:HD2	1.74	0.45
1:B:633:PHE:O	1:B:637:ARG:HG3	2.17	0.45
2:D:59:TYR:CD1	2:D:67:PRO:HG3	2.52	0.45
2:K:182:LEU:HD12	2:K:207:VAL:HG22	1.99	0.45
4:U:264:LYS:HG3	4:U:456:ASN:O	2.16	0.45
4:V:232:LYS:HB2	4:V:233:PRO:HD3	1.99	0.45
2:G:182:LEU:HD12	2:G:207:VAL:HG22	1.99	0.45
4:V:532:LEU:HG	4:V:534:LEU:HG	1.97	0.45
1:A:871:LEU:HD21	1:A:888:ILE:HG23	2.00	0.44
2:D:13:PRO:HG2	2:D:270:ALA:HB2	1.98	0.44
4:R:583:PHE:O	4:R:587:ILE:HG12	2.16	0.44
4:S:111:ASP:HB3	4:S:256:ARG:HH21	1.82	0.44
4:T:205:LYS:HE2	4:T:446:ILE:HD12	2.00	0.44
4:W:17:ILE:HG13	4:W:395:SER:OG	2.17	0.44
2:D:62:PHE:CZ	2:D:293:MET:SD	3.10	0.44
2:F:16:VAL:HG22	2:F:276:ARG:HG2	1.99	0.44
2:H:244:MET:HG2	2:H:249:PHE:HD2	1.81	0.44
2:J:246:ASP:OD1	2:J:246:ASP:N	2.50	0.44
2:K:88:SER:HA	2:K:94:ALA:HB3	1.98	0.44
2:O:27:GLN:O	2:O:31:VAL:HG13	2.17	0.44
4:V:115:GLU:OE1	4:V:256:ARG:NH1	2.51	0.44
4:W:494:TYR:CE1	4:W:568:ARG:HB2	2.52	0.44
4:W:590:LYS:HA	4:W:590:LYS:HD3	1.63	0.44
1:B:576:GLU:CG	1:B:607:ARG:NH1	2.78	0.44
2:D:56:VAL:HG22	2:D:67:PRO:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:225:LEU:HD11	3:P:234:ILE:HD11	1.99	0.44
4:T:531:ILE:HG21	4:T:554:LEU:HD11	1.99	0.44
1:B:46:LYS:HB3	1:B:46:LYS:HE3	1.81	0.44
1:B:816:THR:O	1:B:917:LYS:NZ	2.50	0.44
2:D:59:TYR:HD1	2:D:67:PRO:HG3	1.83	0.44
2:F:22:ASP:OD1	2:F:22:ASP:N	2.48	0.44
2:F:47:ASP:HB3	2:G:112:VAL:HG22	1.99	0.44
2:F:168:ILE:HG23	2:F:268:TYR:CE2	2.51	0.44
3:P:127:LYS:O	3:P:204:ARG:NH2	2.51	0.44
4:S:122:ILE:HG12	4:S:245:ILE:HG23	2.00	0.44
4:U:365:LEU:HD22	4:U:377:LEU:HD23	1.99	0.44
2:O:168:ILE:CG2	2:O:268:TYR:CD2	2.98	0.44
3:Q:233:LEU:HD23	3:Q:233:LEU:HA	1.86	0.44
4:T:230:VAL:HG12	4:T:248:LEU:HD23	2.00	0.44
4:W:38:PRO:HB2	4:W:379:GLY:HA3	2.00	0.44
1:A:642:GLU:H	1:A:642:GLU:HG2	1.59	0.44
2:D:198:LEU:HD22	2:D:205:PHE:CE1	2.53	0.44
4:U:202:ILE:O	4:U:206:GLU:HG2	2.17	0.44
4:W:421:GLU:OE2	4:W:577:ARG:NH2	2.51	0.44
2:I:170:GLU:CD	2:I:224:ARG:HG2	2.38	0.44
4:W:282:ASN:O	4:W:285:GLU:HB2	2.17	0.44
4:W:492:ILE:HD12	4:W:570:TRP:CE2	2.53	0.44
1:A:374:GLN:HE21	1:A:551:PRO:HD3	1.83	0.44
2:F:130:GLU:HG3	2:F:164:ASN:HB3	1.99	0.44
2:H:130:GLU:HG3	2:H:164:ASN:HB3	2.00	0.44
3:Q:63:GLY:HA2	4:W:286:TYR:HH	1.83	0.44
4:T:135:ILE:HD13	4:T:150:LEU:HB3	2.00	0.44
4:U:259:SER:HA	4:U:298:GLN:HG2	1.99	0.44
4:W:515:ASP:N	4:W:515:ASP:OD1	2.50	0.44
2:H:59:TYR:CD2	2:H:67:PRO:HG3	2.52	0.43
4:U:471:GLN:NE2	4:W:207:SER:OG	2.44	0.43
4:V:446:ILE:HD13	4:V:446:ILE:HA	1.85	0.43
1:A:837:MET:SD	1:B:954:ARG:HB2	2.57	0.43
2:I:29:VAL:HG12	2:I:285:LEU:HD23	1.99	0.43
1:B:895:GLU:OE2	1:B:897:ARG:HD2	2.18	0.43
2:F:122:ILE:HD13	2:H:241:GLN:HB2	2.00	0.43
2:K:168:ILE:CD1	2:K:268:TYR:CD2	3.00	0.43
3:P:245:LYS:HB2	3:P:245:LYS:HE2	1.70	0.43
4:R:99:GLN:O	4:R:217:TYR:OH	2.32	0.43
2:I:53:VAL:O	2:I:57:GLN:HG3	2.19	0.43
4:S:89:GLU:HB2	4:S:91:LYS:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:458:LEU:O	4:T:461:THR:HG22	2.18	0.43
4:T:492:ILE:HD12	4:T:570:TRP:CE2	2.53	0.43
4:W:377:LEU:HD23	4:W:377:LEU:HA	1.86	0.43
2:N:131:VAL:HG11	2:N:139:VAL:HG11	2.00	0.43
3:Q:161:ILE:HD13	3:Q:161:ILE:HA	1.84	0.43
4:T:476:TYR:CG	4:T:602:PRO:HG2	2.54	0.43
4:U:124:ARG:HB3	4:U:155:VAL:HB	2.01	0.43
2:F:73:LYS:HB2	2:F:73:LYS:HE2	1.85	0.43
2:M:11:ASP:OD1	2:M:12:ASN:HB2	2.18	0.43
3:P:55:LEU:HD22	3:P:84:HIS:CE1	2.54	0.43
3:P:111:THR:HB	3:P:114:LEU:HD22	2.00	0.43
4:R:61:LEU:HD21	4:T:60:ASP:HB2	2.00	0.43
4:S:514:ILE:HD13	4:S:547:ARG:HE	1.84	0.43
4:V:497:VAL:CG2	4:V:565:LYS:HE3	2.49	0.43
4:V:532:LEU:HD21	4:V:534:LEU:CD1	2.38	0.43
4:W:503:GLU:H	4:W:503:GLU:HG2	1.58	0.43
4:W:547:ARG:HB3	4:W:549:HIS:CE1	2.54	0.43
1:B:359:LYS:HB2	1:B:362:GLU:HG3	2.00	0.43
2:D:187:GLN:OE1	2:D:188:PRO:HD2	2.19	0.43
4:U:129:GLU:O	4:U:133:ASN:ND2	2.52	0.43
2:F:274:ILE:HG22	3:P:50:PRO:HD2	2.01	0.43
2:G:53:VAL:CG1	2:G:54:PRO:HD3	2.48	0.43
2:L:111:THR:O	2:L:111:THR:OG1	2.37	0.43
4:U:51:LYS:CD	4:U:387:LEU:CD1	2.92	0.43
4:W:112:HIS:CE1	4:W:482:LEU:H	2.36	0.43
1:B:109:PHE:HB2	1:B:123:LYS:HG2	2.01	0.43
1:B:866:ASP:OD1	1:B:867:GLY:N	2.52	0.43
2:F:267:GLN:OE1	2:F:276:ARG:HD3	2.19	0.43
2:F:294:ARG:NH1	2:F:297:LEU:O	2.51	0.43
2:L:294:ARG:HA	2:L:294:ARG:HD3	1.85	0.43
2:M:185:LEU:HD23	2:M:185:LEU:HA	1.90	0.43
4:T:73:GLN:NE2	4:T:77:GLU:OE2	2.50	0.43
4:U:133:ASN:O	4:U:137:GLU:HG3	2.19	0.43
4:U:518:LEU:HD12	4:U:518:LEU:HA	1.88	0.43
4:V:463:LEU:HD23	4:V:463:LEU:HA	1.83	0.43
1:A:513:VAL:HA	1:A:516:ASP:OD2	2.19	0.43
1:B:735:LEU:HD23	1:B:735:LEU:HA	1.91	0.43
2:I:116:MET:HA	2:I:228:PRO:HG3	2.01	0.43
2:N:241:GLN:NE2	2:N:258:SER:O	2.52	0.43
2:O:139:VAL:HG22	2:O:151:MET:HG2	2.00	0.43
4:S:251:ILE:HG12	4:S:408:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:PHE:HB3	2:E:261:ASP:OD1	2.19	0.42
2:F:123:PHE:CE2	2:F:225:ILE:HB	2.53	0.42
2:J:70:LEU:HD23	2:J:70:LEU:HA	1.90	0.42
