



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:24 AM UTC

PDB ID : 9R80 / pdb_00009r80
EMDB ID : EMD-53801
Title : RNA-free stacked-ring (r10) 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 : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

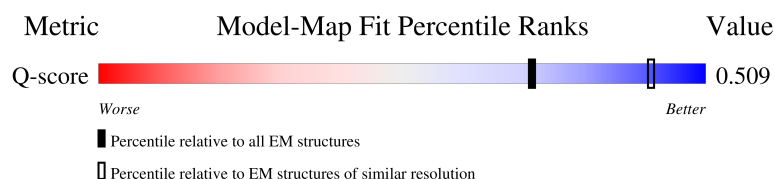
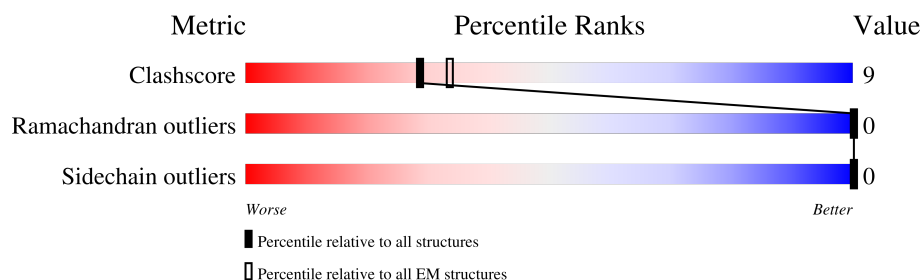
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	269	
1	Ab	269	
1	Ac	269	
1	Ad	269	

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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	
1	Bb	269	
1	Bc	269	

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Mol	Chain	Length	Quality of chain
1	Bd	269	17% 55% 14% 31%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 45120 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	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ab	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ac	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ad	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ae	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Af	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ag	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ah	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ai	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Aj	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ak	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Al	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Am	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	An	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ao	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ap	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Aq	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ar	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	As	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	At	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Au	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Av	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Aw	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ax	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ay	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Az	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Ba	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Bb	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Bc	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		
1	Bd	186	Total	C	N	O	S	0	0
			1504	952	260	279	13		

There are 180 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
An	180	GLU	LYS	engineered mutation	UNP O11986
An	210	ARG	THR	engineered mutation	UNP O11986
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
As	144	GLU	SER	engineered mutation	UNP O11986
As	163	ALA	ARG	engineered mutation	UNP O11986
As	180	GLU	LYS	engineered mutation	UNP O11986
As	210	ARG	THR	engineered mutation	UNP O11986
At	89	GLN	HIS	engineered mutation	UNP O11986
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

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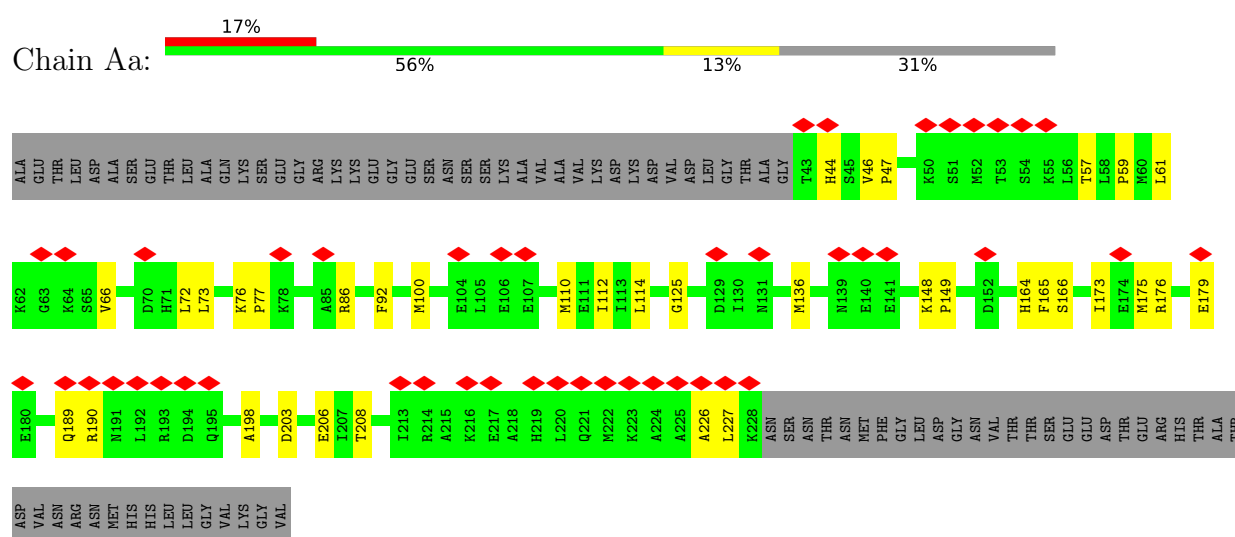
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Chain	Residue	Modelled	Actual	Comment	Reference
Ax	90	SER	GLU	engineered mutation	UNP O11986
Ax	144	GLU	SER	engineered mutation	UNP O11986
Ax	163	ALA	ARG	engineered mutation	UNP O11986
Ax	180	GLU	LYS	engineered mutation	UNP O11986
Ax	210	ARG	THR	engineered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

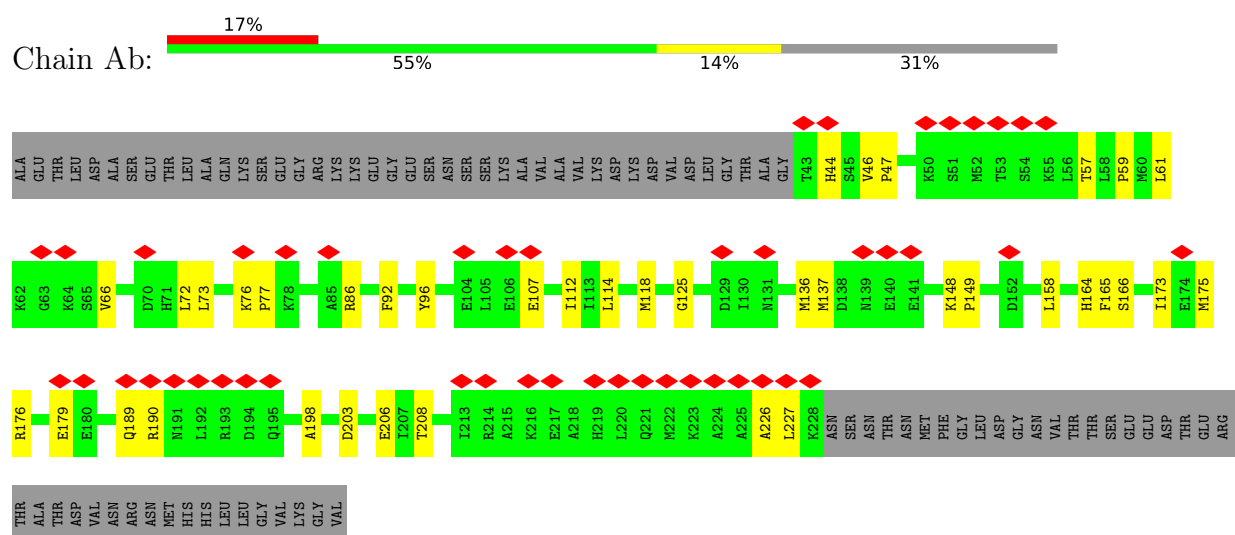
3 Residue-property plots [i](#)

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

• Molecule 1: Genome polyprotein

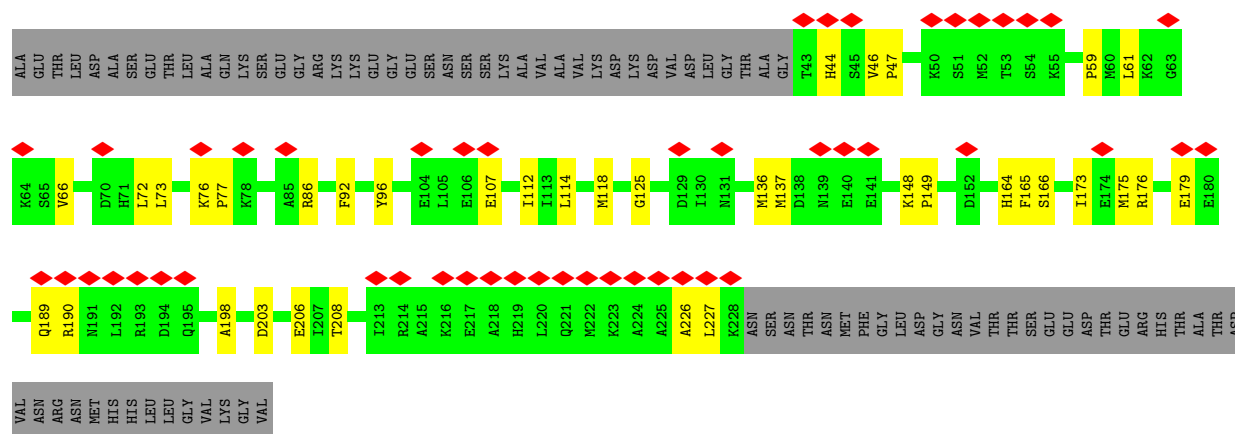


• Molecule 1: Genome polyprotein

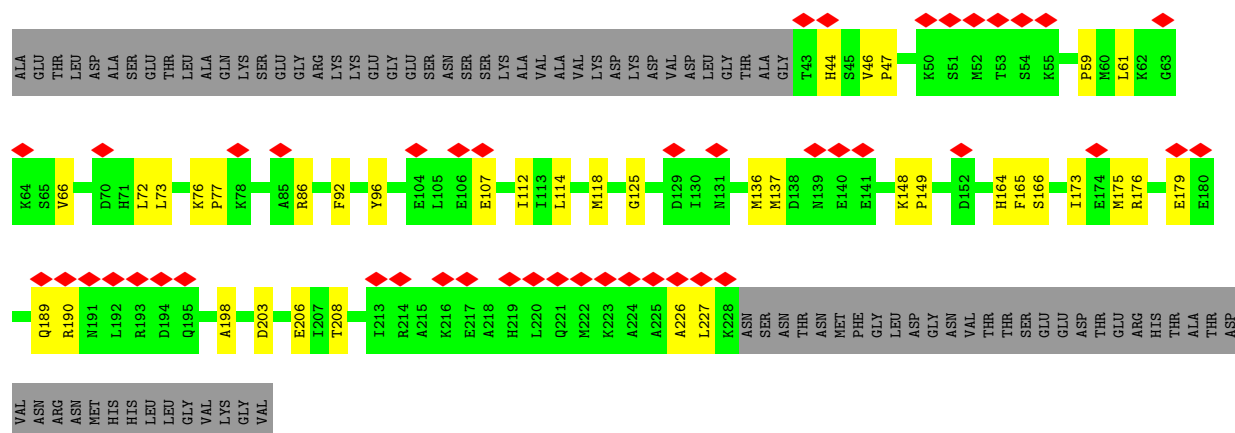


• Molecule 1: Genome polyprotein

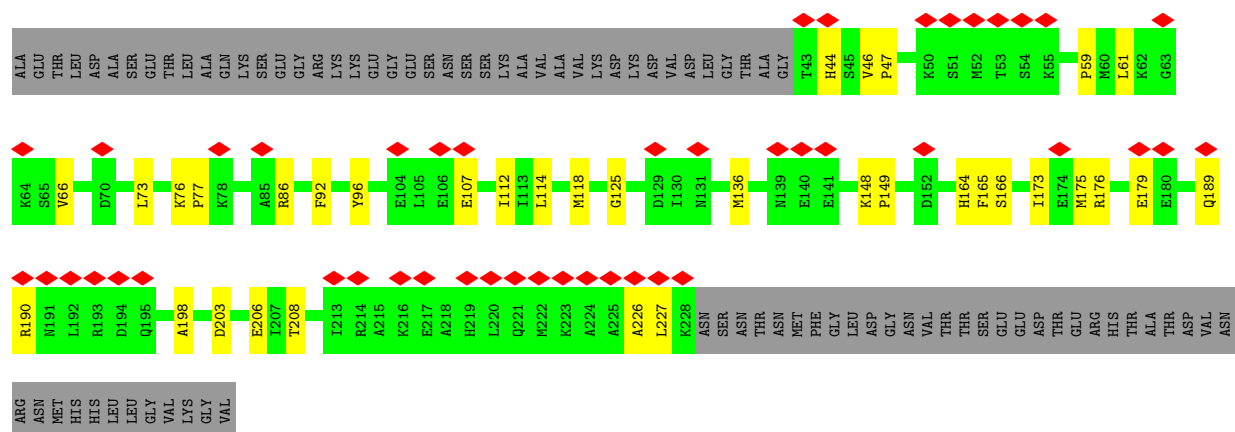




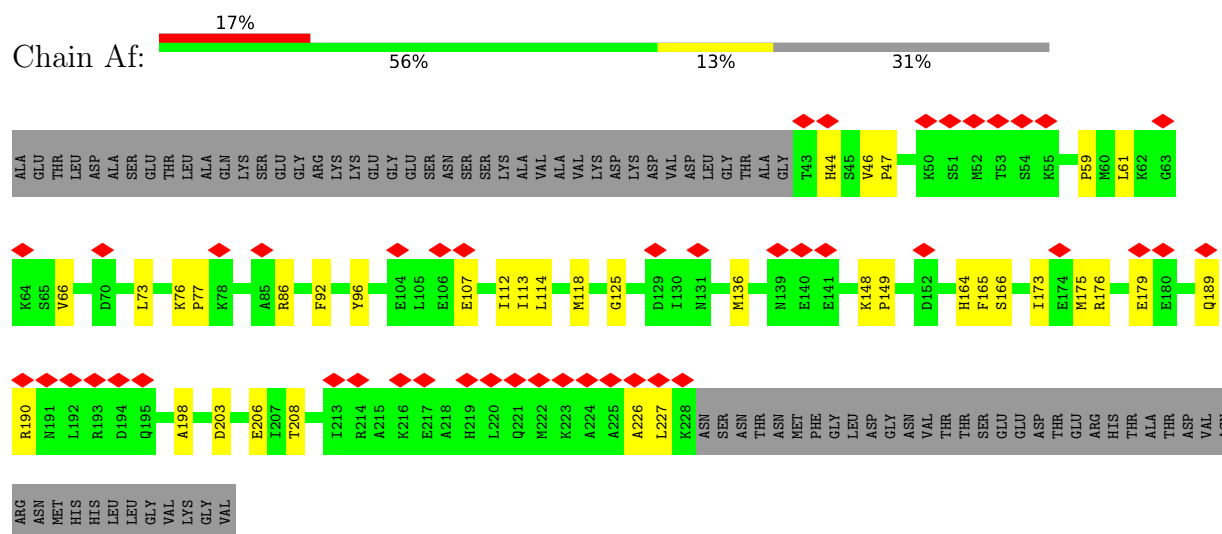
• Molecule 1: Genome polypeptide



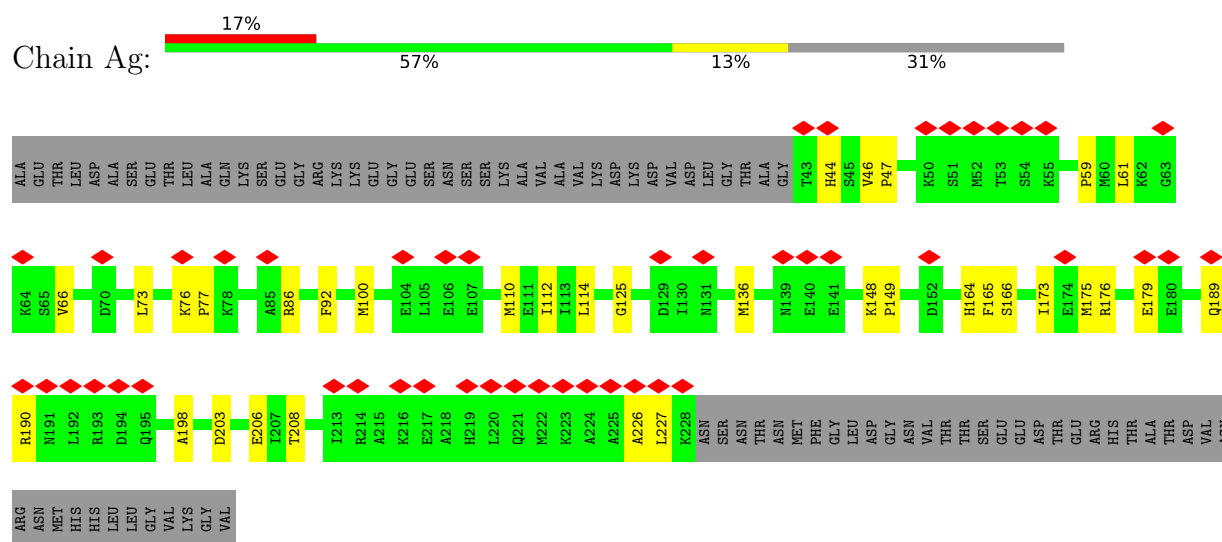
• Molecule 1: Genome polypeptide



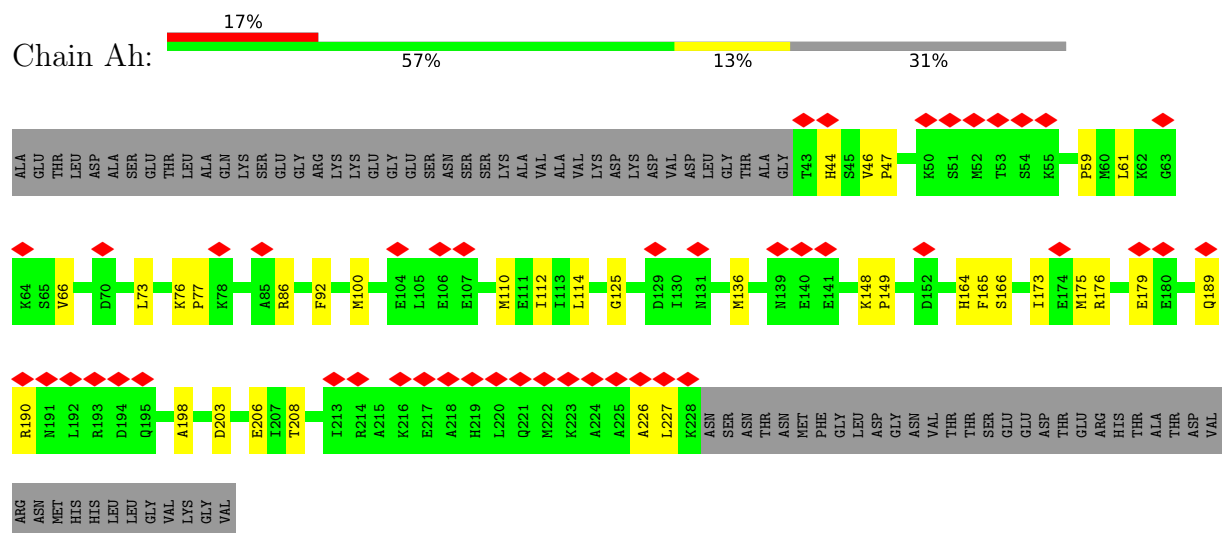
• Molecule 1: Genome polypeptide



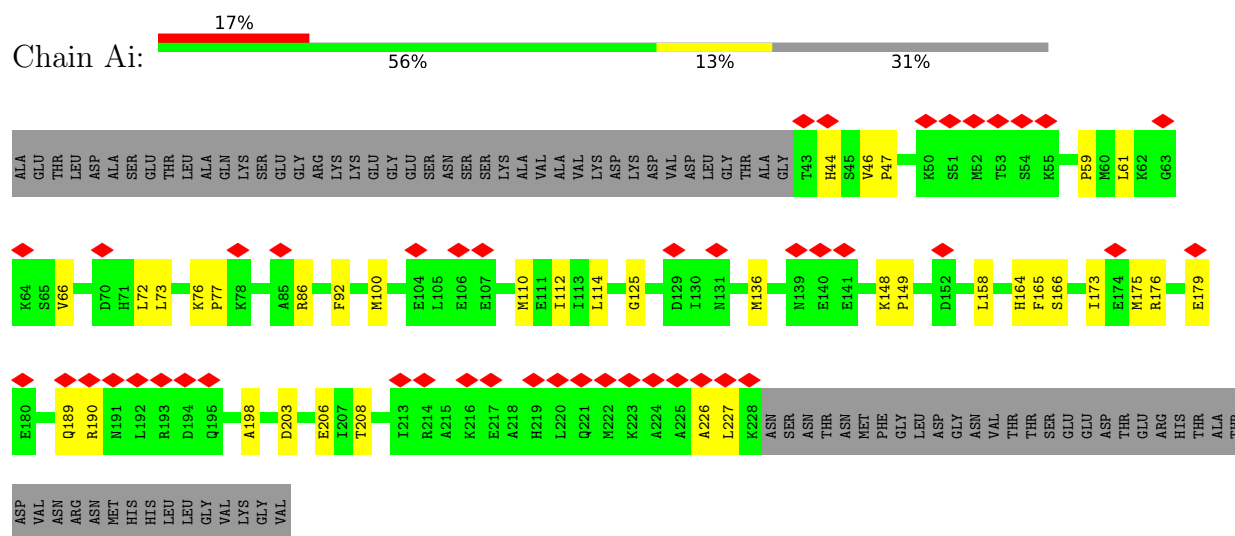
• Molecule 1: Genome polyprotein



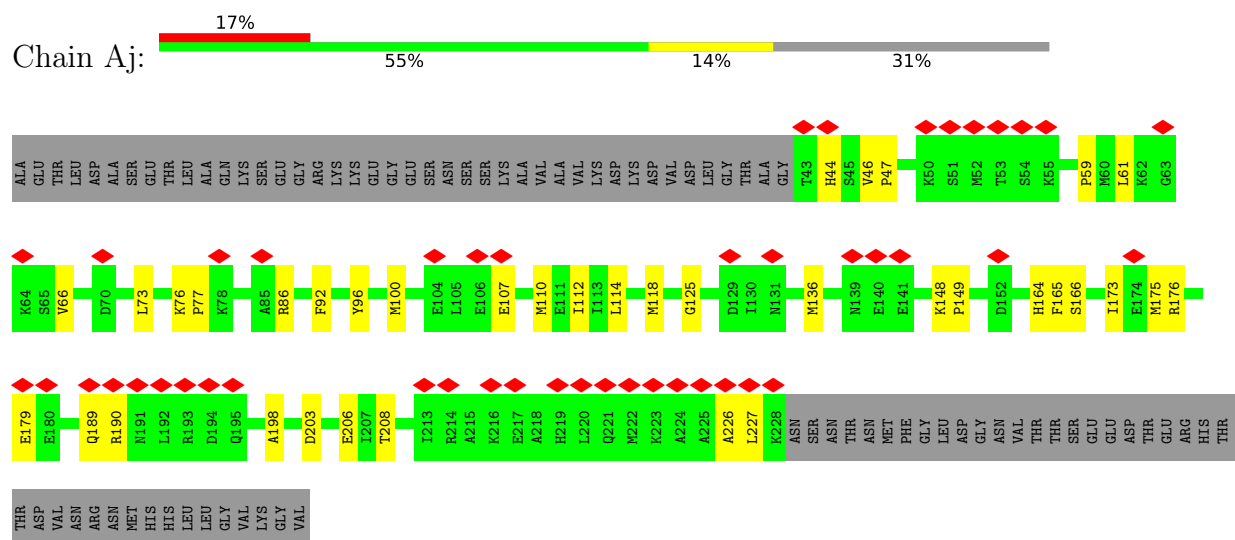
• Molecule 1: Genome polyprotein



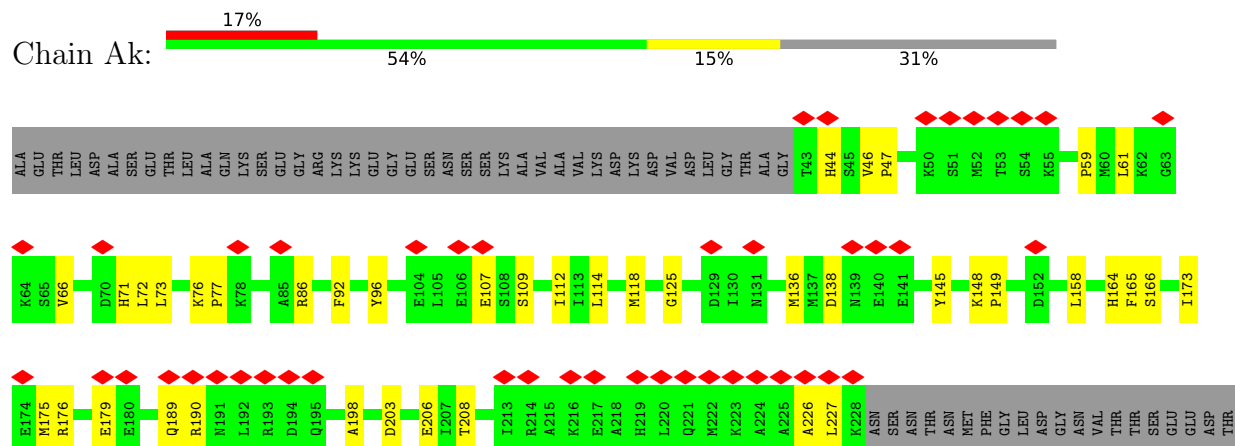
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein

