



Full wwPDB EM Validation Report ⓘ

Mar 18, 2026 – 12:03 AM UTC

PDB ID : 9R81 / pdb_00009r81
EMDB ID : EMD-53802
Title : ssRNA-containing helical virus-like particle composed of PVA coat protein with D138C mutation
Authors : Koritnik, N.; Kezar, A.; Podobnik, M.
Deposited on : 2025-05-15
Resolution : 2.33 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

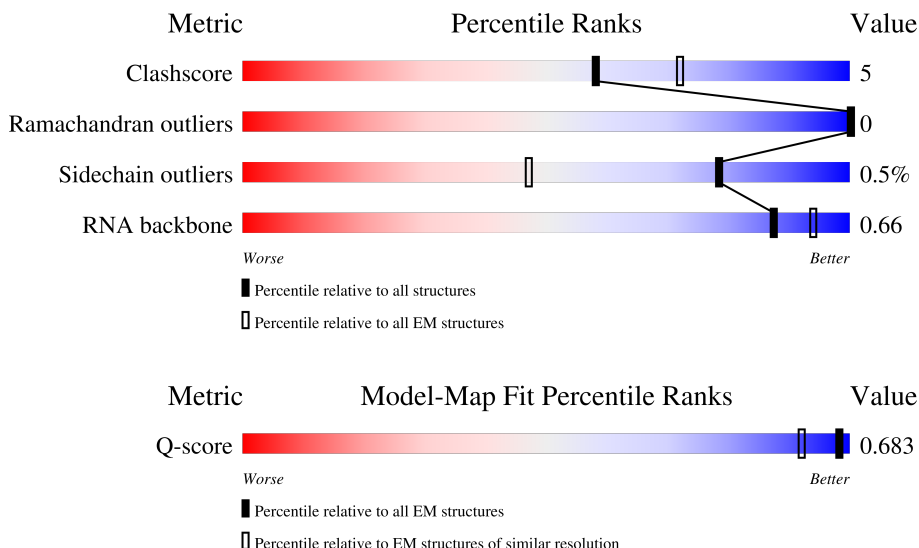
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.33 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	4434 (1.83 - 2.83)

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	20% 75% 9% 16%
1	Ac	269	19% 73% 11% 16%
1	Ae	269	18% 74% 10% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ag	269	
1	Ai	269	
1	Ak	269	
1	Am	269	
1	Ao	269	
1	Aq	269	
1	As	269	
1	Au	269	
1	Aw	269	
1	Ay	269	
1	Ba	269	
1	Bc	269	
1	Be	269	
1	Bg	269	
1	Bi	269	
1	Bk	269	
1	Bm	269	
1	Bo	269	
1	Bq	269	
1	Bs	269	
1	Bu	269	
1	Bw	269	
1	By	269	
1	Ca	269	
1	Cc	269	

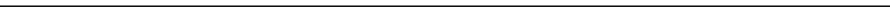
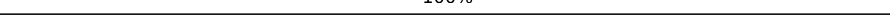
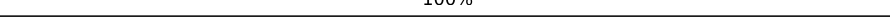
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ce	269	
1	Cg	269	
1	Ci	269	
1	Ck	269	
1	Cm	269	
1	Co	269	
1	Cq	269	
1	Cs	269	
2	Ab	5	
2	Ad	5	
2	Af	5	
2	Ah	5	
2	Aj	5	
2	Al	5	
2	An	5	
2	Ap	5	
2	Ar	5	
2	At	5	
2	Av	5	
2	Ax	5	
2	Az	5	
2	Bb	5	
2	Bd	5	
2	Bf	5	
2	Bh	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Bj	5	 100%
2	Bl	5	 100%
2	Bn	5	 100%
2	Bp	5	 100%
2	Br	5	 100%
2	Bt	5	 80% 20%
2	Bv	5	 60% 40%
2	Bx	5	 80% 20%
2	Bz	5	 80% 20%
2	Cb	5	 100%
2	Cd	5	 100%
2	Cf	5	 80% 20%
2	Ch	5	 60% 40%
2	Cj	5	 100%
2	Cl	5	 100%
2	Cn	5	 100%
2	Cp	5	 60% 40%
2	Cr	5	 80% 20%
2	Ct	5	 100%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 68868 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	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ac	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ae	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ag	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ai	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ak	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Am	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ao	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Aq	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	As	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Au	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Aw	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ay	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ba	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bc	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Be	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bg	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bi	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bk	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bm	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bo	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bq	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bs	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bu	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Bw	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	By	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ca	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Cc	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ce	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Cg	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ci	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Ck	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Cm	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Co	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Cq	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		
1	Cs	226	Total	C	N	O	S	0	0
			1813	1135	321	341	16		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	138	CYS	ASP	engineered mutation	UNP O11986

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Ac	138	CYS	ASP	engineered mutation	UNP O11986
Ae	138	CYS	ASP	engineered mutation	UNP O11986
Ag	138	CYS	ASP	engineered mutation	UNP O11986
Ai	138	CYS	ASP	engineered mutation	UNP O11986
Ak	138	CYS	ASP	engineered mutation	UNP O11986
Am	138	CYS	ASP	engineered mutation	UNP O11986
Ao	138	CYS	ASP	engineered mutation	UNP O11986
Aq	138	CYS	ASP	engineered mutation	UNP O11986
As	138	CYS	ASP	engineered mutation	UNP O11986
Au	138	CYS	ASP	engineered mutation	UNP O11986
Aw	138	CYS	ASP	engineered mutation	UNP O11986
Ay	138	CYS	ASP	engineered mutation	UNP O11986
Ba	138	CYS	ASP	engineered mutation	UNP O11986
Bc	138	CYS	ASP	engineered mutation	UNP O11986
Be	138	CYS	ASP	engineered mutation	UNP O11986
Bg	138	CYS	ASP	engineered mutation	UNP O11986
Bi	138	CYS	ASP	engineered mutation	UNP O11986
Bk	138	CYS	ASP	engineered mutation	UNP O11986
Bm	138	CYS	ASP	engineered mutation	UNP O11986
Bo	138	CYS	ASP	engineered mutation	UNP O11986
Bq	138	CYS	ASP	engineered mutation	UNP O11986
Bs	138	CYS	ASP	engineered mutation	UNP O11986
Bu	138	CYS	ASP	engineered mutation	UNP O11986
Bw	138	CYS	ASP	engineered mutation	UNP O11986
By	138	CYS	ASP	engineered mutation	UNP O11986
Ca	138	CYS	ASP	engineered mutation	UNP O11986
Cc	138	CYS	ASP	engineered mutation	UNP O11986
Ce	138	CYS	ASP	engineered mutation	UNP O11986
Cg	138	CYS	ASP	engineered mutation	UNP O11986
Ci	138	CYS	ASP	engineered mutation	UNP O11986
Ck	138	CYS	ASP	engineered mutation	UNP O11986
Cm	138	CYS	ASP	engineered mutation	UNP O11986
Co	138	CYS	ASP	engineered mutation	UNP O11986
Cq	138	CYS	ASP	engineered mutation	UNP O11986
Cs	138	CYS	ASP	engineered mutation	UNP O11986

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Ab	5	Total	C	N	O	P	
			100	45	10	40	5	0
2	Ad	5	Total	C	N	O	P	
			100	45	10	40	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Af	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ah	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Aj	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Al	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	An	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ap	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ar	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	At	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Av	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ax	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Az	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bb	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bd	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bf	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bh	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bj	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bl	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bn	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bp	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Br	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bt	5	Total 100	C 45	N 10	O 40	P 5	0	0

Continued on next page...

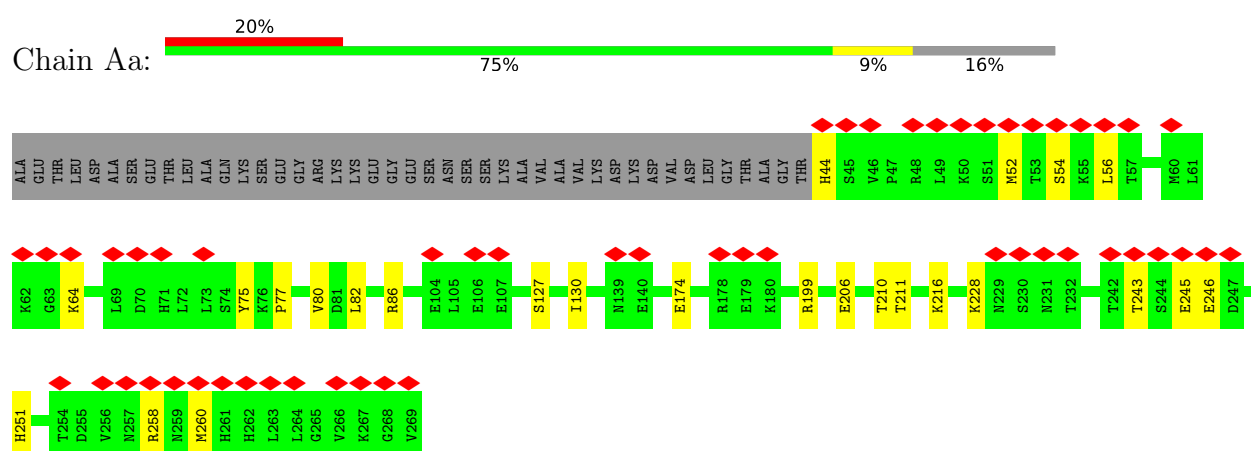
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bv	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bx	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bz	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cb	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cd	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cf	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ch	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cj	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cl	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cn	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cp	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cr	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Ct	5	Total 100	C 45	N 10	O 40	P 5	0	0

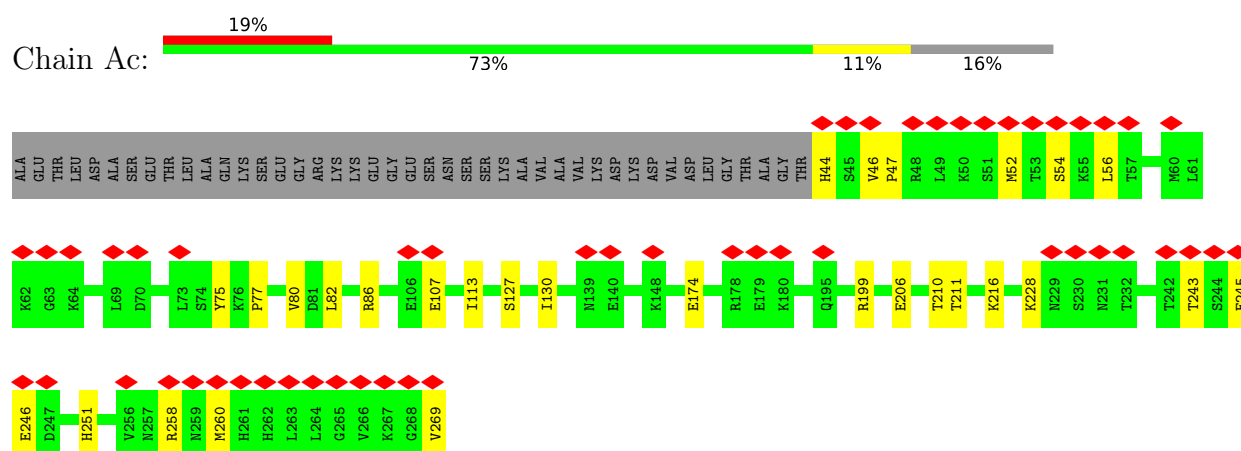
3 Residue-property plots

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

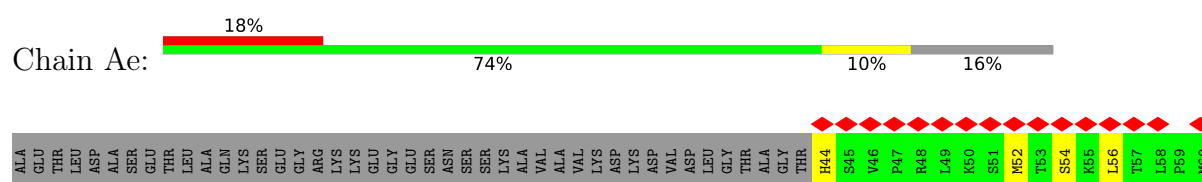
- Molecule 1: Genome polyprotein

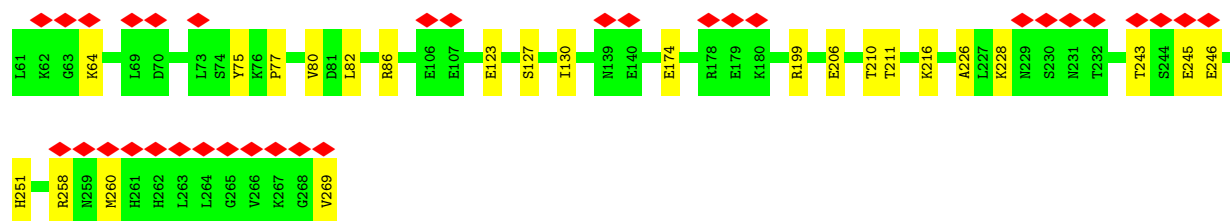


- Molecule 1: Genome polyprotein

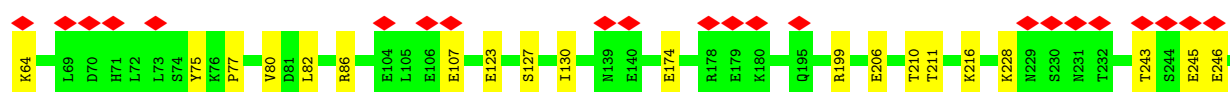
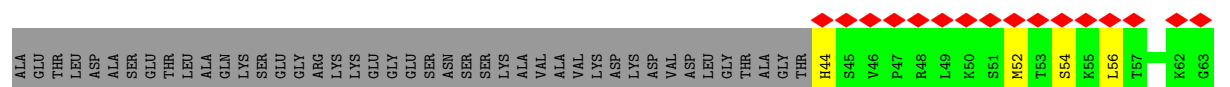
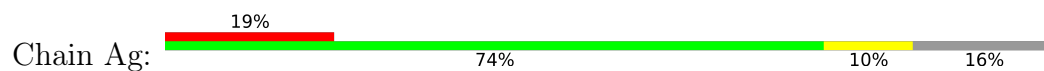


- Molecule 1: Genome polyprotein

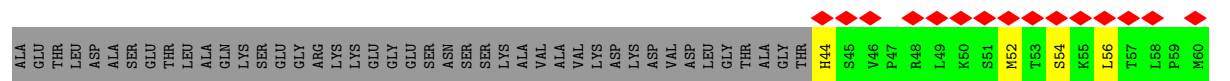
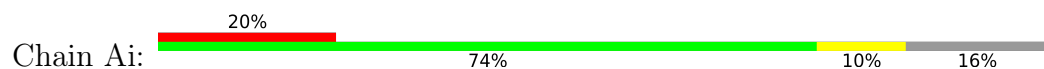




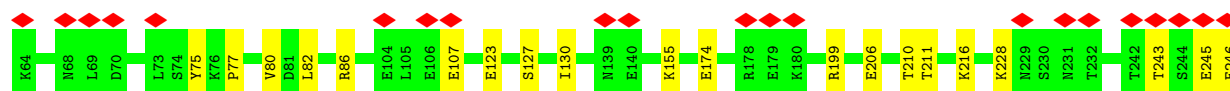
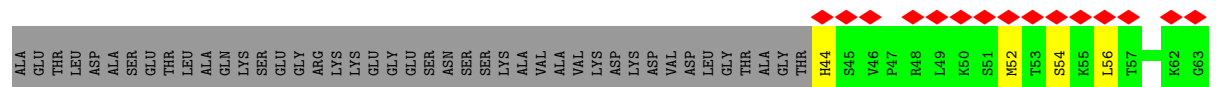
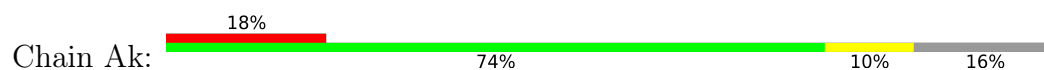
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein

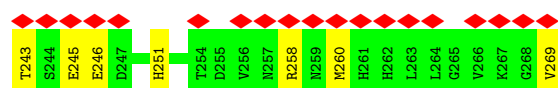
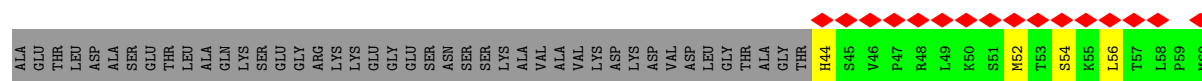
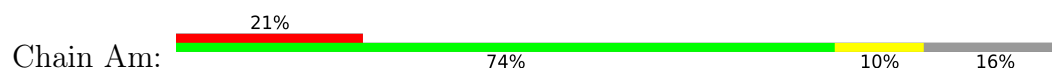


• Molecule 1: Genome polyprotein

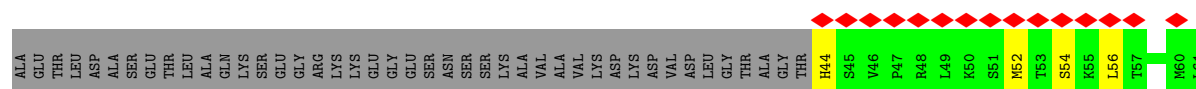
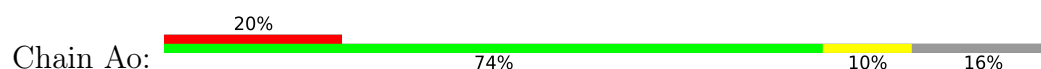




