



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:57 PM UTC

PDB ID : 9R7Y / pdb_00009r7y
EMDB ID : EMD-53799
Title : RNA-free helical (h9.7) virus-like particle composed of PVA coat protein with 6 mutations (H89Q, E90S, S144E, R163A, K180E, and T210R)
Authors : Koritnik, N.; Kezar, A.; Podobnik, M.
Deposited on : 2025-05-15
Resolution : 3.89 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:

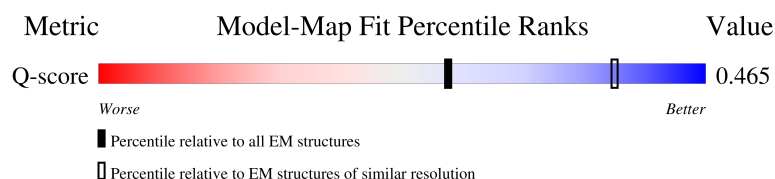
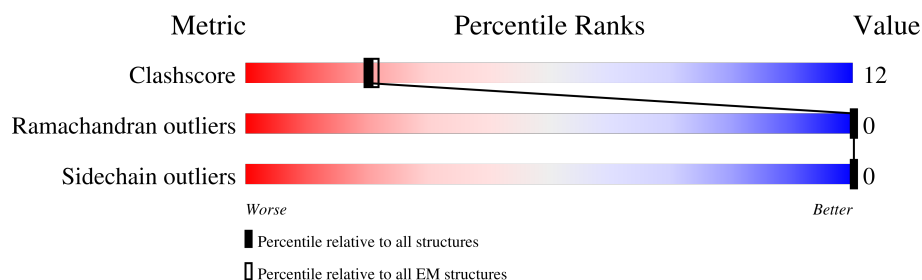
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.89 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	8712 (3.39 - 4.39)

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	269	22% 52% 17% 31%
1	Ab	269	22% 50% 19% 31%
1	Ac	269	22% 50% 19% 31%
1	Ad	269	22% 50% 19% 31%

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Mol	Chain	Length	Quality of chain
1	Ae	269	
1	Af	269	
1	Ag	269	
1	Ah	269	
1	Ai	269	
1	Aj	269	
1	Ak	269	
1	Al	269	
1	Am	269	
1	An	269	
1	Ao	269	
1	Ap	269	
1	Aq	269	
1	Ar	269	
1	As	269	
1	At	269	
1	Au	269	
1	Av	269	
1	Aw	269	
1	Ax	269	
1	Ay	269	
1	Az	269	
1	Ba	269	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 40419 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	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ab	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ac	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ad	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ae	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Af	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ag	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ah	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ai	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Aj	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ak	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Al	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Am	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	An	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ao	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ap	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Aq	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	As	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	At	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Au	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Av	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Aw	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ax	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ay	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Az	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		
1	Ba	185	Total	C	N	O	S	0	0
			1497	948	259	277	13		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	89	GLN	HIS	engineered mutation	UNP O11986
Aa	90	SER	GLU	engineered mutation	UNP O11986
Aa	144	GLU	SER	engineered mutation	UNP O11986
Aa	163	ALA	ARG	engineered mutation	UNP O11986
Aa	180	GLU	LYS	engineered mutation	UNP O11986
Aa	210	ARG	THR	engineered mutation	UNP O11986
Ab	89	GLN	HIS	engineered mutation	UNP O11986
Ab	90	SER	GLU	engineered mutation	UNP O11986
Ab	144	GLU	SER	engineered mutation	UNP O11986
Ab	163	ALA	ARG	engineered mutation	UNP O11986
Ab	180	GLU	LYS	engineered mutation	UNP O11986
Ab	210	ARG	THR	engineered mutation	UNP O11986
Ac	89	GLN	HIS	engineered mutation	UNP O11986
Ac	90	SER	GLU	engineered mutation	UNP O11986
Ac	144	GLU	SER	engineered mutation	UNP O11986
Ac	163	ALA	ARG	engineered mutation	UNP O11986
Ac	180	GLU	LYS	engineered mutation	UNP O11986
Ac	210	ARG	THR	engineered mutation	UNP O11986
Ad	89	GLN	HIS	engineered mutation	UNP O11986

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Chain	Residue	Modelled	Actual	Comment	Reference
Ad	90	SER	GLU	engineered mutation	UNP O11986
Ad	144	GLU	SER	engineered mutation	UNP O11986
Ad	163	ALA	ARG	engineered mutation	UNP O11986
Ad	180	GLU	LYS	engineered mutation	UNP O11986
Ad	210	ARG	THR	engineered mutation	UNP O11986
Ae	89	GLN	HIS	engineered mutation	UNP O11986
Ae	90	SER	GLU	engineered mutation	UNP O11986
Ae	144	GLU	SER	engineered mutation	UNP O11986
Ae	163	ALA	ARG	engineered mutation	UNP O11986
Ae	180	GLU	LYS	engineered mutation	UNP O11986
Ae	210	ARG	THR	engineered mutation	UNP O11986
Af	89	GLN	HIS	engineered mutation	UNP O11986
Af	90	SER	GLU	engineered mutation	UNP O11986
Af	144	GLU	SER	engineered mutation	UNP O11986
Af	163	ALA	ARG	engineered mutation	UNP O11986
Af	180	GLU	LYS	engineered mutation	UNP O11986
Af	210	ARG	THR	engineered mutation	UNP O11986
Ag	89	GLN	HIS	engineered mutation	UNP O11986
Ag	90	SER	GLU	engineered mutation	UNP O11986
Ag	144	GLU	SER	engineered mutation	UNP O11986
Ag	163	ALA	ARG	engineered mutation	UNP O11986
Ag	180	GLU	LYS	engineered mutation	UNP O11986
Ag	210	ARG	THR	engineered mutation	UNP O11986
Ah	89	GLN	HIS	engineered mutation	UNP O11986
Ah	90	SER	GLU	engineered mutation	UNP O11986
Ah	144	GLU	SER	engineered mutation	UNP O11986
Ah	163	ALA	ARG	engineered mutation	UNP O11986
Ah	180	GLU	LYS	engineered mutation	UNP O11986
Ah	210	ARG	THR	engineered mutation	UNP O11986
Ai	89	GLN	HIS	engineered mutation	UNP O11986
Ai	90	SER	GLU	engineered mutation	UNP O11986
Ai	144	GLU	SER	engineered mutation	UNP O11986
Ai	163	ALA	ARG	engineered mutation	UNP O11986
Ai	180	GLU	LYS	engineered mutation	UNP O11986
Ai	210	ARG	THR	engineered mutation	UNP O11986
Aj	89	GLN	HIS	engineered mutation	UNP O11986
Aj	90	SER	GLU	engineered mutation	UNP O11986
Aj	144	GLU	SER	engineered mutation	UNP O11986
Aj	163	ALA	ARG	engineered mutation	UNP O11986
Aj	180	GLU	LYS	engineered mutation	UNP O11986
Aj	210	ARG	THR	engineered mutation	UNP O11986
Ak	89	GLN	HIS	engineered mutation	UNP O11986

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Chain	Residue	Modelled	Actual	Comment	Reference
Ak	90	SER	GLU	engineered mutation	UNP O11986
Ak	144	GLU	SER	engineered mutation	UNP O11986
Ak	163	ALA	ARG	engineered mutation	UNP O11986
Ak	180	GLU	LYS	engineered mutation	UNP O11986
Ak	210	ARG	THR	engineered mutation	UNP O11986
Al	89	GLN	HIS	engineered mutation	UNP O11986
Al	90	SER	GLU	engineered mutation	UNP O11986
Al	144	GLU	SER	engineered mutation	UNP O11986
Al	163	ALA	ARG	engineered mutation	UNP O11986
Al	180	GLU	LYS	engineered mutation	UNP O11986
Al	210	ARG	THR	engineered mutation	UNP O11986
Am	89	GLN	HIS	engineered mutation	UNP O11986
Am	90	SER	GLU	engineered mutation	UNP O11986
Am	144	GLU	SER	engineered mutation	UNP O11986
Am	163	ALA	ARG	engineered mutation	UNP O11986
Am	180	GLU	LYS	engineered mutation	UNP O11986
Am	210	ARG	THR	engineered mutation	UNP O11986
An	89	GLN	HIS	engineered mutation	UNP O11986
An	90	SER	GLU	engineered mutation	UNP O11986
An	144	GLU	SER	engineered mutation	UNP O11986
An	163	ALA	ARG	engineered mutation	UNP O11986
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Ao	89	GLN	HIS	engineered mutation	UNP O11986
Ao	90	SER	GLU	engineered mutation	UNP O11986
Ao	144	GLU	SER	engineered mutation	UNP O11986
Ao	163	ALA	ARG	engineered mutation	UNP O11986
Ao	180	GLU	LYS	engineered mutation	UNP O11986
Ao	210	ARG	THR	engineered mutation	UNP O11986
Ap	89	GLN	HIS	engineered mutation	UNP O11986
Ap	90	SER	GLU	engineered mutation	UNP O11986
Ap	144	GLU	SER	engineered mutation	UNP O11986
Ap	163	ALA	ARG	engineered mutation	UNP O11986
Ap	180	GLU	LYS	engineered mutation	UNP O11986
Ap	210	ARG	THR	engineered mutation	UNP O11986
Aq	89	GLN	HIS	engineered mutation	UNP O11986
Aq	90	SER	GLU	engineered mutation	UNP O11986
Aq	144	GLU	SER	engineered mutation	UNP O11986
Aq	163	ALA	ARG	engineered mutation	UNP O11986
Aq	180	GLU	LYS	engineered mutation	UNP O11986
Aq	210	ARG	THR	engineered mutation	UNP O11986
Ar	89	GLN	HIS	engineered mutation	UNP O11986

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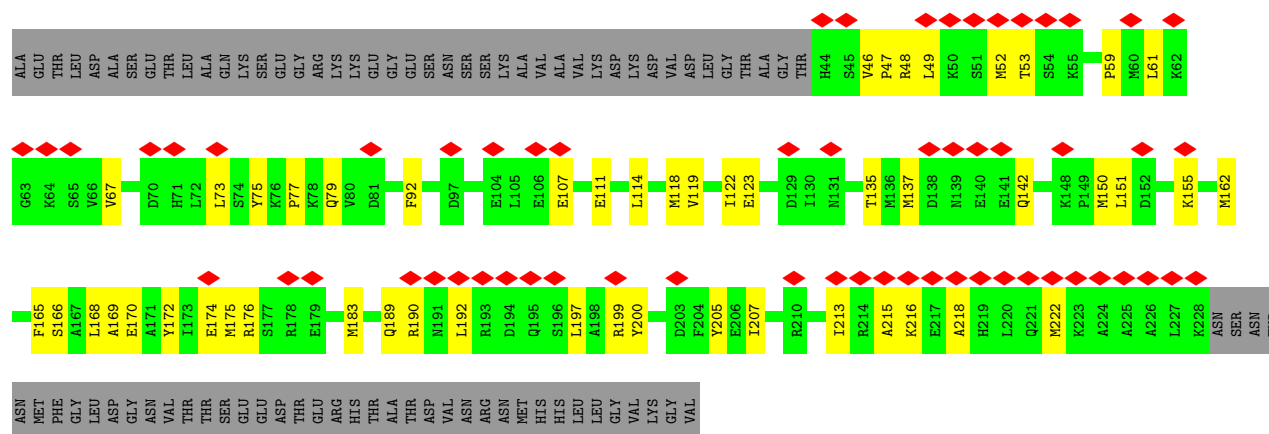
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Chain	Residue	Modelled	Actual	Comment	Reference
Ar	90	SER	GLU	engineered mutation	UNP O11986
Ar	144	GLU	SER	engineered mutation	UNP O11986
Ar	163	ALA	ARG	engineered mutation	UNP O11986
Ar	180	GLU	LYS	engineered mutation	UNP O11986
Ar	210	ARG	THR	engineered mutation	UNP O11986
As	89	GLN	HIS	engineered mutation	UNP O11986
As	90	SER	GLU	engineered mutation	UNP O11986
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As	163	ALA	ARG	engineered mutation	UNP O11986
As	180	GLU	LYS	engineered mutation	UNP O11986
As	210	ARG	THR	engineered mutation	UNP O11986
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At	90	SER	GLU	engineered mutation	UNP O11986
At	144	GLU	SER	engineered mutation	UNP O11986
At	163	ALA	ARG	engineered mutation	UNP O11986
At	180	GLU	LYS	engineered mutation	UNP O11986
At	210	ARG	THR	engineered mutation	UNP O11986
Au	89	GLN	HIS	engineered mutation	UNP O11986
Au	90	SER	GLU	engineered mutation	UNP O11986
Au	144	GLU	SER	engineered mutation	UNP O11986
Au	163	ALA	ARG	engineered mutation	UNP O11986
Au	180	GLU	LYS	engineered mutation	UNP O11986
Au	210	ARG	THR	engineered mutation	UNP O11986
Av	89	GLN	HIS	engineered mutation	UNP O11986
Av	90	SER	GLU	engineered mutation	UNP O11986
Av	144	GLU	SER	engineered mutation	UNP O11986
Av	163	ALA	ARG	engineered mutation	UNP O11986
Av	180	GLU	LYS	engineered mutation	UNP O11986
Av	210	ARG	THR	engineered mutation	UNP O11986
Aw	89	GLN	HIS	engineered mutation	UNP O11986
Aw	90	SER	GLU	engineered mutation	UNP O11986
Aw	144	GLU	SER	engineered mutation	UNP O11986
Aw	163	ALA	ARG	engineered mutation	UNP O11986
Aw	180	GLU	LYS	engineered mutation	UNP O11986
Aw	210	ARG	THR	engineered mutation	UNP O11986
Ax	89	GLN	HIS	engineered mutation	UNP O11986
Ax	90	SER	GLU	engineered mutation	UNP O11986
Ax	144	GLU	SER	engineered mutation	UNP O11986
Ax	163	ALA	ARG	engineered mutation	UNP O11986
Ax	180	GLU	LYS	engineered mutation	UNP O11986
Ax	210	ARG	THR	engineered mutation	UNP O11986
Ay	89	GLN	HIS	engineered mutation	UNP O11986

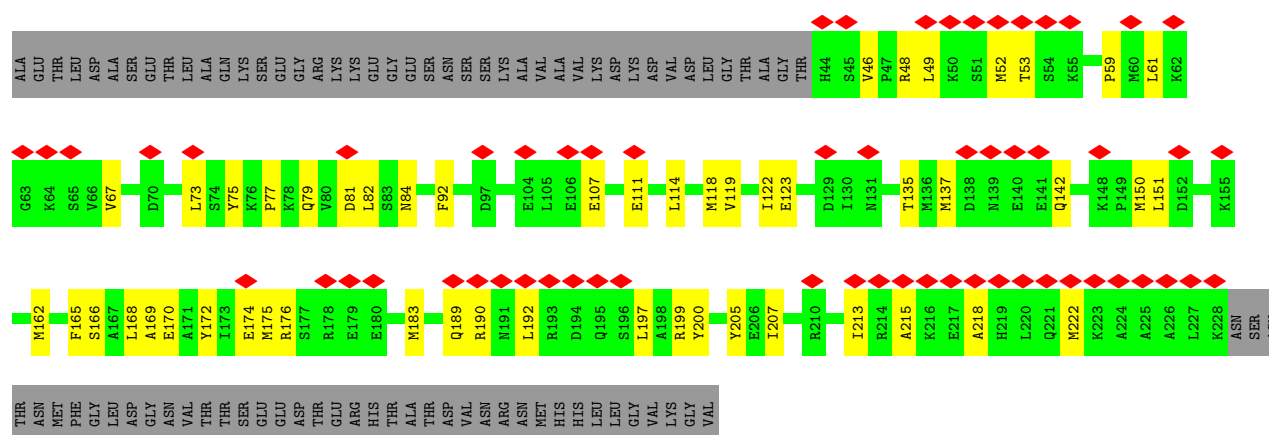
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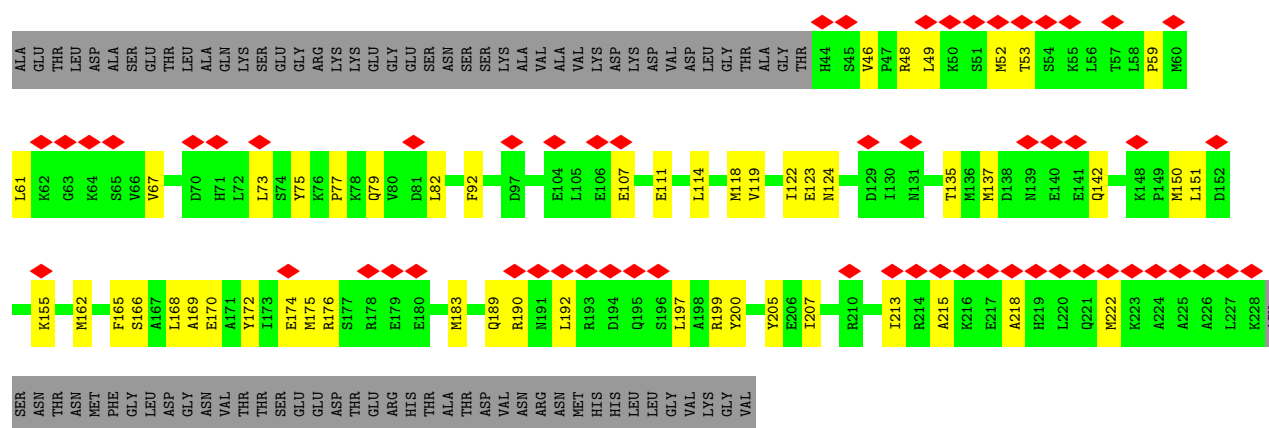
Chain	Residue	Modelled	Actual	Comment	Reference
Ay	90	SER	GLU	engineered mutation	UNP O11986
Ay	144	GLU	SER	engineered mutation	UNP O11986
Ay	163	ALA	ARG	engineered mutation	UNP O11986
Ay	180	GLU	LYS	engineered mutation	UNP O11986
Ay	210	ARG	THR	engineered mutation	UNP O11986
Az	89	GLN	HIS	engineered mutation	UNP O11986
Az	90	SER	GLU	engineered mutation	UNP O11986
Az	144	GLU	SER	engineered mutation	UNP O11986
Az	163	ALA	ARG	engineered mutation	UNP O11986
Az	180	GLU	LYS	engineered mutation	UNP O11986
Az	210	ARG	THR	engineered mutation	UNP O11986
Ba	89	GLN	HIS	engineered mutation	UNP O11986
Ba	90	SER	GLU	engineered mutation	UNP O11986
Ba	144	GLU	SER	engineered mutation	UNP O11986
Ba	163	ALA	ARG	engineered mutation	UNP O11986
Ba	180	GLU	LYS	engineered mutation	UNP O11986
Ba	210	ARG	THR	engineered mutation	UNP O11986