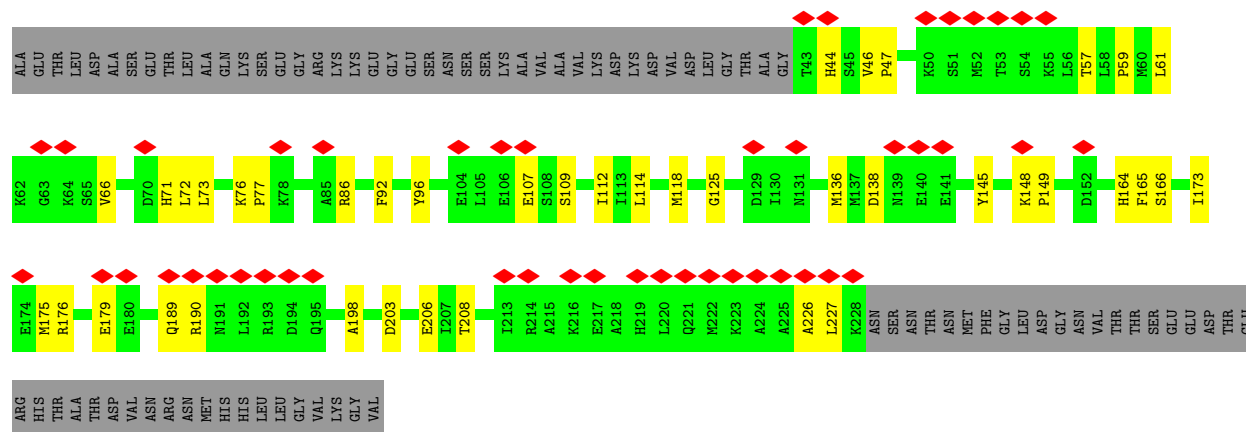


• Molecule 1: Genome polyprotein

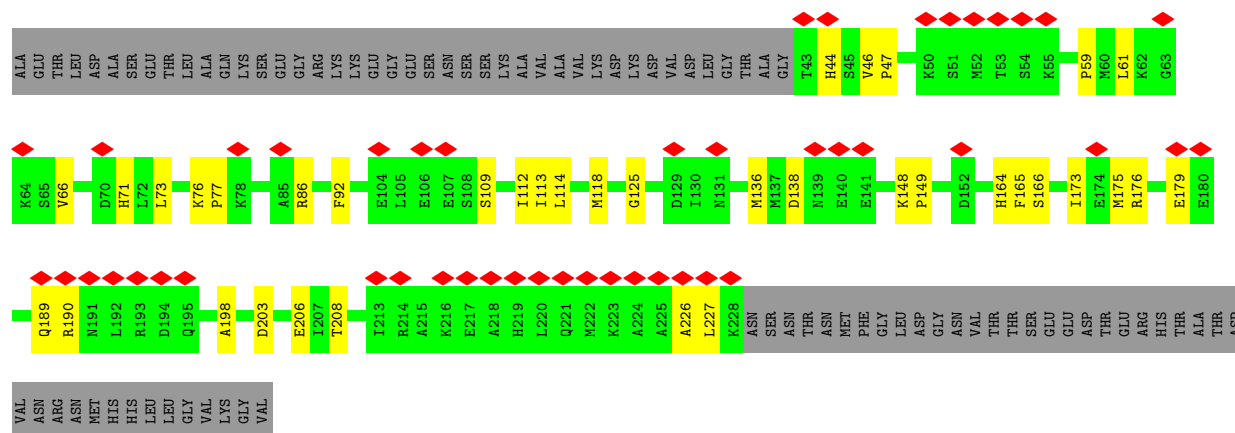


ARG
HIS
THR
ALA
THR
ASP
ASP
VAL
ASN
ARG
ASN
MET
HIS
HIS
LEU
LEU
GLY
VAL
VAL
GLY
VAL

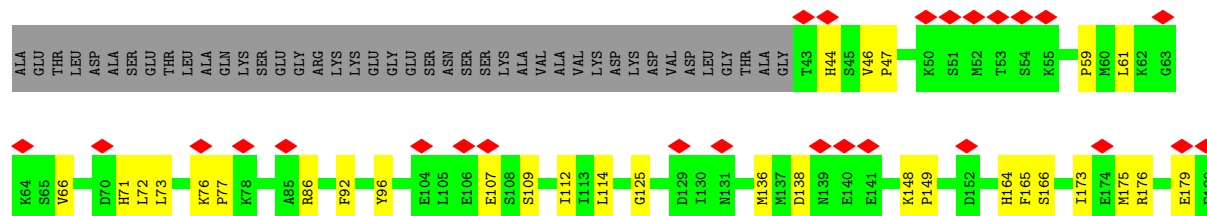
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein

