



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 02:59 AM UTC

PDB ID : 8W9P / pdb_00008w9p
EMDB ID : EMD-37378
Title : Structure of full Banna virus
Authors : Li, Z.; Cao, S.
Deposited on : 2023-09-05
Resolution : 5.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

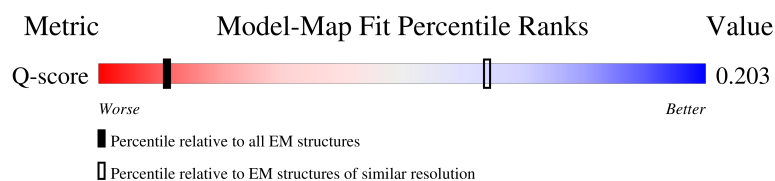
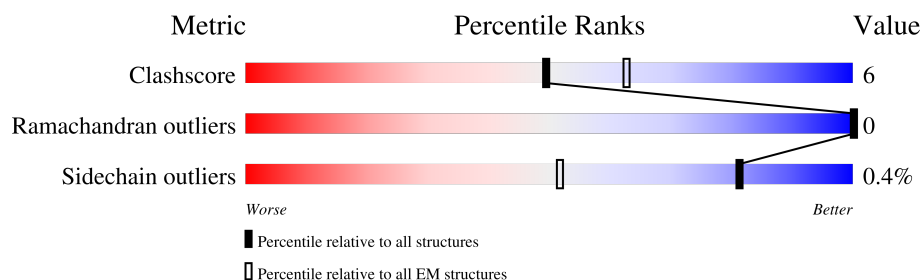
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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.



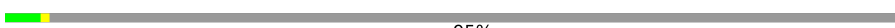
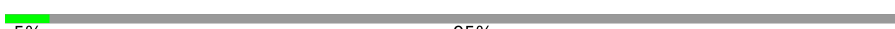
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	503 (5.20 - 6.20)

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	 74% 7% 19%
1	B	955	 87% 8% 5%
2	C	301	 91% 8% .
2	D	301	 85% 14% .

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Mol	Chain	Length	Quality of chain
2	E	301	 89% 10% .
2	F	301	 82% 17% .
2	G	301	 87% 12% .
2	H	301	 85% 14% .
2	I	301	 83% 16% .
2	J	301	 87% 13% .
2	K	301	 90% 9% .
2	L	301	 84% 15% ..
2	M	301	 86% 13% .
2	N	301	 86% 13% .
2	O	301	 92% 6% .
3	P	249	 85% 15%
3	Q	249	 84% 10% 6%
4	R	628	 84% 12% .
4	S	628	 88% 11% .
4	T	628	 83% 15% .
4	U	628	 83% 13% .
4	V	628	 85% 14% .
4	W	628	 80% 17% .
5	r	283	 . . 95%
5	s	283	 5% 95%
5	t	283	 . . 95%
5	u	283	 . . 95%
5	v	283	 5% 95%
5	w	283	 5% 95%

2 Entry composition

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
1	A	774	Total	C	N	O	S	0	0
			6204	3941	1058	1178	27		
1	B	904	Total	C	N	O	S	0	0
			7224	4587	1223	1387	27		

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

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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
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
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
5	t	14	Total	C	N	O	0	0
			110	69	19	22		
5	u	14	Total	C	N	O	0	0
			110	69	19	22		
5	v	14	Total	C	N	O	0	0
			110	69	19	22		
5	w	14	Total	C	N	O	0	0
			110	69	19	22		

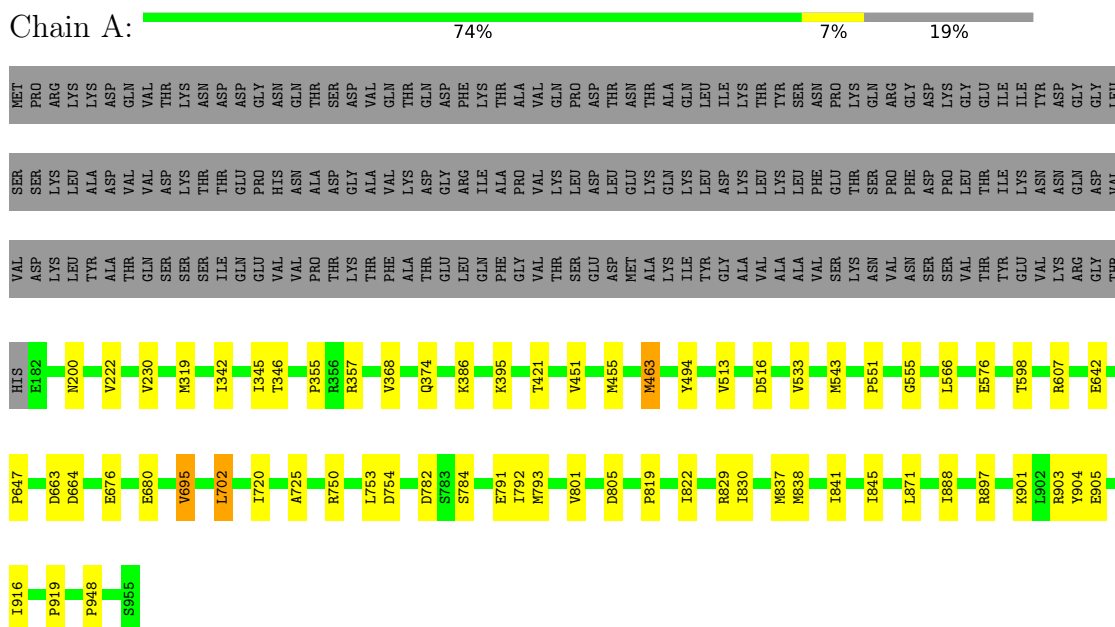
There are 24 discrepancies between the modelled and reference sequences:

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

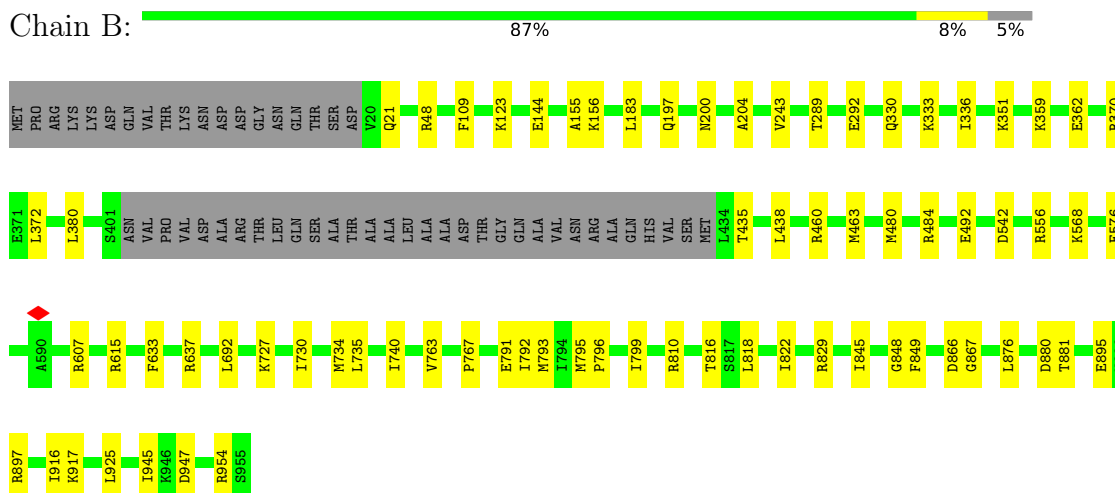
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: VP2



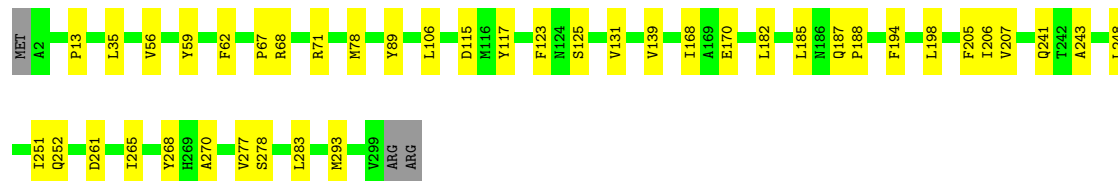
• Molecule 1: VP2



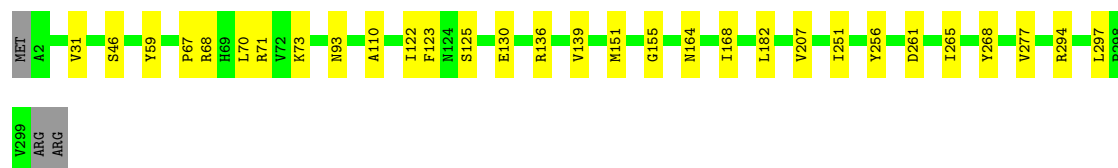
• Molecule 2: VP8

Chain C:  91% 8%

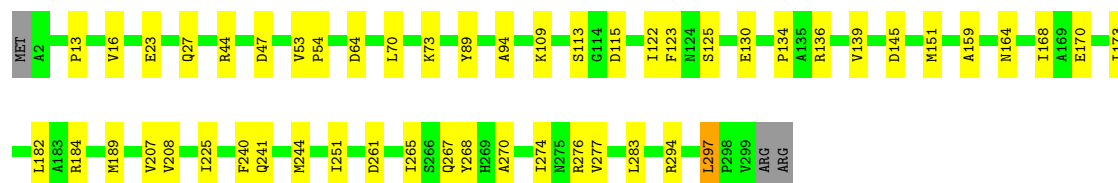
• Molecule 2: VP8

Chain D:  85% 14%

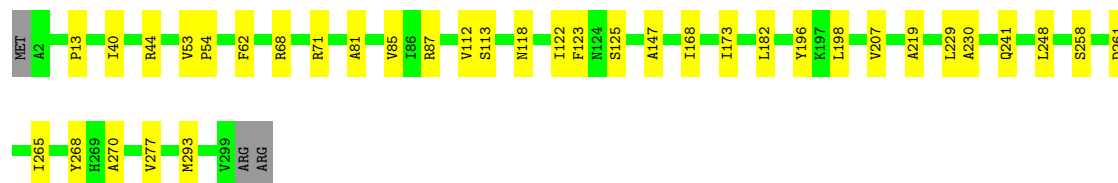
• Molecule 2: VP8

Chain E:  89% 10%

• Molecule 2: VP8

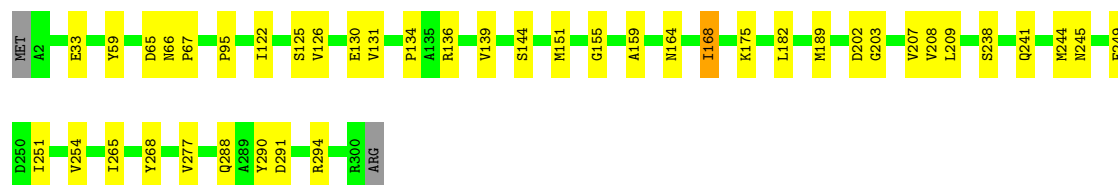
Chain F:  82% 17%

• Molecule 2: VP8

Chain G:  87% 12%

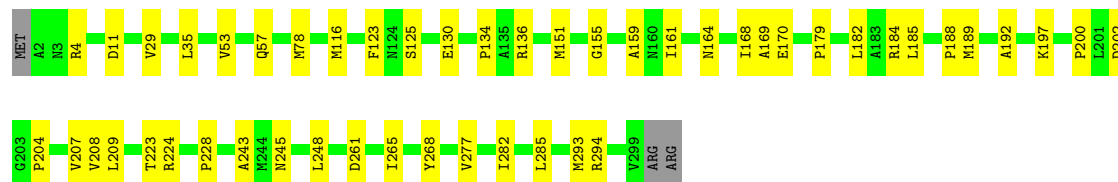
• Molecule 2: VP8

Chain H:  85% 14%



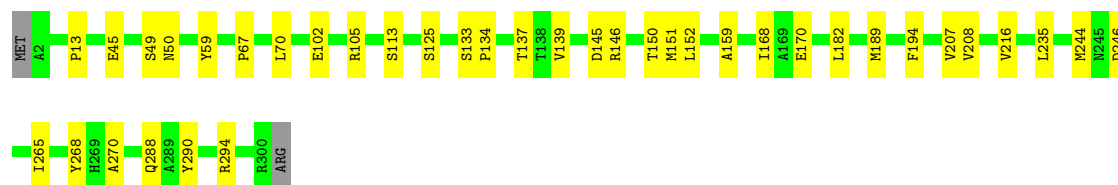
• Molecule 2: VP8

Chain I: 83% 16% .



• Molecule 2: VP8

Chain J: 87% 13% .



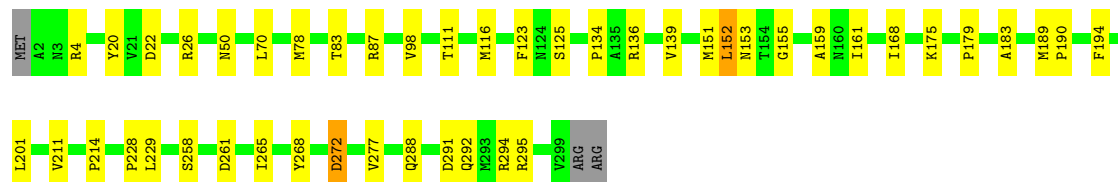
• Molecule 2: VP8

Chain K: 90% 9% .



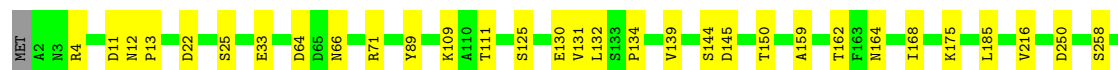
• Molecule 2: VP8

Chain L: 84% 15% ..



• Molecule 2: VP8

Chain M: 86% 13% .





• Molecule 2: VP8

Chain N: 86% 13% .



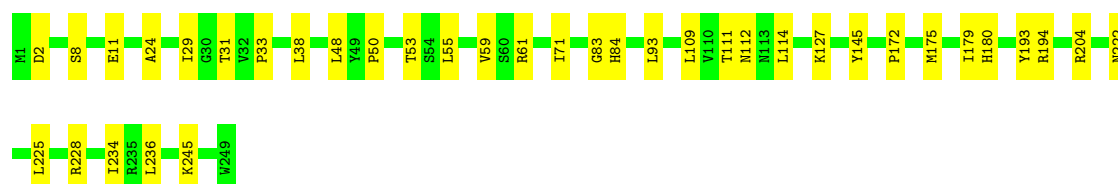
• Molecule 2: VP8

Chain O: 92% 6% .



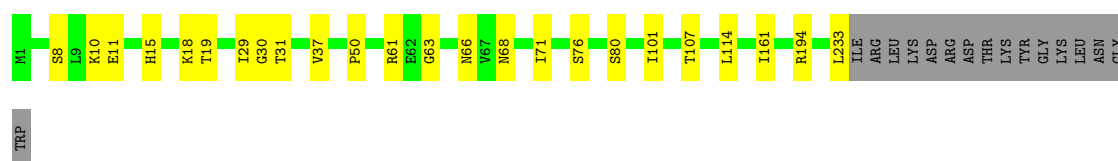
• Molecule 3: VP10

Chain P: 85% 15% .



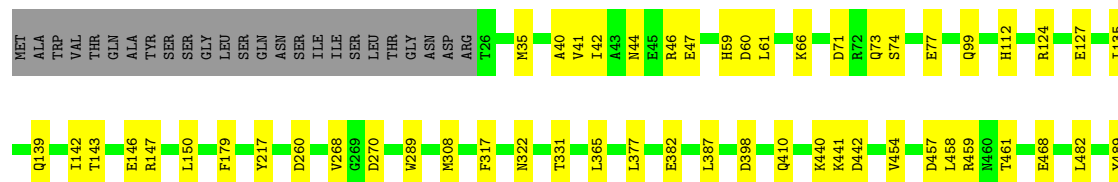
• Molecule 3: VP10

Chain Q: 84% 10% 6% .



• Molecule 4: VP4

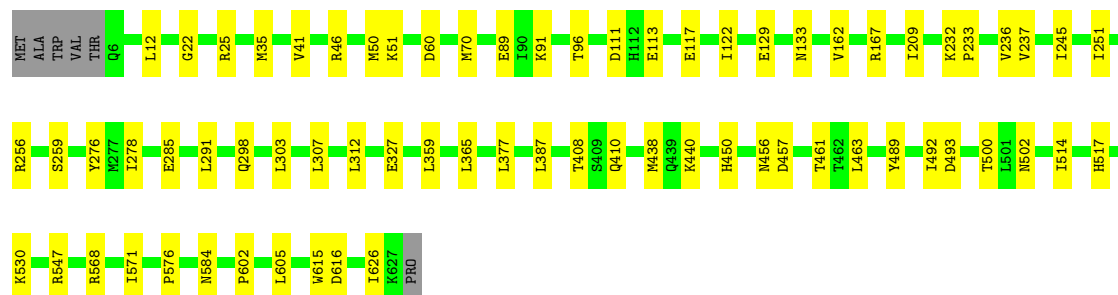
Chain R: 84% 12% .