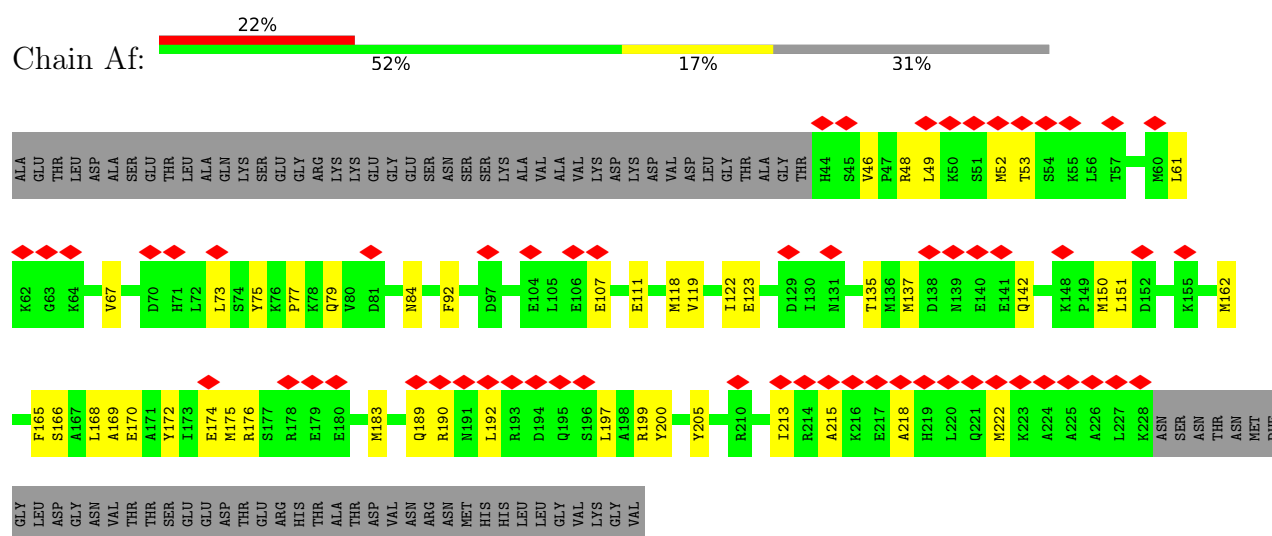
• Molecule 1: Genome polypeptide



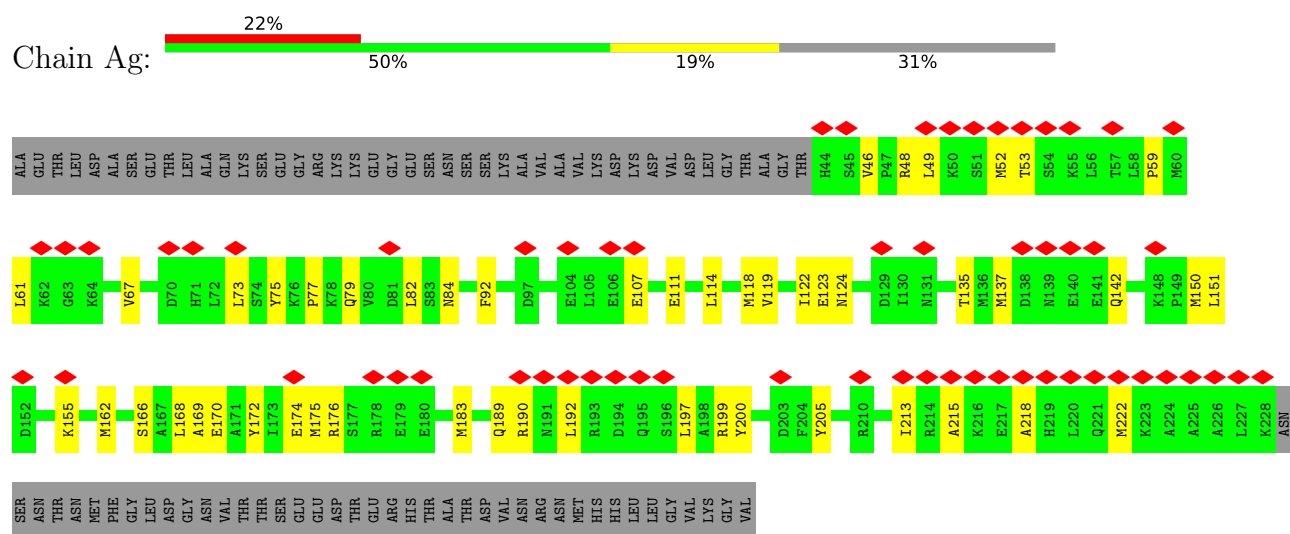
• Molecule 1: Genome polypeptide



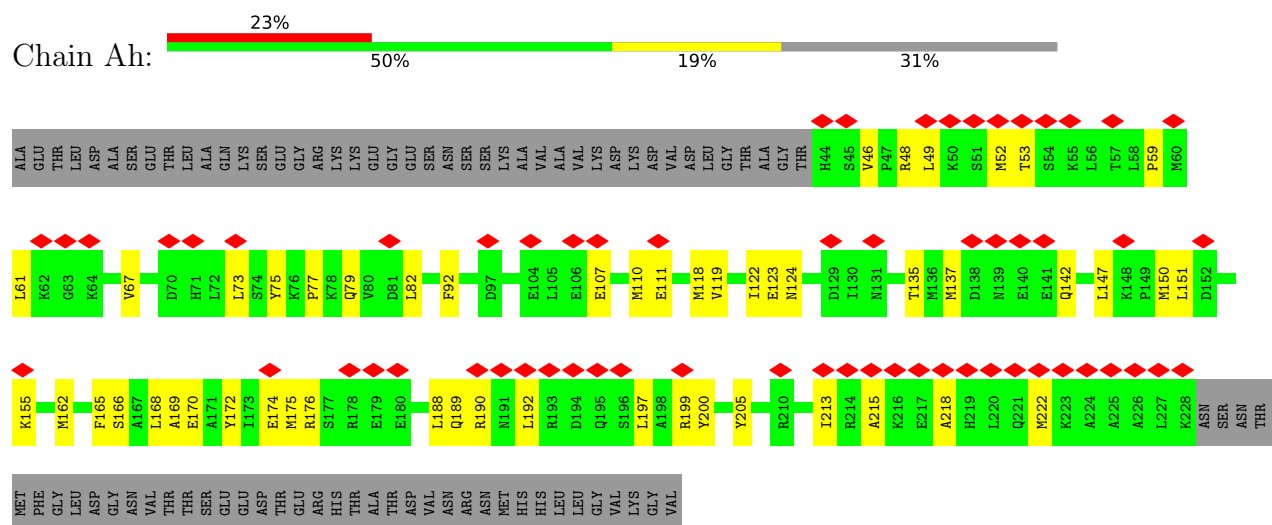
• Molecule 1: Genome polypeptide



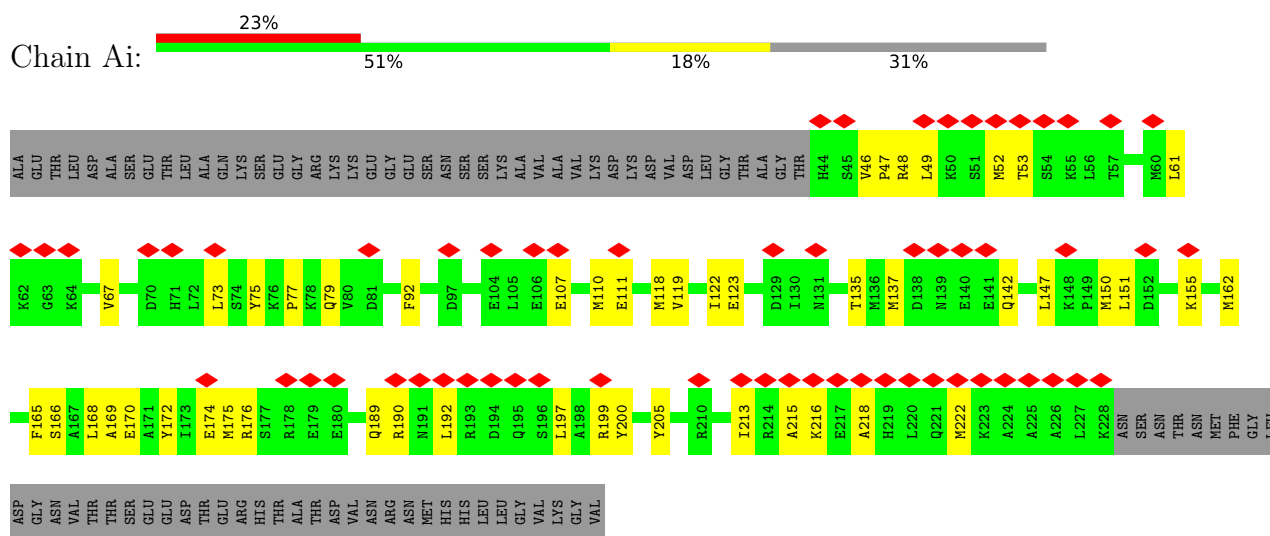
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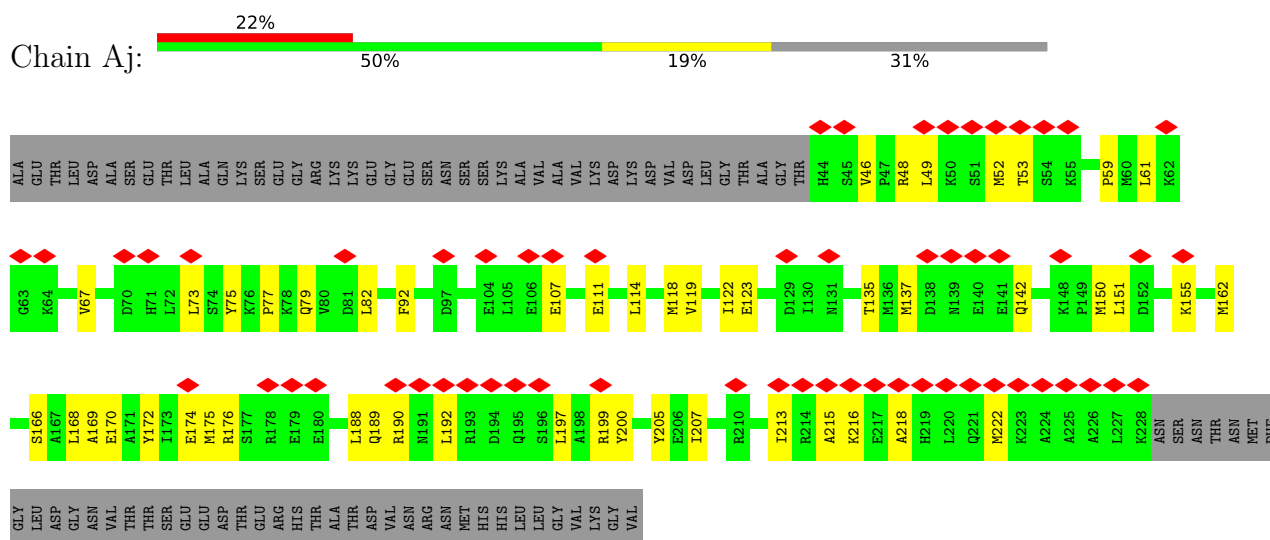
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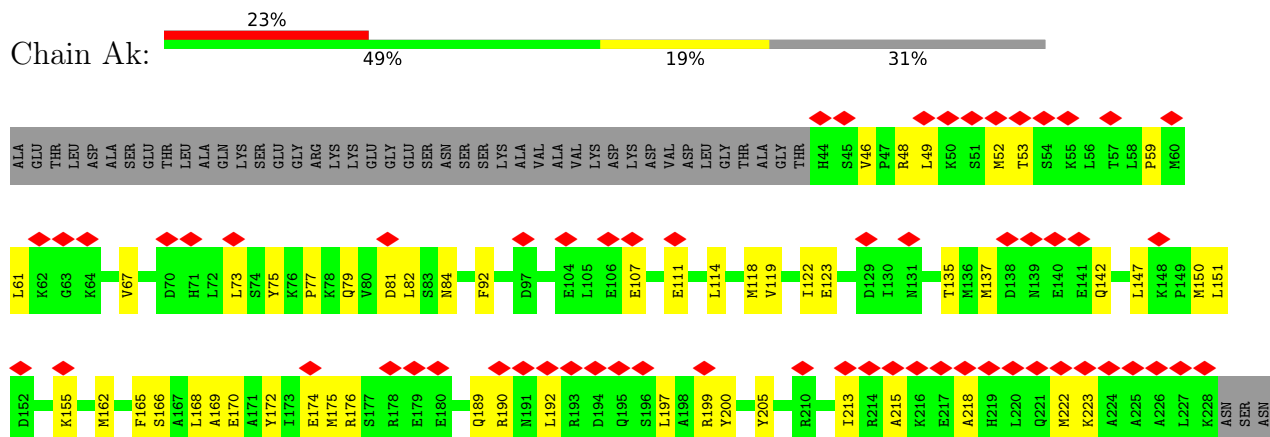
- Molecule 1: Genome polypeptide