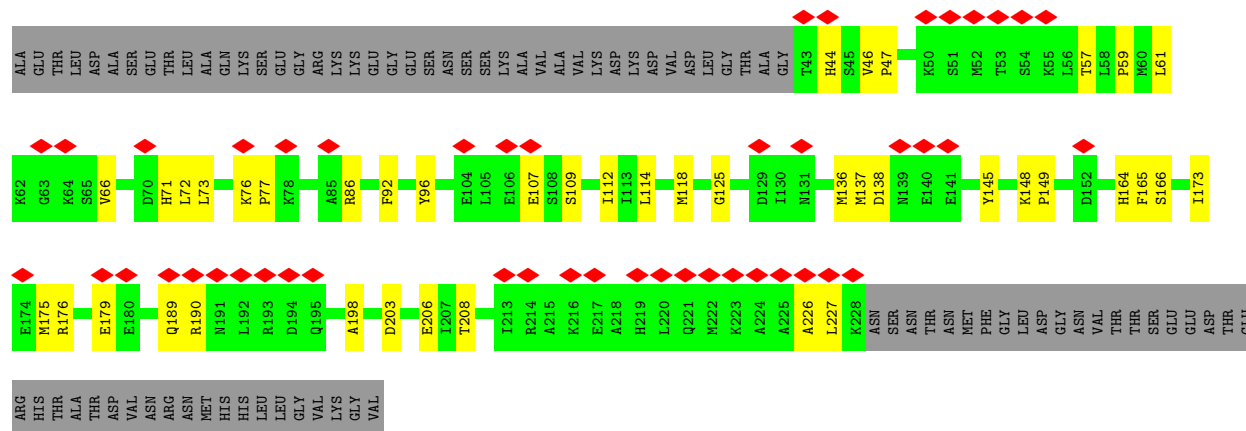


• Molecule 1: Genome polyprotein

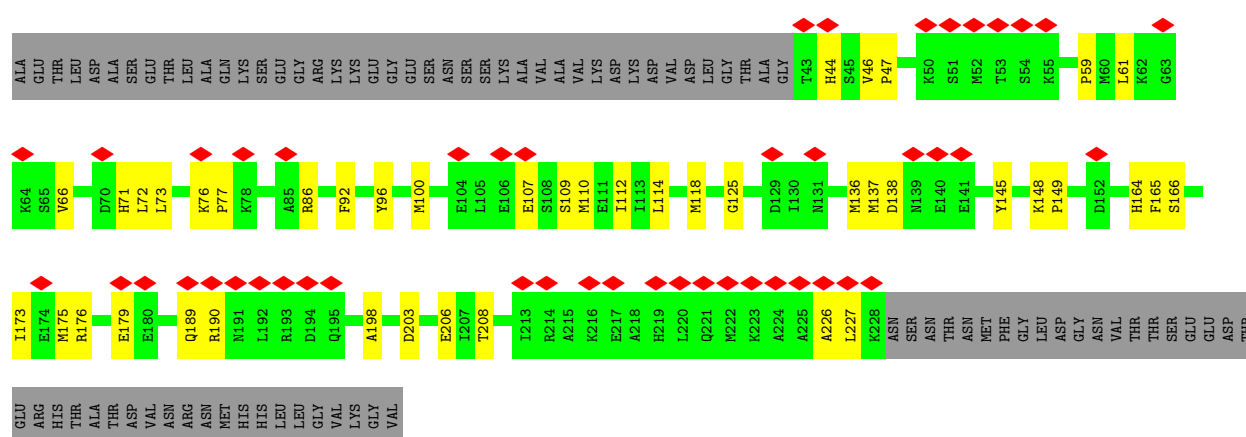




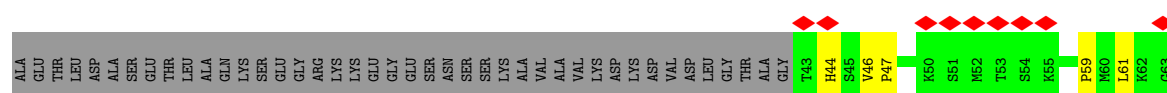
• Molecule 1: Genome polyprotein

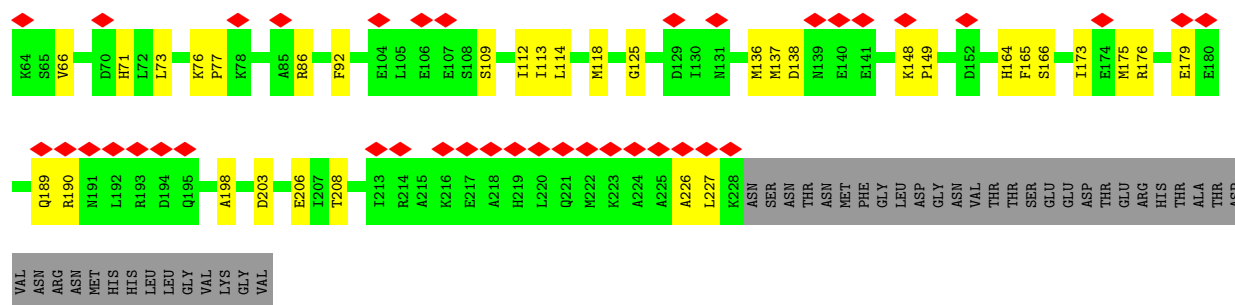


• Molecule 1: Genome polyprotein

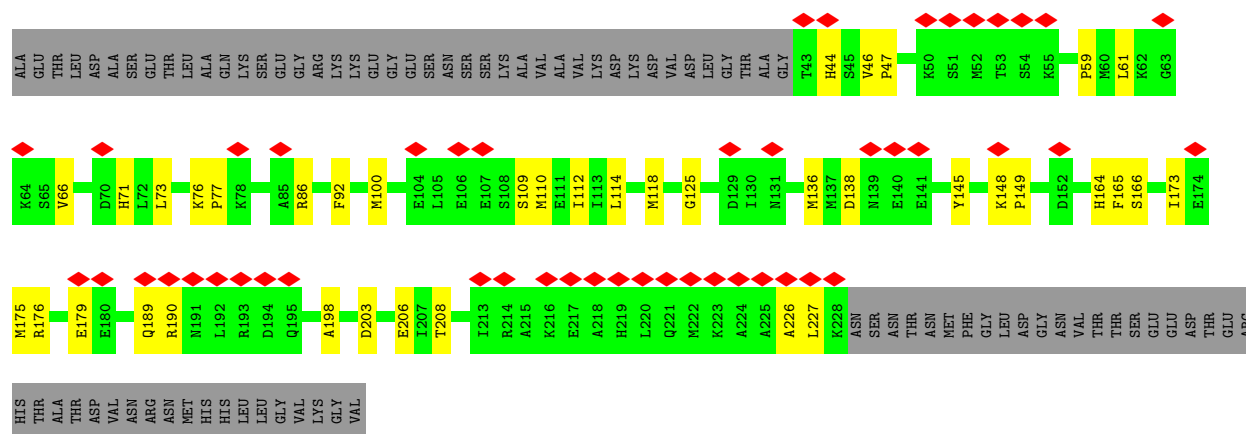


• Molecule 1: Genome polyprotein

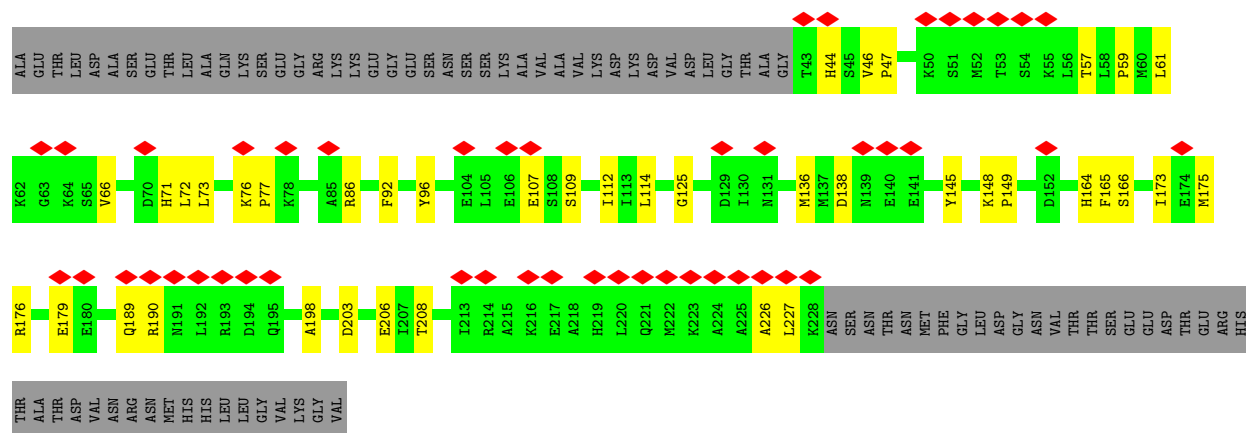




• Molecule 1: Genome polypeptide

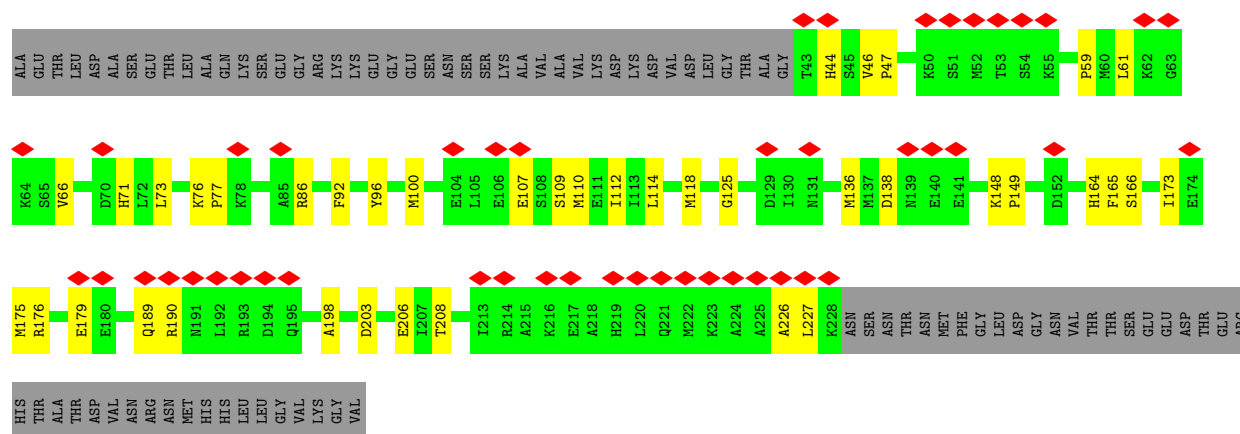


• Molecule 1: Genome polypeptide

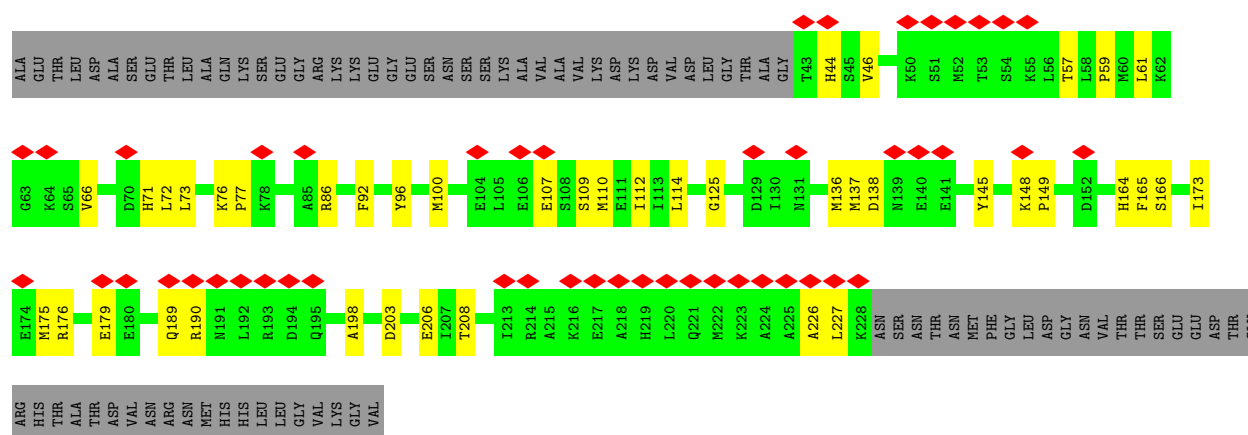


• Molecule 1: Genome polypeptide

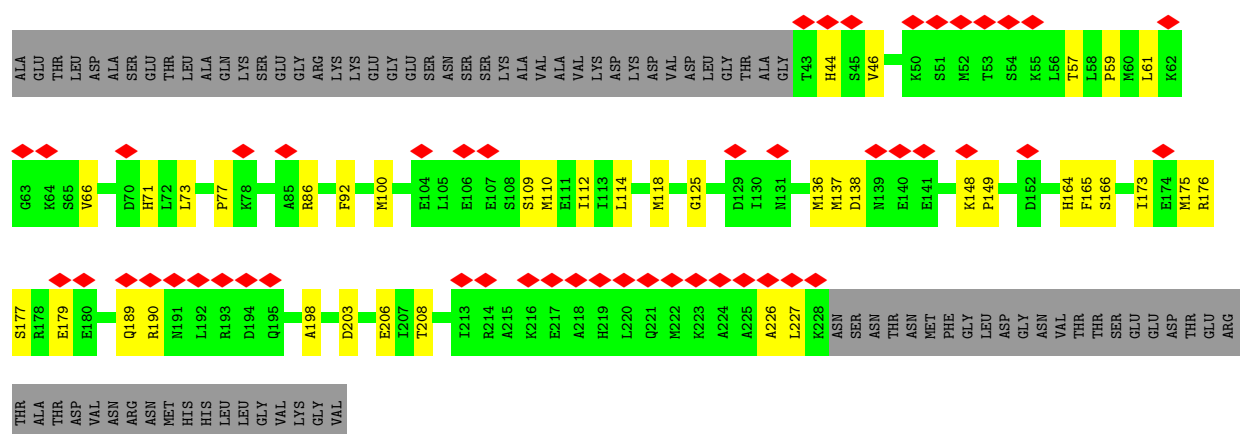




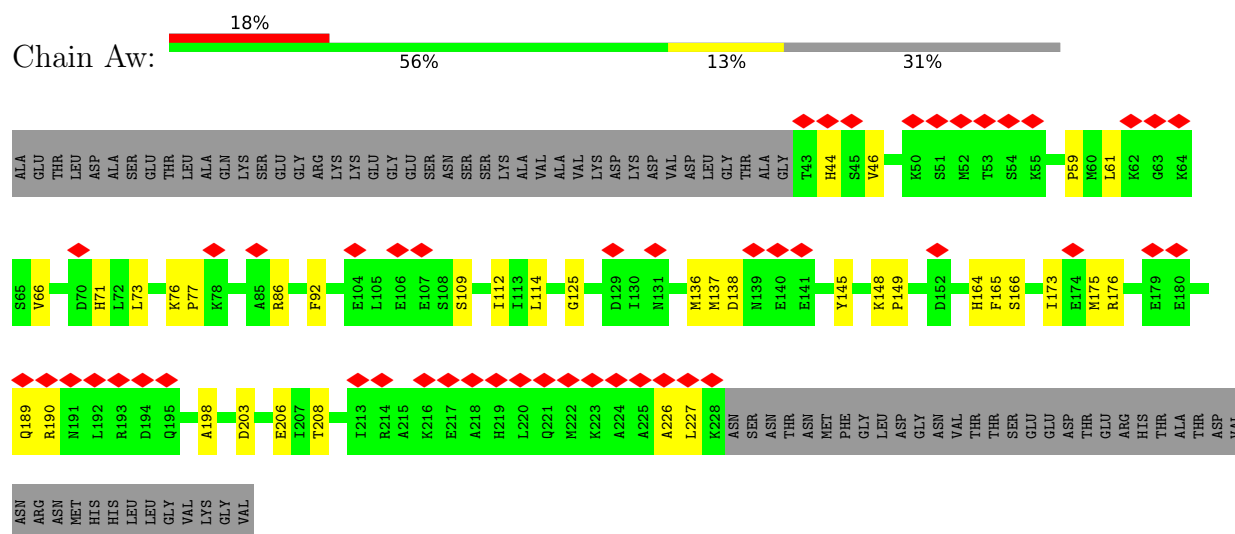
• Molecule 1: Genome polyprotein



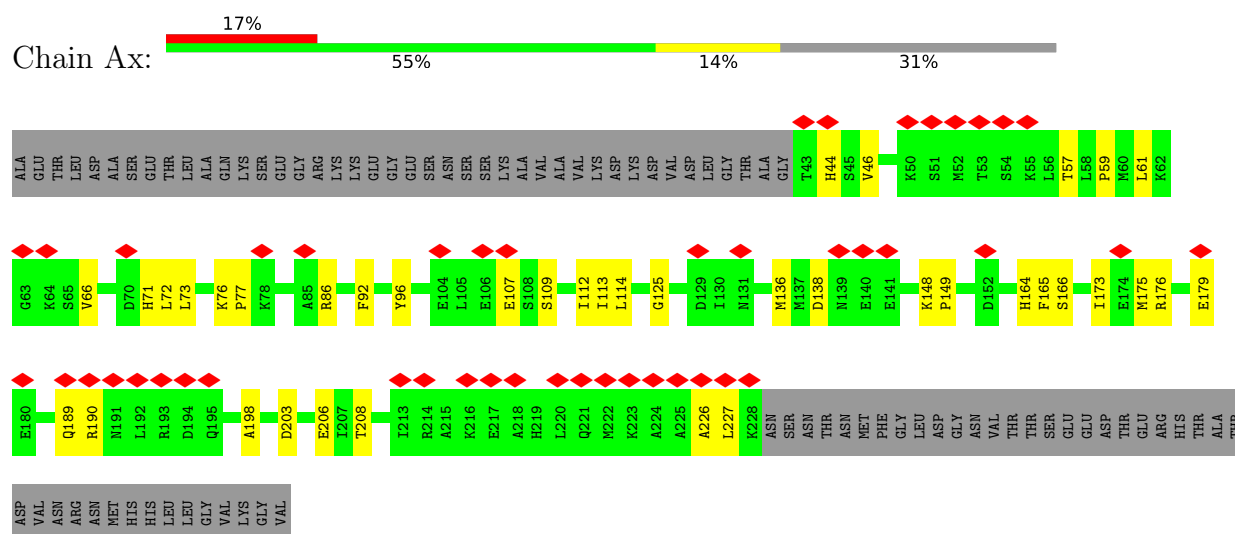
• Molecule 1: Genome polyprotein



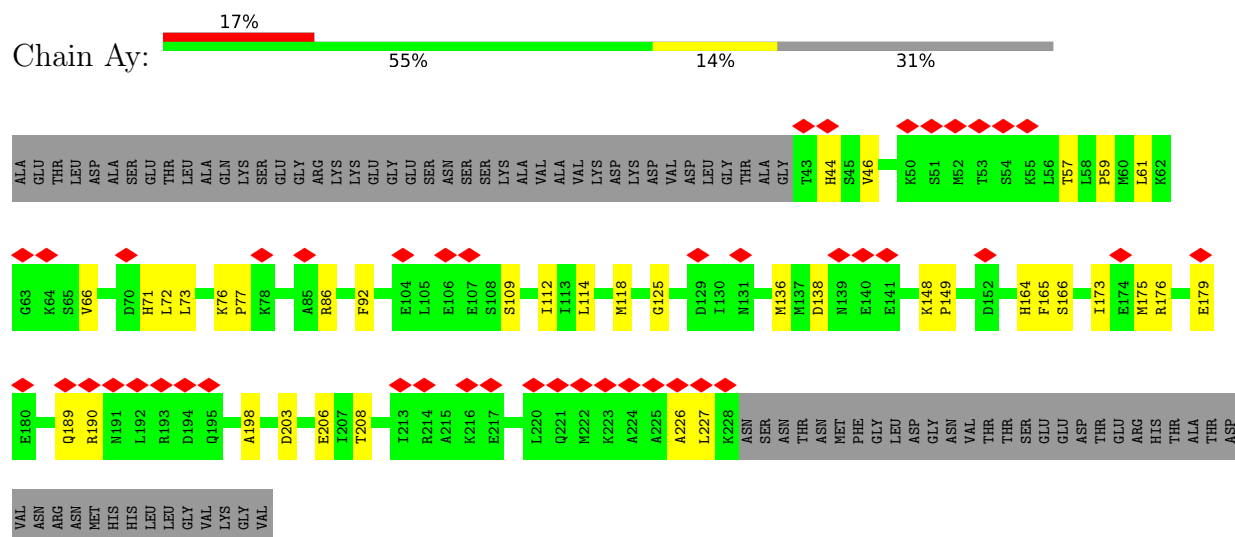
• Molecule 1: Genome polyprotein



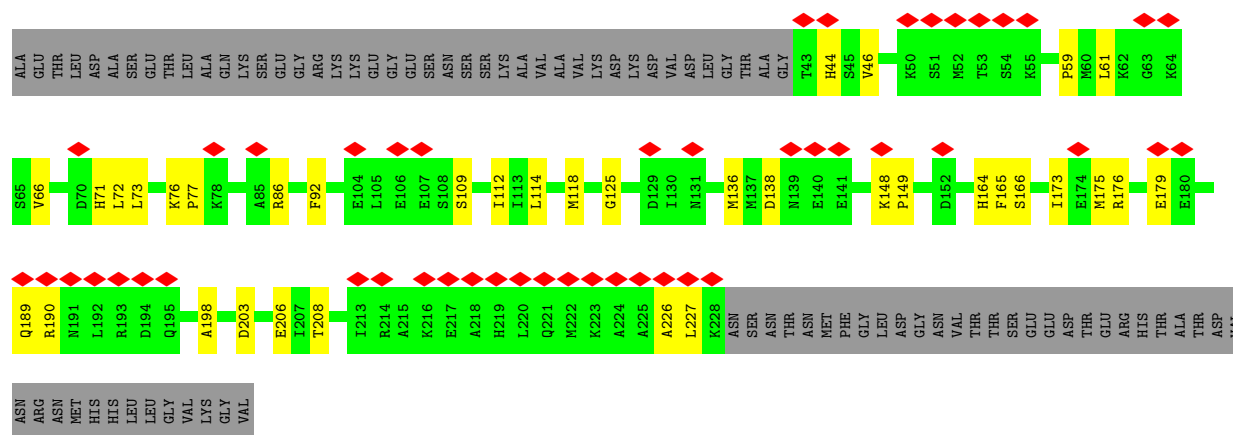
• Molecule 1: Genome polyprotein



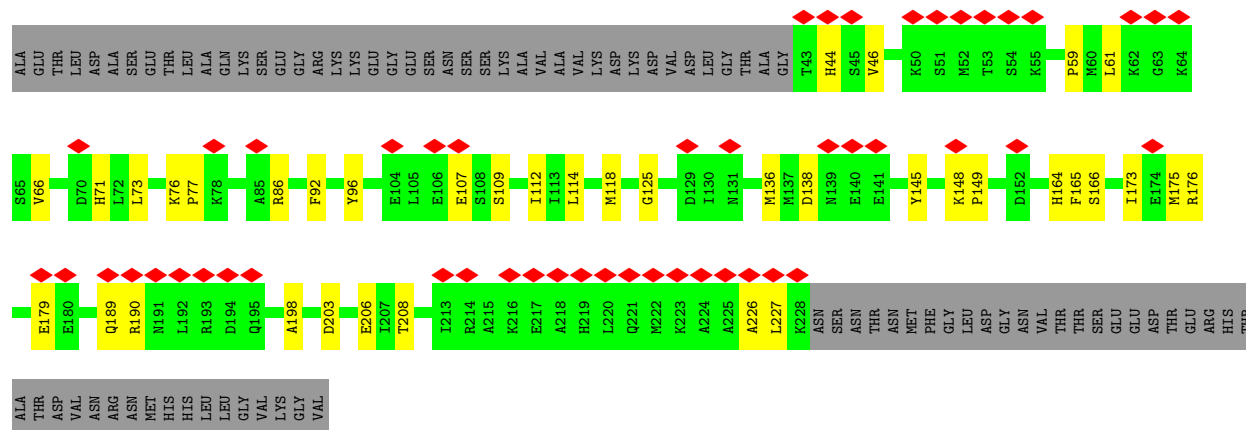
• Molecule 1: Genome polyprotein



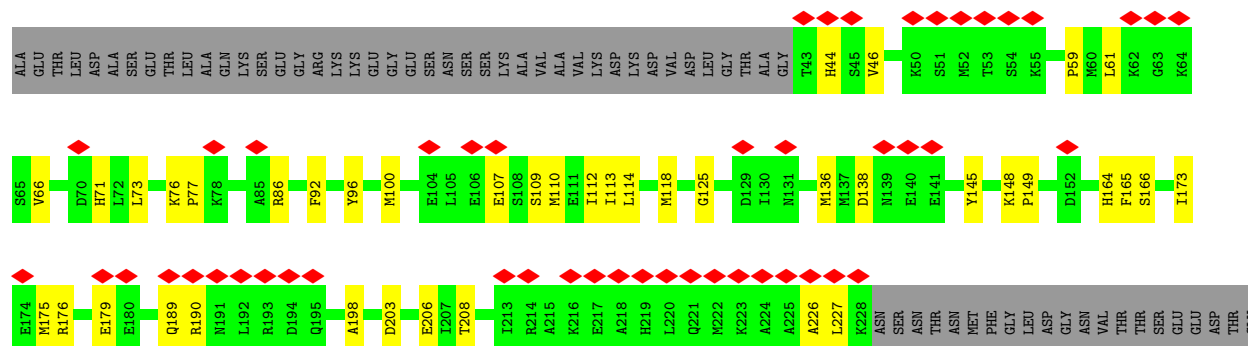
Chain Az:



Chain Ba:

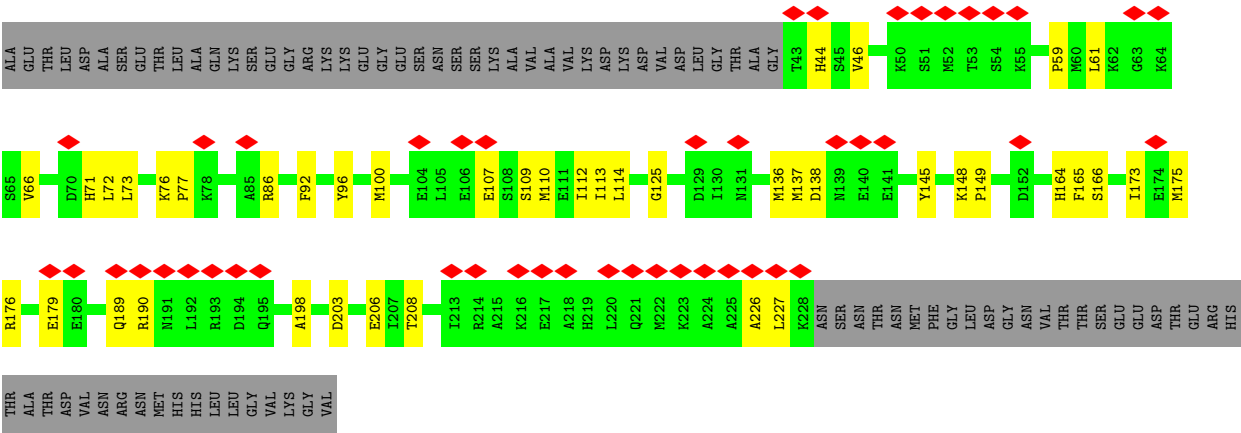


Chain Bb:

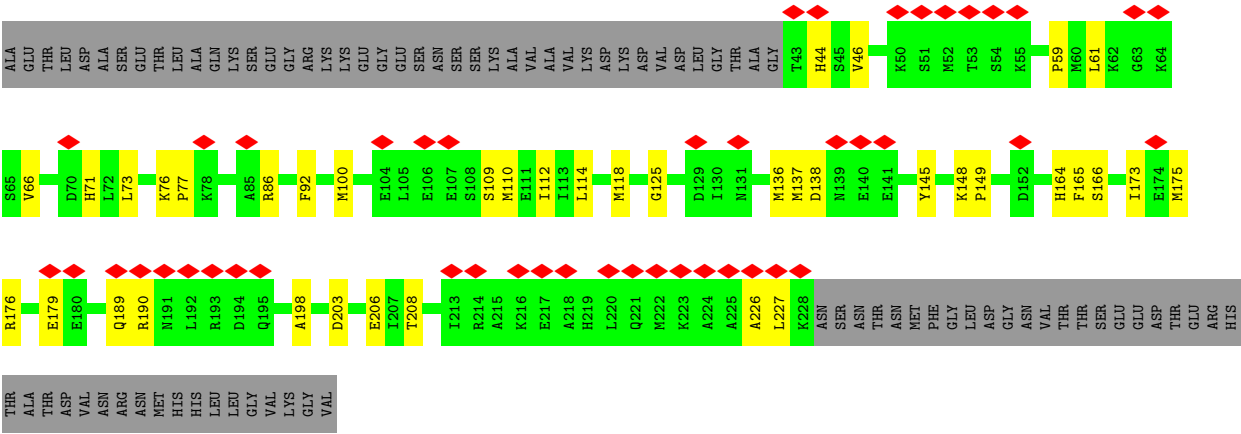


ARG
HIS
THR
ALA
THR
ASP
ASP
VAL
ASN
ARG
ASN
MET
HIS
HIS
LEU
LEU
GLY
VAL
LYS
VAL
GLY
VAL

● Molecule 1: Genome polyprotein



● Molecule 1: Genome polyprotein



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=19.64°, rise=36.33 Å, axial sym=C10	Depositor
Number of segments used	49408	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	6.788	Depositor
Minimum map value	-4.528	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.340	Depositor
Recommended contour level	1.61	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	0.60	0/1538	0.75	0/2077
1	Ab	0.60	0/1538	0.75	0/2077
1	Ac	0.60	0/1538	0.75	0/2077
1	Ad	0.60	0/1538	0.75	0/2077
1	Ae	0.60	0/1538	0.75	0/2077
1	Af	0.60	0/1538	0.75	0/2077
1	Ag	0.60	0/1538	0.75	0/2077
1	Ah	0.60	0/1538	0.75	0/2077
1	Ai	0.60	0/1538	0.75	0/2077
1	Aj	0.60	0/1538	0.75	0/2077
1	Ak	0.60	0/1538	0.75	0/2077
1	Al	0.60	0/1538	0.75	0/2077
1	Am	0.60	0/1538	0.75	0/2077
1	An	0.60	0/1538	0.75	0/2077
1	Ao	0.60	0/1538	0.75	0/2077
1	Ap	0.60	0/1538	0.75	0/2077
1	Aq	0.60	0/1538	0.75	0/2077
1	Ar	0.60	0/1538	0.75	0/2077
1	As	0.60	0/1538	0.75	0/2077
1	At	0.60	0/1538	0.75	0/2077
1	Au	0.60	0/1538	0.75	0/2077
1	Av	0.60	0/1538	0.75	0/2077
1	Aw	0.60	0/1538	0.75	0/2077
1	Ax	0.60	0/1538	0.75	0/2077
1	Ay	0.60	0/1538	0.75	0/2077
1	Az	0.60	0/1538	0.75	0/2077
1	Ba	0.60	0/1538	0.75	0/2077
1	Bb	0.60	0/1538	0.75	0/2077
1	Bc	0.60	0/1538	0.75	0/2077
1	Bd	0.60	0/1538	0.75	0/2077
All	All	0.60	0/46140	0.75	0/62310

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	1504	0	1493	36	0
1	Ab	1504	0	1493	39	0
1	Ac	1504	0	1493	40	0
1	Ad	1504	0	1493	38	0
1	Ae	1504	0	1493	35	0
1	Af	1504	0	1493	37	0
1	Ag	1504	0	1493	35	0
1	Ah	1504	0	1493	35	0
1	Ai	1504	0	1493	38	0
1	Aj	1504	0	1493	38	0
1	Ak	1504	0	1493	43	0
1	Al	1504	0	1493	43	0
1	Am	1504	0	1493	41	0
1	An	1504	0	1493	39	0
1	Ao	1504	0	1493	45	0
1	Ap	1504	0	1493	44	0
1	Aq	1504	0	1493	41	0
1	Ar	1504	0	1493	41	0
1	As	1504	0	1493	42	0
1	At	1504	0	1493	41	0
1	Au	1504	0	1493	40	0
1	Av	1504	0	1493	37	0
1	Aw	1504	0	1493	34	0
1	Ax	1504	0	1493	38	0
1	Ay	1504	0	1493	36	0
1	Az	1504	0	1493	36	0
1	Ba	1504	0	1493	37	0
1	Bb	1504	0	1493	38	0
1	Bc	1504	0	1493	39	0
1	Bd	1504	0	1493	38	0
All	All	45120	0	44790	846	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 9.