3:P:38:LEU:HB3	3:P:48:LEU:HB3	2.01	0.42
4:T:352:LYS:HB3	4:T:352:LYS:HZ2	1.84	0.42
4:U:167:ARG:NH1	4:U:229:ASP:OD1	2.52	0.42
1:A:222:VAL:HG11	2:K:53:VAL:HG21	2.01	0.42
1:B:791:GLU:HB3	1:B:818:LEU:HD12	2.01	0.42
2:J:182:LEU:HD12	2:J:207:VAL:HG22	2.01	0.42
4:W:113:GLU:O	4:W:117:GLU:HG3	2.20	0.42
4:S:463:LEU:HB2	4:S:568:ARG:NH2	2.34	0.42
4:V:330:LYS:HZ2	4:V:331:THR:H	1.67	0.42
4:W:613:HIS:HB2	4:W:618:TYR:OH	2.19	0.42
1:B:818:LEU:HD23	1:B:818:LEU:HA	1.87	0.42
2:J:113:SER:HB3	2:M:71:ARG:CZ	2.49	0.42
2:M:4:ARG:NH1	2:M:130:GLU:HB3	2.34	0.42
2:N:68:ARG:HG3	2:N:71:ARG:HH21	1.84	0.42
4:R:112:HIS:CE1	4:R:482:LEU:H	2.37	0.42
4:R:143:THR:HG22	4:R:398:ASP:OD2	2.18	0.42
4:R:441:LYS:HG2	4:R:442:ASP:OD1	2.19	0.42
4:W:455:PHE:HA	4:W:461:THR:HG23	2.02	0.42
2:L:70:LEU:HD23	2:L:70:LEU:HA	1.91	0.42
3:P:112:ASN:OD1	3:P:112:ASN:N	2.47	0.42
4:S:410:GLN:NE2	4:S:584:ASN:H	2.18	0.42
4:U:90:ILE:HD12	4:U:462:THR:HB	2.01	0.42
4:V:260:ASP:N	4:V:260:ASP:OD1	2.52	0.42
4:W:483:ILE:HD11	4:W:554:LEU:HB3	1.96	0.42
1:B:435:THR:HA	1:B:438:LEU:HD12	2.01	0.42
2:C:22:ASP:OD1	2:C:22:ASP:N	2.46	0.42
3:P:2:ASP:OD1	3:P:2:ASP:N	2.51	0.42
2:I:4:ARG:NH1	2:I:130:GLU:HB3	2.34	0.42
2:J:133:SER:HB2	2:J:137:THR:OG1	2.20	0.42
2:K:89:TYR:HB2	2:K:283:LEU:HD13	2.01	0.42
2:O:77:LYS:HE3	2:O:77:LYS:HB2	1.85	0.42
4:R:621:GLY:HA3	4:T:193:ILE:O	2.19	0.42
4:T:42:ILE:HG12	4:T:386:ASN:HD22	1.85	0.42
4:W:270:ASP:OD1	4:W:270:ASP:N	2.51	0.42
4:R:73:GLN:NE2	4:R:77:GLU:OE2	2.53	0.42
4:R:410:GLN:HE21	4:R:582:MET:CB	2.30	0.42
4:W:544:PHE:CE2	4:W:612:TRP:CZ3	3.07	0.42
1:A:826:ASP:OD2	2:K:77:LYS:NZ	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLN:NE2	1:B:48:ARG:HD2	2.34	0.42
1:B:21:GLN:HE22	1:B:48:ARG:HD2	1.85	0.42
1:B:289:THR:HB	1:B:292:GLU:HG3	2.02	0.42
1:B:319:MET:HE3	1:B:319:MET:HB2	1.95	0.42
4:W:330:LYS:HB2	4:W:330:LYS:NZ	2.34	0.42
2:G:258:SER:OG	2:H:175:LYS:NZ	2.46	0.42
2:I:188:PRO:HG3	4:U:331:THR:HG23	2.02	0.42
4:U:568:ARG:HB3	4:U:568:ARG:NH1	2.34	0.42
4:W:514:ILE:HG21	4:W:547:ARG:HE	1.85	0.42
4:W:519:LEU:HD11	4:W:600:ILE:HD12	2.02	0.42
2:F:27:GLN:OE1	3:P:193:TYR:HB2	2.20	0.41
2:L:22:ASP:O	2:L:26:ARG:HG3	2.20	0.41
2:M:272:ASP:OD1	2:M:275:ASN:HB2	2.19	0.41
2:N:184:ARG:HH11	2:N:202:ASP:HB3	1.84	0.41
1:B:183:LEU:HD22	1:B:243:VAL:HG13	2.02	0.41
4:V:117:GLU:HB3	4:V:227:PRO:HG3	2.01	0.41
4:V:260:ASP:HB3	4:V:457:ASP:OD1	2.20	0.41
1:B:845:ILE:HG13	1:B:849:PHE:HE1	1.84	0.41
2:H:126:VAL:HG12	2:H:144:SER:O	2.20	0.41
2:J:168:ILE:CG2	2:J:268:TYR:HD1	2.09	0.41
4:T:579:LYS:HB3	4:T:579:LYS:HE2	1.77	0.41
4:V:421:GLU:OE2	4:V:577:ARG:NH1	2.54	0.41
4:W:268:VAL:HG23	4:W:270:ASP:OD1	2.21	0.41
4:W:518:LEU:HD12	4:W:518:LEU:HA	1.80	0.41
1:B:333:LYS:HB2	1:B:333:LYS:HE3	1.81	0.41
2:E:70:LEU:O	2:G:118:ASN:ND2	2.52	0.41
2:F:268:TYR:CD1	2:F:277:VAL:CG2	3.03	0.41
2:L:291:ASP:OD1	2:L:295:ARG:HD3	2.20	0.41
3:P:175:MET:O	3:P:179:ILE:HD13	2.20	0.41
4:S:523:SER:O	4:S:523:SER:OG	2.36	0.41
4:T:71:ASP:OD1	4:T:71:ASP:N	2.53	0.41
4:V:532:LEU:HD21	4:V:534:LEU:HD21	2.01	0.41
2:D:35:LEU:HB3	2:D:62:PHE:HD1	1.86	0.41
2:E:73:LYS:HB3	2:E:297:LEU:HD22	2.01	0.41
2:N:233:LYS:HE3	2:N:233:LYS:HB3	1.81	0.41
4:R:503:GLU:OE2	4:R:504:GLU:N	2.51	0.41
4:V:605:LEU:HD23	4:V:605:LEU:HA	1.86	0.41
2:F:23:GLU:O	2:F:27:GLN:HG3	2.20	0.41
2:L:201:LEU:HD23	2:L:201:LEU:HA	1.88	0.41
2:N:83:THR:HG22	2:N:290:TYR:HE1	1.86	0.41
2:N:126:VAL:HA	2:N:127:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:149:VAL:HG22	2:O:217:ILE:HB	2.03	0.41
3:Q:31:THR:OG1	3:Q:61:ARG:NH1	2.54	0.41
4:R:260:ASP:HB3	4:R:457:ASP:OD1	2.21	0.41
4:S:60:ASP:OD2	4:S:60:ASP:N	2.52	0.41
4:S:113:GLU:O	4:S:117:GLU:HG3	2.21	0.41
4:T:440:LYS:HE3	4:T:440:LYS:HB3	1.77	0.41
4:U:614:THR:CG2	4:U:615:TRP:N	2.84	0.41
1:A:576:GLU:N	1:A:576:GLU:OE1	2.54	0.41
1:B:200:ASN:OD1	1:B:200:ASN:N	2.54	0.41
1:B:460:ARG:HH21	3:P:222:ASN:HA	1.86	0.41
2:C:168:ILE:HD12	2:C:268:TYR:CE2	2.53	0.41
2:H:95:PRO:HG3	3:Q:37:VAL:HG21	2.03	0.41
2:H:251:ILE:HB	2:H:254:VAL:HG11	2.02	0.41
2:I:179:PRO:HB2	2:I:192:ALA:HB1	2.03	0.41
2:K:294:ARG:HA	2:K:294:ARG:HD3	1.66	0.41
4:U:282:ASN:ND2	4:V:18:ILE:HD13	2.36	0.41
4:V:607:LEU:HD12	4:V:607:LEU:HA	1.93	0.41
2:E:294:ARG:HA	2:E:294:ARG:HD3	1.81	0.41
2:G:125:SER:HB2	2:G:265:ILE:HG13	2.02	0.41
2:K:198:LEU:HD22	2:K:205:PHE:CE1	2.56	0.41
2:L:179:PRO:HD3	2:L:194:PHE:CZ	2.55	0.41
2:N:91:SER:HB3	2:N:251:ILE:HD13	2.02	0.41
2:N:119:SER:OG	2:N:229:LEU:HD13	2.21	0.41
2:N:175:LYS:HB2	2:N:175:LYS:HE2	1.69	0.41
3:P:29:ILE:HD12	3:P:29:ILE:HA	1.85	0.41
3:Q:18:LYS:HB2	3:Q:18:LYS:HE3	1.82	0.41
4:R:59:HIS:CD2	4:R:179:PHE:H	2.38	0.41
4:R:60:ASP:OD2	4:R:60:ASP:N	2.53	0.41
4:S:96:THR:HG22	4:S:209:ILE:HG22	2.03	0.41
4:V:511:VAL:O	4:V:517:HIS:HA	2.21	0.41
4:W:328:PHE:CE2	4:W:340:THR:HG21	2.55	0.41
2:F:113:SER:HB2	3:P:194:ARG:HH12	1.86	0.41