- Molecule 1: Genome polypeptide

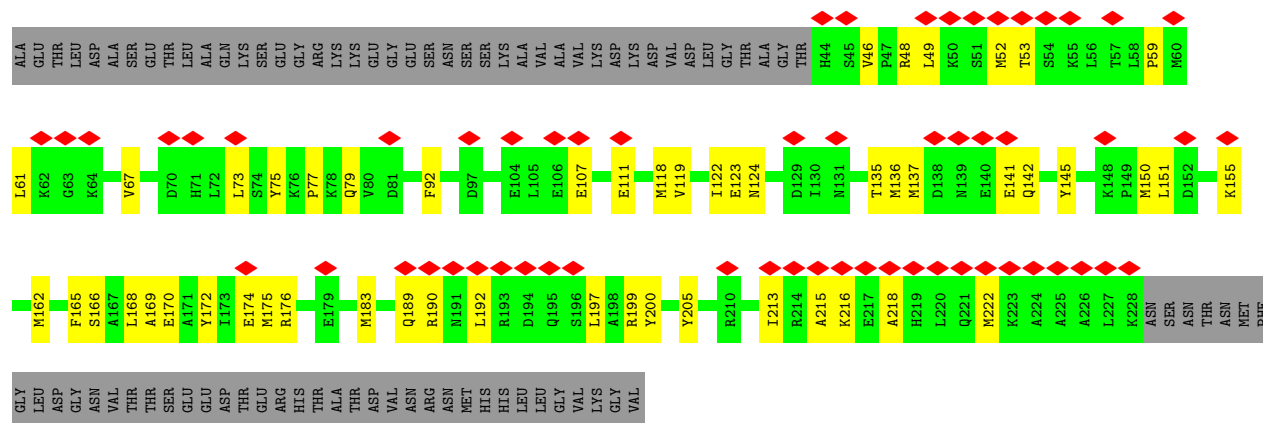


- Molecule 1: Genome polypeptide

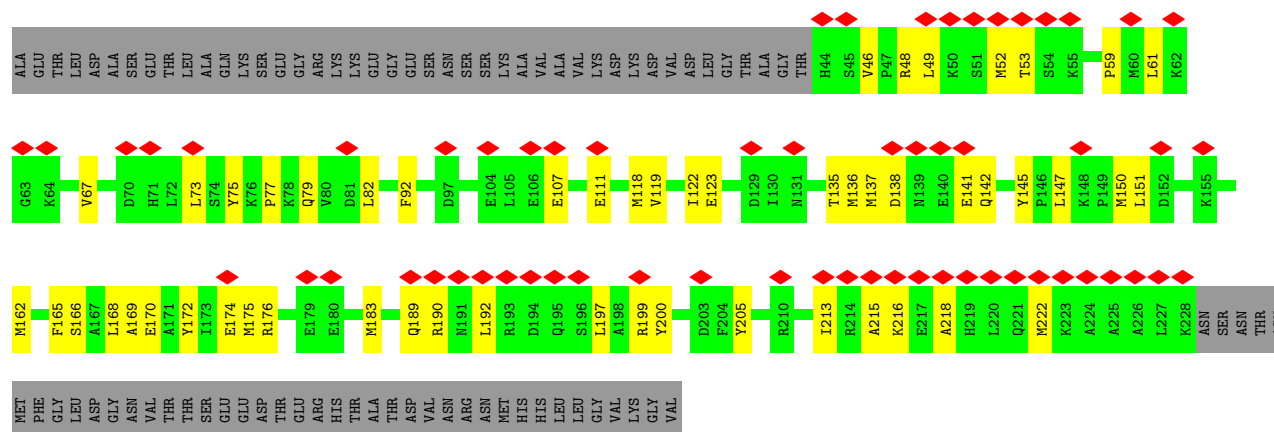


ASN MET PHE GLY LEU ASP ASP GLY VAL THR THR SER GLU GLU ASP THR THR ARG HIS THR ALA GLY VAL

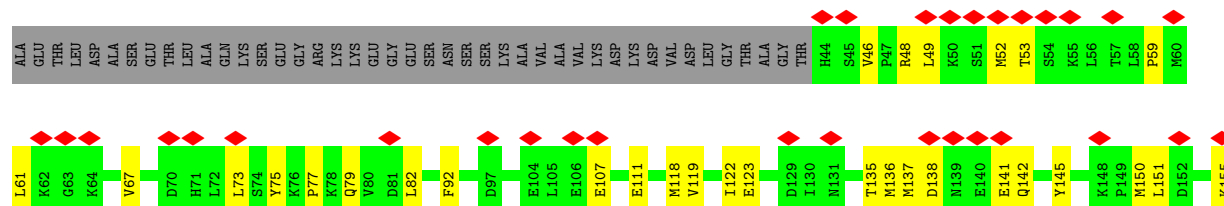
• Molecule 1: Genome polyprotein

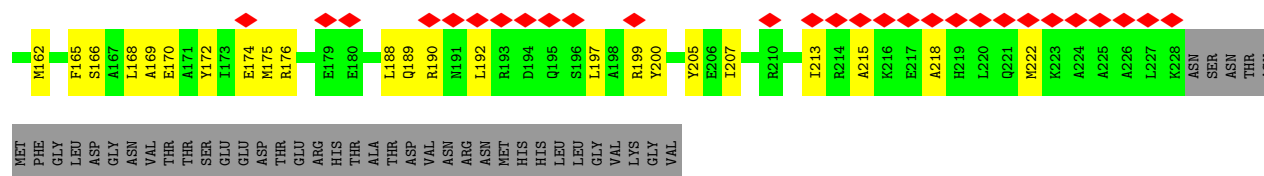


• Molecule 1: Genome polyprotein

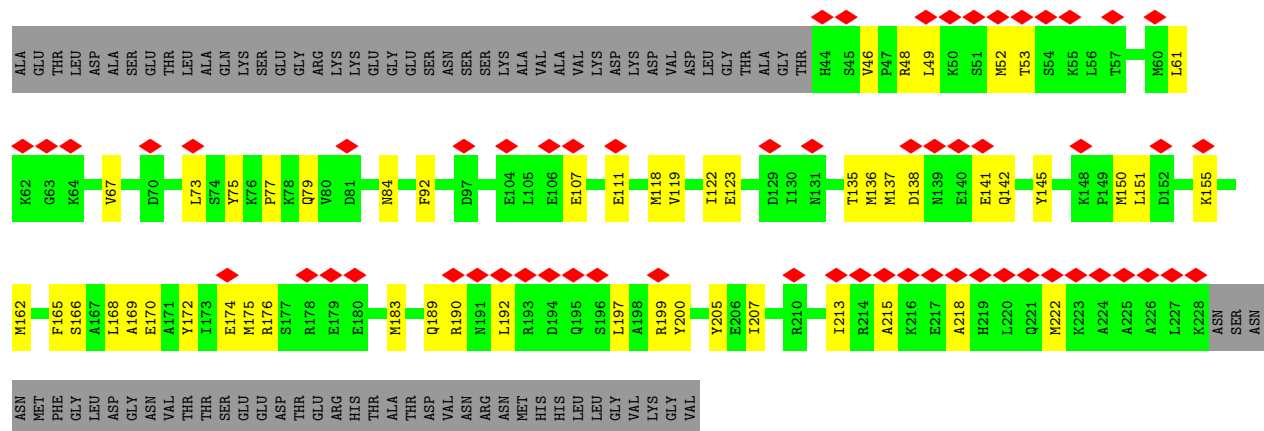


• Molecule 1: Genome polyprotein

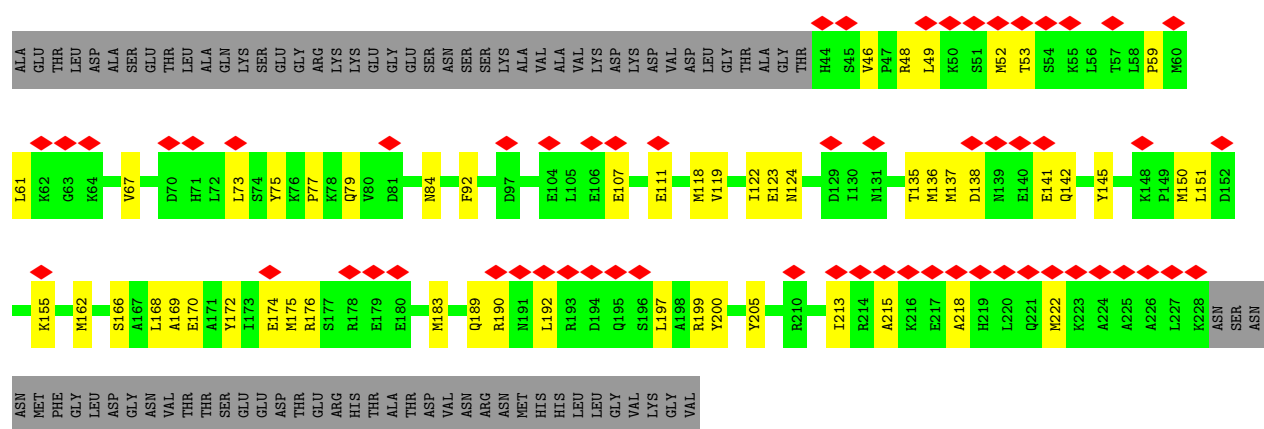




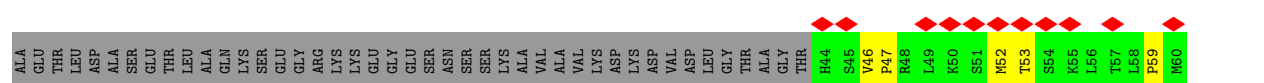
• Molecule 1: Genome polyprotein



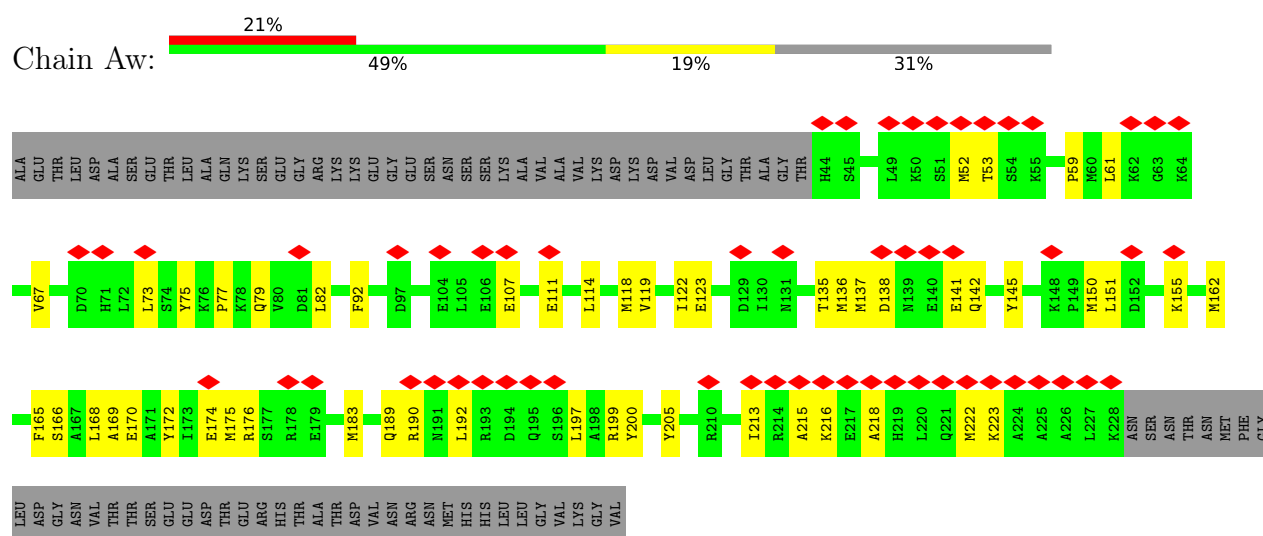
• Molecule 1: Genome polyprotein



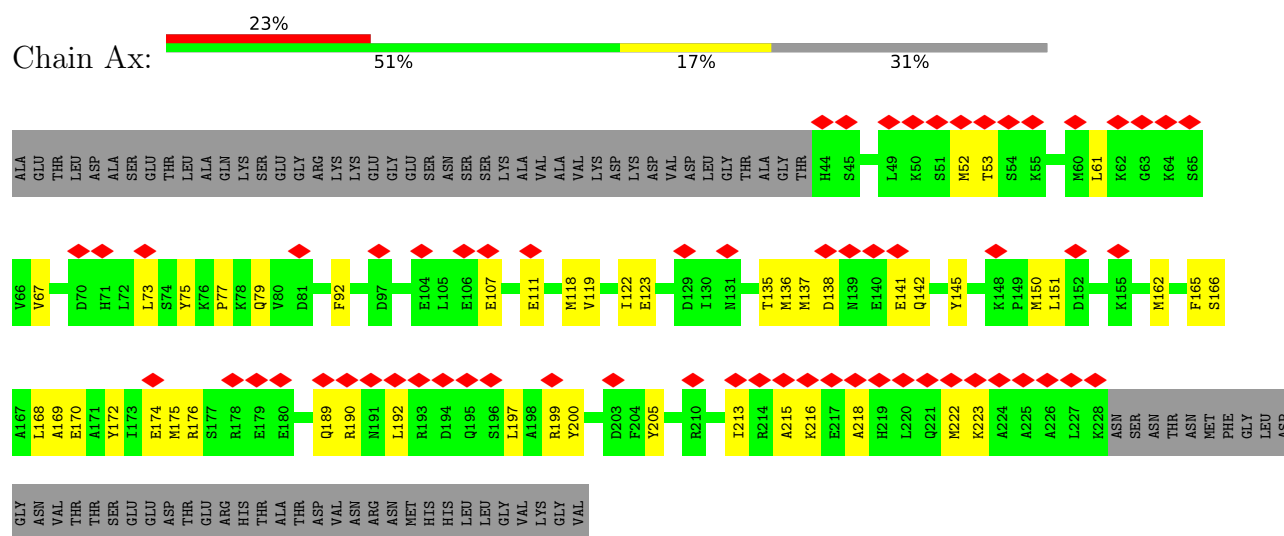
• Molecule 1: Genome polyprotein



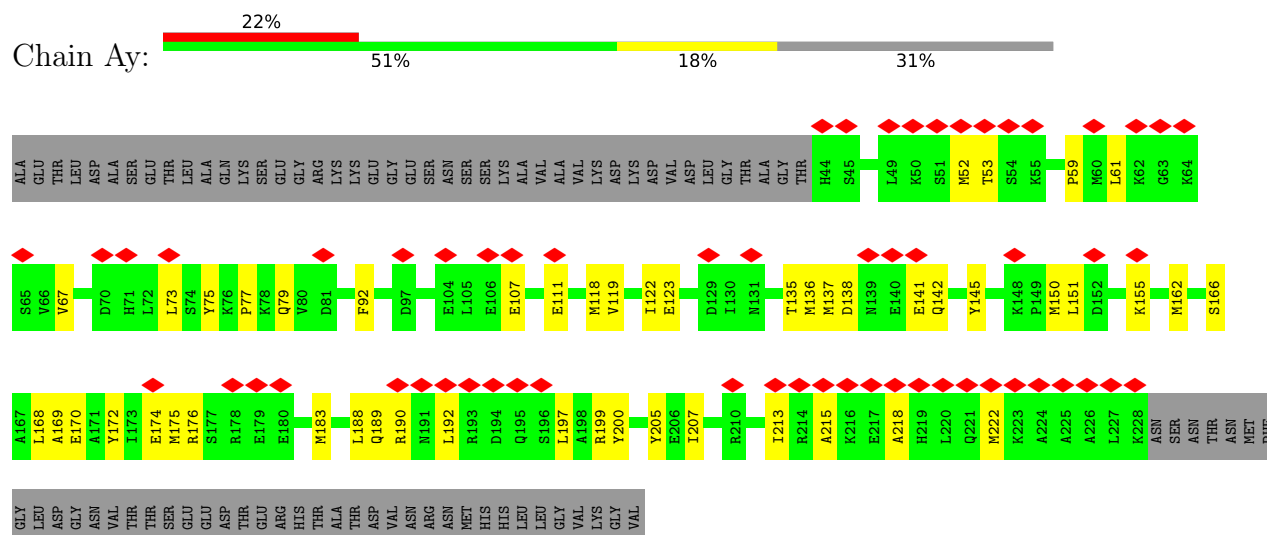




• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-37.08°, rise=3.85 Å, axial sym=C1	Depositor
Number of segments used	122826	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	4.925	Depositor
Minimum map value	-3.137	Depositor
Average map value	0.023	Depositor
Map value standard deviation	0.245	Depositor
Recommended contour level	1.19	Depositor
Map size (Å)	333.55002, 333.55002, 333.55002	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95300007, 0.95300007, 0.95300007	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	Aa	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ab	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ac	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ad	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ae	0.64	0/1531	0.80	1/2067 (0.0%)
1	Af	0.64	0/1531	0.79	1/2067 (0.0%)
1	Ag	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ah	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ai	0.64	0/1531	0.80	1/2067 (0.0%)
1	Aj	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ak	0.64	0/1531	0.80	1/2067 (0.0%)
1	Al	0.64	0/1531	0.80	1/2067 (0.0%)
1	Am	0.64	0/1531	0.80	1/2067 (0.0%)
1	An	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ao	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ap	0.64	0/1531	0.80	1/2067 (0.0%)
1	Aq	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ar	0.64	0/1531	0.80	1/2067 (0.0%)
1	As	0.64	0/1531	0.80	1/2067 (0.0%)
1	At	0.64	0/1531	0.80	1/2067 (0.0%)
1	Au	0.64	0/1531	0.80	1/2067 (0.0%)
1	Av	0.64	0/1531	0.80	1/2067 (0.0%)
1	Aw	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ax	0.64	0/1531	0.79	1/2067 (0.0%)
1	Ay	0.64	0/1531	0.80	1/2067 (0.0%)
1	Az	0.64	0/1531	0.80	1/2067 (0.0%)
1	Ba	0.64	0/1531	0.80	1/2067 (0.0%)
All	All	0.64	0/41337	0.80	27/55809 (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	At	52	MET	N-CA-C	-6.03	105.42	112.89
1	Ao	52	MET	N-CA-C	-6.03	105.42	112.89
1	Ac	52	MET	N-CA-C	-6.02	105.42	112.89
1	Al	52	MET	N-CA-C	-6.01	105.43	112.89
1	Au	52	MET	N-CA-C	-6.01	105.44	112.89
1	Ag	52	MET	N-CA-C	-6.00	105.45	112.89
1	Ap	52	MET	N-CA-C	-6.00	105.45	112.89
1	Ay	52	MET	N-CA-C	-6.00	105.44	112.89
1	Af	52	MET	N-CA-C	-6.00	105.45	112.89
1	An	52	MET	N-CA-C	-6.00	105.45	112.89
1	As	52	MET	N-CA-C	-6.00	105.45	112.89
1	Av	52	MET	N-CA-C	-5.99	105.46	112.89
1	Ak	52	MET	N-CA-C	-5.99	105.47	112.89
1	Ae	52	MET	N-CA-C	-5.99	105.47	112.89
1	Aq	52	MET	N-CA-C	-5.98	105.47	112.89
1	Aw	52	MET	N-CA-C	-5.98	105.47	112.89
1	Aa	52	MET	N-CA-C	-5.98	105.47	112.89
1	Am	52	MET	N-CA-C	-5.97	105.48	112.89
1	Ad	52	MET	N-CA-C	-5.97	105.49	112.89
1	Az	52	MET	N-CA-C	-5.97	105.49	112.89
1	Ab	52	MET	N-CA-C	-5.97	105.49	112.89
1	Ah	52	MET	N-CA-C	-5.96	105.50	112.89
1	Ax	52	MET	N-CA-C	-5.96	105.50	112.89
1	Ba	52	MET	N-CA-C	-5.95	105.51	112.89
1	Ai	52	MET	N-CA-C	-5.95	105.51	112.89
1	Ar	52	MET	N-CA-C	-5.95	105.51	112.89
1	Aj	52	MET	N-CA-C	-5.94	105.52	112.89

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	1497	0	1486	39	0
1	Ab	1497	0	1486	46	0
1	Ac	1497	0	1486	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ad	1497	0	1486	47	0
1	Ae	1497	0	1486	47	0
1	Af	1497	0	1486	43	0
1	Ag	1497	0	1486	46	0
1	Ah	1497	0	1486	48	0
1	Ai	1497	0	1486	45	0
1	Aj	1497	0	1486	44	0
1	Ak	1497	0	1486	50	0
1	Al	1497	0	1486	52	0
1	Am	1497	0	1486	50	0
1	An	1497	0	1486	55	0
1	Ao	1497	0	1486	53	0
1	Ap	1497	0	1486	52	0
1	Aq	1497	0	1486	44	0
1	Ar	1497	0	1486	46	0
1	As	1497	0	1486	47	0
1	At	1497	0	1486	45	0
1	Au	1497	0	1486	42	0
1	Av	1497	0	1486	44	0
1	Aw	1497	0	1486	51	0
1	Ax	1497	0	1486	43	0
1	Ay	1497	0	1486	43	0
1	Az	1497	0	1486	43	0
1	Ba	1497	0	1486	37	0
All	All	40419	0	40122	989	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 12.