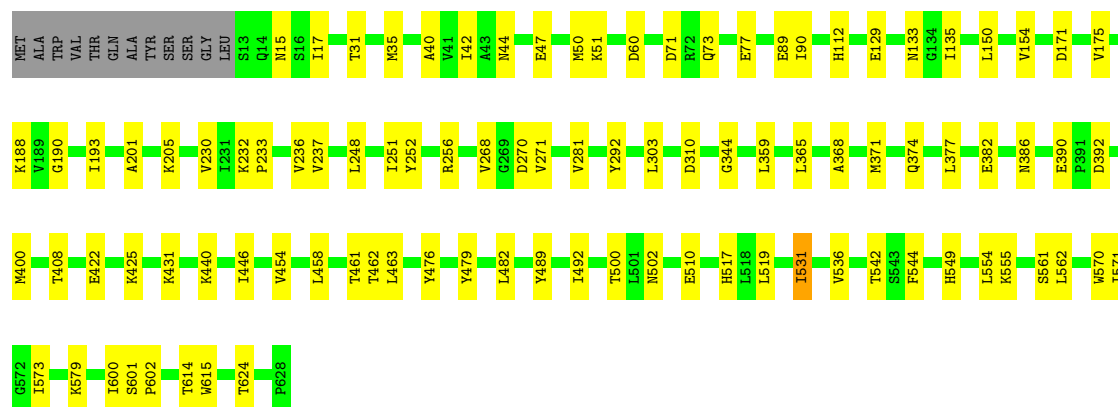
• Molecule 4: VP4

Chain S: 88% 11% .



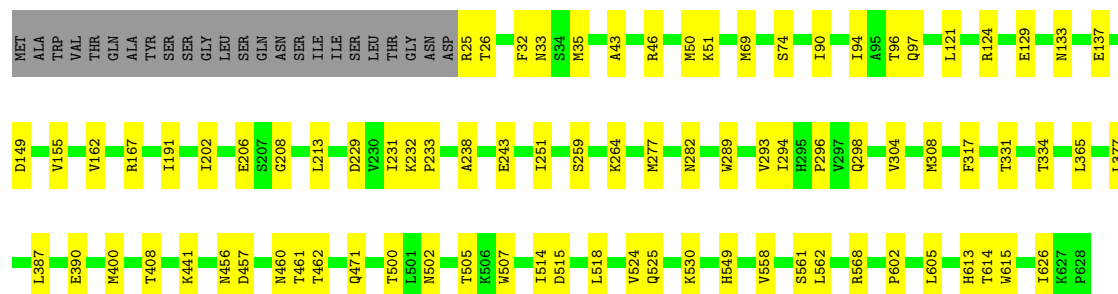
• Molecule 4: VP4

Chain T: 83% 15% .



• Molecule 4: VP4

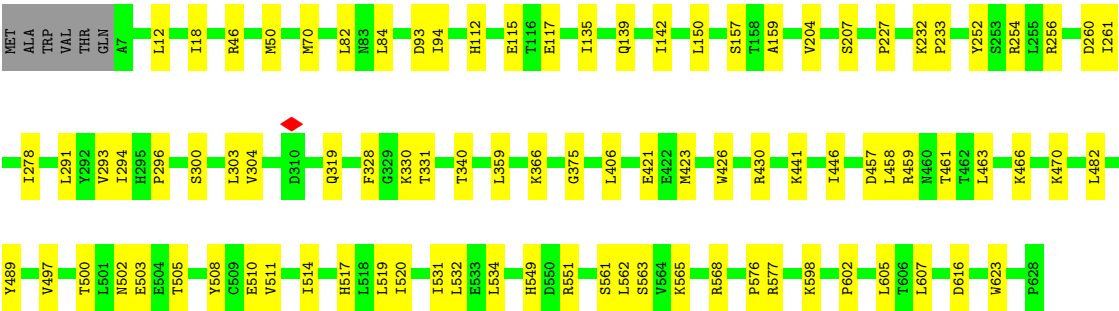
Chain U: 83% 13% .



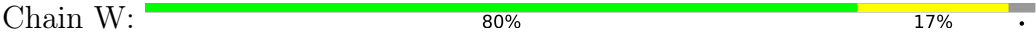
• Molecule 4: VP4

Chain V: 85% 14% .

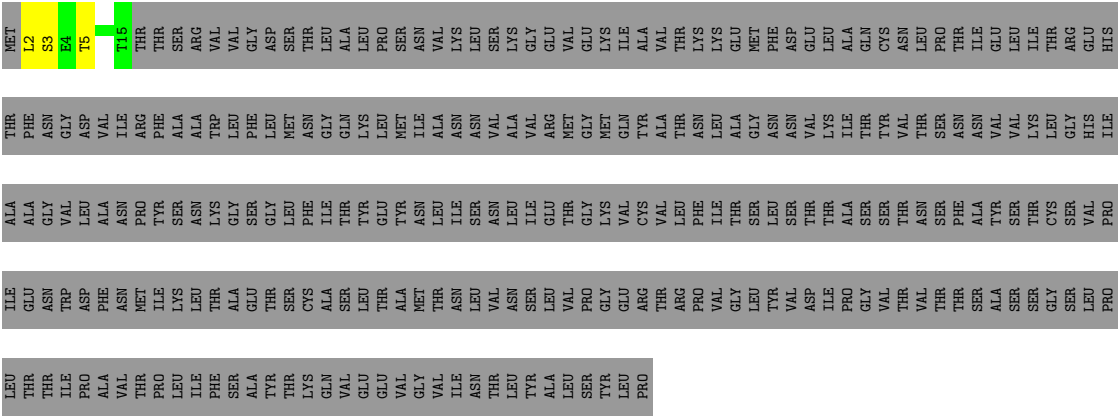




• Molecule 4: VP4



• Molecule 5: VP9



• Molecule 5: VP9



[illegible]

- Molecule 5: VP9

Chain t: 95%

[illegible]

- Molecule 5: VP9

Chain u: 95%

[illegible]

- Molecule 5: VP9

Chain v:

[illegible]

THR	THR	ILE	PRO	ALA	VAL	THR	PRO	LEU	ILE	PHE	SER	ALA	TYR	THR	LYS	GLN	VAL	GLU	GLU	VAL	GLY	VAL	ILE	ASN	THR	LEU	TYR	ALA	LEU	SER	TYR	LEU	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 5: VP9



THR	THR	ILE	PRO	ALA	VAL	THR	PRO	LEU	ILE	PHE	SER	ALA	TYR	THR	LYS	GLN	VAL	GLU	GLU	VAL	GLY	VAL	ILE	ASN	THR	LEU	TYR	ALA	LEU	SER	TYR	LEU	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34342	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	0.124	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	1140.0, 1140.0, 1140.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.85, 2.85, 2.85	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	0.12	0/6339	0.24	0/8607
1	B	0.13	0/7375	0.24	0/10006
2	C	0.13	0/2322	0.24	0/3165
2	D	0.12	0/2322	0.24	0/3165
2	E	0.12	0/2322	0.26	0/3165
2	F	0.13	0/2322	0.26	0/3165
2	G	0.13	0/2322	0.27	0/3165
2	H	0.12	0/2333	0.23	0/3179
2	I	0.12	0/2322	0.25	0/3165
2	J	0.13	0/2333	0.24	0/3179
2	K	0.22	0/2322	0.35	0/3165
2	L	0.13	0/2322	0.25	0/3165
2	M	0.12	0/2322	0.24	0/3165
2	N	0.13	0/2322	0.26	0/3165
2	O	0.21	0/2315	0.34	0/3155
3	P	0.16	0/2050	0.26	0/2772
3	Q	0.11	0/1909	0.23	0/2584
4	R	0.16	0/4806	0.29	0/6525
4	S	0.13	0/4954	0.26	0/6725
4	T	0.17	0/4911	0.31	0/6668
4	U	0.17	0/4825	0.32	0/6551
4	V	0.18	0/4953	0.30	0/6725
4	W	0.20	0/4879	0.35	0/6625
5	r	0.10	0/109	0.11	0/144
5	s	0.09	0/109	0.14	0/144
5	t	0.09	0/109	0.12	0/144
5	u	0.36	0/109	0.41	0/144
5	v	0.15	0/109	0.23	0/144
5	w	0.40	0/109	0.66	0/144
All	All	0.15	0/77856	0.28	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	45	0
1	B	7224	0	7152	69	0
2	C	2277	0	2270	24	0
2	D	2277	0	2270	34	0
2	E	2277	0	2270	24	0
2	F	2277	0	2270	47	0
2	G	2277	0	2270	29	0
2	H	2288	0	2283	32	0
2	I	2277	0	2270	33	0
2	J	2288	0	2283	29	0
2	K	2277	0	2270	22	0
2	L	2277	0	2270	35	0
2	M	2277	0	2270	31	0
2	N	2277	0	2270	28	0
2	O	2270	0	2261	19	0
3	P	2014	0	2036	32	0
3	Q	1876	0	1892	17	0
4	R	4713	0	4656	54	0
4	S	4860	0	4797	49	0
4	T	4817	0	4758	66	0
4	U	4731	0	4676	64	0
4	V	4858	0	4796	73	0
4	W	4786	0	4725	80	0
5	r	110	0	123	3	0
5	s	110	0	123	1	0
5	t	110	0	123	2	0
5	u	110	0	123	4	0
5	v	110	0	123	1	0
5	w	110	0	123	1	0
All	All	76359	0	75874	873	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 6.