All (846) 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:Aj:46:VAL:HG21	1:Al:138:ASP:HB2	1.70	0.73
1:At:46:VAL:HG21	1:Av:138:ASP:HB2	1.71	0.73
1:Ab:46:VAL:HG21	1:An:138:ASP:HB2	1.71	0.72
1:Ae:46:VAL:HG21	1:Aq:138:ASP:HB2	1.72	0.72
1:Ad:46:VAL:HG21	1:Ap:138:ASP:HB2	1.72	0.72
1:Al:46:VAL:HG21	1:Ax:138:ASP:HB2	1.72	0.71
1:Ai:46:VAL:HG21	1:Ak:138:ASP:HB2	1.73	0.71
1:Af:46:VAL:HG21	1:Ar:138:ASP:HB2	1.73	0.71
1:Ao:46:VAL:HG21	1:Ba:138:ASP:HB2	1.72	0.71
1:Ac:46:VAL:HG21	1:Ao:138:ASP:HB2	1.73	0.71
1:Ah:46:VAL:HG21	1:At:138:ASP:HB2	1.73	0.71
1:An:46:VAL:HG21	1:Az:138:ASP:HB2	1.73	0.71
1:Ap:46:VAL:HG21	1:Bb:138:ASP:HB2	1.73	0.71
1:Ar:46:VAL:HG21	1:Bd:138:ASP:HB2	1.73	0.71
1:As:46:VAL:HG21	1:Au:138:ASP:HB2	1.73	0.70
1:Aq:46:VAL:HG21	1:Bc:138:ASP:HB2	1.73	0.70
1:Aa:46:VAL:HG21	1:Am:138:ASP:HB2	1.73	0.70
1:Ag:46:VAL:HG21	1:As:138:ASP:HB2	1.73	0.70
1:Am:46:VAL:HG21	1:Ay:138:ASP:HB2	1.74	0.70
1:Ak:46:VAL:HG21	1:Aw:138:ASP:HB2	1.74	0.69
1:Aw:86:ARG:NH1	1:Aw:164:HIS:HA	2.17	0.59
1:Ba:86:ARG:NH1	1:Ba:164:HIS:HA	2.18	0.59
1:Ap:86:ARG:NH1	1:Ap:164:HIS:HA	2.18	0.59
1:Av:86:ARG:NH1	1:Av:164:HIS:HA	2.18	0.59
1:Ae:86:ARG:NH1	1:Ae:164:HIS:HA	2.18	0.59
1:Af:86:ARG:NH1	1:Af:164:HIS:HA	2.18	0.59
1:Aq:86:ARG:NH1	1:Aq:164:HIS:HA	2.18	0.59
1:Au:86:ARG:NH1	1:Au:164:HIS:HA	2.18	0.59
1:Aa:86:ARG:NH1	1:Aa:164:HIS:HA	2.18	0.59
1:Ax:86:ARG:NH1	1:Ax:164:HIS:HA	2.18	0.59
1:Bb:86:ARG:NH1	1:Bb:164:HIS:HA	2.18	0.59
1:Aj:86:ARG:NH1	1:Aj:164:HIS:HA	2.18	0.59
1:Ab:86:ARG:NH1	1:Ab:164:HIS:HA	2.18	0.59
1:Az:86:ARG:NH1	1:Az:164:HIS:HA	2.18	0.58
1:Ak:86:ARG:NH1	1:Ak:164:HIS:HA	2.18	0.58
1:Bd:86:ARG:NH1	1:Bd:164:HIS:HA	2.18	0.58
1:Ai:86:ARG:NH1	1:Ai:164:HIS:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:86:ARG:NH1	1:Ac:164:HIS:HA	2.18	0.58
1:Ah:86:ARG:NH1	1:Ah:164:HIS:HA	2.18	0.58
1:Am:86:ARG:NH1	1:Am:164:HIS:HA	2.18	0.58
1:Ao:86:ARG:NH1	1:Ao:164:HIS:HA	2.18	0.58
1:Ar:86:ARG:NH1	1:Ar:164:HIS:HA	2.18	0.58
1:Ag:86:ARG:NH1	1:Ag:164:HIS:HA	2.18	0.58
1:Al:86:ARG:NH1	1:Al:164:HIS:HA	2.18	0.58
1:As:86:ARG:NH1	1:As:164:HIS:HA	2.17	0.58
1:At:86:ARG:NH1	1:At:164:HIS:HA	2.18	0.58
1:Ay:86:ARG:NH1	1:Ay:164:HIS:HA	2.18	0.58
1:Bc:86:ARG:NH1	1:Bc:164:HIS:HA	2.17	0.58
1:Ad:86:ARG:NH1	1:Ad:164:HIS:HA	2.18	0.58
1:An:86:ARG:NH1	1:An:164:HIS:HA	2.18	0.58
1:Bb:189:GLN:HB3	1:Bb:190:ARG:HH11	1.70	0.57
1:Am:189:GLN:HB3	1:Am:190:ARG:HH11	1.70	0.57
1:Ab:189:GLN:HB3	1:Ab:190:ARG:HH11	1.70	0.57
1:Ax:189:GLN:HB3	1:Ax:190:ARG:HH11	1.70	0.57
1:Bd:189:GLN:HB3	1:Bd:190:ARG:HH11	1.70	0.57
1:Ad:189:GLN:HB3	1:Ad:190:ARG:HH11	1.70	0.57
1:As:189:GLN:HB3	1:As:190:ARG:HH11	1.70	0.57
1:Bc:59:PRO:HG2	1:Bd:165:PHE:CD1	2.39	0.57
1:Ai:189:GLN:HB3	1:Ai:190:ARG:HH11	1.70	0.57
1:Ao:189:GLN:HB3	1:Ao:190:ARG:HH11	1.70	0.57
1:Aq:189:GLN:HB3	1:Aq:190:ARG:HH11	1.70	0.57
1:At:189:GLN:HB3	1:At:190:ARG:HH11	1.70	0.57
1:Au:189:GLN:HB3	1:Au:190:ARG:HH11	1.70	0.57
1:Av:189:GLN:HB3	1:Av:190:ARG:HH11	1.70	0.57
1:Az:189:GLN:HB3	1:Az:190:ARG:HH11	1.70	0.57
1:Ag:189:GLN:HB3	1:Ag:190:ARG:HH11	1.70	0.57
1:Ah:189:GLN:HB3	1:Ah:190:ARG:HH11	1.70	0.57
1:Ak:189:GLN:HB3	1:Ak:190:ARG:HH11	1.70	0.57
1:Av:59:PRO:HG2	1:Aw:165:PHE:CD1	2.40	0.57
1:Af:59:PRO:HG2	1:Ag:165:PHE:CD1	2.40	0.57
1:Bc:189:GLN:HB3	1:Bc:190:ARG:HH11	1.70	0.56
1:Aj:189:GLN:HB3	1:Aj:190:ARG:HH11	1.70	0.56
1:Af:189:GLN:HB3	1:Af:190:ARG:HH11	1.70	0.56
1:Al:59:PRO:HG2	1:Am:165:PHE:CD1	2.40	0.56
1:Ap:59:PRO:HG2	1:Aq:165:PHE:CD1	2.40	0.56
1:Ar:59:PRO:HG2	1:As:165:PHE:CD1	2.40	0.56
1:Ar:189:GLN:HB3	1:Ar:190:ARG:HH11	1.70	0.56
1:Ab:59:PRO:HG2	1:Ac:165:PHE:CD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:59:PRO:HG2	1:Ae:165:PHE:CD1	2.40	0.56
1:Aw:189:GLN:HB3	1:Aw:190:ARG:HH11	1.70	0.56
1:Ae:189:GLN:HB3	1:Ae:190:ARG:HH11	1.70	0.56
1:Ai:59:PRO:HG2	1:Aj:165:PHE:CD1	2.40	0.56
1:As:59:PRO:HG2	1:At:165:PHE:CD1	2.40	0.56
1:Ay:189:GLN:HB3	1:Ay:190:ARG:HH11	1.70	0.56
1:Az:59:PRO:HG2	1:Ba:165:PHE:CD1	2.40	0.56
1:Ah:59:PRO:HG2	1:Ai:165:PHE:CD1	2.40	0.56
1:Bb:59:PRO:HG2	1:Bc:165:PHE:CD1	2.41	0.56
1:Ac:189:GLN:HB3	1:Ac:190:ARG:HH11	1.70	0.56
1:Ba:59:PRO:HG2	1:Bb:165:PHE:CD1	2.41	0.56
1:Aa:189:GLN:HB3	1:Aa:190:ARG:HH11	1.70	0.56
1:Al:189:GLN:HB3	1:Al:190:ARG:HH11	1.70	0.55
1:Ag:59:PRO:HG2	1:Ah:165:PHE:CD1	2.41	0.55
1:An:59:PRO:HG2	1:Ao:165:PHE:CD1	2.40	0.55
1:Ax:59:PRO:HG2	1:Ay:165:PHE:CD1	2.41	0.55
1:Ae:59:PRO:HG2	1:Af:165:PHE:CD1	2.42	0.55
1:Aq:59:PRO:HG2	1:Ar:165:PHE:CD1	2.41	0.55
1:Ak:59:PRO:HG2	1:Al:165:PHE:CD1	2.41	0.55
1:Ap:189:GLN:HB3	1:Ap:190:ARG:HH11	1.70	0.55
1:Ay:59:PRO:HG2	1:Az:165:PHE:CD1	2.41	0.55
1:Aa:59:PRO:HG2	1:Ab:165:PHE:CD1	2.41	0.55
1:An:189:GLN:HB3	1:An:190:ARG:HH11	1.70	0.55
1:Ao:59:PRO:HG2	1:Ap:165:PHE:CD1	2.42	0.55
1:Au:59:PRO:HG2	1:Av:165:PHE:CD1	2.41	0.55
1:Ba:189:GLN:HB3	1:Ba:190:ARG:HH11	1.70	0.55
1:Aw:59:PRO:HG2	1:Ax:165:PHE:CD1	2.42	0.54
1:Aa:44:HIS:CE1	1:Al:71:HIS:HB2	2.43	0.54
1:Af:44:HIS:CE1	1:Aq:71:HIS:HB2	2.43	0.54
1:Aj:44:HIS:CE1	1:Ak:71:HIS:HB2	2.43	0.54
1:Am:59:PRO:HG2	1:An:165:PHE:CD1	2.42	0.54
1:Ac:44:HIS:CE1	1:An:71:HIS:HB2	2.42	0.54
1:Aa:165:PHE:CD1	1:Aj:59:PRO:HG2	2.42	0.54
1:Aj:44:HIS:HE1	1:Ak:71:HIS:HB2	1.73	0.54
1:Ak:44:HIS:CE1	1:Av:71:HIS:HB2	2.43	0.54
1:Ak:165:PHE:CD1	1:At:59:PRO:HG2	2.42	0.54
1:Ap:44:HIS:CE1	1:Ba:71:HIS:HB2	2.43	0.54
1:Ab:44:HIS:CE1	1:Am:71:HIS:HB2	2.43	0.54
1:Am:44:HIS:CE1	1:Ax:71:HIS:HB2	2.43	0.54
1:At:44:HIS:CE1	1:Au:71:HIS:HB2	2.42	0.54
1:Ac:44:HIS:HE1	1:An:71:HIS:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:59:PRO:HG2	1:Ad:165:PHE:CD1	2.42	0.53
1:Ap:44:HIS:HE1	1:Ba:71:HIS:HB2	1.73	0.53
1:Ad:44:HIS:CE1	1:Ao:71:HIS:HB2	2.44	0.53
1:Ae:44:HIS:CE1	1:Ap:71:HIS:HB2	2.43	0.53
1:Ab:44:HIS:HE1	1:Am:71:HIS:HB2	1.73	0.53
1:At:44:HIS:HE1	1:Au:71:HIS:HB2	1.73	0.53
1:Ao:44:HIS:CE1	1:Az:71:HIS:HB2	2.44	0.53
1:Aq:44:HIS:CE1	1:Bb:71:HIS:HB2	2.44	0.53
1:Ar:44:HIS:CE1	1:Bc:71:HIS:HB2	2.43	0.53
1:Ah:44:HIS:CE1	1:As:71:HIS:HB2	2.44	0.53
1:Au:165:PHE:CD1	1:Bd:59:PRO:HG2	2.42	0.53
1:Al:44:HIS:CE1	1:Aw:71:HIS:HB2	2.44	0.53
1:Af:44:HIS:HE1	1:Aq:71:HIS:HB2	1.74	0.52
1:Ar:44:HIS:HE1	1:Bc:71:HIS:HB2	1.74	0.52
1:Aa:44:HIS:HE1	1:Al:71:HIS:HB2	1.73	0.52
1:Ae:44:HIS:HE1	1:Ap:71:HIS:HB2	1.75	0.52
1:Ah:44:HIS:HE1	1:As:71:HIS:HB2	1.74	0.52
1:Al:44:HIS:HE1	1:Aw:71:HIS:HB2	1.74	0.52
1:Ad:44:HIS:HE1	1:Ao:71:HIS:HB2	1.74	0.52
1:Ak:44:HIS:HE1	1:Av:71:HIS:HB2	1.74	0.52
1:Ag:44:HIS:CE1	1:Ar:71:HIS:HB2	2.44	0.52
1:An:44:HIS:CE1	1:Ay:71:HIS:HB2	2.45	0.52
1:An:44:HIS:HE1	1:Ay:71:HIS:HB2	1.75	0.51
1:Am:44:HIS:HE1	1:Ax:71:HIS:HB2	1.74	0.51
1:Ao:44:HIS:HE1	1:Az:71:HIS:HB2	1.75	0.51
1:Ag:44:HIS:HE1	1:Ar:71:HIS:HB2	1.75	0.51
1:As:44:HIS:CE1	1:Bd:71:HIS:HB2	2.46	0.51
1:Aj:86:ARG:NH2	1:Aj:206:GLU:OE2	2.44	0.51
1:Ap:86:ARG:NH2	1:Ap:206:GLU:OE2	2.44	0.51
1:Ar:86:ARG:NH2	1:Ar:206:GLU:OE2	2.44	0.51
1:Ai:86:ARG:NH2	1:Ai:206:GLU:OE2	2.44	0.51
1:Ao:86:ARG:NH2	1:Ao:206:GLU:OE2	2.44	0.51
1:Aq:44:HIS:HE1	1:Bb:71:HIS:HB2	1.75	0.51
1:Bb:86:ARG:NH2	1:Bb:206:GLU:OE2	2.44	0.51
1:Aa:86:ARG:NH2	1:Aa:206:GLU:OE2	2.44	0.50
1:Af:86:ARG:NH2	1:Af:206:GLU:OE2	2.44	0.50
1:Ah:86:ARG:NH2	1:Ah:206:GLU:OE2	2.44	0.50
1:An:86:ARG:NH2	1:An:206:GLU:OE2	2.44	0.50
1:Au:86:ARG:NH2	1:Au:206:GLU:OE2	2.44	0.50
1:Av:86:ARG:NH2	1:Av:206:GLU:OE2	2.44	0.50
1:Aw:86:ARG:NH2	1:Aw:206:GLU:OE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:86:ARG:NH2	1:Ae:206:GLU:OE2	2.44	0.50
1:Ag:86:ARG:NH2	1:Ag:206:GLU:OE2	2.44	0.50
1:Bd:86:ARG:NH2	1:Bd:206:GLU:OE2	2.44	0.50
1:Aq:86:ARG:NH2	1:Aq:206:GLU:OE2	2.44	0.50
1:Ba:86:ARG:NH2	1:Ba:206:GLU:OE2	2.44	0.50
1:As:86:ARG:NH2	1:As:206:GLU:OE2	2.44	0.50
1:Ax:86:ARG:NH2	1:Ax:206:GLU:OE2	2.44	0.50
1:Aa:176:ARG:NH2	1:Aj:77:PRO:O	2.44	0.50
1:Ai:44:HIS:CE1	1:At:71:HIS:HB2	2.47	0.50
1:Am:86:ARG:NH2	1:Am:206:GLU:OE2	2.44	0.50
1:Ao:77:PRO:O	1:Ap:176:ARG:NH2	2.45	0.50
1:Ak:176:ARG:NH2	1:At:77:PRO:O	2.44	0.50
1:As:44:HIS:HE1	1:Bd:71:HIS:HB2	1.76	0.50
1:Ab:86:ARG:NH2	1:Ab:206:GLU:OE2	2.44	0.50
1:Ad:86:ARG:NH2	1:Ad:206:GLU:OE2	2.44	0.50
1:Ak:86:ARG:NH2	1:Ak:206:GLU:OE2	2.44	0.50
1:At:86:ARG:NH2	1:At:206:GLU:OE2	2.44	0.50
1:Ay:86:ARG:NH2	1:Ay:206:GLU:OE2	2.44	0.50
1:Au:176:ARG:NH2	1:Bd:77:PRO:O	2.44	0.50
1:Ac:86:ARG:NH2	1:Ac:206:GLU:OE2	2.44	0.50
1:Bc:86:ARG:NH2	1:Bc:206:GLU:OE2	2.44	0.50
1:Ay:77:PRO:O	1:Az:176:ARG:NH2	2.45	0.49
1:Bb:46:VAL:HG23	1:Bb:46:VAL:O	2.12	0.49
1:Ac:77:PRO:O	1:Ad:176:ARG:NH2	2.45	0.49
1:Af:46:VAL:HG23	1:Af:46:VAL:O	2.13	0.49
1:Al:86:ARG:NH2	1:Al:206:GLU:OE2	2.44	0.49
1:Aw:77:PRO:O	1:Ax:176:ARG:NH2	2.45	0.49
1:Az:86:ARG:NH2	1:Az:206:GLU:OE2	2.44	0.49
1:Al:112:ILE:HG22	1:Al:136:MET:HE1	1.95	0.49
1:Ab:112:ILE:HG22	1:Ab:136:MET:HE1	1.95	0.49
1:Ac:112:ILE:HG22	1:Ac:136:MET:HE1	1.95	0.49
1:Ad:112:ILE:HG22	1:Ad:136:MET:HE1	1.95	0.49
1:Ak:77:PRO:O	1:Al:176:ARG:NH2	2.45	0.49
1:Am:112:ILE:HG22	1:Am:136:MET:HE1	1.95	0.49
1:Ao:46:VAL:O	1:Ao:46:VAL:HG23	2.13	0.49
1:Au:77:PRO:O	1:Av:176:ARG:NH2	2.45	0.49
1:Av:112:ILE:HG22	1:Av:136:MET:HE1	1.95	0.49
1:Az:112:ILE:HG22	1:Az:136:MET:HE1	1.95	0.49
1:Ai:44:HIS:HE1	1:At:71:HIS:HB2	1.77	0.49
1:Am:77:PRO:O	1:An:176:ARG:NH2	2.45	0.49
1:An:112:ILE:HG22	1:An:136:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ap:46:VAL:HG23	1:Ap:46:VAL:O	2.13	0.49
1:Ap:112:ILE:HG22	1:Ap:136:MET:HE1	1.95	0.49
1:Ay:112:ILE:HG22	1:Ay:136:MET:HE1	1.95	0.49
1:Ae:77:PRO:O	1:Af:176:ARG:NH2	2.45	0.49
1:Af:77:PRO:O	1:Ag:176:ARG:NH2	2.46	0.49
1:Ag:46:VAL:O	1:Ag:46:VAL:HG23	2.13	0.49
1:As:46:VAL:O	1:As:46:VAL:HG23	2.13	0.49
1:Aa:112:ILE:HG22	1:Aa:136:MET:HE1	1.95	0.49
1:Ae:46:VAL:HG23	1:Ae:46:VAL:O	2.12	0.49
1:Ae:112:ILE:HG22	1:Ae:136:MET:HE1	1.95	0.49
1:Ak:112:ILE:HG22	1:Ak:136:MET:HE1	1.95	0.49
1:Ar:46:VAL:HG23	1:Ar:46:VAL:O	2.13	0.49
1:Aw:112:ILE:HG22	1:Aw:136:MET:HE1	1.95	0.49
1:Az:77:PRO:O	1:Ba:176:ARG:NH2	2.46	0.49
1:Ba:46:VAL:HG23	1:Ba:46:VAL:O	2.13	0.49
1:Ba:77:PRO:O	1:Bb:176:ARG:NH2	2.46	0.49
1:Ba:112:ILE:HG22	1:Ba:136:MET:HE1	1.95	0.49
1:Bc:46:VAL:HG23	1:Bc:46:VAL:O	2.13	0.49
1:Aa:77:PRO:O	1:Ab:176:ARG:NH2	2.45	0.49
1:Ao:112:ILE:HG22	1:Ao:136:MET:HE1	1.95	0.49
1:Au:112:ILE:HG22	1:Au:136:MET:HE1	1.95	0.49
1:Ay:46:VAL:HG23	1:Ay:46:VAL:O	2.13	0.49
1:Aq:112:ILE:HG22	1:Aq:136:MET:HE1	1.95	0.49
1:Ax:112:ILE:HG22	1:Ax:136:MET:HE1	1.95	0.49
1:Ag:77:PRO:O	1:Ah:176:ARG:NH2	2.46	0.49
1:Af:112:ILE:HG22	1:Af:136:MET:HE1	1.95	0.48
1:Ai:46:VAL:HG23	1:Ai:46:VAL:O	2.13	0.48
1:Aj:112:ILE:HG22	1:Aj:136:MET:HE1	1.95	0.48
1:Bb:112:ILE:HG22	1:Bb:136:MET:HE1	1.95	0.48
1:Ac:46:VAL:O	1:Ac:46:VAL:HG23	2.13	0.48
1:Ag:112:ILE:HG22	1:Ag:136:MET:HE1	1.95	0.48
1:Ai:112:ILE:HG22	1:Ai:136:MET:HE1	1.95	0.48
1:Ap:77:PRO:O	1:Aq:176:ARG:NH2	2.46	0.48
1:Ah:112:ILE:HG22	1:Ah:136:MET:HE1	1.95	0.48
1:Ar:112:ILE:HG22	1:Ar:136:MET:HE1	1.95	0.48
1:Ax:46:VAL:HG23	1:Ax:46:VAL:O	2.13	0.48
1:Bd:112:ILE:HG22	1:Bd:136:MET:HE1	1.95	0.48
1:At:112:ILE:HG22	1:At:136:MET:HE1	1.95	0.48
1:Aj:46:VAL:HG23	1:Aj:46:VAL:O	2.13	0.48
1:An:46:VAL:HG23	1:An:46:VAL:O	2.13	0.48
1:Aq:46:VAL:HG23	1:Aq:46:VAL:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:112:ILE:HG22	1:As:136:MET:HE1	1.95	0.48
1:Au:46:VAL:HG23	1:Au:46:VAL:O	2.12	0.48
1:Az:46:VAL:HG23	1:Az:46:VAL:O	2.13	0.48
1:Aa:46:VAL:O	1:Aa:46:VAL:HG23	2.12	0.48
1:Ah:77:PRO:O	1:Ai:176:ARG:NH2	2.47	0.48
1:Aq:77:PRO:O	1:Ar:176:ARG:NH2	2.46	0.48
1:Ar:77:PRO:O	1:As:176:ARG:NH2	2.47	0.48
1:Bc:112:ILE:HG22	1:Bc:136:MET:HE1	1.95	0.48
1:Aw:46:VAL:O	1:Aw:46:VAL:HG23	2.12	0.48
1:At:46:VAL:HG23	1:At:46:VAL:O	2.13	0.48
1:Ab:46:VAL:HG23	1:Ab:46:VAL:O	2.13	0.48
1:Ad:46:VAL:HG23	1:Ad:46:VAL:O	2.13	0.48
1:Ah:46:VAL:HG23	1:Ah:46:VAL:O	2.13	0.48
1:Ak:179:GLU:OE2	1:At:76:LYS:NZ	2.47	0.48
1:Al:46:VAL:HG23	1:Al:46:VAL:O	2.13	0.47
1:Bb:77:PRO:O	1:Bc:176:ARG:NH2	2.47	0.47
1:Av:46:VAL:HG23	1:Av:46:VAL:O	2.13	0.47
1:Am:46:VAL:HG23	1:Am:46:VAL:O	2.13	0.47
1:Bd:46:VAL:O	1:Bd:46:VAL:HG23	2.13	0.47
1:Ak:46:VAL:O	1:Ak:46:VAL:HG23	2.12	0.47
1:An:77:PRO:O	1:Ao:176:ARG:NH2	2.48	0.47
1:Bc:66:VAL:HB	1:Bd:114:LEU:CD1	2.45	0.47
1:Ai:66:VAL:HB	1:Aj:114:LEU:CD1	2.45	0.47
1:Am:59:PRO:O	1:Am:66:VAL:HG22	2.15	0.47
1:Ab:59:PRO:O	1:Ab:66:VAL:HG22	2.15	0.47
1:Ab:77:PRO:O	1:Ac:176:ARG:NH2	2.48	0.47
1:Ad:77:PRO:O	1:Ae:176:ARG:NH2	2.48	0.47
1:Af:59:PRO:O	1:Af:66:VAL:HG22	2.15	0.47
1:Aq:59:PRO:O	1:Aq:66:VAL:HG22	2.15	0.47
1:As:77:PRO:O	1:At:176:ARG:NH2	2.48	0.47
1:Ax:59:PRO:O	1:Ax:66:VAL:HG22	2.15	0.47
1:Bb:59:PRO:O	1:Bb:66:VAL:HG22	2.15	0.47
1:Ac:59:PRO:O	1:Ac:66:VAL:HG22	2.15	0.47
1:Az:66:VAL:HB	1:Ba:114:LEU:CD1	2.45	0.47
1:Ai:77:PRO:O	1:Aj:176:ARG:NH2	2.48	0.47
1:Ap:66:VAL:HB	1:Aq:114:LEU:CD1	2.45	0.47
1:Av:77:PRO:O	1:Aw:176:ARG:NH2	2.48	0.47
1:Al:59:PRO:O	1:Al:66:VAL:HG22	2.15	0.47
1:Al:66:VAL:HB	1:Am:114:LEU:CD1	2.45	0.47
1:Ap:59:PRO:O	1:Ap:66:VAL:HG22	2.15	0.47
1:Ar:59:PRO:O	1:Ar:66:VAL:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:59:PRO:O	1:Au:66:VAL:HG22	2.15	0.47
1:Aw:59:PRO:O	1:Aw:66:VAL:HG22	2.15	0.47
1:Ba:59:PRO:O	1:Ba:66:VAL:HG22	2.15	0.47
1:Bc:59:PRO:O	1:Bc:66:VAL:HG22	2.15	0.47
1:Aa:59:PRO:O	1:Aa:66:VAL:HG22	2.15	0.46
1:Ag:59:PRO:O	1:Ag:66:VAL:HG22	2.15	0.46
1:Aj:59:PRO:O	1:Aj:66:VAL:HG22	2.15	0.46
1:An:59:PRO:O	1:An:66:VAL:HG22	2.15	0.46
1:Bc:77:PRO:O	1:Bd:176:ARG:NH2	2.48	0.46
1:Ae:59:PRO:O	1:Ae:66:VAL:HG22	2.15	0.46
1:Af:66:VAL:HB	1:Ag:114:LEU:CD1	2.45	0.46
1:Ah:59:PRO:O	1:Ah:66:VAL:HG22	2.15	0.46
1:Ao:44:HIS:CG	1:Ao:44:HIS:O	2.69	0.46
1:As:59:PRO:O	1:As:66:VAL:HG22	2.15	0.46
1:Ay:59:PRO:O	1:Ay:66:VAL:HG22	2.15	0.46
1:Ba:44:HIS:CG	1:Ba:44:HIS:O	2.69	0.46
1:Ai:44:HIS:O	1:Ai:44:HIS:CG	2.69	0.46
1:Av:66:VAL:HB	1:Aw:114:LEU:CD1	2.45	0.46
1:Ab:44:HIS:CG	1:Ab:44:HIS:O	2.69	0.46
1:Af:76:LYS:NZ	1:Ag:179:GLU:OE2	2.48	0.46
1:Ag:44:HIS:CG	1:Ag:44:HIS:O	2.69	0.46
1:As:66:VAL:HB	1:At:114:LEU:CD1	2.45	0.46
1:At:59:PRO:O	1:At:66:VAL:HG22	2.15	0.46
1:Au:76:LYS:NZ	1:Av:179:GLU:OE2	2.47	0.46
1:Ax:77:PRO:O	1:Ay:176:ARG:NH2	2.48	0.46
1:Az:44:HIS:O	1:Az:44:HIS:CG	2.69	0.46
1:Aa:76:LYS:NZ	1:Ab:179:GLU:OE2	2.47	0.46
1:Ag:76:LYS:NZ	1:Ah:179:GLU:OE2	2.48	0.46
1:As:44:HIS:CG	1:As:44:HIS:O	2.69	0.46
1:Bb:66:VAL:HB	1:Bc:114:LEU:CD1	2.46	0.46
1:Ad:59:PRO:O	1:Ad:66:VAL:HG22	2.15	0.46
1:Ad:66:VAL:HB	1:Ae:114:LEU:CD1	2.46	0.46
1:Ak:66:VAL:HB	1:Al:114:LEU:CD1	2.46	0.46
1:Ap:44:HIS:CG	1:Ap:44:HIS:O	2.69	0.46
1:Ar:66:VAL:HB	1:As:114:LEU:CD1	2.46	0.46
1:Ab:66:VAL:HB	1:Ac:114:LEU:CD1	2.45	0.46
1:Ak:59:PRO:O	1:Ak:66:VAL:HG22	2.15	0.46
1:Al:77:PRO:O	1:Am:176:ARG:NH2	2.48	0.46
1:Aq:66:VAL:HB	1:Ar:114:LEU:CD1	2.46	0.46
1:Aw:76:LYS:NZ	1:Ax:179:GLU:OE2	2.47	0.46
1:Ax:66:VAL:HB	1:Ay:114:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:66:VAL:HB	1:Bb:114:LEU:CD1	2.46	0.46
1:Bb:44:HIS:CG	1:Bb:44:HIS:O	2.69	0.46
1:Bd:44:HIS:CG	1:Bd:44:HIS:O	2.68	0.46
1:Bd:59:PRO:O	1:Bd:66:VAL:HG22	2.15	0.46
1:Ac:44:HIS:CG	1:Ac:44:HIS:O	2.69	0.46
1:Ad:44:HIS:CG	1:Ad:44:HIS:O	2.69	0.46
1:Ah:66:VAL:HB	1:Ai:114:LEU:CD1	2.46	0.46
1:An:44:HIS:CG	1:An:44:HIS:O	2.69	0.46
1:Ao:59:PRO:O	1:Ao:66:VAL:HG22	2.15	0.46
1:Ar:44:HIS:CG	1:Ar:44:HIS:O	2.69	0.46
1:Av:59:PRO:O	1:Av:66:VAL:HG22	2.15	0.46
1:Ax:44:HIS:CG	1:Ax:44:HIS:O	2.69	0.46
1:Bc:44:HIS:CG	1:Bc:44:HIS:O	2.69	0.46
1:Ae:226:ALA:C	1:Ae:227:LEU:HD12	2.41	0.46
1:Ao:76:LYS:NZ	1:Ap:179:GLU:OE2	2.47	0.46
1:Aq:226:ALA:C	1:Aq:227:LEU:HD12	2.41	0.46
1:Af:226:ALA:C	1:Af:227:LEU:HD12	2.41	0.46
1:Ag:226:ALA:C	1:Ag:227:LEU:HD12	2.41	0.46
1:Ap:226:ALA:C	1:Ap:227:LEU:HD12	2.41	0.46
1:At:226:ALA:C	1:At:227:LEU:HD12	2.41	0.46
1:Av:226:ALA:C	1:Av:227:LEU:HD12	2.41	0.46
1:Aw:226:ALA:C	1:Aw:227:LEU:HD12	2.41	0.46
1:Ax:226:ALA:C	1:Ax:227:LEU:HD12	2.41	0.46
1:Bb:226:ALA:C	1:Bb:227:LEU:HD12	2.41	0.46
1:Bc:226:ALA:C	1:Bc:227:LEU:HD12	2.41	0.46
1:Ac:226:ALA:C	1:Ac:227:LEU:HD12	2.41	0.45
1:Ag:66:VAL:HB	1:Ah:114:LEU:CD1	2.46	0.45
1:Ar:226:ALA:C	1:Ar:227:LEU:HD12	2.41	0.45
1:As:226:ALA:C	1:As:227:LEU:HD12	2.41	0.45
1:Az:59:PRO:O	1:Az:66:VAL:HG22	2.15	0.45
1:Ba:226:ALA:C	1:Ba:227:LEU:HD12	2.41	0.45
1:Aa:179:GLU:OE2	1:Aj:76:LYS:NZ	2.47	0.45
1:Ah:44:HIS:CG	1:Ah:44:HIS:O	2.69	0.45
1:Ai:59:PRO:O	1:Ai:66:VAL:HG22	2.15	0.45
1:Ao:226:ALA:C	1:Ao:227:LEU:HD12	2.41	0.45
1:Au:66:VAL:HB	1:Av:114:LEU:CD1	2.46	0.45
1:Aa:66:VAL:HB	1:Ab:114:LEU:CD1	2.46	0.45
1:Ac:76:LYS:NZ	1:Ad:179:GLU:OE2	2.47	0.45
1:Ad:226:ALA:C	1:Ad:227:LEU:HD12	2.42	0.45
1:Ag:47:PRO:HG3	1:As:109:SER:HB3	1.99	0.45
1:Au:226:ALA:C	1:Au:227:LEU:HD12	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:44:HIS:CG	1:Ay:44:HIS:O	2.68	0.45
1:Az:76:LYS:NZ	1:Ba:179:GLU:OE2	2.48	0.45
1:Aa:175:MET:HE2	1:Aj:73:LEU:HA	1.98	0.45
1:Ab:226:ALA:C	1:Ab:227:LEU:HD12	2.41	0.45
1:Ac:47:PRO:O	1:Ao:145:TYR:OH	2.31	0.45
1:Ac:66:VAL:HB	1:Ad:114:LEU:CD1	2.47	0.45
1:Ae:66:VAL:HB	1:Af:114:LEU:CD1	2.46	0.45
1:Ai:166:SER:HB3	1:Ai:206:GLU:HG2	1.99	0.45
1:Ak:226:ALA:C	1:Ak:227:LEU:HD12	2.41	0.45
1:Ao:66:VAL:HB	1:Ap:114:LEU:CD1	2.46	0.45
1:Au:166:SER:HB3	1:Au:206:GLU:HG2	1.99	0.45
1:Aw:44:HIS:CG	1:Aw:44:HIS:O	2.69	0.45
1:Ay:66:VAL:HB	1:Az:114:LEU:CD1	2.47	0.45
1:Aa:114:LEU:CD1	1:Aj:66:VAL:HB	2.47	0.45
1:Ae:44:HIS:CG	1:Ae:44:HIS:O	2.68	0.45
1:Ah:76:LYS:NZ	1:Ai:179:GLU:OE2	2.49	0.45
1:Ah:166:SER:HB3	1:Ah:206:GLU:HG2	1.99	0.45
1:Aj:166:SER:HB3	1:Aj:206:GLU:HG2	1.99	0.45
1:Al:166:SER:HB3	1:Al:206:GLU:HG2	1.99	0.45
1:Ap:73:LEU:HA	1:Aq:175:MET:HE2	1.99	0.45
1:Aq:47:PRO:HG3	1:Bc:109:SER:HB3	1.99	0.45
1:Av:166:SER:HB3	1:Av:206:GLU:HG2	1.99	0.45
1:Az:226:ALA:C	1:Az:227:LEU:HD12	2.42	0.45
1:Bd:166:SER:HB3	1:Bd:206:GLU:HG2	1.99	0.45
1:Bd:226:ALA:C	1:Bd:227:LEU:HD12	2.41	0.45
1:Aa:73:LEU:HA	1:Ab:175:MET:HE2	1.99	0.45
1:Ae:76:LYS:NZ	1:Af:179:GLU:OE2	2.47	0.45
1:Af:73:LEU:HA	1:Ag:175:MET:HE2	1.99	0.45
1:Ah:226:ALA:C	1:Ah:227:LEU:HD12	2.42	0.45
1:Ak:166:SER:HB3	1:Ak:206:GLU:HG2	1.99	0.45
1:Al:226:ALA:C	1:Al:227:LEU:HD12	2.41	0.45
1:Am:76:LYS:NZ	1:An:179:GLU:OE2	2.48	0.45
1:Aq:44:HIS:CG	1:Aq:44:HIS:O	2.69	0.45
1:Aq:76:LYS:NZ	1:Ar:179:GLU:OE2	2.48	0.45
1:As:166:SER:HB3	1:As:206:GLU:HG2	1.99	0.45
1:At:166:SER:HB3	1:At:206:GLU:HG2	1.99	0.45
1:Au:114:LEU:CD1	1:Bd:66:VAL:HB	2.47	0.45
1:Au:175:MET:HE2	1:Bd:73:LEU:HA	1.98	0.45
1:Aw:66:VAL:HB	1:Ax:114:LEU:CD1	2.47	0.45
1:Aa:226:ALA:C	1:Aa:227:LEU:HD12	2.41	0.45
1:Ae:73:LEU:HA	1:Af:175:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aj:226:ALA:C	1:Aj:227:LEU:HD12	2.41	0.45
1:Al:44:HIS:CG	1:Al:44:HIS:O	2.69	0.45
1:An:66:VAL:HB	1:Ao:114:LEU:CD1	2.46	0.45
1:Ay:226:ALA:C	1:Ay:227:LEU:HD12	2.41	0.45
1:Aa:166:SER:HB3	1:Aa:206:GLU:HG2	1.99	0.45
1:Ab:166:SER:HB3	1:Ab:206:GLU:HG2	1.99	0.45
1:Aj:44:HIS:CG	1:Aj:44:HIS:O	2.69	0.45
1:Am:44:HIS:O	1:Am:44:HIS:CG	2.69	0.45
1:Ar:166:SER:HB3	1:Ar:206:GLU:HG2	1.99	0.45
1:Ai:76:LYS:NZ	1:Aj:179:GLU:OE2	2.50	0.45
1:Bc:166:SER:HB3	1:Bc:206:GLU:HG2	1.99	0.45
1:Am:66:VAL:HB	1:An:114:LEU:CD1	2.47	0.45
1:Am:166:SER:HB3	1:Am:206:GLU:HG2	1.99	0.45
1:Aw:166:SER:HB3	1:Aw:206:GLU:HG2	1.99	0.45
1:Ay:76:LYS:NZ	1:Az:179:GLU:OE2	2.47	0.45
1:Az:73:LEU:HA	1:Ba:175:MET:HE2	1.99	0.45
1:Ai:226:ALA:C	1:Ai:227:LEU:HD12	2.41	0.44
1:Ak:73:LEU:HA	1:Al:175:MET:HE2	1.99	0.44
1:Am:226:ALA:C	1:Am:227:LEU:HD12	2.42	0.44
1:An:226:ALA:C	1:An:227:LEU:HD12	2.41	0.44
1:Ao:73:LEU:HA	1:Ap:175:MET:HE2	1.99	0.44
1:Au:44:HIS:CG	1:Au:44:HIS:O	2.69	0.44
1:Aw:73:LEU:HA	1:Ax:175:MET:HE2	1.99	0.44
1:Ak:44:HIS:CG	1:Ak:44:HIS:O	2.69	0.44
1:Ak:114:LEU:CD1	1:At:66:VAL:HB	2.47	0.44
1:Am:47:PRO:HG3	1:Ay:109:SER:HB3	1.99	0.44
1:Au:179:GLU:OE2	1:Bd:76:LYS:NZ	2.47	0.44
1:Bb:166:SER:HB3	1:Bb:206:GLU:HG2	1.99	0.44
1:Bc:76:LYS:NZ	1:Bd:179:GLU:OE2	2.50	0.44
1:Ap:96:TYR:OH	1:Ap:107:GLU:OE1	2.35	0.44
1:Ar:47:PRO:HG3	1:Bd:109:SER:HB3	2.00	0.44
1:As:47:PRO:HG3	1:Au:109:SER:HB3	1.99	0.44
1:Aa:44:HIS:O	1:Aa:44:HIS:CG	2.69	0.44
1:Af:44:HIS:CG	1:Af:44:HIS:O	2.69	0.44
1:Ag:166:SER:HB3	1:Ag:206:GLU:HG2	1.99	0.44
1:Am:73:LEU:HA	1:An:175:MET:HE2	1.99	0.44
1:At:44:HIS:CG	1:At:44:HIS:O	2.69	0.44
1:Ba:73:LEU:HA	1:Bb:175:MET:HE2	2.00	0.44
1:Ac:166:SER:HB3	1:Ac:206:GLU:HG2	1.99	0.44
1:Ah:47:PRO:HG3	1:At:109:SER:HB3	2.00	0.44
1:Ak:175:MET:HE2	1:At:73:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aq:73:LEU:HA	1:Ar:175:MET:HE2	2.00	0.44
1:Af:47:PRO:HG3	1:Ar:109:SER:HB3	2.00	0.44
1:Aq:166:SER:HB3	1:Aq:206:GLU:HG2	1.99	0.44
1:Bb:73:LEU:HA	1:Bc:175:MET:HE2	2.00	0.44
1:Bb:76:LYS:NZ	1:Bc:179:GLU:OE2	2.49	0.44
1:Ac:47:PRO:HG3	1:Ao:109:SER:HB3	2.00	0.44
1:Ao:47:PRO:HG3	1:Ba:109:SER:HB3	2.00	0.44
1:Ao:166:SER:HB3	1:Ao:206:GLU:HG2	1.99	0.44
1:Ap:47:PRO:HG3	1:Bb:109:SER:HB3	2.00	0.44
1:Aq:47:PRO:O	1:Bc:145:TYR:OH	2.31	0.44
1:Ar:173:ILE:HG21	1:Ar:198:ALA:O	2.18	0.44
1:As:173:ILE:HG21	1:As:198:ALA:O	2.18	0.44
1:Bb:173:ILE:HG21	1:Bb:198:ALA:O	2.18	0.44
1:Aa:173:ILE:HG21	1:Aa:198:ALA:O	2.18	0.44
1:Ap:166:SER:HB3	1:Ap:206:GLU:HG2	1.99	0.44
1:Au:173:ILE:HG21	1:Au:198:ALA:O	2.18	0.44
1:Av:173:ILE:HG21	1:Av:198:ALA:O	2.18	0.44
1:An:166:SER:HB3	1:An:206:GLU:HG2	1.99	0.44
