



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:40 PM UTC

PDB ID : 9RA1 / pdb_00009ra1
EMDB ID : EMD-53867
Title : RNA-free helical (h9.6) virus-like particle composed of JGMV coat protein
Authors : Koritnik, N.; Kezar, A.; Podobnik, M.
Deposited on : 2025-05-20
Resolution : 4.02 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:

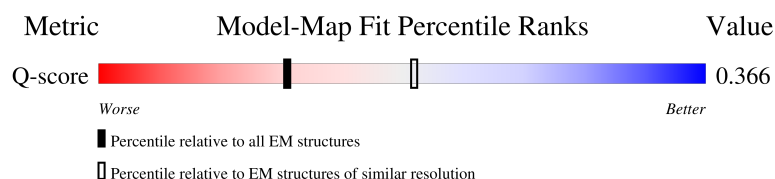
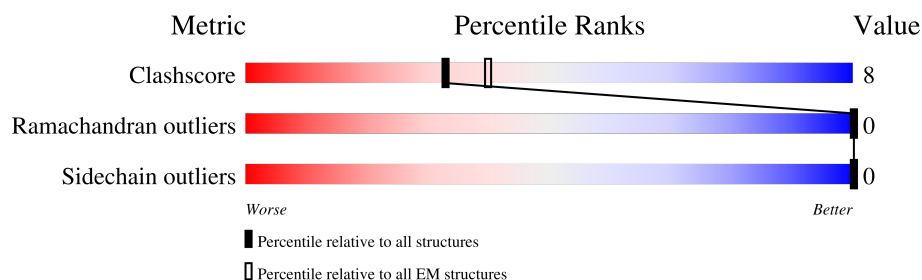
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.02 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	6727 (3.52 - 4.52)

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	Aa	303	22% 49% 10% 41%
1	Ab	303	23% 47% 12% 41%
1	Ac	303	22% 47% 12% 41%
1	Ad	303	21% 47% 12% 41%

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Mol	Chain	Length	Quality of chain			
1	Ae	303	17%	47%	12%	41%
1	Af	303	15%	47%	12%	41%
1	Ag	303	16%	47%	12%	41%
1	Ah	303	18%	47%	12%	41%
1	Ai	303	19%	47%	12%	41%
1	Aj	303	22%	47%	12%	41%
1	Ak	303	23%	47%	12%	41%
1	Al	303	23%	47%	12%	41%
1	Am	303	21%	47%	12%	41%
1	An	303	18%	47%	12%	41%
1	Ao	303	18%	47%	12%	41%
1	Ap	303	16%	47%	12%	41%
1	Aq	303	18%	47%	12%	41%
1	Ar	303	20%	47%	12%	41%
1	As	303	22%	47%	12%	41%
1	At	303	24%	47%	12%	41%
1	Au	303	25%	47%	12%	41%
1	Av	303	24%	47%	12%	41%
1	Aw	303	22%	47%	12%	41%
1	Ax	303	18%	47%	12%	41%
1	Ay	303	18%	47%	12%	41%
1	Az	303	18%	48%	11%	41%
1	Ba	303	20%	49%	10%	41%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 39798 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ab	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ac	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ad	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ae	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Af	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ag	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ah	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ai	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Aj	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ak	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Al	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Am	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	An	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ao	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Ap	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		
1	Aq	178	Total	C	N	O	S	0	0
			1474	932	262	268	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	As	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	At	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	Au	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	Av	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	Aw	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	Ax	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	Ay	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	Az	178	Total 1474	C 932	N 262	O 268	S 12	0	0
1	Ba	178	Total 1474	C 932	N 262	O 268	S 12	0	0

ASN THR
THR GLU
GLU ARG
HIS THR
ALA ALA
ALA ASP
VAL VAL
SER ARG
ASN ARG
VAL VAL
HIS THR
SER SER
TYR THR
ARG ARG
GLY ALA
LYS LYS
ILE

• Molecule 1: Genome polyprotein



SER GLY
ASN THR
GLU ALA
ASP THR
LYS THR
LYS LYS
GLN LYS
SER VAL
SER ASP
ALA VAL
THR VAL
PRO GLY
ALA THR
ALA THR
ASN GLY
GLN THR
THR THR
ALA THR
ALA THR
ASP ASN
LYS LYS
PRO SER
SER SER
ASP ASP
ASN THR
SER THR
SER ASN
ALA THR
GLN GLY
THR THR
SER SER
GLN THR
LYS THR
GLY GLY
GLY GLY
SER GLY
GLY THR

ASN THR
ALA THR
F79 Y80
P82 Y81
K83 L84
K85 K86
Y87 Y88
P89 K90
M91 K92
L93 P94
M95 Y96
Y97 Y98
K99
D105 H106
H107
I108 Q109
Y110 K111
P112 D113
Q114 R115
D116
M119 A120
R121
M132 R133
V134

K135 K136
D139 V140
D141 D142
M145 R146
M150 G151
L152 M153
V154 V155
G156 I157
E158 N159
G160 T161
D164 I165
N166
M171 V172
D173 G174
M175 N176
E187
K190 P191
T192
Q195
H199
D202 A203
A204
A206 Y207
I208
M210 R211
N212 L213
D214 E215

M218 P219
Y220 Y221
G222 L223
L224 R225
M226 L227
N228 D229
K230 S231
L232
F239 Y240
E241
S244
N248 R249
A250 R251
A253 H254
A255 Q256
MET LYS
ALA ALA
ALA ALA
ILE ARG
GLY THR
SER THR
ASN THR
HIS MET
PHE GLY
LEU ASP
ASP ASN
VAL VAL
GLY GLY
SER SER
SER GLU
GLU THR
THR THR
GLU ARG

HIS THR
ALA ALA
ASP THR
VAL VAL
SER ARG
ASN THR
HIS THR
TYR THR
ARG GLY
ALA ALA
LYS LYS
ILE

• Molecule 1: Genome polyprotein



SER GLY
ASN THR
GLU ALA
ASP THR
LYS THR
LYS LYS
GLN LYS
SER VAL
SER ASP
ALA VAL
THR VAL
PRO GLY
ALA THR
ALA THR
ASN GLY
GLN THR
THR THR
ALA THR
ALA THR
ASP ASN
LYS LYS
PRO SER
SER SER
ASP ASP
ASN THR
THR THR
SER ASN
ALA THR
GLN GLY
THR THR
SER SER
GLN THR

ASN THR
ALA THR
F79 Y80
P82 Y81
K83 L84
K85 K86
Y87 Y88
P89 K90
M91 K92
L93 P94
M95 Y96
Y97 Y98
K99
D105 H106
H107
K111 P112
D113 Q114
R115 D116
M119 A120
R121
M132 R133
V134 K135
K136

E137 Y138
D139 D140
D141 D142
M145 R146
M150 G151
W155 C156
I157 N159
G160 T161
D164 I165
N166
M171 V172
D173 G174
N175 N176
E187
K190 P191
T192
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H199
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A204
E205
I208
R211
M212 L213
D214
E215
M218 R219
G222

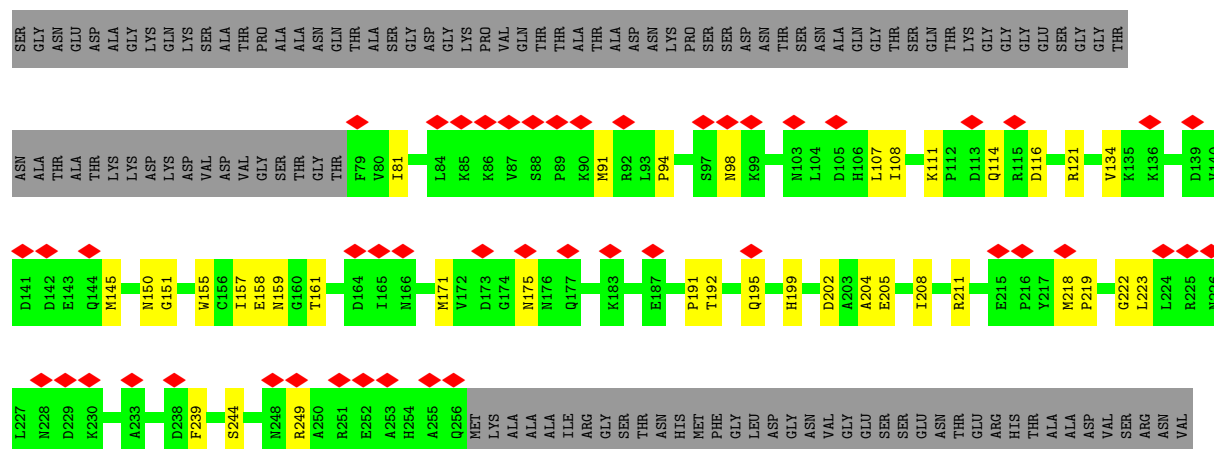
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L227 N228
D229 K230
S231 L232
F239 Y240
E241
S244
N246 R249
A250 R251
E252 A253
H254 A255
Q256
MET LYS
ALA ALA
ALA ALA
ILE ARG
GLY THR
SER SER
THR THR
HIS MET
PHE PHE
GLY LEU
ASP ASP
GLY GLY
ASN VAL
VAL VAL
GLY GLY
SER SER
SER GLU
GLU THR
THR THR
GLU GLU
HIS THR
ALA THR
ALA THR
ASP

VAL SER
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ARG GLY
ALA ALA
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ILE

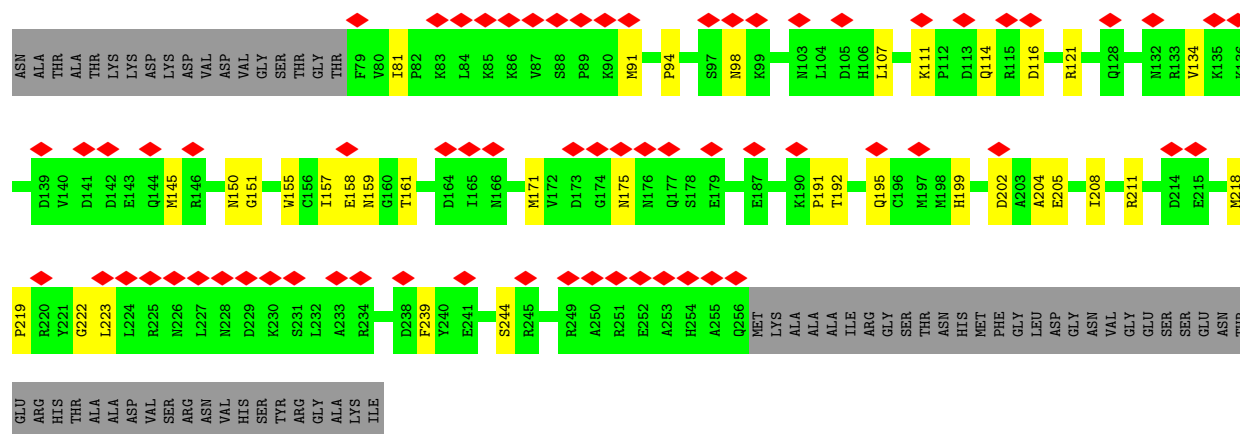
• Molecule 1: Genome polyprotein



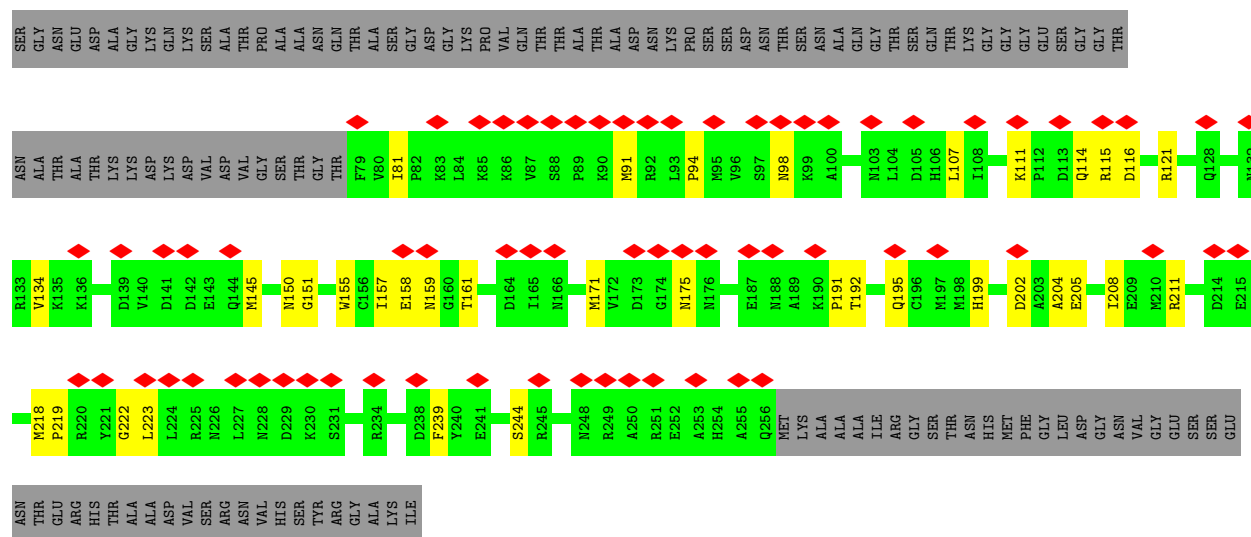
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ASN THR
GLU ALA
ASP THR
LYS THR
LYS LYS
GLN LYS
SER VAL
SER ASP
ALA VAL
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ALA THR
ALA THR
ASN GLY
GLN THR
THR THR
ALA THR
ALA THR
ASP ASN
LYS LYS
PRO SER
SER SER
ASP ASP
ASN THR
THR THR
SER ASN
ALA THR
GLN GLY
THR THR
SER SER
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LYS THR
GLY GLY
GLY GLY
GLU GLU
SER GLY
GLY THR



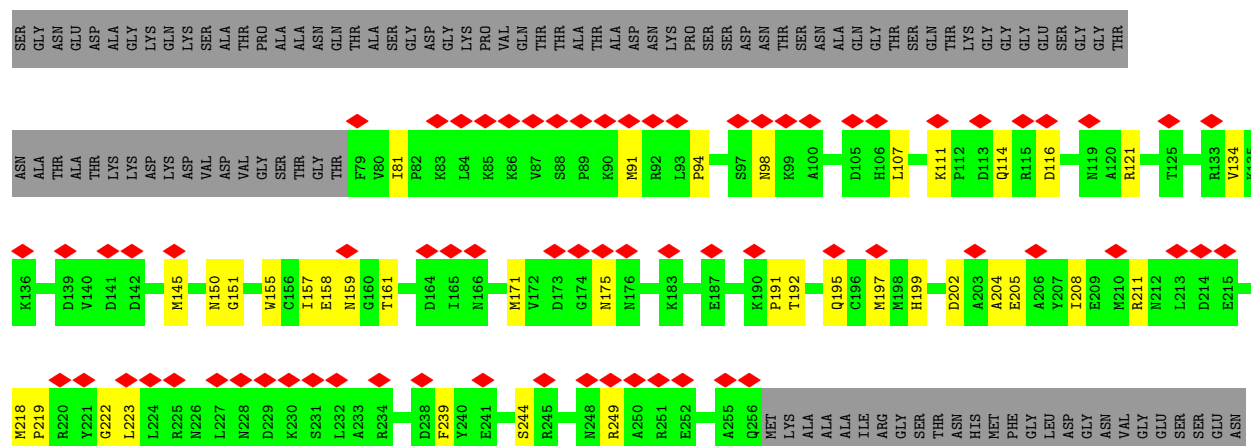
SER	GLY	ASN	GLU	ASP	ALA	GLY	LYS	GLN	LYS	SER	ALA	THR	ASN	GLN	THR	GLY	ASP	GLY	LYS	PRO	VAL	GLN	THR	THR	ALA	ALA	ALA	ASP	ASN	LYS	PRO	SER	SER	ASP	ASN	THR	THR	SER	ASN	ALA	ALA	GLN	GLY	THR	LYS	GLY	GLY	GLU	SER	GLY	THR
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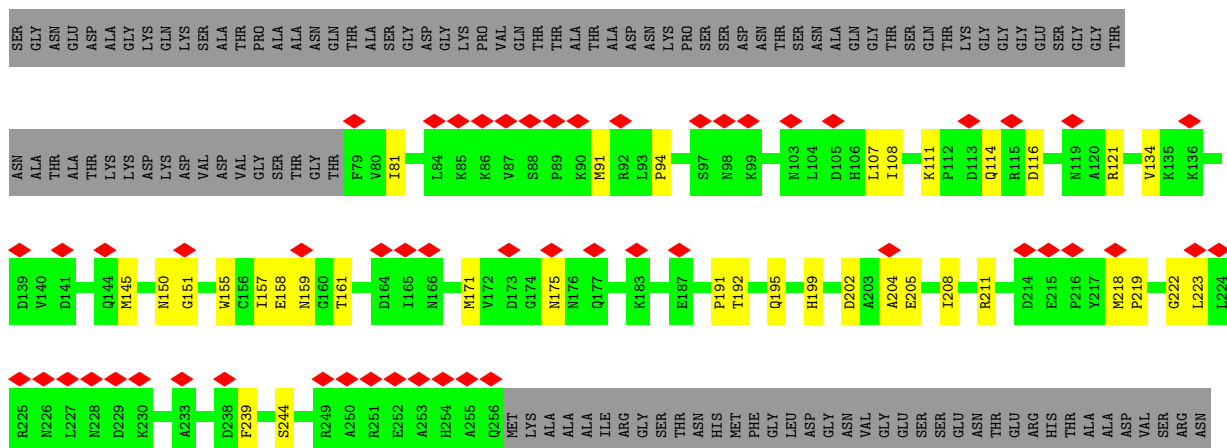
- Molecule 1: Genome polypotein