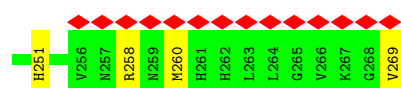
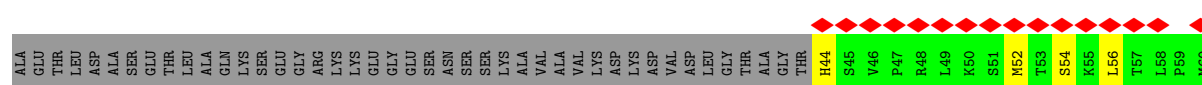
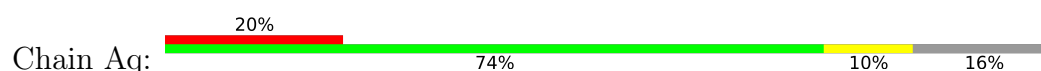
• Molecule 1: Genome polyprotein



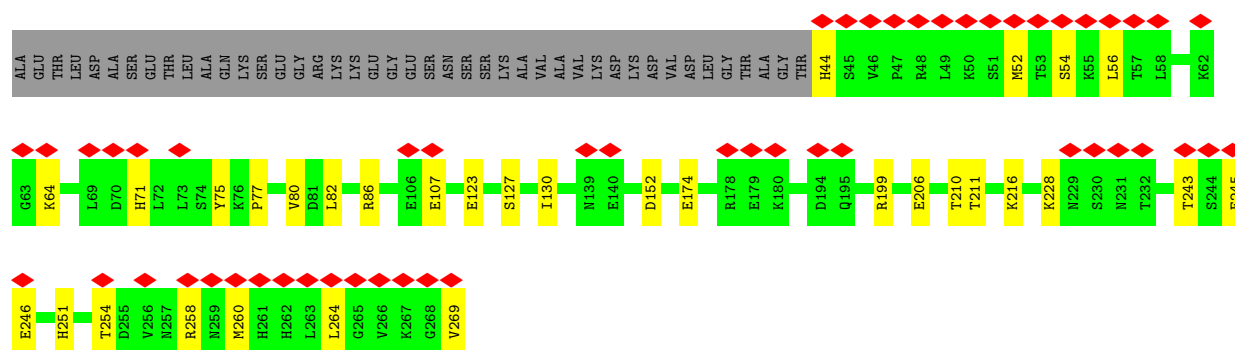
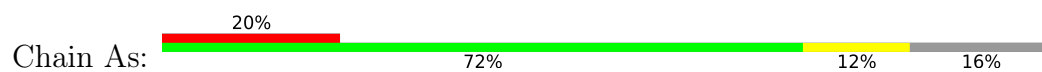
• Molecule 1: Genome polyprotein



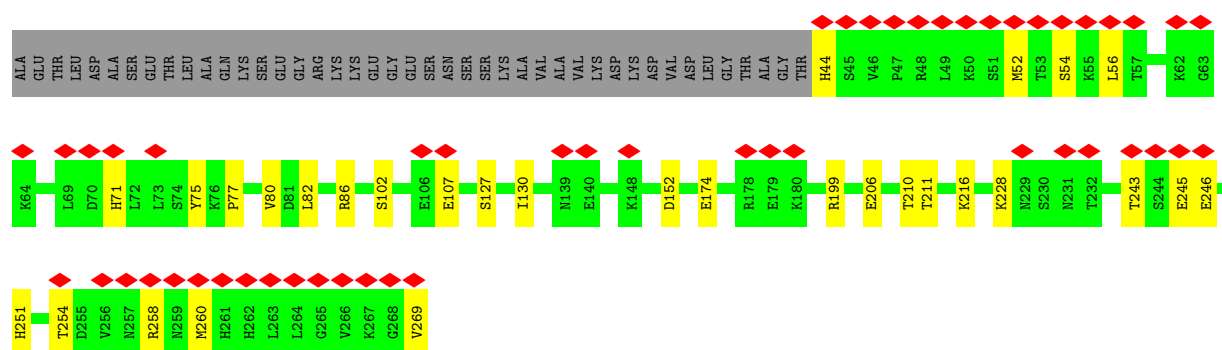
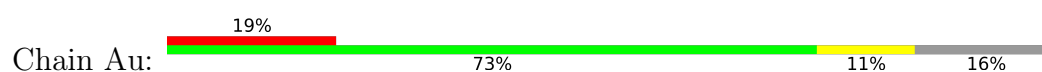
• Molecule 1: Genome polyprotein



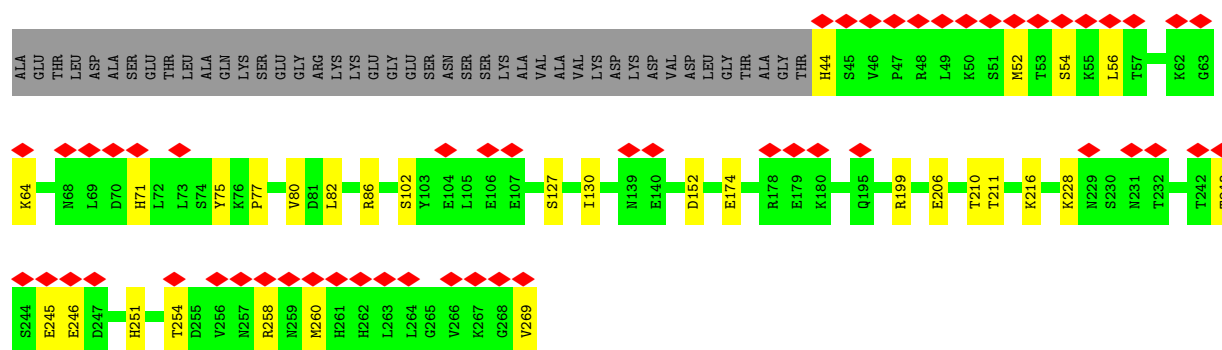
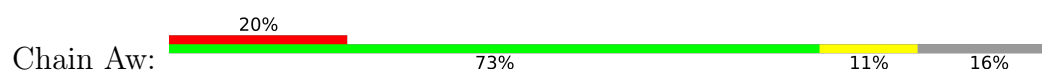
• Molecule 1: Genome polyprotein



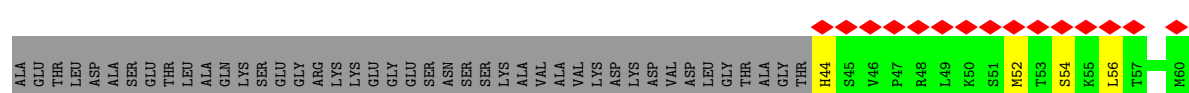
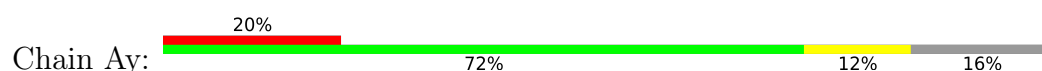
• Molecule 1: Genome polyprotein

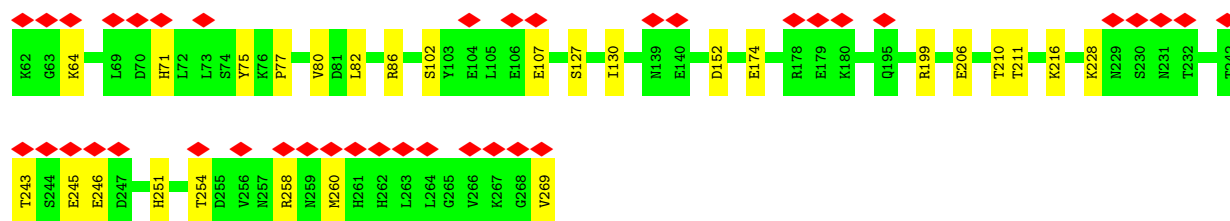


• Molecule 1: Genome polyprotein

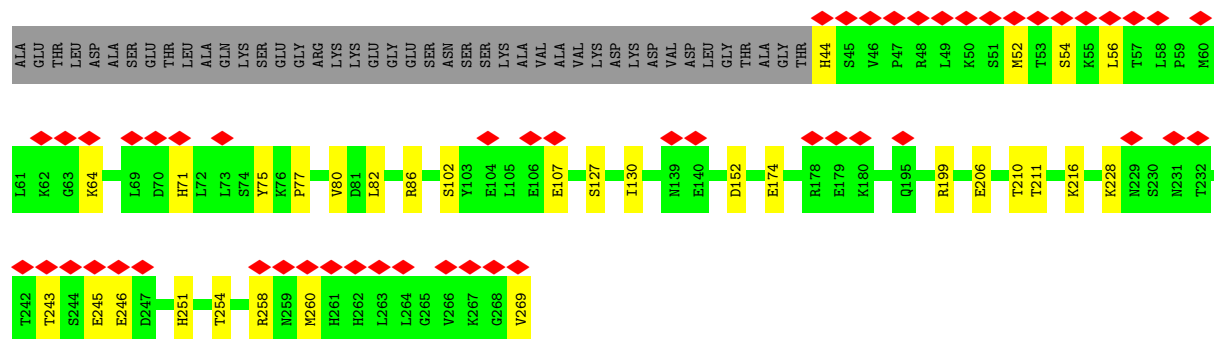
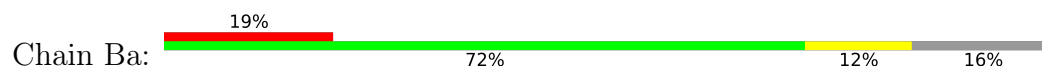


• Molecule 1: Genome polyprotein

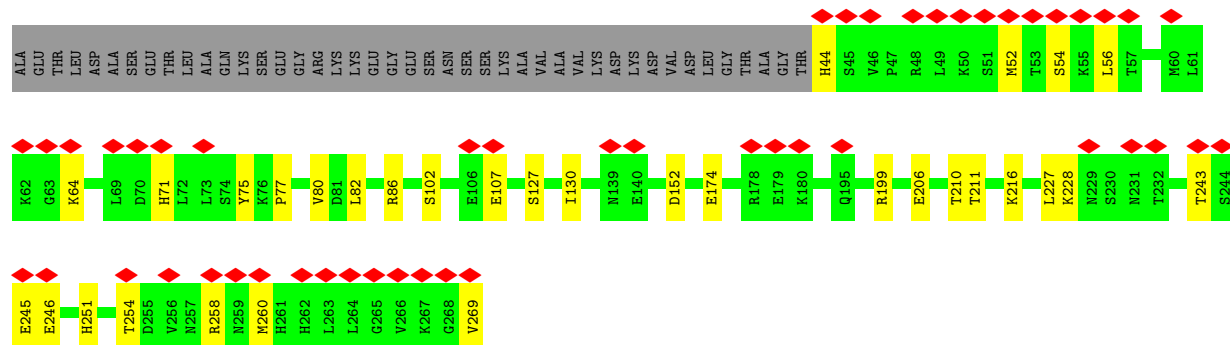
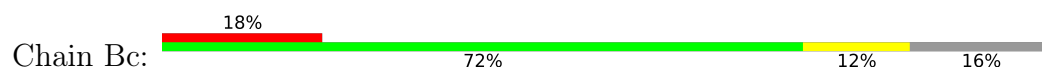




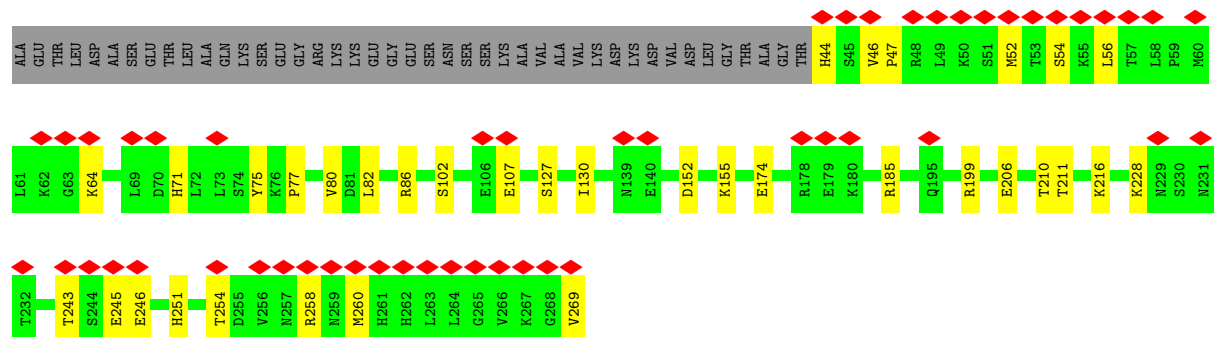
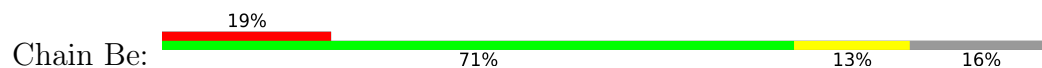
• Molecule 1: Genome polyprotein