All (989) 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:At:75:TYR:CE2	1:At:77:PRO:HD3	2.35	0.62
1:Aa:75:TYR:CE2	1:Aa:77:PRO:HD3	2.35	0.62
1:As:75:TYR:CE2	1:As:77:PRO:HD3	2.35	0.62
1:Ab:75:TYR:CE2	1:Ab:77:PRO:HD3	2.35	0.62
1:Ah:75:TYR:CE2	1:Ah:77:PRO:HD3	2.35	0.62
1:Al:75:TYR:CE2	1:Al:77:PRO:HD3	2.35	0.62
1:Am:75:TYR:CE2	1:Am:77:PRO:HD3	2.35	0.62
1:Ax:75:TYR:CE2	1:Ax:77:PRO:HD3	2.35	0.62
1:Ay:75:TYR:CE2	1:Ay:77:PRO:HD3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:75:TYR:CE2	1:Ai:77:PRO:HD3	2.35	0.62
1:An:75:TYR:CE2	1:An:77:PRO:HD3	2.35	0.62
1:Ba:75:TYR:CE2	1:Ba:77:PRO:HD3	2.35	0.62
1:Au:75:TYR:CE2	1:Au:77:PRO:HD3	2.35	0.62
1:Aw:75:TYR:CE2	1:Aw:77:PRO:HD3	2.35	0.62
1:Ad:75:TYR:CE2	1:Ad:77:PRO:HD3	2.35	0.62
1:Ao:75:TYR:CE2	1:Ao:77:PRO:HD3	2.35	0.62
1:Ar:75:TYR:CE2	1:Ar:77:PRO:HD3	2.35	0.62
1:Ae:75:TYR:CE2	1:Ae:77:PRO:HD3	2.35	0.62
1:Ak:75:TYR:CE2	1:Ak:77:PRO:HD3	2.35	0.62
1:Az:75:TYR:CE2	1:Az:77:PRO:HD3	2.35	0.62
1:Ag:75:TYR:CE2	1:Ag:77:PRO:HD3	2.35	0.61
1:Ap:75:TYR:CE2	1:Ap:77:PRO:HD3	2.35	0.61
1:Ac:75:TYR:CE2	1:Ac:77:PRO:HD3	2.35	0.61
1:Aj:75:TYR:CE2	1:Aj:77:PRO:HD3	2.35	0.61
1:Av:75:TYR:CE2	1:Av:77:PRO:HD3	2.35	0.61
1:Aq:75:TYR:CE2	1:Aq:77:PRO:HD3	2.35	0.61
1:Af:75:TYR:CE2	1:Af:77:PRO:HD3	2.35	0.61
1:Af:46:VAL:HG13	1:Aq:136:MET:HE3	1.83	0.60
1:Ah:46:VAL:HG13	1:As:136:MET:HE3	1.83	0.60
1:An:46:VAL:HG13	1:Ay:136:MET:HE3	1.82	0.60
1:Ap:46:VAL:HG13	1:Ba:136:MET:HE3	1.84	0.59
1:Al:46:VAL:HG13	1:Aw:136:MET:HE3	1.84	0.59
1:Ac:67:VAL:HG21	1:Ad:168:LEU:HD22	1.85	0.59
1:Ag:46:VAL:HG13	1:Ar:136:MET:HE3	1.84	0.59
1:Ad:118:MET:HE2	1:Ad:169:ALA:HA	1.85	0.59
1:Ae:46:VAL:HG13	1:Ap:136:MET:HE3	1.84	0.59
1:Ag:118:MET:HE2	1:Ag:169:ALA:HA	1.85	0.59
1:Ax:118:MET:HE2	1:Ax:169:ALA:HA	1.85	0.59
1:Ac:118:MET:HE2	1:Ac:169:ALA:HA	1.85	0.58
1:Ai:46:VAL:HG13	1:At:136:MET:HE3	1.84	0.58
1:An:118:MET:HE2	1:An:169:ALA:HA	1.85	0.58
1:Ap:118:MET:HE2	1:Ap:169:ALA:HA	1.85	0.58
1:Az:118:MET:HE2	1:Az:169:ALA:HA	1.85	0.58
1:Ab:46:VAL:HG13	1:Am:136:MET:HE3	1.84	0.58
1:Af:118:MET:HE2	1:Af:169:ALA:HA	1.85	0.58
1:Am:118:MET:HE2	1:Am:169:ALA:HA	1.85	0.58
1:Aw:118:MET:HE2	1:Aw:169:ALA:HA	1.85	0.58
1:Ao:118:MET:HE2	1:Ao:169:ALA:HA	1.85	0.58
1:Aq:118:MET:HE2	1:Aq:169:ALA:HA	1.85	0.58
1:Al:118:MET:HE2	1:Al:169:ALA:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:46:VAL:HG13	1:Ax:136:MET:HE3	1.84	0.58
1:Ay:118:MET:HE2	1:Ay:169:ALA:HA	1.85	0.58
1:Ba:118:MET:HE2	1:Ba:169:ALA:HA	1.85	0.58
1:Av:118:MET:HE2	1:Av:169:ALA:HA	1.85	0.58
1:Ab:118:MET:HE2	1:Ab:169:ALA:HA	1.85	0.58
1:Ak:46:VAL:HG13	1:Av:136:MET:HE3	1.85	0.58
1:Ae:118:MET:HE2	1:Ae:169:ALA:HA	1.86	0.58
1:Ag:61:LEU:HD13	1:Ah:92:PHE:HD2	1.69	0.58
1:Ah:118:MET:HE2	1:Ah:169:ALA:HA	1.85	0.58
1:Au:118:MET:HE2	1:Au:169:ALA:HA	1.85	0.58
1:Ac:46:VAL:HG13	1:An:136:MET:HE3	1.85	0.58
1:Ak:118:MET:HE2	1:Ak:169:ALA:HA	1.85	0.58
1:Ap:61:LEU:HD13	1:Aq:92:PHE:HD2	1.69	0.58
1:Ar:118:MET:HE2	1:Ar:169:ALA:HA	1.85	0.58
1:At:118:MET:HE2	1:At:169:ALA:HA	1.85	0.58
1:Aj:118:MET:HE2	1:Aj:169:ALA:HA	1.85	0.57
1:Ay:61:LEU:HD13	1:Az:92:PHE:HD2	1.69	0.57
1:Aa:118:MET:HE2	1:Aa:169:ALA:HA	1.85	0.57
1:Ai:118:MET:HE2	1:Ai:169:ALA:HA	1.86	0.57
1:As:118:MET:HE2	1:As:169:ALA:HA	1.85	0.57
1:Aa:119:VAL:O	1:Aa:122:ILE:HG22	2.05	0.57
1:Aj:119:VAL:O	1:Aj:122:ILE:HG22	2.05	0.57
1:As:119:VAL:O	1:As:122:ILE:HG22	2.05	0.57
1:Av:119:VAL:O	1:Av:122:ILE:HG22	2.05	0.57
1:Ba:119:VAL:O	1:Ba:122:ILE:HG22	2.05	0.57
1:Ac:61:LEU:HD13	1:Ad:92:PHE:HD2	1.69	0.56
1:Ah:61:LEU:HD13	1:Ai:92:PHE:HD2	1.70	0.56
1:Aq:61:LEU:HD13	1:Ar:92:PHE:HD2	1.70	0.56
1:Au:119:VAL:O	1:Au:122:ILE:HG22	2.05	0.56
1:Aa:46:VAL:HG13	1:Al:136:MET:HE3	1.86	0.56
1:Ar:119:VAL:O	1:Ar:122:ILE:HG22	2.05	0.56
1:Af:119:VAL:O	1:Af:122:ILE:HG22	2.05	0.56
1:Ag:119:VAL:O	1:Ag:122:ILE:HG22	2.05	0.56
1:Ai:119:VAL:O	1:Ai:122:ILE:HG22	2.05	0.56
1:Am:119:VAL:O	1:Am:122:ILE:HG22	2.05	0.56
1:An:119:VAL:O	1:An:122:ILE:HG22	2.05	0.56
1:Ao:61:LEU:HD13	1:Ap:92:PHE:HD2	1.70	0.56
1:Au:67:VAL:HG21	1:Av:168:LEU:HD22	1.88	0.56
1:Az:61:LEU:HD13	1:Ba:92:PHE:HD2	1.70	0.56
1:Al:119:VAL:O	1:Al:122:ILE:HG22	2.05	0.56
1:Ao:67:VAL:HG21	1:Ap:168:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:119:VAL:O	1:Ao:122:ILE:HG22	2.05	0.56
1:Ab:119:VAL:O	1:Ab:122:ILE:HG22	2.05	0.56
1:Al:67:VAL:HG21	1:Am:168:LEU:HD22	1.88	0.56
1:Ao:46:VAL:HG13	1:Az:136:MET:HE3	1.85	0.56
1:Az:119:VAL:O	1:Az:122:ILE:HG22	2.05	0.56
1:Ad:49:LEU:HD13	1:Ao:145:TYR:CE1	2.41	0.56
1:Aw:119:VAL:O	1:Aw:122:ILE:HG22	2.05	0.56
1:Ae:49:LEU:HD13	1:Ap:145:TYR:CE1	2.41	0.56
1:Ae:119:VAL:O	1:Ae:122:ILE:HG22	2.05	0.56
1:Ag:49:LEU:HD13	1:Ar:145:TYR:CE1	2.40	0.56
1:Ak:119:VAL:O	1:Ak:122:ILE:HG22	2.05	0.56
1:An:67:VAL:HG21	1:Ao:168:LEU:HD22	1.88	0.56
1:Ax:67:VAL:HG21	1:Ay:168:LEU:HD22	1.88	0.56
1:Ay:119:VAL:O	1:Ay:122:ILE:HG22	2.05	0.56
1:Ad:119:VAL:O	1:Ad:122:ILE:HG22	2.05	0.56
1:Af:61:LEU:HD13	1:Ag:92:PHE:HD2	1.71	0.56
1:Ah:119:VAL:O	1:Ah:122:ILE:HG22	2.05	0.56
1:At:119:VAL:O	1:At:122:ILE:HG22	2.05	0.56
1:Ae:61:LEU:HD13	1:Af:92:PHE:HD2	1.71	0.55
1:Ap:67:VAL:HG21	1:Aq:168:LEU:HD22	1.87	0.55
1:Ay:67:VAL:HG21	1:Az:168:LEU:HD22	1.87	0.55
1:Ac:119:VAL:O	1:Ac:122:ILE:HG22	2.05	0.55
1:An:49:LEU:HD13	1:Ay:145:TYR:CE1	2.41	0.55
1:Ag:67:VAL:HG21	1:Ah:168:LEU:HD22	1.87	0.55
1:Ap:119:VAL:O	1:Ap:122:ILE:HG22	2.05	0.55
1:Au:61:LEU:HD13	1:Av:92:PHE:HD2	1.70	0.55
1:Ax:119:VAL:O	1:Ax:122:ILE:HG22	2.05	0.55
1:Al:61:LEU:HD13	1:Am:92:PHE:HD2	1.70	0.55
1:Aa:61:LEU:HD13	1:Ab:92:PHE:HD2	1.71	0.55
1:Aq:119:VAL:O	1:Aq:122:ILE:HG22	2.05	0.55
1:Aa:67:VAL:HG21	1:Ab:168:LEU:HD22	1.89	0.55
1:Af:67:VAL:HG21	1:Ag:168:LEU:HD22	1.88	0.55
1:Am:61:LEU:HD13	1:An:92:PHE:HD2	1.71	0.55
1:Ap:49:LEU:HD13	1:Ba:145:TYR:CE1	2.42	0.55
1:Av:61:LEU:HD13	1:Aw:92:PHE:HD2	1.71	0.55
1:Av:67:VAL:HG21	1:Aw:168:LEU:HD22	1.89	0.55
1:Ax:61:LEU:HD13	1:Ay:92:PHE:HD2	1.71	0.55
1:Ah:67:VAL:HG21	1:Ai:168:LEU:HD22	1.88	0.55
1:Aw:67:VAL:HG21	1:Ax:168:LEU:HD22	1.89	0.55
1:Ai:61:LEU:HD13	1:Aj:92:PHE:HD2	1.71	0.55
1:Ak:49:LEU:HD13	1:Av:145:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Al:49:LEU:HD13	1:Aw:145:TYR:CE1	2.42	0.55
1:Am:49:LEU:HD13	1:Ax:145:TYR:CE1	2.42	0.55
1:Aj:46:VAL:HG13	1:Au:136:MET:HE3	1.87	0.55
1:Am:67:VAL:HG21	1:An:168:LEU:HD22	1.89	0.55
1:Ai:67:VAL:HG21	1:Aj:168:LEU:HD22	1.88	0.55
1:Aj:67:VAL:HG21	1:Ak:168:LEU:HD22	1.89	0.55
1:As:67:VAL:HG21	1:At:168:LEU:HD22	1.89	0.55
1:Ao:49:LEU:HD13	1:Az:145:TYR:CE1	2.42	0.54
1:Aw:61:LEU:HD13	1:Ax:92:PHE:HD2	1.71	0.54
1:Az:67:VAL:HG21	1:Ba:168:LEU:HD22	1.88	0.54
1:Af:49:LEU:HD13	1:Aq:145:TYR:CE1	2.42	0.54
1:Aq:67:VAL:HG21	1:Ar:168:LEU:HD22	1.88	0.54
1:Ae:67:VAL:HG21	1:Af:168:LEU:HD22	1.89	0.54
1:Ad:61:LEU:HD13	1:Ae:92:PHE:HD2	1.71	0.54
1:Aj:61:LEU:HD13	1:Ak:92:PHE:HD2	1.71	0.54
1:An:61:LEU:HD13	1:Ao:92:PHE:HD2	1.71	0.54
1:Ad:67:VAL:HG21	1:Ae:168:LEU:HD22	1.90	0.54
1:At:67:VAL:HG21	1:Au:168:LEU:HD22	1.90	0.54
1:Ay:53:THR:HG22	1:Ay:73:LEU:HD11	1.90	0.54
1:Az:53:THR:HG22	1:Az:73:LEU:HD11	1.90	0.54
1:Ab:67:VAL:HG21	1:Ac:168:LEU:HD22	1.90	0.54
1:Ak:61:LEU:HD13	1:Al:92:PHE:HD2	1.73	0.54
1:An:53:THR:HG22	1:An:73:LEU:HD11	1.90	0.54
1:At:61:LEU:HD13	1:Au:92:PHE:HD2	1.72	0.54
1:Aa:53:THR:HG22	1:Aa:73:LEU:HD11	1.90	0.54
1:Ao:53:THR:HG22	1:Ao:73:LEU:HD11	1.90	0.54
1:Af:53:THR:HG22	1:Af:73:LEU:HD11	1.90	0.53
1:Ag:53:THR:HG22	1:Ag:73:LEU:HD11	1.90	0.53
1:Ak:53:THR:HG22	1:Ak:73:LEU:HD11	1.90	0.53
1:As:53:THR:HG22	1:As:73:LEU:HD11	1.90	0.53
1:As:61:LEU:HD13	1:At:92:PHE:HD2	1.71	0.53
1:Au:53:THR:HG22	1:Au:73:LEU:HD11	1.90	0.53
1:Ai:49:LEU:HD13	1:At:145:TYR:CE1	2.43	0.53
1:Ak:67:VAL:HG21	1:Al:168:LEU:HD22	1.90	0.53
1:At:53:THR:HG22	1:At:73:LEU:HD11	1.90	0.53
1:Ai:53:THR:HG22	1:Ai:73:LEU:HD11	1.90	0.53
1:Aj:53:THR:HG22	1:Aj:73:LEU:HD11	1.90	0.53
1:Ax:53:THR:HG22	1:Ax:73:LEU:HD11	1.90	0.53
1:Ab:61:LEU:HD13	1:Ac:92:PHE:HD2	1.73	0.53
1:Ah:49:LEU:HD13	1:As:145:TYR:CE1	2.43	0.53
1:An:189:GLN:HE21	1:An:190:ARG:HH12	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:189:GLN:HE21	1:Ao:190:ARG:HH12	1.57	0.53
1:Ac:189:GLN:HE21	1:Ac:190:ARG:HH12	1.57	0.53
1:Am:53:THR:HG22	1:Am:73:LEU:HD11	1.90	0.53
1:Ba:53:THR:HG22	1:Ba:73:LEU:HD11	1.90	0.53
1:Ab:49:LEU:HD13	1:Am:145:TYR:CE1	2.43	0.53
1:Ab:53:THR:HG22	1:Ab:73:LEU:HD11	1.90	0.53
1:Ac:49:LEU:HD13	1:An:145:TYR:CE1	2.43	0.53
1:Ac:53:THR:HG22	1:Ac:73:LEU:HD11	1.90	0.53
1:Ae:53:THR:HG22	1:Ae:73:LEU:HD11	1.90	0.53
1:Ap:53:THR:HG22	1:Ap:73:LEU:HD11	1.90	0.53
1:Aw:189:GLN:HE21	1:Aw:190:ARG:HH12	1.57	0.53
1:Ax:189:GLN:HE21	1:Ax:190:ARG:HH12	1.57	0.53
1:Ae:189:GLN:HE21	1:Ae:190:ARG:HH12	1.57	0.53
1:Al:53:THR:HG22	1:Al:73:LEU:HD11	1.90	0.53
1:Ap:189:GLN:HE21	1:Ap:190:ARG:HH12	1.57	0.53
1:Ar:61:LEU:HD13	1:As:92:PHE:HD2	1.73	0.53
1:Av:189:GLN:HE21	1:Av:190:ARG:HH12	1.57	0.53
1:Ad:53:THR:HG22	1:Ad:73:LEU:HD11	1.90	0.53
1:Ad:189:GLN:HE21	1:Ad:190:ARG:HH12	1.57	0.53
1:Ah:53:THR:HG22	1:Ah:73:LEU:HD11	1.90	0.53
1:Am:189:GLN:HE21	1:Am:190:ARG:HH12	1.57	0.53
1:Ar:67:VAL:HG21	1:As:168:LEU:HD22	1.90	0.53
1:Ad:46:VAL:HG13	1:Ao:136:MET:HE3	1.91	0.52
1:Ar:53:THR:HG22	1:Ar:73:LEU:HD11	1.90	0.52
1:Ab:189:GLN:HE21	1:Ab:190:ARG:HH12	1.57	0.52
1:Ae:170:GLU:OE2	1:Ae:205:TYR:OH	2.27	0.52
1:Af:189:GLN:HE21	1:Af:190:ARG:HH12	1.57	0.52
1:Av:53:THR:HG22	1:Av:73:LEU:HD11	1.90	0.52
1:Aw:170:GLU:OE2	1:Aw:205:TYR:OH	2.27	0.52
1:Ay:189:GLN:HE21	1:Ay:190:ARG:HH12	1.57	0.52
1:Ag:189:GLN:HE21	1:Ag:190:ARG:HH12	1.57	0.52
1:Al:189:GLN:HE21	1:Al:190:ARG:HH12	1.57	0.52
1:Am:170:GLU:OE2	1:Am:205:TYR:OH	2.27	0.52
1:Ao:170:GLU:OE2	1:Ao:205:TYR:OH	2.27	0.52
1:Au:189:GLN:HE21	1:Au:190:ARG:HH12	1.57	0.52
1:Az:189:GLN:HE21	1:Az:190:ARG:HH12	1.57	0.52
1:Ac:170:GLU:OE2	1:Ac:205:TYR:OH	2.27	0.52
1:Ah:170:GLU:OE2	1:Ah:205:TYR:OH	2.27	0.52
1:Aq:189:GLN:HE21	1:Aq:190:ARG:HH12	1.57	0.52
1:Aq:53:THR:HG22	1:Aq:73:LEU:HD11	1.90	0.52
1:Aw:53:THR:HG22	1:Aw:73:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:170:GLU:OE2	1:Ay:205:TYR:OH	2.27	0.52
1:Ah:189:GLN:HE21	1:Ah:190:ARG:HH12	1.57	0.52
1:Aj:49:LEU:HD13	1:Au:145:TYR:CE1	2.44	0.52
1:Aa:189:GLN:HE21	1:Aa:190:ARG:HH12	1.57	0.52
1:Ba:189:GLN:HE21	1:Ba:190:ARG:HH12	1.57	0.52
1:Aj:189:GLN:HE21	1:Aj:190:ARG:HH12	1.57	0.52
1:Ak:189:GLN:HE21	1:Ak:190:ARG:HH12	1.57	0.51
1:Ar:189:GLN:HE21	1:Ar:190:ARG:HH12	1.57	0.51
1:At:189:GLN:HE21	1:At:190:ARG:HH12	1.57	0.51
1:Aa:49:LEU:HD13	1:Al:145:TYR:CE1	2.45	0.51
1:Ai:189:GLN:HE21	1:Ai:190:ARG:HH12	1.57	0.51
1:Ah:192:LEU:HD22	1:Ah:222:MET:SD	2.51	0.51
1:Ak:192:LEU:HD22	1:Ak:222:MET:SD	2.51	0.51
1:An:192:LEU:HD22	1:An:222:MET:SD	2.51	0.51
1:Aw:192:LEU:HD22	1:Aw:222:MET:SD	2.51	0.51
1:Ac:192:LEU:HD22	1:Ac:222:MET:SD	2.51	0.51
1:Ag:118:MET:HE1	1:Ag:122:ILE:HD12	1.93	0.51
1:As:189:GLN:HE21	1:As:190:ARG:HH12	1.57	0.51
1:Az:192:LEU:HD22	1:Az:222:MET:SD	2.51	0.51
1:At:192:LEU:HD22	1:At:222:MET:SD	2.51	0.51
1:Ba:118:MET:HE1	1:Ba:122:ILE:HD12	1.93	0.51
1:Ab:192:LEU:HD22	1:Ab:222:MET:SD	2.51	0.51
1:Ad:192:LEU:HD22	1:Ad:222:MET:SD	2.51	0.51
1:Ae:192:LEU:HD22	1:Ae:222:MET:SD	2.51	0.51
1:Af:170:GLU:OE2	1:Af:205:TYR:OH	2.27	0.51
1:Ag:192:LEU:HD22	1:Ag:222:MET:SD	2.51	0.51
1:Ah:118:MET:HE1	1:Ah:122:ILE:HD12	1.93	0.51
1:Ap:118:MET:HE1	1:Ap:122:ILE:HD12	1.93	0.51
1:Ap:192:LEU:HD22	1:Ap:222:MET:SD	2.51	0.51
1:Aq:192:LEU:HD22	1:Aq:222:MET:SD	2.51	0.51
1:As:192:LEU:HD22	1:As:222:MET:SD	2.51	0.51
1:Az:118:MET:HE1	1:Az:122:ILE:HD12	1.93	0.51
1:Ad:48:ARG:HH21	1:Ao:141:GLU:CD	2.19	0.51
1:An:170:GLU:OE2	1:An:205:TYR:OH	2.27	0.51
1:Av:192:LEU:HD22	1:Av:222:MET:SD	2.51	0.51
1:Ad:170:GLU:OE2	1:Ad:205:TYR:OH	2.27	0.51
1:Af:118:MET:HE1	1:Af:122:ILE:HD12	1.93	0.51
1:Al:150:MET:O	1:Al:151:LEU:HD12	2.11	0.51
1:Al:192:LEU:HD22	1:Al:222:MET:SD	2.51	0.51
1:Am:150:MET:O	1:Am:151:LEU:HD12	2.11	0.51
1:Aq:118:MET:HE1	1:Aq:122:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:170:GLU:OE2	1:Au:205:TYR:OH	2.27	0.51
1:Ax:170:GLU:OE2	1:Ax:205:TYR:OH	2.27	0.51
1:Ab:162:MET:HG3	1:Ab:162:MET:O	2.11	0.51
1:Ac:150:MET:O	1:Ac:151:LEU:HD12	2.11	0.51
1:Ai:192:LEU:HD22	1:Ai:222:MET:SD	2.51	0.51
1:Ak:150:MET:O	1:Ak:151:LEU:HD12	2.11	0.51
1:Ao:118:MET:HE1	1:Ao:122:ILE:HD12	1.93	0.51
1:Ap:170:GLU:OE2	1:Ap:205:TYR:OH	2.27	0.51
1:Ar:118:MET:HE1	1:Ar:122:ILE:HD12	1.93	0.51
1:Au:150:MET:O	1:Au:151:LEU:HD12	2.11	0.51
1:Aw:150:MET:O	1:Aw:151:LEU:HD12	2.11	0.51
1:Aa:150:MET:O	1:Aa:151:LEU:HD12	2.11	0.50
1:Ab:150:MET:O	1:Ab:151:LEU:HD12	2.11	0.50
1:Ad:150:MET:O	1:Ad:151:LEU:HD12	2.11	0.50
1:Ag:170:GLU:OE2	1:Ag:205:TYR:OH	2.27	0.50
1:An:46:VAL:HG13	1:Ay:136:MET:CE	2.41	0.50
1:Ao:192:LEU:HD22	1:Ao:222:MET:SD	2.51	0.50
1:Av:150:MET:O	1:Av:151:LEU:HD12	2.11	0.50
1:Ax:192:LEU:HD22	1:Ax:222:MET:SD	2.51	0.50
1:Ay:192:LEU:HD22	1:Ay:222:MET:SD	2.51	0.50
1:Ba:192:LEU:HD22	1:Ba:222:MET:SD	2.51	0.50
1:Aj:150:MET:O	1:Aj:151:LEU:HD12	2.11	0.50
1:Al:162:MET:O	1:Al:162:MET:HG3	2.11	0.50
1:An:150:MET:O	1:An:151:LEU:HD12	2.11	0.50
1:As:118:MET:HE1	1:As:122:ILE:HD12	1.93	0.50
1:At:150:MET:O	1:At:151:LEU:HD12	2.11	0.50
1:Az:170:GLU:OE2	1:Az:205:TYR:OH	2.27	0.50
1:Ae:118:MET:HE1	1:Ae:122:ILE:HD12	1.93	0.50
1:Aj:192:LEU:HD22	1:Aj:222:MET:SD	2.51	0.50
1:Ak:162:MET:O	1:Ak:162:MET:HG3	2.11	0.50
1:An:118:MET:HE1	1:An:122:ILE:HD12	1.93	0.50
1:Av:162:MET:HG3	1:Av:162:MET:O	2.11	0.50
1:Ay:118:MET:HE1	1:Ay:122:ILE:HD12	1.93	0.50
1:Aa:162:MET:HG3	1:Aa:162:MET:O	2.11	0.50
1:Am:192:LEU:HD22	1:Am:222:MET:SD	2.51	0.50
1:Ax:150:MET:O	1:Ax:151:LEU:HD12	2.11	0.50
1:Ae:150:MET:O	1:Ae:151:LEU:HD12	2.11	0.50
1:Af:46:VAL:HG13	1:Aq:136:MET:CE	2.41	0.50
1:Ai:118:MET:HE1	1:Ai:122:ILE:HD12	1.93	0.50
1:Aq:170:GLU:OE2	1:Aq:205:TYR:OH	2.27	0.50
1:Ax:118:MET:HE1	1:Ax:122:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:170:GLU:OE2	1:Aa:205:TYR:OH	2.27	0.50
1:Aa:192:LEU:HD22	1:Aa:222:MET:SD	2.51	0.50
1:Af:192:LEU:HD22	1:Af:222:MET:SD	2.51	0.50
1:Ao:150:MET:O	1:Ao:151:LEU:HD12	2.11	0.50
1:Ar:166:SER:O	1:Ar:169:ALA:HB3	2.12	0.50
1:Ar:192:LEU:HD22	1:Ar:222:MET:SD	2.51	0.50
1:As:150:MET:O	1:As:151:LEU:HD12	2.11	0.50
1:As:162:MET:O	1:As:162:MET:HG3	2.11	0.50
1:Au:192:LEU:HD22	1:Au:222:MET:SD	2.51	0.50
1:Ad:118:MET:HE1	1:Ad:122:ILE:HD12	1.93	0.50
1:Ag:166:SER:O	1:Ag:169:ALA:HB3	2.12	0.50
1:Ai:150:MET:O	1:Ai:151:LEU:HD12	2.11	0.50
1:Aq:166:SER:O	1:Aq:169:ALA:HB3	2.12	0.50
1:At:118:MET:HE1	1:At:122:ILE:HD12	1.93	0.50
1:Au:162:MET:HG3	1:Au:162:MET:O	2.11	0.50
1:Ai:162:MET:HG3	1:Ai:162:MET:O	2.11	0.50
1:Ai:166:SER:O	1:Ai:169:ALA:HB3	2.12	0.50
1:Am:162:MET:HG3	1:Am:162:MET:O	2.11	0.50
1:Ay:150:MET:O	1:Ay:151:LEU:HD12	2.11	0.50
1:Ay:162:MET:O	1:Ay:162:MET:HG3	2.11	0.50
1:Az:166:SER:O	1:Az:169:ALA:HB3	2.12	0.50
1:Ba:166:SER:O	1:Ba:169:ALA:HB3	2.12	0.50
1:Ac:166:SER:O	1:Ac:169:ALA:HB3	2.12	0.49
1:Ae:162:MET:HG3	1:Ae:162:MET:O	2.11	0.49
1:Ah:166:SER:O	1:Ah:169:ALA:HB3	2.12	0.49
1:Aj:166:SER:O	1:Aj:169:ALA:HB3	2.12	0.49
1:Ao:162:MET:O	1:Ao:162:MET:HG3	2.11	0.49
1:Ar:162:MET:HG3	1:Ar:162:MET:O	2.11	0.49
1:As:166:SER:O	1:As:169:ALA:HB3	2.12	0.49
1:Aw:118:MET:HE1	1:Aw:122:ILE:HD12	1.93	0.49
1:Ab:166:SER:O	1:Ab:169:ALA:HB3	2.12	0.49
1:Ac:162:MET:O	1:Ac:162:MET:HG3	2.11	0.49
1:Af:150:MET:O	1:Af:151:LEU:HD12	2.11	0.49
1:Aj:118:MET:HE1	1:Aj:122:ILE:HD12	1.93	0.49
1:An:166:SER:O	1:An:169:ALA:HB3	2.12	0.49
1:Ar:150:MET:O	1:Ar:151:LEU:HD12	2.11	0.49
1:Aw:162:MET:O	1:Aw:162:MET:HG3	2.11	0.49
1:Aa:118:MET:HE1	1:Aa:122:ILE:HD12	1.93	0.49
1:Ad:166:SER:O	1:Ad:169:ALA:HB3	2.12	0.49
1:Ai:170:GLU:OE2	1:Ai:205:TYR:OH	2.27	0.49
1:Aj:162:MET:HG3	1:Aj:162:MET:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:166:SER:O	1:Ak:169:ALA:HB3	2.12	0.49
1:Ap:150:MET:O	1:Ap:151:LEU:HD12	2.11	0.49
1:At:162:MET:O	1:At:162:MET:HG3	2.11	0.49
1:At:166:SER:O	1:At:169:ALA:HB3	2.12	0.49
1:Ax:166:SER:O	1:Ax:169:ALA:HB3	2.12	0.49
1:Az:162:MET:HG3	1:Az:162:MET:O	2.11	0.49
1:Aa:166:SER:O	1:Aa:169:ALA:HB3	2.12	0.49
1:Ab:118:MET:HE1	1:Ab:122:ILE:HD12	1.93	0.49
1:Ac:118:MET:HE1	1:Ac:122:ILE:HD12	1.93	0.49
1:Af:162:MET:HG3	1:Af:162:MET:O	2.11	0.49
1:Ag:150:MET:O	1:Ag:151:LEU:HD12	2.11	0.49
1:Ah:150:MET:O	1:Ah:151:LEU:HD12	2.11	0.49