4:R:112:HIS:HE1	4:R:482:LEU:H	1.68	0.41
1:B:945:ILE:HD12	1:B:945:ILE:N	2.36	0.40
2:F:44:ARG:HH22	2:G:230:ALA:HB1	1.85	0.40
2:N:77:LYS:HB3	2:N:77:LYS:HE3	1.71	0.40
2:N:274:ILE:HD13	2:N:274:ILE:HA	1.91	0.40
4:R:514:ILE:HD12	4:R:549:HIS:CD2	2.56	0.40
4:R:613:HIS:CE1	4:R:626:ILE:HD11	2.57	0.40
4:S:50:MET:HE2	4:S:50:MET:HB2	1.93	0.40
4:T:571:ILE:HD13	4:T:571:ILE:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:MET:SD	1:A:555:GLY:HA3	2.61	0.40
1:A:703:GLU:HB2	1:A:708:SER:HG	1.87	0.40
1:B:480:MET:HG3	1:B:484:ARG:HG3	2.04	0.40
2:J:59:TYR:CD2	2:J:67:PRO:HG3	2.57	0.40
4:T:50:MET:HE2	4:T:50:MET:HB2	1.89	0.40
4:T:193:ILE:HD13	4:T:193:ILE:HA	1.89	0.40
4:U:33:ASN:OD1	4:W:284:THR:HA	2.20	0.40
4:U:293:VAL:HG22	4:U:304:VAL:HG22	2.04	0.40
4:U:391:PRO:HD2	4:U:400:MET:HE1	2.02	0.40
4:V:293:VAL:HG22	4:V:304:VAL:HG22	2.03	0.40
4:W:398:ASP:OD2	4:W:402:LYS:HE3	2.21	0.40
2:F:89:TYR:HB2	2:F:283:LEU:HD13	2.03	0.40
2:F:240:PHE:CE2	2:F:244:MET:SD	3.14	0.40
2:N:44:ARG:HA	2:N:44:ARG:HD3	1.92	0.40
4:V:426:TRP:CZ2	4:V:430:ARG:HD3	2.57	0.40
1:B:793:MET:CE	1:B:795:MET:SD	3.09	0.40
2:G:40:ILE:O	2:G:44:ARG:HG3	2.21	0.40
2:G:68:ARG:HB2	2:G:71:ARG:HB2	2.03	0.40
2:O:44:ARG:HG3	2:O:44:ARG:NH1	2.36	0.40
4:T:89:GLU:H	4:T:89:GLU:HG3	1.65	0.40
4:T:500:THR:HG22	4:T:502:ASN:H	1.87	0.40
2:E:71:ARG:NE	2:G:113:SER:OG	2.45	0.40
2:E:150:THR:HG23	2:E:216:VAL:HG22	2.03	0.40
2:L:153:ASN:OD1	2:L:211:VAL:HA	2.21	0.40
2:M:89:TYR:HB2	2:M:283:LEU:HD13	2.04	0.40
3:Q:66:ASN:HD21	3:Q:68:ASN:HB2	1.84	0.40
3:Q:101:ILE:HD13	3:Q:107:THR:HG21	2.03	0.40
4:S:12:LEU:HD12	4:S:12:LEU:HA	1.88	0.40
4:T:435:TYR:OH	4:T:448:ASP:OD1	2.28	0.40
4:U:149:ASP:OD1	4:U:162:VAL:HG22	2.22	0.40
4:V:423:MET:HE2	4:V:423:MET:HB2	1.90	0.40
4:W:606:THR:HG22	4:W:608:THR:H	1.87	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	772/955 (81%)	763 (99%)	9 (1%)	0	100	100
1	B	900/955 (94%)	884 (98%)	16 (2%)	0	100	100
2	C	296/302 (98%)	291 (98%)	5 (2%)	0	100	100
2	D	296/302 (98%)	289 (98%)	7 (2%)	0	100	100
2	E	296/302 (98%)	293 (99%)	3 (1%)	0	100	100
2	F	296/302 (98%)	293 (99%)	3 (1%)	0	100	100
2	G	296/302 (98%)	289 (98%)	7 (2%)	0	100	100
2	H	297/302 (98%)	293 (99%)	4 (1%)	0	100	100
2	I	296/302 (98%)	287 (97%)	9 (3%)	0	100	100
2	J	297/302 (98%)	292 (98%)	5 (2%)	0	100	100
2	K	296/302 (98%)	292 (99%)	4 (1%)	0	100	100
2	L	296/302 (98%)	291 (98%)	5 (2%)	0	100	100
2	M	296/302 (98%)	292 (99%)	4 (1%)	0	100	100
2	N	296/302 (98%)	291 (98%)	5 (2%)	0	100	100
2	O	295/302 (98%)	290 (98%)	5 (2%)	0	100	100
3	P	247/249 (99%)	244 (99%)	3 (1%)	0	100	100
3	Q	231/249 (93%)	229 (99%)	2 (1%)	0	100	100
4	R	600/628 (96%)	594 (99%)	6 (1%)	0	100	100
4	S	620/628 (99%)	617 (100%)	3 (0%)	0	100	100
4	T	614/628 (98%)	599 (98%)	15 (2%)	0	100	100
4	U	602/628 (96%)	596 (99%)	6 (1%)	0	100	100
4	V	620/628 (99%)	612 (99%)	8 (1%)	0	100	100
4	W	610/628 (97%)	605 (99%)	5 (1%)	0	100	100
5	r	12/283 (4%)	12 (100%)	0	0	100	100
5	s	12/283 (4%)	12 (100%)	0	0	100	100
5	t	12/283 (4%)	12 (100%)	0	0	100	100
5	u	12/283 (4%)	12 (100%)	0	0	100	100
5	v	12/283 (4%)	12 (100%)	0	0	100	100
5	w	12/283 (4%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	9737/11800 (82%)	9598 (99%)	139 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	687/846 (81%)	687 (100%)	0	100	100
1	B	805/846 (95%)	805 (100%)	0	100	100
2	C	248/252 (98%)	248 (100%)	0	100	100
2	D	248/252 (98%)	248 (100%)	0	100	100
2	E	248/252 (98%)	248 (100%)	0	100	100
2	F	248/252 (98%)	248 (100%)	0	100	100
2	G	248/252 (98%)	248 (100%)	0	100	100
2	H	249/252 (99%)	249 (100%)	0	100	100
2	I	248/252 (98%)	248 (100%)	0	100	100
2	J	249/252 (99%)	249 (100%)	0	100	100
2	K	248/252 (98%)	248 (100%)	0	100	100
2	L	248/252 (98%)	248 (100%)	0	100	100
2	M	248/252 (98%)	248 (100%)	0	100	100
2	N	248/252 (98%)	248 (100%)	0	100	100
2	O	247/252 (98%)	247 (100%)	0	100	100
3	P	225/225 (100%)	225 (100%)	0	100	100
3	Q	211/225 (94%)	211 (100%)	0	100	100
4	R	510/532 (96%)	510 (100%)	0	100	100
4	S	527/532 (99%)	527 (100%)	0	100	100
4	T	523/532 (98%)	523 (100%)	0	100	100
4	U	512/532 (96%)	512 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	V	527/532 (99%)	527 (100%)	0	100	100
4	W	519/532 (98%)	519 (100%)	0	100	100
5	r	13/245 (5%)	13 (100%)	0	100	100
5	s	13/245 (5%)	13 (100%)	0	100	100
5	t	13/245 (5%)	13 (100%)	0	100	100
5	u	13/245 (5%)	13 (100%)	0	100	100
5	v	13/245 (5%)	13 (100%)	0	100	100
5	w	13/245 (5%)	13 (100%)	0	100	100
All	All	8349/10080 (83%)	8349 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	374	GLN
1	B	21	GLN
4	R	44	ASN
4	R	410	GLN
4	S	44	ASN
4	T	517	HIS
4	U	48	HIS
4	U	356	GLN
4	U	410	GLN
4	U	549	HIS
4	W	15	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 monosaccharides 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.