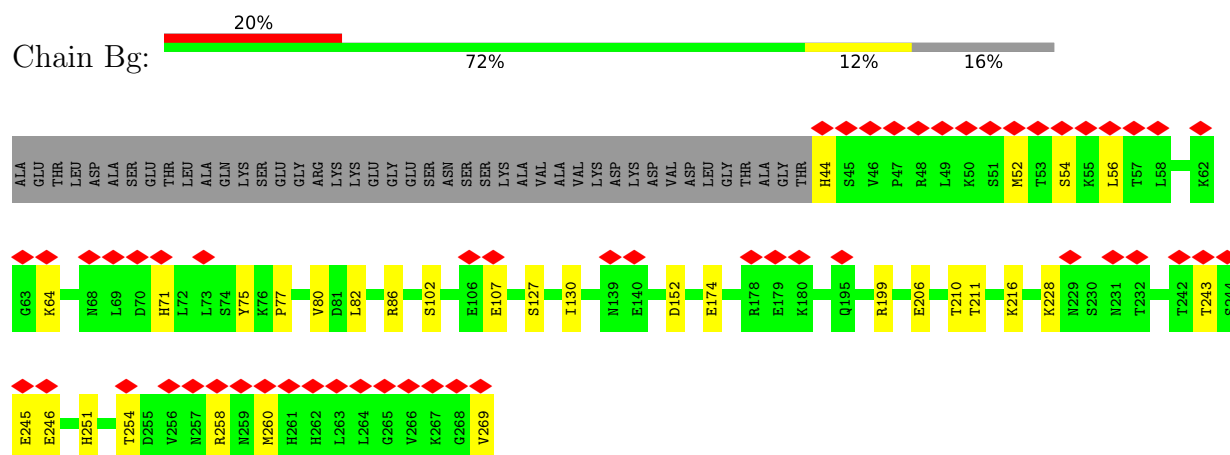
• Molecule 1: Genome polyprotein



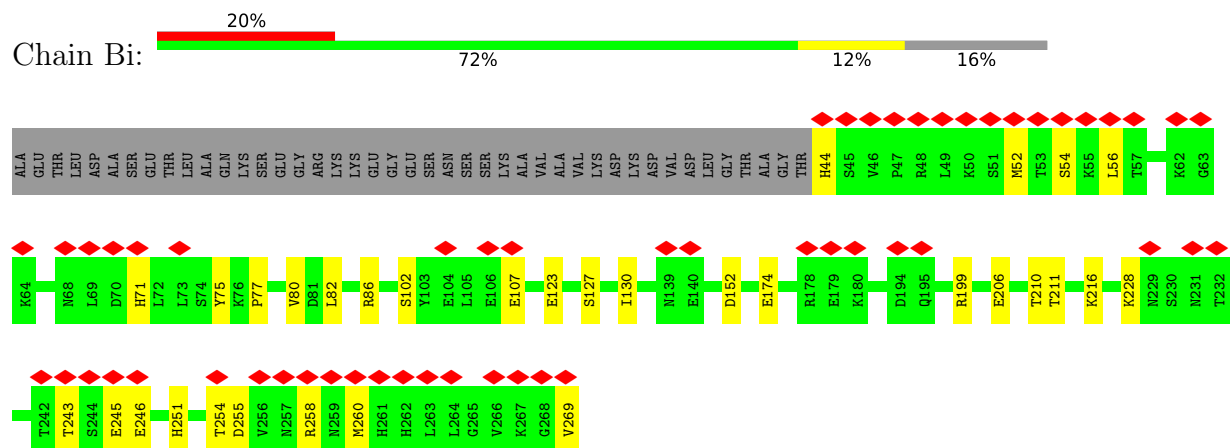
• Molecule 1: Genome polyprotein



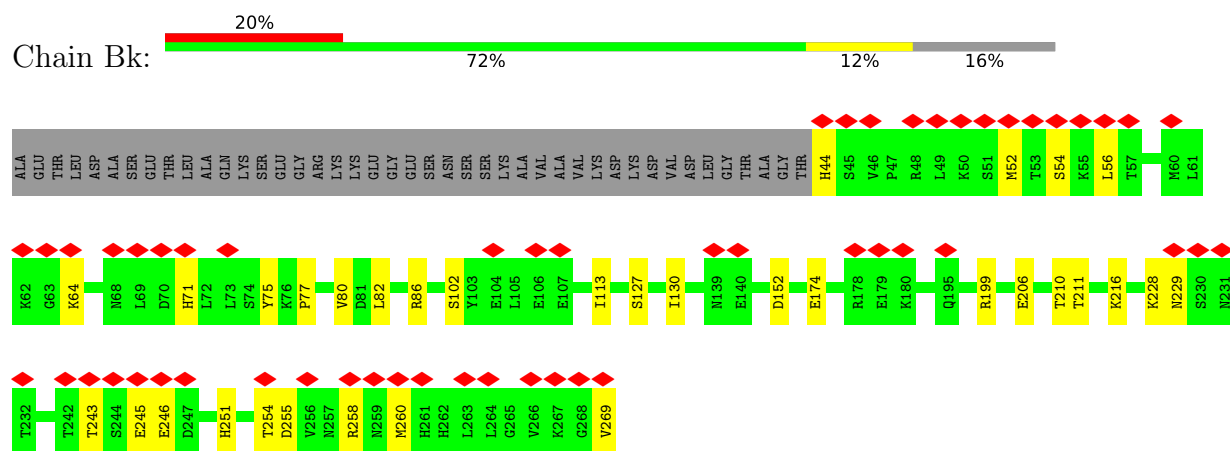
• Molecule 1: Genome polyprotein



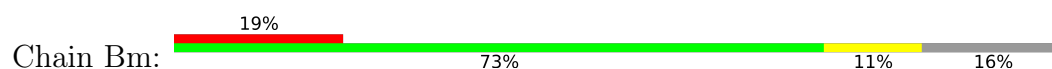
• Molecule 1: Genome polyprotein

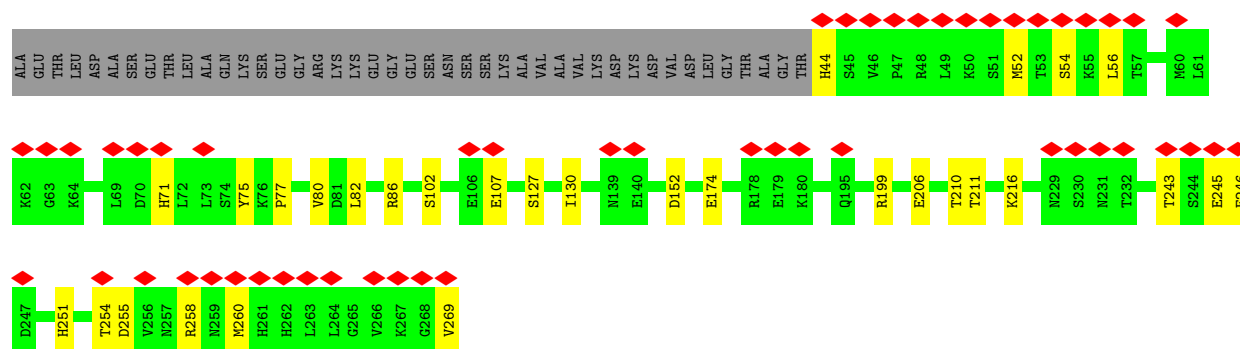


• Molecule 1: Genome polyprotein

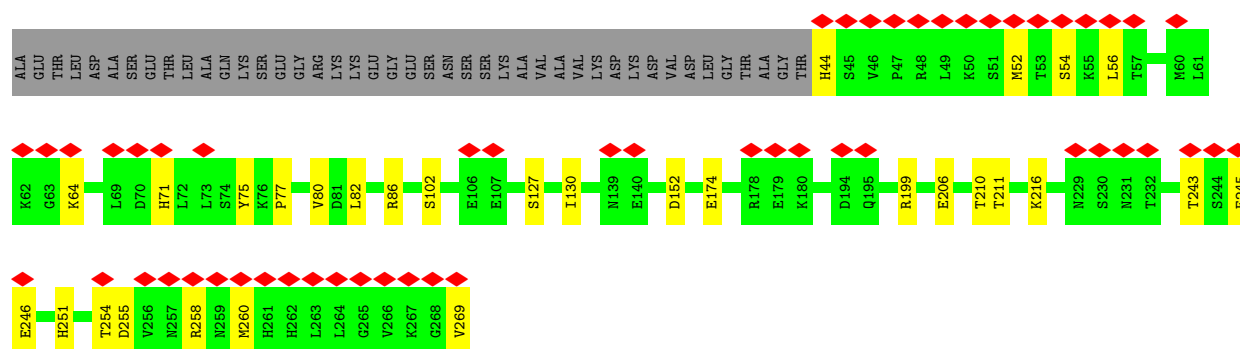
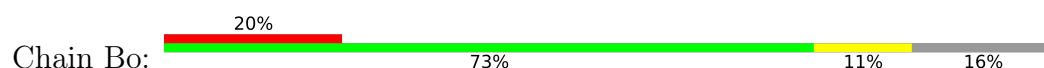


• Molecule 1: Genome polyprotein

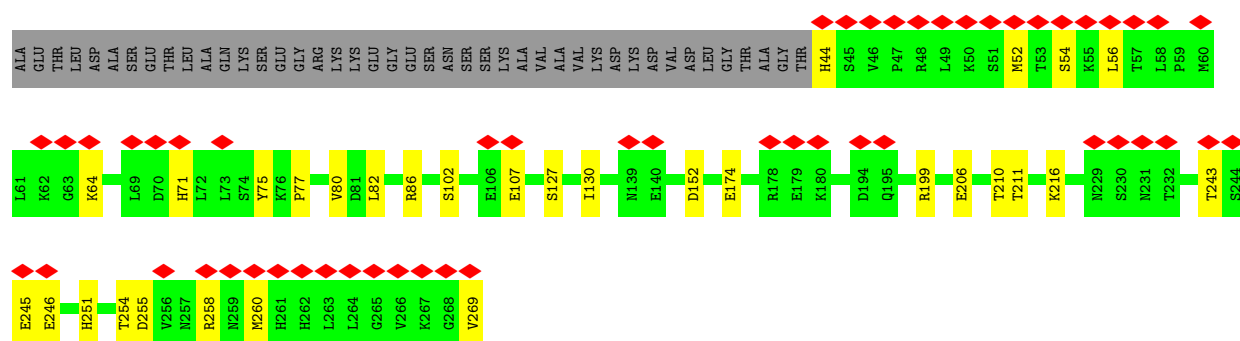
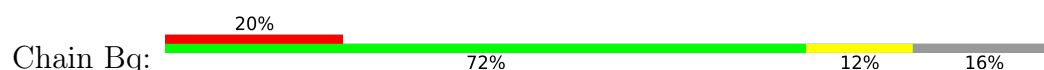




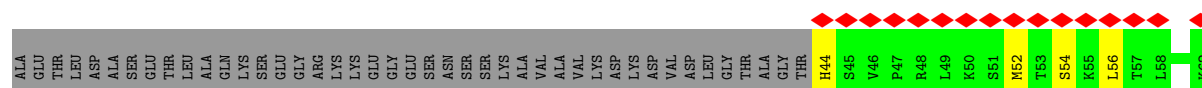
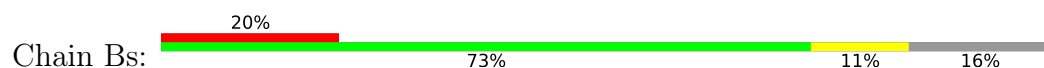
• Molecule 1: Genome polyprotein

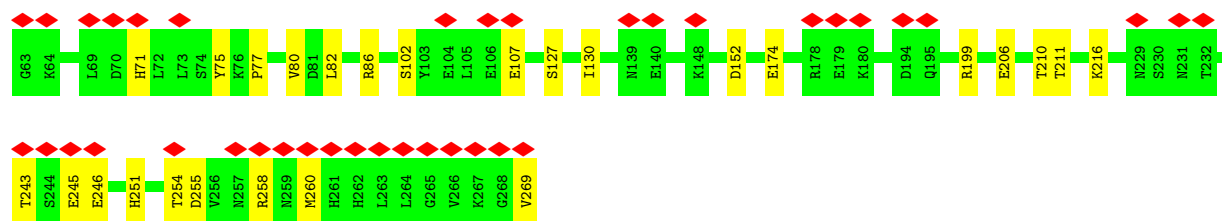


• Molecule 1: Genome polyprotein

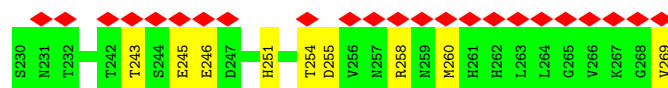
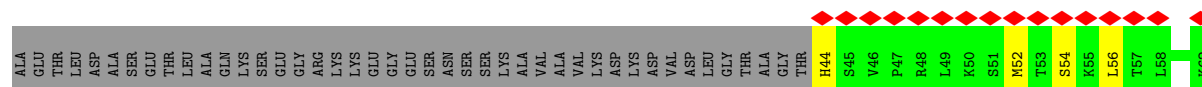
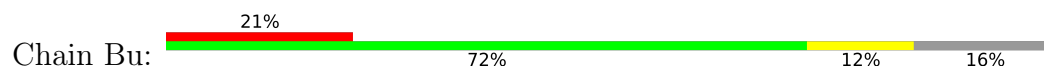


• Molecule 1: Genome polyprotein

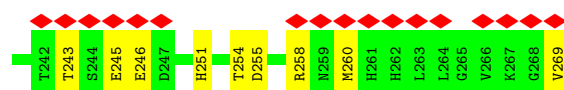
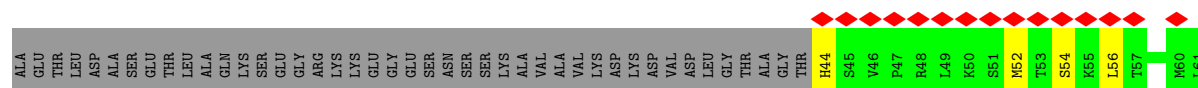
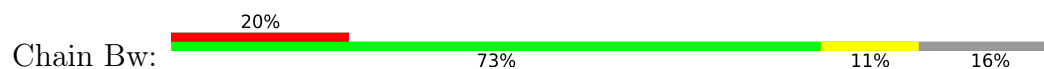




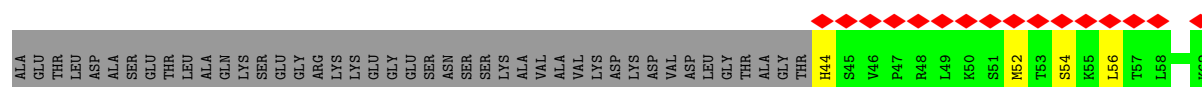
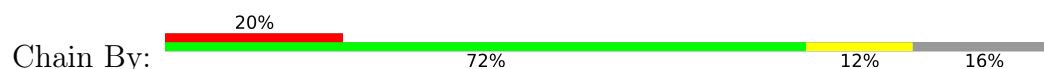
• Molecule 1: Genome polyprotein

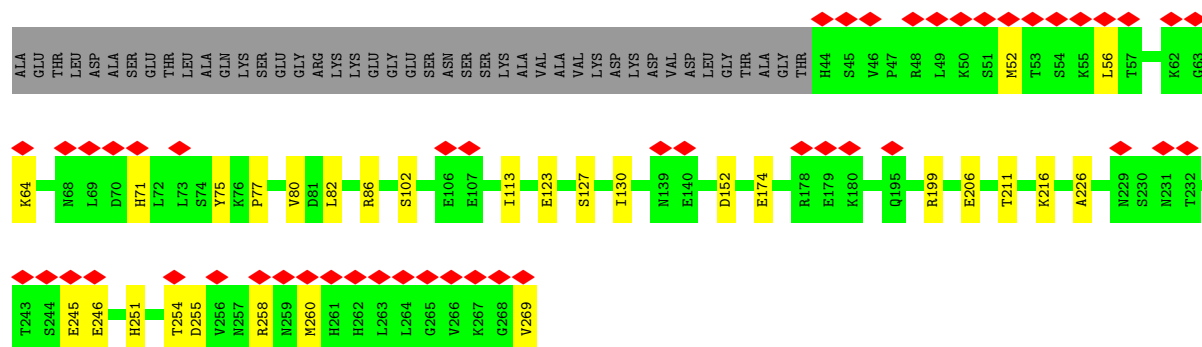
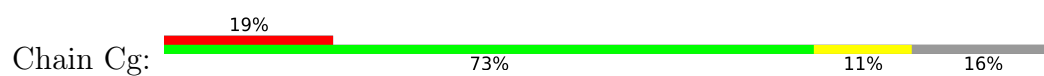


• Molecule 1: Genome polyprotein

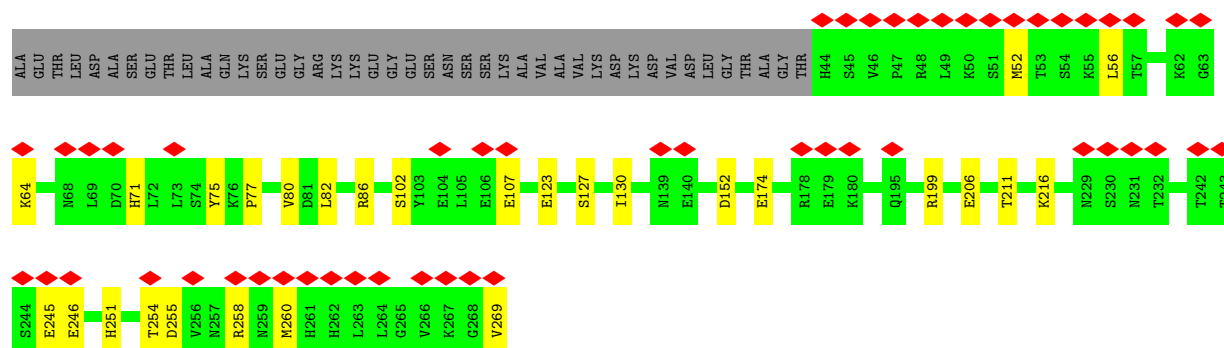
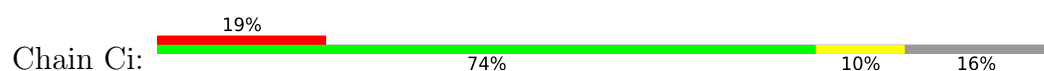


• Molecule 1: Genome polyprotein

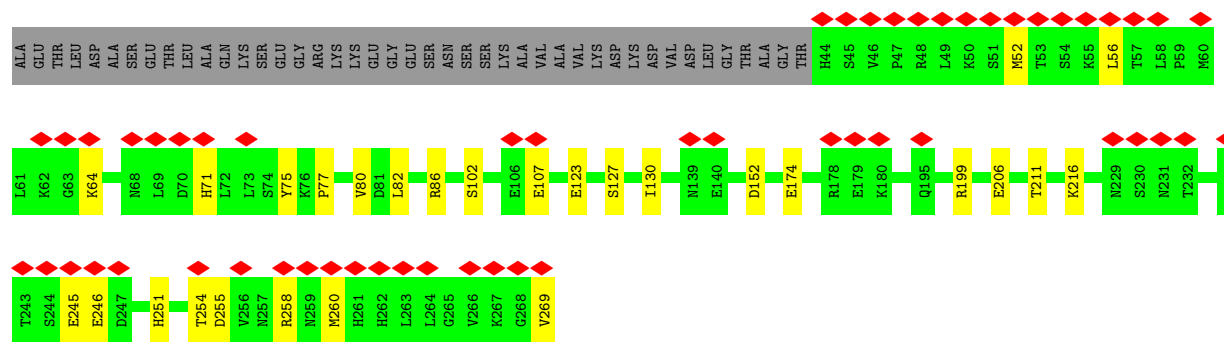
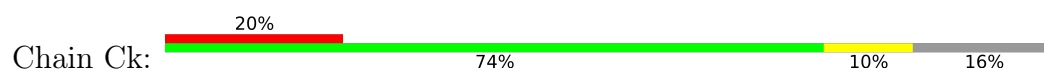




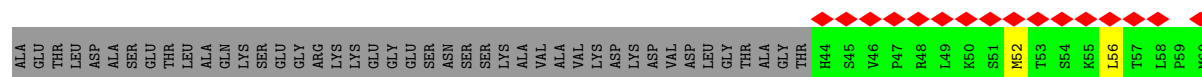
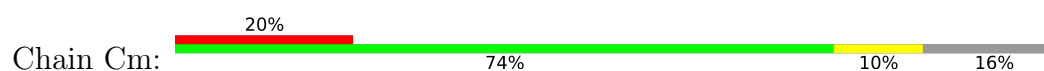
• Molecule 1: Genome polyprotein

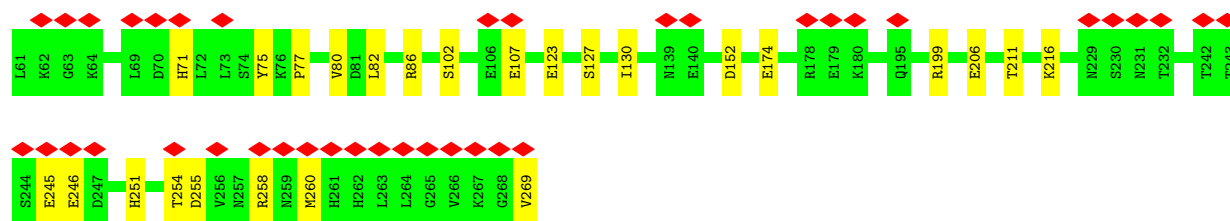


• Molecule 1: Genome polyprotein

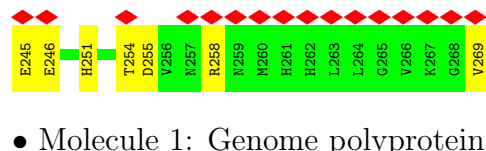
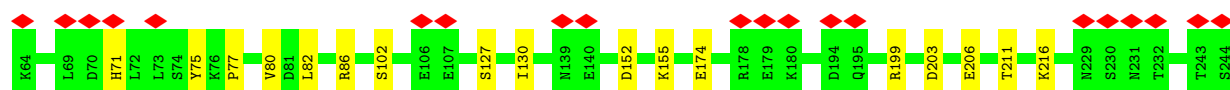
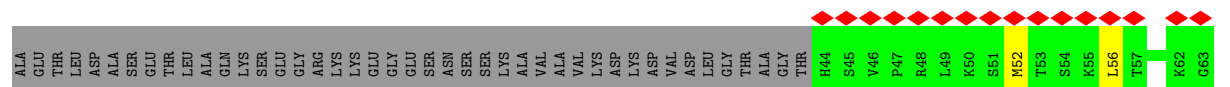
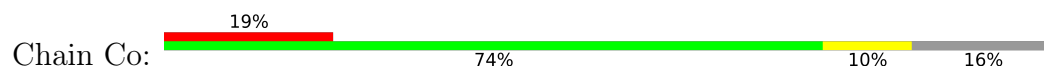