All (873) 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	1.67	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
2:C:268:TYR:HD1	2:C:277:VAL:HG11	1.19	0.94
4:T:517:HIS:CD2	4:T:519:LEU:HD11	2.03	0.94
4:V:497:VAL:CG2	4:V:565:LYS:HB2	1.98	0.93
2:F:244:MET:HE1	2:G:173:ILE:HD11	1.48	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	0.90
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	0.87
2:I:170:GLU:OE2	2:I:224:ARG:HG2	1.77	0.85
4:V:532:LEU:HD11	4:V:534:LEU:HD21	1.58	0.85
3:P:145:TYR:CE1	3:P:172:PRO:HD2	2.12	0.84
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	1.62	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	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:483:ILE:HD11	4:W:554:LEU:HB2	1.62	0.79
2:D:268:TYR:CD1	2:D:277:VAL:CG2	2.61	0.79
4:U:289:TRP:CB	4:U:308:MET:SD	2.73	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
1:B:370:ARG:NH1	1:B:372:LEU:HD21	2.00	0.77
2:O:268:TYR:CD1	2:O:277:VAL:CG1	2.62	0.76
4:U:51:LYS:HD3	4:U:387:LEU:HD11	1.68	0.76
4:T:236:VAL:HG13	4:T:237:VAL:HG13	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	0.73
4:W:483:ILE:HD11	4:W:554:LEU:CB	2.18	0.72
2:H:268:TYR:CD1	2:H:277:VAL:CG2	2.67	0.72
4:R:44:ASN:HD22	4:R:47:GLU:HG3	1.53	0.72
4:U:46:ARG:HH22	4:V:50:MET:HE3	1.54	0.72
2:E:268:TYR:CD1	2:E:277:VAL:HG11	2.25	0.71
4:T:368:ALA:HA	4:T:371:MET:HE3	1.72	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:C:168:ILE:HG21	2:C:268:TYR:CD2	2.26	0.71
2:J:168:ILE:CG2	2:J:268:TYR:CD1	2.73	0.70
1:B:880:ASP:OD1	1:B:881:THR:N	2.25	0.70
4:S:46:ARG:CZ	4:S:50:MET:HE2	2.22	0.70
4:U:294:ILE:HG22	4:U:296:PRO:HD3	1.73	0.70
2:F:168:ILE:HG12	2:F:268:TYR:CE2	2.25	0.69
2:F:189:MET:HE3	2:F:208:VAL:HG23	1.74	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	2.25	0.69
4:V:46:ARG:HG2	4:W:39:ARG:HH21	1.59	0.68
2:F:139:VAL:HG22	2:F:151:MET:HG2	1.75	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
2:I:168:ILE:HG12	2:I:268:TYR:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:390:GLU:HG2	4:W:400:MET:HE1	1.75	0.68
2:J:189:MET:HE2	2:J:208:VAL:HG23	1.75	0.68
4:V:458:LEU:O	4:V:461:THR:HG22	1.94	0.67
1:B:370:ARG:HH12	1:B:372:LEU:CG	2.06	0.67
4:R:410:GLN:HE21	4:R:582:MET:HB3	1.59	0.67
2:D:268:TYR:HD1	2:D:277:VAL:CG2	2.04	0.67
2:D:185:LEU:HD12	2:D:206:ILE:HD11	1.77	0.67
4:R:468:GLU:OE1	4:R:468:GLU:N	2.28	0.67
4:U:74:SER:HB3	5:u:5:THR:HG22	1.76	0.66
1:A:576:GLU:OE2	1:A:607:ARG:NH1	2.29	0.66
1:B:576:GLU:HG2	1:B:607:ARG:NH1	2.10	0.66
4:S:50:MET:SD	4:T:50:MET:SD	2.93	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
2:J:244:MET:HE1	2:K:173:ILE:HD11	1.79	0.65
2:F:173:ILE:HD11	2:H:244:MET:HE1	1.78	0.65
2:F:244:MET:CE	2:G:173:ILE:HD11	2.22	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
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
4:W:70:MET:O	5:w:5:THR:HG21	1.97	0.65
2:G:268:TYR:HD1	2:G:277:VAL:HG21	1.55	0.65
2:N:139:VAL:HG22	2:N:151:MET:HG2	1.78	0.65
1:A:791:GLU:OE2	1:A:829:ARG:NH2	2.27	0.64
1:B:576:GLU:HG2	1:B:607:ARG:HH12	1.62	0.64
4:W:188:LYS:CG	4:W:191:ILE:HD11	2.23	0.64
3:Q:66:ASN:ND2	3:Q:68:ASN:HB2	2.13	0.64
4:W:520:ILE:HD11	4:W:531:ILE:HG22	1.80	0.64
2:F:244:MET:HE1	2:G:173:ILE:CD1	2.23	0.64
2:L:179:PRO:HD3	2:L:194:PHE:CE1	2.32	0.64
4:U:32:PHE:HA	4:U:35:MET:HE2	1.79	0.64
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
4:T:489:TYR:HA	4:T:536:VAL:HG23	1.79	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
4:V:497:VAL:HG23	4:V:565:LYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:454:VAL:HA	4:W:573:ILE:HD11	1.80	0.63
2:G:241:GLN:HB2	2:H:122:ILE:HD13	1.80	0.63
2:N:268:TYR:CD2	2:N:277:VAL:CG2	2.74	0.63
2:G:268:TYR:CD1	2:G:277:VAL:CG2	2.73	0.62
2:H:268:TYR:CE1	2:H:277:VAL:HG21	2.32	0.62
2:L:134:PRO:HG2	2:L:159:ALA:HB1	1.79	0.62
2:M:168:ILE:HG12	2:M:268:TYR:HD2	1.63	0.62
4:S:51:LYS:CD	4:S:387:LEU:CD2	2.77	0.62
2:L:268:TYR:CD1	2:L:277:VAL:CG2	2.74	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
2:C:151:MET:HE3	2:C:209:LEU:HD13	1.81	0.62
2:L:136:ARG:HE	2:L:155:GLY:CA	2.12	0.62
2:O:125:SER:HB2	2:O:265:ILE:HG13	1.82	0.61
2:C:11:ASP:OD2	2:D:194:PHE:HD2	1.82	0.61
1:A:901:LYS:NZ	1:A:905:GLU:OE2	2.31	0.61
2:L:168:ILE:HD12	2:L:268:TYR:CE2	2.35	0.61
1:B:370:ARG:NH1	1:B:372:LEU:CD2	2.63	0.61
4:U:289:TRP:HB2	4:U:308:MET:SD	2.41	0.61
2:I:169:ALA:HA	2:I:223:THR:HG22	1.83	0.61
2:L:123:PHE:HB3	2:L:261:ASP:OD1	2.01	0.61
4:R:459:ARG:HA	4:R:568:ARG:HH21	1.65	0.61
2:H:65:ASP:OD1	2:H:66:ASN: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	0.61
2:J:145:ASP:OD1	2:J:146:ARG:N	2.34	0.60
4:U:46:ARG:NH2	4:V:50:MET:HE3	2.16	0.60
4:R:41:VAL:HG11	4:R:387:LEU:HD11	1.83	0.60
2:F:13:PRO:HB2	2:F:276:ARG:NH1	2.17	0.60
1:B:542:ASP:OD1	1:B:556:ARG:CD	2.49	0.60
2:L:175:LYS:NZ	2:N:262:GLU:OE2	2.32	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	0.59
4:T:461:THR:HG23	4:T:463:LEU:HG	1.82	0.59
4:U:457:ASP:O	4:U:461:THR:HG23	2.02	0.59
2:I:134:PRO:HG2	2:I:159:ALA:HB1	1.83	0.59
4:S:51:LYS:HD3	4:S:387:LEU:HD21	1.84	0.59
4:W:51:LYS:HE2	4:W:386:ASN:CG	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:272:ASP:OD1	2:C:272:ASP:N	2.36	0.59
1:A:903:ARG:HH22	1:A:904:TYR:HE1	1.49	0.59
3:P:31:THR:OG1	3:P:61:ARG:NH1	2.35	0.59
2:F:64:ASP:OD1	2:F:109:LYS:NZ	2.34	0.59
1:A:720:ILE:HG13	1:A:750:ARG:HG3	1.84	0.59
2:E:268:TYR:CE1	2:E:277:VAL:HG21	2.37	0.59
2:N:268:TYR:CE2	2:N:277:VAL:HG21	2.35	0.59
4:R:74:SER:HB3	5:r:5:THR:HG22	1.85	0.59
4:T:365:LEU:HD22	4:T:377:LEU:HD23	1.84	0.59
4:U:602:PRO:HA	4:U:605:LEU:HD12	1.83	0.59
4:V:252:TYR:O	4:V:256:ARG:HG2	2.02	0.59
4:U:514:ILE:H	4:U:549:HIS:CE1	2.21	0.59
2:F:125:SER:HB2	2:F:265:ILE:HG13	1.84	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:F:13:PRO:HB2	2:F:276:ARG:HH12	1.68	0.58
2:J:139:VAL:HG22	2:J:151:MET:HG2	1.83	0.58
4:T:562:LEU:HD22	5:t:7:LEU:HD22	1.85	0.58
2:C:245:ASN:ND2	2:D:170:GLU:OE1	2.35	0.58
4:R:365:LEU:HD22	4:R:377:LEU:HD23	1.85	0.58
1:A:355:PRO:HB2	1:A:357:ARG:HH12	1.69	0.58
1:B:370:ARG:NH1	1:B:372:LEU:CG	2.67	0.58
1:B:791:GLU:OE2	1:B:829:ARG:NH2	2.36	0.58
4:R:143:THR:OG1	4:R:146:GLU:OE1	2.21	0.58
2:G:53:VAL:HG13	2:G:54:PRO:HD3	1.85	0.58
2:H:238:SER:HB3	2:H:291:ASP:OD2	2.04	0.58
2:K:61:LYS:O	2:K:109:LYS:NZ	2.36	0.58
2:M:13:PRO:HG2	2:M:270:ALA:HB2	1.85	0.58
3:P:145:TYR:CG	3:P:172:PRO:HG2	2.38	0.58
4:R:289:TRP:HB3	4:R:308:MET:HE3	1.86	0.58
4:R:505:THR:HG22	4:R:525:GLN:HE21	1.69	0.58
2:I:168:ILE:HG12	2:I:268:TYR:HD2	1.69	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
4:S:162:VAL:O	4:S:167:ARG:NH1	2.37	0.57
2:I:268:TYR:HD1	2:I:277:VAL:HG21	1.65	0.57
4:R:44:ASN:ND2	4:R:47:GLU:HG3	2.20	0.57
2:C:268:TYR:HD1	2:C:277:VAL:CG1	2.07	0.57
2:L:168:ILE:HD12	2:L:268:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:202:ASP:OD1	2:H:203:GLY:N	2.38	0.57
1:A:903:ARG:NH2	1:A:904:TYR:CE1	2.62	0.56
4:R:139:GLN:HB3	4:R:142:ILE:HD11	1.87	0.56
4:S:129:GLU:O	4:S:133:ASN:ND2	2.35	0.56
2:I:197:LYS:NZ	2:K:250:ASP:OD1	2.34	0.56
4:S:500:THR:HG22	4:S:502:ASN:H	1.70	0.56
4:T:112:HIS:CE1	4:T:482:LEU:H	2.23	0.56
2:I:185:LEU:HD22	2:I:204:PRO:HG2	1.87	0.56
4:R:322:ASN:OD1	4:R:322:ASN:O	2.23	0.56
4:R:562:LEU:HD11	5:r:2:LEU:HB3	1.88	0.56
4:S:456:ASN:H	4:S:461:THR:HG22	1.70	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:W:240:THR:HG23	4:W:243:GLU:H	1.70	0.56
2:J:13:PRO:HG2	2:J:270:ALA:HB2	1.87	0.56
4:V:466:LYS:HE2	4:V:563:SER:HB2	1.87	0.56
2:H:189:MET:HE2	2:H:208:VAL:CG2	2.36	0.56
4:S:307:LEU:HD21	4:S:312:LEU:HD12	1.87	0.56
1:B:810:ARG:HB2	1:B:895:GLU:HB2	1.87	0.56
4:T:188:LYS:HE2	4:T:190:GLY:O	2.06	0.56
4:V:300:SER:HA	4:V:423:MET:HE3	1.86	0.56
2:I:188:PRO:HB2	4:U:334:THR:HB	1.88	0.56
4:V:204:VAL:O	4:V:207:SER:OG	2.23	0.56
4:W:115:GLU:OE1	4:W:482:LEU:HD23	2.06	0.56
2:C:268:TYR:CD1	2:C:277:VAL:CG1	2.68	0.56
4:U:46:ARG:NH2	4:V:50:MET:CE	2.69	0.56
2:M:168:ILE:CG2	2:M:268:TYR:CE2	2.89	0.56
4:V:135:ILE:HD13	4:V:150:LEU:HB3	1.87	0.56
4:W:496:VAL:HG22	4:W:566:VAL:HG22	1.87	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:S:278:ILE:HD12	4:S:291:LEU:HD23	1.88	0.55
4:W:115:GLU:OE1	4:W:482:LEU:CD2	2.54	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
1:B:197:GLN:HG3	1:B:204:ALA:HB2	1.87	0.55
2:J:235:LEU:HB3	2:J:288:GLN:HG3	1.89	0.55
2:O:23:GLU:OE1	2:O:26:ARG:NH1	2.40	0.55
4:T:171:ASP:OD2	4:T:175:VAL:CG2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:792:ILE:HG22	1:B:916:ILE:HG22	1.89	0.55
4:V:489:TYR:CE1	4:V:576:PRO:HB2	2.42	0.55
1:B:204:ALA:HB3	1:B:925:LEU:HD22	1.89	0.55
2:L:4:ARG:HG2	2:L:4:ARG:HH11	1.72	0.55
3:P:33:PRO:O	3:P:53:THR:OG1	2.21	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
4:R:42:ILE:HD12	4:R:382:GLU:HG2	1.89	0.54
1:B:793:MET:HE3	1:B:795:MET:SD	2.47	0.54
2:L:268:TYR:HD1	2:L:277:VAL:HG21	1.65	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
2:H:139:VAL:HG22	2:H:151:MET:HG2	1.90	0.54
4:S:493:ASP:HB3	4:S:530:LYS:HZ2	1.72	0.54
1:A:805:ASP:OD1	1:A:805:ASP:N	2.34	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
4:T:51:LYS:HE2	4:T:386:ASN:OD1	2.08	0.54
4:U:514:ILE:H	4:U:549:HIS:HE1	1.56	0.54
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
3:P:145:TYR:CE1	3:P:172:PRO:HG2	2.38	0.54
4:S:492:ILE:HD11	4:S:568:ARG:HG3	1.90	0.54
2:C:238:SER:OG	2:C:291:ASP:OD2	2.24	0.54
4:T:193:ILE:HG12	4:T:205:LYS:HD3	1.89	0.54
4:T:390:GLU:HG2	4:T:400:MET:HE1	1.90	0.54
4:V:497:VAL:HG22	4:V:565:LYS:HB2	1.88	0.54
4:V:500:THR:HG22	4:V:561:SER:HA	1.89	0.54
2:H:136:ARG:HH11	2:H:155:GLY:HA3	1.73	0.54
3:P:71:ILE:HG13	3:P:114:LEU:HD21	1.90	0.53
4:U:507:TRP:HE1	4:U:524:VAL:H	1.56	0.53
4:U:457:ASP:HB2	4:U:460:ASN:HB2	1.90	0.53
2:I:293:MET:HE3	2:I:294:ARG:HG2	1.90	0.53
4:S:365:LEU:HD22	4:S:377:LEU:HD23	1.90	0.53
4:W:259:SER:HA	4:W:298:GLN:HG2	1.89	0.53
3:Q:76:SER:O	3:Q:80:SER:OG	2.23	0.53
4:T:112:HIS:HE1	4:T:482:LEU:H	1.56	0.53
4:T:129:GLU:O	4:T:133:ASN:ND2	2.31	0.53
4:U:456:ASN:H	4:U:461:THR:HG22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:251:ILE:HG13	4:T:408:THR:HG21	1.90	0.53
1:B:542:ASP:OD1	1:B:556:ARG:CG	2.56	0.53
1:B:945:ILE:HG22	1:B:947:ASP:H	1.73	0.53
1:B:336:ILE:CD1	1:B:370:ARG:NE	2.64	0.53
2:C:168:ILE:HD12	2:C:268:TYR:HE2	1.73	0.53
2:J:134:PRO:HG2	2:J:159:ALA:HB1	1.89	0.53
4:W:258:HIS:NE2	4:W:356:GLN:NE2	2.55	0.53
1:B:492:GLU:OE1	1:B:492:GLU:N	2.42	0.53
4:V:510:GLU:HB2	4:V:519:LEU:HD12	1.90	0.53
2:I:11:ASP:OD2	2:J:194:PHE:HD2	1.92	0.52
4:R:139:GLN:O	4:R:147:ARG:NH1	2.36	0.52
1:B:880:ASP:OD1	1:B:881:THR:HG23	2.09	0.52
2:G:196:TYR:HB3	2:G:198:LEU:HD21	1.90	0.52
2:C:168:ILE:HG23	2:C:268:TYR:CE2	2.44	0.52
4:U:317:PHE:HA	4:U:331:THR:HA	1.90	0.52
1:B:727:LYS:HE3	1:B:730:ILE:HD11	1.91	0.52
2:G:87:ARG:HG2	2:G:248:LEU:HB2	1.92	0.52
2:H:182:LEU:HD12	2:H:207:VAL:HG22	1.90	0.52
4:W:356:GLN:HG3	4:W:416:TRP:CZ2	2.45	0.52
2:H:125:SER:HB2	2:H:265:ILE:HG13	1.91	0.52
2:J:125:SER:HB2	2:J:265:ILE:HG13	1.92	0.52
1:A:368:VAL:HG11	1:A:948:PRO:HB3	1.90	0.52
2:H:151:MET:HE2	2:H:209:LEU:HD13	1.91	0.52
1:B:542:ASP:OD1	1:B:556:ARG:HG2	2.10	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
4:W:51:LYS:HE2	4:W:386:ASN:ND2	2.25	0.52
1:A:421:THR:HG21	1:A:598:THR:HA	1.91	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
2:K:130:GLU:HG2	2:K:164:ASN:CB	2.39	0.52
2:M:250:ASP:OD1	2:N:197:LYS:NZ	2.39	0.52
4:U:614:THR:HG22	4:U:615:TRP:N	2.25	0.52
2:F:268:TYR:CD1	2:F:277:VAL:HG21	2.44	0.52
4:V:319:GLN:HB2	4:V:423:MET:HE1	1.92	0.52
2:F:168:ILE:HG12	2:F:268:TYR:CD2	2.44	0.51
2:L:50:ASN:HB2	2:M:111:THR:HG21	1.91	0.51
2:M:168:ILE:CG2	2:M:268:TYR:CD2	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:17:ILE:HD13	4:T:368:ALA:HB2	1.91	0.51
4:T:51:LYS:HD2	4:T:386:ASN:O	2.10	0.51
1:A:841:ILE:O	1:A:845:ILE:HG12	2.10	0.51
2:I:169:ALA:HB3	2:I:200:PRO:HG2	1.92	0.51
2:J:150:THR:HG23	2:J:216:VAL:HG22	1.91	0.51
4:S:493:ASP:HB3	4:S:530:LYS:NZ	2.25	0.51
4:T:31:THR:O	4:T:35:MET:HG3	2.10	0.51
2:M:168:ILE:HD13	2:M:269:HIS:CD2	2.45	0.51