- Molecule 1: Genome polypeptide



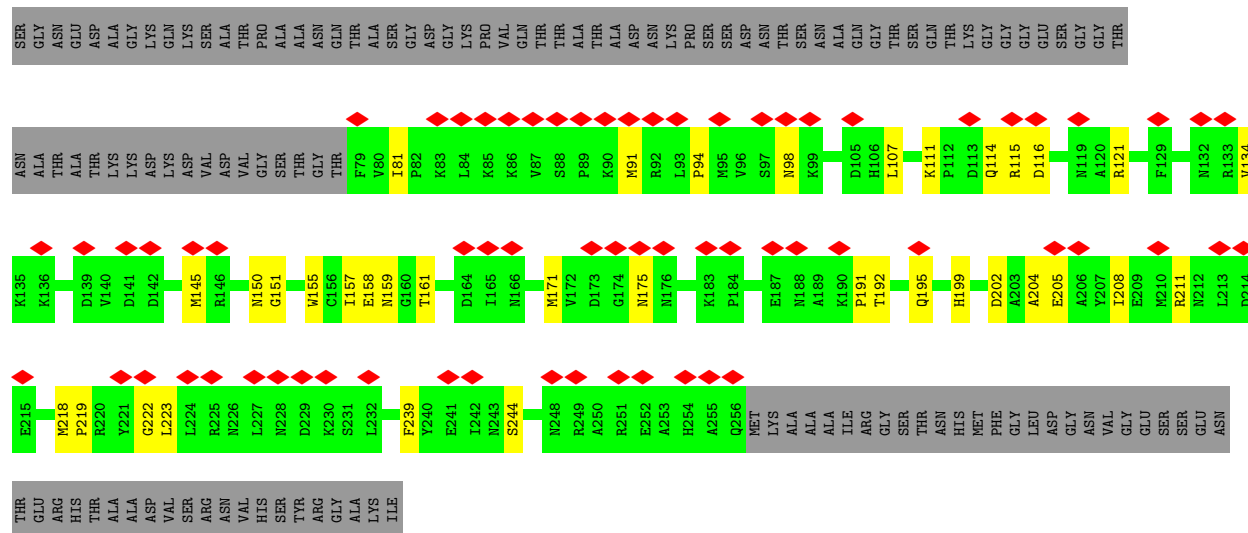
SER	GLY	ASN	GLU	ASP	ALA	GLY	LYS	GLN	LYS	SER	SER	ALA	THR	THR	PRO	ALA	ALA	ASN	GLN	THR	ALA	ALA	SER	GLY	ASP	GLY	LYS	PRO	VAL	GLN	THR	THR	ALA	THR	ALA	ASP	ASN	LYS	LYS	PRO	SER	SER	SER	ASP	ASN	THR	THR	SER	ASN	GLN	ALA	GLN	GLY	THR	THR	SER	GLY	GLY	GLY	GLU	SER	GLY	GLY	THR	THR
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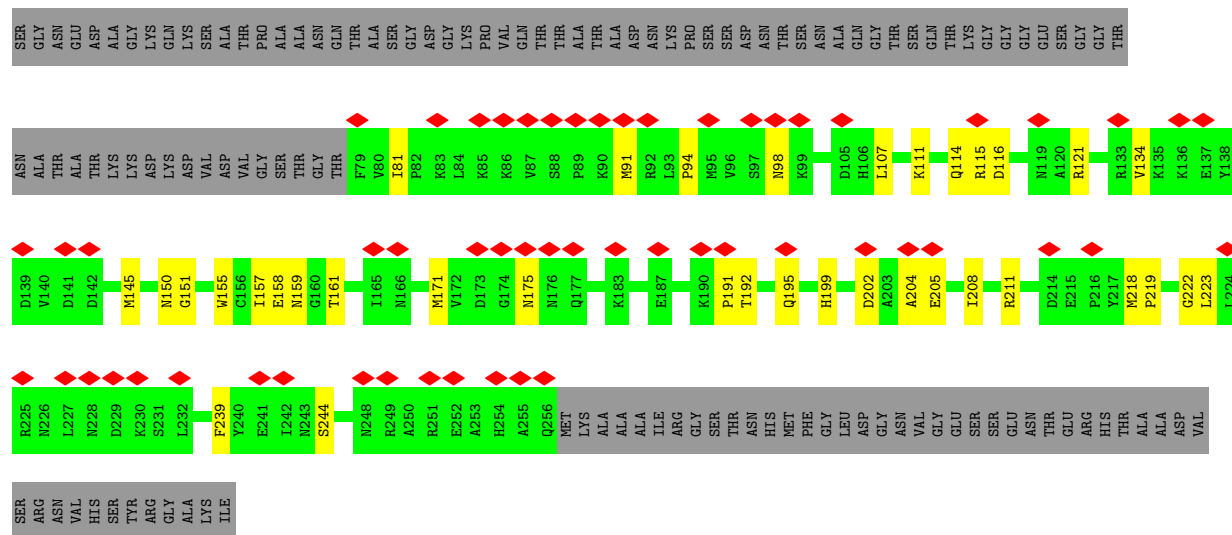
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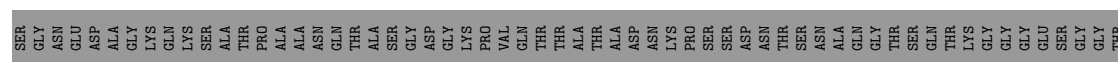
• Molecule 1: Genome polyprotein

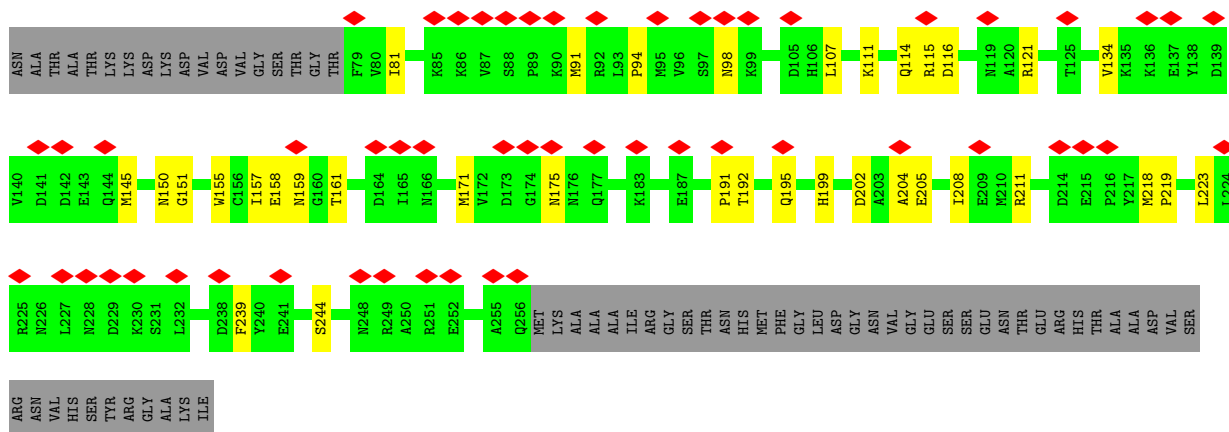


• Molecule 1: Genome polyprotein

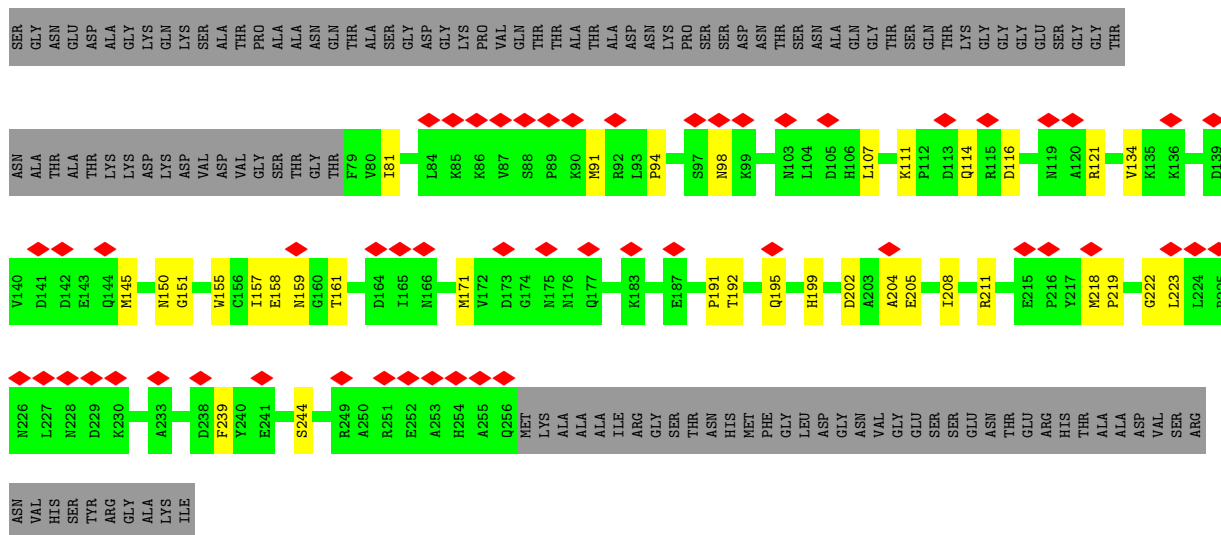


• Molecule 1: Genome polyprotein

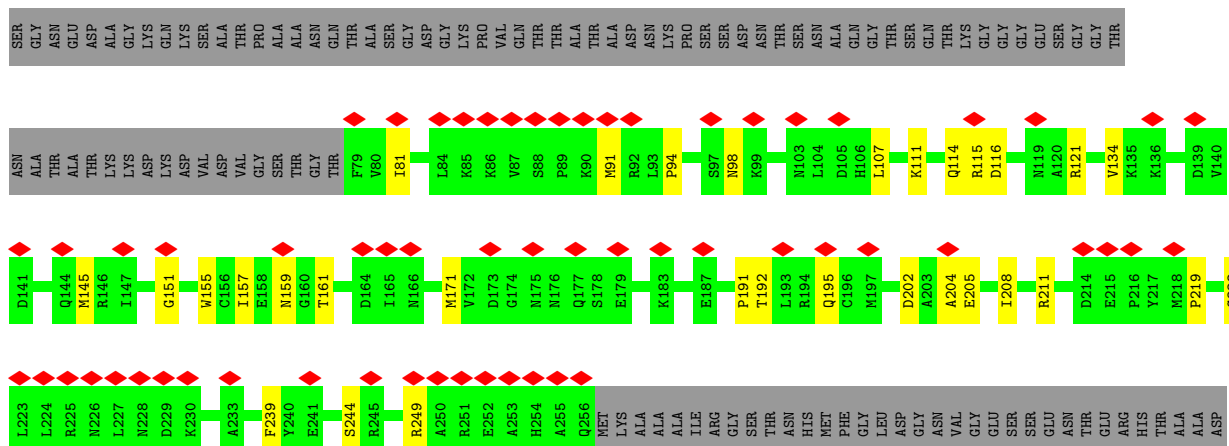




- Molecule 1: Genome polypprotein



- Molecule 1: Genome polypeptide



VAL
SER
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4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-37.65°, rise=4.50 Å, axial sym=C1	Depositor
Number of segments used	81832	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	3.614	Depositor
Minimum map value	-2.374	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.170	Depositor
Recommended contour level	0.88	Depositor
Map size (Å)	332.5, 332.5, 332.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Aa	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ab	0.46	0/1510	0.63	1/2041 (0.0%)
1	Ac	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ad	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ae	0.46	0/1510	0.63	1/2041 (0.0%)
1	Af	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ag	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ah	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ai	0.45	0/1510	0.63	1/2041 (0.0%)
1	Aj	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ak	0.46	0/1510	0.63	1/2041 (0.0%)
1	Al	0.45	0/1510	0.63	1/2041 (0.0%)
1	Am	0.46	0/1510	0.63	1/2041 (0.0%)
1	An	0.46	0/1510	0.63	1/2041 (0.0%)
1	Ao	0.45	0/1510	0.63	1/2041 (0.0%)
1	Ap	0.45	0/1510	0.63	1/2041 (0.0%)
1	Aq	0.46	0/1510	0.63	1/2041 (0.0%)
1	Ar	0.45	0/1510	0.63	1/2041 (0.0%)
1	As	0.45	0/1510	0.63	1/2041 (0.0%)
1	At	0.46	0/1510	0.63	1/2041 (0.0%)
1	Au	0.45	0/1510	0.63	1/2041 (0.0%)
1	Av	0.45	0/1510	0.63	1/2041 (0.0%)
1	Aw	0.46	0/1510	0.63	1/2041 (0.0%)
1	Ax	0.46	0/1510	0.63	1/2041 (0.0%)
1	Ay	0.46	0/1510	0.63	1/2041 (0.0%)
1	Az	0.46	0/1510	0.63	1/2041 (0.0%)
1	Ba	0.46	0/1510	0.63	1/2041 (0.0%)
All	All	0.45	0/40770	0.63	27/55107 (0.0%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Aq	91	MET	N-CA-C	-5.71	101.83	110.28
1	An	91	MET	N-CA-C	-5.70	101.84	110.28
1	Aj	91	MET	N-CA-C	-5.69	101.85	110.28
1	Ay	91	MET	N-CA-C	-5.69	101.85	110.28
1	Ag	91	MET	N-CA-C	-5.69	101.85	110.28
1	Aw	91	MET	N-CA-C	-5.69	101.85	110.28
1	As	91	MET	N-CA-C	-5.69	101.86	110.28
1	Aa	91	MET	N-CA-C	-5.69	101.86	110.28
1	Ae	91	MET	N-CA-C	-5.68	101.87	110.28
1	Ap	91	MET	N-CA-C	-5.68	101.88	110.28
1	Af	91	MET	N-CA-C	-5.67	101.88	110.28
1	Ax	91	MET	N-CA-C	-5.67	101.89	110.28
1	Az	91	MET	N-CA-C	-5.67	101.89	110.28
1	Ad	91	MET	N-CA-C	-5.67	101.89	110.28
1	Ao	91	MET	N-CA-C	-5.67	101.89	110.28
1	Ah	91	MET	N-CA-C	-5.66	101.90	110.28
1	Ar	91	MET	N-CA-C	-5.66	101.90	110.28
1	Av	91	MET	N-CA-C	-5.66	101.90	110.28
1	Ak	91	MET	N-CA-C	-5.66	101.90	110.28
1	Ai	91	MET	N-CA-C	-5.66	101.91	110.28
1	Ac	91	MET	N-CA-C	-5.65	101.91	110.28
1	Ab	91	MET	N-CA-C	-5.65	101.92	110.28
1	Ba	91	MET	N-CA-C	-5.65	101.92	110.28
1	Am	91	MET	N-CA-C	-5.65	101.92	110.28
1	At	91	MET	N-CA-C	-5.65	101.92	110.28
1	Au	91	MET	N-CA-C	-5.64	101.93	110.28
1	Al	91	MET	N-CA-C	-5.63	101.95	110.28

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	Aa	1474	0	1445	24	0
1	Ab	1474	0	1445	35	0
1	Ac	1474	0	1445	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ad	1474	0	1445	37	0
1	Ae	1474	0	1445	35	0
1	Af	1474	0	1445	37	0
1	Ag	1474	0	1445	37	0
1	Ah	1474	0	1445	37	0
1	Ai	1474	0	1445	37	0
1	Aj	1474	0	1445	36	0
1	Ak	1474	0	1445	38	0
1	Al	1474	0	1445	37	0
1	Am	1474	0	1445	37	0
1	An	1474	0	1445	36	0
1	Ao	1474	0	1445	33	0
1	Ap	1474	0	1445	35	0
1	Aq	1474	0	1445	33	0
1	Ar	1474	0	1445	37	0
1	As	1474	0	1445	35	0
1	At	1474	0	1445	38	0
1	Au	1474	0	1445	35	0
1	Av	1474	0	1445	37	0
1	Aw	1474	0	1445	36	0
1	Ax	1474	0	1445	37	0
1	Ay	1474	0	1445	35	0
1	Az	1474	0	1445	33	0
1	Ba	1474	0	1445	26	0
All	All	39798	0	39015	661	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 8.