• Molecule 1: Genome polyprotein

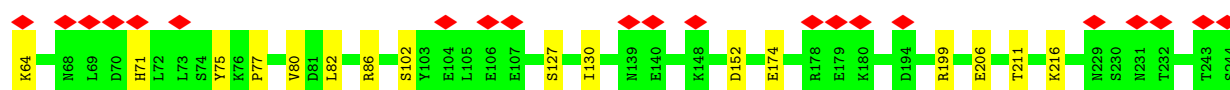
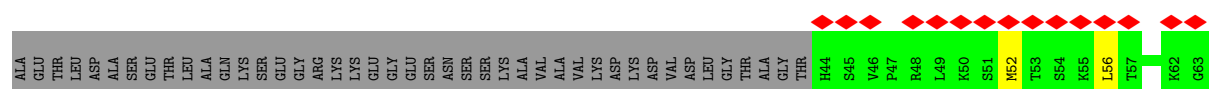
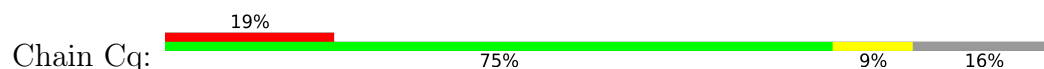




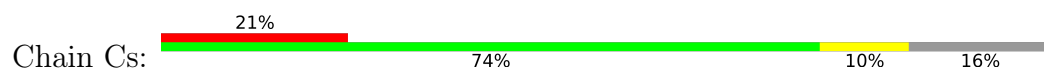
• Molecule 1: Genome polyprotein



• Molecule 1: Genome polyprotein

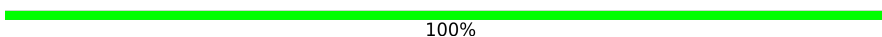


• Molecule 1: Genome polyprotein



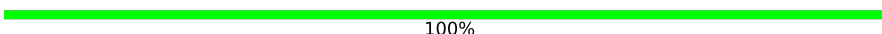


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ab:  100%

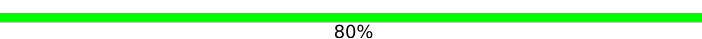
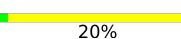
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ad:  100%

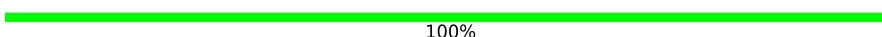
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Af:  80%  20%

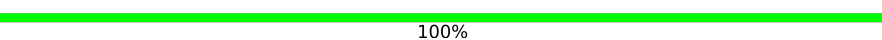


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ah:  100%

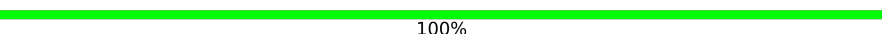
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Aj:  100%

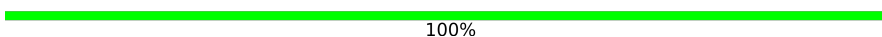
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Al:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain An:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ap:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ar:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain At:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Av:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ax:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Az:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bb:  80% 20%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bd:  60% 40%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bf:  100%

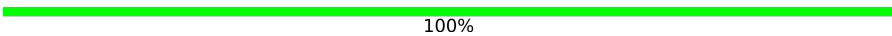
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bh:  100%

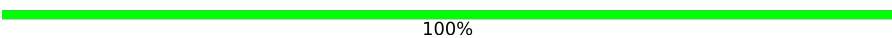
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bj:  100%

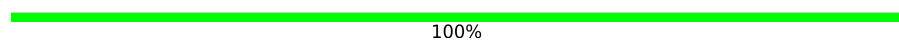
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bl:  100%

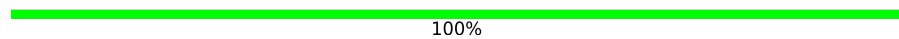
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bn:  100%

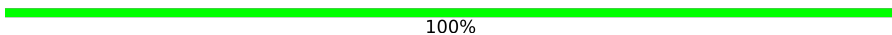
There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bp:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Br:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bt:  80% 20%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bv:  60% 40%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bx:  80% 20%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bz:  80% 20%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cb:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cd:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cf:  80% 20%

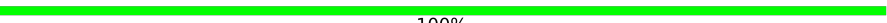


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ch:  60% 40%

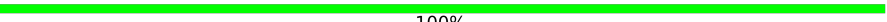


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cj:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cl:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cn:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cp:  60% 40%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cr:  80% 20%



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ct:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-40.95°, rise=3.96 Å, axial sym=C1	Depositor
Number of segments used	319228	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	13.627	Depositor
Minimum map value	-6.109	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.530	Depositor
Recommended contour level	2.39	Depositor
Map size (Å)	332.5, 332.5, 332.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality [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	0.43	0/1852	0.60	0/2500
1	Ac	0.43	0/1852	0.60	0/2500
1	Ae	0.43	0/1852	0.60	0/2500
1	Ag	0.43	0/1852	0.60	0/2500
1	Ai	0.43	0/1852	0.60	0/2500
1	Ak	0.43	0/1852	0.60	0/2500
1	Am	0.43	0/1852	0.60	0/2500
1	Ao	0.43	0/1852	0.60	0/2500
1	Aq	0.43	0/1852	0.60	0/2500
1	As	0.43	0/1852	0.60	0/2500
1	Au	0.43	0/1852	0.60	0/2500
1	Aw	0.43	0/1852	0.60	0/2500
1	Ay	0.43	0/1852	0.60	0/2500
1	Ba	0.43	0/1852	0.60	0/2500
1	Bc	0.43	0/1852	0.60	0/2500
1	Be	0.43	0/1852	0.60	0/2500
1	Bg	0.43	0/1852	0.60	0/2500
1	Bi	0.43	0/1852	0.60	0/2500
1	Bk	0.43	0/1852	0.60	0/2500
1	Bm	0.43	0/1852	0.60	0/2500
1	Bo	0.43	0/1852	0.60	0/2500
1	Bq	0.43	0/1852	0.60	0/2500
1	Bs	0.43	0/1852	0.60	0/2500
1	Bu	0.43	0/1852	0.60	0/2500
1	Bw	0.43	0/1852	0.60	0/2500
1	By	0.43	0/1852	0.60	0/2500
1	Ca	0.43	0/1852	0.60	0/2500
1	Cc	0.43	0/1852	0.60	0/2500
1	Ce	0.43	0/1852	0.60	0/2500
1	Cg	0.43	0/1852	0.60	0/2500
1	Ci	0.43	0/1852	0.60	0/2500
1	Ck	0.43	0/1852	0.60	0/2500
1	Cm	0.43	0/1852	0.60	0/2500
1	Co	0.43	0/1852	0.60	0/2500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Cq	0.43	0/1852	0.60	0/2500
1	Cs	0.43	0/1852	0.60	0/2500
2	Ab	0.30	0/109	0.35	0/166
2	Ad	0.30	0/109	0.35	0/166
2	Af	0.31	0/109	0.35	0/166
2	Ah	0.30	0/109	0.35	0/166
2	Aj	0.30	0/109	0.35	0/166
2	Al	0.30	0/109	0.35	0/166
2	An	0.30	0/109	0.35	0/166
2	Ap	0.30	0/109	0.35	0/166
2	Ar	0.30	0/109	0.35	0/166
2	At	0.30	0/109	0.35	0/166
2	Av	0.30	0/109	0.35	0/166
2	Ax	0.31	0/109	0.35	0/166
2	Az	0.30	0/109	0.35	0/166
2	Bb	0.30	0/109	0.34	0/166
2	Bd	0.30	0/109	0.35	0/166
2	Bf	0.30	0/109	0.35	0/166
2	Bh	0.30	0/109	0.34	0/166
2	Bj	0.30	0/109	0.35	0/166
2	Bl	0.30	0/109	0.35	0/166
2	Bn	0.30	0/109	0.35	0/166
2	Bp	0.30	0/109	0.35	0/166
2	Br	0.30	0/109	0.35	0/166
2	Bt	0.30	0/109	0.34	0/166
2	Bv	0.31	0/109	0.35	0/166
2	Bx	0.31	0/109	0.34	0/166
2	Bz	0.31	0/109	0.35	0/166
2	Cb	0.30	0/109	0.35	0/166
2	Cd	0.30	0/109	0.35	0/166
2	Cf	0.30	0/109	0.35	0/166
2	Ch	0.30	0/109	0.35	0/166
2	Cj	0.30	0/109	0.35	0/166
2	Cl	0.30	0/109	0.35	0/166
2	Cn	0.30	0/109	0.35	0/166
2	Cp	0.31	0/109	0.35	0/166
2	Cr	0.30	0/109	0.35	0/166
2	Ct	0.30	0/109	0.35	0/166
All	All	0.42	0/70596	0.59	0/95976