4:U:191:ILE:HD12	4:U:208:GLY:HA3	1.93	0.51
2:J:168:ILE:CG2	2:J:268:TYR:CE1	2.93	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:F:53:VAL:HG12	2:F:54:PRO:HD3	1.93	0.51
2:H:268:TYR:HD1	2:H:277:VAL:HG21	1.60	0.51
2:M:131:VAL:HG11	2:M:139:VAL:HG11	1.92	0.51
3:P:93:LEU:HD11	3:P:109:LEU:HD13	1.93	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
2:K:275:ASN:HD21	3:Q:50:PRO:HB2	1.75	0.51
4:R:317:PHE:HA	4:R:331:THR:HA	1.92	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	0.51
2:G:13:PRO:HG2	2:G:270:ALA:HB2	1.93	0.51
4:U:43:ALA:HB2	4:U:277:MET:HE1	1.92	0.51
4:U:121:LEU:HD21	4:U:231:ILE:HD12	1.93	0.51
2:F:168:ILE:HG12	2:F:268:TYR:HE2	1.71	0.50
2:M:132:LEU:HB2	2:M:162:THR:HB	1.93	0.50
4:U:238:ALA:HB1	4:U:243:GLU:HB3	1.92	0.50
3:Q:10:LYS:HG3	3:Q:11:GLU:OE1	2.12	0.50
4:T:303:LEU:HD11	4:T:359:LEU:HD13	1.93	0.50
4:V:12:LEU:HD11	4:V:406:LEU:HD13	1.93	0.50
4:V:616:ASP:OD1	4:V:616:ASP:N	2.41	0.50
4:R:135:ILE:HD13	4:R:150:LEU:HB3	1.92	0.50
4:U:515:ASP:OD1	4:U:515:ASP:N	2.44	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
2:I:11:ASP:OD2	2:J:194:PHE:CD2	2.64	0.50
1:A:784:SER:HB3	1:A:919:PRO:HA	1.94	0.50
4:U:558:VAL:HG13	4:U:561:SER:HB2	1.92	0.50
4:S:517:HIS:ND1	4:S:615:TRP:CZ3	2.80	0.50
2:G:147:ALA:HB3	2:G:219:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:145:TYR:CE1	3:P:172:PRO:CG	2.93	0.50
4:U:50:MET:SD	4:W:50:MET:SD	3.10	0.50
2:F:94:ALA:HB2	2:F:251:ILE:HD13	1.94	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
4:S:438:MET:HE1	4:S:450:HIS:ND1	2.27	0.50
4:T:422:GLU:OE2	4:T:425:LYS:NZ	2.45	0.49
2:F:182:LEU:HD12	2:F:207:VAL:HG22	1.92	0.49
2:H:189:MET:HE2	2:H:208:VAL:HG23	1.94	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
4:W:455:PHE:O	4:W:461:THR:OG1	2.22	0.49
1:A:395:LYS:NZ	1:A:680:GLU:OE1	2.46	0.49
2:E:31:VAL:HG22	2:E:110:ALA:HB3	1.94	0.49
4:W:268:VAL:HG12	4:W:431:LYS:HB2	1.94	0.49
4:W:296:PRO:HG2	4:W:355:ALA:HB2	1.95	0.49
1:A:230:VAL:HG11	1:B:155:ALA:HB2	1.93	0.49
1:B:945:ILE:HD12	1:B:945:ILE:H	1.78	0.49
2:D:243:ALA:HB1	2:D:248:LEU:HD11	1.93	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
4:T:193:ILE:HD12	4:T:201:ALA:HB1	1.95	0.49
4:T:252:TYR:O	4:T:256:ARG:HG2	2.12	0.49
4:U:562:LEU:HD13	5:u:7:LEU:HD22	1.94	0.49
1:A:463:MET:HE3	1:A:647:PRO:HA	1.94	0.49
1:A:792:ILE:HG22	1:A:916:ILE:HG22	1.94	0.49
2:D:182:LEU:HD21	2:D:198:LEU:HD21	1.95	0.49
2:O:134:PRO:HG2	2:O:159:ALA:HB1	1.94	0.49
4:S:616:ASP:OD1	4:S:616:ASP:N	2.43	0.49
4:T:536:VAL:HG12	4:T:542:THR:HB	1.95	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
4:V:562:LEU:HD23	5:v:7:LEU:HD22	1.95	0.49
1:B:796:PRO:HD2	1:B:799:ILE:HD12	1.95	0.49
2:D:125:SER:HB2	2:D:265:ILE:HG13	1.95	0.49
2:I:182:LEU:HD12	2:I:207:VAL:HG22	1.94	0.49
2:L:4:ARG:HG2	2:L:4:ARG:NH1	2.28	0.49
4:V:457:ASP:OD1	4:V:458:LEU:N	2.45	0.49
2:J:290:TYR:O	2:J:294:ARG:HG2	2.13	0.49
4:R:613:HIS:CG	4:R:626:ILE:HD11	2.48	0.49
4:S:440:LYS:NZ	4:S:440:LYS:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:94:ILE:HB	4:U:97:GLN:HG3	1.95	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
2:I:170:GLU:CD	2:I:224:ARG:HG2	2.38	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:U:251:ILE:HG12	4:U:408:THR:HG21	1.95	0.48
4:V:330:LYS:HZ3	4:V:331:THR:H	1.60	0.48
4:T:15:ASN:HB3	4:T:371:MET:SD	2.53	0.48
4:U:96:THR:HG23	4:U:213:LEU:HD22	1.95	0.48
4:W:547:ARG:HB3	4:W:549:HIS:HE1	1.78	0.48
1:B:692:LEU:HG	1:B:734:MET:HE1	1.96	0.48
2:E:46:SER:HB2	2:F:70:LEU:HD11	1.94	0.48
2:G:123:PHE:HB3	2:G:261:ASP:OD1	2.13	0.48
2:L:125:SER:HB2	2:L:265:ILE:HG13	1.94	0.48
2:L:272:ASP:OD1	2:L:272:ASP:N	2.32	0.48
2:M:125:SER:HB2	2:M:265:ILE:HG13	1.95	0.48
4:V:514:ILE:HG13	4:V:549:HIS:CD2	2.49	0.48
1:B:795:MET:HE1	1:B:822:ILE:HD13	1.95	0.48
2:D:62:PHE:CE2	2:D:293:MET:SD	3.07	0.48
2:O:44:ARG:HG3	2:O:44:ARG:HH11	1.79	0.48
2:L:183:ALA:HB2	2:L:190:PRO:HD3	1.95	0.48
4:R:522:LYS:NZ	4:R:529:GLU:OE1	2.37	0.48
2:C:152:LEU:HD13	2:C:214:PRO:HG3	1.95	0.48
2:F:123:PHE:HE2	2:F:225:ILE:HB	1.77	0.48
2:I:136:ARG:HE	2:I:155:GLY:HA2	1.79	0.48
2:I:189:MET:HE3	2:I:208:VAL:HG23	1.96	0.48
3:P:24:ALA:O	3:P:83:GLY:HA3	2.13	0.48
4:R:496:VAL:HG22	4:R:566:VAL:HG22	1.94	0.48
4:U:26:THR:OG1	4:W:310:ASP:OD1	2.27	0.48
4:U:69:MET:HE2	4:V:470:LYS:HB3	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
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
2:M:145:ASP:OD1	2:M:145:ASP:N	2.46	0.48
4:S:232:LYS:HB2	4:S:233:PRO:HD3	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:N:189:MET:HG3	2:N:190:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:59:TYR:CD1	2:E:67:PRO:HG3	2.49	0.48
2:F:13:PRO:HG2	2:F:270:ALA:HB2	1.96	0.48
4:S:122:ILE:HG23	4:S:245:ILE:HD13	1.95	0.48
1:B:330:GLN:HB3	1:B:767:PRO:HB3	1.97	0.47
2:D:168:ILE:HG21	2:D:268:TYR:CD2	2.49	0.47
2:F:134:PRO:HG2	2:F:159:ALA:HB1	1.96	0.47
4:R:46:ARG:HG2	4:R:46:ARG:HH11	1.79	0.47
2:D:89:TYR:HB2	2:D:283:LEU:HD13	1.94	0.47
2:D:182:LEU:HD12	2:D:207:VAL:HG22	1.95	0.47
2:I:35:LEU:HD12	2:I:78:MET:HE1	1.96	0.47
2:N:134:PRO:HG2	2:N:159:ALA:HB1	1.95	0.47
4:U:613:HIS:HD2	4:U:626:ILE:HG21	1.77	0.47
2:D:268:TYR:CE1	2:D:277:VAL:HG21	2.36	0.47
2:K:267:GLN:OE1	2:K:276:ARG:NH1	2.41	0.47
2:L:268:TYR:CE1	2:L:277:VAL:HG21	2.44	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:T:392:ASP:OD1	4:T:392:ASP:O	2.32	0.47
1:A:342:ILE:O	1:A:346:THR:HG23	2.13	0.47
4:T:292:TYR:OH	4:T:382:GLU:OE2	2.28	0.47
2:C:197:LYS:HD3	2:E:256:TYR:CD1	2.49	0.47
2:M:150:THR:HG23	2:M:216:VAL:HG22	1.95	0.47
4:T:601:SER:H	4:T:624:THR:CG2	2.27	0.47
4:T:614:THR:HG22	4:T:615:TRP:N	2.29	0.47
4:V:502:ASN:HB2	4:V:505:THR:HG22	1.97	0.47
4:V:503:GLU:HG2	5:u:13:LEU:HD21	1.97	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:V:254:ARG:HD3	4:V:254:ARG:HA	1.61	0.47
1:B:336:ILE:HD11	1:B:370:ARG:HE	1.73	0.47
2:C:35:LEU:HB3	2:C:62:PHE:HD1	1.79	0.47
2:C:168:ILE:CG2	2:C:268:TYR:CE2	2.98	0.47
2:C:189:MET:HE2	2:C:189:MET:HB2	1.75	0.47
2:D:123:PHE:HB3	2:D:261:ASP:OD1	2.15	0.47
4:T:510:GLU:HG2	4:T:555:LYS:HB2	1.95	0.47
4:U:94:ILE:HD12	4:U:206:GLU:OE1	2.15	0.47
4:W:230:VAL:HG12	4:W:248:LEU:HD23	1.97	0.47
4:W:307:LEU:HD23	4:W:378:ILE:HD11	1.97	0.47
1:B:380:LEU:HD11	1:B:740:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ILE:HG13	2:D:252:GLN:H	1.79	0.47
2:F:73:LYS:HB3	2:F:297:LEU:HD22	1.96	0.47
2:L:288:GLN:O	2:L:292:GLN:NE2	2.48	0.47
4:V:328:PHE:CE2	4:V:340:THR:HG21	2.50	0.47
4:W:232:LYS:HB2	4:W:233:PRO:HD3	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:L:83:THR:O	2:L:87:ARG:HG3	2.14	0.47
4:V:330:LYS:NZ	4:V:331:THR:H	2.13	0.47
4:V:482:LEU:HD21	4:V:551:ARG:HD3	1.97	0.47
2:H:131:VAL:HG11	2:H:139:VAL:HG11	1.97	0.47
2:I:245:ASN:ND2	2:J:170:GLU:OE1	2.48	0.47
3:P:8:SER:OG	3:P:11:GLU:HG3	2.15	0.47
4:U:232:LYS:HB2	4:U:233:PRO:HD3	1.97	0.47
4:V:598:LYS:HD3	4:V:623:TRP:CE2	2.51	0.47
1:A:801:VAL:HG12	1:A:822:ILE:HD12	1.97	0.46
2:G:81:ALA:O	2:G:85:VAL:HG23	2.16	0.46
2:I:184:ARG:NH1	2:I:202:ASP:O	2.47	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:W:115:GLU:OE2	4:W:551:ARG:NH1	2.48	0.46
4:V:508:TYR:CD1	4:V:602:PRO:HB3	2.50	0.46
2:C:101:VAL:HG21	3:P:180:HIS:O	2.14	0.46
2:E:136:ARG:NH1	2:E:155:GLY:HA3	2.31	0.46
2:E:139:VAL:HG22	2:E:151:MET:HG2	1.96	0.46
2:M:144:SER:OG	2:M:262:GLU:HG2	2.15	0.46
2:O:168:ILE:HG23	2:O:268:TYR:CE2	2.50	0.46
4:R:66:LYS:HB3	4:R:66:LYS:HE2	1.60	0.46
4:V:278:ILE:HD12	4:V:291:LEU:HD23	1.97	0.46
1:A:663:ASP:OD1	1:A:664:ASP:N	2.48	0.46
2:F:123:PHE:HB3	2:F:261:ASP:OD1	2.15	0.46
2:K:168:ILE:CD1	2:K:268:TYR:HD2	2.24	0.46
4:S:236:VAL:HG23	4:S:237:VAL:HG13	1.96	0.46
4:T:232:LYS:HB2	4:T:233:PRO:HD3	1.98	0.46
4:U:390:GLU:HG3	4:U:400:MET:HE1	1.97	0.46
2:C:26:ARG:HD2	2:C:116:MET:HG3	1.98	0.46
2:I:161:ILE:HD11	2:I:209:LEU:HD22	1.98	0.46
2:M:64:ASP:OD1	2:M:109:LYS:HE3	2.16	0.46
2:N:189:MET:HE2	2:N:189:MET:HB2	1.78	0.46
4:U:530:LYS:HB2	4:U:530:LYS:NZ	2.30	0.46
2:G:62:PHE:CE2	2:G:293:MET:SD	3.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:15:HIS:O	3:Q:19:THR:OG1	2.26	0.46
4:V:112:HIS:CE1	4:V:482:LEU:H	2.33	0.46
2:C:11:ASP:OD1	2:C:12:ASN:HB2	2.16	0.46
2:H:168:ILE:HG12	2:H:268:TYR:HD2	1.76	0.46
2:L:152:LEU:HD12	2:L:214:PRO:HG3	1.98	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
1:A:451:VAL:HG12	1:A:455:MET:HE2	1.97	0.46
4:V:423:MET:HE2	4:V:423:MET:HB2	1.86	0.46
2:G:268:TYR:CE1	2:G:277:VAL:HG21	2.46	0.46
2:H:134:PRO:HG2	2:H:159:ALA:HB1	1.98	0.46
2:L:134:PRO:HD2	2:L:161:ILE:HD13	1.97	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:M:130:GLU:OE2	2:M:164:ASN:ND2	2.46	0.46
4:T:42:ILE:HG12	4:T:386:ASN:ND2	2.31	0.46
2:F:170:GLU:OE1	2:H:245:ASN:ND2	2.49	0.45
2:H:33:GLU:OE2	2:H:288:GLN:NE2	2.50	0.45
3:Q:29:ILE:HD12	3:Q:30:GLY:O	2.16	0.45
3:Q:194:ARG:HE	3:Q:194:ARG:HB2	1.52	0.45
4:S:489:TYR:CZ	4:S:576:PRO:HB2	2.51	0.45
4:U:441:LYS:HE2	4:U:441:LYS:HB2	1.67	0.45
4:U:500:THR:HG22	4:U:502:ASN:H	1.82	0.45
2:L:258:SER:OG	2:M:175:LYS:NZ	2.49	0.45
4:W:489:TYR:CE1	4:W:576:PRO:HB2	2.51	0.45
2:O:59:TYR:CD1	2:O:67:PRO:HG3	2.50	0.45
3:Q:71:ILE:HG13	3:Q:114:LEU:HD11	1.98	0.45
4:T:479:TYR:OH	4:T:561:SER:OG	2.22	0.45
4:V:139:GLN:HB3	4:V:142:ILE:HD11	1.98	0.45
4:V:375:GLY:HA3	4:W:30:GLY:O	2.16	0.45
4:V:532:LEU:CD2	4:V:534:LEU:HD11	2.38	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
4:R:459:ARG:CA	4:R:568:ARG:HH21	2.29	0.45
4:V:520:ILE:HD11	4:V:531:ILE:HG23	1.97	0.45
1:A:386:LYS:HE3	1:A:386:LYS:HB3	1.73	0.45
2:K:53:VAL:CG1	2:K:54:PRO:HD3	2.47	0.45
2:L:139:VAL:HG22	2:L:151:MET:HG2	1.97	0.45
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	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:19:SER:OG	4:W:376:GLU:OE2	2.30	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:O:149:VAL:HG23	2:O:149:VAL:O	2.15	0.45
4:R:35:MET:HE3	4:T:40:ALA:HB2	1.98	0.45
4:W:489:TYR:CZ	4:W:576:PRO:HB2	2.52	0.45
2:N:150:THR:HG23	2:N:216:VAL:HG22	1.99	0.45
4:T:230:VAL:HG21	4:T:252:TYR:CE1	2.51	0.45
4:W:188:LYS:HE2	4:W:191:ILE:CD1	2.46	0.45
4:W:410:GLN:HE21	4:W:584:ASN:H	1.65	0.45
1:B:633:PHE:O	1:B:637:ARG:HG3	2.17	0.45
2:N:116:MET:SD	2:N:228:PRO:HG3	2.57	0.45
4:T:44:ASN:HB3	4:T:47:GLU:HB2	1.98	0.45
4:W:492:ILE:HD11	4:W:568:ARG:HG3	1.98	0.45
2:D:13:PRO:HG2	2:D:270:ALA:HB2	1.98	0.45
2:K:88:SER:HA	2:K:94:ALA:HB3	1.98	0.45
4:V:232:LYS:HB2	4:V:233:PRO:HD3	1.99	0.45
4:V:497:VAL:CG2	4:V:565:LYS:CB	2.85	0.45
2:D:59:TYR:CD1	2:D:67:PRO:HG3	2.52	0.45
2:G:182:LEU:HD12	2:G:207:VAL:HG22	1.99	0.45
2:K:182:LEU:HD12	2:K:207:VAL:HG22	1.99	0.45
2:M:22:ASP:OD1	2:M:22:ASP:N	2.46	0.45
4:V:532:LEU:HG	4:V:534:LEU:HG	1.97	0.45
4:W:17:ILE:HG13	4:W:395:SER:OG	2.17	0.45
4:W:24:ASP:OD1	4:W:24:ASP:N	2.49	0.45
1:A:871:LEU:HD21	1:A:888:ILE:HG23	2.00	0.44
1:A:897:ARG:HA	1:A:897:ARG:HD2	1.73	0.44
2:D:62:PHE:CZ	2:D:293:MET:SD	3.10	0.44
4:R:71:ASP:OD1	5:r:3:SER:OG	2.32	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:U:264:LYS:HG3	4:U:456:ASN:O	2.16	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
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
2:D:59:TYR:HD1	2:D:67:PRO:HG3	1.83	0.44
2:O:27:GLN:O	2:O:31:VAL:HG13	2.17	0.44
2:O:168:ILE:CG2	2:O:268:TYR:CD2	2.98	0.44
3:P:127:LYS:O	3:P:204:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:230:VAL:HG12	4:T:248:LEU:HD23	2.00	0.44
4:U:365:LEU:HD22	4:U:377:LEU:HD23	1.99	0.44
5:t:12:LYS:HB3	5:t:12:LYS:HE2	1.83	0.44
1:B:576:GLU:CG	1:B:607:ARG:NH1	2.78	0.44
2:E:68:ARG:HD2	2:E:68:ARG:HA	1.83	0.44
4:R:40:ALA:HB2	4:S:35:MET:HE2	1.98	0.44
4:S:122:ILE:HG12	4:S:245:ILE:HG23	2.00	0.44
4:T:531:ILE:HG21	4:T:554:LEU:HD11	1.99	0.44
4:V:446:ILE:HD13	4:V:446:ILE:HA	1.85	0.44
1:A:793:MET:HE1	1:A:819:PRO:HD2	2.00	0.44
1:B:816:THR:O	1:B:917:LYS:NZ	2.50	0.44
2:D:56:VAL:HG22	2:D:67:PRO:HG2	1.98	0.44
2:F:47:ASP:HB3	2:G:112:VAL:HG22	1.99	0.44
3:P:225:LEU:HD11	3:P:234:ILE:HD11	2.00	0.44
4:W:38:PRO:HB2	4:W:379:GLY:HA3	2.00	0.44
2:D:198:LEU:HD22	2:D:205:PHE:CE1	2.53	0.44