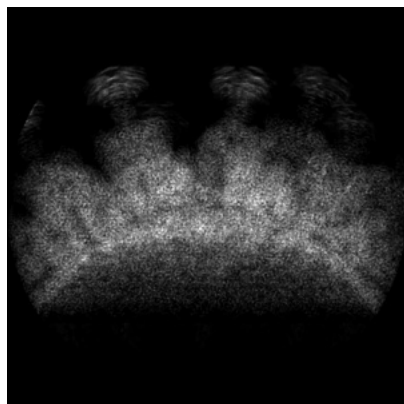
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36870. These allow visual inspection of the internal detail of the map and identification of artifacts.

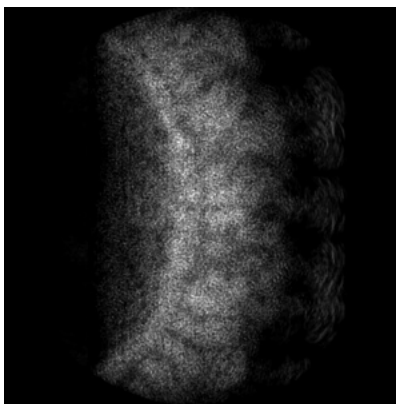
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

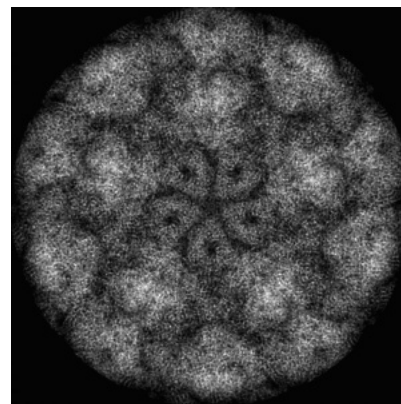
6.1.1 Primary map



X

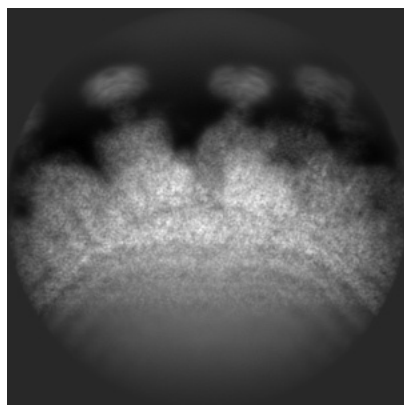


Y

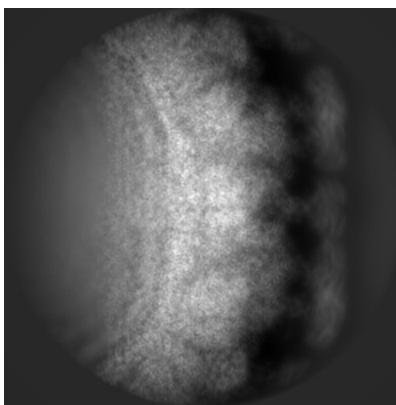


Z

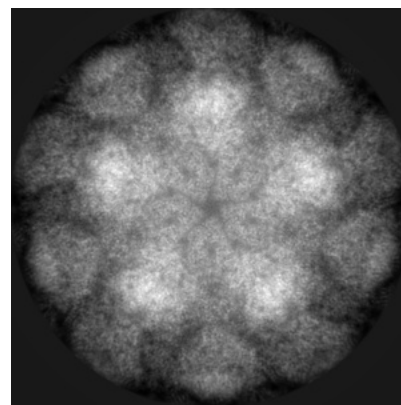
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

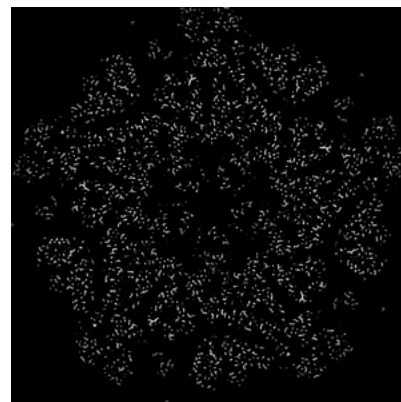
6.2.1 Primary map



X Index: 240

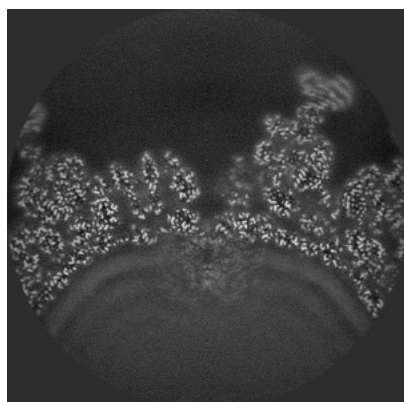


Y Index: 240

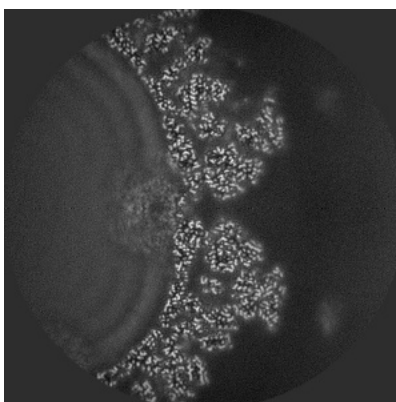


Z Index: 240

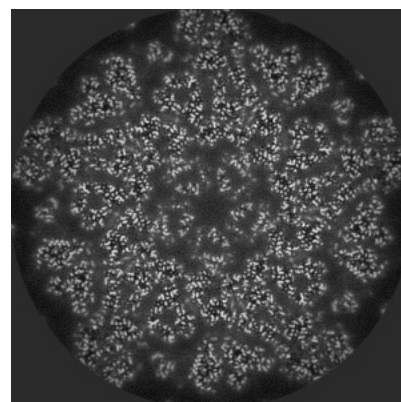
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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: 247

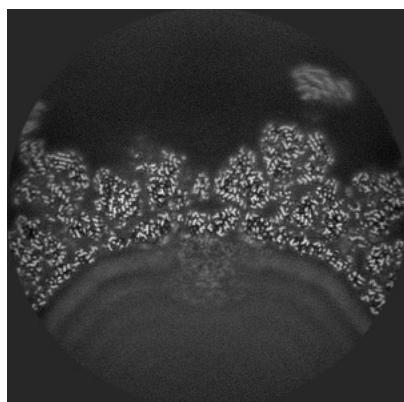


Y Index: 296

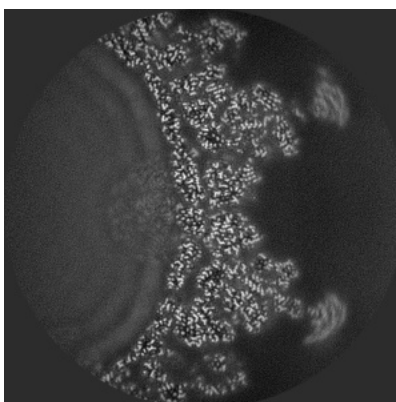


Z Index: 213

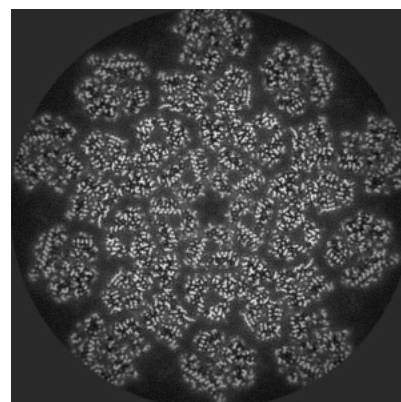
6.3.2 Raw map



X Index: 256



Y Index: 266

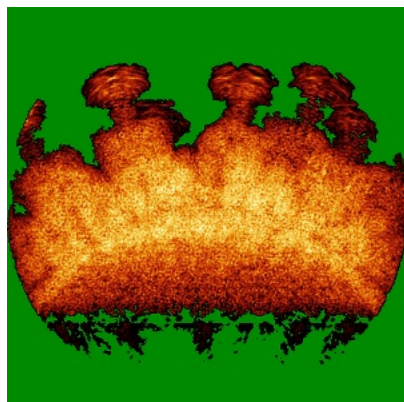


Z Index: 250

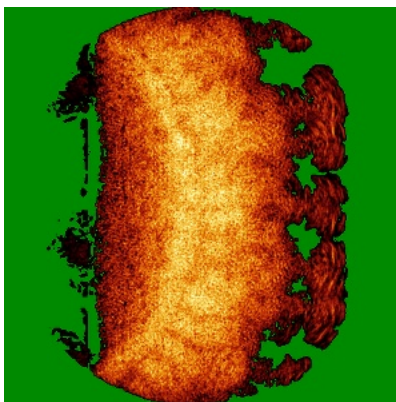
The images above show the largest variance slices of the map in three orthogonal directions.