All (661) 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)
1:Av:175:ASN:HB2	1:Ax:98:ASN:HD21	1.62	0.65
1:Ak:175:ASN:HB2	1:Am:98:ASN:HD21	1.61	0.65
1:Ad:175:ASN:HB2	1:Af:98:ASN:HD21	1.62	0.65
1:Ab:175:ASN:HB2	1:Ad:98:ASN:HD21	1.61	0.64
1:At:175:ASN:HB2	1:Av:98:ASN:HD21	1.61	0.64
1:Ah:175:ASN:HB2	1:Aj:98:ASN:HD21	1.62	0.64
1:Am:175:ASN:HB2	1:Ao:98:ASN:HD21	1.62	0.64
1:Ar:175:ASN:HB2	1:At:98:ASN:HD21	1.62	0.64
1:An:175:ASN:HB2	1:Ap:98:ASN:HD21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ax:175:ASN:HB2	1:Az:98:ASN:HD21	1.62	0.63
1:Af:175:ASN:HB2	1:Ah:98:ASN:HD21	1.62	0.63
1:Ag:175:ASN:HB2	1:Ai:98:ASN:HD21	1.62	0.63
1:Aa:175:ASN:HB2	1:Ac:98:ASN:HD21	1.63	0.63
1:Aq:175:ASN:HB2	1:As:98:ASN:HD21	1.63	0.63
1:Ay:175:ASN:HB2	1:Ba:98:ASN:HD21	1.63	0.63
1:Ap:175:ASN:HB2	1:Ar:98:ASN:HD21	1.62	0.63
1:Al:175:ASN:HB2	1:An:98:ASN:HD21	1.64	0.62
1:Ai:175:ASN:HB2	1:Ak:98:ASN:HD21	1.63	0.62
1:As:175:ASN:HB2	1:Au:98:ASN:HD21	1.63	0.62
1:Au:175:ASN:HB2	1:Aw:98:ASN:HD21	1.64	0.62
1:Aw:175:ASN:HB2	1:Ay:98:ASN:HD21	1.63	0.62
1:Ae:175:ASN:HB2	1:Ag:98:ASN:HD21	1.63	0.62
1:Ak:158:GLU:OE2	1:Al:114:GLN:HG3	2.00	0.61
1:At:158:GLU:OE2	1:Au:114:GLN:HG3	2.00	0.61
1:Ac:175:ASN:HB2	1:Ae:98:ASN:HD21	1.65	0.61
1:Ah:158:GLU:OE2	1:Ai:114:GLN:HG3	2.00	0.61
1:Aj:175:ASN:HB2	1:Al:98:ASN:HD21	1.64	0.61
1:Av:158:GLU:OE2	1:Aw:114:GLN:HG3	2.01	0.60
1:Am:158:GLU:OE2	1:An:114:GLN:HG3	2.01	0.60
1:Ar:158:GLU:OE2	1:As:114:GLN:HG3	2.01	0.60
1:Ab:158:GLU:OE2	1:Ac:114:GLN:HG3	2.01	0.60
1:Aq:158:GLU:OE2	1:Ar:114:GLN:HG3	2.01	0.60
1:Az:158:GLU:OE2	1:Ba:114:GLN:HG3	2.00	0.60
1:Ac:211:ARG:NH1	1:Ad:111:LYS:HB3	2.17	0.59
1:Ap:158:GLU:OE2	1:Aq:114:GLN:HG3	2.01	0.59
1:Ag:211:ARG:NH1	1:Ah:111:LYS:HB3	2.17	0.59
1:Aw:158:GLU:OE2	1:Ax:114:GLN:HG3	2.02	0.59
1:An:158:GLU:OE2	1:Ao:114:GLN:HG3	2.02	0.59
1:Ad:158:GLU:OE2	1:Ae:114:GLN:HG3	2.01	0.59
1:Ay:211:ARG:NH1	1:Az:111:LYS:HB3	2.17	0.59
1:Ao:158:GLU:OE2	1:Ap:114:GLN:HG3	2.02	0.59
1:As:211:ARG:NH1	1:At:111:LYS:HB3	2.18	0.59
1:Ax:158:GLU:OE2	1:Ay:114:GLN:HG3	2.02	0.59
1:Al:158:GLU:OE2	1:Am:114:GLN:HG3	2.03	0.59
1:Ai:158:GLU:OE2	1:Aj:114:GLN:HG3	2.03	0.58
1:Aj:211:ARG:NH1	1:Ak:111:LYS:HB3	2.18	0.58
1:Au:158:GLU:OE2	1:Av:114:GLN:HG3	2.03	0.58
1:Af:158:GLU:OE2	1:Ag:114:GLN:HG3	2.02	0.58
1:Ae:158:GLU:OE2	1:Af:114:GLN:HG3	2.02	0.58
1:Aq:211:ARG:NH1	1:Ar:111:LYS:HB3	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:211:ARG:NH1	1:Aj:111:LYS:HB3	2.19	0.58
1:Ac:158:GLU:OE2	1:Ad:114:GLN:HG3	2.04	0.58
1:Aa:158:GLU:OE2	1:Ab:114:GLN:HG3	2.04	0.58
1:Aa:211:ARG:NH1	1:Ab:111:LYS:HB3	2.18	0.58
1:Au:211:ARG:NH1	1:Av:111:LYS:HB3	2.19	0.58
1:Az:211:ARG:NH1	1:Ba:111:LYS:HB3	2.19	0.58
1:Aj:158:GLU:OE2	1:Ak:114:GLN:HG3	2.04	0.57
1:Am:211:ARG:NH1	1:An:111:LYS:HB3	2.19	0.57
1:As:158:GLU:OE2	1:At:114:GLN:HG3	2.04	0.57
1:Ad:211:ARG:NH1	1:Ae:111:LYS:HB3	2.19	0.57
1:Av:211:ARG:NH1	1:Aw:111:LYS:HB3	2.19	0.57
1:Ay:161:THR:HG21	1:Ay:239:PHE:HD1	1.69	0.57
1:Ap:161:THR:HG21	1:Ap:239:PHE:HD1	1.69	0.57
1:Af:161:THR:HG21	1:Af:239:PHE:HD1	1.70	0.57
1:Ag:211:ARG:CZ	1:Ah:111:LYS:HB3	2.34	0.57
1:At:211:ARG:NH1	1:Au:111:LYS:HB3	2.20	0.57
1:Af:211:ARG:NH1	1:Ag:111:LYS:HB3	2.20	0.57
1:Ag:161:THR:HG21	1:Ag:239:PHE:HD1	1.69	0.57
1:Ah:211:ARG:NH1	1:Ai:111:LYS:HB3	2.19	0.57
1:Al:211:ARG:NH1	1:Am:111:LYS:HB3	2.19	0.57
1:Ao:161:THR:HG21	1:Ao:239:PHE:HD1	1.70	0.57
1:Ax:161:THR:HG21	1:Ax:239:PHE:HD1	1.70	0.57
1:Ay:211:ARG:CZ	1:Az:111:LYS:HB3	2.34	0.57
1:Ai:161:THR:HG21	1:Ai:239:PHE:HD1	1.70	0.57
1:Ac:161:THR:HG21	1:Ac:239:PHE:HD1	1.69	0.57
1:Ac:211:ARG:CZ	1:Ad:111:LYS:HB3	2.35	0.57
1:Ah:161:THR:HG21	1:Ah:239:PHE:HD1	1.70	0.57
1:Aj:211:ARG:CZ	1:Ak:111:LYS:HB3	2.35	0.57
1:Ar:161:THR:HG21	1:Ar:239:PHE:HD1	1.70	0.57
1:Aw:161:THR:HG21	1:Aw:239:PHE:HD1	1.69	0.57
1:Aa:161:THR:HG21	1:Aa:239:PHE:HD1	1.70	0.57
1:Av:161:THR:HG21	1:Av:239:PHE:HD1	1.70	0.57
1:Aa:211:ARG:CZ	1:Ab:111:LYS:HB3	2.35	0.57
1:Al:161:THR:HG21	1:Al:239:PHE:HD1	1.70	0.57
1:Ao:211:ARG:NH1	1:Ap:111:LYS:HB3	2.20	0.57
1:Ar:211:ARG:NH1	1:As:111:LYS:HB3	2.20	0.57
1:Ad:161:THR:HG21	1:Ad:239:PHE:HD1	1.70	0.56
1:Ak:211:ARG:NH1	1:Al:111:LYS:HB3	2.20	0.56
1:Am:161:THR:HG21	1:Am:239:PHE:HD1	1.69	0.56
1:Ba:161:THR:HG21	1:Ba:239:PHE:HD1	1.70	0.56
1:Ab:161:THR:HG21	1:Ab:239:PHE:HD1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:211:ARG:CZ	1:Aj:111:LYS:HB3	2.36	0.56
1:Aj:134:VAL:HG12	1:Aj:145:MET:HE1	1.87	0.56
1:Aj:161:THR:HG21	1:Aj:239:PHE:HD1	1.70	0.56
1:Aq:161:THR:HG21	1:Aq:239:PHE:HD1	1.70	0.56
1:As:161:THR:HG21	1:As:239:PHE:HD1	1.70	0.56
1:Au:161:THR:HG21	1:Au:239:PHE:HD1	1.69	0.56
1:Aa:134:VAL:HG12	1:Aa:145:MET:HE1	1.87	0.56
1:Ab:211:ARG:NH1	1:Ac:111:LYS:HB3	2.20	0.56
1:Ae:161:THR:HG21	1:Ae:239:PHE:HD1	1.70	0.56
1:Ae:211:ARG:NH1	1:Af:111:LYS:HB3	2.20	0.56
1:Ak:161:THR:HG21	1:Ak:239:PHE:HD1	1.70	0.56
1:An:161:THR:HG21	1:An:239:PHE:HD1	1.70	0.56
1:As:134:VAL:HG12	1:As:145:MET:HE1	1.88	0.56
1:At:161:THR:HG21	1:At:239:PHE:HD1	1.69	0.56
1:Aw:211:ARG:NH1	1:Ax:111:LYS:HB3	2.20	0.56
1:Ai:134:VAL:HG12	1:Ai:145:MET:HE1	1.87	0.56
1:Ar:134:VAL:HG12	1:Ar:145:MET:HE1	1.87	0.56
1:As:211:ARG:CZ	1:At:111:LYS:HB3	2.35	0.56
1:At:134:VAL:HG12	1:At:145:MET:HE1	1.87	0.56
1:Ax:211:ARG:NH1	1:Ay:111:LYS:HB3	2.20	0.56
1:Az:161:THR:HG21	1:Az:239:PHE:HD1	1.70	0.56
1:Au:134:VAL:HG12	1:Au:145:MET:HE1	1.88	0.56
1:Ag:158:GLU:OE2	1:Ah:114:GLN:HG3	2.05	0.56
1:Ak:134:VAL:HG12	1:Ak:145:MET:HE1	1.88	0.56
1:Ao:211:ARG:CZ	1:Ap:111:LYS:HB3	2.36	0.56
1:Ay:158:GLU:OE2	1:Az:114:GLN:HG3	2.05	0.56
1:Ba:134:VAL:HG12	1:Ba:145:MET:HE1	1.87	0.56
1:Ab:134:VAL:HG12	1:Ab:145:MET:HE1	1.88	0.56
1:Ah:134:VAL:HG12	1:Ah:145:MET:HE1	1.87	0.56
1:Al:211:ARG:CZ	1:Am:111:LYS:HB3	2.36	0.56
1:An:211:ARG:NH1	1:Ao:111:LYS:HB3	2.20	0.56
1:Aq:199:HIS:O	1:Ar:94:PRO:HG3	2.05	0.56
1:Al:134:VAL:HG12	1:Al:145:MET:HE1	1.87	0.56
1:Av:134:VAL:HG12	1:Av:145:MET:HE1	1.87	0.56
1:Ai:211:ARG:CG	1:Ai:211:ARG:O	2.55	0.55
1:As:211:ARG:O	1:As:211:ARG:CG	2.55	0.55
1:Ah:211:ARG:CZ	1:Ai:111:LYS:HB3	2.37	0.55
1:Ak:211:ARG:CZ	1:Al:111:LYS:HB3	2.37	0.55
1:Ao:134:VAL:HG12	1:Ao:145:MET:HE1	1.87	0.55
1:Ab:211:ARG:CG	1:Ab:211:ARG:O	2.55	0.55
1:Ad:211:ARG:CZ	1:Ae:111:LYS:HB3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:134:VAL:HG12	1:Ac:145:MET:HE1	1.87	0.55
1:Ag:134:VAL:HG12	1:Ag:145:MET:HE1	1.87	0.55
1:Al:211:ARG:CG	1:Al:211:ARG:O	2.55	0.55
1:Am:134:VAL:HG12	1:Am:145:MET:HE1	1.87	0.55
1:An:134:VAL:HG12	1:An:145:MET:HE1	1.87	0.55
1:Ar:211:ARG:CG	1:Ar:211:ARG:O	2.55	0.55
1:Au:211:ARG:CZ	1:Av:111:LYS:HB3	2.36	0.55
1:Af:211:ARG:CZ	1:Ag:111:LYS:HB3	2.36	0.55
1:Aq:134:VAL:HG12	1:Aq:145:MET:HE1	1.87	0.55
1:Ar:211:ARG:CZ	1:As:111:LYS:HB3	2.36	0.55
1:Ah:211:ARG:CG	1:Ah:211:ARG:O	2.55	0.55
1:Am:211:ARG:CZ	1:An:111:LYS:HB3	2.36	0.55
1:At:211:ARG:CZ	1:Au:111:LYS:HB3	2.37	0.55
1:Ay:134:VAL:HG12	1:Ay:145:MET:HE1	1.87	0.55
1:Ay:199:HIS:O	1:Az:94:PRO:HG3	2.07	0.55
1:Az:211:ARG:CG	1:Az:211:ARG:O	2.55	0.55
1:Ab:211:ARG:CZ	1:Ac:111:LYS:HB3	2.37	0.55
1:Ae:211:ARG:CZ	1:Af:111:LYS:HB3	2.37	0.55
1:Ap:211:ARG:CG	1:Ap:211:ARG:O	2.55	0.55
1:Aw:134:VAL:HG12	1:Aw:145:MET:HE1	1.87	0.55
1:Ax:211:ARG:CZ	1:Ay:111:LYS:HB3	2.36	0.55
1:Az:134:VAL:HG12	1:Az:145:MET:HE1	1.87	0.55
1:Aa:211:ARG:CG	1:Aa:211:ARG:O	2.55	0.55
1:Ad:134:VAL:HG12	1:Ad:145:MET:HE1	1.87	0.55
1:Ak:211:ARG:O	1:Ak:211:ARG:CG	2.55	0.55
1:Ap:134:VAL:HG12	1:Ap:145:MET:HE1	1.88	0.55
1:Au:211:ARG:CG	1:Au:211:ARG:O	2.55	0.55
1:Az:211:ARG:CZ	1:Ba:111:LYS:HB3	2.37	0.55
1:Ae:134:VAL:HG12	1:Ae:145:MET:HE1	1.87	0.54
1:Af:134:VAL:HG12	1:Af:145:MET:HE1	1.87	0.54
1:Ax:134:VAL:HG12	1:Ax:145:MET:HE1	1.88	0.54
1:An:211:ARG:CZ	1:Ao:111:LYS:HB3	2.37	0.54
1:Af:211:ARG:CG	1:Af:211:ARG:O	2.55	0.54
1:Ak:192:THR:HG22	1:Ak:195:GLN:HG3	1.89	0.54
1:Av:192:THR:HG22	1:Av:195:GLN:HG3	1.89	0.54
1:Av:211:ARG:CZ	1:Aw:111:LYS:HB3	2.36	0.54
1:Ab:192:THR:HG22	1:Ab:195:GLN:HG3	1.89	0.54
1:Ab:199:HIS:O	1:Ac:94:PRO:HG3	2.08	0.54
1:Ad:211:ARG:CG	1:Ad:211:ARG:O	2.55	0.54
1:Ae:211:ARG:CG	1:Ae:211:ARG:O	2.55	0.54
1:Ag:199:HIS:O	1:Ah:94:PRO:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:192:THR:HG22	1:Ac:195:GLN:HG3	1.89	0.54
1:Ak:223:LEU:HD11	1:Al:244:SER:HA	1.90	0.54
1:An:211:ARG:CG	1:An:211:ARG:O	2.55	0.54
1:At:211:ARG:CG	1:At:211:ARG:O	2.55	0.54
1:Ak:202:ASP:HA	1:Ak:205:GLU:HG2	1.90	0.54
1:Ao:211:ARG:O	1:Ao:211:ARG:CG	2.55	0.54
1:At:223:LEU:HD11	1:Au:244:SER:HA	1.90	0.54
1:Ab:202:ASP:HA	1:Ab:205:GLU:HG2	1.90	0.54
1:As:199:HIS:O	1:At:94:PRO:HG3	2.08	0.54
1:Au:199:HIS:O	1:Av:94:PRO:HG3	2.08	0.54
1:Av:211:ARG:CG	1:Av:211:ARG:O	2.55	0.54
1:Am:192:THR:HG22	1:Am:195:GLN:HG3	1.90	0.54
1:Am:211:ARG:CG	1:Am:211:ARG:O	2.55	0.54
1:As:192:THR:HG22	1:As:195:GLN:HG3	1.89	0.54
1:Ax:211:ARG:CG	1:Ax:211:ARG:O	2.55	0.54
1:Ay:202:ASP:HA	1:Ay:205:GLU:HG2	1.90	0.54
1:Ba:211:ARG:O	1:Ba:211:ARG:CG	2.55	0.54
1:Ag:192:THR:HG22	1:Ag:195:GLN:HG3	1.89	0.53
1:An:192:THR:HG22	1:An:195:GLN:HG3	1.89	0.53
1:Ap:192:THR:HG22	1:Ap:195:GLN:HG3	1.89	0.53
1:At:202:ASP:HA	1:At:205:GLU:HG2	1.90	0.53
1:Au:192:THR:HG22	1:Au:195:GLN:HG3	1.89	0.53
1:Aw:211:ARG:CG	1:Aw:211:ARG:O	2.55	0.53
1:Ay:211:ARG:CG	1:Ay:211:ARG:O	2.55	0.53
1:Az:199:HIS:O	1:Ba:94:PRO:HG3	2.08	0.53
1:Aa:199:HIS:O	1:Ab:94:PRO:HG3	2.08	0.53
1:Aa:202:ASP:HA	1:Aa:205:GLU:HG2	1.90	0.53
1:Ac:211:ARG:O	1:Ac:211:ARG:CG	2.55	0.53
1:Ae:199:HIS:O	1:Af:94:PRO:HG3	2.09	0.53
1:Al:202:ASP:HA	1:Al:205:GLU:HG2	1.90	0.53
1:Aq:211:ARG:CG	1:Aq:211:ARG:O	2.55	0.53
1:At:192:THR:HG22	1:At:195:GLN:HG3	1.89	0.53
1:Au:202:ASP:HA	1:Au:205:GLU:HG2	1.90	0.53
1:Aw:211:ARG:CZ	1:Ax:111:LYS:HB3	2.37	0.53
1:Aj:192:THR:HG22	1:Aj:195:GLN:HG3	1.89	0.53
1:Ao:202:ASP:HA	1:Ao:205:GLU:HG2	1.90	0.53
1:Aq:192:THR:HG22	1:Aq:195:GLN:HG3	1.89	0.53
1:Ah:199:HIS:O	1:Ai:94:PRO:HG3	2.08	0.53
1:Aj:202:ASP:HA	1:Aj:205:GLU:HG2	1.90	0.53
1:Al:199:HIS:O	1:Am:94:PRO:HG3	2.08	0.53
1:Am:223:LEU:HD11	1:An:244:SER:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:199:HIS:O	1:Ao:94:PRO:HG3	2.08	0.53
1:Ar:199:HIS:O	1:As:94:PRO:HG3	2.08	0.53
1:At:158:GLU:CD	1:Au:114:GLN:HG3	2.34	0.53
1:Ay:192:THR:HG22	1:Ay:195:GLN:HG3	1.89	0.53
1:Az:192:THR:HG22	1:Az:195:GLN:HG3	1.89	0.53
1:Ac:199:HIS:O	1:Ad:94:PRO:HG3	2.08	0.53
1:Ac:202:ASP:HA	1:Ac:205:GLU:HG2	1.90	0.53
1:Ad:223:LEU:HD11	1:Ae:244:SER:HA	1.91	0.53
1:Ae:202:ASP:HA	1:Ae:205:GLU:HG2	1.90	0.53
1:Ah:192:THR:HG22	1:Ah:195:GLN:HG3	1.89	0.53
1:Ah:202:ASP:HA	1:Ah:205:GLU:HG2	1.90	0.53
1:Av:202:ASP:HA	1:Av:205:GLU:HG2	1.90	0.53
1:Aj:211:ARG:CG	1:Aj:211:ARG:O	2.55	0.53
1:Al:192:THR:HG22	1:Al:195:GLN:HG3	1.89	0.53
1:Am:202:ASP:HA	1:Am:205:GLU:HG2	1.90	0.53
1:Aw:192:THR:HG22	1:Aw:195:GLN:HG3	1.89	0.53
1:Ba:192:THR:HG22	1:Ba:195:GLN:HG3	1.90	0.53
1:Ag:211:ARG:O	1:Ag:211:ARG:CG	2.55	0.53
1:Aq:202:ASP:HA	1:Aq:205:GLU:HG2	1.90	0.53
1:As:202:ASP:HA	1:As:205:GLU:HG2	1.90	0.53
1:Av:223:LEU:HD11	1:Aw:244:SER:HA	1.91	0.53
1:Ab:223:LEU:HD11	1:Ac:244:SER:HA	1.91	0.53
1:Af:192:THR:HG22	1:Af:195:GLN:HG3	1.90	0.53
1:Af:202:ASP:HA	1:Af:205:GLU:HG2	1.90	0.53
1:Ag:202:ASP:HA	1:Ag:205:GLU:HG2	1.90	0.53
1:Am:199:HIS:O	1:An:94:PRO:HG3	2.09	0.53
1:Av:199:HIS:O	1:Aw:94:PRO:HG3	2.09	0.53
1:Ax:223:LEU:HD11	1:Ay:244:SER:HA	1.91	0.53
1:Ab:158:GLU:CD	1:Ac:114:GLN:HG3	2.34	0.53
1:Ap:202:ASP:HA	1:Ap:205:GLU:HG2	1.90	0.53
1:Aq:211:ARG:CZ	1:Ar:111:LYS:HB3	2.39	0.53
1:Ar:175:ASN:CB	1:At:98:ASN:HD21	2.22	0.53
1:Ar:202:ASP:HA	1:Ar:205:GLU:HG2	1.90	0.53
1:Ax:199:HIS:O	1:Ay:94:PRO:HG3	2.09	0.53
1:Ba:202:ASP:HA	1:Ba:205:GLU:HG2	1.90	0.53
1:Ae:192:THR:HG22	1:Ae:195:GLN:HG3	1.89	0.53
1:Ao:192:THR:HG22	1:Ao:195:GLN:HG3	1.90	0.53
1:Ar:158:GLU:CD	1:As:114:GLN:HG3	2.34	0.53
1:Aa:192:THR:HG22	1:Aa:195:GLN:HG3	1.89	0.52
1:Ad:199:HIS:O	1:Ae:94:PRO:HG3	2.09	0.52
1:Ai:202:ASP:HA	1:Ai:205:GLU:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:199:HIS:O	1:Ak:94:PRO:HG3	2.08	0.52
1:Ar:192:THR:HG22	1:Ar:195:GLN:HG3	1.90	0.52
1:Az:202:ASP:HA	1:Az:205:GLU:HG2	1.90	0.52
1:Ac:223:LEU:HD11	1:Ad:244:SER:HA	1.92	0.52
1:Ad:202:ASP:HA	1:Ad:205:GLU:HG2	1.90	0.52
1:Ao:223:LEU:HD11	1:Ap:244:SER:HA	1.91	0.52
1:Aw:199:HIS:O	1:Ax:94:PRO:HG3	2.09	0.52
1:Az:158:GLU:CD	1:Ba:114:GLN:HG3	2.34	0.52
1:Ah:158:GLU:CD	1:Ai:114:GLN:HG3	2.34	0.52
1:Ap:211:ARG:NH1	1:Aq:111:LYS:HB3	2.24	0.52
1:Aw:202:ASP:HA	1:Aw:205:GLU:HG2	1.90	0.52
1:Af:199:HIS:O	1:Ag:94:PRO:HG3	2.09	0.52
1:Af:223:LEU:HD11	1:Ag:244:SER:HA	1.91	0.52
1:At:175:ASN:CB	1:Av:98:ASN:HD21	2.22	0.52
1:Ax:192:THR:HG22	1:Ax:195:GLN:HG3	1.90	0.52
1:Az:223:LEU:HD11	1:Ba:244:SER:HA	1.90	0.52
1:Ai:192:THR:HG22	1:Ai:195:GLN:HG3	1.90	0.52
1:Ak:155:TRP:O	1:Ak:159:ASN:ND2	2.43	0.52
1:Ak:158:GLU:CD	1:Al:114:GLN:HG3	2.34	0.52
1:Ax:202:ASP:HA	1:Ax:205:GLU:HG2	1.90	0.52
1:Ab:155:TRP:O	1:Ab:159:ASN:ND2	2.43	0.52
1:Ak:199:HIS:O	1:Al:94:PRO:HG3	2.09	0.52
1:Ao:199:HIS:O	1:Ap:94:PRO:HG3	2.09	0.52
1:At:155:TRP:O	1:At:159:ASN:ND2	2.43	0.52
1:Av:155:TRP:O	1:Av:159:ASN:ND2	2.43	0.52
1:Ab:175:ASN:CB	1:Ad:98:ASN:HD21	2.22	0.52
1:Ac:155:TRP:O	1:Ac:159:ASN:ND2	2.43	0.52
1:Ad:192:THR:HG22	1:Ad:195:GLN:HG3	1.90	0.52
1:Ah:223:LEU:HD11	1:Ai:244:SER:HA	1.90	0.52
1:Av:158:GLU:CD	1:Aw:114:GLN:HG3	2.35	0.52
1:Ah:175:ASN:CB	1:Aj:98:ASN:HD21	2.23	0.52
1:Ai:199:HIS:O	1:Aj:94:PRO:HG3	2.09	0.52
1:An:202:ASP:HA	1:An:205:GLU:HG2	1.90	0.52
1:Ad:158:GLU:CD	1:Ae:114:GLN:HG3	2.35	0.52
1:Af:158:GLU:CD	1:Ag:114:GLN:HG3	2.35	0.52
1:At:199:HIS:O	1:Au:94:PRO:HG3	2.09	0.52
1:Ao:158:GLU:CD	1:Ap:114:GLN:HG3	2.35	0.51
1:Al:223:LEU:HD11	1:Am:244:SER:HA	1.93	0.51
1:Ar:223:LEU:HD11	1:As:244:SER:HA	1.91	0.51
1:Ax:158:GLU:CD	1:Ay:114:GLN:HG3	2.35	0.51
1:Aa:155:TRP:O	1:Aa:159:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:223:LEU:HD11	1:Af:244:SER:HA	1.92	0.51
1:An:223:LEU:HD11	1:Ao:244:SER:HA	1.92	0.51
1:Au:223:LEU:HD11	1:Av:244:SER:HA	1.92	0.51
1:Al:155:TRP:O	1:Al:159:ASN:ND2	2.43	0.51
1:Aw:223:LEU:HD11	1:Ax:244:SER:HA	1.92	0.51
1:Ae:158:GLU:CD	1:Af:114:GLN:HG3	2.35	0.51
1:Ad:155:TRP:O	1:Ad:159:ASN:ND2	2.43	0.51
1:Am:158:GLU:CD	1:An:114:GLN:HG3	2.35	0.51
1:An:158:GLU:CD	1:Ao:114:GLN:HG3	2.36	0.51
1:Aw:158:GLU:CD	1:Ax:114:GLN:HG3	2.36	0.51
1:Ai:158:GLU:CD	1:Aj:114:GLN:HG3	2.36	0.51
1:Ai:223:LEU:HD11	1:Aj:244:SER:HA	1.91	0.51
1:Am:175:ASN:CB	1:Ao:98:ASN:HD21	2.23	0.51
1:Au:155:TRP:O	1:Au:159:ASN:ND2	2.43	0.51
1:Ay:223:LEU:HD11	1:Az:244:SER:HA	1.93	0.51
1:Aa:223:LEU:HD11	1:Ab:244:SER:HA	1.93	0.50
1:Ag:175:ASN:CB	1:Ai:98:ASN:HD21	2.24	0.50
1:Al:158:GLU:CD	1:Am:114:GLN:HG3	2.36	0.50
1:Aj:223:LEU:HD11	1:Ak:244:SER:HA	1.93	0.50
1:Ax:175:ASN:CB	1:Az:98:ASN:HD21	2.22	0.50
1:Ag:223:LEU:HD11	1:Ah:244:SER:HA	1.93	0.50
1:Ak:175:ASN:CB	1:Am:98:ASN:HD21	2.22	0.50
1:Am:155:TRP:O	1:Am:159:ASN:ND2	2.43	0.50
1:Ay:175:ASN:CB	1:Ba:98:ASN:HD21	2.24	0.50
1:Af:175:ASN:CB	1:Ah:98:ASN:HD21	2.22	0.50
1:Aq:158:GLU:CD	1:Ar:114:GLN:HG3	2.37	0.50
1:Ae:155:TRP:O	1:Ae:159:ASN:ND2	2.42	0.50
1:Ai:175:ASN:CB	1:Ak:98:ASN:HD21	2.23	0.50
1:As:223:LEU:HD11	1:At:244:SER:HA	1.93	0.50
1:Au:158:GLU:CD	1:Av:114:GLN:HG3	2.36	0.50
1:Ad:175:ASN:CB	1:Af:98:ASN:HD21	2.23	0.49
1:Ae:175:ASN:CB	1:Ag:98:ASN:HD21	2.25	0.49
1:Aj:155:TRP:O	1:Aj:159:ASN:ND2	2.43	0.49
1:Av:175:ASN:CB	1:Ax:98:ASN:HD21	2.23	0.49
1:Aj:158:GLU:CD	1:Ak:114:GLN:HG3	2.38	0.49
1:Aj:175:ASN:CB	1:Al:98:ASN:HD21	2.25	0.49
1:Ac:158:GLU:CD	1:Ad:114:GLN:HG3	2.37	0.49
1:Aw:175:ASN:CB	1:Ay:98:ASN:HD21	2.25	0.49
1:Ay:158:GLU:CD	1:Az:114:GLN:HG3	2.38	0.49
1:Ag:158:GLU:CD	1:Ah:114:GLN:HG3	2.38	0.49
1:Ap:158:GLU:CD	1:Aq:114:GLN:HG3	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:175:ASN:CB	1:Ac:98:ASN:HD21	2.24	0.48
1:Aa:158:GLU:CD	1:Ab:114:GLN:HG3	2.38	0.48
1:Az:155:TRP:O	1:Az:159:ASN:ND2	2.43	0.48
1:Ah:81:ILE:H	1:Ah:81:ILE:HD12	1.79	0.48
1:Ap:155:TRP:O	1:Ap:159:ASN:ND2	2.43	0.48
1:Aq:155:TRP:O	1:Aq:159:ASN:ND2	2.43	0.48
1:Ar:81:ILE:HD12	1:Ar:81:ILE:H	1.79	0.48
1:Ab:81:ILE:HD12	1:Ab:81:ILE:H	1.79	0.48
1:Af:155:TRP:O	1:Af:159:ASN:ND2	2.42	0.48
1:An:155:TRP:O	1:An:159:ASN:ND2	2.42	0.48
1:As:155:TRP:O	1:As:159:ASN:ND2	2.43	0.48
1:Ay:155:TRP:O	1:Ay:159:ASN:ND2	2.42	0.48
1:Al:81:ILE:H	1:Al:81:ILE:HD12	1.79	0.48
1:Ap:211:ARG:CZ	1:Aq:111:LYS:HB3	2.43	0.48
1:Av:81:ILE:HD12	1:Av:81:ILE:H	1.79	0.48
1:Aw:81:ILE:HD12	1:Aw:81:ILE:H	1.79	0.48
1:Ay:81:ILE:HD12	1:Ay:81:ILE:H	1.79	0.48
1:Ag:155:TRP:O	1:Ag:159:ASN:ND2	2.42	0.48
1:Am:81:ILE:HD12	1:Am:81:ILE:H	1.79	0.48
1:Ap:175:ASN:CB	1:Ar:98:ASN:HD21	2.24	0.48
1:Ah:155:TRP:O	1:Ah:159:ASN:ND2	2.43	0.48
1:Ak:81:ILE:HD12	1:Ak:81:ILE:H	1.79	0.48
1:Ao:81:ILE:HD12	1:Ao:81:ILE:H	1.79	0.48
1:Aq:175:ASN:CB	1:As:98:ASN:HD21	2.27	0.48
1:Ba:81:ILE:HD12	1:Ba:81:ILE:H	1.79	0.48
1:Aa:81:ILE:HD12	1:Aa:81:ILE:H	1.79	0.47
1:Ac:81:ILE:HD12	1:Ac:81:ILE:H	1.79	0.47