1:Ap:47:PRO:O	1:Bb:145:TYR:OH	2.30	0.44
1:Ar:73:LEU:HA	1:As:175:MET:HE2	2.00	0.44
1:Av:44:HIS:CG	1:Av:44:HIS:O	2.69	0.44
1:Ax:166:SER:HB3	1:Ax:206:GLU:HG2	1.99	0.44
1:Ad:47:PRO:O	1:Ap:145:TYR:OH	2.30	0.43
1:Ae:47:PRO:HG3	1:Aq:109:SER:HB3	2.00	0.43
1:Ag:73:LEU:HA	1:Ah:175:MET:HE2	2.00	0.43
1:Ai:47:PRO:HG3	1:Ak:109:SER:HB3	2.00	0.43
1:Ai:173:ILE:HG21	1:Ai:198:ALA:O	2.18	0.43
1:Aj:47:PRO:O	1:Al:145:TYR:OH	2.29	0.43
1:Ak:47:PRO:O	1:Aw:145:TYR:OH	2.32	0.43
1:Ak:173:ILE:HG21	1:Ak:198:ALA:O	2.18	0.43
1:An:47:PRO:HG3	1:Az:109:SER:HB3	2.00	0.43
1:Ap:76:LYS:NZ	1:Aq:179:GLU:OE2	2.48	0.43
1:Aq:173:ILE:HG21	1:Aq:198:ALA:O	2.18	0.43
1:Au:73:LEU:HA	1:Av:175:MET:HE2	1.99	0.43
1:Ba:166:SER:HB3	1:Ba:206:GLU:HG2	1.99	0.43
1:Bd:173:ILE:HG21	1:Bd:198:ALA:O	2.18	0.43
1:Ad:47:PRO:HG3	1:Ap:109:SER:HB3	2.00	0.43
1:Ad:166:SER:HB3	1:Ad:206:GLU:HG2	1.99	0.43
1:Af:173:ILE:HG21	1:Af:198:ALA:O	2.18	0.43
1:Ah:173:ILE:HG21	1:Ah:198:ALA:O	2.18	0.43
1:Am:173:ILE:HG21	1:Am:198:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:47:PRO:O	1:Au:145:TYR:OH	2.32	0.43
1:At:173:ILE:HG21	1:At:198:ALA:O	2.18	0.43
1:Az:166:SER:HB3	1:Az:206:GLU:HG2	1.99	0.43
1:Ai:47:PRO:O	1:Ak:145:TYR:OH	2.32	0.43
1:Aw:173:ILE:HG21	1:Aw:198:ALA:O	2.18	0.43
1:Ay:73:LEU:HA	1:Az:175:MET:HE2	1.99	0.43
1:Af:166:SER:HB3	1:Af:206:GLU:HG2	1.99	0.43
1:Ak:47:PRO:HG3	1:Aw:109:SER:HB3	2.00	0.43
1:Ao:118:MET:HE2	1:Ao:118:MET:HB3	1.94	0.43
1:At:47:PRO:HG3	1:Av:109:SER:HB3	2.00	0.43
1:Ay:166:SER:HB3	1:Ay:206:GLU:HG2	1.99	0.43
1:Bc:96:TYR:OH	1:Bc:107:GLU:OE1	2.35	0.43
1:Ab:76:LYS:NZ	1:Ac:179:GLU:OE2	2.50	0.43
1:Ab:173:ILE:HG21	1:Ab:198:ALA:O	2.18	0.43
1:Ac:73:LEU:HA	1:Ad:175:MET:HE2	1.99	0.43
1:Ah:73:LEU:HA	1:Ai:175:MET:HE2	2.00	0.43
1:Ap:173:ILE:HG21	1:Ap:198:ALA:O	2.18	0.43
1:Aq:137:MET:HE3	1:Aq:137:MET:HB3	1.96	0.43
1:Ar:47:PRO:O	1:Bd:145:TYR:OH	2.32	0.43
1:Bc:173:ILE:HG21	1:Bc:198:ALA:O	2.18	0.43
1:Ac:173:ILE:HG21	1:Ac:198:ALA:O	2.18	0.43
1:Af:125:GLY:HA2	1:Af:203:ASP:HB2	2.01	0.43
1:Ak:76:LYS:NZ	1:Al:179:GLU:OE2	2.47	0.43
1:Aq:125:GLY:HA2	1:Aq:203:ASP:HB2	2.01	0.43
1:Ae:166:SER:HB3	1:Ae:206:GLU:HG2	1.99	0.43
1:Ae:173:ILE:HG21	1:Ae:198:ALA:O	2.18	0.43
1:Ag:173:ILE:HG21	1:Ag:198:ALA:O	2.18	0.43
1:Ax:173:ILE:HG21	1:Ax:198:ALA:O	2.18	0.43
1:Ad:173:ILE:HG21	1:Ad:198:ALA:O	2.18	0.43
1:Af:96:TYR:OH	1:Af:107:GLU:OE1	2.35	0.43
1:Ak:96:TYR:OH	1:Ak:107:GLU:OE1	2.35	0.43
1:Al:57:THR:O	1:Al:57:THR:OG1	2.35	0.43
1:Ay:173:ILE:HG21	1:Ay:198:ALA:O	2.18	0.43
1:Bb:125:GLY:HA2	1:Bb:203:ASP:HB2	2.01	0.43
1:Aj:173:ILE:HG21	1:Aj:198:ALA:O	2.18	0.43
1:Al:173:ILE:HG21	1:Al:198:ALA:O	2.18	0.43
1:Am:118:MET:HE2	1:Am:118:MET:HB3	1.94	0.43
1:Ae:125:GLY:HA2	1:Ae:203:ASP:HB2	2.01	0.43
1:Al:73:LEU:HA	1:Am:175:MET:HE2	2.01	0.43
1:Ap:125:GLY:HA2	1:Ap:203:ASP:HB2	2.01	0.43
1:Ay:189:GLN:CG	1:Ay:190:ARG:NH1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:189:GLN:CG	1:Ad:190:ARG:NH1	2.82	0.42
1:Ae:189:GLN:CG	1:Ae:190:ARG:NH1	2.82	0.42
1:Ai:148:LYS:HB2	1:Ai:149:PRO:HD3	2.01	0.42
1:Aj:226:ALA:O	1:Aj:227:LEU:HD12	2.19	0.42
1:Al:96:TYR:OH	1:Al:107:GLU:OE1	2.35	0.42
1:Ao:189:GLN:CG	1:Ao:190:ARG:NH1	2.82	0.42
1:Ar:189:GLN:CG	1:Ar:190:ARG:NH1	2.82	0.42
1:At:148:LYS:HB2	1:At:149:PRO:HD3	2.01	0.42
1:Av:226:ALA:O	1:Av:227:LEU:HD12	2.20	0.42
1:Ay:125:GLY:HA2	1:Ay:203:ASP:HB2	2.01	0.42
1:Az:173:ILE:HG21	1:Az:198:ALA:O	2.18	0.42
1:Ba:125:GLY:HA2	1:Ba:203:ASP:HB2	2.01	0.42
1:Ba:173:ILE:HG21	1:Ba:198:ALA:O	2.18	0.42
1:Ac:226:ALA:O	1:Ac:227:LEU:HD12	2.19	0.42
1:Ag:125:GLY:HA2	1:Ag:203:ASP:HB2	2.01	0.42
1:Ah:189:GLN:CG	1:Ah:190:ARG:NH1	2.82	0.42
1:Ak:92:PHE:CE2	1:At:61:LEU:HD23	2.54	0.42
1:An:76:LYS:NZ	1:Ao:179:GLU:OE2	2.50	0.42
1:An:125:GLY:HA2	1:An:203:ASP:HB2	2.01	0.42
1:Ao:173:ILE:HG21	1:Ao:198:ALA:O	2.18	0.42
1:Ap:61:LEU:HD23	1:Aq:92:PHE:CE2	2.54	0.42
1:As:76:LYS:NZ	1:At:179:GLU:OE2	2.50	0.42
1:Bb:148:LYS:HB2	1:Bb:149:PRO:HD3	2.01	0.42
1:Bb:189:GLN:CG	1:Bb:190:ARG:NH1	2.82	0.42
1:Bc:189:GLN:CG	1:Bc:190:ARG:NH1	2.83	0.42
1:Aa:59:PRO:HG3	1:Ab:165:PHE:HA	2.01	0.42
1:Ab:73:LEU:HA	1:Ac:175:MET:HE2	2.01	0.42
1:Ac:125:GLY:HA2	1:Ac:203:ASP:HB2	2.01	0.42
1:Ac:189:GLN:CG	1:Ac:190:ARG:NH1	2.83	0.42
1:Ai:189:GLN:CG	1:Ai:190:ARG:NH1	2.82	0.42
1:Aj:148:LYS:HB2	1:Aj:149:PRO:HD3	2.01	0.42
1:An:189:GLN:CG	1:An:190:ARG:NH1	2.82	0.42
1:Ap:189:GLN:CG	1:Ap:190:ARG:NH1	2.83	0.42
1:Aq:148:LYS:HB2	1:Aq:149:PRO:HD3	2.01	0.42
1:Aq:189:GLN:CG	1:Aq:190:ARG:NH1	2.82	0.42
1:Ar:125:GLY:HA2	1:Ar:203:ASP:HB2	2.01	0.42
1:As:189:GLN:CG	1:As:190:ARG:NH1	2.83	0.42
1:Au:61:LEU:HD23	1:Av:92:PHE:CE2	2.55	0.42
1:Au:148:LYS:HB2	1:Au:149:PRO:HD3	2.01	0.42
1:Ax:125:GLY:HA2	1:Ax:203:ASP:HB2	2.01	0.42
1:Bc:73:LEU:HA	1:Bd:175:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bd:189:GLN:CG	1:Bd:190:ARG:NH1	2.82	0.42
1:Ad:76:LYS:NZ	1:Ae:179:GLU:OE2	2.50	0.42
1:Ad:137:MET:HE3	1:Ad:137:MET:HB3	1.96	0.42
1:Ak:148:LYS:HB2	1:Ak:149:PRO:HD3	2.01	0.42
1:Ak:226:ALA:O	1:Ak:227:LEU:HD12	2.20	0.42
1:Al:226:ALA:O	1:Al:227:LEU:HD12	2.20	0.42
1:Am:125:GLY:HA2	1:Am:203:ASP:HB2	2.01	0.42
1:Am:226:ALA:O	1:Am:227:LEU:HD12	2.20	0.42
1:An:173:ILE:HG21	1:An:198:ALA:O	2.18	0.42
1:At:96:TYR:OH	1:At:107:GLU:OE1	2.35	0.42
1:At:226:ALA:O	1:At:227:LEU:HD12	2.20	0.42
1:Au:92:PHE:CE2	1:Bd:61:LEU:HD23	2.54	0.42
1:Av:61:LEU:HD23	1:Aw:92:PHE:CE2	2.55	0.42
1:Ba:61:LEU:HD23	1:Bb:92:PHE:CE2	2.55	0.42
1:Ba:189:GLN:CG	1:Ba:190:ARG:NH1	2.82	0.42
1:Aa:61:LEU:HD23	1:Ab:92:PHE:CE2	2.55	0.42
1:Ab:61:LEU:HD23	1:Ac:92:PHE:CE2	2.55	0.42
1:Ad:73:LEU:HA	1:Ae:175:MET:HE2	2.01	0.42
1:Af:61:LEU:HD23	1:Ag:92:PHE:CE2	2.54	0.42
1:Af:189:GLN:CG	1:Af:190:ARG:NH1	2.83	0.42
1:Ao:57:THR:O	1:Ao:57:THR:OG1	2.35	0.42
1:Ao:61:LEU:HD23	1:Ap:92:PHE:CE2	2.55	0.42
1:Aq:61:LEU:HD23	1:Ar:92:PHE:CE2	2.55	0.42
1:Ar:206:GLU:O	1:Ar:208:THR:HG23	2.20	0.42
1:Ax:73:LEU:HA	1:Ay:175:MET:HE2	2.01	0.42
1:Az:61:LEU:HD23	1:Ba:92:PHE:CE2	2.54	0.42
1:Az:189:GLN:CG	1:Az:190:ARG:NH1	2.83	0.42
1:Ba:206:GLU:O	1:Ba:208:THR:HG23	2.20	0.42
1:Ab:59:PRO:HG3	1:Ac:165:PHE:HA	2.02	0.42
1:Ab:189:GLN:CG	1:Ab:190:ARG:NH1	2.82	0.42
1:Af:148:LYS:HB2	1:Af:149:PRO:HD3	2.01	0.42
1:Ag:148:LYS:HB2	1:Ag:149:PRO:HD3	2.01	0.42
1:Ak:59:PRO:HG3	1:Al:165:PHE:HA	2.01	0.42
1:Ak:61:LEU:HD23	1:Al:92:PHE:CE2	2.55	0.42
1:Al:47:PRO:HG3	1:Ax:109:SER:HB3	2.01	0.42
1:Aq:113:ILE:HD13	1:Aq:113:ILE:HA	1.89	0.42
1:As:206:GLU:O	1:As:208:THR:HG23	2.20	0.42
1:As:226:ALA:O	1:As:227:LEU:HD12	2.19	0.42
1:Aw:226:ALA:O	1:Aw:227:LEU:HD12	2.19	0.42
1:Ax:57:THR:O	1:Ax:57:THR:OG1	2.35	0.42
1:Ax:76:LYS:NZ	1:Ay:179:GLU:OE2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ax:96:TYR:OH	1:Ax:107:GLU:OE1	2.35	0.42
1:Ax:226:ALA:O	1:Ax:227:LEU:HD12	2.19	0.42
1:Ba:148:LYS:HB2	1:Ba:149:PRO:HD3	2.01	0.42
1:Ab:57:THR:O	1:Ab:57:THR:OG1	2.35	0.42
1:Ab:125:GLY:HA2	1:Ab:203:ASP:HB2	2.01	0.42
1:Af:59:PRO:HG3	1:Ag:165:PHE:HA	2.01	0.42
1:Ai:226:ALA:O	1:Ai:227:LEU:HD12	2.19	0.42
1:Al:189:GLN:CG	1:Al:190:ARG:NH1	2.82	0.42
1:Ar:148:LYS:HB2	1:Ar:149:PRO:HD3	2.01	0.42
1:As:73:LEU:HA	1:At:175:MET:HE2	2.01	0.42
1:Au:189:GLN:CG	1:Au:190:ARG:NH1	2.82	0.42
1:Av:73:LEU:HA	1:Aw:175:MET:HE2	2.01	0.42
1:Av:148:LYS:HB2	1:Av:149:PRO:HD3	2.01	0.42
1:Ax:189:GLN:CG	1:Ax:190:ARG:NH1	2.82	0.42
1:Ay:226:ALA:O	1:Ay:227:LEU:HD12	2.20	0.42
1:Az:206:GLU:O	1:Az:208:THR:HG23	2.20	0.42
1:Bb:61:LEU:HD23	1:Bc:92:PHE:CE2	2.55	0.42
1:Bb:96:TYR:OH	1:Bb:107:GLU:OE1	2.35	0.42
1:Aa:47:PRO:HG3	1:Am:109:SER:HB3	2.01	0.42
1:Aa:226:ALA:O	1:Aa:227:LEU:HD12	2.20	0.42
1:Ab:96:TYR:OH	1:Ab:107:GLU:OE1	2.35	0.42
1:Ae:206:GLU:O	1:Ae:208:THR:HG23	2.20	0.42
1:Al:76:LYS:NZ	1:Am:179:GLU:OE2	2.50	0.42
1:Am:189:GLN:CG	1:Am:190:ARG:NH1	2.83	0.42
1:At:206:GLU:O	1:At:208:THR:HG23	2.20	0.42
1:Au:226:ALA:O	1:Au:227:LEU:HD12	2.20	0.42
1:Av:137:MET:HE3	1:Av:137:MET:HB3	1.96	0.42
1:Av:189:GLN:CG	1:Av:190:ARG:NH1	2.83	0.42
1:Bb:113:ILE:HD13	1:Bb:113:ILE:HA	1.89	0.42
1:Bb:206:GLU:O	1:Bb:208:THR:HG23	2.20	0.42
1:Bc:125:GLY:HA2	1:Bc:203:ASP:HB2	2.01	0.42
1:Bc:148:LYS:HB2	1:Bc:149:PRO:HD3	2.01	0.42
1:Aa:189:GLN:CG	1:Aa:190:ARG:NH1	2.82	0.42
1:Ab:226:ALA:O	1:Ab:227:LEU:HD12	2.20	0.42
1:Ae:96:TYR:OH	1:Ae:107:GLU:OE1	2.35	0.42
1:Ag:61:LEU:HD23	1:Ah:92:PHE:CE2	2.55	0.42
1:Ag:189:GLN:CG	1:Ag:190:ARG:NH1	2.82	0.42
1:Ai:206:GLU:O	1:Ai:208:THR:HG23	2.20	0.42
1:Aj:47:PRO:HG3	1:Al:109:SER:HB3	2.01	0.42
1:Aj:206:GLU:O	1:Aj:208:THR:HG23	2.20	0.42
1:Ak:118:MET:HE2	1:Ak:118:MET:HB3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:189:GLN:CG	1:Ak:190:ARG:NH1	2.82	0.42
1:Ap:148:LYS:HB2	1:Ap:149:PRO:HD3	2.01	0.42
1:Ar:61:LEU:HD23	1:As:92:PHE:CE2	2.55	0.42
1:Au:59:PRO:HG3	1:Av:165:PHE:HA	2.01	0.42
1:Av:59:PRO:HG3	1:Aw:165:PHE:HA	2.02	0.42
1:Aw:125:GLY:HA2	1:Aw:203:ASP:HB2	2.01	0.42
1:Bc:226:ALA:O	1:Bc:227:LEU:HD12	2.19	0.42
1:Bd:148:LYS:HB2	1:Bd:149:PRO:HD3	2.01	0.42
1:Aa:57:THR:O	1:Aa:57:THR:OG1	2.35	0.42
1:Aa:92:PHE:CE2	1:Aj:61:LEU:HD23	2.54	0.42
1:Ac:61:LEU:HD23	1:Ad:92:PHE:CE2	2.55	0.42
1:Ac:118:MET:HE2	1:Ac:118:MET:HB3	1.94	0.42
1:Ad:125:GLY:HA2	1:Ad:203:ASP:HB2	2.01	0.42
1:Ad:206:GLU:O	1:Ad:208:THR:HG23	2.20	0.42
1:Af:113:ILE:HD13	1:Af:113:ILE:HA	1.89	0.42
1:Af:206:GLU:O	1:Af:208:THR:HG23	2.20	0.42
1:Aj:189:GLN:CG	1:Aj:190:ARG:NH1	2.82	0.42
1:Al:125:GLY:HA2	1:Al:203:ASP:HB2	2.01	0.42
1:Ao:96:TYR:OH	1:Ao:107:GLU:OE1	2.35	0.42
1:Ao:125:GLY:HA2	1:Ao:203:ASP:HB2	2.01	0.42
1:Aq:206:GLU:O	1:Aq:208:THR:HG23	2.20	0.42
1:As:148:LYS:HB2	1:As:149:PRO:HD3	2.01	0.42
1:Bc:206:GLU:O	1:Bc:208:THR:HG23	2.20	0.42
1:Ae:61:LEU:HD23	1:Af:92:PHE:CE2	2.55	0.41
1:Ah:206:GLU:O	1:Ah:208:THR:HG23	2.20	0.41
1:Al:59:PRO:HG3	1:Am:165:PHE:HA	2.02	0.41
1:Ap:59:PRO:HG3	1:Aq:165:PHE:HA	2.01	0.41
1:Aw:61:LEU:HD23	1:Ax:92:PHE:CE2	2.55	0.41
1:Aa:125:GLY:HA2	1:Aa:203:ASP:HB2	2.01	0.41
1:Ad:226:ALA:O	1:Ad:227:LEU:HD12	2.20	0.41
1:Ae:148:LYS:HB2	1:Ae:149:PRO:HD3	2.01	0.41
1:Ak:125:GLY:HA2	1:Ak:203:ASP:HB2	2.01	0.41
1:At:189:GLN:CG	1:At:190:ARG:NH1	2.82	0.41
1:Av:125:GLY:HA2	1:Av:203:ASP:HB2	2.01	0.41
1:Av:177:SER:O	1:Av:177:SER:OG	2.37	0.41
1:Ay:206:GLU:O	1:Ay:208:THR:HG23	2.20	0.41
1:Ba:226:ALA:O	1:Ba:227:LEU:HD12	2.20	0.41
1:Bd:226:ALA:O	1:Bd:227:LEU:HD12	2.19	0.41
1:Aa:148:LYS:HB2	1:Aa:149:PRO:HD3	2.01	0.41
1:Aa:165:PHE:HA	1:Aj:59:PRO:HG3	2.02	0.41
1:Ac:206:GLU:O	1:Ac:208:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ah:61:LEU:HD23	1:Ai:92:PHE:CE2	2.55	0.41
1:Ah:148:LYS:HB2	1:Ah:149:PRO:HD3	2.01	0.41
1:Aj:96:TYR:OH	1:Aj:107:GLU:OE1	2.35	0.41
1:Aj:125:GLY:HA2	1:Aj:203:ASP:HB2	2.01	0.41
1:Al:61:LEU:HD23	1:Am:92:PHE:CE2	2.55	0.41
1:Am:206:GLU:O	1:Am:208:THR:HG23	2.20	0.41
1:An:72:LEU:HD21	1:Ao:118:MET:HE1	2.03	0.41
1:Ao:47:PRO:O	1:Ba:145:TYR:OH	2.30	0.41
1:Ao:226:ALA:O	1:Ao:227:LEU:HD12	2.20	0.41
1:Ap:137:MET:HE3	1:Ap:137:MET:HB3	1.96	0.41
1:Aw:189:GLN:CG	1:Aw:190:ARG:NH1	2.82	0.41
1:Ax:59:PRO:HG3	1:Ay:165:PHE:HA	2.02	0.41
1:Ay:148:LYS:HB2	1:Ay:149:PRO:HD3	2.01	0.41
1:Az:59:PRO:HG3	1:Ba:165:PHE:HA	2.01	0.41
1:Az:125:GLY:HA2	1:Az:203:ASP:HB2	2.01	0.41
1:Aa:206:GLU:O	1:Aa:208:THR:HG23	2.20	0.41
1:Ab:72:LEU:HD21	1:Ac:118:MET:HE1	2.03	0.41
1:Ag:226:ALA:O	1:Ag:227:LEU:HD12	2.19	0.41
1:An:148:LYS:HB2	1:An:149:PRO:HD3	2.01	0.41
1:Ao:137:MET:HE3	1:Ao:137:MET:HB3	1.96	0.41
1:Ap:226:ALA:O	1:Ap:227:LEU:HD12	2.19	0.41
1:At:125:GLY:HA2	1:At:203:ASP:HB2	2.01	0.41
1:Aw:137:MET:HE3	1:Aw:137:MET:HB3	1.96	0.41
1:Ax:148:LYS:HB2	1:Ax:149:PRO:HD3	2.01	0.41
1:Ay:59:PRO:HG3	1:Az:165:PHE:HA	2.02	0.41
1:Bb:226:ALA:O	1:Bb:227:LEU:HD12	2.20	0.41
1:Bd:118:MET:HE2	1:Bd:118:MET:HB3	1.93	0.41
1:Ab:47:PRO:HG3	1:An:109:SER:HB3	2.02	0.41
1:Ad:72:LEU:HD21	1:Ae:118:MET:HE1	2.03	0.41
1:Ad:148:LYS:HB2	1:Ad:149:PRO:HD3	2.01	0.41
1:Ag:47:PRO:O	1:As:145:TYR:OH	2.32	0.41
1:Ag:59:PRO:HG3	1:Ah:165:PHE:HA	2.02	0.41
1:Ak:206:GLU:O	1:Ak:208:THR:HG23	2.20	0.41
1:Al:148:LYS:HB2	1:Al:149:PRO:HD3	2.01	0.41
1:Al:206:GLU:O	1:Al:208:THR:HG23	2.20	0.41
1:Au:125:GLY:HA2	1:Au:203:ASP:HB2	2.01	0.41
1:Au:137:MET:HE3	1:Au:137:MET:HB3	1.96	0.41
1:Aw:59:PRO:HG3	1:Ax:165:PHE:HA	2.03	0.41
1:Ab:206:GLU:O	1:Ab:208:THR:HG23	2.20	0.41
1:Ak:165:PHE:HA	1:At:59:PRO:HG3	2.02	0.41
1:Am:61:LEU:HD23	1:An:92:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:An:59:PRO:HG3	1:Ao:165:PHE:HA	2.03	0.41
1:An:73:LEU:HA	1:Ao:175:MET:HE2	2.01	0.41
1:Aq:59:PRO:HG3	1:Ar:165:PHE:HA	2.02	0.41
1:As:57:THR:O	1:As:57:THR:OG1	2.35	0.41
1:As:96:TYR:OH	1:As:107:GLU:OE1	2.35	0.41
1:Ay:61:LEU:HD23	1:Az:92:PHE:CE2	2.55	0.41
1:Az:226:ALA:O	1:Az:227:LEU:HD12	2.20	0.41
1:Bb:59:PRO:HG3	1:Bc:165:PHE:HA	2.02	0.41
1:Bc:61:LEU:HD23	1:Bd:92:PHE:CE2	2.56	0.41
1:Bd:137:MET:HE3	1:Bd:137:MET:HB3	1.96	0.41
1:Aa:72:LEU:HD21	1:Ab:118:MET:HE1	2.02	0.41
1:Ac:59:PRO:HG3	1:Ad:165:PHE:HA	2.02	0.41
1:Af:226:ALA:O	1:Af:227:LEU:HD12	2.20	0.41
1:Ah:125:GLY:HA2	1:Ah:203:ASP:HB2	2.01	0.41
1:Ai:73:LEU:HA	1:Aj:175:MET:HE2	2.01	0.41
1:Ai:125:GLY:HA2	1:Ai:203:ASP:HB2	2.01	0.41
1:Am:59:PRO:HG3	1:An:165:PHE:HA	2.02	0.41
1:Am:148:LYS:HB2	1:Am:149:PRO:HD3	2.01	0.41
1:Ao:59:PRO:HG3	1:Ap:165:PHE:HA	2.02	0.41
1:Ao:148:LYS:HB2	1:Ao:149:PRO:HD3	2.01	0.41
1:Ap:206:GLU:O	1:Ap:208:THR:HG23	2.20	0.41
1:Ar:59:PRO:HG3	1:As:165:PHE:HA	2.02	0.41
1:Au:57:THR:O	1:Au:57:THR:OG1	2.35	0.41
1:Ax:72:LEU:HD21	1:Ay:118:MET:HE1	2.03	0.41
1:Ax:206:GLU:O	1:Ax:208:THR:HG23	2.20	0.41
1:Ba:76:LYS:NZ	1:Bb:179:GLU:OE2	2.48	0.41
1:Af:118:MET:HE2	1:Af:118:MET:HB3	1.94	0.41
1:Ah:226:ALA:O	1:Ah:227:LEU:HD12	2.20	0.41
1:An:61:LEU:HD23	1:Ao:92:PHE:CE2	2.56	0.41
1:As:61:LEU:HD23	1:At:92:PHE:CE2	2.56	0.41
1:At:100:MET:HA	1:At:110:MET:HE3	2.03	0.41
1:Au:206:GLU:O	1:Au:208:THR:HG23	2.20	0.41
1:Av:206:GLU:O	1:Av:208:THR:HG23	2.20	0.41
1:Aw:148:LYS:HB2	1:Aw:149:PRO:HD3	2.01	0.41
1:Ay:57:THR:O	1:Ay:57:THR:OG1	2.35	0.41
1:Az:72:LEU:HD21	1:Ba:118:MET:HE1	2.03	0.41
1:Bd:100:MET:HA	1:Bd:110:MET:HE3	2.03	0.41
1:Ab:137:MET:HE3	1:Ab:137:MET:HB3	1.96	0.41
1:Ab:148:LYS:HB2	1:Ab:149:PRO:HD3	2.01	0.41
1:Ac:148:LYS:HB2	1:Ac:149:PRO:HD3	2.01	0.41
1:Ad:59:PRO:HG3	1:Ae:165:PHE:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ad:96:TYR:OH	1:Ad:107:GLU:OE1	2.35	0.41
1:Ae:226:ALA:O	1:Ae:227:LEU:HD12	2.20	0.41
1:Af:47:PRO:O	1:Ar:145:TYR:OH	2.30	0.41
1:Ag:100:MET:HA	1:Ag:110:MET:HE3	2.03	0.41
1:Ag:206:GLU:O	1:Ag:208:THR:HG23	2.20	0.41
1:Ah:59:PRO:HG3	1:Ai:165:PHE:HA	2.02	0.41
1:Ai:100:MET:HA	1:Ai:110:MET:HE3	2.03	0.41
1:Ak:158:LEU:HD12	1:Ak:158:LEU:HA	1.92	0.41
1:Al:72:LEU:HD21	1:Am:118:MET:HE1	2.03	0.41
1:An:206:GLU:O	1:An:208:THR:HG23	2.20	0.41
1:An:226:ALA:O	1:An:227:LEU:HD12	2.20	0.41
1:Ao:206:GLU:O	1:Ao:208:THR:HG23	2.20	0.41
1:Aq:226:ALA:O	1:Aq:227:LEU:HD12	2.20	0.41
1:Ar:100:MET:HA	1:Ar:110:MET:HE3	2.03	0.41
1:As:125:GLY:HA2	1:As:203:ASP:HB2	2.01	0.41
1:Au:165:PHE:HA	1:Bd:59:PRO:HG3	2.02	0.41
1:Ax:113:ILE:HD13	1:Ax:113:ILE:HA	1.89	0.41
1:Az:148:LYS:HB2	1:Az:149:PRO:HD3	2.01	0.41
1:Ba:59:PRO:HG3	1:Bb:165:PHE:HA	2.02	0.41
1:Bb:100:MET:HA	1:Bb:110:MET:HE3	2.03	0.41
1:Bb:118:MET:HE2	1:Bb:118:MET:HB3	1.94	0.41
1:Bc:137:MET:HE3	1:Bc:137:MET:HB3	1.96	0.41
1:Bd:125:GLY:HA2	1:Bd:203:ASP:HB2	2.01	0.41
1:Bd:206:GLU:O	1:Bd:208:THR:HG23	2.20	0.41
1:Ad:61:LEU:HD23	1:Ae:92:PHE:CE2	2.56	0.41
1:Ae:59:PRO:HG3	1:Af:165:PHE:HA	2.02	0.41
1:Ai:189:GLN:HB3	1:Ai:190:ARG:NH1	2.36	0.41
1:Am:189:GLN:HB3	1:Am:190:ARG:NH1	2.36	0.41
1:At:189:GLN:HB3	1:At:190:ARG:NH1	2.36	0.41
1:Au:189:GLN:HB3	1:Au:190:ARG:NH1	2.36	0.41
1:Aw:206:GLU:O	1:Aw:208:THR:HG23	2.20	0.41
1:Ah:189:GLN:HB3	1:Ah:190:ARG:NH1	2.36	0.40
1:Ai:158:LEU:HD12	1:Ai:158:LEU:HA	1.92	0.40
1:Ar:76:LYS:NZ	1:As:179:GLU:OE2	2.49	0.40
1:Ar:226:ALA:O	1:Ar:227:LEU:HD12	2.20	0.40
1:As:72:LEU:HD21	1:At:118:MET:HE1	2.02	0.40
1:Ax:189:GLN:HB3	1:Ax:190:ARG:NH1	2.36	0.40
1:Ba:96:TYR:OH	1:Ba:107:GLU:OE1	2.35	0.40
1:Am:113:ILE:HD13	1:Am:113:ILE:HA	1.89	0.40
1:Ap:72:LEU:HD21	1:Aq:118:MET:HE1	2.02	0.40
1:Ar:118:MET:HE2	1:Ar:118:MET:HB3	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:96:TYR:OH	1:Au:107:GLU:OE1	2.35	0.40
1:Au:100:MET:HA	1:Au:110:MET:HE3	2.03	0.40
1:Av:100:MET:HA	1:Av:110:MET:HE3	2.03	0.40
1:Ax:61:LEU:HD23	1:Ay:92:PHE:CE2	2.56	0.40
1:Ab:158:LEU:HD12	1:Ab:158:LEU:HA	1.92	0.40
1:Ac:137:MET:HE3	1:Ac:137:MET:HB3	1.96	0.40
1:Ai:72:LEU:HD21	1:Aj:118:MET:HE1	2.02	0.40
1:Aj:46:VAL:HG21	1:Al:138:ASP:CB	2.48	0.40
1:Aj:100:MET:HA	1:Aj:110:MET:HE3	2.03	0.40
1:An:96:TYR:OH	1:An:107:GLU:OE1	2.35	0.40
1:Au:72:LEU:HD21	1:Av:118:MET:HE1	2.02	0.40
1:Av:57:THR:O	1:Av:57:THR:OG1	2.35	0.40
1:Ac:96:TYR:OH	1:Ac:107:GLU:OE1	2.35	0.40
1:Ai:59:PRO:HG3	1:Aj:165:PHE:HA	2.03	0.40
1:Ai:61:LEU:HD23	1:Aj:92:PHE:CE2	2.56	0.40
1:Ao:72:LEU:HD21	1:Ap:118:MET:HE1	2.03	0.40
1:Ap:100:MET:HA	1:Ap:110:MET:HE3	2.03	0.40
1:Ay:72:LEU:HD21	1:Az:118:MET:HE1	2.04	0.40
1:Az:118:MET:HE2	1:Az:118:MET:HB3	1.94	0.40
1:Ba:118:MET:HE2	1:Ba:118:MET:HB3	1.93	0.40
1:Bc:59:PRO:HG3	1:Bd:165:PHE:HA	2.02	0.40
1:Bc:100:MET:HA	1:Bc:110:MET:HE3	2.03	0.40
1:Bc:113:ILE:HD13	1:Bc:113:ILE:HA	1.89	0.40
1:Aa:100:MET:HA	1:Aa:110:MET:HE3	2.03	0.40
1:Ac:72:LEU:HD21	1:Ad:118:MET:HE1	2.04	0.40
1:Ac:189:GLN:HB3	1:Ac:190:ARG:NH1	2.36	0.40
1:Ah:100:MET:HA	1:Ah:110:MET:HE3	2.03	0.40
1:Ak:72:LEU:HD21	1:Al:118:MET:HE1	2.02	0.40
1:As:59:PRO:HG3	1:At:165:PHE:HA	2.02	0.40
1:Bc:72:LEU:HD21	1:Bd:118:MET:HE1	2.02	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	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ab	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ac	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ad	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ae	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Af	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ag	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ah	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ai	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Aj	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ak	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Al	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Am	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	An	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ao	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ap	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Aq	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ar	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	As	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	At	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Au	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Av	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Aw	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ax	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ay	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Az	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Ba	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Bb	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Bc	184/269 (68%)	173 (94%)	11 (6%)	0	100	100
1	Bd	184/269 (68%)	173 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5520/8070 (68%)	5190 (94%)	330 (6%)	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	164/232 (71%)	164 (100%)	0	100	100
1	Ab	164/232 (71%)	164 (100%)	0	100	100
1	Ac	164/232 (71%)	164 (100%)	0	100	100
1	Ad	164/232 (71%)	164 (100%)	0	100	100
1	Ae	164/232 (71%)	164 (100%)	0	100	100
1	Af	164/232 (71%)	164 (100%)	0	100	100
1	Ag	164/232 (71%)	164 (100%)	0	100	100
1	Ah	164/232 (71%)	164 (100%)	0	100	100
1	Ai	164/232 (71%)	164 (100%)	0	100	100
1	Aj	164/232 (71%)	164 (100%)	0	100	100
1	Ak	164/232 (71%)	164 (100%)	0	100	100
1	Al	164/232 (71%)	164 (100%)	0	100	100
1	Am	164/232 (71%)	164 (100%)	0	100	100
1	An	164/232 (71%)	164 (100%)	0	100	100
1	Ao	164/232 (71%)	164 (100%)	0	100	100
1	Ap	164/232 (71%)	164 (100%)	0	100	100
1	Aq	164/232 (71%)	164 (100%)	0	100	100
1	Ar	164/232 (71%)	164 (100%)	0	100	100
1	As	164/232 (71%)	164 (100%)	0	100	100
1	At	164/232 (71%)	164 (100%)	0	100	100
1	Au	164/232 (71%)	164 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Av	164/232 (71%)	164 (100%)	0	100	100
1	Aw	164/232 (71%)	164 (100%)	0	100	100
1	Ax	164/232 (71%)	164 (100%)	0	100	100
1	Ay	164/232 (71%)	164 (100%)	0	100	100
1	Az	164/232 (71%)	164 (100%)	0	100	100
1	Ba	164/232 (71%)	164 (100%)	0	100	100
1	Bb	164/232 (71%)	164 (100%)	0	100	100
1	Bc	164/232 (71%)	164 (100%)	0	100	100
1	Bd	164/232 (71%)	164 (100%)	0	100	100
All	All	4920/6960 (71%)	4920 (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 (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	44	HIS
1	Aa	115	ASN
1	Ab	44	HIS
1	Ab	115	ASN
1	Ac	44	HIS
1	Ac	115	ASN
1	Ac	219	HIS
1	Ad	44	HIS
1	Ad	115	ASN
1	Ae	44	HIS
1	Ae	115	ASN
1	Af	44	HIS
1	Af	115	ASN
1	Ag	44	HIS
1	Ag	115	ASN
1	Ah	44	HIS
1	Ah	115	ASN
1	Ai	44	HIS
1	Ai	115	ASN
1	Aj	44	HIS
1	Aj	115	ASN
1	Ak	44	HIS
1	Ak	115	ASN