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

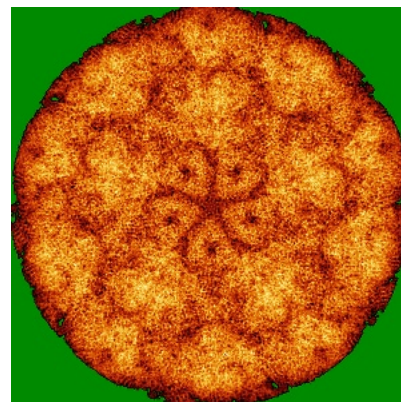
6.4.1 Primary map



X

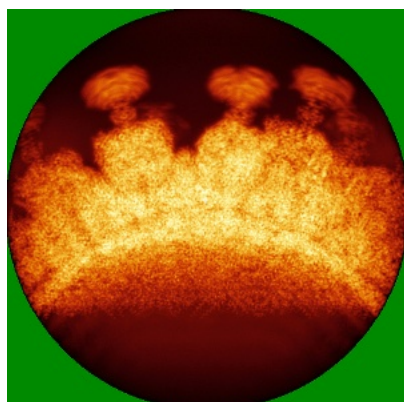


Y

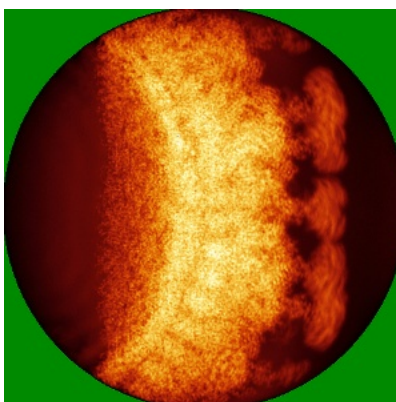


Z

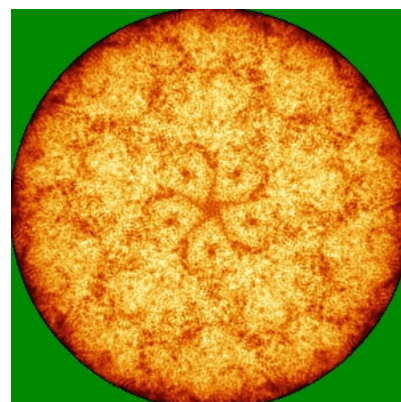
6.4.2 Raw map



X



Y

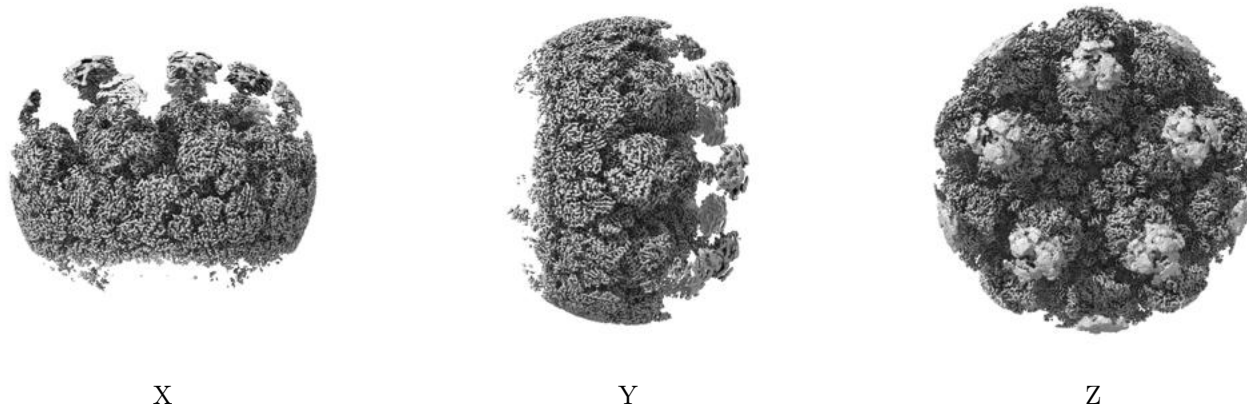


Z

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.

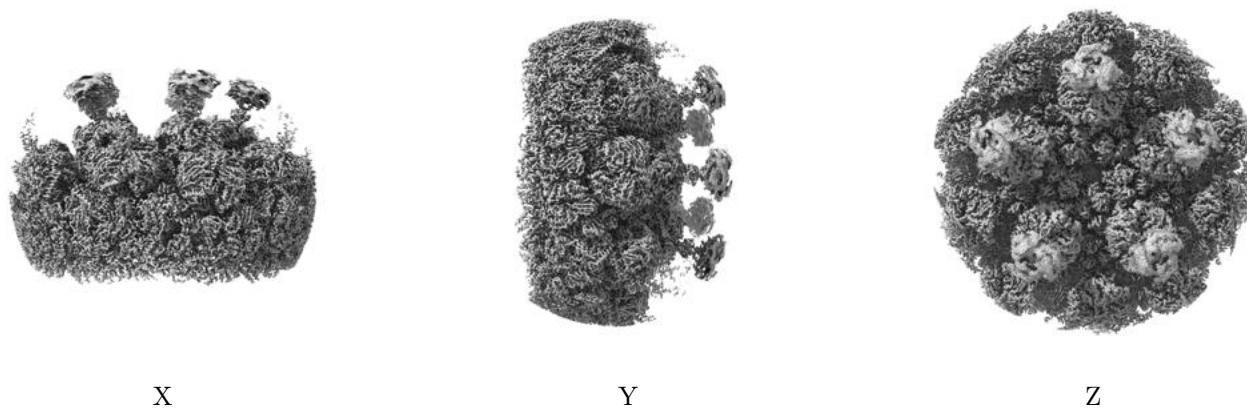
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