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	1813	0	1786	18	0
1	Ac	1813	0	1786	21	0
1	Ae	1813	0	1786	23	0
1	Ag	1813	0	1786	22	0
1	Ai	1813	0	1786	21	0
1	Ak	1813	0	1786	21	0
1	Am	1813	0	1786	20	0
1	Ao	1813	0	1786	21	0
1	Aq	1813	0	1786	22	0
1	As	1813	0	1786	25	0
1	Au	1813	0	1786	24	0
1	Aw	1813	0	1786	25	0
1	Ay	1813	0	1786	25	0
1	Ba	1813	0	1786	26	0
1	Bc	1813	0	1786	26	0
1	Be	1813	0	1786	27	0
1	Bg	1813	0	1786	25	0
1	Bi	1813	0	1786	26	0
1	Bk	1813	0	1786	27	0
1	Bm	1813	0	1786	25	0
1	Bo	1813	0	1786	25	0
1	Bq	1813	0	1786	25	0
1	Bs	1813	0	1786	24	0
1	Bu	1813	0	1786	25	0
1	Bw	1813	0	1786	23	0
1	By	1813	0	1786	26	0
1	Ca	1813	0	1786	24	0
1	Cc	1813	0	1786	21	0
1	Ce	1813	0	1786	21	0
1	Cg	1813	0	1786	25	0
1	Ci	1813	0	1786	22	0
1	Ck	1813	0	1786	21	0
1	Cm	1813	0	1786	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Co	1813	0	1786	19	0
1	Cq	1813	0	1786	19	0
1	Cs	1813	0	1786	21	0
2	Ab	100	0	51	0	0
2	Ad	100	0	51	0	0
2	Af	100	0	51	2	0
2	Ah	100	0	51	0	0
2	Aj	100	0	51	0	0
2	Al	100	0	51	0	0
2	An	100	0	51	0	0
2	Ap	100	0	51	0	0
2	Ar	100	0	51	0	0
2	At	100	0	51	0	0
2	Av	100	0	51	0	0
2	Ax	100	0	51	0	0
2	Az	100	0	51	0	0
2	Bb	100	0	51	2	0
2	Bd	100	0	51	3	0
2	Bf	100	0	51	0	0
2	Bh	100	0	51	0	0
2	Bj	100	0	51	0	0
2	Bl	100	0	51	0	0
2	Bn	100	0	51	0	0
2	Bp	100	0	51	0	0
2	Br	100	0	51	0	0
2	Bt	100	0	51	1	0
2	Bv	100	0	51	2	0
2	Bx	100	0	51	1	0
2	Bz	100	0	51	1	0
2	Cb	100	0	51	0	0
2	Cd	100	0	51	0	0
2	Cf	100	0	51	1	0
2	Ch	100	0	51	3	0
2	Cj	100	0	51	0	0
2	Cl	100	0	51	0	0
2	Cn	100	0	51	0	0
2	Cp	100	0	51	2	0
2	Cr	100	0	51	1	0
2	Ct	100	0	51	0	0
All	All	68868	0	66132	636	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (636) 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:Ao:251:HIS:CD2	1:Ao:258:ARG:HD2	2.32	0.65
1:By:251:HIS:CD2	1:By:258:ARG:HD2	2.32	0.65
1:Co:251:HIS:CD2	1:Co:258:ARG:HD2	2.32	0.65
1:Cq:251:HIS:CD2	1:Cq:258:ARG:HD2	2.32	0.65
1:Aa:251:HIS:CD2	1:Aa:258:ARG:HD2	2.32	0.65
1:Ca:251:HIS:CD2	1:Ca:258:ARG:HD2	2.32	0.65
1:Aq:251:HIS:CD2	1:Aq:258:ARG:HD2	2.32	0.64
1:As:251:HIS:CD2	1:As:258:ARG:HD2	2.32	0.64
1:Bw:251:HIS:CD2	1:Bw:258:ARG:HD2	2.32	0.64
1:Be:251:HIS:CD2	1:Be:258:ARG:HD2	2.32	0.64
1:Bg:251:HIS:CD2	1:Bg:258:ARG:HD2	2.32	0.64
1:Bi:251:HIS:CD2	1:Bi:258:ARG:HD2	2.32	0.64
1:Ac:251:HIS:CD2	1:Ac:258:ARG:HD2	2.32	0.64
1:Am:251:HIS:CD2	1:Am:258:ARG:HD2	2.32	0.64
1:Bk:251:HIS:CD2	1:Bk:258:ARG:HD2	2.32	0.64
1:Cm:251:HIS:CD2	1:Cm:258:ARG:HD2	2.32	0.64
1:Cc:251:HIS:CD2	1:Cc:258:ARG:HD2	2.32	0.64
1:Ay:251:HIS:CD2	1:Ay:258:ARG:HD2	2.32	0.64
1:Cg:251:HIS:CD2	1:Cg:258:ARG:HD2	2.32	0.64
1:Cs:251:HIS:CD2	1:Cs:258:ARG:HD2	2.32	0.64
1:Ba:251:HIS:CD2	1:Ba:258:ARG:HD2	2.32	0.64
1:Ci:251:HIS:CD2	1:Ci:258:ARG:HD2	2.32	0.64
1:Ak:251:HIS:CD2	1:Ak:258:ARG:HD2	2.32	0.63
1:Ae:251:HIS:CD2	1:Ae:258:ARG:HD2	2.32	0.63
1:Ag:251:HIS:CD2	1:Ag:258:ARG:HD2	2.32	0.63
1:Au:251:HIS:CD2	1:Au:258:ARG:HD2	2.32	0.63
1:Bc:251:HIS:CD2	1:Bc:258:ARG:HD2	2.32	0.63
1:Bm:251:HIS:CD2	1:Bm:258:ARG:HD2	2.32	0.63
1:Bu:251:HIS:CD2	1:Bu:258:ARG:HD2	2.32	0.63
1:Ce:251:HIS:CD2	1:Ce:258:ARG:HD2	2.32	0.63
1:Ai:251:HIS:CD2	1:Ai:258:ARG:HD2	2.32	0.63
1:Aw:251:HIS:CD2	1:Aw:258:ARG:HD2	2.32	0.63
1:Bo:251:HIS:CD2	1:Bo:258:ARG:HD2	2.32	0.63
1:Bs:251:HIS:CD2	1:Bs:258:ARG:HD2	2.32	0.63
1:Bq:251:HIS:CD2	1:Bq:258:ARG:HD2	2.32	0.63
1:Ck:251:HIS:CD2	1:Ck:258:ARG:HD2	2.32	0.63
1:Be:260:MET:HE1	1:Bk:269:VAL:HB	1.82	0.61
1:Bs:211:THR:HG22	1:Bs:216:LYS:HG3	1.83	0.60
1:Ck:211:THR:HG22	1:Ck:216:LYS:HG3	1.83	0.60
1:Ai:211:THR:HG22	1:Ai:216:LYS:HG3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:211:THR:HG22	1:Ay:216:LYS:HG3	1.84	0.60
1:Bq:211:THR:HG22	1:Bq:216:LYS:HG3	1.83	0.60
1:Bc:211:THR:HG22	1:Bc:216:LYS:HG3	1.84	0.60
1:Cg:211:THR:HG22	1:Cg:216:LYS:HG3	1.84	0.60
1:Ak:211:THR:HG22	1:Ak:216:LYS:HG3	1.84	0.60
1:Ae:211:THR:HG22	1:Ae:216:LYS:HG3	1.84	0.60
1:Aw:211:THR:HG22	1:Aw:216:LYS:HG3	1.84	0.60
1:Ci:211:THR:HG22	1:Ci:216:LYS:HG3	1.84	0.60
1:Cm:211:THR:HG22	1:Cm:216:LYS:HG3	1.83	0.60
1:Ba:211:THR:HG22	1:Ba:216:LYS:HG3	1.83	0.60
1:Bo:211:THR:HG22	1:Bo:216:LYS:HG3	1.83	0.60
1:Ag:211:THR:HG22	1:Ag:216:LYS:HG3	1.84	0.60
1:Am:211:THR:HG22	1:Am:216:LYS:HG3	1.83	0.60
1:Bm:211:THR:HG22	1:Bm:216:LYS:HG3	1.84	0.60
1:Be:211:THR:HG22	1:Be:216:LYS:HG3	1.83	0.60
1:Bw:211:THR:HG22	1:Bw:216:LYS:HG3	1.83	0.60
1:Ce:211:THR:HG22	1:Ce:216:LYS:HG3	1.83	0.60
1:Bu:211:THR:HG22	1:Bu:216:LYS:HG3	1.84	0.59
1:Cg:260:MET:HE1	1:Cm:269:VAL:HB	1.85	0.59
1:Ae:260:MET:HE1	1:Ak:269:VAL:HB	1.85	0.59
1:Bg:260:MET:HE1	1:Bm:269:VAL:HB	1.83	0.59
1:Bo:260:MET:HE1	1:Bu:269:VAL:HB	1.85	0.59
1:Ac:211:THR:HG22	1:Ac:216:LYS:HG3	1.84	0.59
1:Aw:260:MET:HE1	1:Bc:269:VAL:HB	1.85	0.59
1:Ao:211:THR:HG22	1:Ao:216:LYS:HG3	1.83	0.59
1:Au:211:THR:HG22	1:Au:216:LYS:HG3	1.84	0.59
1:Cc:211:THR:HG22	1:Cc:216:LYS:HG3	1.84	0.59
1:Bu:54:SER:HB2	1:Co:102:SER:O	2.03	0.59
1:Co:211:THR:HG22	1:Co:216:LYS:HG3	1.83	0.59
1:As:211:THR:HG22	1:As:216:LYS:HG3	1.84	0.59
1:Bg:211:THR:HG22	1:Bg:216:LYS:HG3	1.83	0.59
1:Bs:54:SER:HB2	1:Cm:102:SER:O	2.03	0.59
1:Bi:211:THR:HG22	1:Bi:216:LYS:HG3	1.83	0.59
1:Ca:211:THR:HG22	1:Ca:216:LYS:HG3	1.83	0.59
1:Bk:211:THR:HG22	1:Bk:216:LYS:HG3	1.84	0.58
1:Cq:211:THR:HG22	1:Cq:216:LYS:HG3	1.84	0.58
1:Aa:211:THR:HG22	1:Aa:216:LYS:HG3	1.84	0.58
1:Ay:260:MET:HE1	1:Be:269:VAL:HB	1.86	0.58
1:By:211:THR:HG22	1:By:216:LYS:HG3	1.84	0.58
1:Cs:211:THR:HG22	1:Cs:216:LYS:HG3	1.83	0.58
1:Aq:211:THR:HG22	1:Aq:216:LYS:HG3	1.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:260:MET:HE1	1:Ao:269:VAL:HB	1.86	0.58
1:Bq:260:MET:HE1	1:Bw:269:VAL:HB	1.86	0.58
1:Ci:260:MET:HE1	1:Co:269:VAL:HB	1.85	0.58
1:Ac:260:MET:HE1	1:Ai:269:VAL:HB	1.86	0.58
1:Ag:260:MET:HE1	1:Am:269:VAL:HB	1.86	0.58
1:Bm:260:MET:HE1	1:Bs:269:VAL:HB	1.86	0.58
1:Ao:260:MET:HE1	1:Au:269:VAL:HB	1.85	0.58
1:Bs:260:MET:HE1	1:By:269:VAL:HB	1.86	0.58
1:Ce:260:MET:HE1	1:Ck:269:VAL:HB	1.86	0.58
1:Ck:260:MET:HE1	1:Cq:269:VAL:HB	1.86	0.58
1:Ba:260:MET:HE1	1:Bg:269:VAL:HB	1.86	0.58
1:Au:260:MET:HE1	1:Ba:269:VAL:HB	1.86	0.57
1:Bc:260:MET:HE1	1:Bi:269:VAL:HB	1.86	0.57
1:Ak:260:MET:HE1	1:Aq:269:VAL:HB	1.86	0.57
1:Am:260:MET:HE1	1:As:269:VAL:HB	1.85	0.57
1:As:260:MET:HE1	1:Ay:269:VAL:HB	1.87	0.57
1:Ae:226:ALA:HB1	2:Af:4:U:H1'	1.87	0.57
1:Cc:260:MET:HE1	1:Ci:269:VAL:HB	1.87	0.57
1:Cm:260:MET:HE1	1:Cs:269:VAL:HB	1.86	0.57
1:Bk:260:MET:HE1	1:Bq:269:VAL:HB	1.87	0.57
1:Bu:260:MET:HE1	1:Ca:269:VAL:HB	1.86	0.57
1:Aa:260:MET:HE1	1:Ag:269:VAL:HB	1.87	0.57
1:Be:54:SER:HB2	1:By:102:SER:O	2.05	0.57
1:Ai:54:SER:HB2	1:Bc:102:SER:O	2.05	0.57
1:Bw:54:SER:HB2	1:Cq:102:SER:O	2.05	0.57
1:Bc:54:SER:HB2	1:Bw:102:SER:O	2.05	0.57
1:By:260:MET:HE1	1:Ce:269:VAL:HB	1.86	0.57
1:As:54:SER:HB2	1:Bm:102:SER:O	2.04	0.56
1:Bw:260:MET:HE1	1:Cc:269:VAL:HB	1.86	0.56
1:Aq:260:MET:HE1	1:Aw:269:VAL:HB	1.87	0.56
1:Ca:260:MET:HE1	1:Cg:269:VAL:HB	1.87	0.56
1:Ak:54:SER:HB2	1:Be:102:SER:O	2.05	0.56
1:Bq:54:SER:HB2	1:Ck:102:SER:O	2.06	0.56
1:Bi:260:MET:HE1	1:Bo:269:VAL:HB	1.88	0.56
1:Bi:54:SER:HB2	1:Cc:102:SER:O	2.05	0.56
1:Au:54:SER:HB2	1:Bo:102:SER:O	2.05	0.55
1:Aq:54:SER:HB2	1:Bk:102:SER:O	2.05	0.55
1:Am:54:SER:HB2	1:Bg:102:SER:O	2.06	0.55
1:Ag:54:SER:HB2	1:Ba:102:SER:O	2.06	0.55
1:Ba:54:SER:HB2	1:Bu:102:SER:O	2.07	0.55
1:Ba:44:HIS:ND1	1:Bs:71:HIS:HB2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:54:SER:HB2	1:Ca:102:SER:O	2.06	0.55
1:Bm:44:HIS:ND1	1:Ce:71:HIS:HB2	2.22	0.54
1:Ac:54:SER:HB2	1:Aw:102:SER:O	2.06	0.54
1:Aq:44:HIS:ND1	1:Bi:71:HIS:HB2	2.22	0.54
1:Aa:54:SER:HB2	1:Au:102:SER:O	2.07	0.54
1:Aa:44:HIS:ND1	1:As:71:HIS:HB2	2.23	0.54
1:Ao:44:HIS:ND1	1:Bg:71:HIS:HB2	2.23	0.54
1:Bo:44:HIS:ND1	1:Cg:71:HIS:HB2	2.23	0.54
1:Bo:54:SER:HB2	1:Ci:102:SER:O	2.07	0.54
1:Bc:44:HIS:ND1	1:Bu:71:HIS:HB2	2.23	0.54
1:Ca:44:HIS:ND1	1:Cs:71:HIS:HB2	2.23	0.53
1:Ac:44:HIS:ND1	1:Au:71:HIS:HB2	2.23	0.53
1:Bk:44:HIS:ND1	1:Cc:71:HIS:HB2	2.23	0.53
1:Be:44:HIS:ND1	1:Bw:71:HIS:HB2	2.23	0.53
1:Ae:54:SER:HB2	1:Ay:102:SER:O	2.07	0.53
1:Bk:54:SER:HB2	1:Ce:102:SER:O	2.08	0.53
1:Am:44:HIS:ND1	1:Be:71:HIS:HB2	2.24	0.53
1:Bq:44:HIS:ND1	1:Ci:71:HIS:HB2	2.24	0.53
1:Aw:54:SER:HB2	1:Bq:102:SER:O	2.08	0.52
1:Bm:54:SER:HB2	1:Cg:102:SER:O	2.07	0.52
1:Ay:44:HIS:ND1	1:Bq:71:HIS:HB2	2.23	0.52
1:Bg:44:HIS:ND1	1:By:71:HIS:HB2	2.25	0.52
1:Ag:44:HIS:ND1	1:Ay:71:HIS:HB2	2.25	0.52
1:Ai:44:HIS:ND1	1:Ba:71:HIS:HB2	2.25	0.52
1:Ay:54:SER:HB2	1:Bs:102:SER:O	2.08	0.52
1:Bi:44:HIS:ND1	1:Ca:71:HIS:HB2	2.25	0.52
1:Ao:54:SER:HB2	1:Bi:102:SER:O	2.10	0.52
1:By:54:SER:HB2	1:Cs:102:SER:O	2.08	0.52
1:Cm:56:LEU:N	1:Cm:56:LEU:HD12	2.25	0.52
1:Aa:80:VAL:HB	1:Aa:86:ARG:NH1	2.25	0.52
1:Ba:80:VAL:HB	1:Ba:86:ARG:NH1	2.25	0.52
1:By:44:HIS:ND1	1:Cq:71:HIS:HB2	2.25	0.52
1:Ac:80:VAL:HB	1:Ac:86:ARG:NH1	2.25	0.51
1:Ak:44:HIS:ND1	1:Bc:71:HIS:HB2	2.25	0.51
1:Ak:80:VAL:HB	1:Ak:86:ARG:NH1	2.26	0.51
1:Aw:56:LEU:N	1:Aw:56:LEU:HD12	2.26	0.51
1:Bm:80:VAL:HB	1:Bm:86:ARG:NH1	2.25	0.51
1:Bs:56:LEU:N	1:Bs:56:LEU:HD12	2.25	0.51
1:Bu:56:LEU:HD12	1:Bu:56:LEU:N	2.25	0.51
1:By:80:VAL:HB	1:By:86:ARG:NH1	2.25	0.51
1:Ck:56:LEU:HD12	1:Ck:56:LEU:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:44:HIS:ND1	1:Aw:71:HIS:HB2	2.24	0.51
1:Ae:56:LEU:HD12	1:Ae:56:LEU:N	2.26	0.51
1:Ae:226:ALA:CB	2:Af:4:U:H1'	2.39	0.51
1:Aw:44:HIS:ND1	1:Bo:71:HIS:HB2	2.25	0.51
1:Ay:56:LEU:N	1:Ay:56:LEU:HD12	2.26	0.51
1:Bq:56:LEU:N	1:Bq:56:LEU:HD12	2.26	0.51
1:Bq:80:VAL:HB	1:Bq:86:ARG:NH1	2.26	0.51
1:Bs:44:HIS:ND1	1:Ck:71:HIS:HB2	2.25	0.51
1:Ag:56:LEU:N	1:Ag:56:LEU:HD12	2.26	0.51
1:Bk:80:VAL:HB	1:Bk:86:ARG:NH1	2.26	0.51
1:Bo:56:LEU:N	1:Bo:56:LEU:HD12	2.25	0.51
1:Bs:80:VAL:HB	1:Bs:86:ARG:NH1	2.25	0.51
1:Ca:80:VAL:HB	1:Ca:86:ARG:NH1	2.26	0.51
1:Cc:80:VAL:HB	1:Cc:86:ARG:NH1	2.25	0.51
1:Ai:80:VAL:HB	1:Ai:86:ARG:NH1	2.25	0.51
1:Ba:56:LEU:N	1:Ba:56:LEU:HD12	2.26	0.51
1:Bc:80:VAL:HB	1:Bc:86:ARG:NH1	2.25	0.51
1:Bo:80:VAL:HB	1:Bo:86:ARG:NH1	2.25	0.51
1:Bw:44:HIS:ND1	1:Co:71:HIS:HB2	2.26	0.51
1:Bw:80:VAL:HB	1:Bw:86:ARG:NH1	2.25	0.51
1:Ci:56:LEU:N	1:Ci:56:LEU:HD12	2.26	0.51
1:Ci:80:VAL:HB	1:Ci:86:ARG:NH1	2.26	0.51
1:Ao:80:VAL:HB	1:Ao:86:ARG:NH1	2.25	0.51
1:Au:56:LEU:HD12	1:Au:56:LEU:N	2.25	0.51
1:Bc:56:LEU:HD12	1:Bc:56:LEU:N	2.25	0.51
1:Bi:80:VAL:HB	1:Bi:86:ARG:NH1	2.26	0.51
1:Cg:80:VAL:HB	1:Cg:86:ARG:NH1	2.26	0.51
1:Ac:56:LEU:N	1:Ac:56:LEU:HD12	2.25	0.51
1:Am:80:VAL:HB	1:Am:86:ARG:NH1	2.25	0.51
1:Au:44:HIS:ND1	1:Bm:71:HIS:HB2	2.25	0.51
1:Bi:56:LEU:HD12	1:Bi:56:LEU:N	2.25	0.51
1:Ae:80:VAL:HB	1:Ae:86:ARG:NH1	2.25	0.51
1:Ai:56:LEU:HD12	1:Ai:56:LEU:N	2.26	0.51
1:Ce:80:VAL:HB	1:Ce:86:ARG:NH1	2.25	0.51
1:Co:56:LEU:HD12	1:Co:56:LEU:N	2.26	0.51
1:Co:80:VAL:HB	1:Co:86:ARG:NH1	2.25	0.51
1:Cq:56:LEU:N	1:Cq:56:LEU:HD12	2.25	0.51
1:Aq:56:LEU:HD12	1:Aq:56:LEU:N	2.25	0.51
1:Aq:80:VAL:HB	1:Aq:86:ARG:NH1	2.26	0.51
1:Ay:80:VAL:HB	1:Ay:86:ARG:NH1	2.26	0.51
1:Cg:56:LEU:HD12	1:Cg:56:LEU:N	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cm:80:VAL:HB	1:Cm:86:ARG:NH1	2.26	0.51
1:Cs:56:LEU:HD12	1:Cs:56:LEU:N	2.25	0.51
1:Aw:80:VAL:HB	1:Aw:86:ARG:NH1	2.25	0.51
1:Bg:80:VAL:HB	1:Bg:86:ARG:NH1	2.25	0.51
1:Bm:56:LEU:N	1:Bm:56:LEU:HD12	2.25	0.51
1:Bu:44:HIS:ND1	1:Cm:71:HIS:HB2	2.26	0.51
1:Bw:56:LEU:N	1:Bw:56:LEU:HD12	2.26	0.51
1:Ck:80:VAL:HB	1:Ck:86:ARG:NH1	2.25	0.51
1:Aa:56:LEU:HD12	1:Aa:56:LEU:N	2.26	0.50
1:Ao:56:LEU:N	1:Ao:56:LEU:HD12	2.26	0.50
1:As:44:HIS:ND1	1:Bk:71:HIS:HB2	2.26	0.50
1:Ba:127:SER:O	1:Ba:130:ILE:HG12	2.11	0.50
1:Ci:127:SER:O	1:Ci:130:ILE:HG12	2.11	0.50
1:Cq:80:VAL:HB	1:Cq:86:ARG:NH1	2.25	0.50
1:Ag:127:SER:O	1:Ag:130:ILE:HG12	2.11	0.50
1:As:80:VAL:HB	1:As:86:ARG:NH1	2.25	0.50
1:Bk:56:LEU:N	1:Bk:56:LEU:HD12	2.26	0.50
1:Cc:56:LEU:N	1:Cc:56:LEU:HD12	2.26	0.50
1:Ai:127:SER:O	1:Ai:130:ILE:HG12	2.11	0.50
1:Bu:80:VAL:HB	1:Bu:86:ARG:NH1	2.26	0.50
1:Bu:127:SER:O	1:Bu:130:ILE:HG12	2.11	0.50
1:Aa:127:SER:O	1:Aa:130:ILE:HG12	2.11	0.50
1:Ak:56:LEU:N	1:Ak:56:LEU:HD12	2.25	0.50
1:Be:80:VAL:HB	1:Be:86:ARG:NH1	2.25	0.50
1:Cg:127:SER:O	1:Cg:130:ILE:HG12	2.11	0.50
1:Cs:80:VAL:HB	1:Cs:86:ARG:NH1	2.26	0.50
1:Cs:127:SER:O	1:Cs:130:ILE:HG12	2.11	0.50
1:Am:56:LEU:HD12	1:Am:56:LEU:N	2.26	0.50
1:Am:127:SER:O	1:Am:130:ILE:HG12	2.11	0.50
1:Aq:127:SER:O	1:Aq:130:ILE:HG12	2.11	0.50
1:As:56:LEU:N	1:As:56:LEU:HD12	2.26	0.50
1:Au:80:VAL:HB	1:Au:86:ARG:NH1	2.26	0.50
1:Ay:127:SER:O	1:Ay:130:ILE:HG12	2.11	0.50
1:Bs:127:SER:O	1:Bs:130:ILE:HG12	2.11	0.50
1:By:56:LEU:HD12	1:By:56:LEU:N	2.26	0.50
1:Be:56:LEU:N	1:Be:56:LEU:HD12	2.26	0.50
1:Bo:127:SER:O	1:Bo:130:ILE:HG12	2.11	0.50
1:Cc:127:SER:O	1:Cc:130:ILE:HG12	2.11	0.50
1:Ag:80:VAL:HB	1:Ag:86:ARG:NH1	2.26	0.50
1:Ak:127:SER:O	1:Ak:130:ILE:HG12	2.11	0.50
1:Ao:127:SER:O	1:Ao:130:ILE:HG12	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:127:SER:O	1:Bi:130:ILE:HG12	2.11	0.50
1:Ce:56:LEU:N	1:Ce:56:LEU:HD12	2.25	0.50
1:Bg:127:SER:O	1:Bg:130:ILE:HG12	2.11	0.50
1:Bq:127:SER:O	1:Bq:130:ILE:HG12	2.11	0.50
1:Ca:56:LEU:N	1:Ca:56:LEU:HD12	2.26	0.50
1:Bc:127:SER:O	1:Bc:130:ILE:HG12	2.11	0.50
1:Bg:56:LEU:HD12	1:Bg:56:LEU:N	2.26	0.50
1:Co:127:SER:O	1:Co:130:ILE:HG12	2.11	0.50
1:Ae:127:SER:O	1:Ae:130:ILE:HG12	2.11	0.49
1:Bm:127:SER:O	1:Bm:130:ILE:HG12	2.11	0.49
1:Ck:127:SER:O	1:Ck:130:ILE:HG12	2.11	0.49
1:Ce:127:SER:O	1:Ce:130:ILE:HG12	2.11	0.49
1:Cm:127:SER:O	1:Cm:130:ILE:HG12	2.11	0.49
1:Cq:127:SER:O	1:Cq:130:ILE:HG12	2.11	0.49
1:Ac:127:SER:O	1:Ac:130:ILE:HG12	2.11	0.49
1:Bk:127:SER:O	1:Bk:130:ILE:HG12	2.11	0.49
1:As:127:SER:O	1:As:130:ILE:HG12	2.11	0.49
1:Aw:127:SER:O	1:Aw:130:ILE:HG12	2.11	0.49
1:Bw:127:SER:O	1:Bw:130:ILE:HG12	2.11	0.49
1:Ca:127:SER:O	1:Ca:130:ILE:HG12	2.11	0.49
1:Ca:210:THR:HB	1:Cs:152:ASP:OD2	2.12	0.49
1:Au:127:SER:O	1:Au:130:ILE:HG12	2.11	0.49
1:By:127:SER:O	1:By:130:ILE:HG12	2.11	0.49
1:Be:127:SER:O	1:Be:130:ILE:HG12	2.11	0.49
1:Bk:210:THR:HB	1:Cc:152:ASP:OD2	2.13	0.49
1:Aq:210:THR:HB	1:Bi:152:ASP:OD2	2.13	0.49
1:Ao:210:THR:HB	1:Bg:152:ASP:OD2	2.13	0.49
1:Ay:210:THR:HB	1:Bq:152:ASP:OD2	2.12	0.49
1:By:210:THR:HB	1:Cq:152:ASP:OD2	2.13	0.48
1:Aw:210:THR:HB	1:Bo:152:ASP:OD2	2.13	0.48
1:Aa:210:THR:HB	1:As:152:ASP:OD2	2.13	0.48
1:Bc:227:LEU:CD2	2:Bd:3:U:H2'	2.43	0.48
1:Am:210:THR:HB	1:Be:152:ASP:OD2	2.13	0.48
1:Bg:75:TYR:CZ	1:Bg:77:PRO:HG3	2.49	0.48
1:Bi:75:TYR:CZ	1:Bi:77:PRO:HG3	2.49	0.48
1:Bq:75:TYR:CZ	1:Bq:77:PRO:HG3	2.49	0.48
1:Ce:75:TYR:CZ	1:Ce:77:PRO:HG3	2.49	0.48
1:Ae:75:TYR:CZ	1:Ae:77:PRO:HG3	2.49	0.48
1:Ag:75:TYR:CZ	1:Ag:77:PRO:HG3	2.49	0.48
1:Au:75:TYR:CZ	1:Au:77:PRO:HG3	2.49	0.48
1:Ay:75:TYR:CZ	1:Ay:77:PRO:HG3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:By:75:TYR:CZ	1:By:77:PRO:HG3	2.49	0.48
1:Cs:75:TYR:CZ	1:Cs:77:PRO:HG3	2.49	0.48
1:As:75:TYR:CZ	1:As:77:PRO:HG3	2.49	0.48
1:Ca:75:TYR:CZ	1:Ca:77:PRO:HG3	2.49	0.48
1:Cg:75:TYR:CZ	1:Cg:77:PRO:HG3	2.49	0.48
1:Cq:75:TYR:CZ	1:Cq:77:PRO:HG3	2.49	0.48
1:Ac:75:TYR:CZ	1:Ac:77:PRO:HG3	2.49	0.47
2:Bd:1:U:P	1:Be:185:ARG:HH12	2.37	0.47
1:Bo:75:TYR:CZ	1:Bo:77:PRO:HG3	2.49	0.47
1:Bs:75:TYR:CZ	1:Bs:77:PRO:HG3	2.49	0.47
1:Ac:210:THR:HB	1:Au:152:ASP:OD2	2.15	0.47
1:Aw:75:TYR:CZ	1:Aw:77:PRO:HG3	2.49	0.47
1:Cc:75:TYR:CZ	1:Cc:77:PRO:HG3	2.49	0.47
1:Ai:75:TYR:CZ	1:Ai:77:PRO:HG3	2.49	0.47
1:Aq:75:TYR:CZ	1:Aq:77:PRO:HG3	2.49	0.47
1:Be:75:TYR:CZ	1:Be:77:PRO:HG3	2.49	0.47
1:Bk:75:TYR:CZ	1:Bk:77:PRO:HG3	2.49	0.47
1:Aa:75:TYR:CZ	1:Aa:77:PRO:HG3	2.49	0.47
1:Ao:75:TYR:CZ	1:Ao:77:PRO:HG3	2.49	0.47
1:Ba:210:THR:HB	1:Bs:152:ASP:OD2	2.14	0.47
1:Bm:210:THR:HB	1:Ce:152:ASP:OD2	2.15	0.47
1:Bu:75:TYR:CZ	1:Bu:77:PRO:HG3	2.49	0.47
1:Bw:75:TYR:CZ	1:Bw:77:PRO:HG3	2.49	0.47
1:Ci:75:TYR:CZ	1:Ci:77:PRO:HG3	2.49	0.47
1:Bc:75:TYR:CZ	1:Bc:77:PRO:HG3	2.49	0.47
1:Au:210:THR:HB	1:Bm:152:ASP:OD2	2.14	0.47
1:Bw:210:THR:HB	1:Co:152:ASP:OD2	2.14	0.47
1:Ae:210:THR:HB	1:Aw:152:ASP:OD2	2.15	0.47
1:Ak:75:TYR:CZ	1:Ak:77:PRO:HG3	2.49	0.47
1:Ba:75:TYR:CZ	1:Ba:77:PRO:HG3	2.49	0.47
1:Bg:243:THR:HG22	1:By:254:THR:HG22	1.97	0.47
1:Ck:75:TYR:CZ	1:Ck:77:PRO:HG3	2.49	0.47
1:Co:75:TYR:CZ	1:Co:77:PRO:HG3	2.49	0.47
1:Ag:210:THR:HB	1:Ay:152:ASP:OD2	2.15	0.47
1:Am:75:TYR:CZ	1:Am:77:PRO:HG3	2.49	0.47
1:As:210:THR:HB	1:Bk:152:ASP:OD2	2.15	0.47
1:Ba:86:ARG:HD2	1:Ba:206:GLU:OE1	2.15	0.47
1:Bc:210:THR:HB	1:Bu:152:ASP:OD2	2.15	0.47
1:Bk:86:ARG:HD2	1:Bk:206:GLU:OE1	2.15	0.47
1:Ac:86:ARG:HD2	1:Ac:206:GLU:OE1	2.15	0.47
1:Ak:210:THR:HB	1:Bc:152:ASP:OD2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:86:ARG:HD2	1:Am:206:GLU:OE1	2.15	0.47
1:Bm:75:TYR:CZ	1:Bm:77:PRO:HG3	2.49	0.47
1:Bo:210:THR:HB	1:Cg:152:ASP:OD2	2.15	0.47
1:By:86:ARG:HD2	1:By:206:GLU:OE1	2.15	0.47
1:Ci:86:ARG:HD2	1:Ci:206:GLU:OE1	2.15	0.47
1:Ao:86:ARG:HD2	1:Ao:206:GLU:OE1	2.15	0.46
1:As:86:ARG:HD2	1:As:206:GLU:OE1	2.15	0.46
1:Ca:86:ARG:HD2	1:Ca:206:GLU:OE1	2.15	0.46
1:Cm:86:ARG:HD2	1:Cm:206:GLU:OE1	2.15	0.46
1:Ak:86:ARG:HD2	1:Ak:206:GLU:OE1	2.15	0.46
1:Ce:86:ARG:HD2	1:Ce:206:GLU:OE1	2.15	0.46
1:Cs:86:ARG:HD2	1:Cs:206:GLU:OE1	2.15	0.46
1:Aa:86:ARG:HD2	1:Aa:206:GLU:OE1	2.15	0.46
1:Bs:86:ARG:HD2	1:Bs:206:GLU:OE1	2.16	0.46
1:Bw:86:ARG:HD2	1:Bw:206:GLU:OE1	2.16	0.46
1:Cm:75:TYR:CZ	1:Cm:77:PRO:HG3	2.49	0.46
1:Aa:228:LYS:NZ	1:Bi:255:ASP:OD1	2.49	0.46
1:Ag:86:ARG:HD2	1:Ag:206:GLU:OE1	2.15	0.46
1:Aq:86:ARG:HD2	1:Aq:206:GLU:OE1	2.15	0.46
1:Aw:86:ARG:HD2	1:Aw:206:GLU:OE1	2.15	0.46
1:Bo:86:ARG:HD2	1:Bo:206:GLU:OE1	2.15	0.46
1:Ck:86:ARG:HD2	1:Ck:206:GLU:OE1	2.15	0.46
1:Co:86:ARG:HD2	1:Co:206:GLU:OE1	2.16	0.46