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Mol	Chain	Res	Type
1	Al	44	HIS
1	Al	115	ASN
1	Am	44	HIS
1	Am	115	ASN
1	An	44	HIS
1	An	115	ASN
1	Ao	44	HIS
1	Ao	115	ASN
1	Ap	44	HIS
1	Ap	115	ASN
1	Aq	44	HIS
1	Aq	115	ASN
1	Ar	44	HIS
1	Ar	115	ASN
1	As	44	HIS
1	As	115	ASN
1	At	44	HIS
1	At	115	ASN
1	Au	115	ASN
1	Av	115	ASN
1	Aw	115	ASN
1	Aw	219	HIS
1	Ax	115	ASN
1	Ay	115	ASN
1	Az	115	ASN
1	Ba	115	ASN
1	Bb	115	ASN
1	Bc	115	ASN
1	Bd	115	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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.

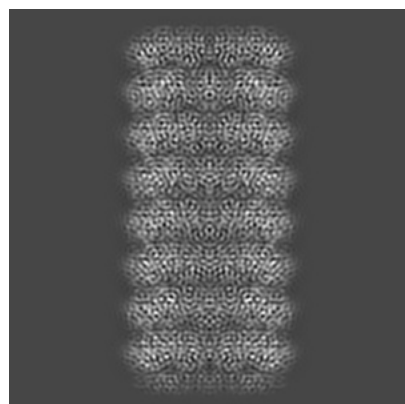
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53801. These allow visual inspection of the internal detail of the map and identification of artifacts.