1:Ah:162:MET:O	1:Ah:162:MET:HG3	2.11	0.49
1:Al:166:SER:O	1:Al:169:ALA:HB3	2.12	0.49
1:Am:118:MET:HE1	1:Am:122:ILE:HD12	1.93	0.49
1:Am:166:SER:O	1:Am:169:ALA:HB3	2.12	0.49
1:Ap:162:MET:O	1:Ap:162:MET:HG3	2.11	0.49
1:As:170:GLU:OE2	1:As:205:TYR:OH	2.27	0.49
1:Av:170:GLU:OE2	1:Av:205:TYR:OH	2.27	0.49
1:Ay:166:SER:O	1:Ay:169:ALA:HB3	2.12	0.49
1:Aq:150:MET:O	1:Aq:151:LEU:HD12	2.11	0.49
1:Au:118:MET:HE1	1:Au:122:ILE:HD12	1.93	0.49
1:Av:118:MET:HE1	1:Av:122:ILE:HD12	1.93	0.49
1:Ae:166:SER:O	1:Ae:169:ALA:HB3	2.12	0.49
1:Ak:118:MET:HE1	1:Ak:122:ILE:HD12	1.93	0.49
1:Ao:166:SER:O	1:Ao:169:ALA:HB3	2.12	0.49
1:Az:150:MET:O	1:Az:151:LEU:HD12	2.11	0.49
1:Af:166:SER:O	1:Af:169:ALA:HB3	2.12	0.49
1:Al:118:MET:HE1	1:Al:122:ILE:HD12	1.93	0.49
1:Ap:166:SER:O	1:Ap:169:ALA:HB3	2.12	0.49
1:Au:166:SER:O	1:Au:169:ALA:HB3	2.12	0.49
1:Ba:150:MET:O	1:Ba:151:LEU:HD12	2.11	0.49
1:Ab:46:VAL:HG13	1:Am:136:MET:CE	2.43	0.49
1:Al:46:VAL:HG13	1:Aw:136:MET:CE	2.43	0.49
1:Al:170:GLU:OE2	1:Al:205:TYR:OH	2.27	0.49
1:Av:166:SER:O	1:Av:169:ALA:HB3	2.12	0.49
1:Ag:162:MET:O	1:Ag:162:MET:HG3	2.11	0.49
1:Aw:166:SER:O	1:Aw:169:ALA:HB3	2.12	0.49
1:Ba:162:MET:O	1:Ba:162:MET:HG3	2.11	0.49
1:Ab:170:GLU:OE2	1:Ab:205:TYR:OH	2.27	0.48
1:Ac:46:VAL:HG13	1:An:136:MET:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ap:213:ILE:H	1:Ap:213:ILE:HD12	1.78	0.48
1:Ad:213:ILE:H	1:Ad:213:ILE:HD12	1.78	0.48
1:Ah:46:VAL:HG13	1:As:136:MET:CE	2.41	0.48
1:Ah:213:ILE:H	1:Ah:213:ILE:HD12	1.78	0.48
1:Am:46:VAL:HG13	1:Ax:136:MET:CE	2.43	0.48
1:Am:213:ILE:HD12	1:Am:213:ILE:H	1.79	0.48
1:Aq:118:MET:CE	1:Aq:122:ILE:HD12	2.43	0.48
1:Aq:162:MET:HG3	1:Aq:162:MET:O	2.11	0.48
1:Ae:46:VAL:HG13	1:Ap:136:MET:CE	2.43	0.48
1:Ae:213:ILE:HD12	1:Ae:213:ILE:H	1.79	0.48
1:Ah:118:MET:CE	1:Ah:122:ILE:HD12	2.44	0.48
1:Aj:213:ILE:HD12	1:Aj:213:ILE:H	1.78	0.48
1:An:135:THR:HB	1:An:142:GLN:OE1	2.14	0.48
1:Ax:135:THR:HB	1:Ax:142:GLN:OE1	2.14	0.48
1:Ax:213:ILE:H	1:Ax:213:ILE:HD12	1.78	0.48
1:Ad:135:THR:HB	1:Ad:142:GLN:OE1	2.14	0.48
1:Ag:213:ILE:HD12	1:Ag:213:ILE:H	1.78	0.48
1:Ak:213:ILE:HD12	1:Ak:213:ILE:H	1.78	0.48
1:Av:135:THR:HB	1:Av:142:GLN:OE1	2.14	0.48
1:Ay:213:ILE:HD12	1:Ay:213:ILE:H	1.79	0.48
1:Az:118:MET:CE	1:Az:122:ILE:HD12	2.44	0.48
1:Ba:118:MET:CE	1:Ba:122:ILE:HD12	2.44	0.48
1:Ba:213:ILE:HD12	1:Ba:213:ILE:H	1.78	0.48
1:Af:135:THR:HB	1:Af:142:GLN:OE1	2.14	0.48
1:Ag:48:ARG:HH21	1:Ar:141:GLU:CD	2.22	0.48
1:Ap:135:THR:HB	1:Ap:142:GLN:OE1	2.14	0.48
1:Az:135:THR:HB	1:Az:142:GLN:OE1	2.14	0.48
1:Al:213:ILE:HD12	1:Al:213:ILE:H	1.78	0.48
1:Au:213:ILE:HD12	1:Au:213:ILE:H	1.79	0.48
1:Ax:162:MET:O	1:Ax:162:MET:HG3	2.11	0.48
1:Ac:135:THR:HB	1:Ac:142:GLN:OE1	2.14	0.48
1:Ad:48:ARG:NH2	1:Ao:141:GLU:CD	2.72	0.48
1:Ag:118:MET:CE	1:Ag:122:ILE:HD12	2.44	0.48
1:Al:135:THR:HB	1:Al:142:GLN:OE1	2.14	0.48
1:An:162:MET:HG3	1:An:162:MET:O	2.11	0.48
1:Ap:118:MET:CE	1:Ap:122:ILE:HD12	2.44	0.48
1:At:213:ILE:H	1:At:213:ILE:HD12	1.79	0.48
1:Aa:213:ILE:HD12	1:Aa:213:ILE:H	1.79	0.48
1:Ab:135:THR:HB	1:Ab:142:GLN:OE1	2.14	0.48
1:Ae:135:THR:HB	1:Ae:142:GLN:OE1	2.14	0.48
1:Ag:135:THR:HB	1:Ag:142:GLN:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:118:MET:CE	1:Aj:122:ILE:HD12	2.44	0.48
1:Aq:135:THR:HB	1:Aq:142:GLN:OE1	2.14	0.48
1:Aq:213:ILE:HD12	1:Aq:213:ILE:H	1.78	0.48
1:Av:213:ILE:HD12	1:Av:213:ILE:H	1.78	0.48
1:Ba:135:THR:HB	1:Ba:142:GLN:OE1	2.14	0.48
1:Aa:46:VAL:HG13	1:Al:136:MET:CE	2.44	0.48
1:Ab:213:ILE:HD12	1:Ab:213:ILE:H	1.78	0.48
1:Af:118:MET:CE	1:Af:122:ILE:HD12	2.44	0.48
1:Ak:46:VAL:HG13	1:Av:136:MET:CE	2.44	0.48
1:Ap:46:VAL:HG13	1:Ba:136:MET:CE	2.43	0.48
1:As:118:MET:CE	1:As:122:ILE:HD12	2.44	0.48
1:As:213:ILE:HD12	1:As:213:ILE:H	1.79	0.48
1:Ad:46:VAL:HB	1:Ao:138:ASP:OD1	2.14	0.48
1:Ad:162:MET:O	1:Ad:162:MET:HG3	2.11	0.48
1:Ae:118:MET:CE	1:Ae:122:ILE:HD12	2.44	0.48
1:Ai:46:VAL:HG13	1:At:136:MET:CE	2.43	0.48
1:Ai:135:THR:HB	1:Ai:142:GLN:OE1	2.14	0.48
1:Ai:213:ILE:HD12	1:Ai:213:ILE:H	1.79	0.48
1:Am:135:THR:HB	1:Am:142:GLN:OE1	2.14	0.48
1:An:213:ILE:HD12	1:An:213:ILE:H	1.79	0.48
1:Ao:213:ILE:HD12	1:Ao:213:ILE:H	1.78	0.48
1:Ar:213:ILE:HD12	1:Ar:213:ILE:H	1.79	0.48
1:As:135:THR:HB	1:As:142:GLN:OE1	2.14	0.48
1:At:118:MET:CE	1:At:122:ILE:HD12	2.44	0.48
1:Ac:213:ILE:HD12	1:Ac:213:ILE:H	1.78	0.47
1:Ao:118:MET:CE	1:Ao:122:ILE:HD12	2.44	0.47
1:Ar:118:MET:CE	1:Ar:122:ILE:HD12	2.44	0.47
1:Av:118:MET:CE	1:Av:122:ILE:HD12	2.44	0.47
1:Aw:175:MET:HG3	1:Aw:176:ARG:N	2.29	0.47
1:Aa:118:MET:CE	1:Aa:122:ILE:HD12	2.44	0.47
1:Ah:174:GLU:HG2	1:Ah:199:ARG:HH22	1.79	0.47
1:Ak:135:THR:HB	1:Ak:142:GLN:OE1	2.14	0.47
1:Am:175:MET:HG3	1:Am:176:ARG:N	2.30	0.47
1:Au:118:MET:CE	1:Au:122:ILE:HD12	2.44	0.47
1:Au:135:THR:HB	1:Au:142:GLN:OE1	2.14	0.47
1:Ax:118:MET:CE	1:Ax:122:ILE:HD12	2.44	0.47
1:Aa:135:THR:HB	1:Aa:142:GLN:OE1	2.14	0.47
1:Ah:135:THR:HB	1:Ah:142:GLN:OE1	2.14	0.47
1:Aj:174:GLU:HG2	1:Aj:199:ARG:HH22	1.79	0.47
1:As:174:GLU:HG2	1:As:199:ARG:HH22	1.79	0.47
1:At:174:GLU:HG2	1:At:199:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:174:GLU:HG2	1:Au:199:ARG:HH22	1.79	0.47
1:Ab:118:MET:CE	1:Ab:122:ILE:HD12	2.44	0.47
1:Ab:175:MET:HG3	1:Ab:176:ARG:N	2.30	0.47
1:Ac:118:MET:CE	1:Ac:122:ILE:HD12	2.44	0.47
1:Ac:175:MET:HG3	1:Ac:176:ARG:N	2.30	0.47
1:Ad:118:MET:CE	1:Ad:122:ILE:HD12	2.44	0.47
1:Ag:46:VAL:HG13	1:Ar:136:MET:CE	2.43	0.47
1:Ag:48:ARG:NH2	1:Ar:141:GLU:CD	2.72	0.47
1:Aq:174:GLU:HG2	1:Aq:199:ARG:HH22	1.79	0.47
1:Ar:135:THR:HB	1:Ar:142:GLN:OE1	2.14	0.47
1:Ba:174:GLU:HG2	1:Ba:199:ARG:HH22	1.79	0.47
1:Ae:175:MET:HG3	1:Ae:176:ARG:N	2.29	0.47
1:An:197:LEU:HD23	1:An:218:ALA:HB2	1.97	0.47
1:Ao:135:THR:HB	1:Ao:142:GLN:OE1	2.14	0.47
1:Ao:197:LEU:HD23	1:Ao:218:ALA:HB2	1.97	0.47
1:Aw:135:THR:HB	1:Aw:142:GLN:OE1	2.14	0.47
1:Ax:197:LEU:HD23	1:Ax:218:ALA:HB2	1.97	0.47
1:Ay:135:THR:HB	1:Ay:142:GLN:OE1	2.14	0.47
1:Ac:79:GLN:HG2	1:Ad:123:GLU:OE2	2.14	0.47
1:Ad:197:LEU:HD23	1:Ad:218:ALA:HB2	1.97	0.47
1:Ai:118:MET:CE	1:Ai:122:ILE:HD12	2.44	0.47
1:Al:175:MET:HG3	1:Al:176:ARG:N	2.29	0.47
1:An:118:MET:CE	1:An:122:ILE:HD12	2.44	0.47
1:Aw:118:MET:CE	1:Aw:122:ILE:HD12	2.44	0.47
1:Aw:197:LEU:HD23	1:Aw:218:ALA:HB2	1.97	0.47
1:Aw:213:ILE:HD12	1:Aw:213:ILE:H	1.79	0.47
1:Ac:197:LEU:HD23	1:Ac:218:ALA:HB2	1.97	0.47
1:Ae:48:ARG:HH21	1:Ap:141:GLU:CD	2.23	0.47
1:Ae:197:LEU:HD23	1:Ae:218:ALA:HB2	1.97	0.47
1:Af:213:ILE:HD12	1:Af:213:ILE:H	1.78	0.47
1:Ak:118:MET:CE	1:Ak:122:ILE:HD12	2.44	0.47
1:Ak:174:GLU:HG2	1:Ak:199:ARG:HH22	1.79	0.47
1:Al:118:MET:CE	1:Al:122:ILE:HD12	2.44	0.47
1:Al:174:GLU:HG2	1:Al:199:ARG:HH22	1.79	0.47
1:Ao:46:VAL:HG13	1:Az:136:MET:CE	2.45	0.47
1:Ao:175:MET:HG3	1:Ao:176:ARG:N	2.29	0.47
1:Ap:197:LEU:HD23	1:Ap:218:ALA:HB2	1.96	0.47
1:At:135:THR:HB	1:At:142:GLN:OE1	2.14	0.47
1:Av:174:GLU:HG2	1:Av:199:ARG:HH22	1.79	0.47
1:Av:175:MET:HG3	1:Av:176:ARG:N	2.29	0.47
1:Ay:118:MET:CE	1:Ay:122:ILE:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:170:GLU:OE2	1:Ba:205:TYR:OH	2.27	0.47
1:Ae:174:GLU:HG2	1:Ae:199:ARG:HH22	1.79	0.47
1:Af:174:GLU:HG2	1:Af:199:ARG:HH22	1.79	0.47
1:Af:197:LEU:HD23	1:Af:218:ALA:HB2	1.97	0.47
1:Aj:135:THR:HB	1:Aj:142:GLN:OE1	2.14	0.47
1:Av:137:MET:HE3	1:Av:137:MET:HB3	1.82	0.47
1:Af:175:MET:HG3	1:Af:176:ARG:N	2.29	0.47
1:Am:48:ARG:HH21	1:Ax:141:GLU:CD	2.23	0.47
1:Am:197:LEU:HD23	1:Am:218:ALA:HB2	1.96	0.47
1:Az:213:ILE:HD12	1:Az:213:ILE:H	1.78	0.47
1:Ac:174:GLU:HG2	1:Ac:199:ARG:HH22	1.79	0.47
1:Ag:174:GLU:HG2	1:Ag:199:ARG:HH22	1.79	0.47
1:Ak:48:ARG:HH21	1:Av:141:GLU:CD	2.22	0.47
1:Am:174:GLU:HG2	1:Am:199:ARG:HH22	1.79	0.47
1:An:174:GLU:HG2	1:An:199:ARG:HH22	1.79	0.47
1:At:175:MET:HG3	1:At:176:ARG:N	2.30	0.47
1:Av:197:LEU:HD23	1:Av:218:ALA:HB2	1.97	0.47
1:Aw:174:GLU:HG2	1:Aw:199:ARG:HH22	1.79	0.47
1:Ay:197:LEU:HD23	1:Ay:218:ALA:HB2	1.97	0.47
1:Az:197:LEU:HD23	1:Az:218:ALA:HB2	1.97	0.47
1:Ab:174:GLU:HG2	1:Ab:199:ARG:HH22	1.79	0.46
1:Ad:174:GLU:HG2	1:Ad:199:ARG:HH22	1.79	0.46
1:Ag:197:LEU:HD23	1:Ag:218:ALA:HB2	1.97	0.46
1:Ax:175:MET:HG3	1:Ax:176:ARG:N	2.30	0.46
1:Aa:174:GLU:HG2	1:Aa:199:ARG:HH22	1.79	0.46
1:Ab:197:LEU:HD23	1:Ab:218:ALA:HB2	1.96	0.46
1:Af:79:GLN:HG2	1:Ag:123:GLU:OE2	2.15	0.46
1:Ah:137:MET:HE3	1:Ah:137:MET:HB3	1.82	0.46
1:Ah:175:MET:HG3	1:Ah:176:ARG:N	2.30	0.46
1:Am:118:MET:CE	1:Am:122:ILE:HD12	2.44	0.46
1:Ap:48:ARG:HH21	1:Ba:141:GLU:CD	2.23	0.46
1:Ap:175:MET:HG3	1:Ap:176:ARG:N	2.30	0.46
1:Ar:174:GLU:HG2	1:Ar:199:ARG:HH22	1.79	0.46
1:Ar:175:MET:HG3	1:Ar:176:ARG:N	2.30	0.46
1:Ai:174:GLU:HG2	1:Ai:199:ARG:HH22	1.79	0.46
1:Aj:79:GLN:HG2	1:Ak:123:GLU:OE2	2.16	0.46
1:Ak:48:ARG:NH2	1:Av:141:GLU:CD	2.73	0.46
1:Al:197:LEU:HD23	1:Al:218:ALA:HB2	1.97	0.46
1:An:48:ARG:HH21	1:Ay:141:GLU:CD	2.23	0.46
1:An:175:MET:HG3	1:An:176:ARG:N	2.29	0.46
1:Ao:174:GLU:HG2	1:Ao:199:ARG:HH22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:79:GLN:HG2	1:At:123:GLU:OE2	2.15	0.46
1:Au:137:MET:HE3	1:Au:137:MET:HB3	1.82	0.46
1:Au:175:MET:HG3	1:Au:176:ARG:N	2.30	0.46
1:Az:175:MET:HG3	1:Az:176:ARG:N	2.29	0.46
1:Aj:175:MET:HG3	1:Aj:176:ARG:N	2.30	0.46
1:Aq:197:LEU:HD23	1:Aq:218:ALA:HB2	1.96	0.46
1:Aw:137:MET:HE3	1:Aw:137:MET:HB3	1.82	0.46
1:Ay:174:GLU:HG2	1:Ay:199:ARG:HH22	1.79	0.46
1:Ay:175:MET:HG3	1:Ay:176:ARG:N	2.30	0.46
1:Aa:79:GLN:HG2	1:Ab:123:GLU:OE2	2.15	0.46
1:Az:174:GLU:HG2	1:Az:199:ARG:HH22	1.79	0.46
1:Ba:197:LEU:HD23	1:Ba:218:ALA:HB2	1.96	0.46
1:Ap:174:GLU:HG2	1:Ap:199:ARG:HH22	1.79	0.46
1:Ax:174:GLU:HG2	1:Ax:199:ARG:HH22	1.79	0.46
1:Az:79:GLN:HG2	1:Ba:123:GLU:OE2	2.16	0.46
1:Ad:175:MET:HG3	1:Ad:176:ARG:N	2.29	0.46
1:Al:79:GLN:HG2	1:Am:123:GLU:OE2	2.16	0.46
1:Ah:197:LEU:HD23	1:Ah:218:ALA:HB2	1.96	0.46
1:Ak:175:MET:HG3	1:Ak:176:ARG:N	2.30	0.46
1:Ak:197:LEU:HD23	1:Ak:218:ALA:HB2	1.96	0.46
1:Al:48:ARG:HH21	1:Aw:141:GLU:CD	2.23	0.46
1:Ap:48:ARG:NH2	1:Ba:141:GLU:CD	2.74	0.46
1:At:197:LEU:HD23	1:At:218:ALA:HB2	1.97	0.46
1:Au:197:LEU:HD23	1:Au:218:ALA:HB2	1.97	0.46
1:Ac:77:PRO:HD2	1:Ad:176:ARG:HH12	1.81	0.46
1:As:175:MET:HG3	1:As:176:ARG:N	2.29	0.46
1:Ah:79:GLN:HG2	1:Ai:123:GLU:OE2	2.16	0.46
1:Ai:197:LEU:HD23	1:Ai:218:ALA:HB2	1.96	0.46
1:Am:48:ARG:NH2	1:Ax:141:GLU:CD	2.73	0.46
1:Am:79:GLN:HG2	1:An:123:GLU:OE2	2.16	0.46
1:Aa:137:MET:HE3	1:Aa:137:MET:HB3	1.81	0.45
1:Ae:48:ARG:NH2	1:Ap:141:GLU:CD	2.74	0.45
1:Ag:137:MET:HE3	1:Ag:137:MET:HB3	1.82	0.45
1:Ai:175:MET:HG3	1:Ai:176:ARG:N	2.30	0.45
1:Aa:175:MET:HG3	1:Aa:176:ARG:N	2.30	0.45
1:Ab:137:MET:HE3	1:Ab:137:MET:HB3	1.82	0.45
1:Ac:137:MET:HE3	1:Ac:137:MET:HB3	1.82	0.45
1:Ak:79:GLN:HG2	1:Al:123:GLU:OE2	2.17	0.45
1:An:48:ARG:NH2	1:Ay:141:GLU:CD	2.74	0.45
1:At:170:GLU:OE2	1:At:205:TYR:OH	2.27	0.45
1:Aa:197:LEU:HD23	1:Aa:218:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:137:MET:HE3	1:Ad:137:MET:HB3	1.81	0.45
1:Ai:79:GLN:HG2	1:Aj:123:GLU:OE2	2.16	0.45
1:Aj:197:LEU:HD23	1:Aj:218:ALA:HB2	1.97	0.45
1:Aq:175:MET:HG3	1:Aq:176:ARG:N	2.29	0.45
1:Ar:197:LEU:HD23	1:Ar:218:ALA:HB2	1.96	0.45
1:Ax:137:MET:HE3	1:Ax:137:MET:HB3	1.82	0.45
1:Ae:137:MET:HE3	1:Ae:137:MET:HB3	1.82	0.45
1:Ag:175:MET:HG3	1:Ag:176:ARG:N	2.30	0.45
1:Aj:46:VAL:HG13	1:Au:136:MET:CE	2.46	0.45
1:Al:137:MET:HE3	1:Al:137:MET:HB3	1.82	0.45
1:An:79:GLN:HG2	1:Ao:123:GLU:OE2	2.16	0.45
1:Ao:48:ARG:HH21	1:Az:141:GLU:CD	2.24	0.45
1:Ar:79:GLN:HG2	1:As:123:GLU:OE2	2.17	0.45
1:As:197:LEU:HD23	1:As:218:ALA:HB2	1.97	0.45
1:At:79:GLN:HG2	1:Au:123:GLU:OE2	2.17	0.45
1:Ax:79:GLN:HG2	1:Ay:123:GLU:OE2	2.15	0.45
1:Ba:175:MET:HG3	1:Ba:176:ARG:N	2.30	0.45
1:Aj:170:GLU:OE2	1:Aj:205:TYR:OH	2.27	0.45
1:Au:79:GLN:HG2	1:Av:123:GLU:OE2	2.16	0.45
1:Af:137:MET:HE3	1:Af:137:MET:HB3	1.82	0.45
1:Al:48:ARG:NH2	1:Aw:141:GLU:CD	2.75	0.45
1:Am:137:MET:HE3	1:Am:137:MET:HB3	1.81	0.45
1:Ao:79:GLN:HG2	1:Ap:123:GLU:OE2	2.17	0.45
1:Ae:79:GLN:HG2	1:Af:123:GLU:OE2	2.17	0.45
1:Aq:79:GLN:HG2	1:Ar:123:GLU:OE2	2.16	0.45
1:Av:79:GLN:HG2	1:Aw:123:GLU:OE2	2.16	0.45
1:Ay:137:MET:HE3	1:Ay:137:MET:HB3	1.82	0.45
1:Ab:79:GLN:HG2	1:Ac:123:GLU:OE2	2.17	0.45
1:Ag:79:GLN:HG2	1:Ah:123:GLU:OE2	2.18	0.45
1:At:137:MET:HE3	1:At:137:MET:HB3	1.82	0.44
1:Ae:172:TYR:O	1:Ae:175:MET:HG2	2.18	0.44
1:Aj:48:ARG:HH21	1:Au:141:GLU:CD	2.24	0.44
1:Ao:48:ARG:NH2	1:Az:141:GLU:CD	2.75	0.44
1:Ao:172:TYR:O	1:Ao:175:MET:HG2	2.18	0.44
1:Am:172:TYR:O	1:Am:175:MET:HG2	2.18	0.44
1:Ap:137:MET:HE3	1:Ap:137:MET:HB3	1.81	0.44
1:Aw:172:TYR:O	1:Aw:175:MET:HG2	2.18	0.44
1:Ay:172:TYR:O	1:Ay:175:MET:HG2	2.18	0.44
1:Ac:172:TYR:O	1:Ac:175:MET:HG2	2.18	0.44
1:Aj:48:ARG:NH2	1:Au:141:GLU:CD	2.76	0.44
1:An:137:MET:HE3	1:An:137:MET:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aw:79:GLN:HG2	1:Ax:123:GLU:OE2	2.17	0.44
1:Ax:172:TYR:O	1:Ax:175:MET:HG2	2.18	0.44
1:Ak:137:MET:HE3	1:Ak:137:MET:HB3	1.82	0.44
1:Ap:79:GLN:HG2	1:Aq:123:GLU:OE2	2.18	0.44
1:Ac:48:ARG:HH21	1:An:141:GLU:CD	2.26	0.44
1:Ad:49:LEU:HD13	1:Ao:145:TYR:HE1	1.80	0.44
1:Ao:137:MET:HE3	1:Ao:137:MET:HB3	1.82	0.44
1:Al:172:TYR:O	1:Al:175:MET:HG2	2.18	0.43
1:An:172:TYR:O	1:An:175:MET:HG2	2.18	0.43
1:Av:172:TYR:O	1:Av:175:MET:HG2	2.18	0.43
1:Ax:77:PRO:HD2	1:Ay:176:ARG:HH12	1.83	0.43
1:Ay:79:GLN:HG2	1:Az:123:GLU:OE2	2.18	0.43
1:Ab:172:TYR:O	1:Ab:175:MET:HG2	2.18	0.43
1:Ae:183:MET:HE2	1:Ae:183:MET:HB2	1.96	0.43
1:Af:77:PRO:HD2	1:Ag:176:ARG:HH12	1.83	0.43
1:Ao:77:PRO:HD2	1:Ap:176:ARG:HH12	1.83	0.43
1:As:172:TYR:O	1:As:175:MET:HG2	2.18	0.43
1:Ad:82:LEU:HD21	1:Ae:137:MET:HG2	1.99	0.43
1:Af:172:TYR:O	1:Af:175:MET:HG2	2.18	0.43
1:Ag:172:TYR:O	1:Ag:175:MET:HG2	2.18	0.43
1:Ai:172:TYR:O	1:Ai:175:MET:HG2	2.18	0.43
1:Ap:172:TYR:O	1:Ap:175:MET:HG2	2.18	0.43
1:Ar:172:TYR:O	1:Ar:175:MET:HG2	2.18	0.43
1:As:188:LEU:HD23	1:As:188:LEU:HA	1.87	0.43
1:Aw:183:MET:HE2	1:Aw:183:MET:HB2	1.96	0.43
1:Az:216:LYS:HE3	1:Az:216:LYS:HB2	1.85	0.43
1:Ab:175:MET:CG	1:Ab:176:ARG:N	2.82	0.43
1:Ad:183:MET:HE2	1:Ad:183:MET:HB2	1.96	0.43
1:Al:77:PRO:HD2	1:Am:176:ARG:HH12	1.84	0.43
1:Aq:172:TYR:O	1:Aq:175:MET:HG2	2.18	0.43
1:Az:172:TYR:O	1:Az:175:MET:HG2	2.18	0.43
1:Ae:175:MET:CG	1:Ae:176:ARG:N	2.82	0.43
1:Ah:48:ARG:HH21	1:As:141:GLU:CD	2.26	0.43
1:Aj:172:TYR:O	1:Aj:175:MET:HG2	2.18	0.43
1:Ak:114:LEU:HD23	1:Ak:114:LEU:HA	1.92	0.43
1:Al:175:MET:CG	1:Al:176:ARG:N	2.82	0.43
1:Ar:170:GLU:OE2	1:Ar:205:TYR:OH	2.27	0.43
1:Au:172:TYR:O	1:Au:175:MET:HG2	2.18	0.43
1:Aw:175:MET:CG	1:Aw:176:ARG:N	2.82	0.43
1:Ad:172:TYR:O	1:Ad:175:MET:HG2	2.18	0.43
1:Af:48:ARG:NH2	1:Aq:141:GLU:CD	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ah:59:PRO:HG2	1:Ai:165:PHE:CD1	2.54	0.43
1:Ah:172:TYR:O	1:Ah:175:MET:HG2	2.18	0.43
1:Am:175:MET:CG	1:Am:176:ARG:N	2.82	0.43
1:An:77:PRO:HD2	1:Ao:176:ARG:HH12	1.84	0.43
1:Ao:175:MET:CG	1:Ao:176:ARG:N	2.82	0.43
1:At:172:TYR:O	1:At:175:MET:HG2	2.18	0.43
1:At:175:MET:CG	1:At:176:ARG:N	2.82	0.43
1:Av:175:MET:CG	1:Av:176:ARG:N	2.82	0.43
1:Ba:172:TYR:O	1:Ba:175:MET:HG2	2.18	0.43
1:Ab:48:ARG:HH21	1:Am:141:GLU:CD	2.25	0.43
1:Af:48:ARG:HH21	1:Aq:141:GLU:CD	2.26	0.43
1:Am:183:MET:HE2	1:Am:183:MET:HB2	1.96	0.43
1:Ao:183:MET:HE2	1:Ao:183:MET:HB2	1.96	0.43
1:Ap:77:PRO:HD2	1:Aq:176:ARG:HH12	1.84	0.43
1:Ac:175:MET:CG	1:Ac:176:ARG:N	2.82	0.43
1:Aq:59:PRO:HG2	1:Ar:165:PHE:CD1	2.54	0.43
1:Ax:216:LYS:HE3	1:Ax:216:LYS:HB2	1.85	0.43
1:Ac:207:ILE:HD13	1:Ac:207:ILE:HA	1.93	0.43
1:Ai:48:ARG:HH21	1:At:141:GLU:CD	2.26	0.43
1:Aj:175:MET:CG	1:Aj:176:ARG:N	2.82	0.43
1:Ak:172:TYR:O	1:Ak:175:MET:HG2	2.18	0.43
1:As:175:MET:CG	1:As:176:ARG:N	2.82	0.43
1:Ay:77:PRO:HD2	1:Az:176:ARG:HH12	1.84	0.43
1:Aa:172:TYR:O	1:Aa:175:MET:HG2	2.18	0.43
1:Ab:207:ILE:HD13	1:Ab:207:ILE:HA	1.93	0.43
1:Ac:114:LEU:HD23	1:Ac:114:LEU:HA	1.92	0.43
1:Ad:79:GLN:HG2	1:Ae:123:GLU:OE2	2.19	0.43
1:Af:175:MET:CG	1:Af:176:ARG:N	2.82	0.43
1:Ag:46:VAL:HB	1:Ar:138:ASP:OD1	2.19	0.43
1:Ai:175:MET:CG	1:Ai:176:ARG:N	2.82	0.43
1:Ap:175:MET:CG	1:Ap:176:ARG:N	2.82	0.43
1:Aq:77:PRO:HD2	1:Ar:176:ARG:HH12	1.84	0.43
1:At:82:LEU:HD21	1:Au:137:MET:HG2	2.01	0.43
1:Ay:175:MET:CG	1:Ay:176:ARG:N	2.82	0.43
1:Az:59:PRO:HG2	1:Ba:165:PHE:CD1	2.54	0.43
1:Az:175:MET:CG	1:Az:176:ARG:N	2.82	0.43
1:Ab:48:ARG:NH2	1:Am:141:GLU:CD	2.76	0.42