1:Aq:81:ILE:HD12	1:Aq:81:ILE:H	1.79	0.47
1:Ae:81:ILE:HD12	1:Ae:81:ILE:H	1.79	0.47
1:Al:175:ASN:CB	1:An:98:ASN:HD21	2.26	0.47
1:As:158:GLU:CD	1:At:114:GLN:HG3	2.38	0.47
1:Ab:218:MET:O	1:Ac:114:GLN:NE2	2.47	0.47
1:Ak:218:MET:O	1:Al:114:GLN:NE2	2.47	0.47
1:An:175:ASN:CB	1:Ap:98:ASN:HD21	2.25	0.47
1:Au:81:ILE:HD12	1:Au:81:ILE:H	1.79	0.47
1:Ag:81:ILE:HD12	1:Ag:81:ILE:H	1.79	0.47
1:Aq:175:ASN:OD1	1:As:98:ASN:ND2	2.48	0.47
1:Au:175:ASN:CB	1:Aw:98:ASN:HD21	2.26	0.47
1:Af:175:ASN:OD1	1:Ah:98:ASN:ND2	2.47	0.47
1:An:81:ILE:HD12	1:An:81:ILE:H	1.79	0.47
1:Ao:155:TRP:O	1:Ao:159:ASN:ND2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Az:218:MET:O	1:Ba:114:GLN:NE2	2.46	0.47
1:Ac:175:ASN:CB	1:Ae:98:ASN:HD21	2.26	0.47
1:Ad:81:ILE:H	1:Ad:81:ILE:HD12	1.79	0.47
1:Af:81:ILE:HD12	1:Af:81:ILE:H	1.79	0.47
1:Am:218:MET:O	1:An:114:GLN:NE2	2.48	0.47
1:As:175:ASN:CB	1:Au:98:ASN:HD21	2.25	0.47
1:Ax:81:ILE:H	1:Ax:81:ILE:HD12	1.79	0.47
1:Ax:175:ASN:OD1	1:Az:98:ASN:ND2	2.47	0.47
1:Ba:155:TRP:O	1:Ba:159:ASN:ND2	2.43	0.47
1:Ah:218:MET:O	1:Ai:114:GLN:NE2	2.46	0.47
1:Aj:81:ILE:HD12	1:Aj:81:ILE:H	1.79	0.47
1:Ak:175:ASN:OD1	1:Am:98:ASN:ND2	2.48	0.47
1:Ap:81:ILE:H	1:Ap:81:ILE:HD12	1.79	0.47
1:At:81:ILE:H	1:At:81:ILE:HD12	1.79	0.47
1:Az:81:ILE:HD12	1:Az:81:ILE:H	1.79	0.47
1:Ad:218:MET:O	1:Ae:114:GLN:NE2	2.48	0.47
1:Ax:208:ILE:HD11	1:Ax:219:PRO:HD3	1.97	0.47
1:Ai:175:ASN:OD1	1:Ak:98:ASN:ND2	2.49	0.46
1:Ac:218:MET:O	1:Ad:114:GLN:NE2	2.48	0.46
1:Ak:150:ASN:HD21	1:Al:107:LEU:HA	1.81	0.46
1:Ap:223:LEU:HD11	1:Aq:244:SER:HA	1.97	0.46
1:Aq:223:LEU:HD11	1:Ar:244:SER:HA	1.96	0.46
1:Aw:208:ILE:HD11	1:Aw:219:PRO:HD3	1.97	0.46
1:Ay:208:ILE:HD11	1:Ay:219:PRO:HD3	1.97	0.46
1:Ai:81:ILE:HD12	1:Ai:81:ILE:H	1.79	0.46
1:At:175:ASN:OD1	1:Av:98:ASN:ND2	2.48	0.46
1:Ab:175:ASN:OD1	1:Ad:98:ASN:ND2	2.48	0.46
1:Aw:155:TRP:O	1:Aw:159:ASN:ND2	2.42	0.46
1:Ar:175:ASN:OD1	1:At:98:ASN:ND2	2.48	0.46
1:Au:218:MET:O	1:Av:114:GLN:NE2	2.49	0.46
1:Ax:155:TRP:O	1:Ax:159:ASN:ND2	2.42	0.46
1:Az:208:ILE:HD11	1:Az:219:PRO:HD3	1.97	0.46
1:Ae:208:ILE:HD11	1:Ae:219:PRO:HD3	1.97	0.46
1:Af:208:ILE:HD11	1:Af:219:PRO:HD3	1.97	0.46
1:Ar:155:TRP:O	1:Ar:159:ASN:ND2	2.43	0.46
1:At:218:MET:O	1:Au:114:GLN:NE2	2.47	0.46
1:Av:218:MET:O	1:Aw:114:GLN:NE2	2.48	0.46
1:An:208:ILE:HD11	1:An:219:PRO:HD3	1.97	0.46
1:Ar:150:ASN:HD21	1:As:107:LEU:HA	1.81	0.46
1:Aw:218:MET:O	1:Ax:114:GLN:NE2	2.49	0.46
1:Ag:208:ILE:HD11	1:Ag:219:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:208:ILE:HD11	1:Ao:219:PRO:HD3	1.97	0.46
1:As:81:ILE:HD12	1:As:81:ILE:H	1.79	0.46
1:Aa:175:ASN:OD1	1:Ac:98:ASN:ND2	2.49	0.46
1:Aq:218:MET:O	1:Ar:114:GLN:NE2	2.48	0.46
1:Ar:218:MET:O	1:As:114:GLN:NE2	2.48	0.46
1:As:208:ILE:HD11	1:As:219:PRO:HD3	1.97	0.46
1:At:208:ILE:HD11	1:At:219:PRO:HD3	1.97	0.46
1:Av:208:ILE:HD11	1:Av:219:PRO:HD3	1.97	0.46
1:Aw:150:ASN:HD21	1:Ax:107:LEU:HA	1.81	0.46
1:Aa:208:ILE:HD11	1:Aa:219:PRO:HD3	1.97	0.46
1:Ah:175:ASN:OD1	1:Aj:98:ASN:ND2	2.49	0.46
1:Am:208:ILE:HD11	1:Am:219:PRO:HD3	1.97	0.46
1:Ax:150:ASN:HD21	1:Ay:107:LEU:HA	1.81	0.46
1:Ae:150:ASN:HD21	1:Af:107:LEU:HA	1.81	0.45
1:Ao:150:ASN:HD21	1:Ap:107:LEU:HA	1.81	0.45
1:Aa:218:MET:O	1:Ab:114:GLN:NE2	2.49	0.45
1:Ad:208:ILE:HD11	1:Ad:219:PRO:HD3	1.97	0.45
1:Ai:155:TRP:O	1:Ai:159:ASN:ND2	2.43	0.45
1:At:150:ASN:HD21	1:Au:107:LEU:HA	1.81	0.45
1:Ax:218:MET:O	1:Ay:114:GLN:NE2	2.49	0.45
1:Ah:208:ILE:HD11	1:Ah:219:PRO:HD3	1.97	0.45
1:Aj:208:ILE:HD11	1:Aj:219:PRO:HD3	1.97	0.45
1:Al:208:ILE:HD11	1:Al:219:PRO:HD3	1.97	0.45
1:Al:218:MET:O	1:Am:114:GLN:NE2	2.49	0.45
1:Am:175:ASN:OD1	1:Ao:98:ASN:ND2	2.50	0.45
1:Ao:218:MET:O	1:Ap:114:GLN:NE2	2.49	0.45
1:Au:208:ILE:HD11	1:Au:219:PRO:HD3	1.97	0.45
1:Ba:208:ILE:HD11	1:Ba:219:PRO:HD3	1.97	0.45
1:Ab:150:ASN:HD21	1:Ac:107:LEU:HA	1.81	0.45
1:Ab:208:ILE:HD11	1:Ab:219:PRO:HD3	1.97	0.45
1:Ae:218:MET:O	1:Af:114:GLN:NE2	2.49	0.45
1:Af:218:MET:O	1:Ag:114:GLN:NE2	2.49	0.45
1:Ap:208:ILE:HD11	1:Ap:219:PRO:HD3	1.97	0.45
1:Ar:208:ILE:HD11	1:Ar:219:PRO:HD3	1.97	0.45
1:Ay:218:MET:O	1:Az:114:GLN:NE2	2.49	0.45
1:Az:150:ASN:HD21	1:Ba:107:LEU:HA	1.81	0.45
1:Ac:175:ASN:OD1	1:Ae:98:ASN:ND2	2.50	0.45
1:Ad:150:ASN:HD21	1:Ae:107:LEU:HA	1.82	0.45
1:Ai:208:ILE:HD11	1:Ai:219:PRO:HD3	1.97	0.45
1:Ak:208:ILE:HD11	1:Ak:219:PRO:HD3	1.97	0.45
1:An:218:MET:O	1:Ao:114:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:218:MET:O	1:Ah:114:GLN:NE2	2.49	0.45
1:Aw:151:GLY:HA3	1:Aw:171:MET:SD	2.57	0.45
1:Ah:150:ASN:HD21	1:Ai:107:LEU:HA	1.81	0.45
1:Ah:151:GLY:HA3	1:Ah:171:MET:SD	2.57	0.45
1:Ar:151:GLY:HA3	1:Ar:171:MET:SD	2.57	0.45
1:Av:151:GLY:HA3	1:Av:171:MET:SD	2.57	0.45
1:Ay:175:ASN:OD1	1:Ba:98:ASN:ND2	2.50	0.45
1:Ab:151:GLY:HA3	1:Ab:171:MET:SD	2.57	0.45
1:Ai:151:GLY:HA3	1:Ai:171:MET:SD	2.57	0.45
1:As:151:GLY:HA3	1:As:171:MET:SD	2.57	0.45
1:Ai:218:MET:O	1:Aj:114:GLN:NE2	2.49	0.45
1:Al:150:ASN:HD21	1:Am:107:LEU:HA	1.82	0.45
1:An:151:GLY:HA3	1:An:171:MET:SD	2.57	0.45
1:Ap:175:ASN:OD1	1:Ar:98:ASN:ND2	2.50	0.45
1:As:218:MET:O	1:At:114:GLN:NE2	2.49	0.45
1:Ax:151:GLY:HA3	1:Ax:171:MET:SD	2.57	0.45
1:Ac:151:GLY:HA3	1:Ac:171:MET:SD	2.57	0.45
1:Ac:208:ILE:HD11	1:Ac:219:PRO:HD3	1.97	0.45
1:Af:157:ILE:HD11	1:Af:204:ALA:HB1	1.99	0.45
1:Ag:175:ASN:OD1	1:Ai:98:ASN:ND2	2.50	0.45
1:Ao:151:GLY:HA3	1:Ao:171:MET:SD	2.57	0.45
1:Aq:157:ILE:HD11	1:Aq:204:ALA:HB1	1.99	0.45
1:Ar:157:ILE:HD11	1:Ar:204:ALA:HB1	1.99	0.45
1:Ag:151:GLY:HA3	1:Ag:171:MET:SD	2.57	0.44
1:Ba:151:GLY:HA3	1:Ba:171:MET:SD	2.57	0.44
1:Ad:175:ASN:OD1	1:Af:98:ASN:ND2	2.50	0.44
1:Ag:157:ILE:HD11	1:Ag:204:ALA:HB1	2.00	0.44
1:Am:150:ASN:HD21	1:An:107:LEU:HA	1.82	0.44
1:An:150:ASN:HD21	1:Ao:107:LEU:HA	1.81	0.44
1:Aq:151:GLY:HA3	1:Aq:171:MET:SD	2.57	0.44
1:Aq:208:ILE:HD11	1:Aq:219:PRO:HD3	1.97	0.44
1:As:157:ILE:HD11	1:As:204:ALA:HB1	1.99	0.44
1:Aa:151:GLY:HA3	1:Aa:171:MET:SD	2.57	0.44
1:Ae:157:ILE:HD11	1:Ae:204:ALA:HB1	1.99	0.44
1:Af:150:ASN:HD21	1:Ag:107:LEU:HA	1.81	0.44
1:Ap:157:ILE:HD11	1:Ap:204:ALA:HB1	2.00	0.44
1:Av:150:ASN:HD21	1:Aw:107:LEU:HA	1.82	0.44
1:Ah:157:ILE:HD11	1:Ah:204:ALA:HB1	1.99	0.44
1:Am:151:GLY:HA3	1:Am:171:MET:SD	2.57	0.44
1:Au:151:GLY:HA3	1:Au:171:MET:SD	2.57	0.44
1:Av:175:ASN:OD1	1:Ax:98:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:151:GLY:HA3	1:Ay:171:MET:SD	2.57	0.44
1:Ad:151:GLY:HA3	1:Ad:171:MET:SD	2.57	0.44
1:Ad:219:PRO:O	1:Ad:222:GLY:N	2.50	0.44
1:Af:116:ASP:HA	1:Af:121:ARG:NH2	2.33	0.44
1:Ag:116:ASP:HA	1:Ag:121:ARG:NH2	2.33	0.44
1:Ah:116:ASP:HA	1:Ah:121:ARG:NH2	2.33	0.44
1:Ab:219:PRO:O	1:Ab:222:GLY:N	2.50	0.44
1:Ag:219:PRO:O	1:Ag:222:GLY:N	2.50	0.44
1:Ai:116:ASP:HA	1:Ai:121:ARG:NH2	2.33	0.44
1:Ai:150:ASN:HD21	1:Aj:107:LEU:HA	1.82	0.44
1:Aj:151:GLY:HA3	1:Aj:171:MET:SD	2.57	0.44
1:Aj:218:MET:O	1:Ak:114:GLN:NE2	2.49	0.44
1:Am:219:PRO:O	1:Am:222:GLY:N	2.50	0.44
1:Ao:157:ILE:HD11	1:Ao:204:ALA:HB1	1.99	0.44
1:At:157:ILE:HD11	1:At:204:ALA:HB1	1.99	0.44
1:Ad:157:ILE:HD11	1:Ad:204:ALA:HB1	1.99	0.44
1:Ae:151:GLY:HA3	1:Ae:171:MET:SD	2.57	0.44
1:Ae:175:ASN:OD1	1:Ag:98:ASN:ND2	2.51	0.44
1:Ak:151:GLY:HA3	1:Ak:171:MET:SD	2.57	0.44
1:Ap:116:ASP:HA	1:Ap:121:ARG:NH2	2.33	0.44
1:Aq:116:ASP:HA	1:Aq:121:ARG:NH2	2.33	0.44
1:Aw:175:ASN:OD1	1:Ay:98:ASN:ND2	2.51	0.44
1:Ba:157:ILE:HD11	1:Ba:204:ALA:HB1	1.99	0.44
1:Aa:157:ILE:HD11	1:Aa:204:ALA:HB1	2.00	0.44
1:Ae:116:ASP:HA	1:Ae:121:ARG:NH2	2.33	0.44
1:Al:151:GLY:HA3	1:Al:171:MET:SD	2.57	0.44
1:Ao:116:ASP:HA	1:Ao:121:ARG:NH2	2.33	0.44
1:Ap:151:GLY:HA3	1:Ap:171:MET:SD	2.57	0.44
1:At:151:GLY:HA3	1:At:171:MET:SD	2.57	0.44
1:Av:219:PRO:O	1:Av:222:GLY:N	2.50	0.44
1:Aj:116:ASP:HA	1:Aj:121:ARG:NH2	2.33	0.43
1:Ak:219:PRO:O	1:Ak:222:GLY:N	2.50	0.43
1:Ar:116:ASP:HA	1:Ar:121:ARG:NH2	2.33	0.43
1:Au:150:ASN:HD21	1:Av:107:LEU:HA	1.82	0.43
1:Au:175:ASN:OD1	1:Aw:98:ASN:ND2	2.51	0.43
1:Ax:157:ILE:HD11	1:Ax:204:ALA:HB1	1.99	0.43
1:Az:151:GLY:HA3	1:Az:171:MET:SD	2.57	0.43
1:Ac:116:ASP:HA	1:Ac:121:ARG:NH2	2.33	0.43
1:Ai:157:ILE:HD11	1:Ai:204:ALA:HB1	2.00	0.43
1:An:116:ASP:HA	1:An:121:ARG:NH2	2.33	0.43
1:Ay:116:ASP:HA	1:Ay:121:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ab:157:ILE:HD11	1:Ab:204:ALA:HB1	2.00	0.43
1:Ac:157:ILE:HD11	1:Ac:204:ALA:HB1	1.99	0.43
1:Aj:150:ASN:HD21	1:Ak:107:LEU:HA	1.83	0.43
1:Ao:219:PRO:O	1:Ao:222:GLY:N	2.50	0.43
1:Ax:219:PRO:O	1:Ax:222:GLY:N	2.50	0.43
1:Az:116:ASP:HA	1:Az:121:ARG:NH2	2.33	0.43
1:Ab:116:ASP:HA	1:Ab:121:ARG:NH2	2.33	0.43
1:Ac:150:ASN:HD21	1:Ad:107:LEU:HA	1.84	0.43
1:Af:151:GLY:HA3	1:Af:171:MET:SD	2.57	0.43
1:Ag:150:ASN:HD21	1:Ah:107:LEU:HA	1.84	0.43
1:Ak:116:ASP:HA	1:Ak:121:ARG:NH2	2.33	0.43
1:As:116:ASP:HA	1:As:121:ARG:NH2	2.33	0.43
1:Aw:157:ILE:HD11	1:Aw:204:ALA:HB1	1.99	0.43
1:Ay:157:ILE:HD11	1:Ay:204:ALA:HB1	2.00	0.43
1:Ac:191:PRO:HD2	1:Ac:195:GLN:HB2	2.00	0.43
1:Ad:116:ASP:HA	1:Ad:121:ARG:NH2	2.33	0.43
1:Af:219:PRO:O	1:Af:222:GLY:N	2.50	0.43
1:Aj:175:ASN:OD1	1:Al:98:ASN:ND2	2.52	0.43
1:Al:116:ASP:HA	1:Al:121:ARG:NH2	2.33	0.43
1:As:150:ASN:HD21	1:At:107:LEU:HA	1.83	0.43
1:As:175:ASN:OD1	1:Au:98:ASN:ND2	2.52	0.43
1:At:219:PRO:O	1:At:222:GLY:N	2.50	0.43
1:Au:157:ILE:HD11	1:Au:204:ALA:HB1	2.00	0.43
1:Az:157:ILE:HD11	1:Az:204:ALA:HB1	1.99	0.43
1:Ba:219:PRO:O	1:Ba:222:GLY:N	2.50	0.43
1:Ab:191:PRO:HD2	1:Ab:195:GLN:HB2	2.00	0.43
1:Af:191:PRO:HD2	1:Af:195:GLN:HB2	2.00	0.43
1:Am:116:ASP:HA	1:Am:121:ARG:NH2	2.33	0.43
1:Am:191:PRO:HD2	1:Am:195:GLN:HB2	2.00	0.43
1:An:157:ILE:HD11	1:An:204:ALA:HB1	2.00	0.43
1:Ag:191:PRO:HD2	1:Ag:195:GLN:HB2	2.00	0.43
1:Aq:191:PRO:HD2	1:Aq:195:GLN:HB2	2.00	0.43
1:Ar:219:PRO:O	1:Ar:222:GLY:N	2.50	0.43
1:Av:157:ILE:HD11	1:Av:204:ALA:HB1	2.00	0.43
1:Az:191:PRO:HD2	1:Az:195:GLN:HB2	2.00	0.43
1:Ah:219:PRO:O	1:Ah:222:GLY:N	2.50	0.43
1:Ai:219:PRO:O	1:Ai:222:GLY:N	2.50	0.43
1:Al:191:PRO:HD2	1:Al:195:GLN:HB2	2.00	0.43
1:Ao:191:PRO:HD2	1:Ao:195:GLN:HB2	2.00	0.43
1:Ap:191:PRO:HD2	1:Ap:195:GLN:HB2	2.00	0.43
1:As:219:PRO:O	1:As:222:GLY:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:At:191:PRO:HD2	1:At:195:GLN:HB2	2.00	0.43
1:Ax:116:ASP:HA	1:Ax:121:ARG:NH2	2.33	0.43
1:Ba:116:ASP:HA	1:Ba:121:ARG:NH2	2.33	0.43
1:Aa:116:ASP:HA	1:Aa:121:ARG:NH2	2.33	0.43
1:Aj:157:ILE:HD11	1:Aj:204:ALA:HB1	1.99	0.43
1:Aj:219:PRO:O	1:Aj:222:GLY:N	2.50	0.43
1:As:191:PRO:HD2	1:As:195:GLN:HB2	2.00	0.43
1:At:116:ASP:HA	1:At:121:ARG:NH2	2.33	0.43
1:Av:191:PRO:HD2	1:Av:195:GLN:HB2	2.00	0.43
1:Aw:191:PRO:HD2	1:Aw:195:GLN:HB2	2.00	0.43
1:Ba:191:PRO:HD2	1:Ba:195:GLN:HB2	2.00	0.43
1:Au:116:ASP:HA	1:Au:121:ARG:NH2	2.33	0.43
1:Aa:219:PRO:O	1:Aa:222:GLY:N	2.50	0.42
1:Ad:191:PRO:HD2	1:Ad:195:GLN:HB2	2.00	0.42
1:Aj:191:PRO:HD2	1:Aj:195:GLN:HB2	2.00	0.42
1:Al:175:ASN:OD1	1:An:98:ASN:ND2	2.51	0.42
1:Aw:116:ASP:HA	1:Aw:121:ARG:NH2	2.33	0.42
1:Ay:191:PRO:HD2	1:Ay:195:GLN:HB2	2.00	0.42
1:Ah:191:PRO:HD2	1:Ah:195:GLN:HB2	2.00	0.42
1:Am:157:ILE:HD11	1:Am:204:ALA:HB1	1.99	0.42
1:An:175:ASN:OD1	1:Ap:98:ASN:ND2	2.51	0.42
1:Ax:191:PRO:HD2	1:Ax:195:GLN:HB2	2.00	0.42
1:Ae:191:PRO:HD2	1:Ae:195:GLN:HB2	2.00	0.42
1:Ai:191:PRO:HD2	1:Ai:195:GLN:HB2	2.00	0.42
1:Ar:191:PRO:HD2	1:Ar:195:GLN:HB2	2.00	0.42
1:Ax:175:ASN:CG	1:Az:98:ASN:HD21	2.27	0.42
1:Aq:219:PRO:O	1:Aq:222:GLY:N	2.50	0.42
1:Ak:157:ILE:HD11	1:Ak:204:ALA:HB1	2.00	0.42
1:Al:157:ILE:HD11	1:Al:204:ALA:HB1	1.99	0.42
1:An:191:PRO:HD2	1:An:195:GLN:HB2	2.00	0.42
1:Aa:150:ASN:HD21	1:Ab:107:LEU:HA	1.83	0.42
1:Aa:191:PRO:HD2	1:Aa:195:GLN:HB2	2.00	0.42
1:Ap:199:HIS:O	1:Aq:94:PRO:HG3	2.19	0.42
1:Au:191:PRO:HD2	1:Au:195:GLN:HB2	2.00	0.42
1:Ak:191:PRO:HD2	1:Ak:195:GLN:HB2	2.00	0.42
1:Av:116:ASP:HA	1:Av:121:ARG:NH2	2.33	0.42
1:Az:219:PRO:O	1:Az:222:GLY:N	2.50	0.42
1:Ak:175:ASN:CG	1:Am:98:ASN:HD21	2.28	0.42
1:Ab:175:ASN:CG	1:Ad:98:ASN:HD21	2.28	0.42
1:Ab:249:ARG:HE	1:Ab:249:ARG:HB2	1.77	0.42
1:Af:175:ASN:CG	1:Ah:98:ASN:HD21	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ar:175:ASN:CG	1:At:98:ASN:HD21	2.28	0.42
1:At:175:ASN:CG	1:Av:98:ASN:HD21	2.28	0.42
1:Au:219:PRO:O	1:Au:222:GLY:N	2.50	0.42
1:Ay:150:ASN:HD21	1:Az:107:LEU:HA	1.84	0.42
1:Al:219:PRO:O	1:Al:222:GLY:N	2.50	0.41
1:Ai:175:ASN:CG	1:Ak:98:ASN:HD21	2.28	0.41
1:Ap:218:MET:O	1:Aq:114:GLN:NE2	2.52	0.41
1:Ba:249:ARG:HE	1:Ba:249:ARG:HB2	1.77	0.41
1:Ap:150:ASN:HD21	1:Aq:107:LEU:HA	1.86	0.41
1:Ac:219:PRO:O	1:Ac:222:GLY:N	2.50	0.41
1:Ad:115:ARG:O	1:Ad:121:ARG:NH2	2.54	0.41
1:Ag:249:ARG:HE	1:Ag:249:ARG:HB2	1.77	0.41
1:Am:115:ARG:O	1:Am:121:ARG:NH2	2.54	0.41
1:Av:115:ARG:O	1:Av:121:ARG:NH2	2.54	0.41
1:Al:249:ARG:HE	1:Al:249:ARG:HB2	1.77	0.41
1:Ax:115:ARG:O	1:Ax:121:ARG:NH2	2.54	0.41
1:Ah:175:ASN:CG	1:Aj:98:ASN:HD21	2.29	0.41
1:An:219:PRO:O	1:An:222:GLY:N	2.50	0.41
1:Ao:115:ARG:O	1:Ao:121:ARG:NH2	2.54	0.41
1:Aq:150:ASN:HD21	1:Ar:107:LEU:HA	1.84	0.41
1:Aw:115:ARG:O	1:Aw:121:ARG:NH2	2.54	0.41
1:Af:115:ARG:O	1:Af:121:ARG:NH2	2.54	0.40
1:Ai:115:ARG:O	1:Ai:121:ARG:NH2	2.54	0.40
1:Ay:115:ARG:O	1:Ay:121:ARG:NH2	2.54	0.40
1:Ab:115:ARG:O	1:Ab:121:ARG:NH2	2.54	0.40
1:Ac:115:ARG:O	1:Ac:121:ARG:NH2	2.54	0.40
1:Ar:115:ARG:O	1:Ar:121:ARG:NH2	2.54	0.40
1:Aw:219:PRO:O	1:Aw:222:GLY:N	2.50	0.40
1:Ag:108:ILE:HD13	1:Ag:108:ILE:HA	1.96	0.40
1:Al:197:MET:HE3	1:Al:197:MET:HB3	1.91	0.40
1:An:115:ARG:O	1:An:121:ARG:NH2	2.54	0.40
1:Ap:115:ARG:O	1:Ap:121:ARG:NH2	2.54	0.40
1:Ak:115:ARG:O	1:Ak:121:ARG:NH2	2.54	0.40
1:Aq:108:ILE:HD13	1:Aq:108:ILE:HA	1.96	0.40
1:Ba:115:ARG:O	1:Ba:121:ARG:NH2	2.54	0.40
1:Ae:115:ARG:O	1:Ae:121:ARG:NH2	2.54	0.40
1:At:115:ARG:O	1:At:121:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ab	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ac	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ad	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ae	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Af	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ag	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ah	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ai	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Aj	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ak	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Al	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Am	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	An	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ao	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ap	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Aq	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ar	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	As	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	At	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Au	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Av	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Aw	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ax	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ay	176/303 (58%)	168 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Az	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
1	Ba	176/303 (58%)	168 (96%)	8 (4%)	0	100	100
All	All	4752/8181 (58%)	4536 (96%)	216 (4%)	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	Aa	161/253 (64%)	161 (100%)	0	100	100
1	Ab	161/253 (64%)	161 (100%)	0	100	100
1	Ac	161/253 (64%)	161 (100%)	0	100	100
1	Ad	161/253 (64%)	161 (100%)	0	100	100
1	Ae	161/253 (64%)	161 (100%)	0	100	100
1	Af	161/253 (64%)	161 (100%)	0	100	100
1	Ag	161/253 (64%)	161 (100%)	0	100	100
1	Ah	161/253 (64%)	161 (100%)	0	100	100
1	Ai	161/253 (64%)	161 (100%)	0	100	100
1	Aj	161/253 (64%)	161 (100%)	0	100	100
1	Ak	161/253 (64%)	161 (100%)	0	100	100
1	Al	161/253 (64%)	161 (100%)	0	100	100
1	Am	161/253 (64%)	161 (100%)	0	100	100
1	An	161/253 (64%)	161 (100%)	0	100	100
1	Ao	161/253 (64%)	161 (100%)	0	100	100
1	Ap	161/253 (64%)	161 (100%)	0	100	100
1	Aq	161/253 (64%)	161 (100%)	0	100	100
1	Ar	161/253 (64%)	161 (100%)	0	100	100
1	As	161/253 (64%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	At	161/253 (64%)	161 (100%)	0	100	100
1	Au	161/253 (64%)	161 (100%)	0	100	100
1	Av	161/253 (64%)	161 (100%)	0	100	100
1	Aw	161/253 (64%)	161 (100%)	0	100	100
1	Ax	161/253 (64%)	161 (100%)	0	100	100
1	Ay	161/253 (64%)	161 (100%)	0	100	100
1	Az	161/253 (64%)	161 (100%)	0	100	100
1	Ba	161/253 (64%)	161 (100%)	0	100	100
All	All	4347/6831 (64%)	4347 (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 (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	98	ASN
1	Aa	176	ASN
1	Aa	228	ASN
1	Ab	98	ASN
1	Ab	176	ASN
1	Ab	228	ASN
1	Ac	98	ASN
1	Ac	176	ASN
1	Ac	228	ASN
1	Ad	98	ASN
1	Ad	176	ASN
1	Ad	228	ASN
1	Ae	98	ASN
1	Ae	176	ASN
1	Ae	228	ASN
1	Af	98	ASN
1	Af	176	ASN
1	Af	228	ASN
1	Ag	98	ASN
1	Ag	176	ASN
1	Ag	228	ASN
1	Ah	98	ASN
1	Ah	176	ASN
1	Ah	228	ASN