2:F:168:ILE:HG23	2:F:268:TYR:CE2	2.51	0.44
4:W:282:ASN:O	4:W:285:GLU:HB2	2.17	0.44
4:W:421:GLU:OE2	4:W:577:ARG:NH2	2.51	0.44
2:F:130:GLU:HG3	2:F:164:ASN:HB3	1.99	0.44
2:H:59:TYR:CD2	2:H:67:PRO:HG3	2.52	0.44
4:T:135:ILE:HD13	4:T:150:LEU:HB3	2.00	0.44
4:W:492:ILE:HD12	4:W:570:TRP:CE2	2.53	0.44
4:W:515:ASP:OD1	4:W:515:ASP:N	2.50	0.44
1:A:374:GLN:HE21	1:A:551:PRO:HD3	1.83	0.44
2:H:130:GLU:HG3	2:H:164:ASN:HB3	1.99	0.44
4:S:70:MET:HE2	4:S:70:MET:HB2	1.92	0.44
4:U:202:ILE:O	4:U:206:GLU:HG2	2.17	0.44
4:U:259:SER:HA	4:U:298:GLN:HG2	1.99	0.44
4:W:43:ALA:HB2	4:W:277:MET:HE1	2.00	0.44
4:W:590:LYS:HA	4:W:590:LYS:HD3	1.63	0.44
1:A:642:GLU:H	1:A:642:GLU:HG2	1.59	0.43
2:N:31:VAL:HG12	2:N:78:MET:HE1	1.99	0.43
1:A:837:MET:SD	1:B:954:ARG:HB2	2.57	0.43
3:Q:233:LEU:HD23	3:Q:233:LEU:HA	1.86	0.43
4:U:471:GLN:NE2	4:W:207:SER:OG	2.44	0.43
4:W:503:GLU:H	4:W:503:GLU:HG2	1.58	0.43
2:K:168:ILE:CD1	2:K:268:TYR:CD2	3.00	0.43
2:L:20:TYR:OH	2:L:98:VAL:O	2.28	0.43
4:R:99:GLN:O	4:R:217:TYR:OH	2.32	0.43
1:B:895:GLU:OE2	1:B:897:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:LYS:HB2	2:F:73:LYS:HE2	1.85	0.43
2:F:122:ILE:HD13	2:H:241:GLN:HB2	2.00	0.43
2:I:29:VAL:HG12	2:I:285:LEU:HD23	2.00	0.43
2:I:53:VAL:O	2:I:57:GLN:HG3	2.19	0.43
4:S:46:ARG:NH2	4:S:50:MET:HE2	2.34	0.43
4:S:89:GLU:HB2	4:S:91:LYS:HZ2	1.83	0.43
2:N:131:VAL:HG11	2:N:139:VAL:HG11	2.00	0.43
3:P:111:THR:HB	3:P:114:LEU:HD22	2.00	0.43
3:Q:161:ILE:HD13	3:Q:161:ILE:HA	1.83	0.43
4:R:61:LEU:HD21	4:T:60:ASP:HB2	2.00	0.43
4:R:459:ARG:C	4:R:568:ARG:HH21	2.25	0.43
4:T:476:TYR:CG	4:T:602:PRO:HG2	2.53	0.43
4:U:124:ARG:HB3	4:U:155:VAL:HB	2.01	0.43
2:D:187:GLN:OE1	2:D:188:PRO:HD2	2.19	0.43
4:S:514:ILE:HD13	4:S:547:ARG:HE	1.84	0.43
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: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
2:J:246:ASP:OD1	2:J:246:ASP:N	2.50	0.43
3:P:55:LEU:HD22	3:P:84:HIS:CE1	2.54	0.43
3:P:245:LYS:HB2	3:P:245:LYS:HE2	1.69	0.43
4:U:129:GLU:O	4:U:133:ASN:ND2	2.52	0.43
1:B:109:PHE:HB2	1:B:123:LYS:HG2	2.00	0.43
1:B:359:LYS:HB2	1:B:362:GLU:HG3	2.00	0.43
1:B:866:ASP:OD1	1:B:867:GLY:N	2.52	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
2:M:11:ASP:OD1	2:M:12:ASN:HB2	2.18	0.43
4:T:73:GLN:NE2	4:T:77:GLU:OE2	2.50	0.43
4:W:112:HIS:CE1	4:W:482:LEU:H	2.36	0.43
4:W:377:LEU:HD23	4:W:377:LEU:HA	1.86	0.43
4:W:547:ARG:HB3	4:W:549:HIS:CE1	2.54	0.43
1:A:830:ILE:HD13	1:A:838:MET:HE1	2.01	0.43
2:F:267:GLN:OE1	2:F:276:ARG:HD3	2.19	0.43
2:F:274:ILE:HG22	3:P:50:PRO:HD2	2.01	0.43
2:O:139:VAL:HG22	2:O:151:MET:HG2	2.00	0.43
4:U:51:LYS:CD	4:U:387:LEU:CD1	2.92	0.43
5:u:13:LEU:HD23	5:u:13:LEU:HA	1.79	0.43
1:A:513:VAL:HA	1:A:516:ASP:OD2	2.19	0.43
2:F:294:ARG:NH1	2:F:297:LEU:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:294:ARG:HA	2:L:294:ARG:HD3	1.85	0.43
3:P:38:LEU:HB3	3:P:48:LEU:HB3	2.01	0.43
4:S:571:ILE:HD13	4:S:571:ILE:HA	1.91	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
2:C:168:ILE:CG2	2:C:268:TYR:CD2	2.98	0.42
2:F:123:PHE:CE2	2:F:225:ILE:HB	2.53	0.42
2:N:241:GLN:NE2	2:N:258:SER:O	2.52	0.42
4:S:251:ILE:HG12	4:S:408:THR:HG21	2.01	0.42
4:U:167:ARG:NH1	4:U:229:ASP:OD1	2.52	0.42
4:W:113:GLU:O	4:W:117:GLU:HG3	2.19	0.42
1:A:222:VAL:HG11	2:K:53:VAL:HG21	2.01	0.42
1:A:793:MET:HE1	1:A:819:PRO:HG2	2.01	0.42
1:B:735:LEU:HD23	1:B:735:LEU:HA	1.91	0.42
2:C:22:ASP:OD1	2:C:22:ASP:N	2.46	0.42
2:I:116:MET:HA	2:I:228:PRO:HG3	2.02	0.42
2:J:182:LEU:HD12	2:J:207:VAL:HG22	2.01	0.42
2:N:68:ARG:HG3	2:N:71:ARG:HH21	1.84	0.42
4:R:143:THR:HG22	4:R:398:ASP:OD2	2.18	0.42
4:U:507:TRP:NE1	4:U:524:VAL:H	2.18	0.42
4:V:463:LEU:HD23	4:V:463:LEU:HA	1.83	0.42
4:W:483:ILE:HD11	4:W:554:LEU:HB3	1.96	0.42
1:A:319:MET:HE1	1:A:782:ASP:HB2	2.01	0.42
1:B:791:GLU:HB3	1:B:818:LEU:HD12	2.01	0.42
2:E:123:PHE:HB3	2:E:261:ASP:OD1	2.19	0.42
2:J:70:LEU:HD23	2:J:70:LEU:HA	1.90	0.42
2:N:151:MET:HE3	2:N:151:MET:HB2	1.84	0.42
4:W:455:PHE:HA	4:W:461:THR:HG23	2.02	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:M:4:ARG:NH1	2:M:130:GLU:HB3	2.34	0.42
3:P:112:ASN:OD1	3:P:112:ASN:N	2.47	0.42
4:R:441:LYS:HG2	4:R:442:ASP:OD1	2.19	0.42
4:S:463:LEU:HB2	4:S:568:ARG:NH2	2.34	0.42
2:J:113:SER:HB3	2:M:71:ARG:CZ	2.49	0.42
2:M:185:LEU:HD23	2:M:185:LEU:HA	1.90	0.42
4:R:112:HIS:CE1	4:R:482:LEU:H	2.37	0.42
4:R:410:GLN:HE21	4:R:582:MET:CB	2.29	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
2:D:78:MET:HE3	2:D:106:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:89:TYR:HB2	2:K:283:LEU:HD13	2.01	0.42
4:R:621:GLY:HA3	4:T:193:ILE:O	2.19	0.42
4:S:410:GLN:NE2	4:S:584:ASN:H	2.17	0.42
1:B:435:THR:HA	1:B:438:LEU:HD12	2.01	0.42
3:P:2:ASP:OD1	3:P:2:ASP:N	2.51	0.42
4:R:73:GLN:NE2	4:R:77:GLU:OE2	2.53	0.42
4:W:270:ASP:OD1	4:W:270: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:O:77:LYS:HE3	2:O:77:LYS:HB2	1.85	0.42
4:T:42:ILE:HG12	4:T:386:ASN:HD22	1.85	0.42
4:T:579:LYS:HB3	4:T:579:LYS:HE2	1.77	0.42
4:W:544:PHE:CE2	4:W:612:TRP:CZ3	3.07	0.42
1:B:21:GLN:NE2	1:B:48:ARG:HD2	2.34	0.42
1:B:289:THR:HB	1:B:292:GLU:HG3	2.02	0.42
4:W:330:LYS:HB2	4:W:330:LYS:NZ	2.34	0.42
4:W:514:ILE:HG21	4:W:547:ARG:HE	1.85	0.42
1:B:21:GLN:HE22	1:B:48:ARG:HD2	1.85	0.42
1:B:370:ARG:HH12	1:B:372:LEU:CD2	2.29	0.42
2:I:188:PRO:HG3	4:U:331:THR:HG23	2.02	0.42
2:L:22:ASP:O	2:L:26:ARG:HG3	2.20	0.42
2:L:70:LEU:HD23	2:L:70:LEU:HA	1.91	0.42
4:U:46:ARG:HH22	4:V:50:MET:CE	2.26	0.42
4:U:568:ARG:HB3	4:U:568:ARG:NH1	2.34	0.42
2:F:27:GLN:OE1	3:P:193:TYR:HB2	2.20	0.41
2:F:115:ASP:C	2:F:115:ASP:OD1	2.63	0.41
2:M:272:ASP:OD1	2:M:275:ASN:HB2	2.19	0.41
2:N:126:VAL:HA	2:N:127:PRO:HD3	1.91	0.41
2:N:184:ARG:HH11	2:N:202:ASP:HB3	1.84	0.41
4:T:440:LYS:HE3	4:T:440:LYS:HB3	1.77	0.41
4:W:519:LEU:HD11	4:W:600:ILE:HD12	2.02	0.41
2:F:268:TYR:CD1	2:F:277:VAL:CG2	3.03	0.41
2:H:126:VAL:HG12	2:H:144:SER:O	2.20	0.41
2:I:116:MET:HE2	2:I:282:ILE:HA	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
2:G:258:SER:OG	2:H:175:LYS:NZ	2.46	0.41
2:L:291:ASP:OD1	2:L:295:ARG:HD3	2.20	0.41
3:Q:18:LYS:HB2	3:Q:18:LYS:HE3	1.82	0.41
4:T:71:ASP:OD1	4:T:71:ASP:N	2.53	0.41
4:V:421:GLU:OE2	4:V:577:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:532:LEU:HD21	4:V:534:LEU:HD21	2.01	0.41
4:W:268:VAL:HG23	4:W:270:ASP:OD1	2.21	0.41
1:B:183:LEU:HD22	1:B:243:VAL:HG13	2.02	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:E:73:LYS:HB3	2:E:297:LEU:HD22	2.01	0.41
2:N:115:ASP:OD1	2:N:115:ASP:C	2.64	0.41
2:N:233:LYS:HE3	2:N:233:LYS:HB3	1.81	0.41
1:B:845:ILE:HG13	1:B:849:PHE:HE1	1.84	0.41
2:D:35:LEU:HB3	2:D:62:PHE:HD1	1.86	0.41
2:E:294:ARG:HA	2:E:294:ARG:HD3	1.81	0.41
3:P:175:MET:O	3:P:179:ILE:HD13	2.20	0.41
4:S:276:TYR:OH	4:S:327:GLU:OE2	2.29	0.41
4:V:157:SER:C	4:V:159:ALA:H	2.28	0.41
1:A:576:GLU:N	1:A:576:GLU:OE1	2.54	0.41
1:B:460:ARG:HH21	3:P:222:ASN:HA	1.86	0.41
2:F:23:GLU:O	2:F:27:GLN:HG3	2.20	0.41
2:H:251:ILE:HB	2:H:254:VAL:HG11	2.02	0.41
2:J:168:ILE:CG2	2:J:268:TYR:HD1	2.09	0.41
2:M:22:ASP:OD1	2:M:25:SER:OG	2.32	0.41
2:N:83:THR:HG22	2:N:290:TYR:HE1	1.85	0.41
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:503:GLU:OE2	4:R:504:GLU:N	2.51	0.41
4:S:113:GLU:O	4:S:117:GLU:HG3	2.21	0.41
4:V:607:LEU:HD12	4:V:607:LEU:HA	1.93	0.41
4:W:371:MET:HE2	4:W:371:MET:HB3	1.97	0.41
1:B:200:ASN:OD1	1:B:200:ASN:N	2.54	0.41
2:C:168:ILE:HD12	2:C:268:TYR:CE2	2.53	0.41
4:R:60:ASP:OD2	4:R:60:ASP:N	2.53	0.41
4:R:260:ASP:HB3	4:R:457:ASP:OD1	2.21	0.41
4:U:282:ASN:ND2	4:V:18:ILE:HD13	2.36	0.41
4:U:614:THR:CG2	4:U:615:TRP:N	2.84	0.41
4:V:70:MET:HE3	4:V:70:MET:HB3	1.96	0.41
4:V:605:LEU:HD23	4:V:605:LEU:HA	1.86	0.41
4:W:328:PHE:CE2	4:W:340:THR:HG21	2.55	0.41
4:W:398:ASP:OD2	4:W:402:LYS:NZ	2.50	0.41
1:A:319:MET:HE2	1:A:319:MET:HB2	1.95	0.41
1:B:480:MET:HG3	1:B:484:ARG:HG3	2.03	0.41
2:D:115:ASP:OD1	2:D:115:ASP:C	2.63	0.41
2:F:113:SER:HB2	3:P:194:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:125:SER:HB2	2:G:265:ILE:HG13	2.02	0.41
2:H:95:PRO:HG3	3:Q:37:VAL:HG21	2.03	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
2:L:179:PRO:HD3	2:L:194:PHE:CZ	2.55	0.41
2:L:189:MET:HE2	2:L:189:MET:HB2	1.93	0.41
2:L:201:LEU:HD23	2:L:201:LEU:HA	1.88	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
3:P:29:ILE:HD12	3:P:29:ILE:HA	1.85	0.41
4:R:59:HIS:CD2	4:R:179:PHE:H	2.38	0.41
4:S:60:ASP:OD2	4:S:60:ASP:N	2.52	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:518:LEU:HD12	4:W:518:LEU:HA	1.80	0.41
5:s:2:LEU:HD12	5:s:2:LEU:HA	1.89	0.41
1:B:945:ILE:HD12	1:B:945:ILE:N	2.36	0.41
2:E:71:ARG:NE	2:G:113:SER:OG	2.45	0.41
2:J:59:TYR:CD2	2:J:67:PRO:HG3	2.56	0.41
2:K:198:LEU:HD22	2:K:205:PHE:CE1	2.56	0.41
4:R:112:HIS:HE1	4:R:482:LEU:H	1.68	0.41
4:S:285:GLU:H	4:S:285:GLU:HG3	1.64	0.41
4:T:89:GLU:H	4:T:89:GLU:HG3	1.65	0.41
1:A:543:MET:SD	1:A:555:GLY:HA3	2.61	0.40
2:F:44:ARG:HH22	2:G:230:ALA:HB1	1.85	0.40
2:N:175:LYS:HB2	2:N:175:LYS:HE2	1.69	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:12:LEU:HD12	4:S:12:LEU:HA	1.88	0.40
4:U:33:ASN:OD1	4:W:284:THR:HA	2.20	0.40
1:B:793:MET:CE	1:B:795:MET:SD	3.09	0.40
2:F:89:TYR:HB2	2:F:283:LEU:HD13	2.03	0.40
2:G:68:ARG:HB2	2:G:71:ARG:HB2	2.03	0.40
4:R:579:LYS:HD2	4:R:579:LYS:HA	1.80	0.40
4:U:293:VAL:HG22	4:U:304:VAL:HG22	2.04	0.40
1:B:336:ILE:HD13	1:B:370:ARG:NE	2.10	0.40
2:L:153:ASN:OD1	2:L:211:VAL:HA	2.21	0.40
2:N:77:LYS:HB3	2:N:77:LYS:HE3	1.71	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
4:W:463:LEU:C	4:W:463:LEU:HD12	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:40:ILE:O	2:G:44:ARG:HG3	2.21	0.40
2:M:89:TYR:HB2	2:M:283:LEU:HD13	2.04	0.40
2:O:44:ARG:HG3	2:O:44:ARG:NH1	2.36	0.40
3:P:93:LEU:HD23	3:P:93:LEU:HA	1.83	0.40
4:V:426:TRP:CZ2	4:V:430:ARG:HD3	2.57	0.40
4:W:616:ASP:OD1	4:W:617:GLN:N	2.54	0.40
1:A:494:TYR:OH	1:A:533:VAL:O	2.35	0.40
2:F:240:PHE:CE2	2:F:244:MET:SD	3.14	0.40
3:Q:101:ILE:HD13	3:Q:107:THR:HG21	2.03	0.40
4:T:500:THR:HG22	4:T:502:ASN:H	1.87	0.40
4:T:571:ILE:HD13	4:T:571:ILE:HA	1.89	0.40
4:U:149:ASP:OD1	4:U:162:VAL:HG22	2.22	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	296/301 (98%)	291 (98%)	5 (2%)	0	100	100
2	D	296/301 (98%)	289 (98%)	7 (2%)	0	100	100
2	E	296/301 (98%)	293 (99%)	3 (1%)	0	100	100
2	F	296/301 (98%)	293 (99%)	3 (1%)	0	100	100
2	G	296/301 (98%)	289 (98%)	7 (2%)	0	100	100
2	H	297/301 (99%)	293 (99%)	4 (1%)	0	100	100
2	I	296/301 (98%)	287 (97%)	9 (3%)	0	100	100
2	J	297/301 (99%)	292 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	296/301 (98%)	292 (99%)	4 (1%)	0	100	100
2	L	296/301 (98%)	291 (98%)	5 (2%)	0	100	100
2	M	296/301 (98%)	292 (99%)	4 (1%)	0	100	100
2	N	296/301 (98%)	291 (98%)	5 (2%)	0	100	100
2	O	295/301 (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
All	All	9737/11787 (83%)	9598 (99%)	139 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	687/846 (81%)	682 (99%)	5 (1%)	76	80
1	B	805/846 (95%)	802 (100%)	3 (0%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	248/251 (99%)	247 (100%)	1 (0%)	84	83
2	D	248/251 (99%)	248 (100%)	0	100	100
2	E	248/251 (99%)	248 (100%)	0	100	100
2	F	248/251 (99%)	246 (99%)	2 (1%)	73	79
2	G	248/251 (99%)	247 (100%)	1 (0%)	84	83
2	H	249/251 (99%)	248 (100%)	1 (0%)	84	83
2	I	248/251 (99%)	247 (100%)	1 (0%)	84	83
2	J	249/251 (99%)	248 (100%)	1 (0%)	84	83
2	K	248/251 (99%)	248 (100%)	0	100	100
2	L	248/251 (99%)	244 (98%)	4 (2%)	55	69
2	M	248/251 (99%)	247 (100%)	1 (0%)	84	83
2	N	248/251 (99%)	246 (99%)	2 (1%)	73	79
2	O	247/251 (98%)	247 (100%)	0	100	100
3	P	225/225 (100%)	222 (99%)	3 (1%)	61	73
3	Q	211/225 (94%)	211 (100%)	0	100	100
4	R	510/532 (96%)	509 (100%)	1 (0%)	87	86
4	S	527/532 (99%)	526 (100%)	1 (0%)	87	86
4	T	523/532 (98%)	521 (100%)	2 (0%)	84	83
4	U	512/532 (96%)	512 (100%)	0	100	100
4	V	527/532 (99%)	524 (99%)	3 (1%)	78	82
4	W	519/532 (98%)	516 (99%)	3 (1%)	78	82
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	8349/10067 (83%)	8314 (100%)	35 (0%)	81	83