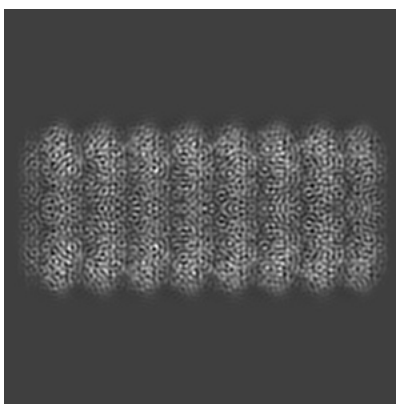
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

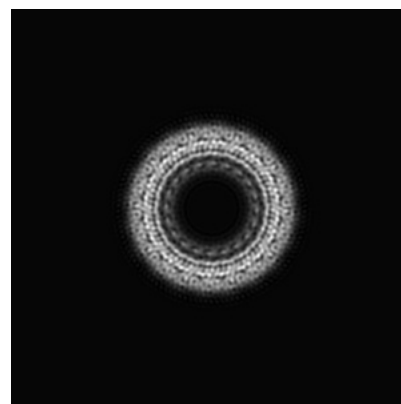
6.1.1 Primary map



X

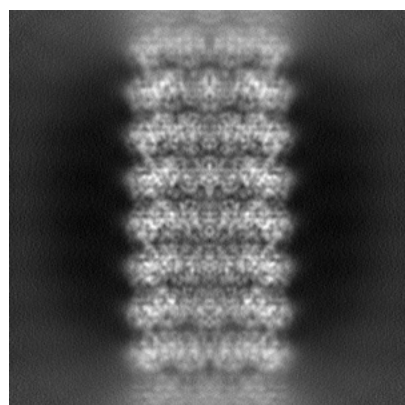


Y

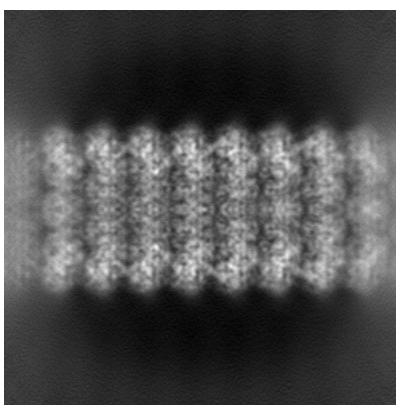


Z

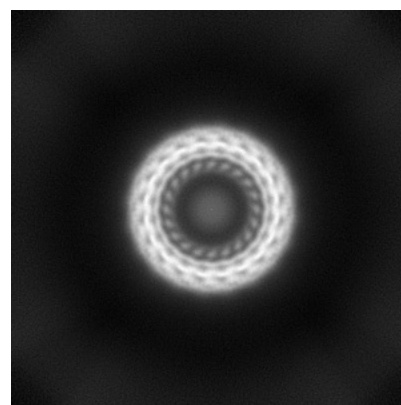
6.1.2 Raw map



X



Y

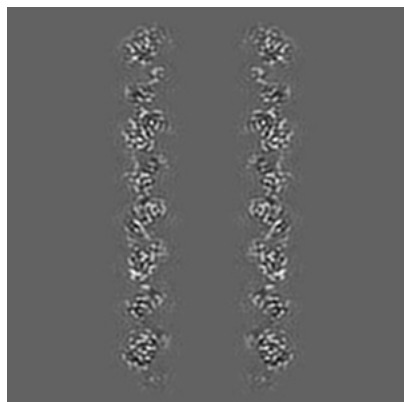


Z

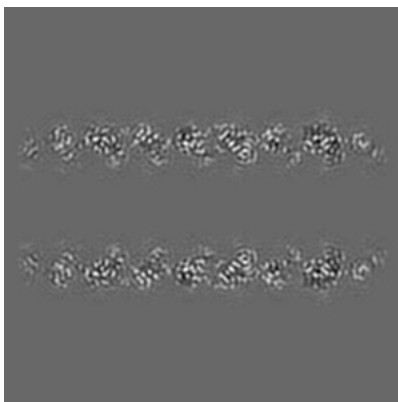
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

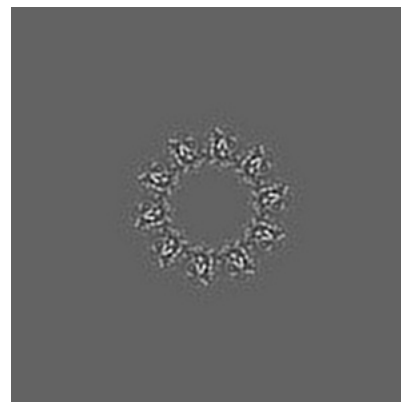
6.2.1 Primary map



X Index: 175

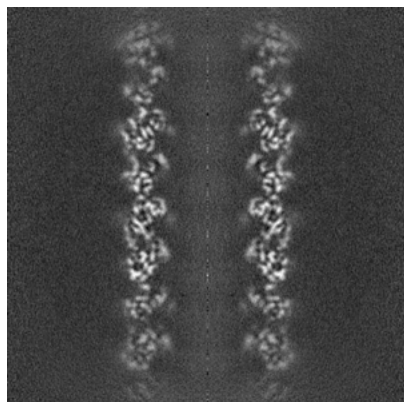


Y Index: 175

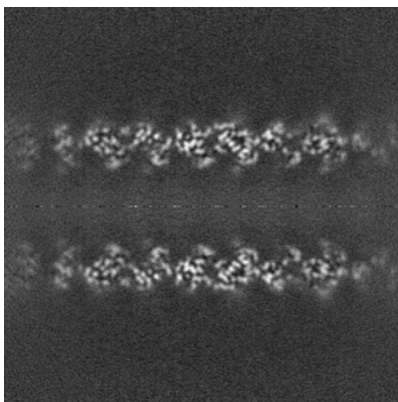


Z Index: 175

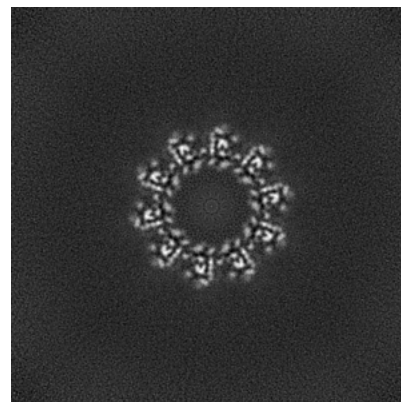
6.2.2 Raw map



X Index: 175



Y Index: 175

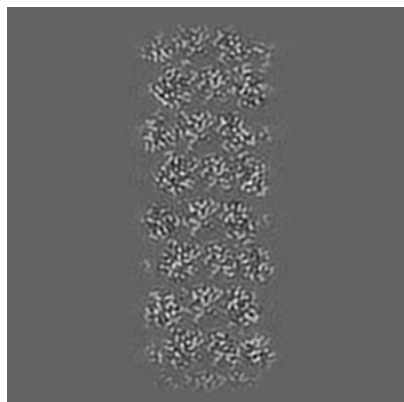


Z Index: 175

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

6.3 Largest variance slices [i](#)

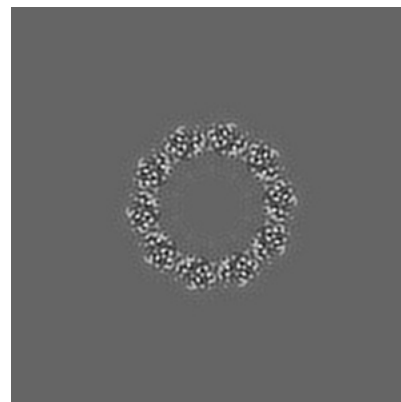
6.3.1 Primary map



X Index: 128

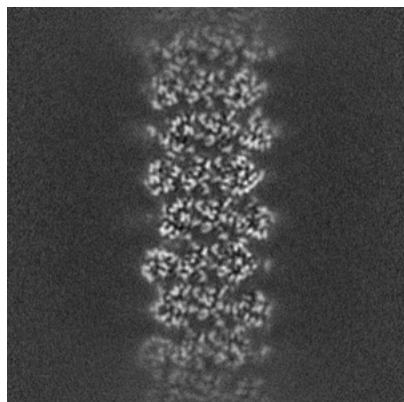


Y Index: 127

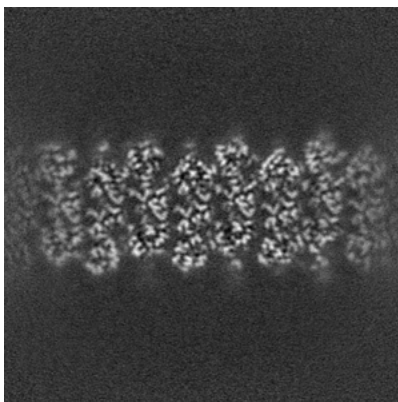


Z Index: 83

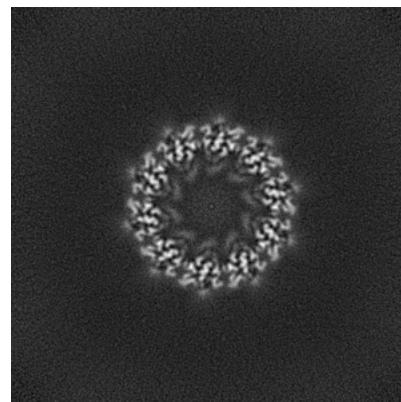
6.3.2 Raw map



X Index: 224



Y Index: 127

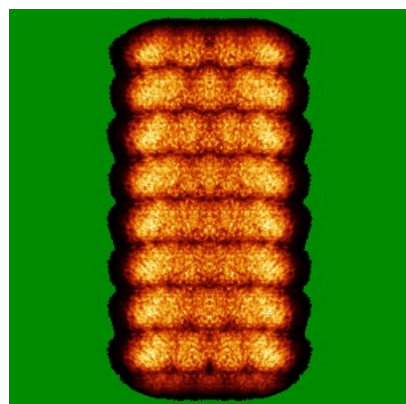


Z Index: 165

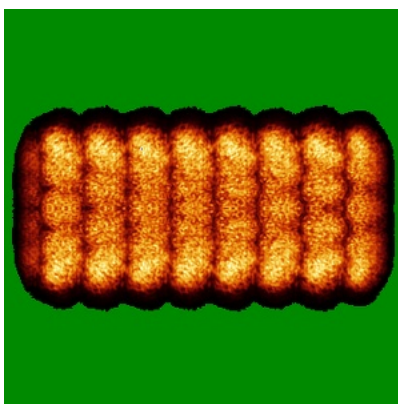
The images above show the largest variance slices of the map in three orthogonal directions.

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

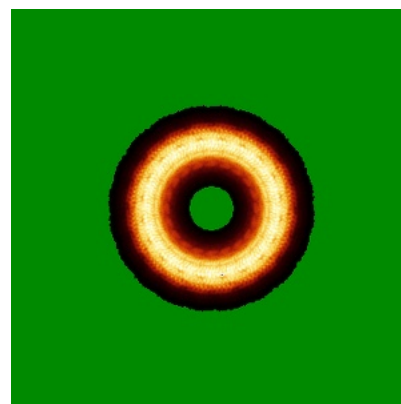
6.4.1 Primary map



X

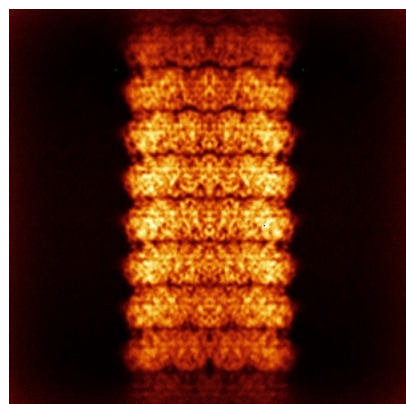


Y

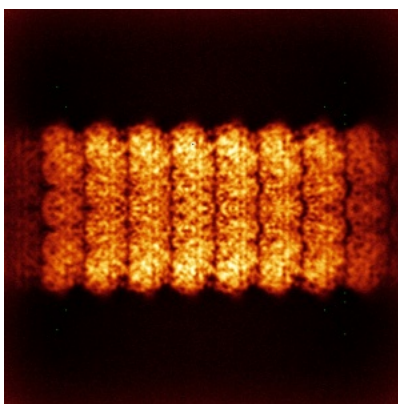


Z

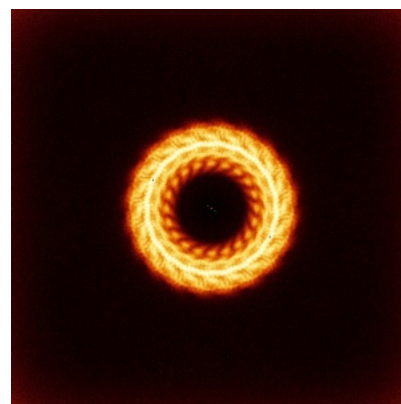
6.4.2 Raw map



X



Y

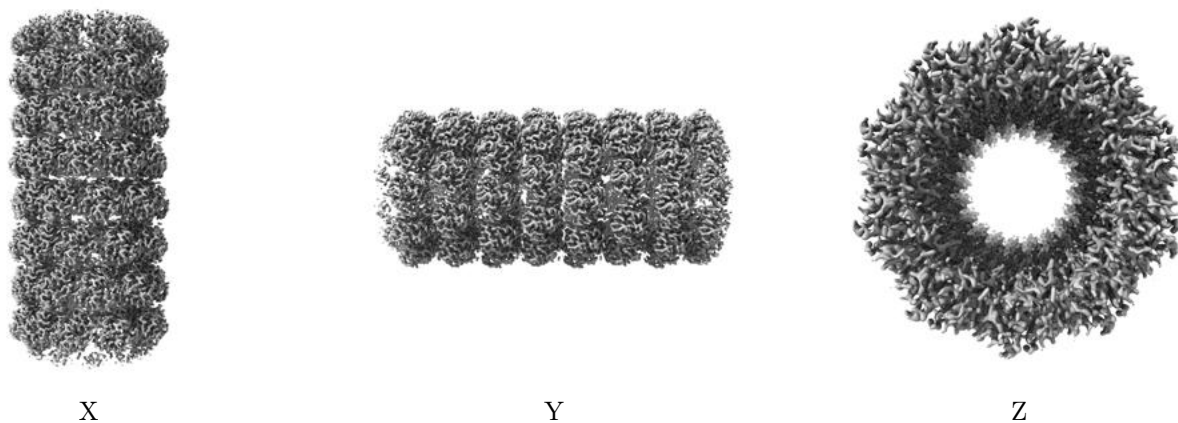


Z

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.

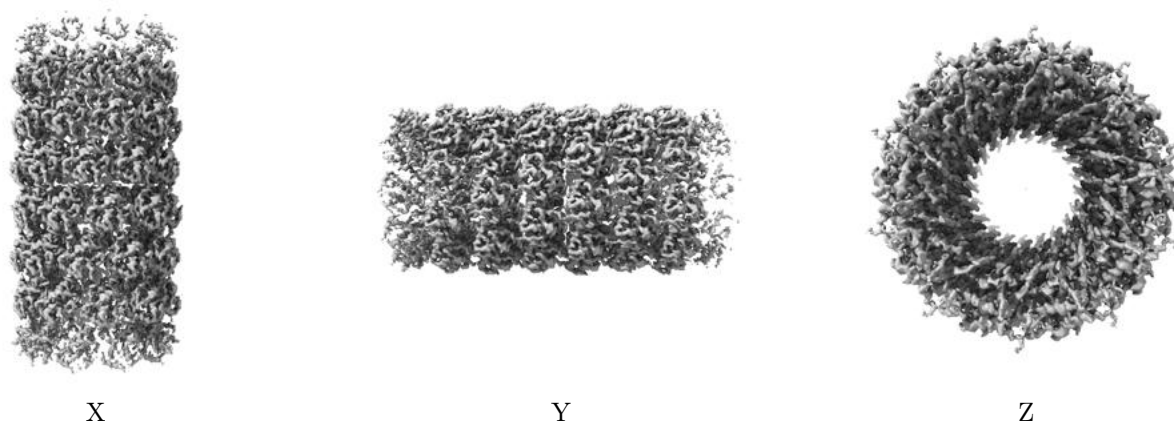
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.61. 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.