1:Ae:46:VAL:HB	1:Ap:138:ASP:OD1	2.19	0.42
1:Ai:107:GLU:OE2	1:Ai:111:GLU:HG3	2.19	0.42
1:Ak:46:VAL:HB	1:Av:138:ASP:OD1	2.18	0.42
1:Aa:107:GLU:OE2	1:Aa:111:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:175:MET:CG	1:Aa:176:ARG:N	2.82	0.42
1:Ad:175:MET:CG	1:Ad:176:ARG:N	2.82	0.42
1:Ae:155:LYS:HA	1:Ae:155:LYS:HD3	1.89	0.42
1:Ah:48:ARG:NH2	1:As:141:GLU:CD	2.76	0.42
1:Ai:48:ARG:NH2	1:At:141:GLU:CD	2.77	0.42
1:Aj:107:GLU:OE2	1:Aj:111:GLU:HG3	2.20	0.42
1:Ao:46:VAL:HB	1:Az:138:ASP:OD1	2.19	0.42
1:Ao:49:LEU:HD13	1:Az:145:TYR:HE1	1.84	0.42
1:Ar:107:GLU:OE2	1:Ar:111:GLU:HG3	2.19	0.42
1:As:200:TYR:CD2	1:As:215:ALA:HB2	2.54	0.42
1:Au:77:PRO:HD2	1:Av:176:ARG:HH12	1.84	0.42
1:Ab:114:LEU:HD23	1:Ab:114:LEU:HA	1.92	0.42
1:Aj:188:LEU:HD23	1:Aj:188:LEU:HA	1.87	0.42
1:As:107:GLU:OE2	1:As:111:GLU:HG3	2.20	0.42
1:At:107:GLU:OE2	1:At:111:GLU:HG3	2.20	0.42
1:At:200:TYR:CD2	1:At:215:ALA:HB2	2.54	0.42
1:Au:200:TYR:CD2	1:Au:215:ALA:HB2	2.54	0.42
1:Ab:107:GLU:OE2	1:Ab:111:GLU:HG3	2.19	0.42
1:Af:183:MET:HE2	1:Af:183:MET:HB2	1.96	0.42
1:Ag:77:PRO:HD2	1:Ah:176:ARG:HH12	1.84	0.42
1:Ah:107:GLU:OE2	1:Ah:111:GLU:HG3	2.19	0.42
1:Ai:77:PRO:HD2	1:Aj:176:ARG:HH12	1.84	0.42
1:Ak:49:LEU:HD13	1:Av:145:TYR:HE1	1.83	0.42
1:Ak:175:MET:CG	1:Ak:176:ARG:N	2.82	0.42
1:Al:107:GLU:OE2	1:Al:111:GLU:HG3	2.19	0.42
1:Am:216:LYS:HE3	1:Am:216:LYS:HB2	1.85	0.42
1:An:46:VAL:HB	1:Ay:138:ASP:OD1	2.20	0.42
1:Ar:200:TYR:CD2	1:Ar:215:ALA:HB2	2.54	0.42
1:Ax:175:MET:CG	1:Ax:176:ARG:N	2.82	0.42
1:Ba:200:TYR:CD2	1:Ba:215:ALA:HB2	2.55	0.42
1:Aa:48:ARG:HH21	1:Al:141:GLU:CD	2.27	0.42
1:Ad:114:LEU:HD23	1:Ad:114:LEU:HA	1.92	0.42
1:Ak:223:LYS:HD3	1:Ak:223:LYS:HA	1.92	0.42
1:An:175:MET:CG	1:An:176:ARG:N	2.82	0.42
1:An:207:ILE:HD13	1:An:207:ILE:HA	1.93	0.42
1:At:155:LYS:HD3	1:At:155:LYS:HA	1.89	0.42
1:Au:175:MET:CG	1:Au:176:ARG:N	2.82	0.42
1:Av:107:GLU:OE2	1:Av:111:GLU:HG3	2.19	0.42
1:Av:183:MET:HE2	1:Av:183:MET:HB2	1.96	0.42
1:Av:216:LYS:HB2	1:Av:216:LYS:HE3	1.85	0.42
1:Ax:107:GLU:OE2	1:Ax:111:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:183:MET:HE2	1:Ay:183:MET:HB2	1.96	0.42
1:Ay:200:TYR:CD2	1:Ay:215:ALA:HB2	2.55	0.42
1:Ba:107:GLU:OE2	1:Ba:111:GLU:HG3	2.19	0.42
1:Aa:216:LYS:HE3	1:Aa:216:LYS:HB2	1.85	0.42
1:Ac:48:ARG:NH2	1:An:141:GLU:CD	2.77	0.42
1:Ac:107:GLU:OE2	1:Ac:111:GLU:HG3	2.19	0.42
1:Ad:200:TYR:CD2	1:Ad:215:ALA:HB2	2.54	0.42
1:Ae:114:LEU:HD23	1:Ae:114:LEU:HA	1.92	0.42
1:Ah:77:PRO:HD2	1:Ai:176:ARG:HH12	1.84	0.42
1:Ai:147:LEU:HD12	1:Ai:147:LEU:HA	1.86	0.42
1:Ai:216:LYS:HE3	1:Ai:216:LYS:HB2	1.85	0.42
1:Ak:82:LEU:HD21	1:Al:137:MET:HG2	2.01	0.42
1:Ak:107:GLU:OE2	1:Ak:111:GLU:HG3	2.20	0.42
1:Am:107:GLU:OE2	1:Am:111:GLU:HG3	2.19	0.42
1:Aq:107:GLU:OE2	1:Aq:111:GLU:HG3	2.19	0.42
1:Ar:216:LYS:HE3	1:Ar:216:LYS:HB2	1.85	0.42
1:Au:188:LEU:HD23	1:Au:188:LEU:HA	1.87	0.42
1:Av:200:TYR:CD2	1:Av:215:ALA:HB2	2.54	0.42
1:Aw:107:GLU:OE2	1:Aw:111:GLU:HG3	2.19	0.42
1:Az:200:TYR:CD2	1:Az:215:ALA:HB2	2.54	0.42
1:Ac:200:TYR:CD2	1:Ac:215:ALA:HB2	2.54	0.42
1:Ad:46:VAL:CG2	1:Ao:138:ASP:OD1	2.67	0.42
1:Ah:110:MET:HE3	1:Ah:110:MET:HB3	1.91	0.42
1:Ah:175:MET:CG	1:Ah:176:ARG:N	2.82	0.42
1:Ai:200:TYR:CD2	1:Ai:215:ALA:HB2	2.54	0.42
1:Aj:200:TYR:CD2	1:Aj:215:ALA:HB2	2.54	0.42
1:Ak:147:LEU:HD12	1:Ak:147:LEU:HA	1.86	0.42
1:Ak:200:TYR:CD2	1:Ak:215:ALA:HB2	2.55	0.42
1:Al:200:TYR:CD2	1:Al:215:ALA:HB2	2.54	0.42
1:An:46:VAL:CG1	1:Ay:136:MET:HE3	2.48	0.42
1:An:59:PRO:HG2	1:Ao:165:PHE:CD1	2.55	0.42
1:Ap:49:LEU:HD13	1:Ba:145:TYR:HE1	1.85	0.42
1:Ap:200:TYR:CD2	1:Ap:215:ALA:HB2	2.54	0.42
1:Aq:200:TYR:CD2	1:Aq:215:ALA:HB2	2.54	0.42
1:Aw:59:PRO:HG2	1:Ax:165:PHE:CD1	2.55	0.42
1:Ay:107:GLU:OE2	1:Ay:111:GLU:HG3	2.19	0.42
1:Ay:188:LEU:HD23	1:Ay:188:LEU:HA	1.87	0.42
1:Az:107:GLU:OE2	1:Az:111:GLU:HG3	2.19	0.42
1:Ba:175:MET:CG	1:Ba:176:ARG:N	2.82	0.42
1:Aa:200:TYR:CD2	1:Aa:215:ALA:HB2	2.54	0.42
1:Ac:183:MET:HE2	1:Ac:183:MET:HB2	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:137:MET:HE3	1:Aj:137:MET:HB3	1.81	0.42
1:Am:200:TYR:CD2	1:Am:215:ALA:HB2	2.54	0.42
1:An:107:GLU:OE2	1:An:111:GLU:HG3	2.19	0.42
1:Az:110:MET:HE3	1:Az:110:MET:HB3	1.91	0.42
1:Ae:59:PRO:HG2	1:Af:165:PHE:CD1	2.55	0.42
1:Ao:107:GLU:OE2	1:Ao:111:GLU:HG3	2.19	0.42
1:Ap:107:GLU:OE2	1:Ap:111:GLU:HG3	2.20	0.42
1:Aq:110:MET:HE3	1:Aq:110:MET:HB3	1.91	0.42
1:Aq:175:MET:CG	1:Aq:176:ARG:N	2.82	0.42
1:Aw:200:TYR:CD2	1:Aw:215:ALA:HB2	2.54	0.42
1:Ay:155:LYS:HA	1:Ay:155:LYS:HD3	1.89	0.42
1:Ad:207:ILE:HD13	1:Ad:207:ILE:HA	1.93	0.42
1:Ag:107:GLU:OE2	1:Ag:111:GLU:HG3	2.20	0.42
1:Ah:200:TYR:CD2	1:Ah:215:ALA:HB2	2.54	0.42
1:Ai:46:VAL:HA	1:Ai:47:PRO:HD3	1.94	0.42
1:Al:46:VAL:HB	1:Aw:138:ASP:OD1	2.19	0.42
1:Ao:84:ASN:HB2	1:Ap:124:ASN:OD1	2.20	0.42
1:Ao:200:TYR:CD2	1:Ao:215:ALA:HB2	2.55	0.42
1:As:223:LYS:HD3	1:As:223:LYS:HA	1.93	0.42
1:Ba:216:LYS:HE3	1:Ba:216:LYS:HB2	1.85	0.42
1:Aa:48:ARG:NH2	1:Al:141:GLU:CD	2.78	0.41
1:Al:155:LYS:HA	1:Al:155:LYS:HD3	1.89	0.41
1:Al:216:LYS:HB2	1:Al:216:LYS:HE3	1.85	0.41
1:Ap:155:LYS:HA	1:Ap:155:LYS:HD3	1.89	0.41
1:Ar:175:MET:CG	1:Ar:176:ARG:N	2.82	0.41
1:As:137:MET:HE3	1:As:137:MET:HB3	1.81	0.41
1:Aw:77:PRO:HD2	1:Ax:176:ARG:HH12	1.85	0.41
1:Ax:200:TYR:CD2	1:Ax:215:ALA:HB2	2.55	0.41
1:Az:77:PRO:HD2	1:Ba:176:ARG:HH12	1.84	0.41
1:Aa:207:ILE:HD13	1:Aa:207:ILE:HA	1.93	0.41
1:Ab:82:LEU:HD21	1:Ac:137:MET:HG2	2.01	0.41
1:Ab:188:LEU:HD23	1:Ab:188:LEU:HA	1.87	0.41
1:Ab:200:TYR:CD2	1:Ab:215:ALA:HB2	2.54	0.41
1:Ad:118:MET:HE1	1:Ad:169:ALA:CB	2.51	0.41
1:Af:107:GLU:OE2	1:Af:111:GLU:HG3	2.19	0.41
1:Ag:175:MET:CG	1:Ag:176:ARG:N	2.82	0.41
1:Ag:200:TYR:CD2	1:Ag:215:ALA:HB2	2.54	0.41
1:Ar:84:ASN:HB2	1:As:124:ASN:OD1	2.20	0.41
1:Au:107:GLU:OE2	1:Au:111:GLU:HG3	2.19	0.41
1:Ae:107:GLU:OE2	1:Ae:111:GLU:HG3	2.19	0.41
1:Af:200:TYR:CD2	1:Af:215:ALA:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:59:PRO:HG2	1:At:165:PHE:CD1	2.55	0.41
1:At:118:MET:HE1	1:At:169:ALA:CB	2.51	0.41
1:Aw:216:LYS:HE3	1:Aw:216:LYS:HB2	1.85	0.41
1:Ay:59:PRO:HG2	1:Az:165:PHE:CD1	2.55	0.41
1:Ay:118:MET:HE1	1:Ay:169:ALA:CB	2.51	0.41
1:Ba:147:LEU:HD12	1:Ba:147:LEU:HA	1.86	0.41
1:Aa:118:MET:HE1	1:Aa:169:ALA:CB	2.51	0.41
1:Ab:46:VAL:HB	1:Am:138:ASP:OD1	2.20	0.41
1:Ab:118:MET:CE	1:Ab:169:ALA:HA	2.51	0.41
1:Ab:216:LYS:HE3	1:Ab:216:LYS:HB2	1.85	0.41
1:Ag:59:PRO:HG2	1:Ah:165:PHE:CD1	2.55	0.41
1:Ai:118:MET:HE1	1:Ai:169:ALA:CB	2.51	0.41
1:Aj:46:VAL:HB	1:Au:138:ASP:OD1	2.20	0.41
1:Aj:207:ILE:HD13	1:Aj:207:ILE:HA	1.93	0.41
1:Ak:118:MET:CE	1:Ak:169:ALA:HA	2.50	0.41
1:An:155:LYS:HA	1:An:155:LYS:HD3	1.89	0.41
1:An:200:TYR:CD2	1:An:215:ALA:HB2	2.54	0.41
1:Ap:183:MET:HE2	1:Ap:183:MET:HB2	1.96	0.41
1:Ad:59:PRO:HG2	1:Ae:165:PHE:CD1	2.55	0.41
1:Ae:200:TYR:CD2	1:Ae:215:ALA:HB2	2.54	0.41
1:Ah:82:LEU:HD21	1:Ai:137:MET:HG2	2.02	0.41
1:Aj:77:PRO:HD2	1:Ak:176:ARG:HH12	1.85	0.41
1:Aj:114:LEU:HD23	1:Aj:114:LEU:HA	1.92	0.41
1:Ak:155:LYS:HA	1:Ak:155:LYS:HD3	1.89	0.41
1:Ak:170:GLU:OE2	1:Ak:205:TYR:OH	2.27	0.41
1:Al:118:MET:HE1	1:Al:169:ALA:CB	2.51	0.41
1:An:118:MET:HE1	1:An:169:ALA:CB	2.51	0.41
1:An:118:MET:CE	1:An:169:ALA:HA	2.51	0.41
1:Ao:118:MET:HE1	1:Ao:169:ALA:CB	2.51	0.41
1:Ar:155:LYS:HD3	1:Ar:155:LYS:HA	1.89	0.41
1:As:77:PRO:HD2	1:At:176:ARG:HH12	1.85	0.41
1:As:114:LEU:HD23	1:As:114:LEU:HA	1.92	0.41
1:At:118:MET:CE	1:At:169:ALA:HA	2.50	0.41
1:Av:59:PRO:HG2	1:Aw:165:PHE:CD1	2.55	0.41
1:Av:77:PRO:HD2	1:Aw:176:ARG:HH12	1.85	0.41
1:Aw:82:LEU:HD21	1:Ax:137:MET:HG2	2.02	0.41
1:Aw:192:LEU:HD12	1:Aw:192:LEU:HA	1.93	0.41
1:Ax:118:MET:HE1	1:Ax:169:ALA:CB	2.51	0.41
1:Ac:46:VAL:HA	1:Ac:47:PRO:HD3	1.94	0.41
1:Ac:155:LYS:HA	1:Ac:155:LYS:HD3	1.89	0.41
1:Ac:216:LYS:HB2	1:Ac:216:LYS:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:107:GLU:OE2	1:Ad:111:GLU:HG3	2.19	0.41
1:Ag:118:MET:CE	1:Ag:169:ALA:HA	2.50	0.41
1:Ah:118:MET:HE1	1:Ah:169:ALA:CB	2.51	0.41
1:Aj:155:LYS:HA	1:Aj:155:LYS:HD3	1.89	0.41
1:Al:183:MET:HE2	1:Al:183:MET:HB2	1.96	0.41
1:An:188:LEU:HD23	1:An:188:LEU:HA	1.87	0.41
1:Ap:59:PRO:HG2	1:Aq:165:PHE:CD1	2.55	0.41
1:Ar:188:LEU:HA	1:Ar:188:LEU:HD23	1.87	0.41
1:As:82:LEU:HD21	1:At:137:MET:HG2	2.02	0.41
1:Aw:118:MET:CE	1:Aw:169:ALA:HA	2.51	0.41
1:Aa:114:LEU:HD23	1:Aa:114:LEU:HA	1.92	0.41
1:Ae:118:MET:HE1	1:Ae:169:ALA:CB	2.51	0.41
1:Af:118:MET:CE	1:Af:169:ALA:HA	2.51	0.41
1:Aj:59:PRO:HG2	1:Ak:165:PHE:CD1	2.55	0.41
1:Ak:192:LEU:HD12	1:Ak:192:LEU:HA	1.93	0.41
1:Am:46:VAL:HB	1:Ax:138:ASP:OD1	2.21	0.41
1:An:82:LEU:HD21	1:Ao:137:MET:HG2	2.02	0.41
1:Ap:46:VAL:HB	1:Ba:138:ASP:OD1	2.20	0.41
1:Aq:46:VAL:HA	1:Aq:47:PRO:HD3	1.94	0.41
1:Aq:118:MET:HE1	1:Aq:169:ALA:CB	2.51	0.41
1:Ar:82:LEU:HD21	1:As:137:MET:HG2	2.02	0.41
1:At:216:LYS:HB2	1:At:216:LYS:HE3	1.85	0.41
1:Az:118:MET:HE1	1:Az:169:ALA:CB	2.51	0.41
1:Aa:59:PRO:HG2	1:Ab:165:PHE:CD1	2.55	0.41
1:Aa:77:PRO:HD2	1:Ab:176:ARG:HH12	1.85	0.41
1:Ab:46:VAL:CG1	1:Am:136:MET:HE3	2.50	0.41
1:Ab:118:MET:HE1	1:Ab:169:ALA:CB	2.51	0.41
1:Ac:118:MET:HE1	1:Ac:169:ALA:CB	2.51	0.41
1:Ae:49:LEU:HD13	1:Ap:145:TYR:HE1	1.84	0.41
1:Ag:114:LEU:HD23	1:Ag:114:LEU:HA	1.92	0.41
1:Ai:46:VAL:HB	1:At:138:ASP:OD1	2.21	0.41
1:Ai:155:LYS:HA	1:Ai:155:LYS:HD3	1.89	0.41
1:Aj:118:MET:HE1	1:Aj:169:ALA:CB	2.51	0.41
1:Aj:216:LYS:HB2	1:Aj:216:LYS:HE3	1.85	0.41
1:Am:82:LEU:HD21	1:An:137:MET:HG2	2.02	0.41
1:Ao:118:MET:CE	1:Ao:169:ALA:HA	2.50	0.41
1:Ab:59:PRO:HG2	1:Ac:165:PHE:CD1	2.56	0.41
1:Ac:59:PRO:HG2	1:Ad:165:PHE:CD1	2.55	0.41
1:Ad:81:ASP:HB3	1:Ae:137:MET:SD	2.61	0.41
1:Ae:77:PRO:HD2	1:Af:176:ARG:HH12	1.85	0.41
1:Ae:82:LEU:HD21	1:Af:137:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Af:46:VAL:CG1	1:Aq:136:MET:HE3	2.48	0.41
1:Af:84:ASN:HB2	1:Ag:124:ASN:OD1	2.21	0.41
1:Ag:84:ASN:HB2	1:Ah:124:ASN:OD1	2.21	0.41
1:Ah:118:MET:CE	1:Ah:169:ALA:HA	2.51	0.41
1:Ah:155:LYS:HA	1:Ah:155:LYS:HD3	1.89	0.41
1:Ah:188:LEU:HA	1:Ah:188:LEU:HD23	1.87	0.41
1:Aj:82:LEU:HD21	1:Ak:137:MET:HG2	2.02	0.41
1:Am:59:PRO:HG2	1:An:165:PHE:CD1	2.55	0.41
1:Am:118:MET:HE1	1:Am:169:ALA:CB	2.51	0.41
1:Ao:155:LYS:HD3	1:Ao:155:LYS:HA	1.89	0.41
1:Ap:118:MET:HE1	1:Ap:169:ALA:CB	2.51	0.41
1:Ar:77:PRO:HD2	1:As:176:ARG:HH12	1.86	0.41
1:Ar:118:MET:HE1	1:Ar:169:ALA:CB	2.51	0.41
1:At:59:PRO:HG2	1:Au:165:PHE:CD1	2.56	0.41
1:At:81:ASP:HB3	1:Au:137:MET:SD	2.61	0.41
1:Au:118:MET:HE1	1:Au:169:ALA:CB	2.51	0.41
1:Av:82:LEU:HD21	1:Aw:137:MET:HG2	2.02	0.41
1:Aw:114:LEU:HD23	1:Aw:114:LEU:HA	1.92	0.41
1:Aw:118:MET:HE1	1:Aw:169:ALA:CB	2.51	0.41
1:Ac:46:VAL:HB	1:An:138:ASP:OD1	2.20	0.41
1:Ak:81:ASP:HB3	1:Al:137:MET:SD	2.61	0.41
1:Ak:118:MET:HE1	1:Ak:169:ALA:CB	2.51	0.41
1:Al:46:VAL:CG1	1:Aw:136:MET:HE3	2.50	0.41
1:Aq:82:LEU:HD21	1:Ar:137:MET:HG2	2.02	0.41
1:At:77:PRO:HD2	1:Au:176:ARG:HH12	1.86	0.41
1:Aw:155:LYS:HA	1:Aw:155:LYS:HD3	1.89	0.41
1:Aw:223:LYS:HD3	1:Aw:223:LYS:HA	1.92	0.41
1:Ac:46:VAL:CG1	1:An:136:MET:HE3	2.51	0.40
1:Af:118:MET:HE1	1:Af:169:ALA:CB	2.51	0.40
1:Ag:49:LEU:HD13	1:Ar:145:TYR:HE1	1.83	0.40
1:Ak:77:PRO:HD2	1:Al:176:ARG:HH12	1.86	0.40
1:Ar:81:ASP:HB3	1:As:137:MET:SD	2.61	0.40
1:As:118:MET:HE1	1:As:169:ALA:CB	2.51	0.40
1:As:207:ILE:HD13	1:As:207:ILE:HA	1.93	0.40
1:Au:59:PRO:HG2	1:Av:165:PHE:CD1	2.56	0.40
1:Aw:150:MET:C	1:Aw:151:LEU:HD12	2.46	0.40
1:Ax:223:LYS:HD3	1:Ax:223:LYS:HA	1.93	0.40
1:Az:147:LEU:HD12	1:Az:147:LEU:HA	1.86	0.40
1:Ba:118:MET:HE1	1:Ba:169:ALA:CB	2.51	0.40
1:Ad:84:ASN:HB2	1:Ae:124:ASN:OD1	2.21	0.40
1:Ag:118:MET:HE1	1:Ag:169:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ah:59:PRO:HG2	1:Ai:165:PHE:CE1	2.57	0.40
1:Ah:147:LEU:HD12	1:Ah:147:LEU:HA	1.86	0.40
1:Ak:59:PRO:HG2	1:Al:165:PHE:CD1	2.56	0.40
1:Am:77:PRO:HD2	1:An:176:ARG:HH12	1.85	0.40
1:Ap:46:VAL:CG1	1:Ba:136:MET:HE3	2.50	0.40
1:Av:46:VAL:HA	1:Av:47:PRO:HD3	1.94	0.40
1:Av:118:MET:HE1	1:Av:169:ALA:CB	2.51	0.40
1:Aa:110:MET:HE3	1:Aa:110:MET:HB3	1.91	0.40
1:Ac:49:LEU:HD13	1:An:145:TYR:HE1	1.86	0.40
1:Ag:82:LEU:HD21	1:Ah:137:MET:HG2	2.03	0.40
1:Ah:46:VAL:HB	1:As:138:ASP:OD1	2.22	0.40
1:Ai:150:MET:C	1:Ai:151:LEU:HD12	2.46	0.40
1:Ap:84:ASN:HB2	1:Aq:124:ASN:OD1	2.21	0.40
1:Ap:118:MET:CE	1:Ap:169:ALA:HA	2.50	0.40
1:Ax:118:MET:CE	1:Ax:169:ALA:HA	2.50	0.40
1:Ax:150:MET:C	1:Ax:151:LEU:HD12	2.46	0.40
1:Ac:118:MET:CE	1:Ac:169:ALA:HA	2.51	0.40
1:Ae:207:ILE:HD13	1:Ae:207:ILE:HA	1.93	0.40
1:Af:46:VAL:HB	1:Aq:138:ASP:OD1	2.22	0.40
1:Ag:155:LYS:HA	1:Ag:155:LYS:HD3	1.89	0.40
1:Ag:183:MET:HE2	1:Ag:183:MET:HB2	1.96	0.40
1:Ai:110:MET:HE3	1:Ai:110:MET:HB3	1.91	0.40
1:Al:49:LEU:HD13	1:Aw:145:TYR:HE1	1.84	0.40
1:Al:59:PRO:HG2	1:Am:165:PHE:CD1	2.56	0.40
1:Am:147:LEU:HD12	1:Am:147:LEU:HA	1.86	0.40
1:An:150:MET:C	1:An:151:LEU:HD12	2.46	0.40
1:Ao:207:ILE:HD13	1:Ao:207:ILE:HA	1.93	0.40
1:Ay:207:ILE:HD13	1:Ay:207:ILE:HA	1.93	0.40
1:Az:150:MET:C	1:Az:151:LEU:HD12	2.46	0.40
1:Aa:72:LEU:HB2	1:Ab:115:ASN:OD1	2.22	0.40
1:Aa:150:MET:C	1:Aa:151:LEU:HD12	2.46	0.40
1:Ac:150:MET:C	1:Ac:151:LEU:HD12	2.46	0.40
1:Ad:48:ARG:NH2	1:Ao:141:GLU:OE1	2.54	0.40
1:Ad:150:MET:C	1:Ad:151:LEU:HD12	2.46	0.40
1:Ak:84:ASN:HB2	1:Al:124:ASN:OD1	2.22	0.40
1:Aq:59:PRO:HG2	1:Ar:165:PHE:CE1	2.57	0.40
1:As:185:ARG:NH1	1:As:189:GLN:OE1	2.55	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	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ab	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ac	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ad	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ae	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Af	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ag	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ah	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ai	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Aj	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ak	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Al	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Am	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	An	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ao	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ap	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Aq	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ar	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	As	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	At	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Au	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Av	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Aw	183/269 (68%)	174 (95%)	9 (5%)	0	100	100
1	Ax	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ay	183/269 (68%)	175 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Az	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
1	Ba	183/269 (68%)	175 (96%)	8 (4%)	0	100	100
All	All	4941/7263 (68%)	4724 (96%)	217 (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	163/232 (70%)	163 (100%)	0	100	100
1	Ab	163/232 (70%)	163 (100%)	0	100	100
1	Ac	163/232 (70%)	163 (100%)	0	100	100
1	Ad	163/232 (70%)	163 (100%)	0	100	100
1	Ae	163/232 (70%)	163 (100%)	0	100	100
1	Af	163/232 (70%)	163 (100%)	0	100	100
1	Ag	163/232 (70%)	163 (100%)	0	100	100
1	Ah	163/232 (70%)	163 (100%)	0	100	100
1	Ai	163/232 (70%)	163 (100%)	0	100	100
1	Aj	163/232 (70%)	163 (100%)	0	100	100
1	Ak	163/232 (70%)	163 (100%)	0	100	100
1	Al	163/232 (70%)	163 (100%)	0	100	100
1	Am	163/232 (70%)	163 (100%)	0	100	100
1	An	163/232 (70%)	163 (100%)	0	100	100
1	Ao	163/232 (70%)	163 (100%)	0	100	100
1	Ap	163/232 (70%)	163 (100%)	0	100	100
1	Aq	163/232 (70%)	163 (100%)	0	100	100
1	Ar	163/232 (70%)	163 (100%)	0	100	100
1	As	163/232 (70%)	163 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	At	163/232 (70%)	163 (100%)	0	100	100
1	Au	163/232 (70%)	163 (100%)	0	100	100
1	Av	163/232 (70%)	163 (100%)	0	100	100
1	Aw	163/232 (70%)	163 (100%)	0	100	100
1	Ax	163/232 (70%)	163 (100%)	0	100	100
1	Ay	163/232 (70%)	163 (100%)	0	100	100
1	Az	163/232 (70%)	163 (100%)	0	100	100
1	Ba	163/232 (70%)	163 (100%)	0	100	100
All	All	4401/6264 (70%)	4401 (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. There are no such sidechains identified.