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Mol	Chain	Res	Type
1	Ai	98	ASN
1	Ai	176	ASN
1	Ai	228	ASN
1	Aj	98	ASN
1	Aj	176	ASN
1	Aj	228	ASN
1	Ak	98	ASN
1	Ak	176	ASN
1	Ak	228	ASN
1	Al	98	ASN
1	Al	176	ASN
1	Al	228	ASN
1	Am	98	ASN
1	Am	176	ASN
1	Am	228	ASN
1	An	98	ASN
1	An	176	ASN
1	An	228	ASN
1	Ao	98	ASN
1	Ao	176	ASN
1	Ao	228	ASN
1	Ap	98	ASN
1	Ap	176	ASN
1	Ap	228	ASN
1	Aq	176	ASN
1	Aq	228	ASN
1	Ar	98	ASN
1	Ar	176	ASN
1	Ar	228	ASN
1	As	98	ASN
1	As	176	ASN
1	As	228	ASN
1	At	98	ASN
1	At	176	ASN
1	At	228	ASN
1	Au	98	ASN
1	Au	176	ASN
1	Au	228	ASN
1	Av	98	ASN
1	Av	176	ASN
1	Av	228	ASN
1	Aw	98	ASN

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Mol	Chain	Res	Type
1	Aw	176	ASN
1	Aw	228	ASN
1	Ax	98	ASN
1	Ax	176	ASN
1	Ax	228	ASN
1	Ay	98	ASN
1	Ay	176	ASN
1	Ay	228	ASN
1	Az	98	ASN
1	Az	176	ASN
1	Az	228	ASN
1	Ba	98	ASN
1	Ba	176	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.