1:Aa:174:GLU:HG3	1:Aa:199:ARG:NH1	2.31	0.46
1:Au:174:GLU:HG3	1:Au:199:ARG:NH1	2.31	0.46
1:Be:86:ARG:HD2	1:Be:206:GLU:OE1	2.15	0.46
1:Bi:243:THR:HG22	1:Ca:254:THR:HG22	1.98	0.46
1:Bq:210:THR:HB	1:Ci:152:ASP:OD2	2.16	0.46
1:Bu:210:THR:HB	1:Cm:152:ASP:OD2	2.15	0.46
1:Ai:210:THR:HB	1:Ba:152:ASP:OD2	2.15	0.46
1:As:174:GLU:HG3	1:As:199:ARG:NH1	2.31	0.46
1:Be:210:THR:HB	1:Bw:152:ASP:OD2	2.16	0.46
1:Bm:174:GLU:HG3	1:Bm:199:ARG:NH1	2.31	0.46
1:Bs:243:THR:HG22	1:Ck:254:THR:HG22	1.97	0.46
1:Bu:86:ARG:HD2	1:Bu:206:GLU:OE1	2.15	0.46
1:Cq:86:ARG:HD2	1:Cq:206:GLU:OE1	2.15	0.46
1:Ac:174:GLU:HG3	1:Ac:199:ARG:NH1	2.31	0.46
1:Ai:86:ARG:HD2	1:Ai:206:GLU:OE1	2.15	0.46
1:Aw:174:GLU:HG3	1:Aw:199:ARG:NH1	2.31	0.46
1:Bg:86:ARG:HD2	1:Bg:206:GLU:OE1	2.15	0.46
1:Bo:174:GLU:HG3	1:Bo:199:ARG:NH1	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bq:86:ARG:HD2	1:Bq:206:GLU:OE1	2.15	0.46
1:Co:174:GLU:HG3	1:Co:199:ARG:NH1	2.31	0.46
1:Cq:174:GLU:HG3	1:Cq:199:ARG:NH1	2.31	0.46
1:Au:86:ARG:HD2	1:Au:206:GLU:OE1	2.15	0.46
1:Bi:174:GLU:HG3	1:Bi:199:ARG:NH1	2.31	0.46
1:Ca:174:GLU:HG3	1:Ca:199:ARG:NH1	2.31	0.46
1:Cc:86:ARG:HD2	1:Cc:206:GLU:OE1	2.15	0.46
1:Cc:174:GLU:HG3	1:Cc:199:ARG:NH1	2.31	0.46
1:Aq:174:GLU:HG3	1:Aq:199:ARG:NH1	2.31	0.46
1:Bi:86:ARG:HD2	1:Bi:206:GLU:OE1	2.15	0.46
1:Bk:228:LYS:NZ	1:Cs:255:ASP:OD1	2.49	0.46
1:Bw:174:GLU:HG3	1:Bw:199:ARG:NH1	2.31	0.46
2:Cp:1:U:P	2:Cr:5:U:O3'	2.74	0.46
1:Ak:228:LYS:NZ	1:Bs:255:ASP:OD1	2.49	0.46
1:Bc:86:ARG:HD2	1:Bc:206:GLU:OE1	2.15	0.46
1:Bi:211:THR:CG2	1:Bi:216:LYS:HG3	2.46	0.46
1:Bk:174:GLU:HG3	1:Bk:199:ARG:NH1	2.31	0.46
1:Bm:86:ARG:HD2	1:Bm:206:GLU:OE1	2.15	0.46
1:Ce:174:GLU:HG3	1:Ce:199:ARG:NH1	2.31	0.46
1:Cg:174:GLU:HG3	1:Cg:199:ARG:NH1	2.31	0.46
1:Ae:174:GLU:HG3	1:Ae:199:ARG:NH1	2.31	0.45
1:Ao:211:THR:CG2	1:Ao:216:LYS:HG3	2.47	0.45
1:Aq:211:THR:CG2	1:Aq:216:LYS:HG3	2.46	0.45
1:Ba:130:ILE:HG22	2:Bb:5:U:H1'	1.98	0.45
1:Bg:174:GLU:HG3	1:Bg:199:ARG:NH1	2.31	0.45
1:Bk:211:THR:CG2	1:Bk:216:LYS:HG3	2.47	0.45
1:Cm:174:GLU:HG3	1:Cm:199:ARG:NH1	2.31	0.45
1:Cs:211:THR:CG2	1:Cs:216:LYS:HG3	2.46	0.45
1:Ac:211:THR:CG2	1:Ac:216:LYS:HG3	2.47	0.45
1:Ay:86:ARG:HD2	1:Ay:206:GLU:OE1	2.15	0.45
1:Bg:210:THR:HB	1:By:152:ASP:OD2	2.16	0.45
1:Bq:174:GLU:HG3	1:Bq:199:ARG:NH1	2.31	0.45
1:Bs:210:THR:HB	1:Ck:152:ASP:OD2	2.16	0.45
1:Bw:211:THR:CG2	1:Bw:216:LYS:HG3	2.47	0.45
1:By:174:GLU:HG3	1:By:199:ARG:NH1	2.31	0.45
1:Cq:211:THR:CG2	1:Cq:216:LYS:HG3	2.47	0.45
1:Cs:174:GLU:HG3	1:Cs:199:ARG:NH1	2.31	0.45
1:Ae:86:ARG:HD2	1:Ae:206:GLU:OE1	2.15	0.45
1:Ay:174:GLU:HG3	1:Ay:199:ARG:NH1	2.31	0.45
1:Bu:174:GLU:HG3	1:Bu:199:ARG:NH1	2.31	0.45
1:Bu:243:THR:HG22	1:Cm:254:THR:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:211:THR:CG2	1:Aa:216:LYS:HG3	2.47	0.45
1:Ao:174:GLU:HG3	1:Ao:199:ARG:NH1	2.31	0.45
1:Ce:211:THR:CG2	1:Ce:216:LYS:HG3	2.47	0.45
1:Ci:174:GLU:HG3	1:Ci:199:ARG:NH1	2.31	0.45
1:Ck:174:GLU:HG3	1:Ck:199:ARG:NH1	2.31	0.45
1:Co:211:THR:CG2	1:Co:216:LYS:HG3	2.47	0.45
1:Am:211:THR:CG2	1:Am:216:LYS:HG3	2.47	0.45
1:Ba:174:GLU:HG3	1:Ba:199:ARG:NH1	2.31	0.45
1:Be:243:THR:HG22	1:Bw:254:THR:HG22	1.97	0.45
1:Bi:210:THR:HB	1:Ca:152:ASP:OD2	2.15	0.45
1:Bs:174:GLU:HG3	1:Bs:199:ARG:NH1	2.31	0.45
1:Cc:211:THR:CG2	1:Cc:216:LYS:HG3	2.47	0.45
1:Ae:211:THR:CG2	1:Ae:216:LYS:HG3	2.47	0.45
1:Bu:211:THR:CG2	1:Bu:216:LYS:HG3	2.47	0.45
1:By:211:THR:CG2	1:By:216:LYS:HG3	2.47	0.45
1:Cg:86:ARG:HD2	1:Cg:206:GLU:OE1	2.15	0.45
1:Bm:211:THR:CG2	1:Bm:216:LYS:HG3	2.47	0.45
1:Bq:243:THR:HG22	1:Ci:254:THR:HG22	1.98	0.45
1:Co:203:ASP:OD1	2:Cp:4:U:O2'	2.31	0.45
1:Ac:243:THR:HG22	1:Au:254:THR:HG22	1.99	0.45
1:Ag:174:GLU:HG3	1:Ag:199:ARG:NH1	2.31	0.45
1:Ak:174:GLU:HG3	1:Ak:199:ARG:NH1	2.31	0.45
1:Be:174:GLU:HG3	1:Be:199:ARG:NH1	2.31	0.45
1:Bg:211:THR:CG2	1:Bg:216:LYS:HG3	2.47	0.45
1:Bs:130:ILE:HG22	2:Bt:5:U:H1'	1.98	0.45
1:Ae:243:THR:HG22	1:Aw:254:THR:HG22	1.99	0.45
1:Am:174:GLU:HG3	1:Am:199:ARG:NH1	2.31	0.45
1:As:243:THR:HG22	1:Bk:254:THR:HG22	1.98	0.45
1:Ba:211:THR:CG2	1:Ba:216:LYS:HG3	2.47	0.45
1:Bc:174:GLU:HG3	1:Bc:199:ARG:NH1	2.31	0.45
1:Bc:211:THR:CG2	1:Bc:216:LYS:HG3	2.47	0.45
1:Cg:211:THR:CG2	1:Cg:216:LYS:HG3	2.47	0.45
1:As:211:THR:CG2	1:As:216:LYS:HG3	2.47	0.45
1:Aw:211:THR:CG2	1:Aw:216:LYS:HG3	2.47	0.45
1:Ay:211:THR:CG2	1:Ay:216:LYS:HG3	2.47	0.45
1:Cg:226:ALA:HB1	2:Ch:4:U:H1'	1.99	0.45
1:Be:211:THR:CG2	1:Be:216:LYS:HG3	2.46	0.44
1:Bs:211:THR:CG2	1:Bs:216:LYS:HG3	2.46	0.44
1:Ca:211:THR:CG2	1:Ca:216:LYS:HG3	2.46	0.44
1:Au:211:THR:CG2	1:Au:216:LYS:HG3	2.47	0.44
1:Ci:211:THR:CG2	1:Ci:216:LYS:HG3	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:211:THR:CG2	1:Ag:216:LYS:HG3	2.47	0.44
1:Cm:211:THR:CG2	1:Cm:216:LYS:HG3	2.47	0.44
1:Aa:243:THR:HG22	1:As:254:THR:HG22	2.00	0.44
2:Cf:1:U:P	2:Ch:5:U:O3'	2.76	0.44
1:Ck:211:THR:CG2	1:Ck:216:LYS:HG3	2.46	0.44
1:Ai:174:GLU:HG3	1:Ai:199:ARG:NH1	2.31	0.44
1:Ak:211:THR:CG2	1:Ak:216:LYS:HG3	2.47	0.44
1:Bc:228:LYS:NZ	1:Ck:255:ASP:OD1	2.50	0.44
1:Bc:243:THR:HG22	1:Bu:254:THR:HG22	1.99	0.44
1:Ak:243:THR:HG22	1:Bc:254:THR:HG22	1.99	0.44
1:Ao:228:LYS:NZ	1:Bw:255:ASP:OD1	2.50	0.44
1:Ao:243:THR:HG22	1:Bg:254:THR:HG22	2.00	0.44
1:Bo:243:THR:HG22	1:Cg:254:THR:HG22	1.98	0.44
1:Am:243:THR:HG22	1:Be:254:THR:HG22	2.00	0.44
1:Ba:228:LYS:NZ	1:Ci:255:ASP:OD1	2.51	0.44
1:Bo:211:THR:CG2	1:Bo:216:LYS:HG3	2.47	0.44
1:Ai:243:THR:HG22	1:Ba:254:THR:HG22	1.98	0.44
1:Bq:211:THR:CG2	1:Bq:216:LYS:HG3	2.46	0.44
1:Ai:211:THR:CG2	1:Ai:216:LYS:HG3	2.47	0.43
1:Au:243:THR:HG22	1:Bm:254:THR:HG22	2.00	0.43
1:Bm:243:THR:HG22	1:Ce:254:THR:HG22	1.99	0.43
1:Bw:243:THR:HG22	1:Co:254:THR:HG22	2.00	0.43
1:Ac:228:LYS:NZ	1:Bk:255:ASP:OD1	2.51	0.43
1:Ai:228:LYS:NZ	1:Bq:255:ASP:OD1	2.51	0.43
1:Bi:245:GLU:HG2	1:Bi:246:GLU:N	2.34	0.43
1:Cc:245:GLU:HG2	1:Cc:246:GLU:N	2.34	0.43
1:Aq:245:GLU:HG2	1:Aq:246:GLU:N	2.34	0.43
1:Ae:245:GLU:HG2	1:Ae:246:GLU:N	2.33	0.43
1:Ao:245:GLU:HG2	1:Ao:246:GLU:N	2.34	0.43
1:As:228:LYS:NZ	1:Ca:255:ASP:OD1	2.51	0.43
1:Bu:124:ASN:O	2:Bv:5:U:O2'	2.34	0.43
1:Ca:245:GLU:HG2	1:Ca:246:GLU:N	2.34	0.43
1:Am:228:LYS:NZ	1:Bu:255:ASP:OD1	2.51	0.43
1:Bk:245:GLU:HG2	1:Bk:246:GLU:N	2.34	0.43
1:Aq:243:THR:HG22	1:Bi:254:THR:HG22	2.01	0.43
1:Bg:245:GLU:HG2	1:Bg:246:GLU:N	2.34	0.43
1:Bk:243:THR:HG22	1:Cc:254:THR:HG22	2.01	0.43
1:Cg:226:ALA:CB	2:Ch:4:U:H1'	2.49	0.43
1:Cs:245:GLU:HG2	1:Cs:246:GLU:N	2.34	0.43
1:Ac:245:GLU:HG2	1:Ac:246:GLU:N	2.33	0.43
1:Ag:243:THR:HG22	1:Ay:254:THR:HG22	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aw:245:GLU:HG2	1:Aw:246:GLU:N	2.34	0.43
1:Bg:228:LYS:NZ	1:Co:255:ASP:OD1	2.52	0.43
1:Cm:245:GLU:HG2	1:Cm:246:GLU:N	2.33	0.43
1:Ce:245:GLU:HG2	1:Ce:246:GLU:N	2.34	0.43
1:As:245:GLU:HG2	1:As:246:GLU:N	2.34	0.43
1:Co:245:GLU:HG2	1:Co:246:GLU:N	2.34	0.43
1:Ae:228:LYS:NZ	1:Bm:255:ASP:OD1	2.52	0.42
1:Ag:245:GLU:HG2	1:Ag:246:GLU:N	2.34	0.42
1:Au:228:LYS:NZ	1:Cc:255:ASP:OD1	2.51	0.42
1:Ay:245:GLU:HG2	1:Ay:246:GLU:N	2.34	0.42
1:Ba:243:THR:HG22	1:Bs:254:THR:HG22	2.00	0.42
1:By:245:GLU:HG2	1:By:246:GLU:N	2.34	0.42
1:Am:245:GLU:HG2	1:Am:246:GLU:N	2.34	0.42
1:Bo:245:GLU:HG2	1:Bo:246:GLU:N	2.34	0.42
1:Bu:245:GLU:HG2	1:Bu:246:GLU:N	2.34	0.42
1:Ao:269:VAL:HA	1:Aq:269:VAL:HG22	2.02	0.42
1:Aw:228:LYS:NZ	1:Ce:255:ASP:OD1	2.52	0.42
1:Ay:228:LYS:NZ	1:Cg:255:ASP:OD1	2.52	0.42
1:Bg:269:VAL:HA	1:Bi:269:VAL:HG22	2.01	0.42
1:Bm:245:GLU:HG2	1:Bm:246:GLU:N	2.33	0.42
1:Cq:269:VAL:HA	1:Cs:269:VAL:HG22	2.02	0.42
1:Au:245:GLU:HG2	1:Au:246:GLU:N	2.33	0.42
1:Bq:245:GLU:HG2	1:Bq:246:GLU:N	2.34	0.42
1:Bs:245:GLU:HG2	1:Bs:246:GLU:N	2.34	0.42
1:Ck:245:GLU:HG2	1:Ck:246:GLU:N	2.34	0.42
1:Ag:228:LYS:NZ	1:Bo:255:ASP:OD1	2.53	0.42
1:Aw:243:THR:HG22	1:Bo:254:THR:HG22	2.01	0.42
2:Bx:1:U:P	2:Bz:5:U:O3'	2.78	0.42
1:Ba:245:GLU:HG2	1:Ba:246:GLU:N	2.34	0.42
1:Be:245:GLU:HG2	1:Be:246:GLU:N	2.34	0.42
1:Bw:245:GLU:HG2	1:Bw:246:GLU:N	2.34	0.42
1:Aa:245:GLU:HG2	1:Aa:246:GLU:N	2.34	0.42
1:Bg:64:LYS:HE3	1:Bi:107:GLU:OE1	2.20	0.42
1:Cq:64:LYS:HE3	1:Cs:107:GLU:OE1	2.20	0.42
1:Cq:245:GLU:HG2	1:Cq:246:GLU:N	2.34	0.42
1:Aq:113:ILE:HD13	1:Aq:113:ILE:HA	1.96	0.42
1:Bk:64:LYS:HE3	1:Bm:107:GLU:OE1	2.20	0.42
1:Cg:77:PRO:HG2	1:Cg:82:LEU:HD11	2.02	0.42
1:Aa:64:LYS:HE3	1:Ac:107:GLU:OE1	2.20	0.42
1:Ae:269:VAL:HA	1:Ag:269:VAL:HG22	2.02	0.42
1:Ag:77:PRO:HG2	1:Ag:82:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:245:GLU:HG2	1:Bc:246:GLU:N	2.34	0.42
1:Bu:203:ASP:OD1	2:Bv:4:U:O2'	2.27	0.42
1:By:243:THR:HG22	1:Cq:254:THR:HG22	2.01	0.42
1:Ci:245:GLU:HG2	1:Ci:246:GLU:N	2.34	0.42
1:Ai:245:GLU:HG2	1:Ai:246:GLU:N	2.34	0.42
1:Bo:77:PRO:HG2	1:Bo:82:LEU:HD11	2.02	0.42
1:Bq:77:PRO:HG2	1:Bq:82:LEU:HD11	2.02	0.42
1:Ce:77:PRO:HG2	1:Ce:82:LEU:HD11	2.02	0.42
1:Ci:77:PRO:HG2	1:Ci:82:LEU:HD11	2.02	0.42
1:Ca:64:LYS:HE3	1:Cc:107:GLU:OE1	2.20	0.41
1:Ca:243:THR:HG22	1:Cs:254:THR:HG22	2.02	0.41
1:Ae:77:PRO:HG2	1:Ae:82:LEU:HD11	2.02	0.41
1:Aw:77:PRO:HG2	1:Aw:82:LEU:HD11	2.02	0.41
1:Bk:113:ILE:HD13	1:Bk:113:ILE:HA	1.96	0.41
1:Bm:77:PRO:HG2	1:Bm:82:LEU:HD11	2.02	0.41
1:Cg:245:GLU:HG2	1:Cg:246:GLU:N	2.34	0.41
1:Ai:77:PRO:HG2	1:Ai:82:LEU:HD11	2.02	0.41
1:Ao:77:PRO:HG2	1:Ao:82:LEU:HD11	2.02	0.41
1:Ay:64:LYS:HE3	1:Ba:107:GLU:OE1	2.20	0.41
1:Ay:77:PRO:HG2	1:Ay:82:LEU:HD11	2.02	0.41
1:Bw:77:PRO:HG2	1:Bw:82:LEU:HD11	2.02	0.41
1:Cg:269:VAL:HA	1:Ci:269:VAL:HG22	2.02	0.41
1:Ci:64:LYS:HE3	1:Ck:107:GLU:OE1	2.20	0.41
1:Ac:269:VAL:HA	1:Ae:269:VAL:HG22	2.03	0.41
1:Ao:64:LYS:HE3	1:Aq:107:GLU:OE1	2.20	0.41
1:Bg:77:PRO:HG2	1:Bg:82:LEU:HD11	2.02	0.41
1:Bi:77:PRO:HG2	1:Bi:82:LEU:HD11	2.02	0.41
1:Bm:269:VAL:HA	1:Bo:269:VAL:HG22	2.03	0.41
1:Ce:269:VAL:HA	1:Cg:269:VAL:HG22	2.03	0.41
1:Ae:64:LYS:HE3	1:Ag:107:GLU:OE1	2.21	0.41
1:Am:77:PRO:HG2	1:Am:82:LEU:HD11	2.02	0.41
1:Bi:228:LYS:NZ	1:Cq:255:ASP:OD1	2.54	0.41
1:Bo:64:LYS:HE3	1:Bq:107:GLU:OE1	2.21	0.41
1:By:64:LYS:HE3	1:Ca:107:GLU:OE1	2.20	0.41
1:By:77:PRO:HG2	1:By:82:LEU:HD11	2.02	0.41
1:Ck:77:PRO:HG2	1:Ck:82:LEU:HD11	2.02	0.41
1:Cq:77:PRO:HG2	1:Cq:82:LEU:HD11	2.02	0.41
1:Aq:64:LYS:HE3	1:As:107:GLU:OE1	2.21	0.41
1:Au:77:PRO:HG2	1:Au:82:LEU:HD11	2.02	0.41
1:Aw:269:VAL:HA	1:Ay:269:VAL:HG22	2.02	0.41
1:Ba:130:ILE:CG2	2:Bb:5:U:H1'	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:227:LEU:HD22	2:Bd:3:U:H2'	2.02	0.41
1:Be:228:LYS:NZ	1:Cm:255:ASP:OD1	2.53	0.41
1:Bs:77:PRO:HG2	1:Bs:82:LEU:HD11	2.02	0.41
1:By:113:ILE:HD13	1:By:113:ILE:HA	1.96	0.41
1:By:269:VAL:HA	1:Ca:269:VAL:HG22	2.02	0.41
1:Cc:77:PRO:HG2	1:Cc:82:LEU:HD11	2.02	0.41
1:Cm:77:PRO:HG2	1:Cm:82:LEU:HD11	2.02	0.41
1:Ac:77:PRO:HG2	1:Ac:82:LEU:HD11	2.02	0.41
1:Ak:245:GLU:HG2	1:Ak:246:GLU:N	2.34	0.41
1:Aq:228:LYS:NZ	1:By:255:ASP:OD1	2.53	0.41
1:Ba:77:PRO:HG2	1:Ba:82:LEU:HD11	2.02	0.41
1:Ay:243:THR:HG22	1:Bq:254:THR:HG22	2.02	0.41
1:Co:77:PRO:HG2	1:Co:82:LEU:HD11	2.02	0.41
1:Cs:77:PRO:HG2	1:Cs:82:LEU:HD11	2.02	0.41
1:Aq:77:PRO:HG2	1:Aq:82:LEU:HD11	2.02	0.41
1:As:64:LYS:HE3	1:Au:107:GLU:OE1	2.20	0.41
1:As:77:PRO:HG2	1:As:82:LEU:HD11	2.02	0.41
1:Bc:77:PRO:HG2	1:Bc:82:LEU:HD11	2.02	0.41
1:Be:46:VAL:HA	1:Be:47:PRO:HD3	1.96	0.41
1:Be:77:PRO:HG2	1:Be:82:LEU:HD11	2.02	0.41
1:Bk:77:PRO:HG2	1:Bk:82:LEU:HD11	2.02	0.41
1:Bo:269:VAL:HA	1:Bq:269:VAL:HG22	2.02	0.41
1:Bq:64:LYS:HE3	1:Bs:107:GLU:OE1	2.20	0.41
1:Cc:64:LYS:HE3	1:Ce:107:GLU:OE1	2.20	0.41
1:Co:155:LYS:HB3	1:Co:155:LYS:HE2	1.95	0.41
1:Ac:46:VAL:HA	1:Ac:47:PRO:HD3	1.96	0.41
1:Bk:229:ASN:HD21	1:Cs:254:THR:HG21	1.86	0.41
1:Cg:113:ILE:HD13	1:Cg:113:ILE:HA	1.96	0.41
1:Ak:77:PRO:HG2	1:Ak:82:LEU:HD11	2.02	0.40
1:Ak:123:GLU:HA	1:Ak:123:GLU:OE1	2.22	0.40
1:Ba:64:LYS:HE3	1:Bc:107:GLU:OE1	2.22	0.40
1:Be:64:LYS:HE3	1:Bg:107:GLU:OE1	2.21	0.40
1:Ca:77:PRO:HG2	1:Ca:82:LEU:HD11	2.02	0.40
1:Aa:77:PRO:HG2	1:Aa:82:LEU:HD11	2.02	0.40
1:Ai:123:GLU:HA	1:Ai:123:GLU:OE1	2.22	0.40
1:Bc:64:LYS:HE3	1:Be:107:GLU:OE1	2.22	0.40
1:Be:155:LYS:HB3	1:Be:155:LYS:HE2	1.94	0.40
1:Bk:269:VAL:HA	1:Bm:269:VAL:HG22	2.04	0.40
1:Bu:77:PRO:HG2	1:Bu:82:LEU:HD11	2.02	0.40
1:Bw:64:LYS:HE3	1:By:107:GLU:OE1	2.21	0.40
1:Ci:123:GLU:HA	1:Ci:123:GLU:OE1	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ck:123:GLU:HA	1:Ck:123:GLU:OE1	2.22	0.40
1:Ag:64:LYS:HE3	1:Ai:107:GLU:OE1	2.20	0.40
1:Ag:123:GLU:HA	1:Ag:123:GLU:OE1	2.22	0.40
1:Am:64:LYS:HE3	1:Ao:107:GLU:OE1	2.21	0.40
1:Cg:64:LYS:HE3	1:Ci:107:GLU:OE1	2.21	0.40
1:Cg:123:GLU:HA	1:Cg:123:GLU:OE1	2.22	0.40
1:Cs:123:GLU:OE1	1:Cs:123:GLU:HA	2.22	0.40
1:Ae:123:GLU:HA	1:Ae:123:GLU:OE1	2.22	0.40
1:Am:123:GLU:HA	1:Am:123:GLU:OE1	2.22	0.40
1:As:264:LEU:HD12	1:As:264:LEU:HA	1.94	0.40
1:Aw:64:LYS:HE3	1:Ay:107:GLU:OE1	2.21	0.40
1:Bi:123:GLU:OE1	1:Bi:123:GLU:HA	2.22	0.40
1:Bu:123:GLU:HA	1:Bu:123:GLU:OE1	2.22	0.40
1:Cm:123:GLU:HA	1:Cm:123:GLU:OE1	2.22	0.40
1:Ac:113:ILE:HD13	1:Ac:113:ILE:HA	1.96	0.40
1:Ai:64:LYS:HE3	1:Ak:107:GLU:OE1	2.21	0.40
1:Ak:155:LYS:HE2	1:Ak:155:LYS:HB3	1.95	0.40
1:As:123:GLU:OE1	1:As:123:GLU:HA	2.22	0.40
1:Au:269:VAL:HA	1:Aw:269:VAL:HG22	2.03	0.40
1:Cc:123:GLU:OE1	1:Cc:123:GLU:HA	2.22	0.40
1:Ce:123:GLU:HA	1:Ce:123:GLU:OE1	2.21	0.40
1:Ck:64:LYS:HE3	1:Cm:107:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ac	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ae	224/269 (83%)	221 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ag	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ai	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Ak	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Am	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Ao	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Aq	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	As	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Au	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Aw	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ay	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ba	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Bc	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Be	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Bg	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bi	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Bk	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bm	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bo	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bq	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bs	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bu	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Bw	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	By	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Ca	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Cc	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ce	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Cg	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ci	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ck	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Cm	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
1	Co	224/269 (83%)	220 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Cq	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Cs	224/269 (83%)	220 (98%)	4 (2%)	0	100	100
All	All	8064/9684 (83%)	7942 (98%)	122 (2%)	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	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ac	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ae	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ag	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ai	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ak	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Am	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ao	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Aq	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	As	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Au	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Aw	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ay	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ba	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bc	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Be	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bg	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bi	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bk	200/233 (86%)	199 (100%)	1 (0%)	81	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bm	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bo	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bq	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bs	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bu	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Bw	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	By	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ca	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Cc	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ce	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Cg	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ci	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Ck	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Cm	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Co	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Cq	200/233 (86%)	199 (100%)	1 (0%)	81	88
1	Cs	200/233 (86%)	199 (100%)	1 (0%)	81	88
All	All	7200/8388 (86%)	7164 (100%)	36 (0%)	78	88