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 ⓘ

There are no chain breaks in this entry.

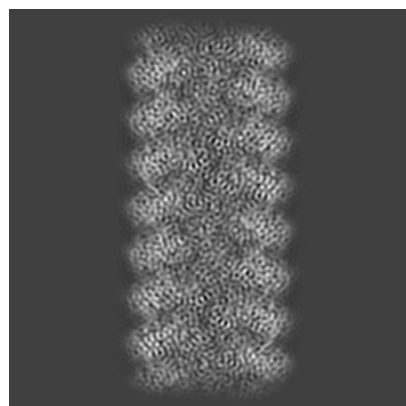
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53799. These allow visual inspection of the internal detail of the map and identification of artifacts.

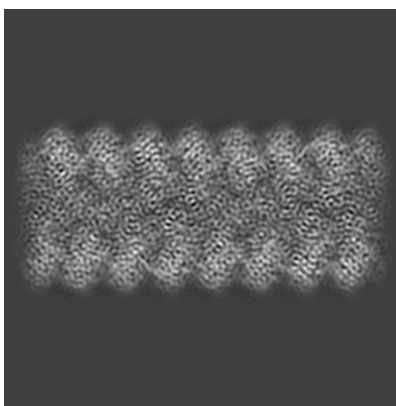
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

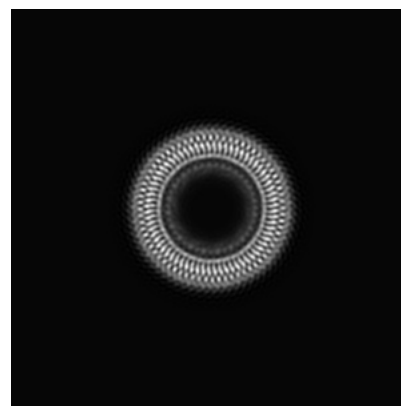
6.1.1 Primary map



X

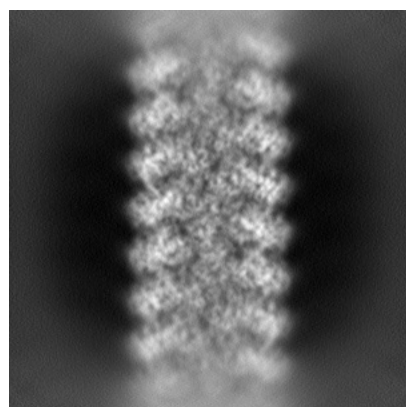


Y

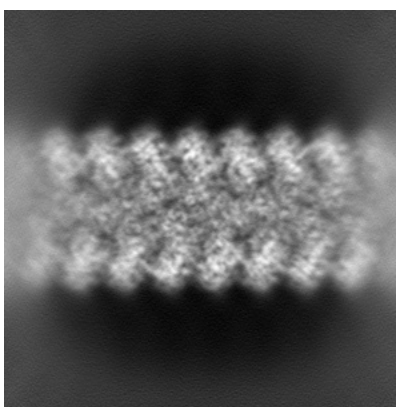


Z

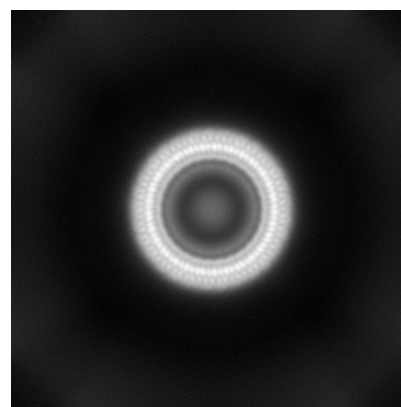
6.1.2 Raw map



X



Y

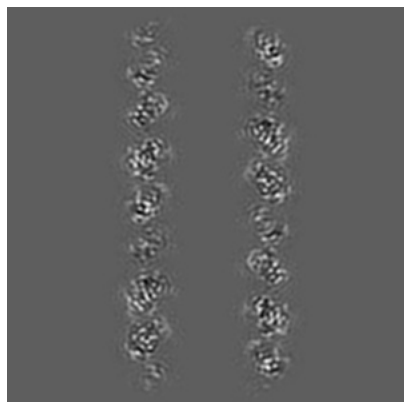


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 175

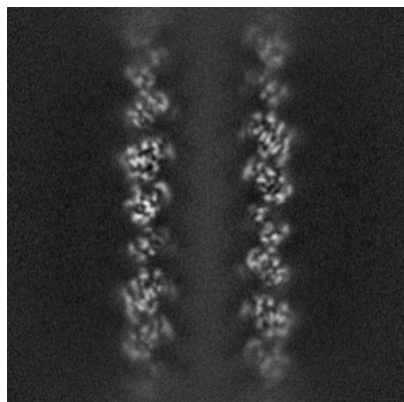


Y Index: 175

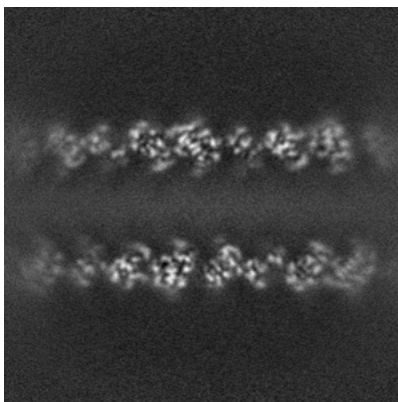


Z Index: 175

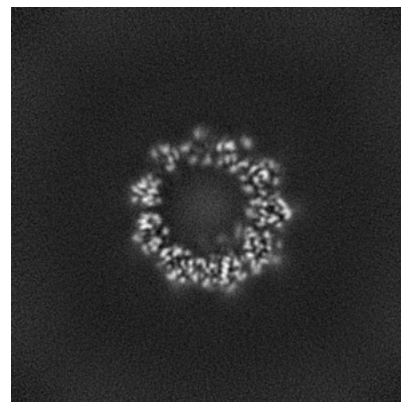
6.2.2 Raw map



X Index: 175



Y Index: 175

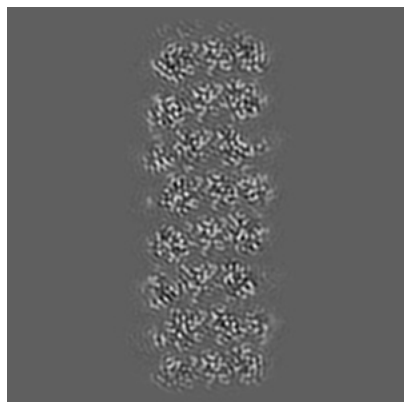


Z Index: 175

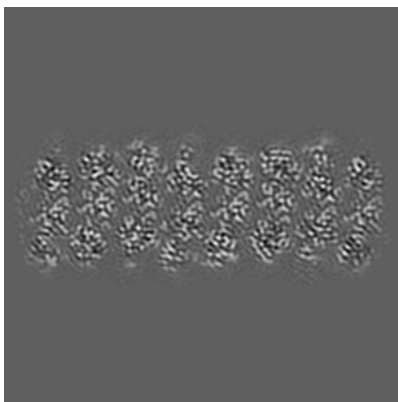
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 129

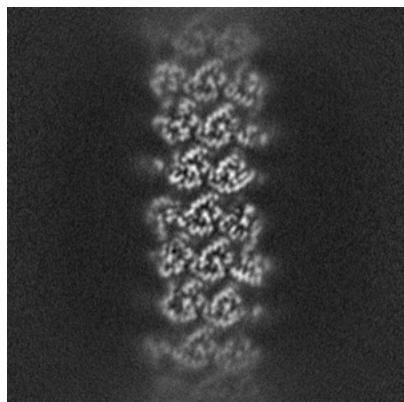


Y Index: 221

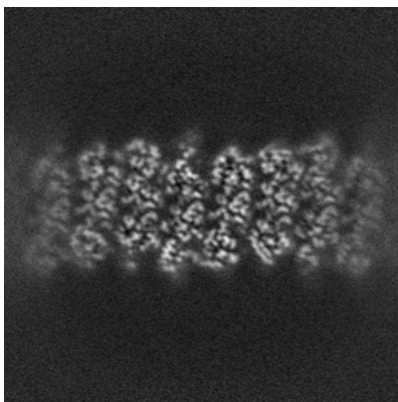


Z Index: 111

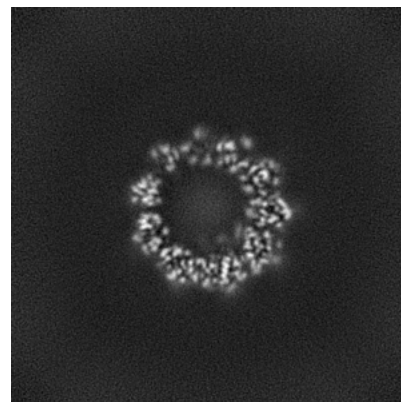
6.3.2 Raw map



X Index: 228



Y Index: 221

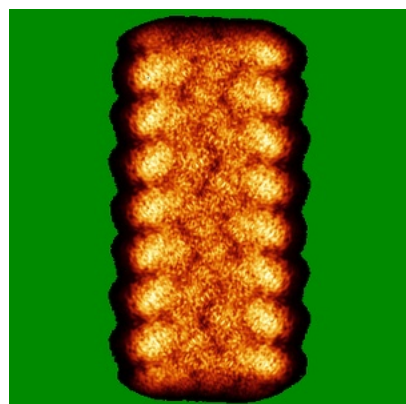


Z Index: 175

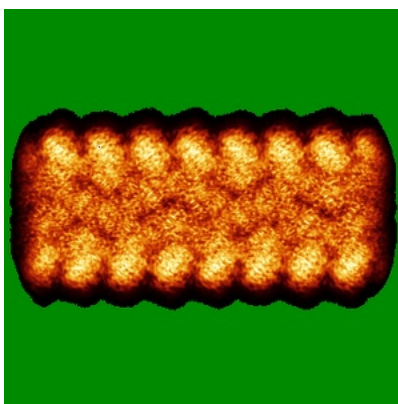
The images above show the largest variance slices of the map in three orthogonal directions.

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

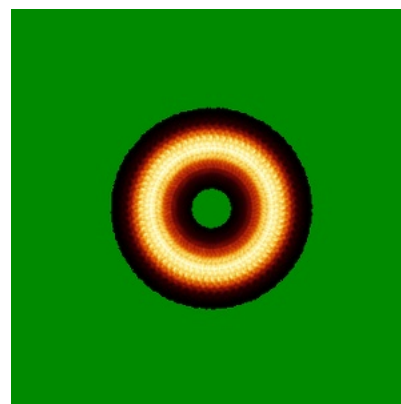
6.4.1 Primary map



X

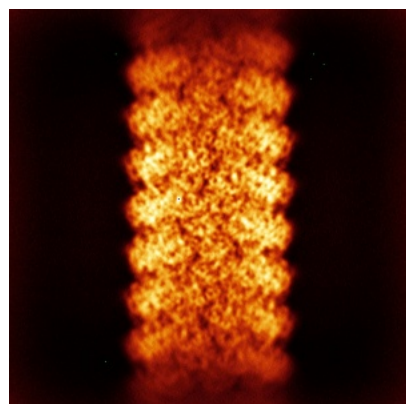


Y

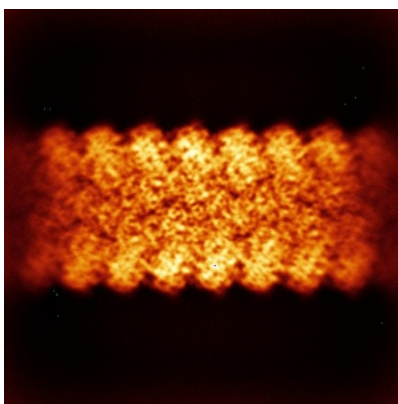


Z

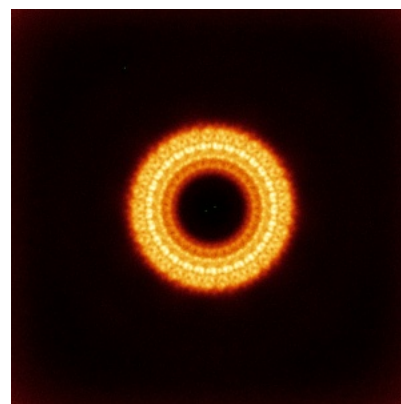
6.4.2 Raw map



X



Y

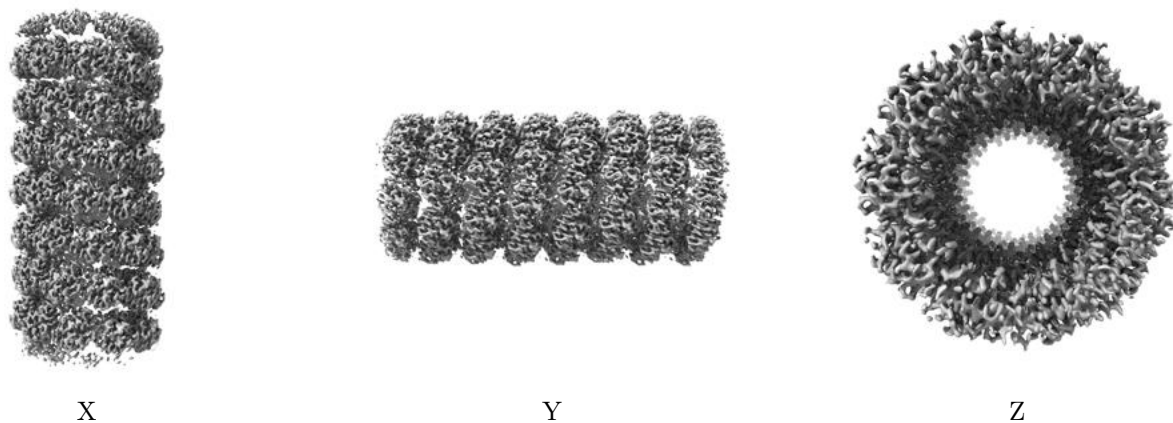


Z

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.

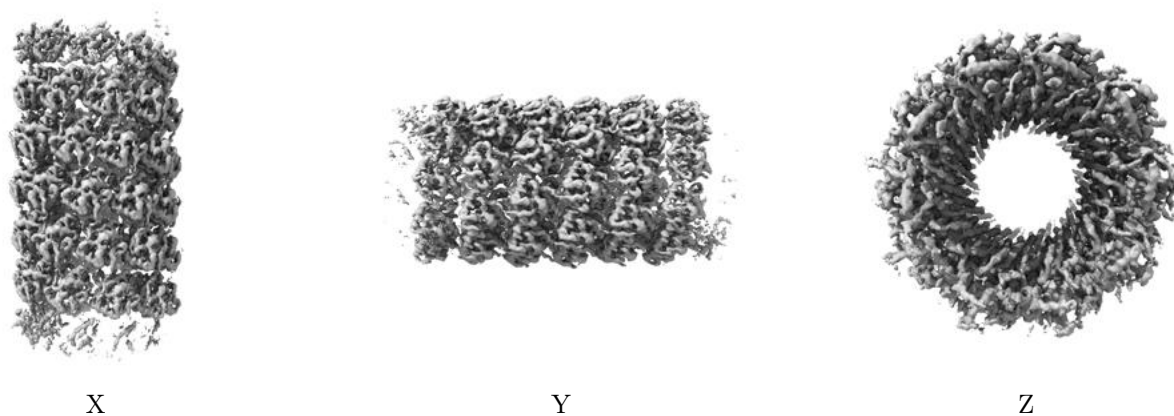
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.19. 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.