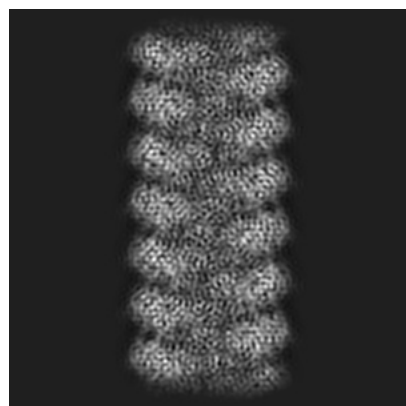
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53867. These allow visual inspection of the internal detail of the map and identification of artifacts.

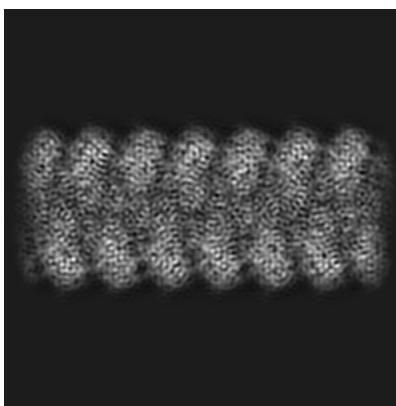
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

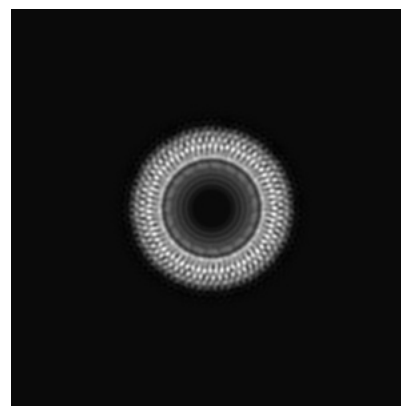
6.1.1 Primary map



X

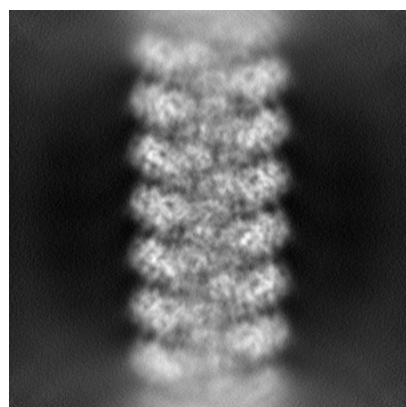


Y

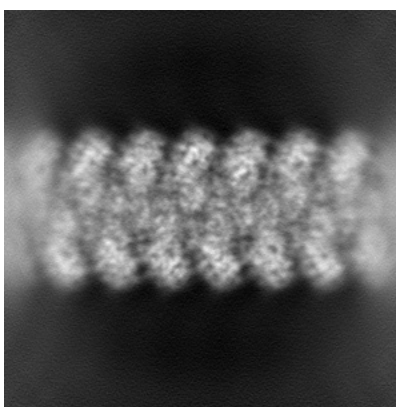


Z

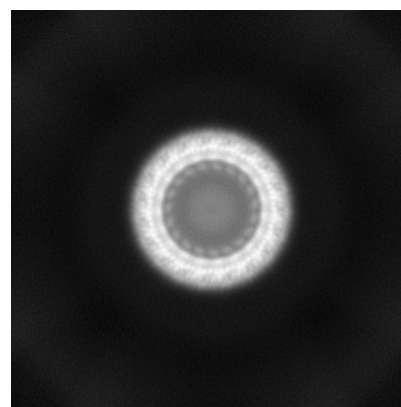
6.1.2 Raw map



X



Y

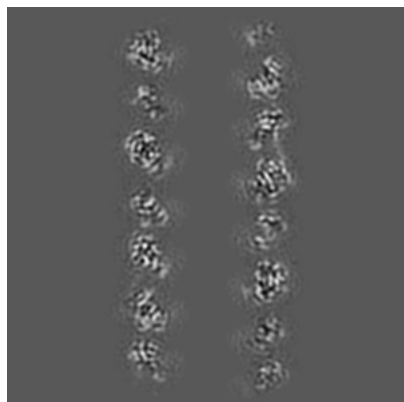


Z

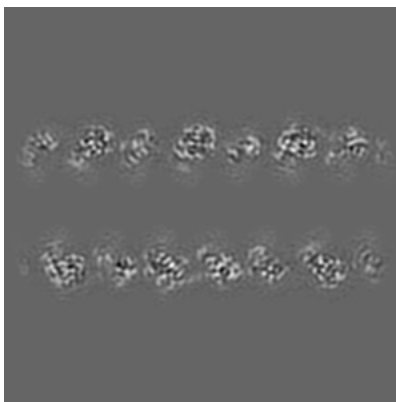
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

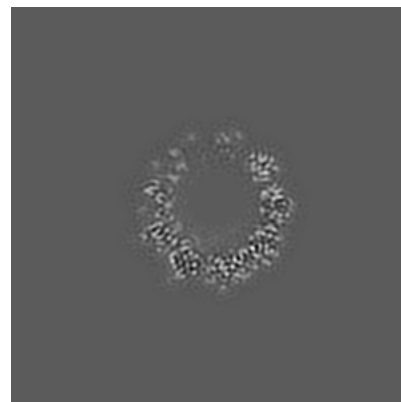
6.2.1 Primary map



X Index: 175

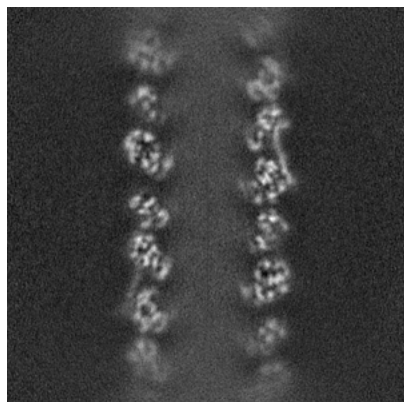


Y Index: 175

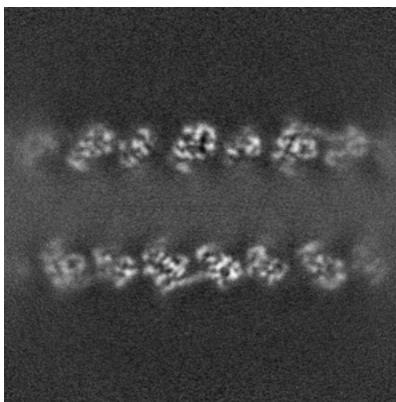


Z Index: 175

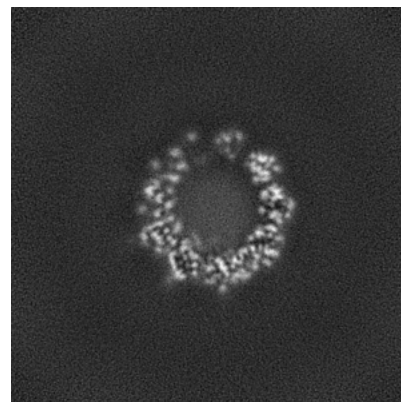
6.2.2 Raw map



X Index: 175



Y Index: 175

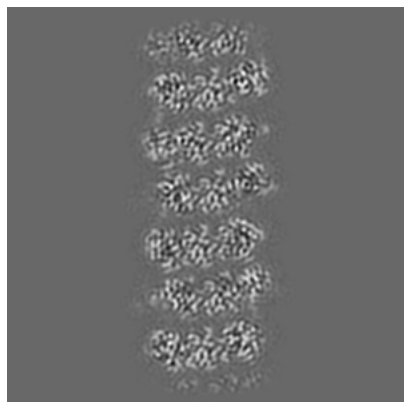


Z Index: 175

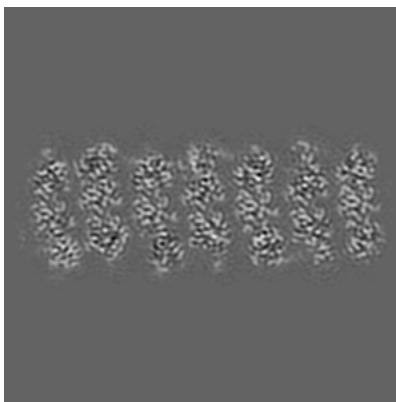
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 130