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	52	MET
1	Ac	52	MET
1	Ae	52	MET
1	Ag	52	MET
1	Ai	52	MET
1	Ak	52	MET
1	Am	52	MET
1	Ao	52	MET
1	Aq	52	MET
1	As	52	MET
1	Au	52	MET
1	Aw	52	MET
1	Ay	52	MET
1	Ba	52	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bc	52	MET
1	Be	52	MET
1	Bg	52	MET
1	Bi	52	MET
1	Bk	52	MET
1	Bm	52	MET
1	Bo	52	MET
1	Bq	52	MET
1	Bs	52	MET
1	Bu	52	MET
1	Bw	52	MET
1	By	52	MET
1	Ca	52	MET
1	Cc	52	MET
1	Ce	52	MET
1	Cg	52	MET
1	Ci	52	MET
1	Ck	52	MET
1	Cm	52	MET
1	Co	52	MET
1	Cq	52	MET
1	Cs	52	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	79	GLN
1	Aa	89	HIS
1	Aa	229	ASN
1	Aa	240	ASN
1	Aa	251	HIS
1	Ac	79	GLN
1	Ac	89	HIS
1	Ac	240	ASN
1	Ae	79	GLN
1	Ae	89	HIS
1	Ae	240	ASN
1	Ag	79	GLN
1	Ag	89	HIS
1	Ag	229	ASN
1	Ag	240	ASN
1	Ai	79	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ai	89	HIS
1	Ai	240	ASN
1	Ak	79	GLN
1	Ak	89	HIS
1	Ak	153	HIS
1	Ak	229	ASN
1	Ak	240	ASN
1	Am	79	GLN
1	Am	89	HIS
1	Am	240	ASN
1	Ao	79	GLN
1	Ao	240	ASN
1	Aq	79	GLN
1	Aq	240	ASN
1	As	79	GLN
1	As	89	HIS
1	As	240	ASN
1	Au	79	GLN
1	Au	89	HIS
1	Au	229	ASN
1	Aw	79	GLN
1	Aw	89	HIS
1	Aw	240	ASN
1	Ay	79	GLN
1	Ay	89	HIS
1	Ay	240	ASN
1	Ba	79	GLN
1	Ba	89	HIS
1	Ba	240	ASN
1	Bc	79	GLN
1	Bc	89	HIS
1	Bc	229	ASN
1	Bc	240	ASN
1	Be	79	GLN
1	Be	89	HIS
1	Be	240	ASN
1	Bg	79	GLN
1	Bg	89	HIS
1	Bg	240	ASN
1	Bi	79	GLN
1	Bi	89	HIS
1	Bi	240	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bk	79	GLN
1	Bk	89	HIS
1	Bk	229	ASN
1	Bk	240	ASN
1	Bm	79	GLN
1	Bm	89	HIS
1	Bm	240	ASN
1	Bo	79	GLN
1	Bo	89	HIS
1	Bo	240	ASN
1	Bq	79	GLN
1	Bq	89	HIS
1	Bq	240	ASN
1	Bs	79	GLN
1	Bs	89	HIS
1	Bs	240	ASN
1	Bu	79	GLN
1	Bu	89	HIS
1	Bu	240	ASN
1	Bw	79	GLN
1	Bw	240	ASN
1	By	79	GLN
1	By	240	ASN
1	Ca	79	GLN
1	Ca	89	HIS
1	Ca	240	ASN
1	Cc	79	GLN
1	Cc	89	HIS
1	Cc	240	ASN
1	Ce	79	GLN
1	Ce	89	HIS
1	Ce	240	ASN
1	Cg	79	GLN
1	Cg	89	HIS
1	Cg	240	ASN
1	Ci	79	GLN
1	Ci	191	ASN
1	Ci	240	ASN
1	Ck	79	GLN
1	Ck	89	HIS
1	Ck	191	ASN
1	Ck	240	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Cm	79	GLN
1	Cm	89	HIS
1	Cm	191	ASN
1	Cm	240	ASN
1	Co	79	GLN
1	Co	89	HIS
1	Co	240	ASN
1	Cq	79	GLN
1	Cq	89	HIS
1	Cq	240	ASN
1	Cs	79	GLN
1	Cs	240	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Ab	4/5 (80%)	0	0
2	Ad	4/5 (80%)	0	0
2	Af	4/5 (80%)	0	0
2	Ah	4/5 (80%)	0	0
2	Aj	4/5 (80%)	0	0
2	Al	4/5 (80%)	0	0
2	An	4/5 (80%)	0	0
2	Ap	4/5 (80%)	0	0
2	Ar	4/5 (80%)	0	0
2	At	4/5 (80%)	0	0
2	Av	4/5 (80%)	0	0
2	Ax	4/5 (80%)	0	0
2	Az	4/5 (80%)	0	0
2	Bb	4/5 (80%)	0	0
2	Bd	4/5 (80%)	0	0
2	Bf	4/5 (80%)	0	0
2	Bh	4/5 (80%)	0	0
2	Bj	4/5 (80%)	0	0
2	Bl	4/5 (80%)	0	0
2	Bn	4/5 (80%)	0	0
2	Bp	4/5 (80%)	0	0
2	Br	4/5 (80%)	0	0
2	Bt	4/5 (80%)	0	0
2	Bv	4/5 (80%)	0	0
2	Bx	4/5 (80%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Bz	4/5 (80%)	0	0
2	Cb	4/5 (80%)	0	0
2	Cd	4/5 (80%)	0	0
2	Cf	4/5 (80%)	0	0
2	Ch	4/5 (80%)	0	0
2	Cj	4/5 (80%)	0	0
2	Cl	4/5 (80%)	0	0
2	Cn	4/5 (80%)	0	0
2	Cp	4/5 (80%)	0	0
2	Cr	4/5 (80%)	0	0
2	Ct	4/5 (80%)	0	0
All	All	144/180 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