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	463	MET

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Mol	Chain	Res	Type
1	A	566	LEU
1	A	676	GLU
1	A	695	VAL
1	A	702	LEU
1	B	463	MET
1	B	763	VAL
1	B	876	LEU
2	C	201	LEU
2	F	184	ARG
2	F	297	LEU
2	G	229	LEU
2	H	168	ILE
2	I	151	MET
2	J	152	LEU
2	L	78	MET
2	L	152	LEU
2	L	229	LEU
2	L	272	ASP
2	M	66	ASN
2	N	27	GLN
2	N	152	LEU
3	P	59	VAL
3	P	228	ARG
3	P	236	LEU
4	R	597	ASP
4	S	626	ILE
4	T	154	VAL
4	T	531	ILE
4	V	261	ILE
4	V	366	LYS
4	V	441	LYS
4	W	47	GLU
4	W	50	MET
4	W	626	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	ASN
1	A	373	ASN
1	A	374	GLN
1	A	411	GLN

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Mol	Chain	Res	Type
1	A	493	GLN
1	A	825	ASN
1	B	21	GLN
1	B	37	GLN
1	B	118	GLN
1	B	279	GLN
1	B	309	ASN
1	B	562	ASN
1	B	659	GLN
1	B	717	ASN
1	B	751	ASN
1	B	800	ASN
1	B	825	ASN
1	B	889	HIS
2	D	27	GLN
2	D	80	ASN
2	D	292	GLN
2	F	124	ASN
2	G	84	ASN
2	G	93	ASN
2	G	226	GLN
2	G	275	ASN
2	H	19	ASN
2	H	164	ASN
2	H	232	ASN
2	H	241	GLN
2	H	292	GLN
2	I	93	ASN
2	I	245	ASN
2	J	100	GLN
2	J	181	GLN
2	J	288	GLN
2	K	269	HIS
2	L	3	ASN
2	L	66	ASN
2	L	164	ASN
2	L	292	GLN
2	M	19	ASN
2	M	167	GLN
2	M	187	GLN
3	P	15	HIS
3	P	35	GLN

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Mol	Chain	Res	Type
3	P	68	ASN
3	Q	112	ASN
3	Q	165	GLN
3	Q	182	GLN
4	R	33	ASN
4	R	44	ASN
4	R	73	GLN
4	R	98	HIS
4	R	128	ASN
4	R	214	ASN
4	R	319	GLN
4	R	339	ASN
4	R	410	GLN
4	R	545	ASN
4	S	44	ASN
4	S	62	ASN
4	S	73	GLN
4	S	128	ASN
4	S	214	ASN
4	S	356	GLN
4	T	48	HIS
4	T	98	HIS
4	T	290	GLN
4	T	397	GLN
4	T	488	HIS
4	T	517	HIS
4	T	622	ASN
4	U	48	HIS
4	U	101	ASN
4	U	128	ASN
4	U	306	GLN
4	U	464	HIS
4	U	471	GLN
4	U	549	HIS
4	U	622	ASN
4	V	15	ASN
4	V	23	ASN
4	V	101	ASN
4	V	128	ASN
4	V	212	GLN
4	V	319	GLN
4	V	350	GLN

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Mol	Chain	Res	Type
4	V	405	HIS
4	V	456	ASN
4	V	545	ASN
4	V	604	HIS
4	W	15	ASN
4	W	73	GLN
4	W	101	ASN
4	W	218	HIS
4	W	397	GLN
4	W	405	HIS
4	W	526	HIS
4	W	622	ASN
4	W	625	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

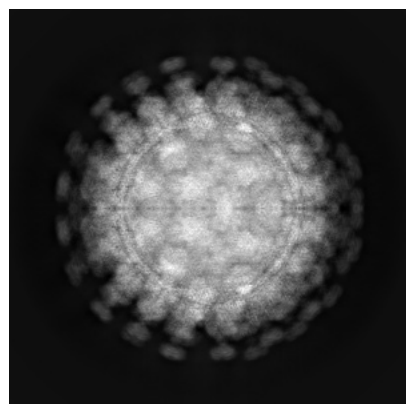
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37378. These allow visual inspection of the internal detail of the map and identification of artifacts.

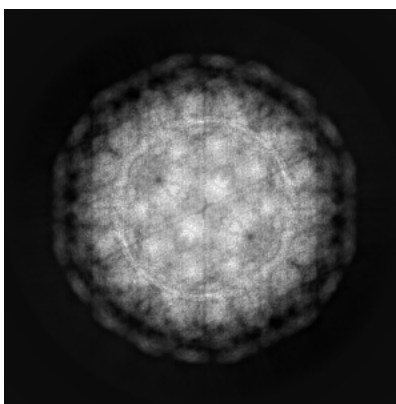
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

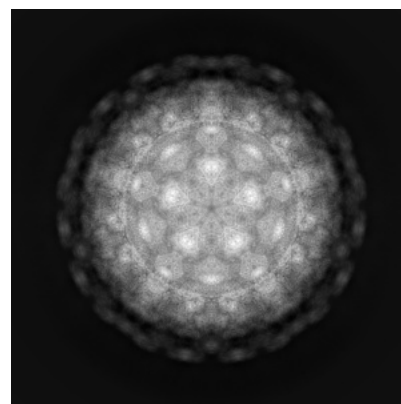
6.1.1 Primary map



X

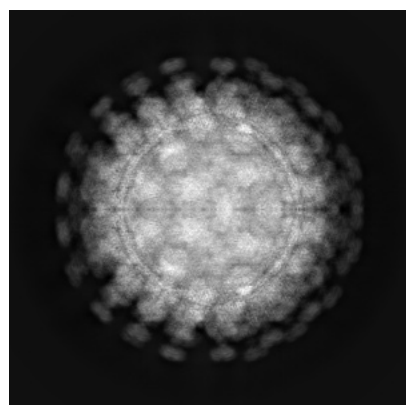


Y

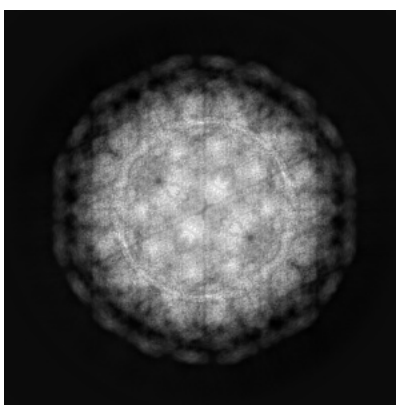


Z

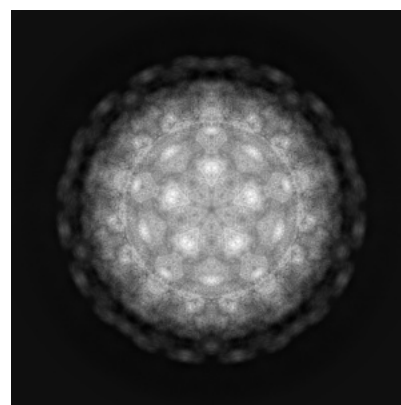
6.1.2 Raw map



X



Y

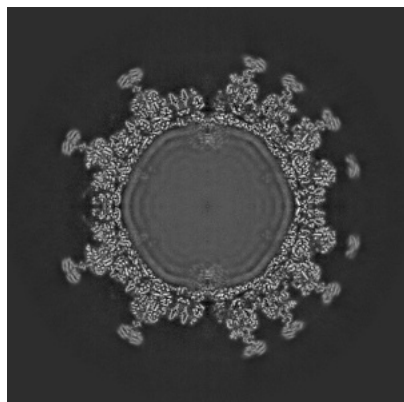


Z

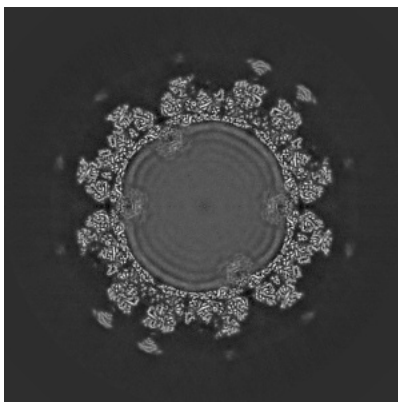
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

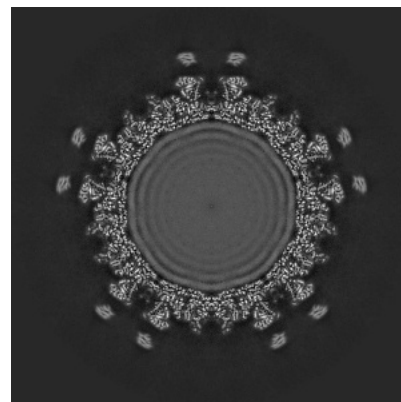
6.2.1 Primary map



X Index: 200

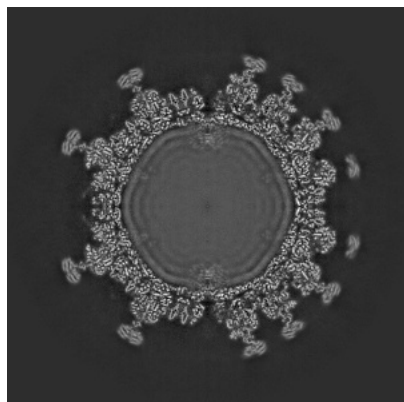


Y Index: 200

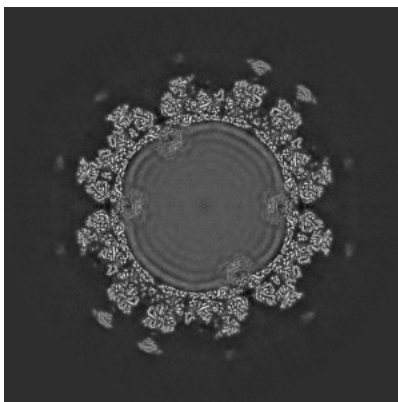


Z Index: 200

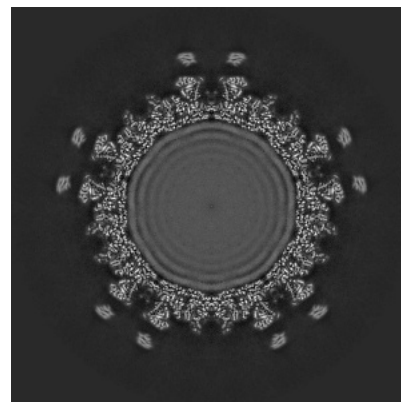
6.2.2 Raw map



X Index: 200



Y Index: 200

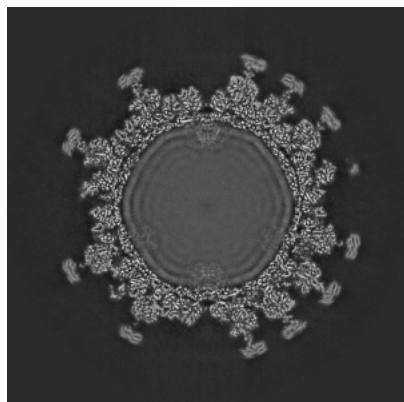


Z Index: 200

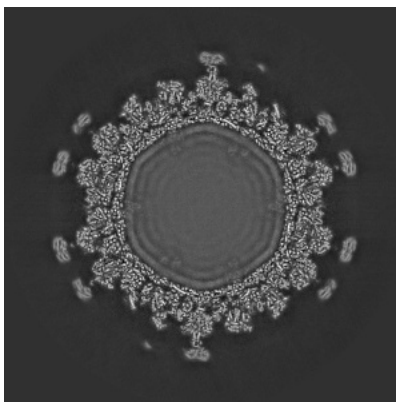
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

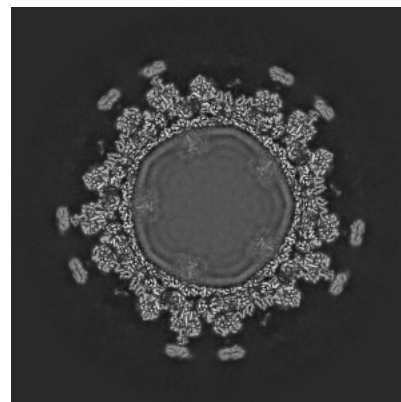
6.3.1 Primary map



X Index: 203

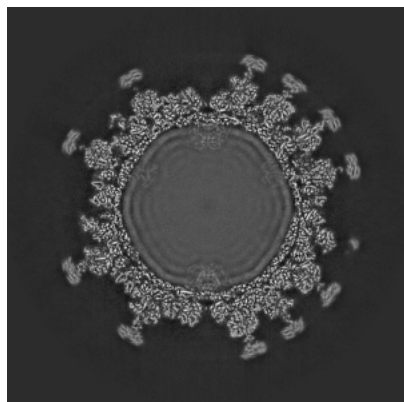


Y Index: 219

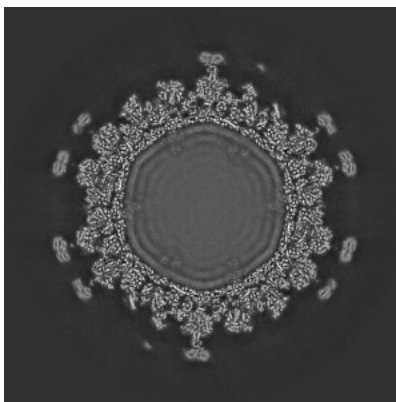


Z Index: 224

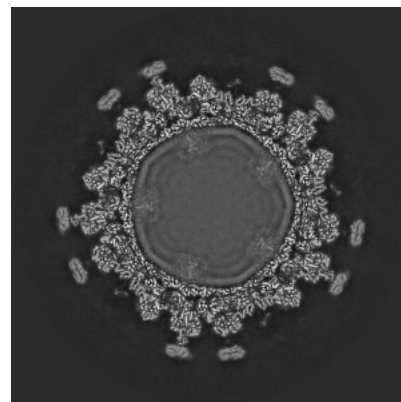
6.3.2 Raw map



X Index: 197



Y Index: 219

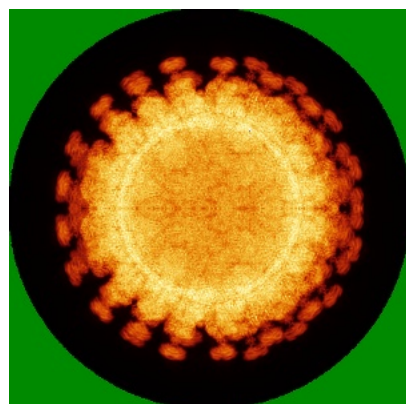


Z Index: 224

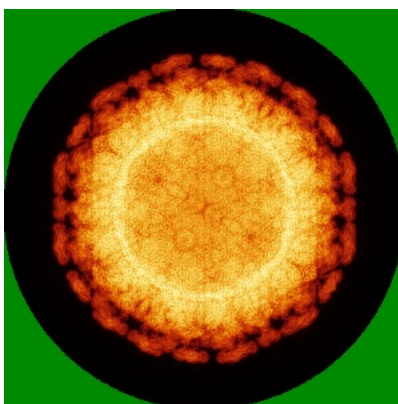
The images above show the largest variance slices of the map in three orthogonal directions.