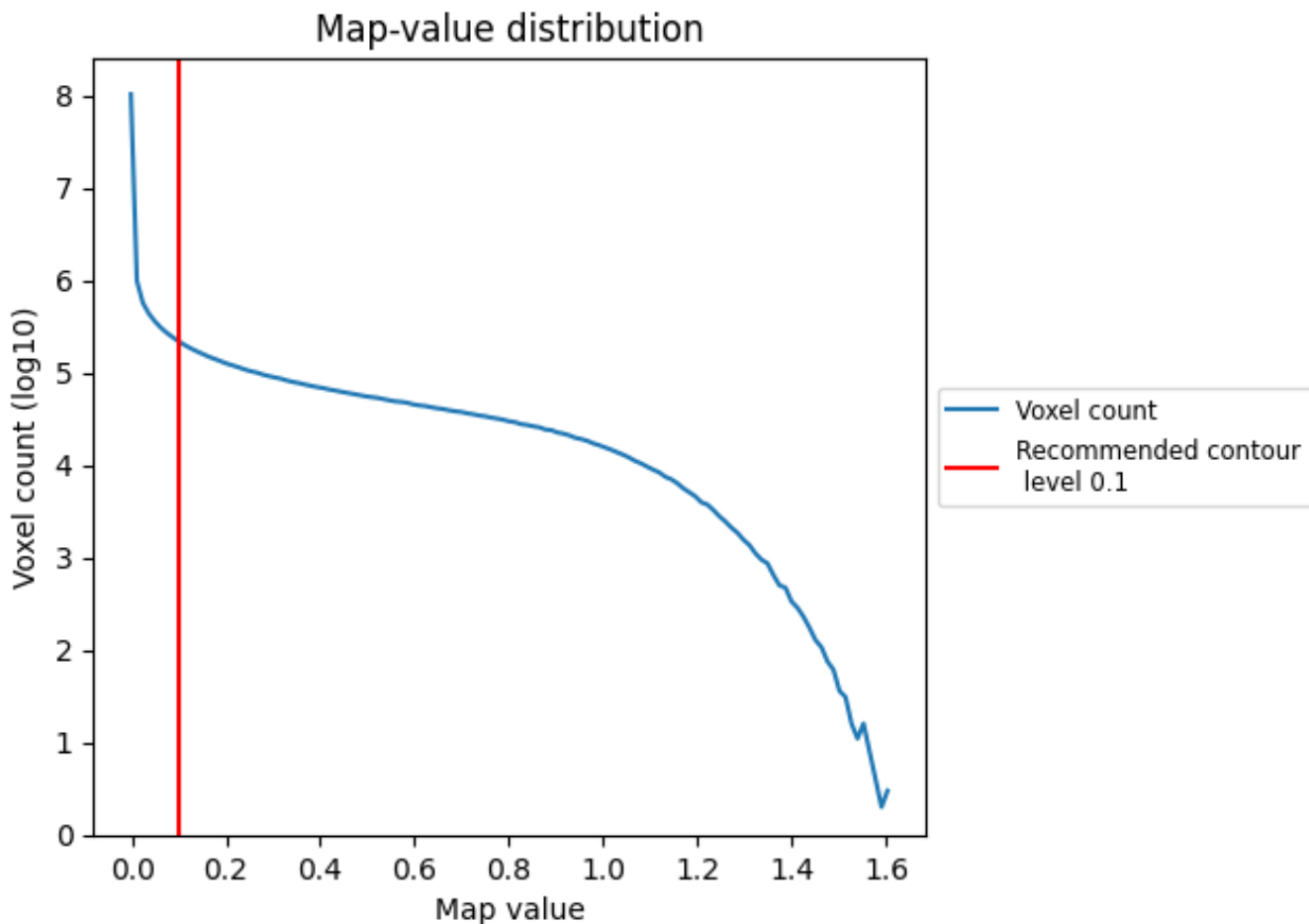
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

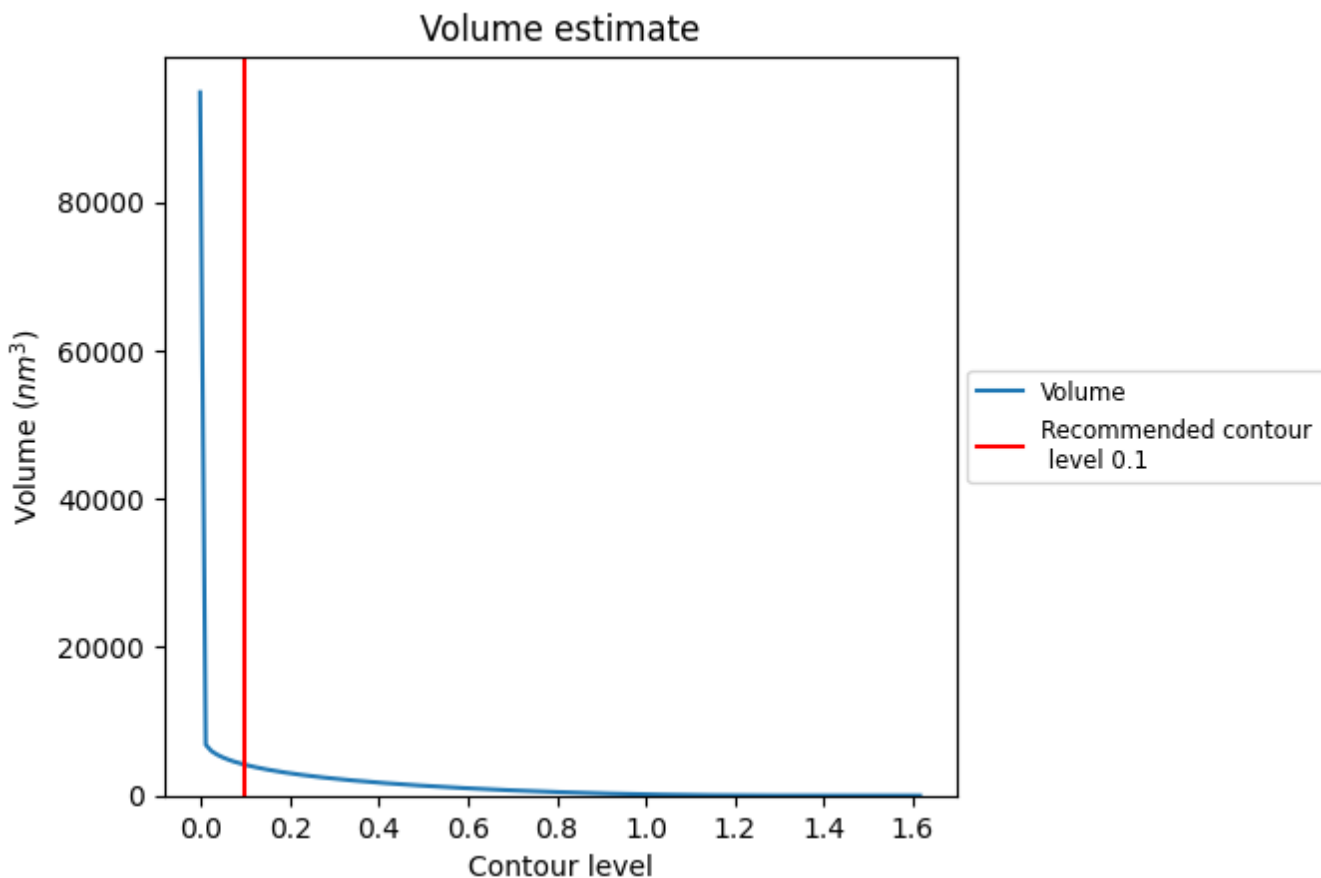
This section contains the results of statistical analysis of the map.

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.

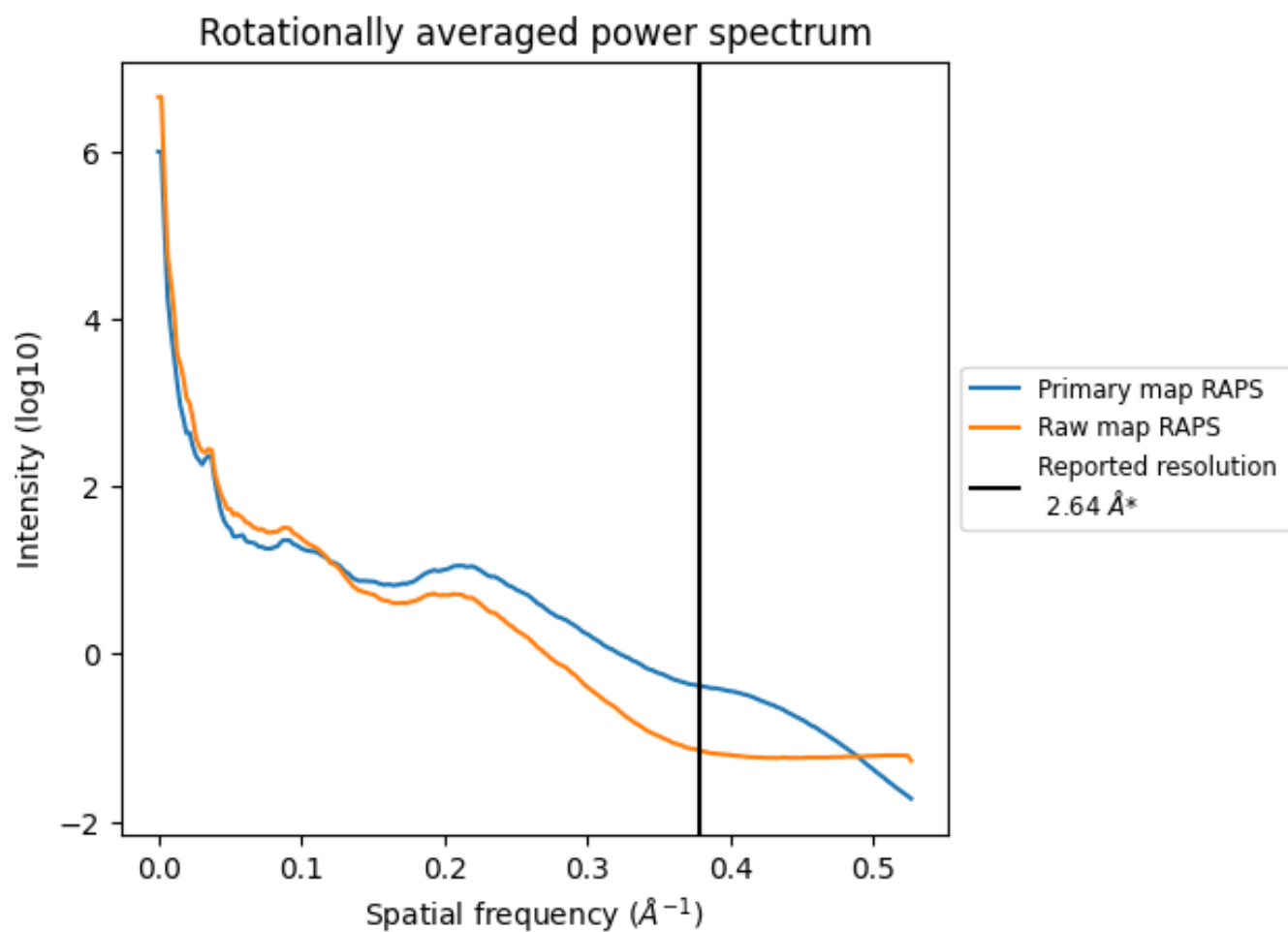
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4144 nm³; this corresponds to an approximate mass of 3744 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