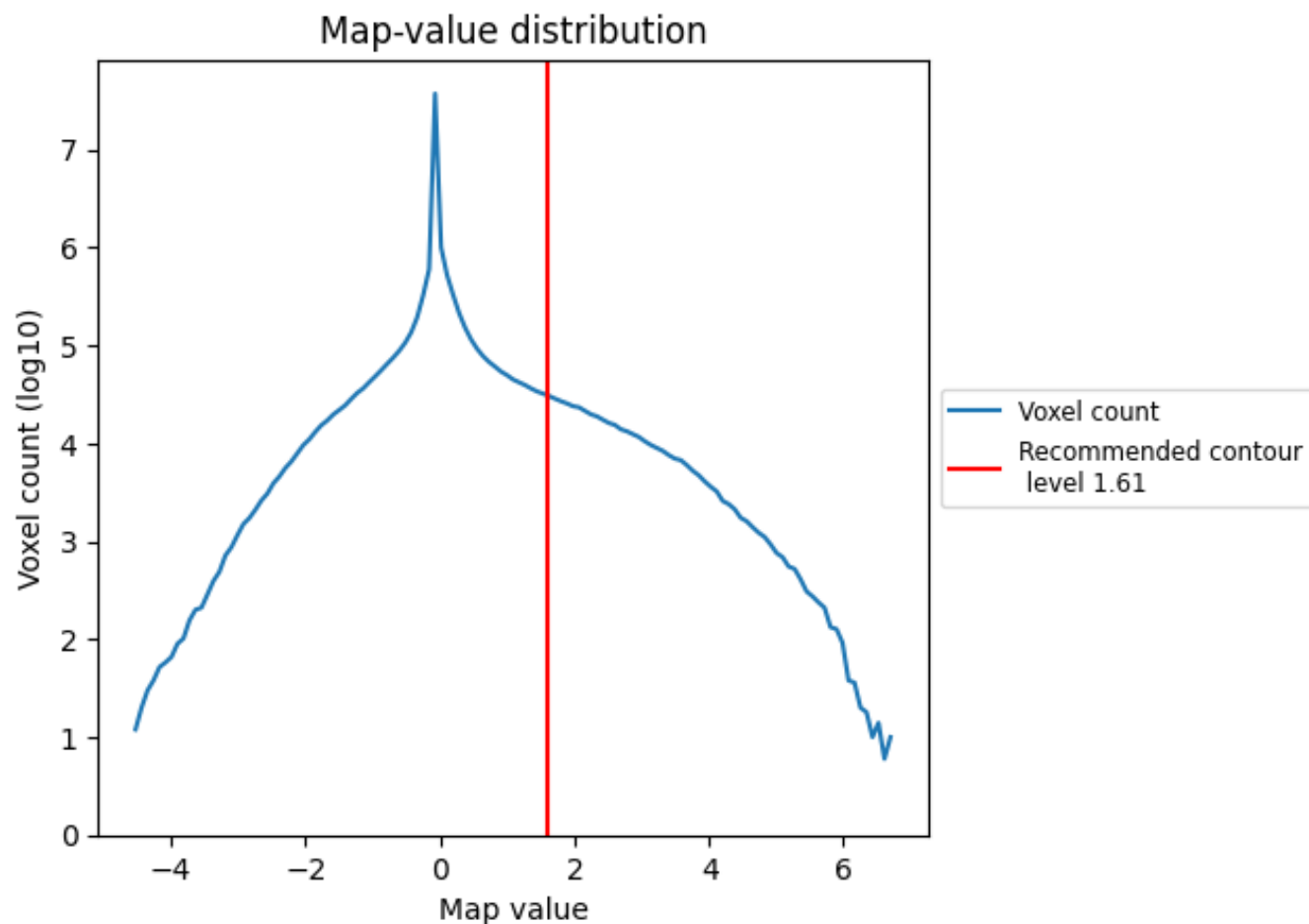
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

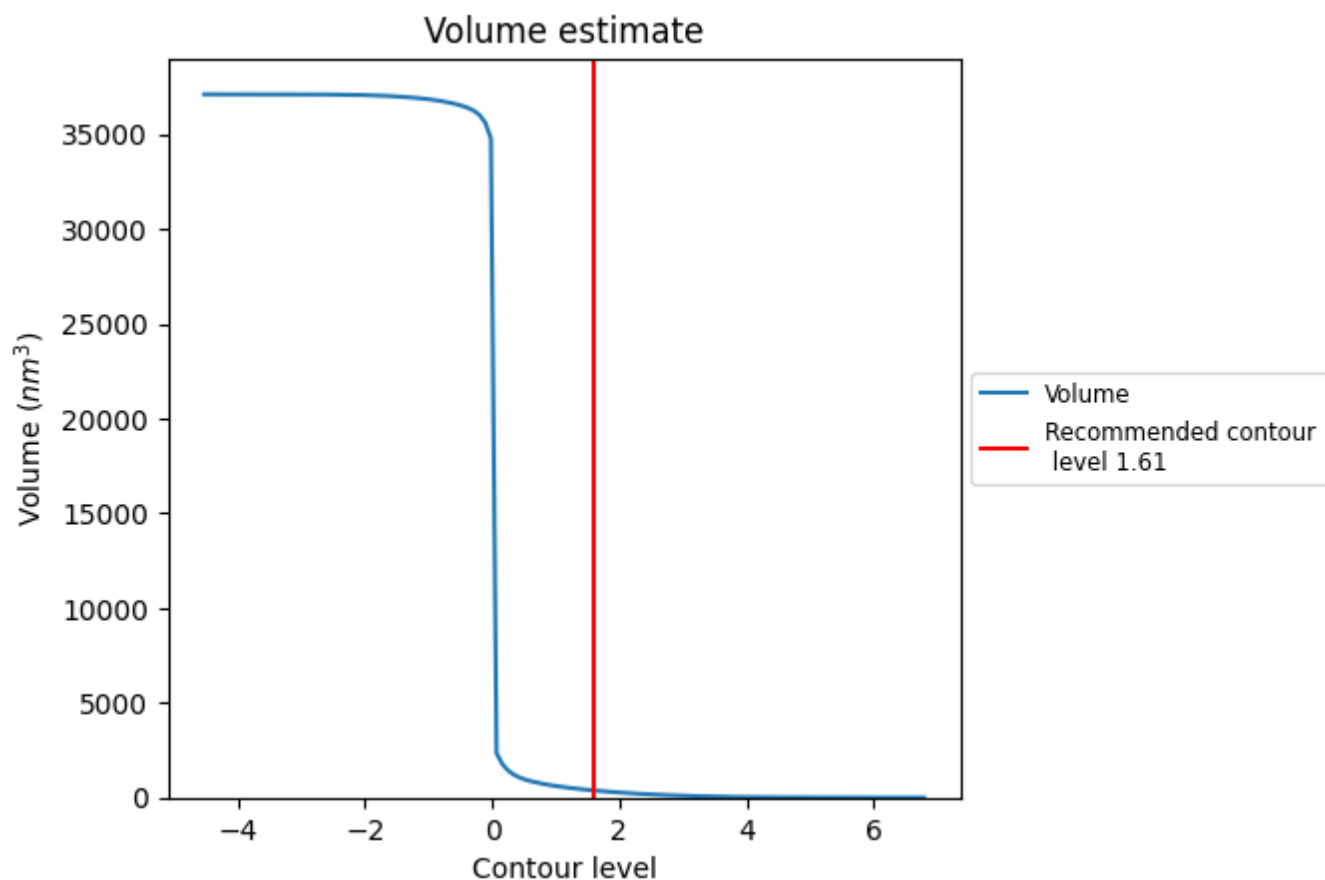
This section contains the results of statistical analysis of the map.

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.

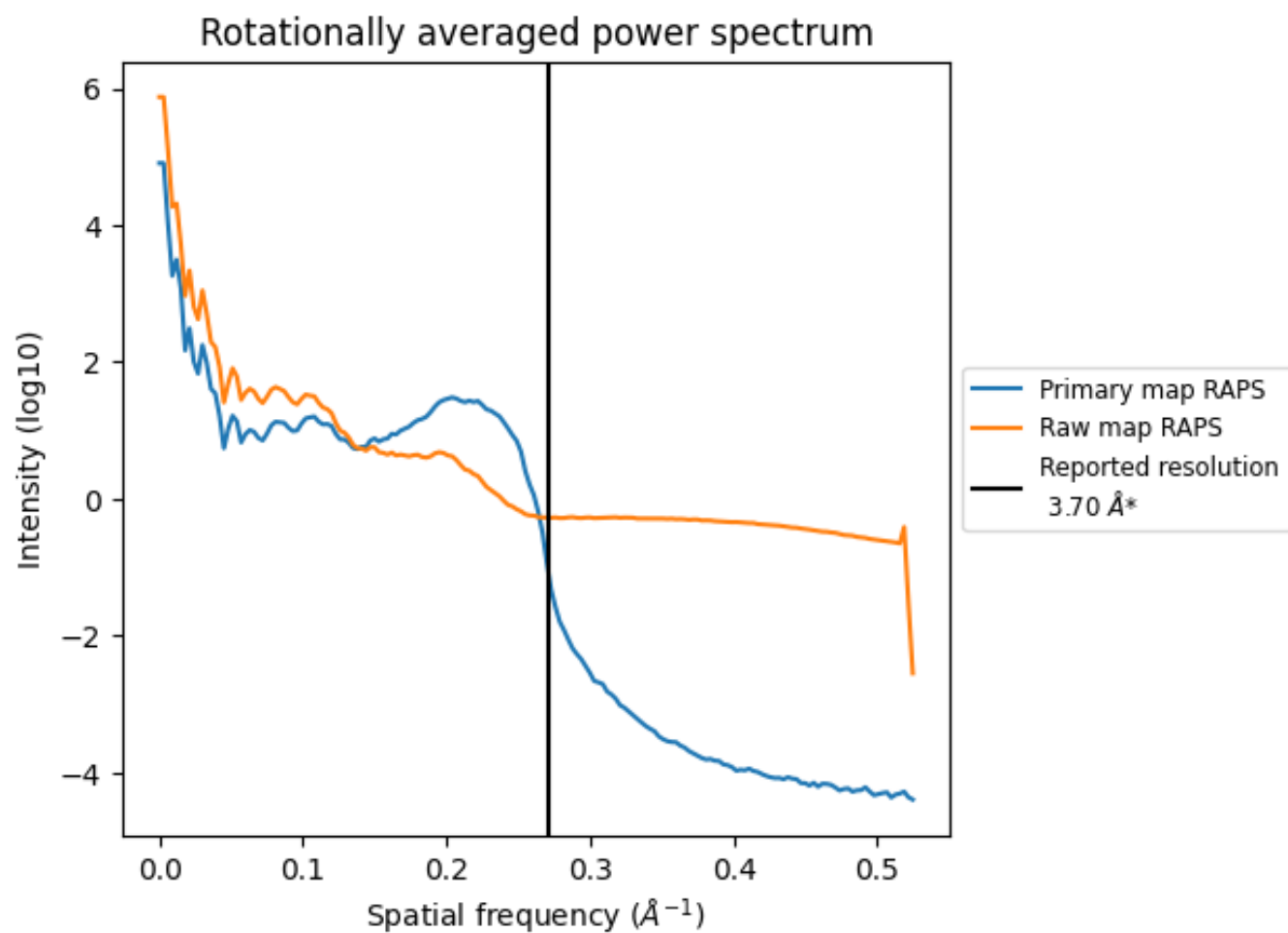
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 372 nm³; this corresponds to an approximate mass of 336 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 ⓘ

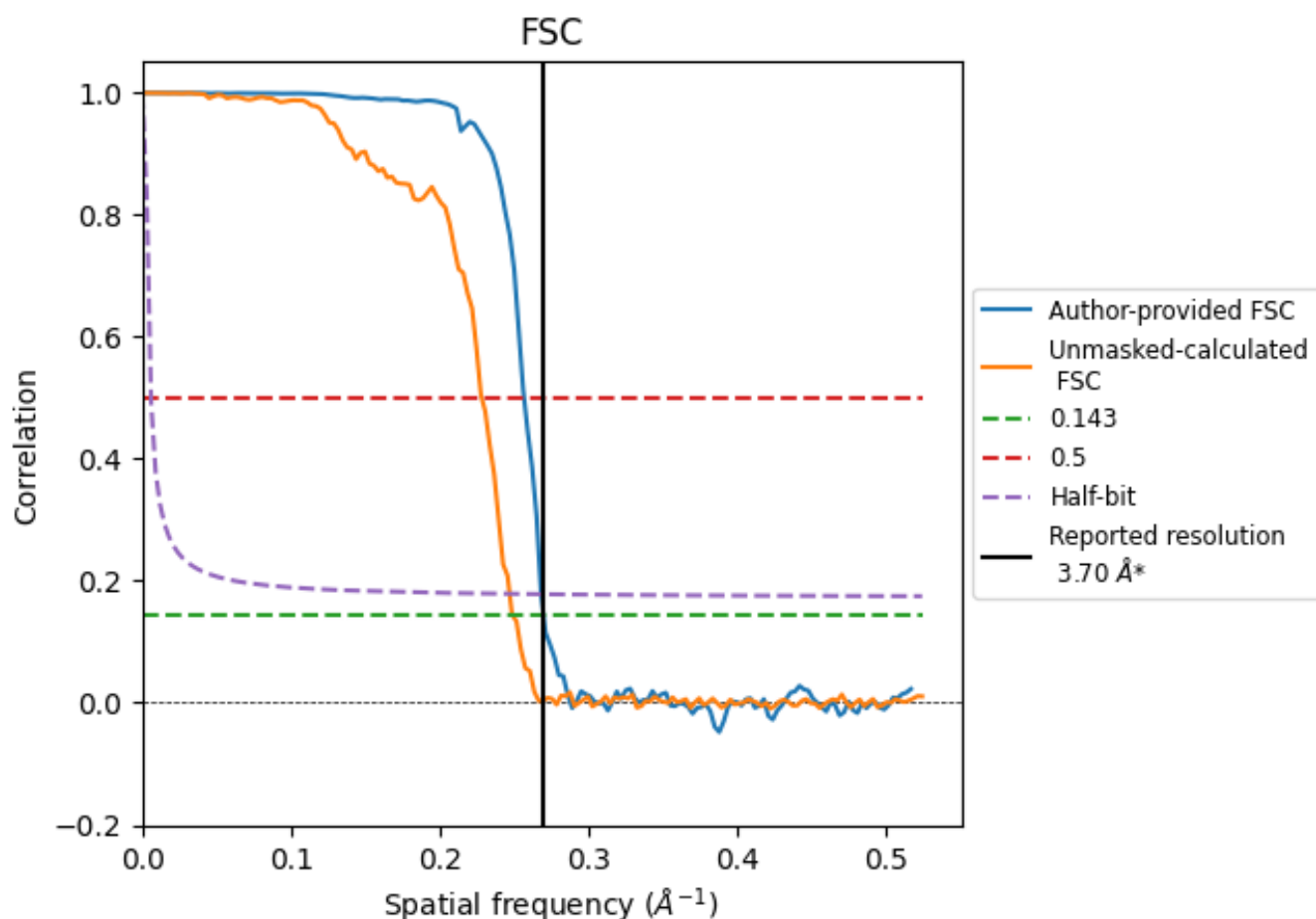


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 $0.270 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.70	3.89	3.73
Unmasked-calculated*	4.01	4.38	4.05

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

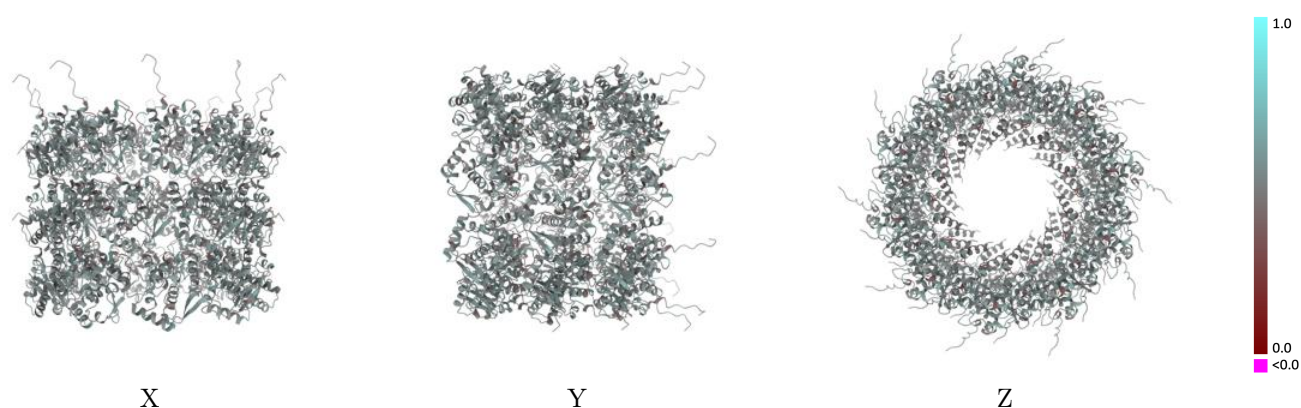
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-53801 and PDB model 9R80. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

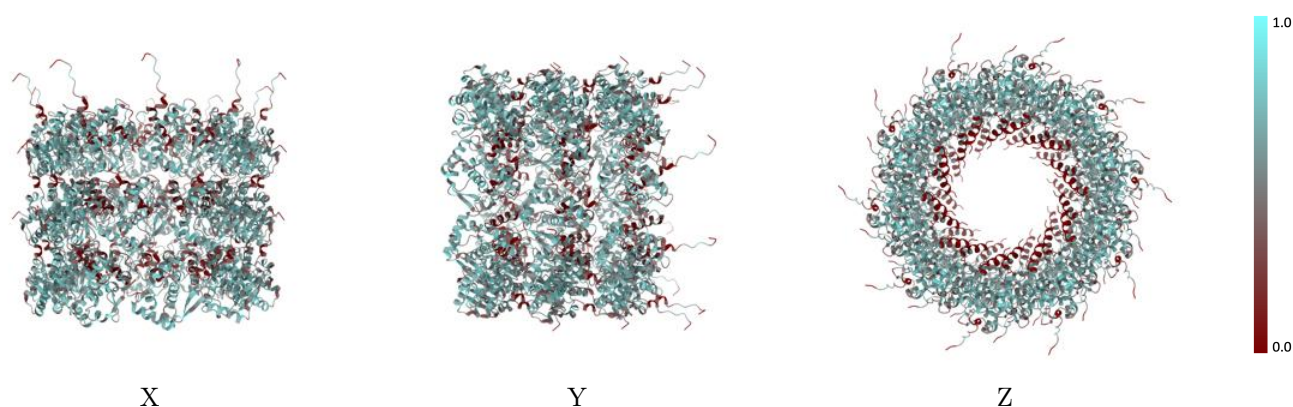
This section was not generated.

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



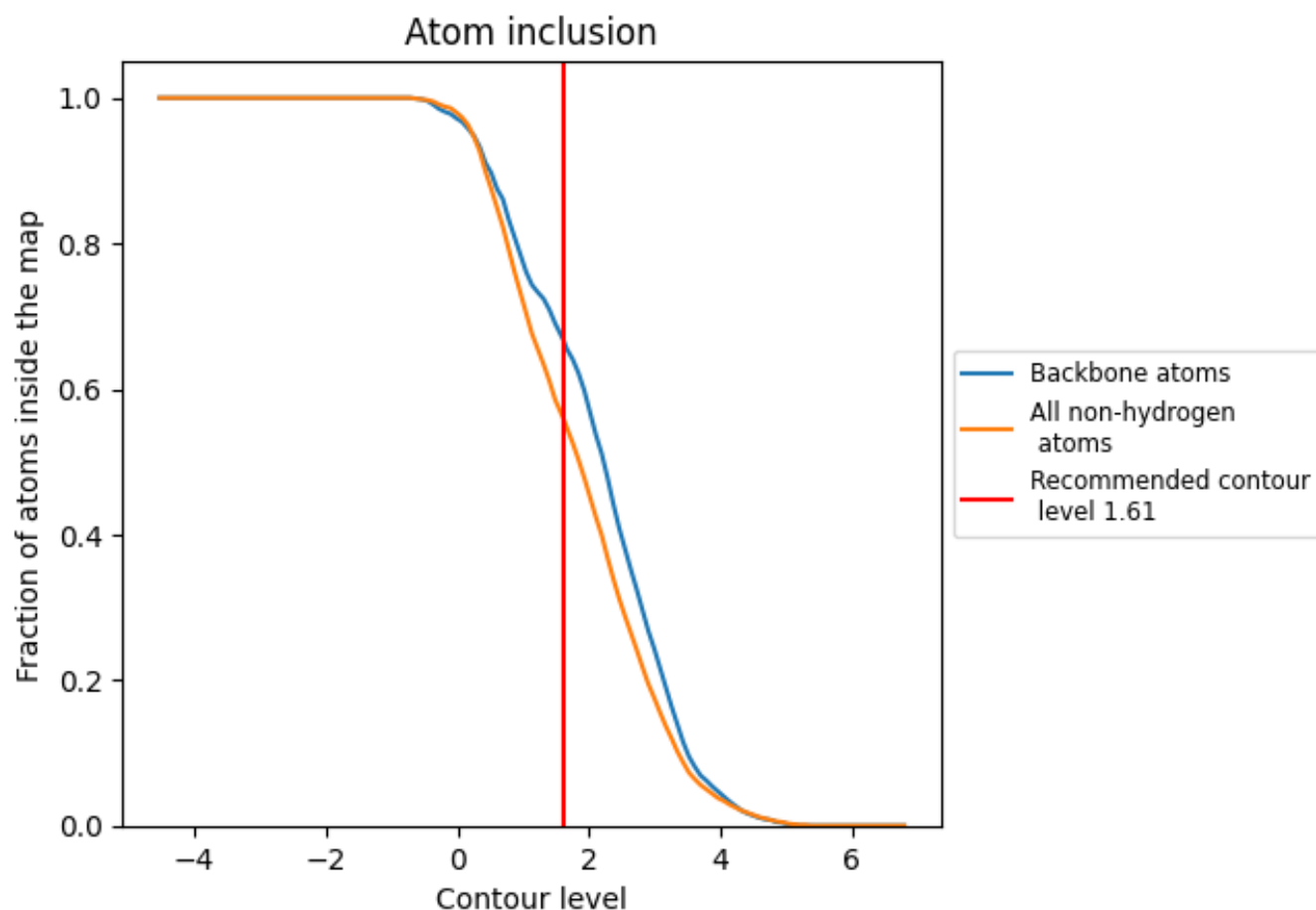
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.61).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 56% 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 (1.61) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5590	 0.5090
Aa	 0.5630	 0.5090
Ab	 0.5580	 0.5100
Ac	 0.5560	 0.5100
Ad	 0.5580	 0.5090
Ae	 0.5600	 0.5100
Af	 0.5630	 0.5090
Ag	 0.5580	 0.5110
Ah	 0.5560	 0.5090
Ai	 0.5580	 0.5080
Aj	 0.5600	 0.5100
Ak	 0.5630	 0.5100
Al	 0.5560	 0.5090
Am	 0.5580	 0.5100
An	 0.5600	 0.5080
Ao	 0.5560	 0.5090
Ap	 0.5620	 0.5100
Aq	 0.5550	 0.5100
Ar	 0.5580	 0.5090
As	 0.5590	 0.5090
At	 0.5580	 0.5100
Au	 0.5580	 0.5100
Av	 0.5560	 0.5080
Aw	 0.5580	 0.5090
Ax	 0.5630	 0.5100
Ay	 0.5610	 0.5090
Az	 0.5580	 0.5100
Ba	 0.5580	 0.5090
Bb	 0.5600	 0.5100
Bc	 0.5630	 0.5090
Bd	 0.5600	 0.5080