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

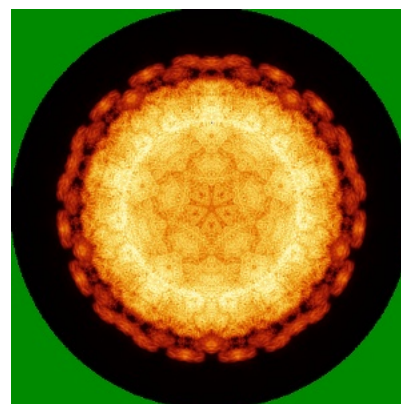
6.4.1 Primary map



X

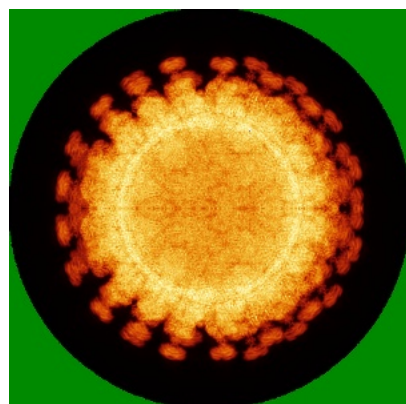


Y

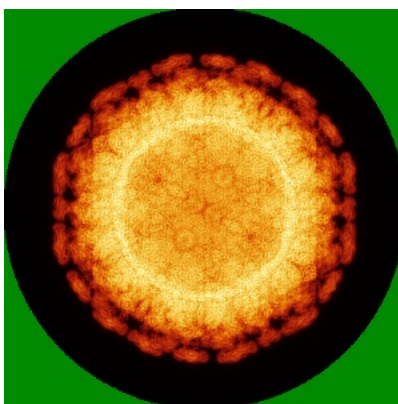


Z

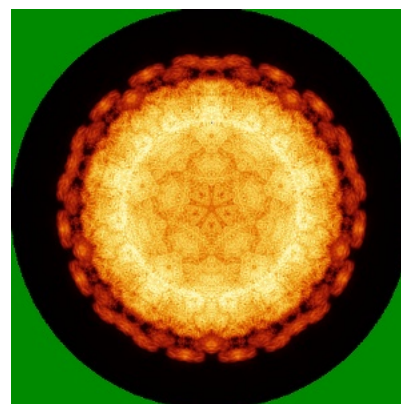
6.4.2 Raw map



X



Y



Z

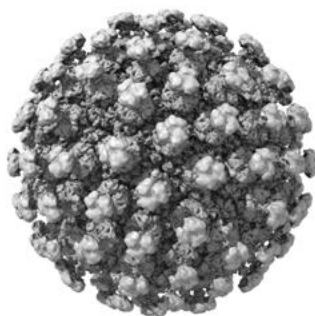
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

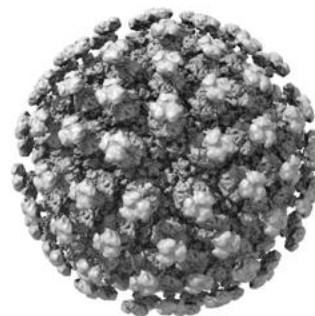
6.5.1 Primary map



X



Y



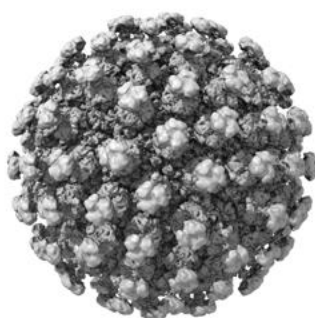
Z

The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

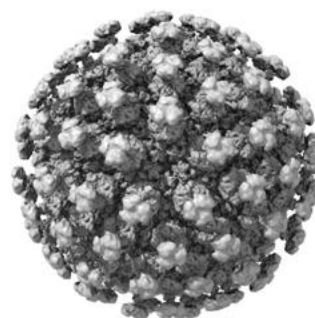
6.5.2 Raw map



X



Y



Z

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.

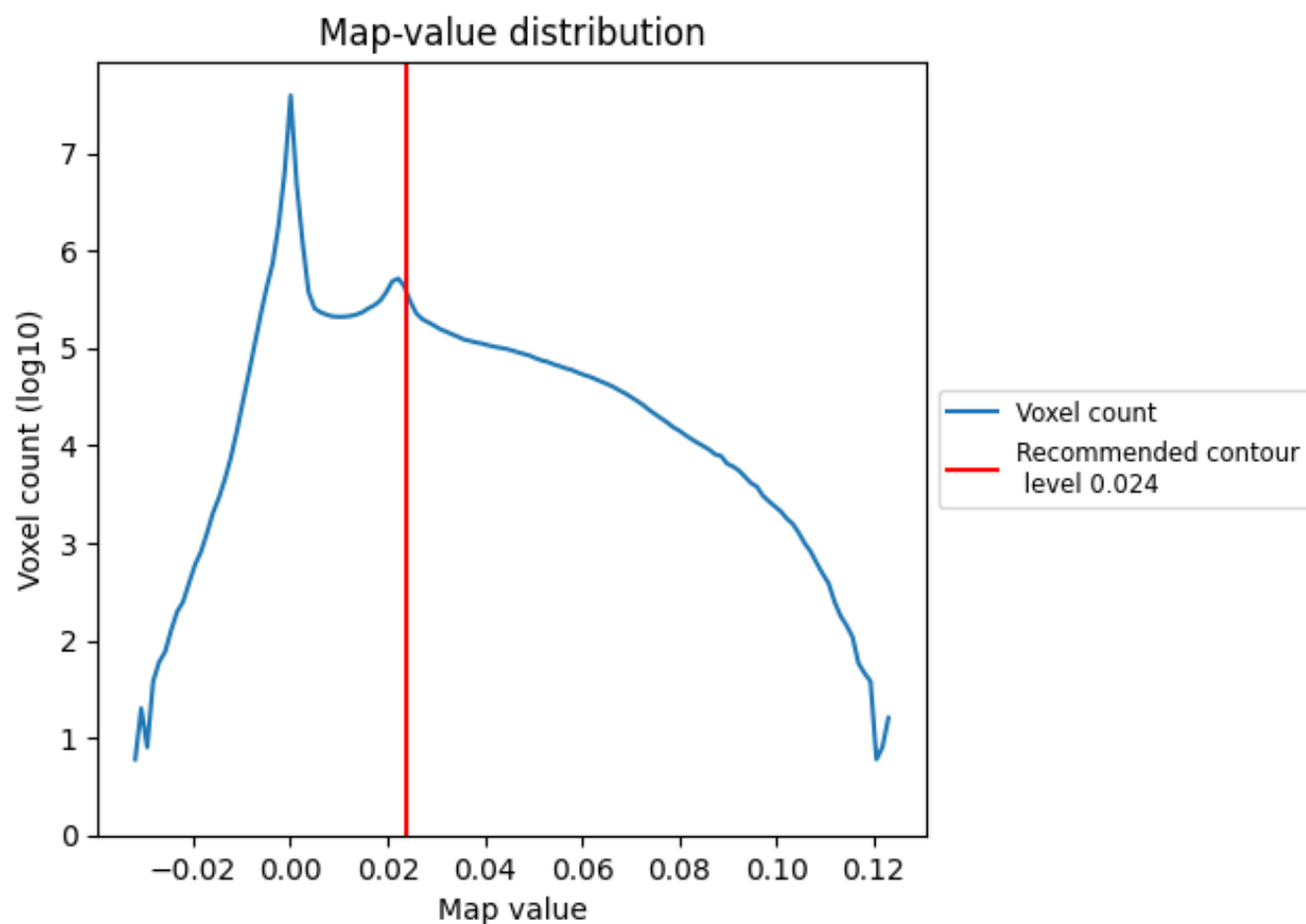
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

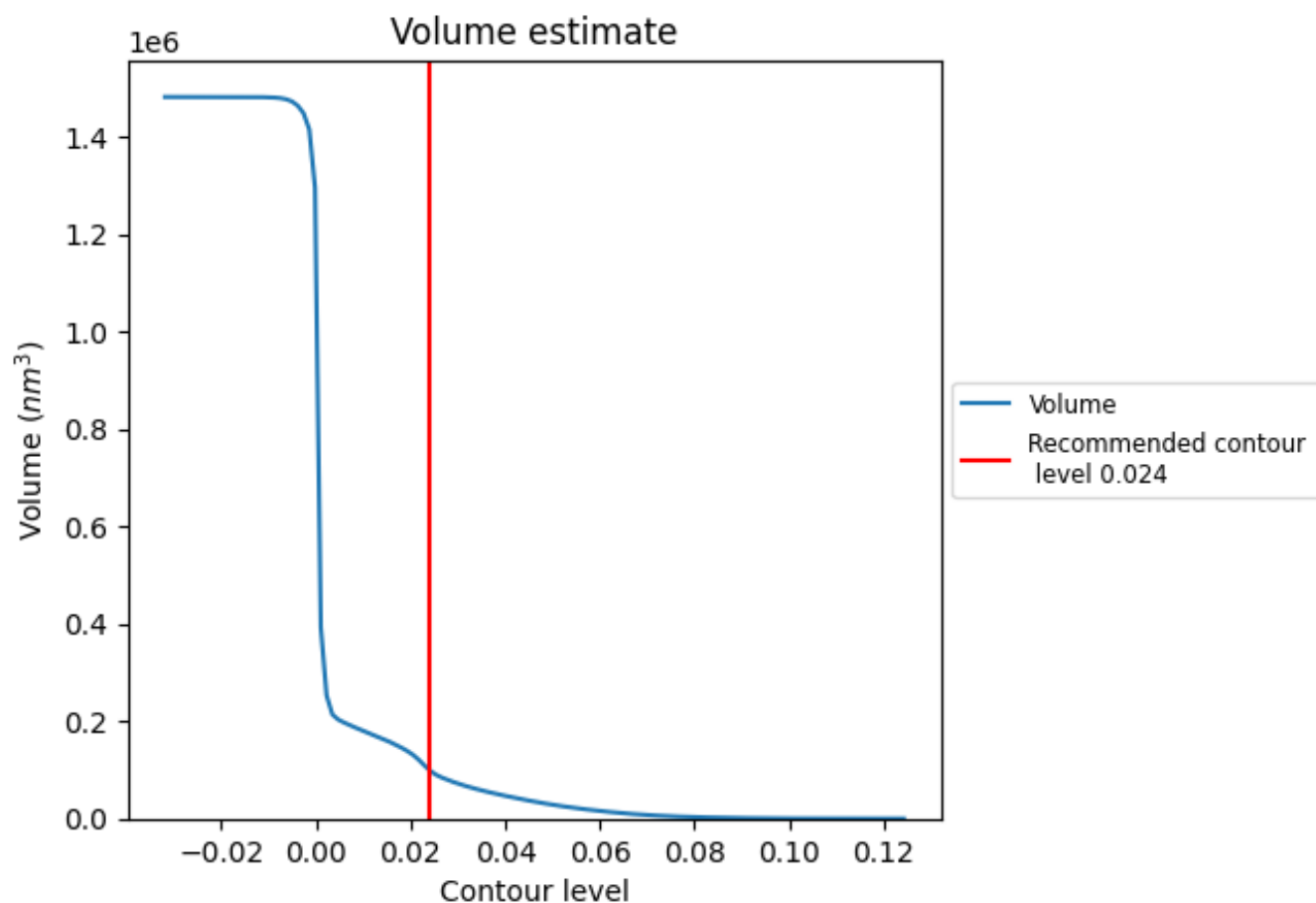
This section contains the results of statistical analysis of the map.

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.

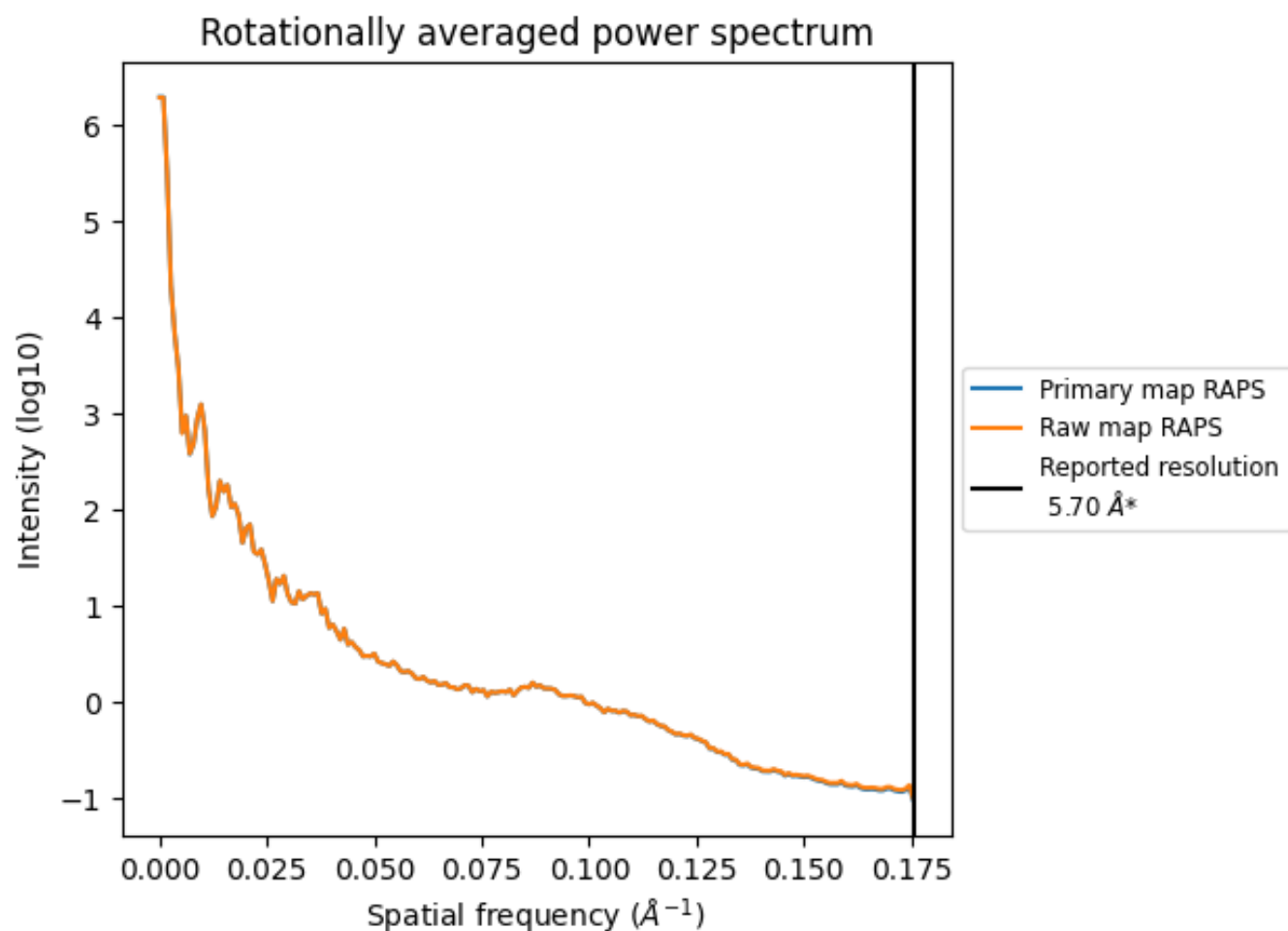
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 99702 nm³; this corresponds to an approximate mass of 90063 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