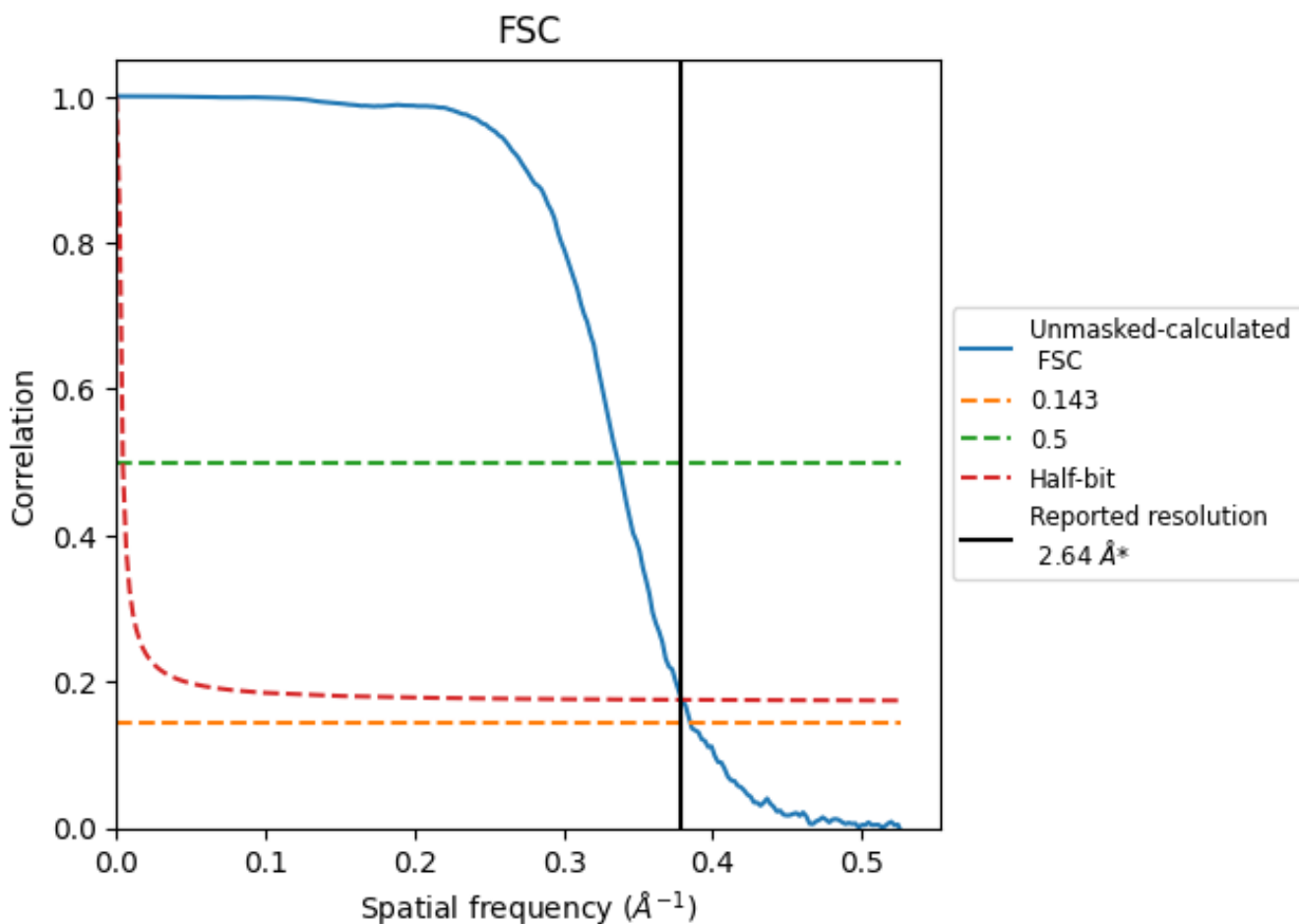


*Reported resolution corresponds to spatial frequency of 0.379 Å⁻¹

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 0.379 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.60	2.97	2.64

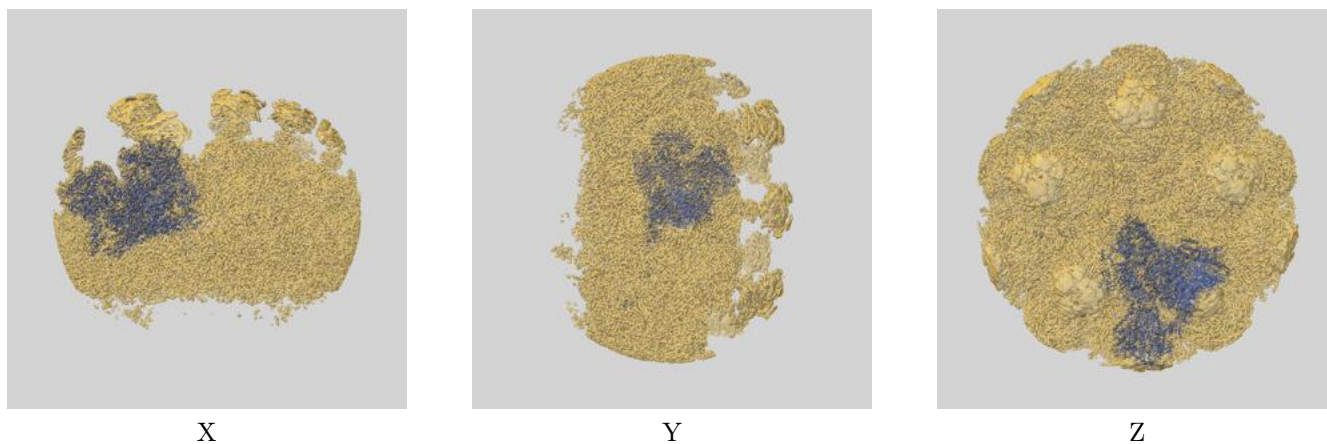
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

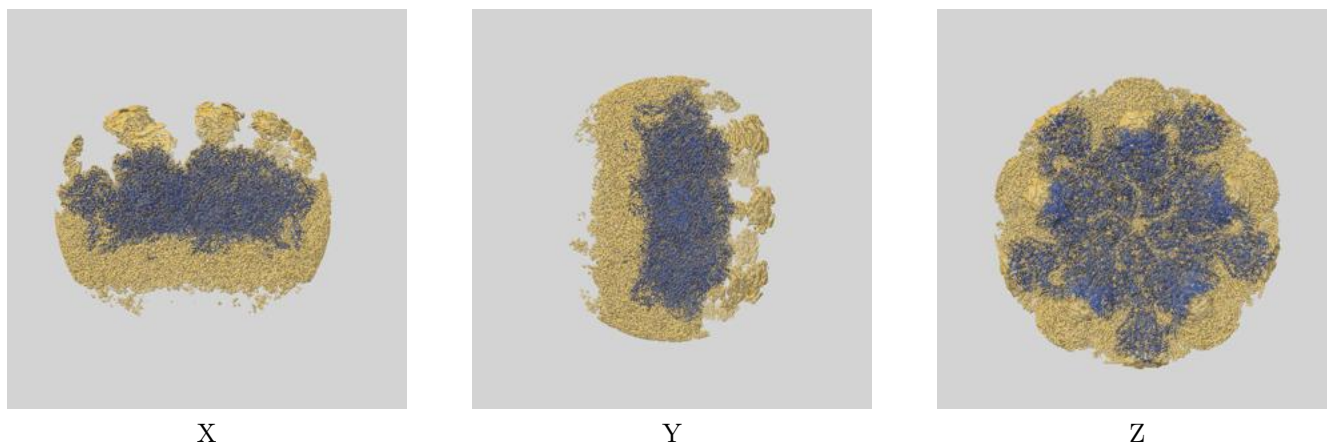
This section contains information regarding the fit between EMDB map EMD-36870 and PDB model 8K42. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