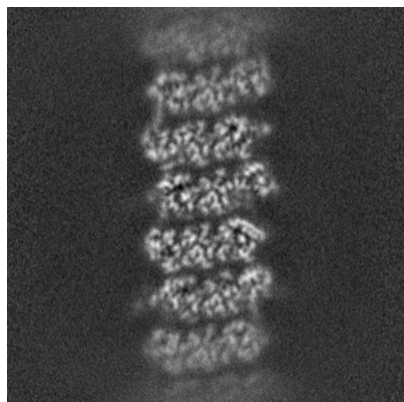


Y Index: 130

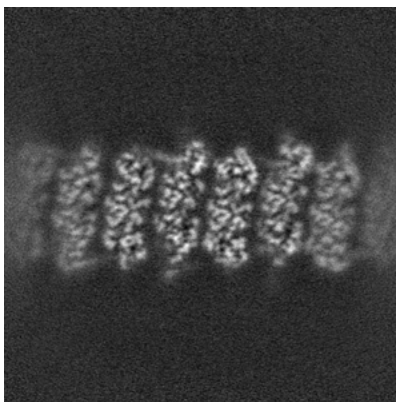


Z Index: 107

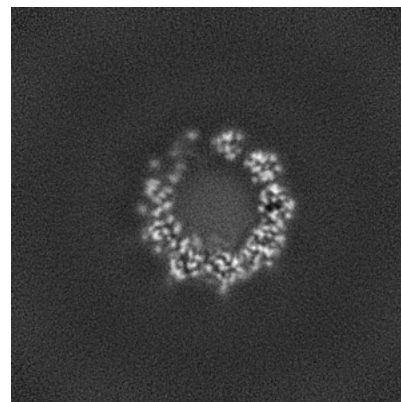
6.3.2 Raw map



X Index: 130



Y Index: 220

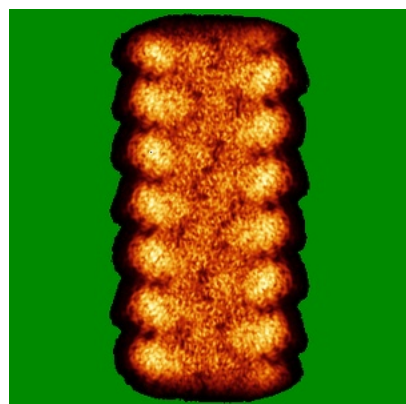


Z Index: 173

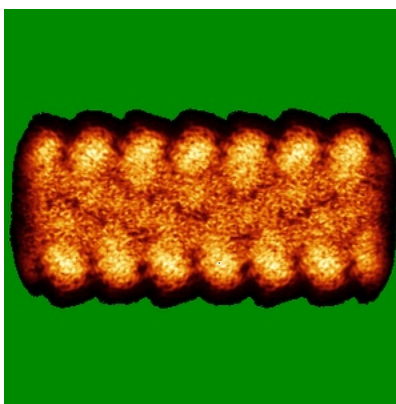
The images above show the largest variance slices of the map in three orthogonal directions.

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

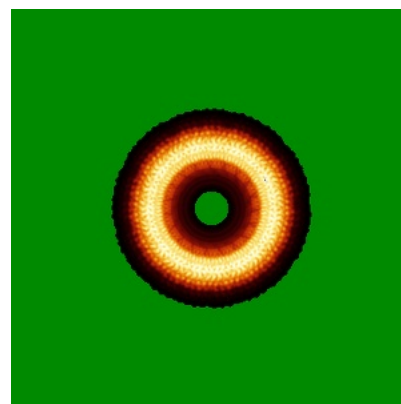
6.4.1 Primary map



X

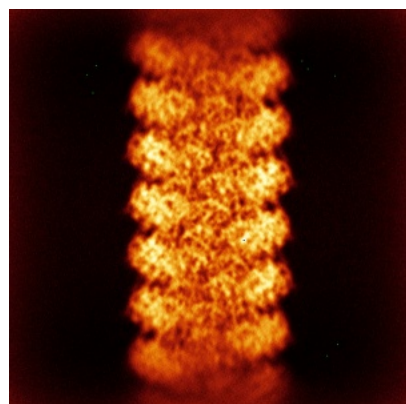


Y

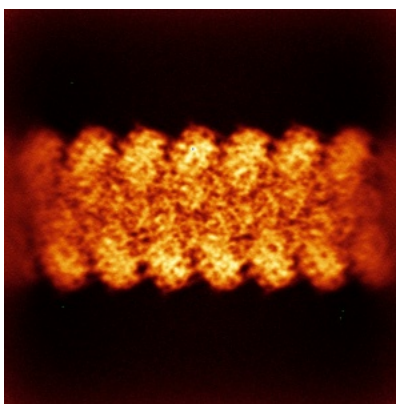


Z

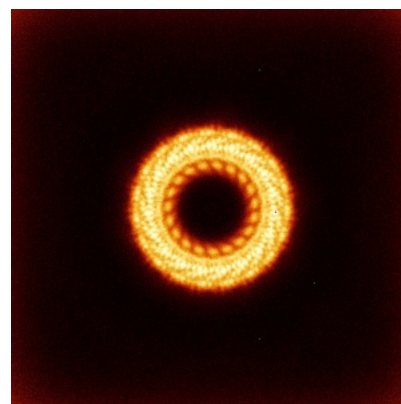
6.4.2 Raw map



X



Y

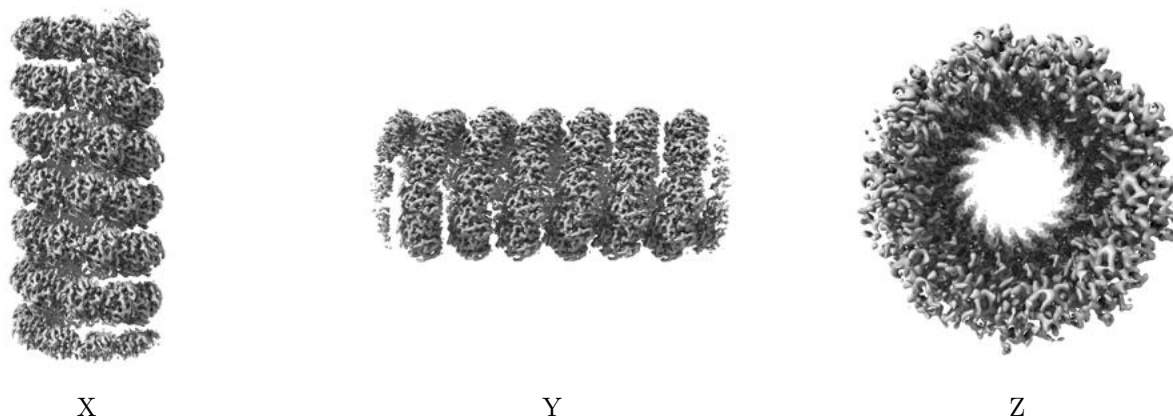


Z

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.

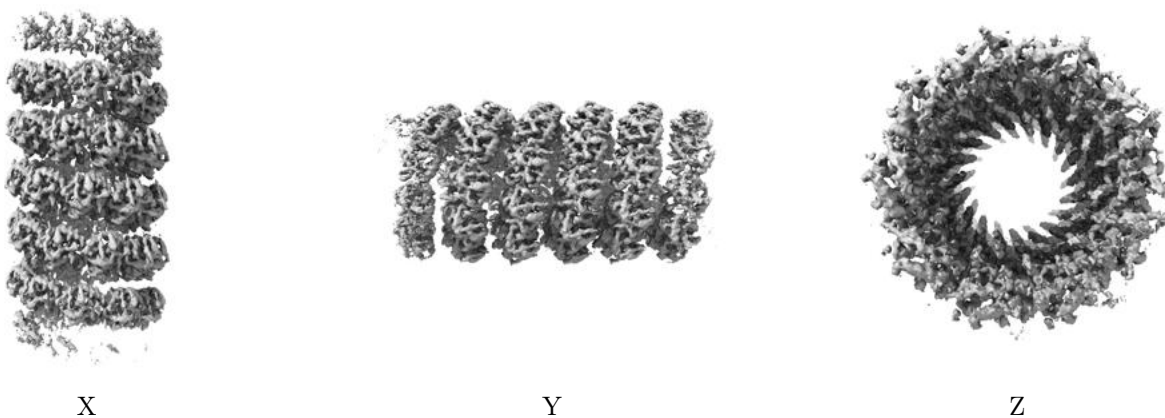
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.88. 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.

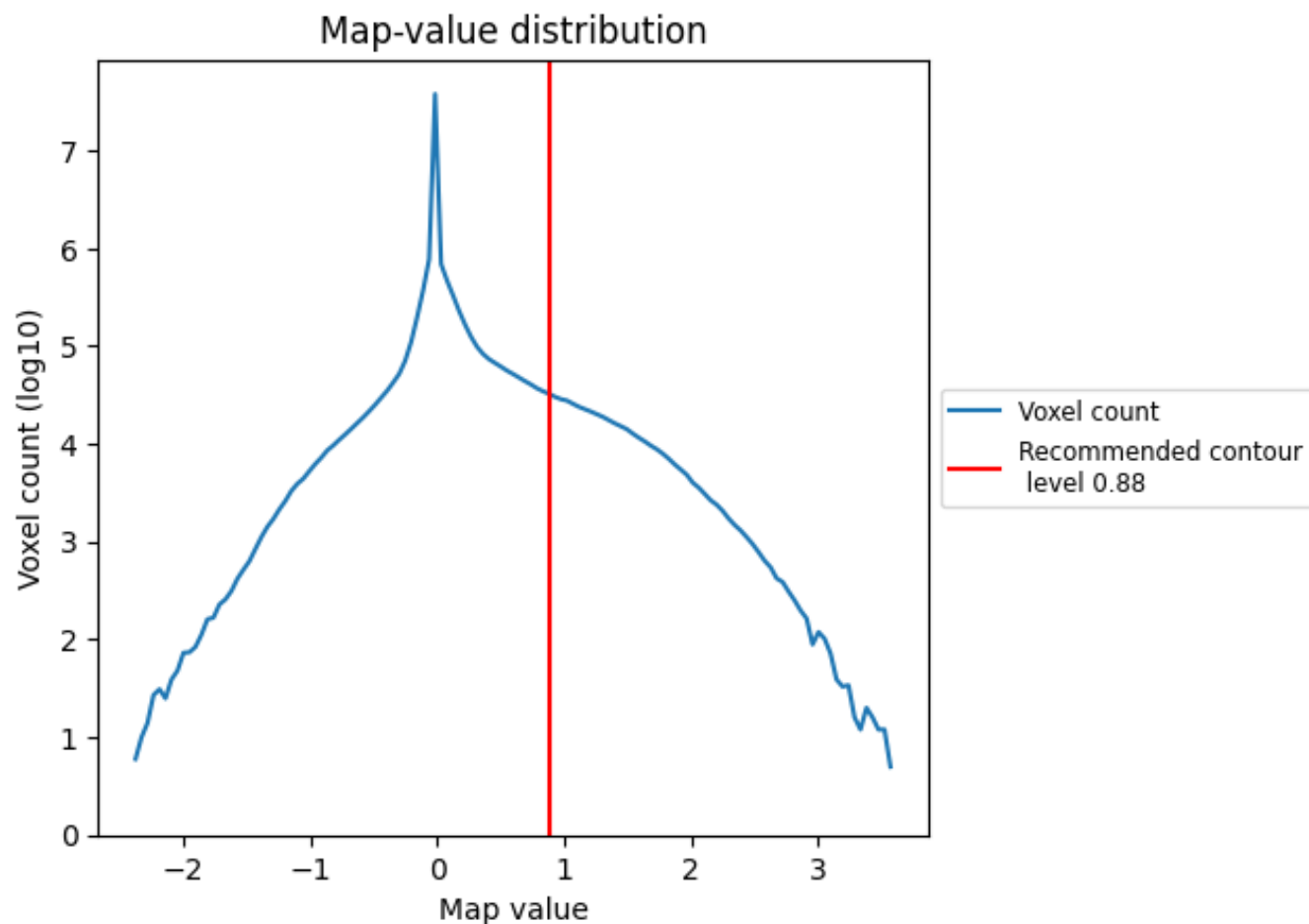
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

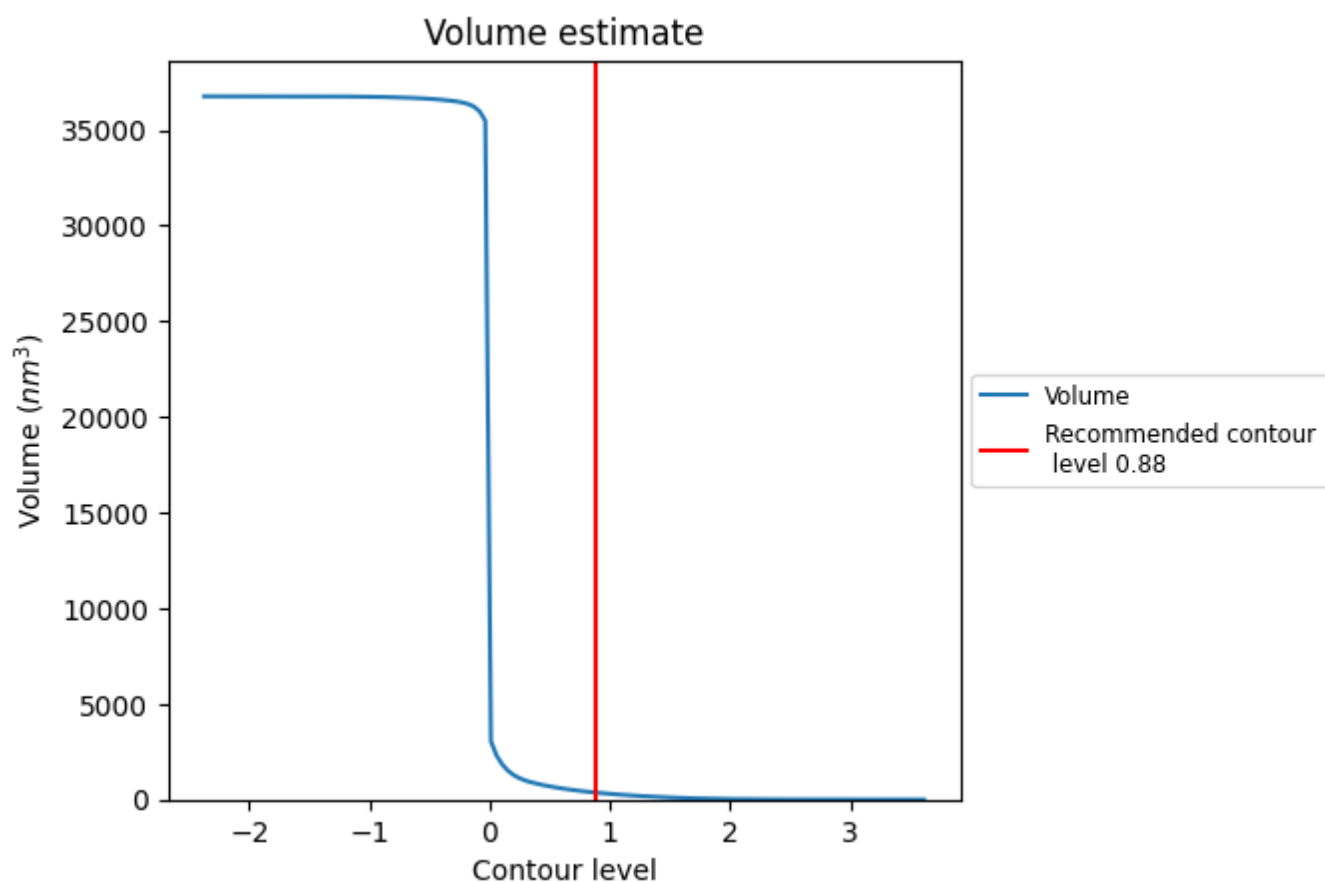
This section contains the results of statistical analysis of the map.

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.