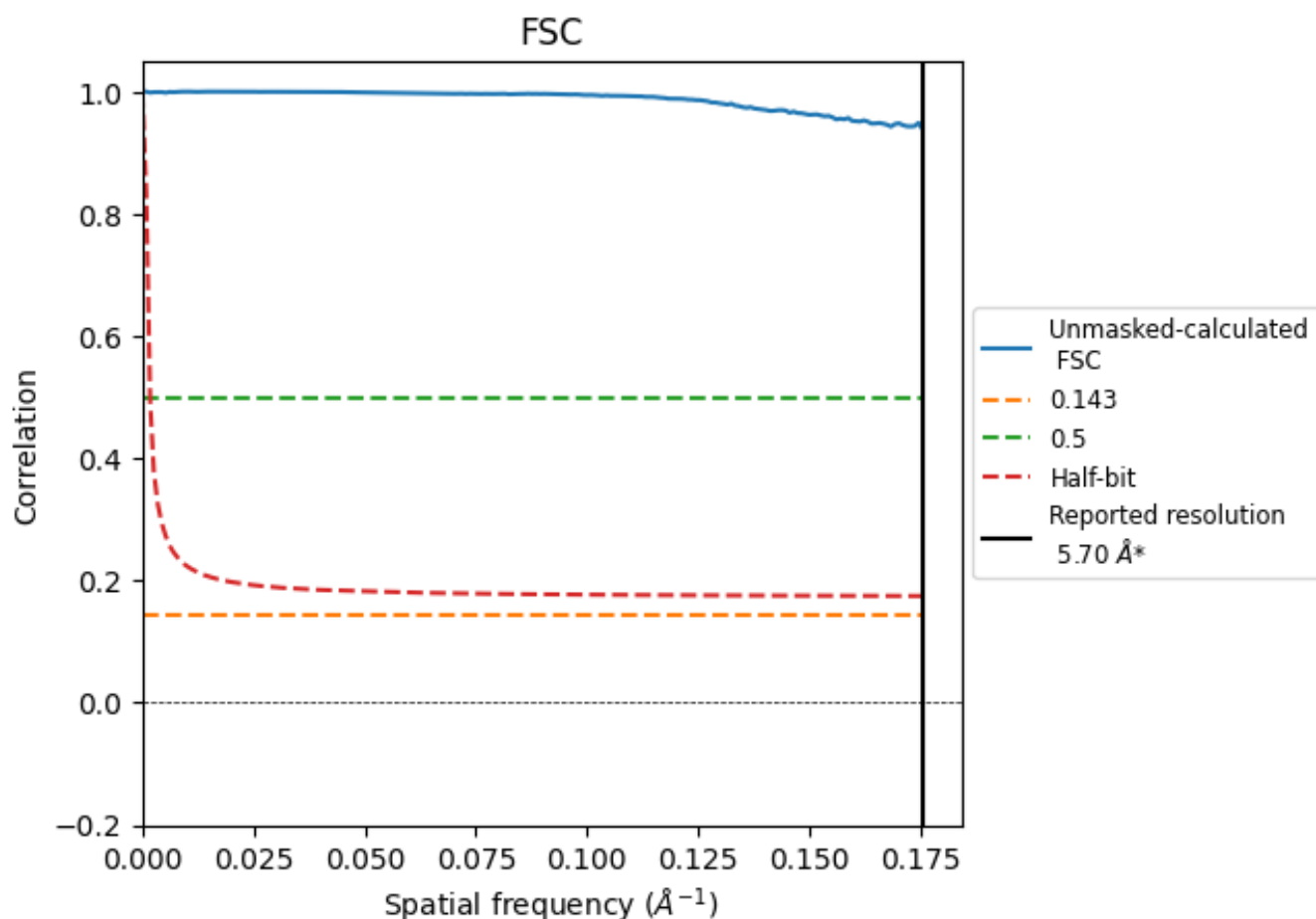


*Reported resolution corresponds to spatial frequency of 0.175 Å⁻¹

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 0.175 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

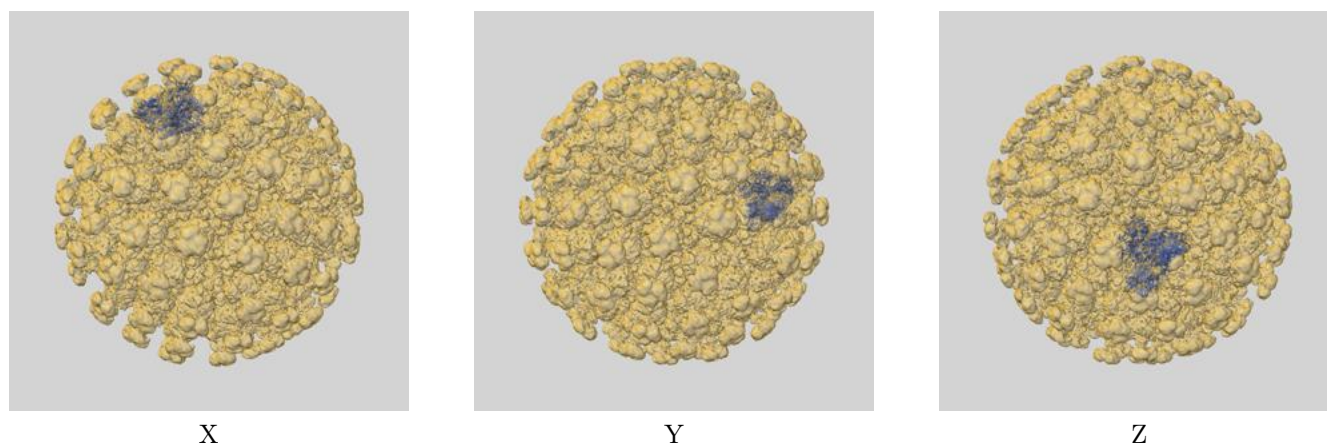
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

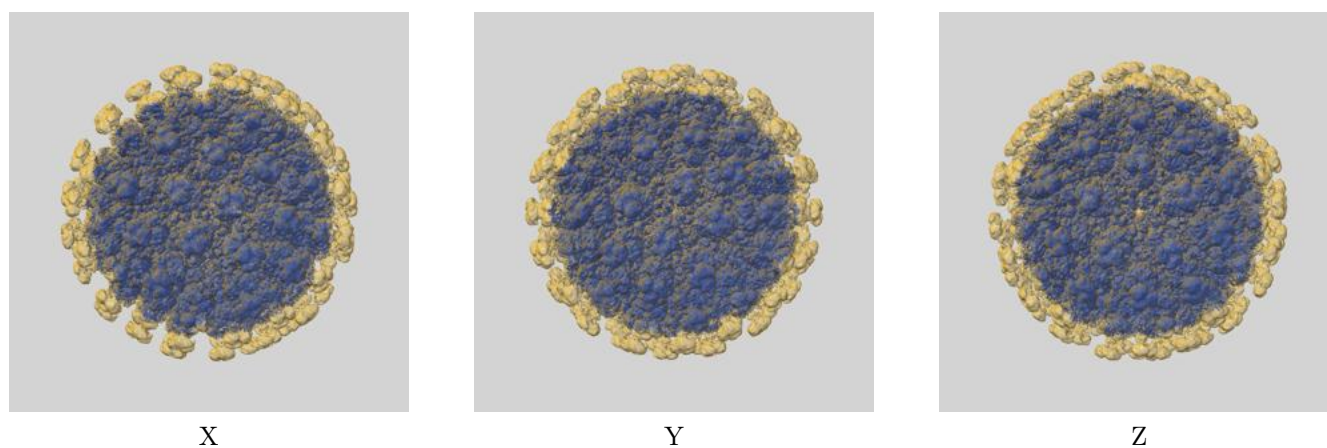
This section contains information regarding the fit between EMDB map EMD-37378 and PDB model 8W9P. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

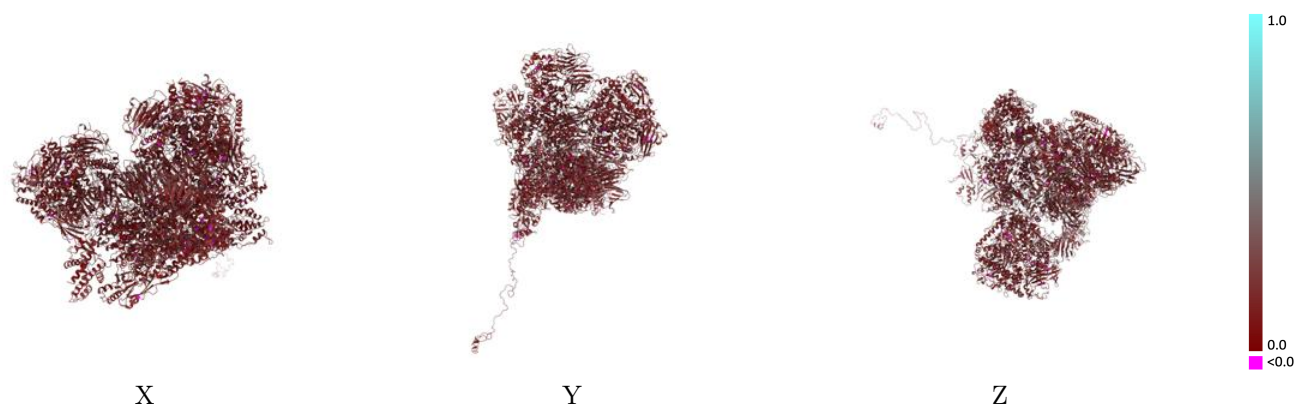


9.1.2 Map-model assembly overlay [i](#)



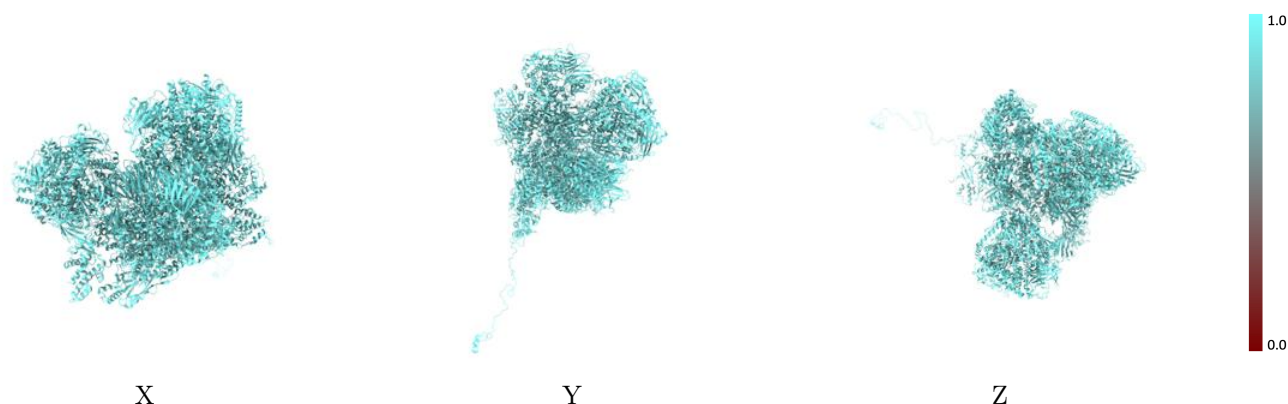
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



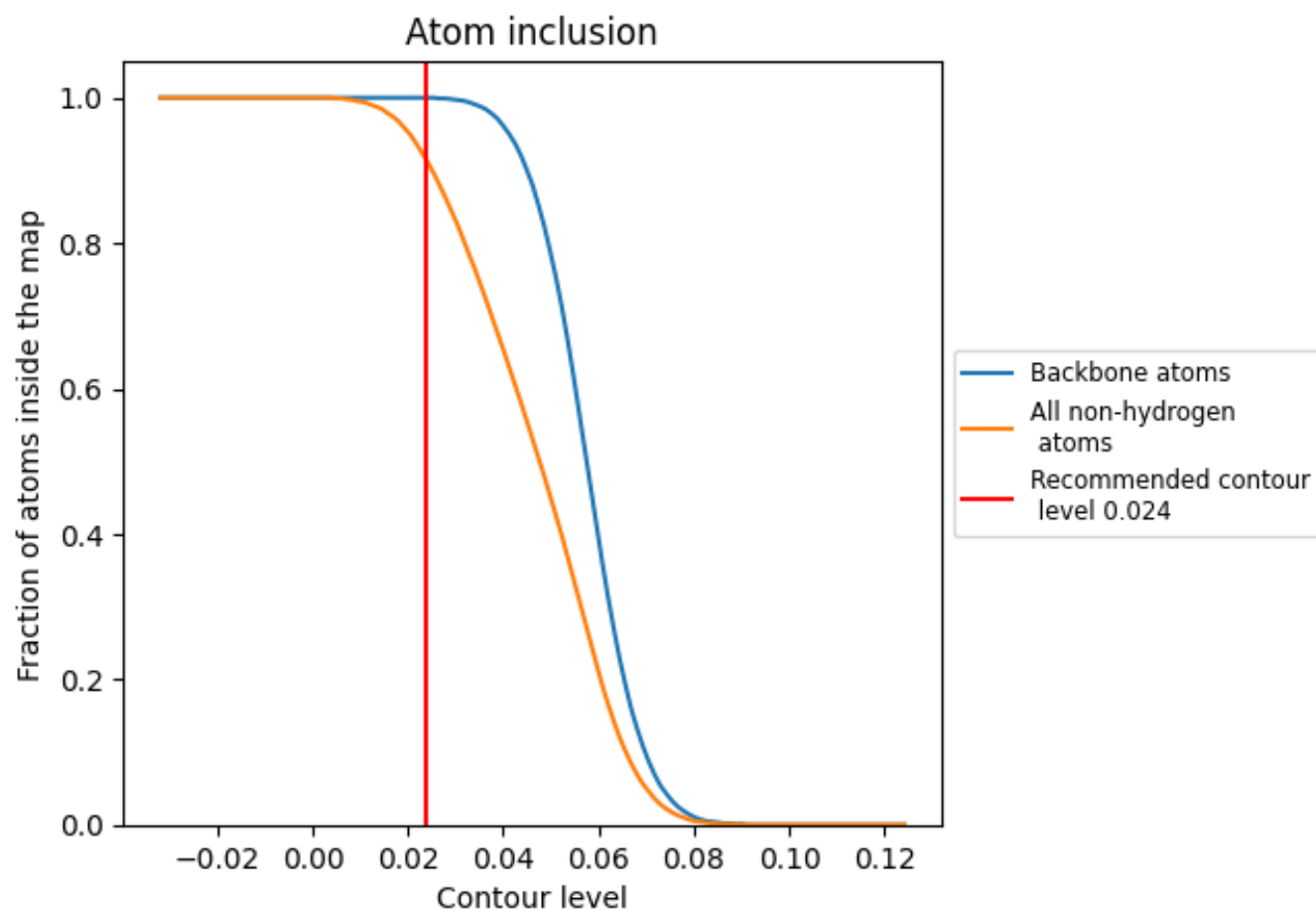
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.024).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9130	 0.2030
A	 0.8950	 0.2020
B	 0.8940	 0.2060
C	 0.9060	 0.2050
D	 0.9120	 0.2050
E	 0.9220	 0.2070
F	 0.8970	 0.2040
G	 0.9030	 0.1990
H	 0.9000	 0.2070
I	 0.9140	 0.2110
J	 0.9230	 0.2080
K	 0.9140	 0.2110
L	 0.9290	 0.2090
M	 0.9220	 0.2020
N	 0.9210	 0.2060
O	 0.9030	 0.2090
P	 0.8890	 0.1910
Q	 0.8780	 0.1940
R	 0.9300	 0.1990
S	 0.9380	 0.2030
T	 0.9390	 0.1990
U	 0.9190	 0.2000
V	 0.9100	 0.2020
W	 0.9190	 0.2030
r	 0.9170	 0.1620
s	 0.9260	 0.1610
t	 0.9350	 0.1720
u	 0.9170	 0.1920
v	 0.9070	 0.1530
w	 0.8520	 0.1790