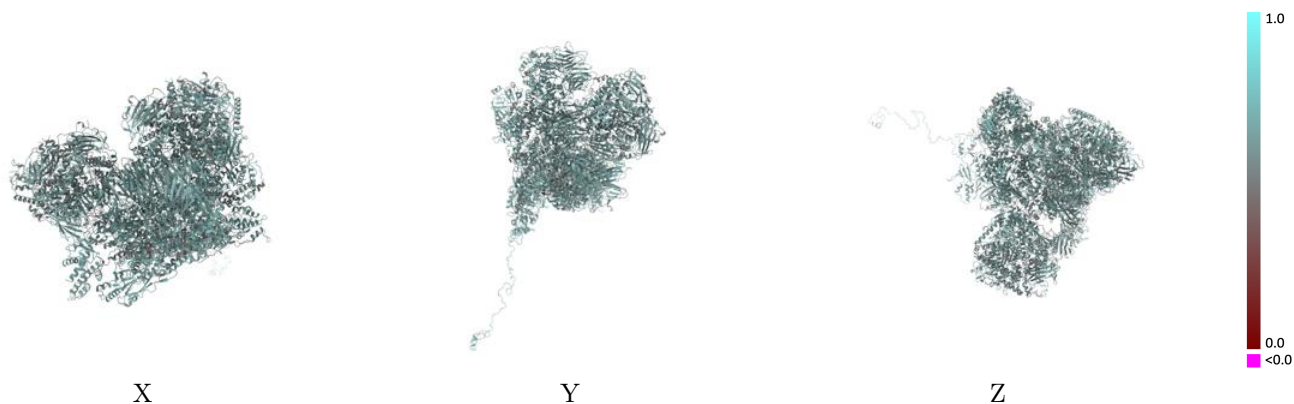


9.1.2 Map-model assembly overlay [i](#)



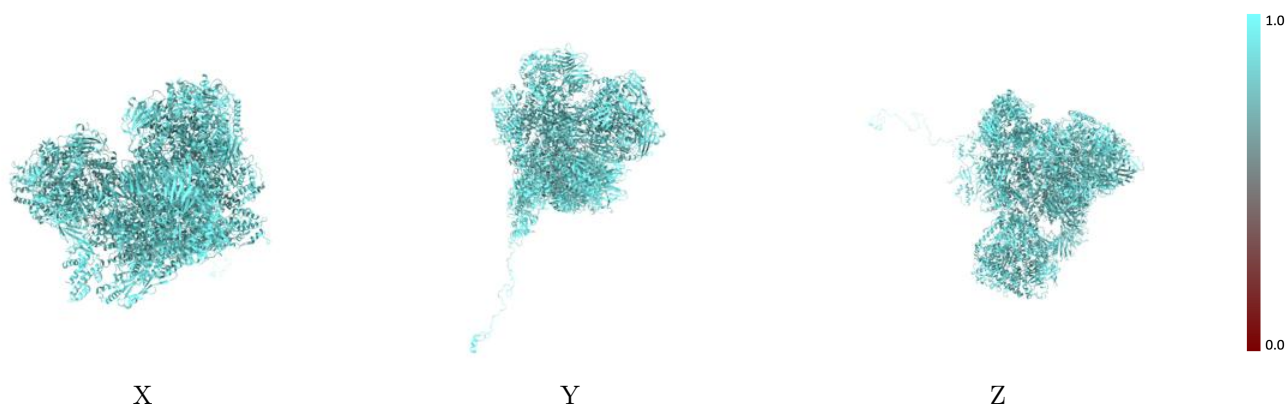
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



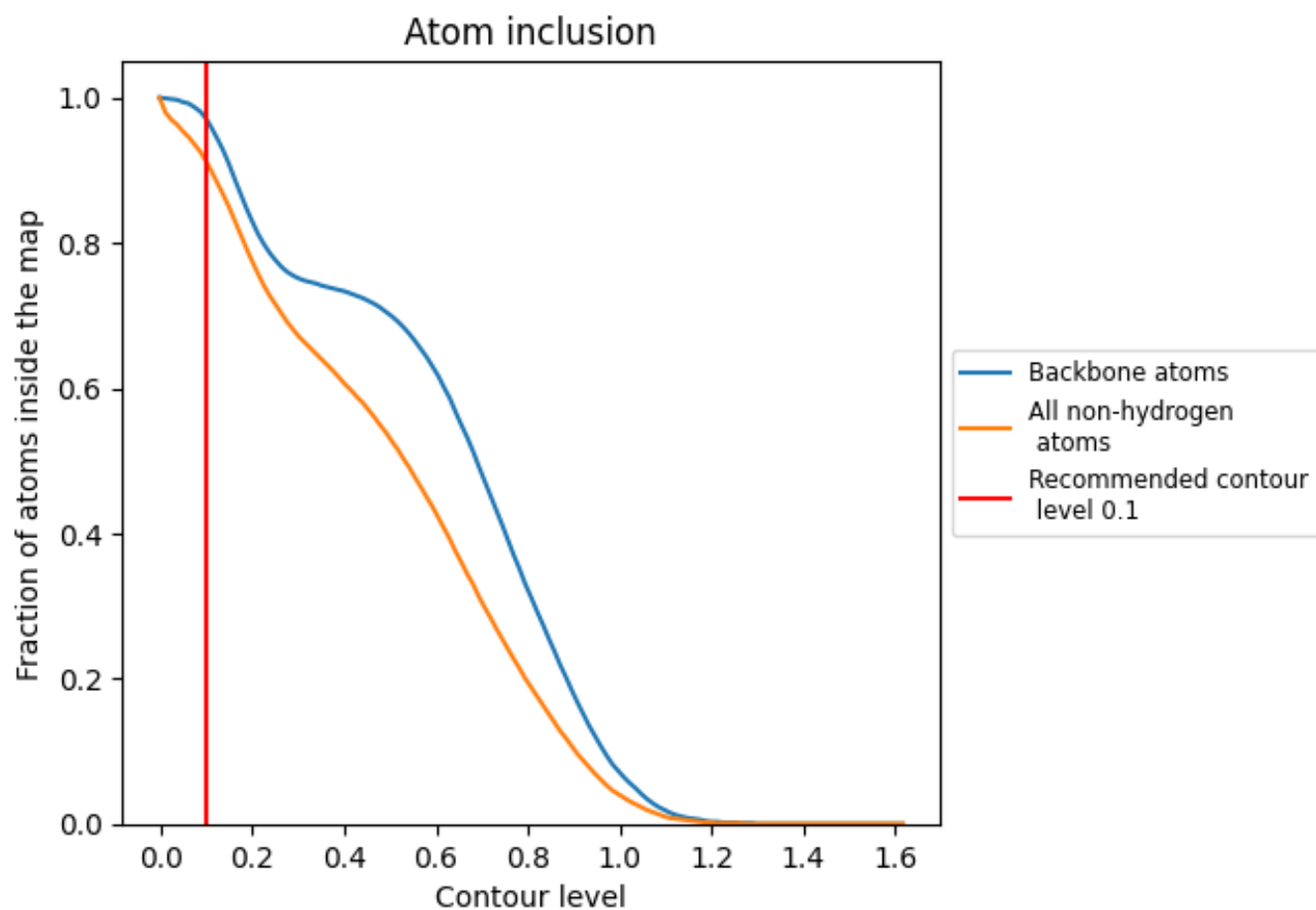
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.5900
A	 0.9280	 0.6060
B	 0.9200	 0.5980
C	 0.9360	 0.6080
D	 0.9200	 0.5940
E	 0.9160	 0.5910
F	 0.9230	 0.5980
G	 0.9180	 0.5930
H	 0.9120	 0.5890
I	 0.9230	 0.5990
J	 0.9250	 0.5990
K	 0.9380	 0.6140
L	 0.9230	 0.5890
M	 0.9180	 0.5950
N	 0.9290	 0.5940
O	 0.9230	 0.5890
P	 0.9160	 0.6010
Q	 0.9130	 0.5910
R	 0.9080	 0.5850
S	 0.9040	 0.5850
T	 0.8970	 0.5790
U	 0.8970	 0.5790
V	 0.8800	 0.5700
W	 0.8890	 0.5730
r	 0.8700	 0.5740
s	 0.8520	 0.5640
t	 0.8890	 0.5630
u	 0.8700	 0.5510
v	 0.8240	 0.5560
w	 0.8330	 0.5300