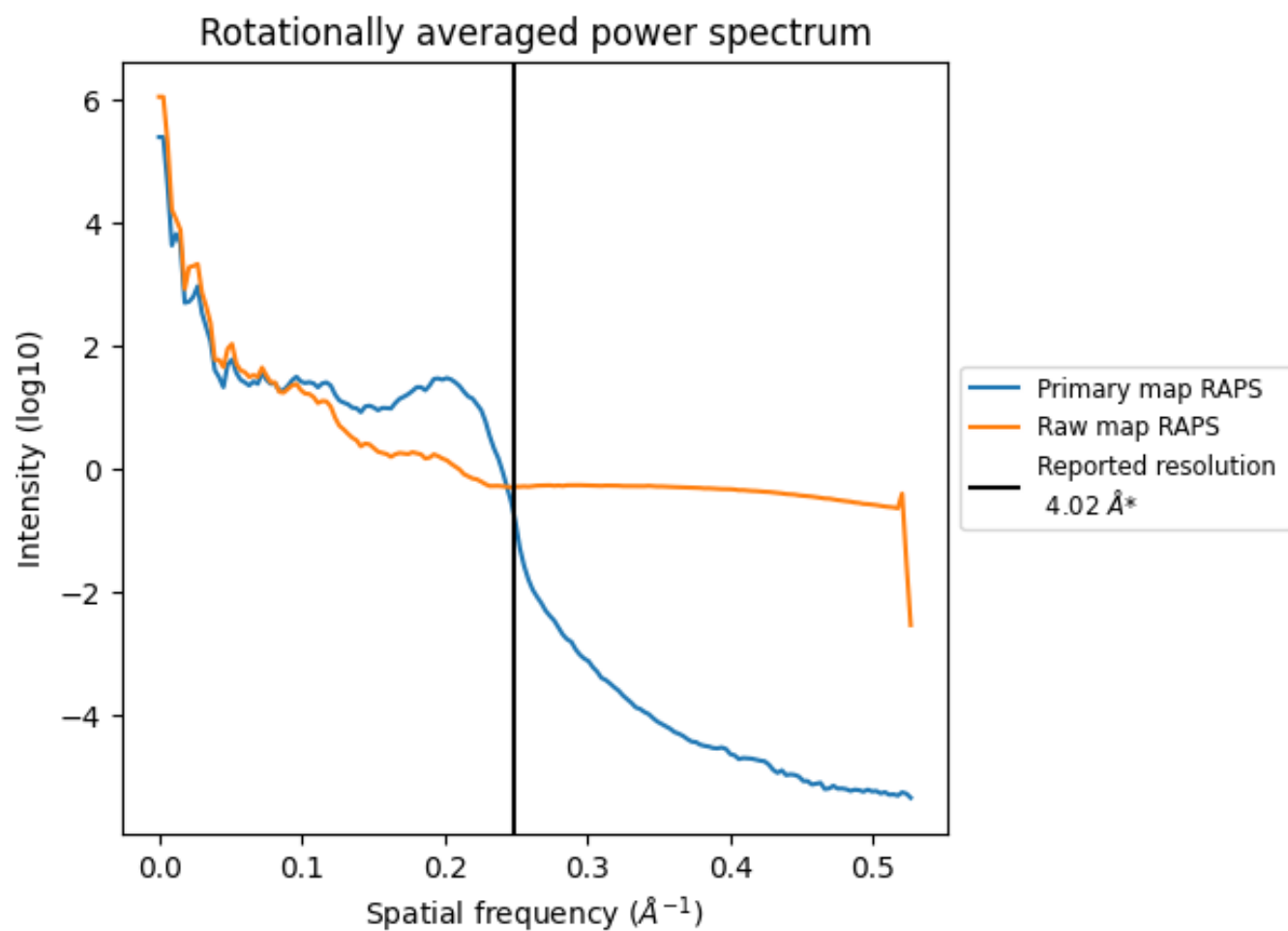
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 367 nm³; this corresponds to an approximate mass of 332 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 ⓘ

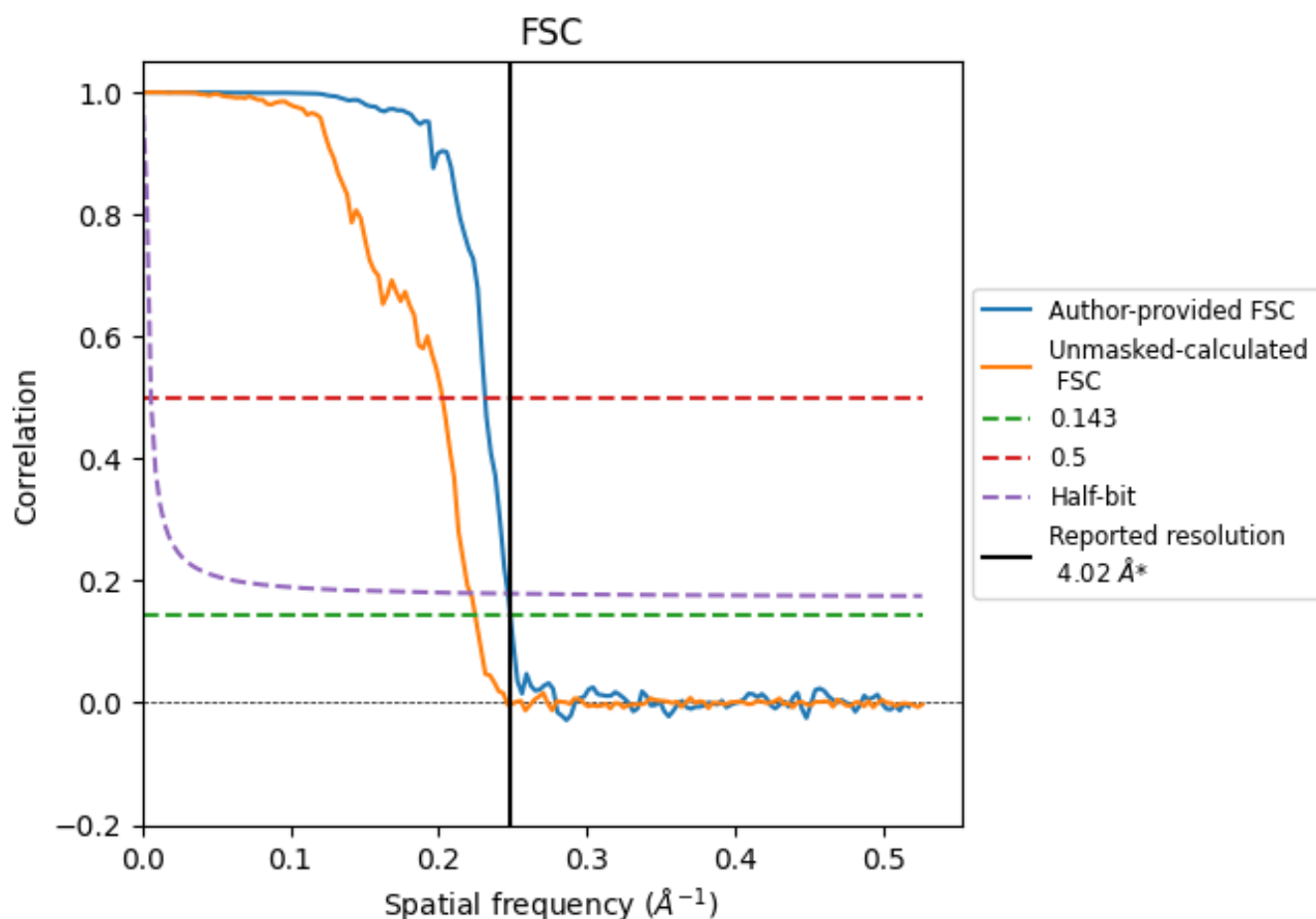


*Reported resolution corresponds to spatial frequency of 0.249 Å⁻¹

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 0.249 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

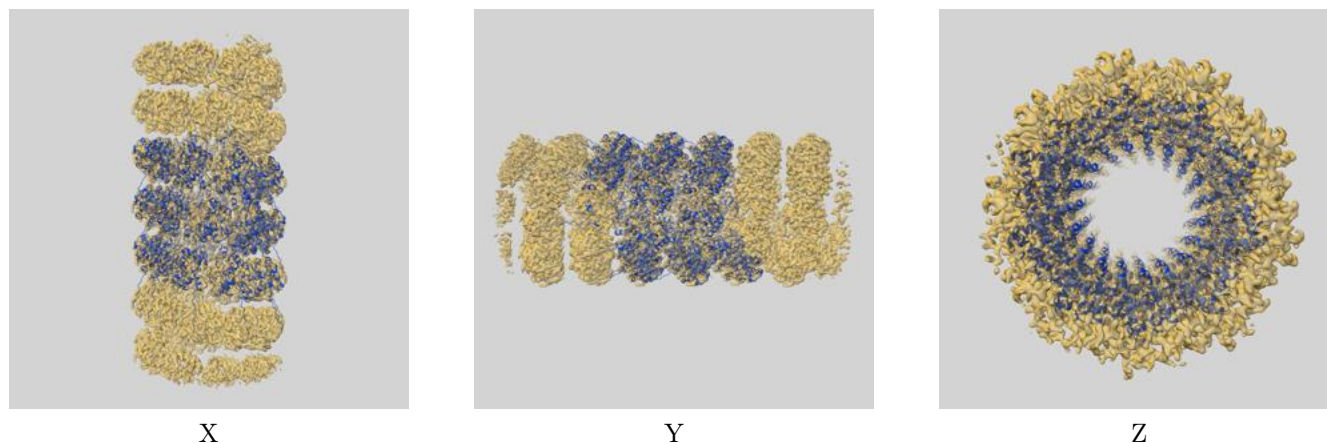
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.02	-	-
Author-provided FSC curve	4.02	4.32	4.05
Unmasked-calculated*	4.45	4.94	4.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.45 differs from the reported value 4.02 by more than 10 %

9 Map-model fit [i](#)

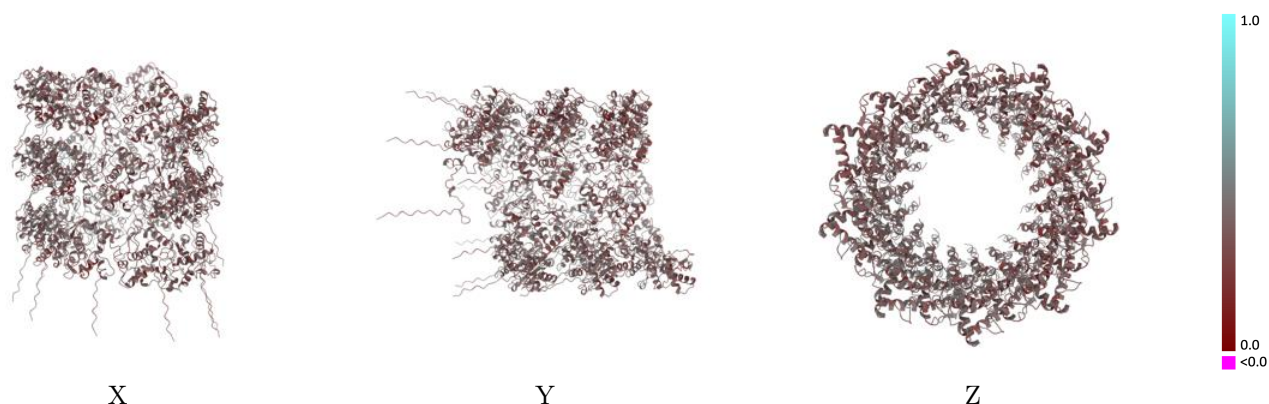
This section contains information regarding the fit between EMDB map EMD-53867 and PDB model 9RA1. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



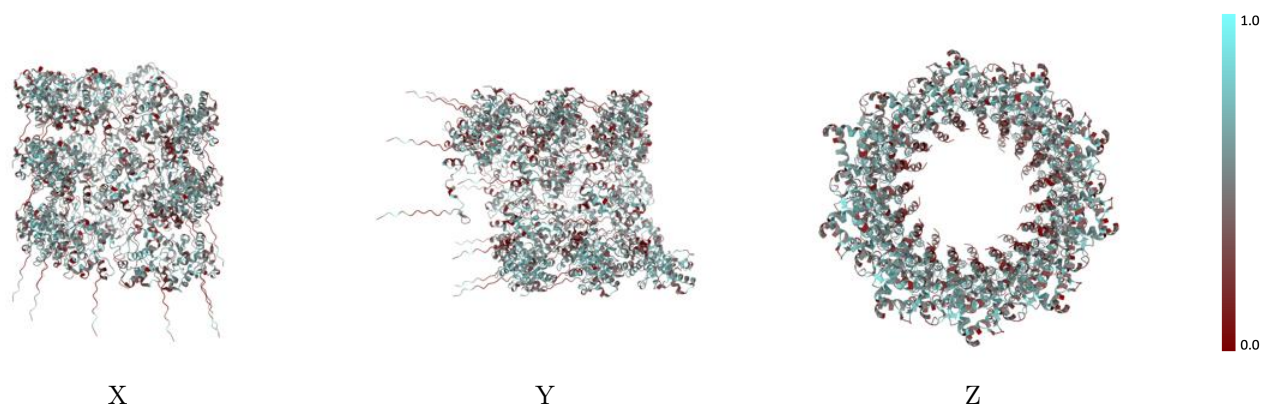
The images above show the 3D surface view of the map at the recommended contour level 0.88 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



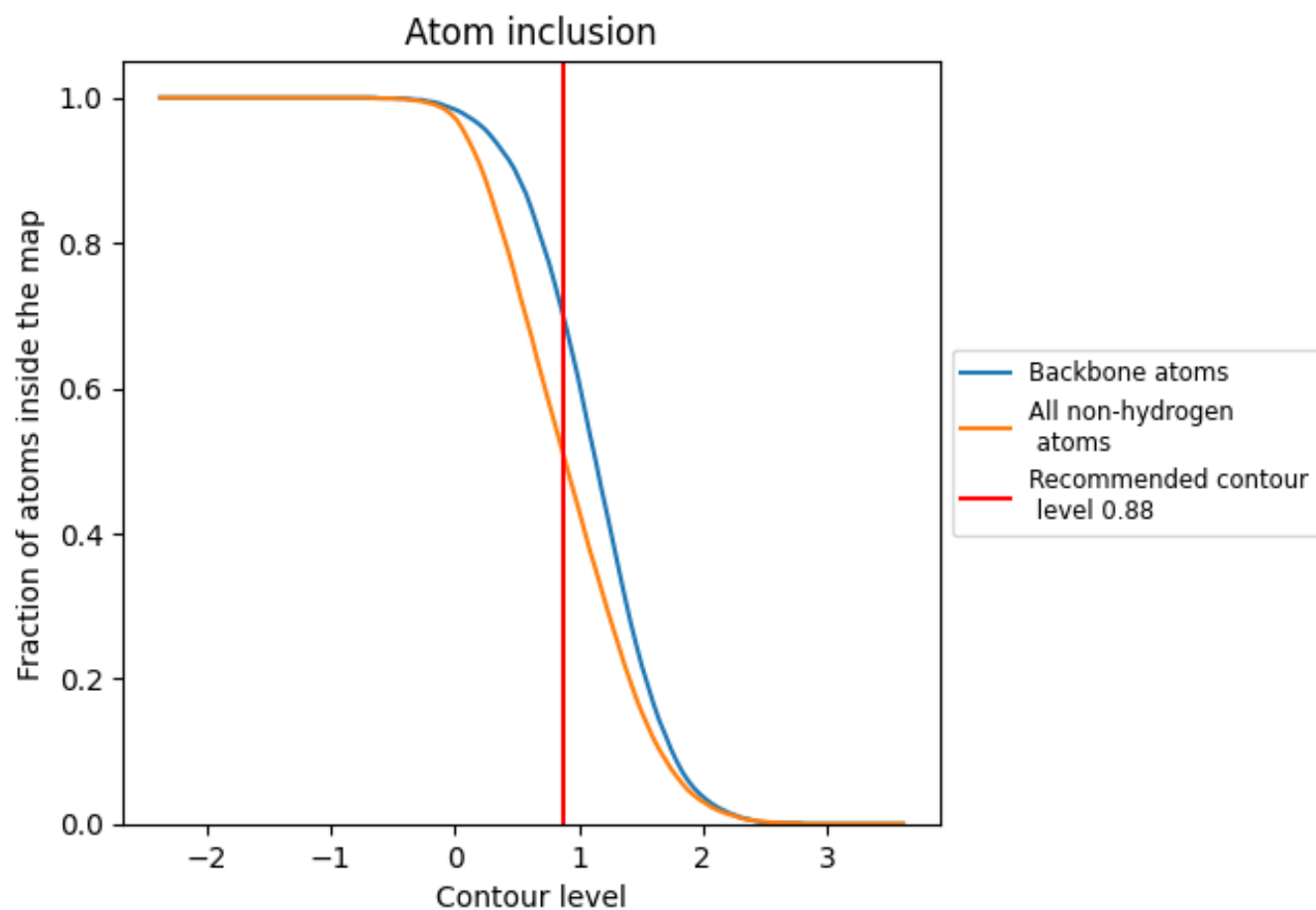
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.88).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 50% 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 (0.88) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5050	 0.3660
Aa	 0.4990	 0.3620
Ab	 0.4940	 0.3600
Ac	 0.4910	 0.3540
Ad	 0.5150	 0.3720
Ae	 0.5330	 0.3930
Af	 0.5460	 0.4080
Ag	 0.5420	 0.4020
Ah	 0.5220	 0.3750
Ai	 0.5050	 0.3620
Aj	 0.4930	 0.3550
Ak	 0.4800	 0.3510
Al	 0.4830	 0.3470
Am	 0.4870	 0.3540
An	 0.5140	 0.3710
Ao	 0.5330	 0.3930
Ap	 0.5410	 0.4010
Aq	 0.5250	 0.3820
Ar	 0.5020	 0.3590
As	 0.4960	 0.3470
At	 0.4780	 0.3380
Au	 0.4620	 0.3330
Av	 0.4620	 0.3300
Aw	 0.4760	 0.3440
Ax	 0.5090	 0.3680
Ay	 0.5210	 0.3860
Az	 0.5210	 0.3840
Ba	 0.5030	 0.3610