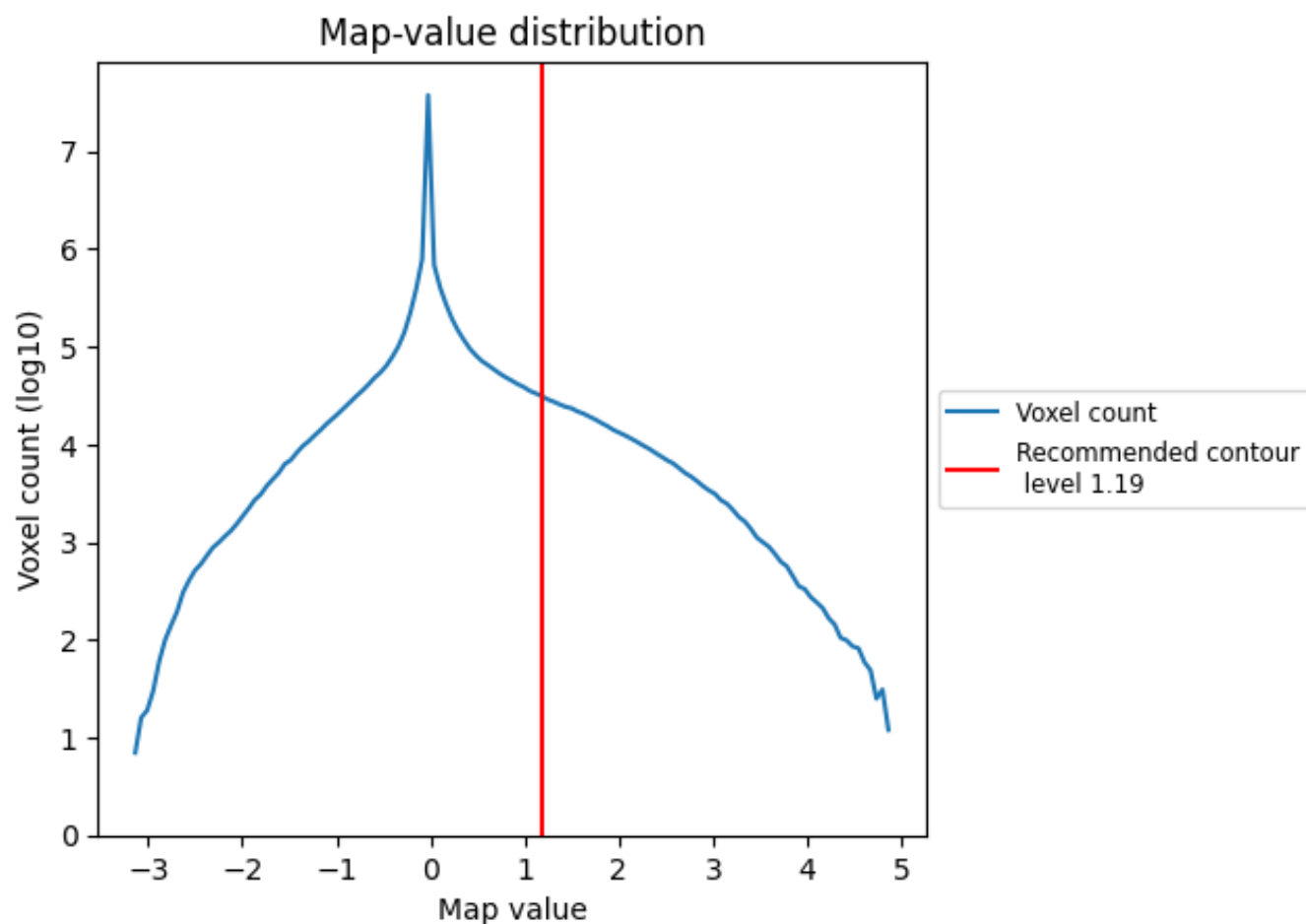
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

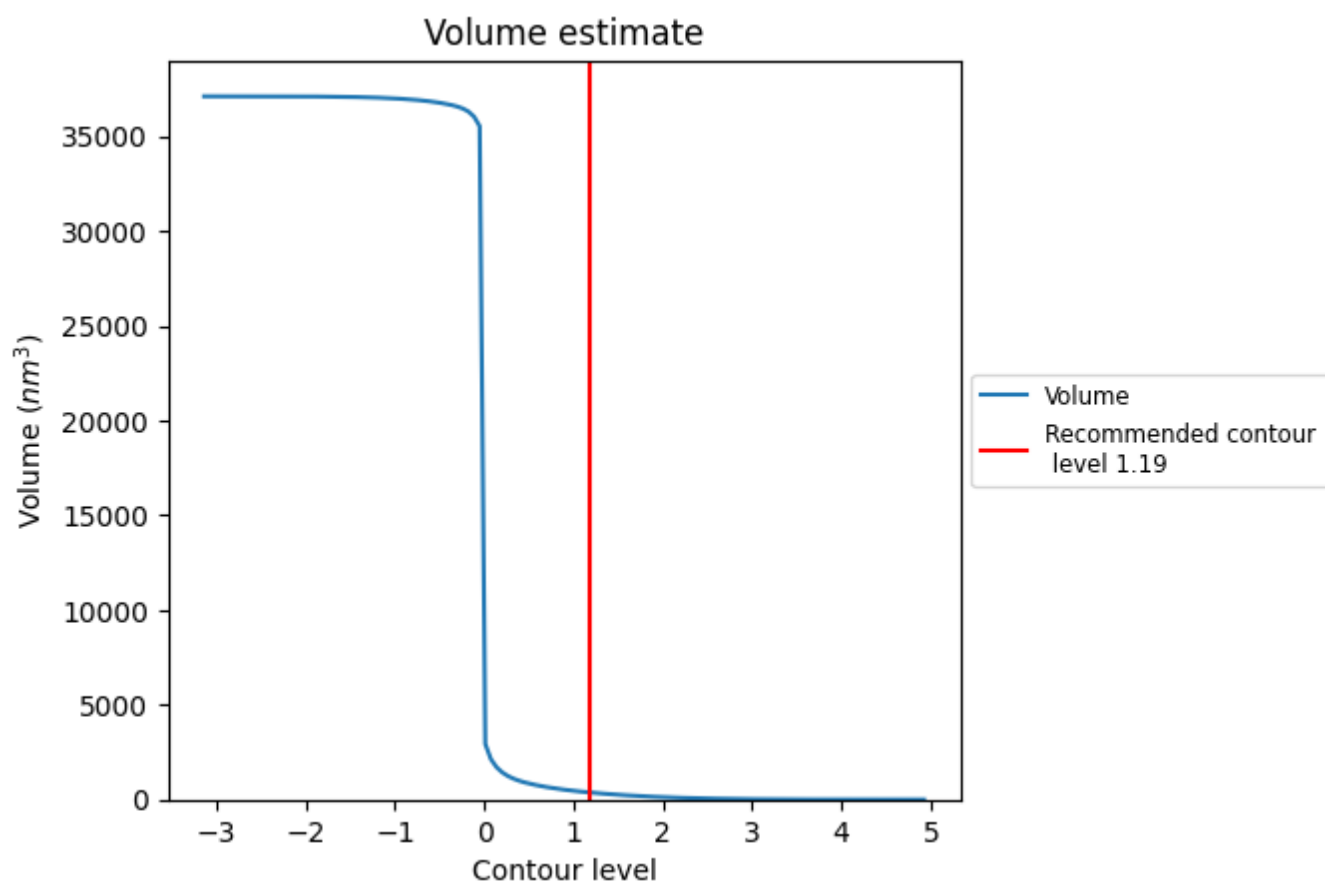
This section contains the results of statistical analysis of the map.

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.

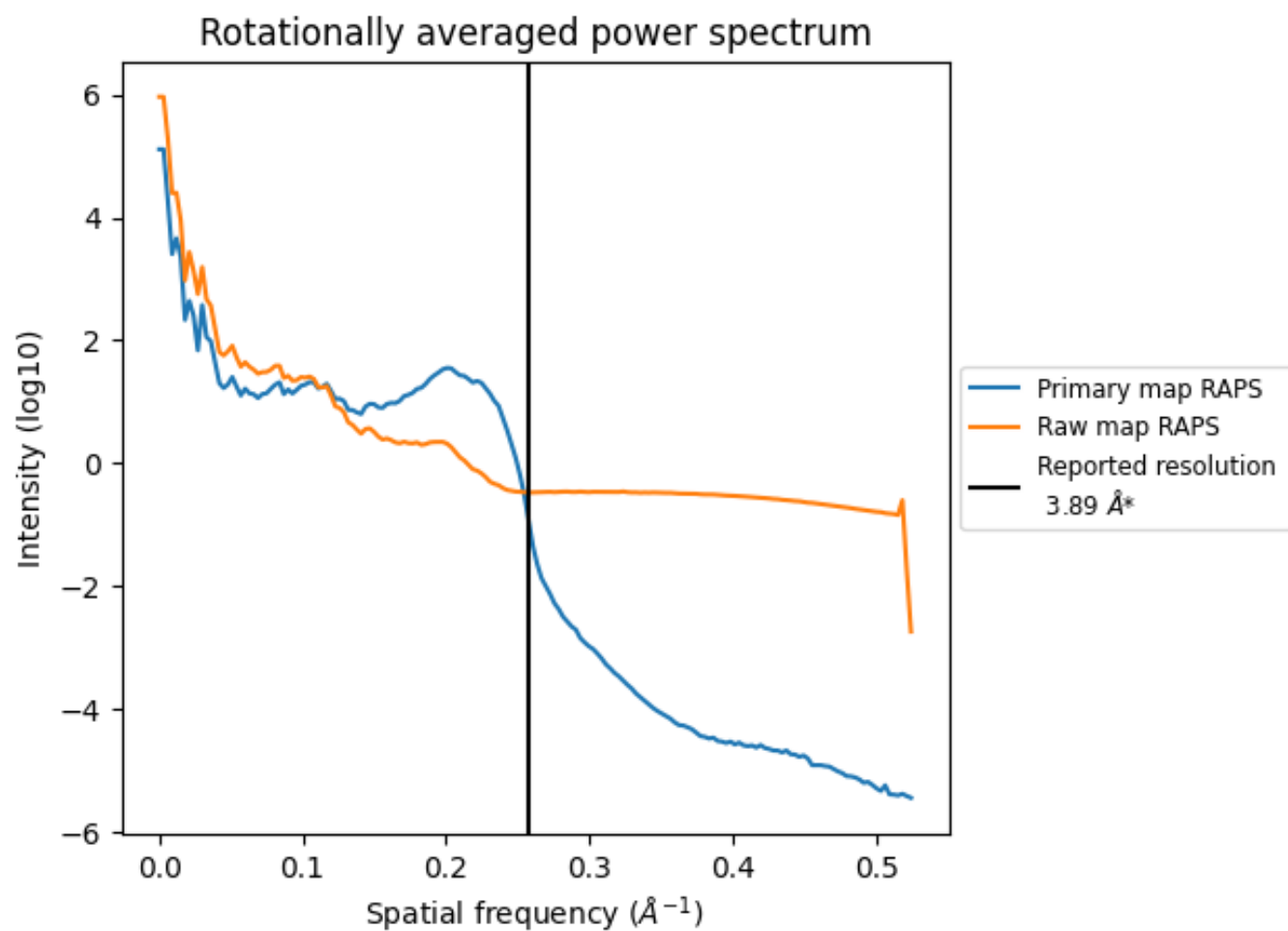
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm³; this corresponds to an approximate mass of 334 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 ⓘ

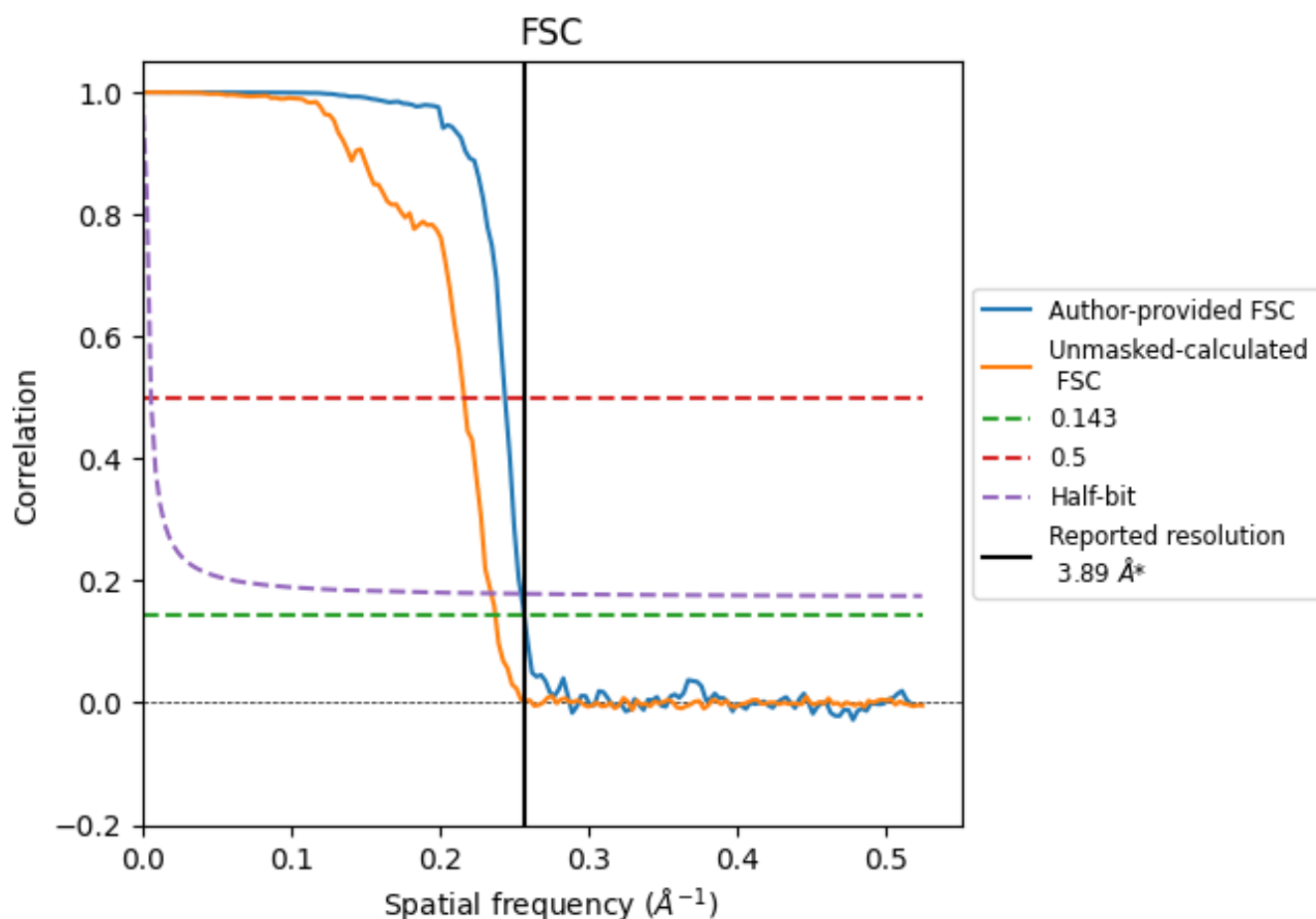


*Reported resolution corresponds to spatial frequency of 0.257 $\text{\AA}^{-1}$

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 $0.257 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

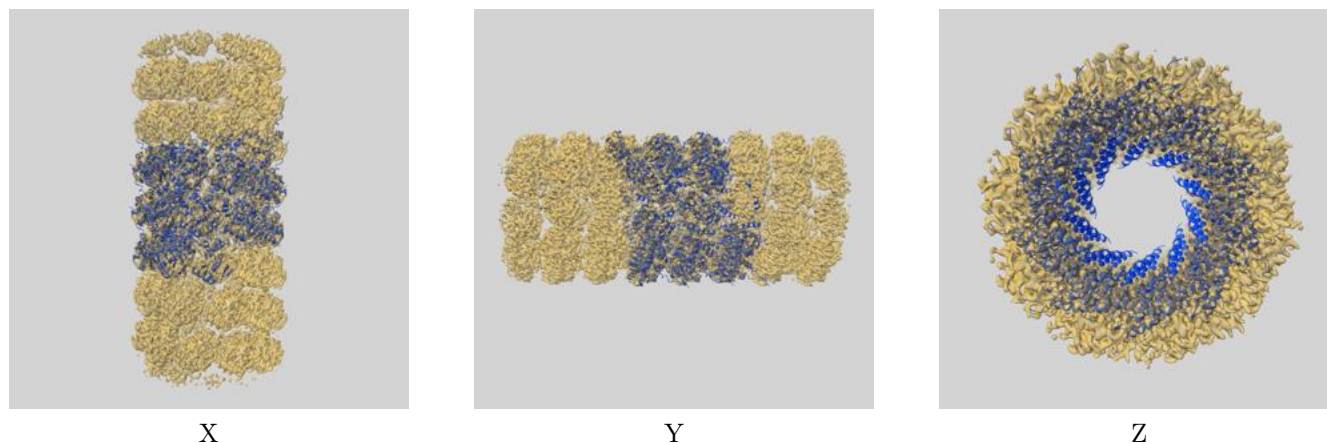
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.89	-	-
Author-provided FSC curve	3.89	4.10	3.92
Unmasked-calculated*	4.21	4.62	4.26

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

9 Map-model fit [i](#)

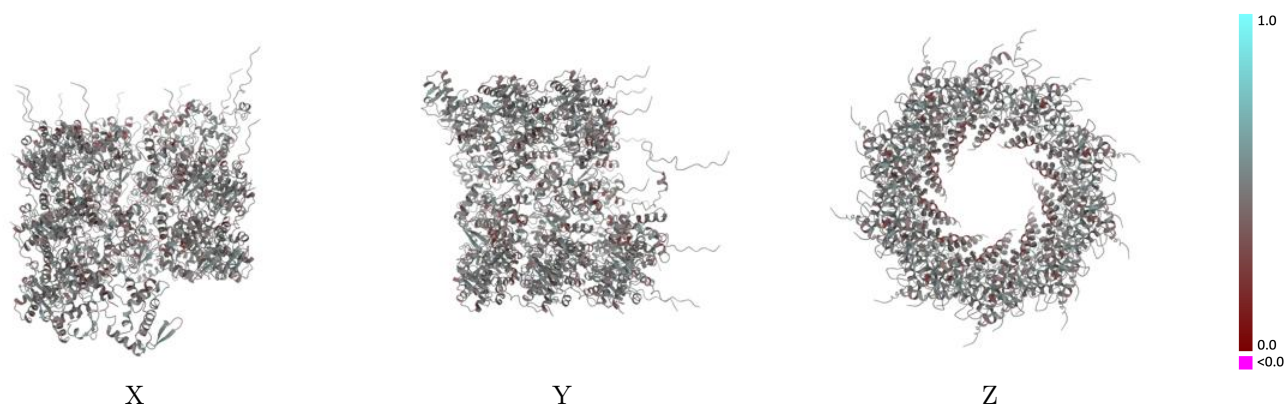
This section contains information regarding the fit between EMDB map EMD-53799 and PDB model 9R7Y. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



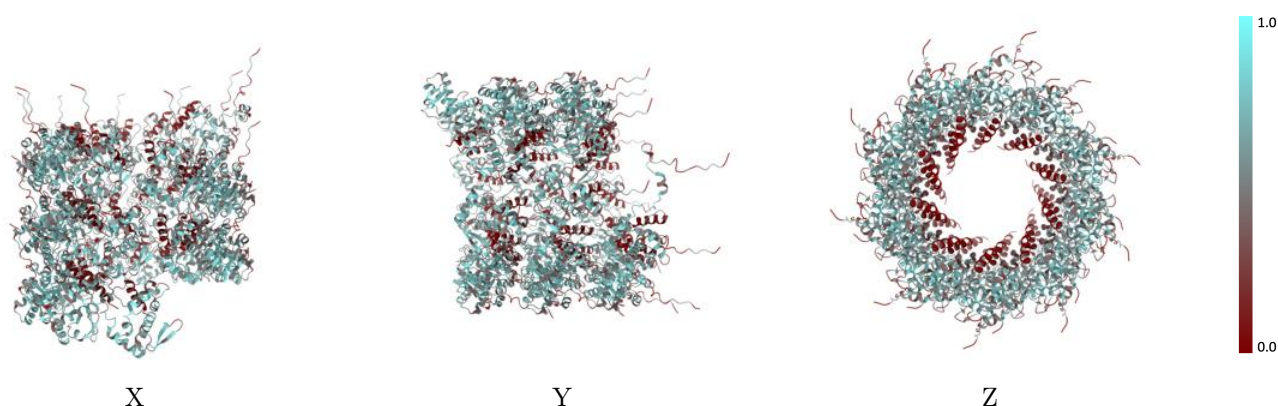
The images above show the 3D surface view of the map at the recommended contour level 1.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



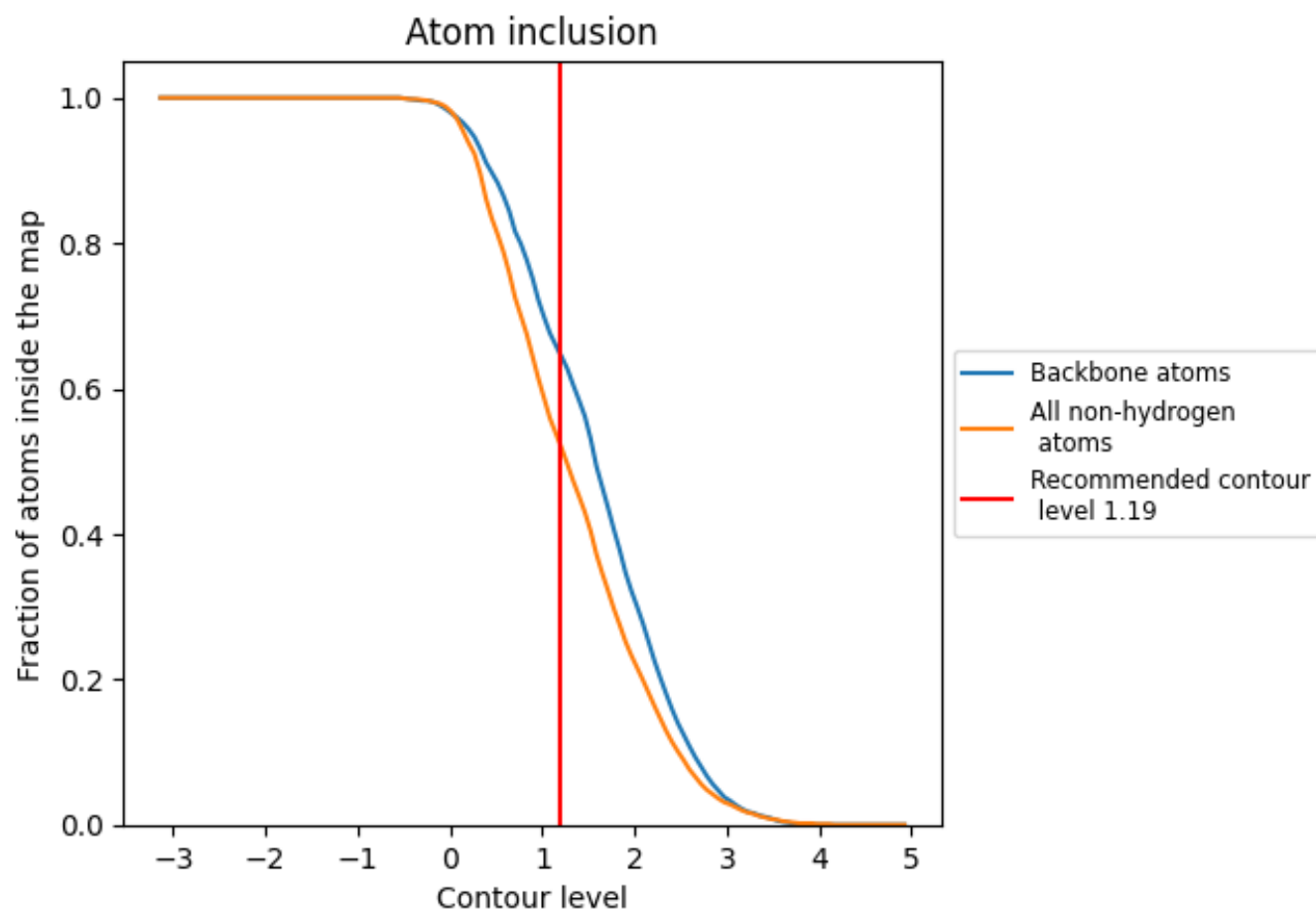
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.19).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5240	 0.4650
Aa	 0.5230	 0.4640
Ab	 0.5210	 0.4640
Ac	 0.5250	 0.4640
Ad	 0.5240	 0.4640
Ae	 0.5260	 0.4640
Af	 0.5210	 0.4640
Ag	 0.5210	 0.4650
Ah	 0.5210	 0.4640
Ai	 0.5210	 0.4660
Aj	 0.5240	 0.4640
Ak	 0.5210	 0.4650
Al	 0.5230	 0.4640
Am	 0.5250	 0.4630
An	 0.5220	 0.4650
Ao	 0.5280	 0.4660
Ap	 0.5240	 0.4650
Aq	 0.5210	 0.4650
Ar	 0.5260	 0.4650
As	 0.5260	 0.4650
At	 0.5240	 0.4640
Au	 0.5270	 0.4660
Av	 0.5260	 0.4640
Aw	 0.5270	 0.4630
Ax	 0.5240	 0.4640
Ay	 0.5250	 0.4640
Az	 0.5260	 0.4660
Ba	 0.5240	 0.4650