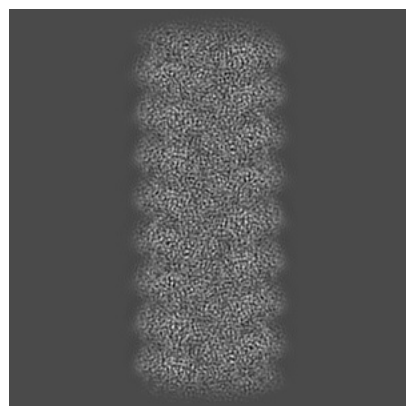
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53802. These allow visual inspection of the internal detail of the map and identification of artifacts.

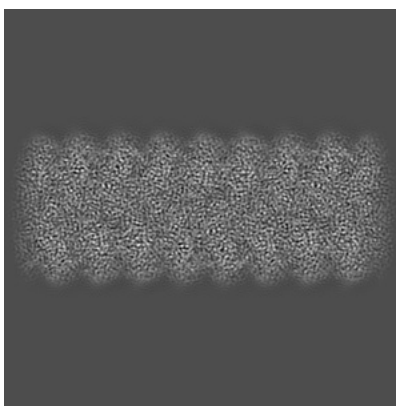
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

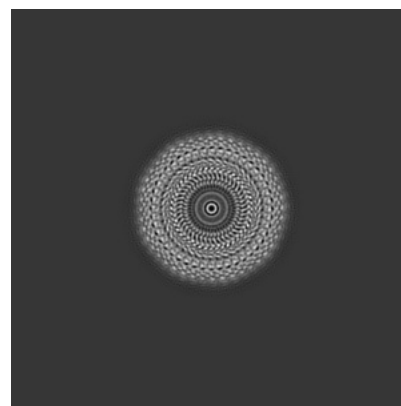
6.1.1 Primary map



X

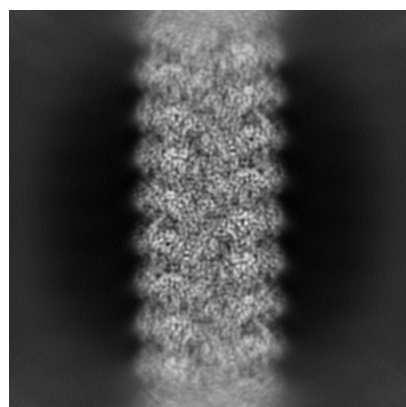


Y

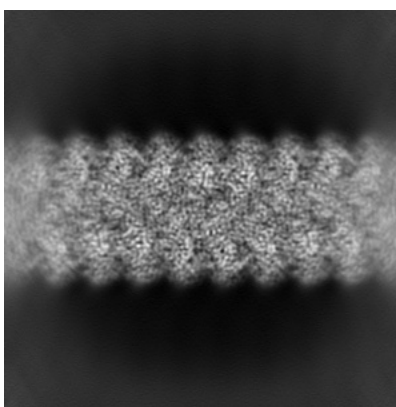


Z

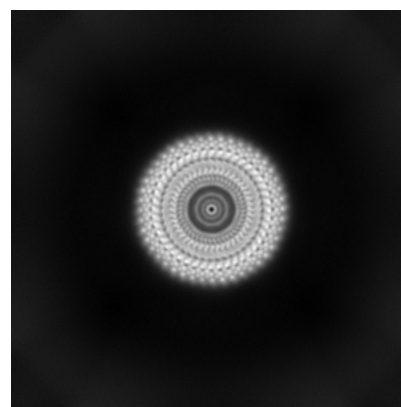
6.1.2 Raw map



X



Y

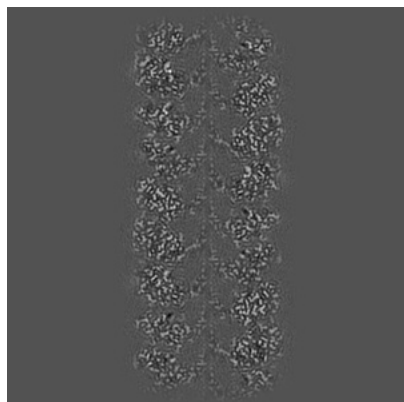


Z

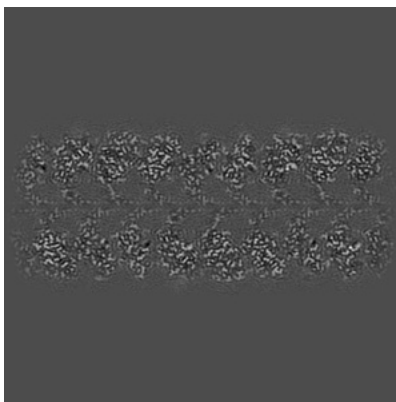
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

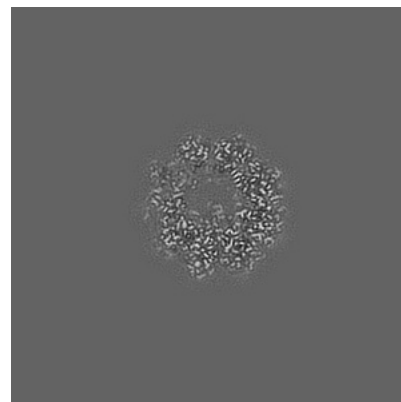
6.2.1 Primary map



X Index: 175

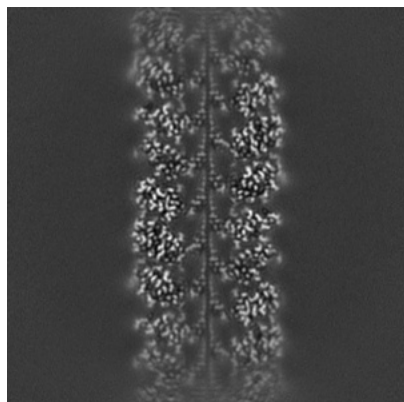


Y Index: 175

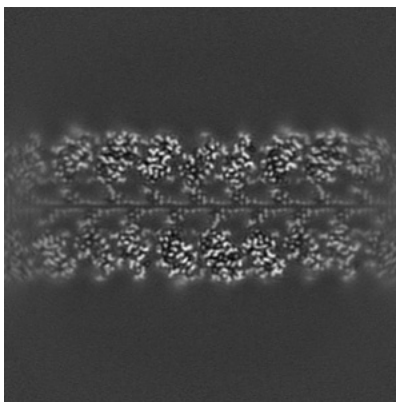


Z Index: 175

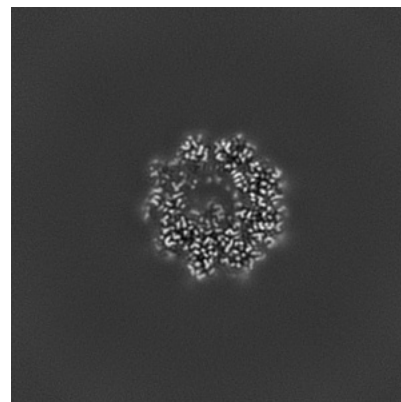
6.2.2 Raw map



X Index: 175



Y Index: 175

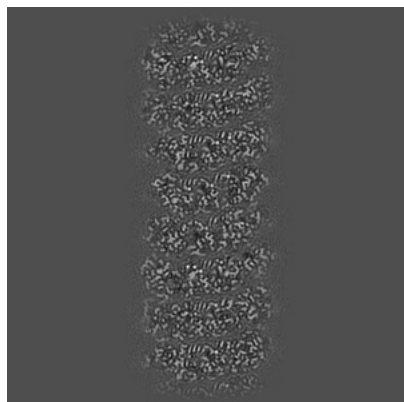


Z Index: 175

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

6.3 Largest variance slices [i](#)

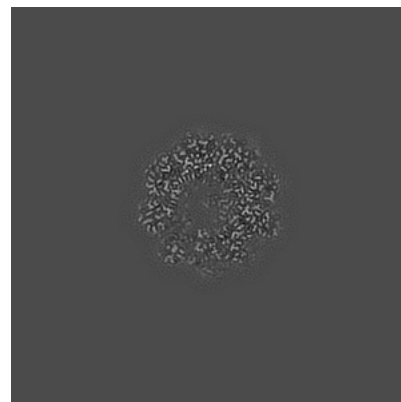
6.3.1 Primary map



X Index: 143

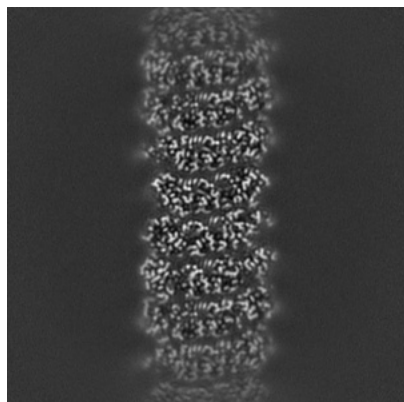


Y Index: 143

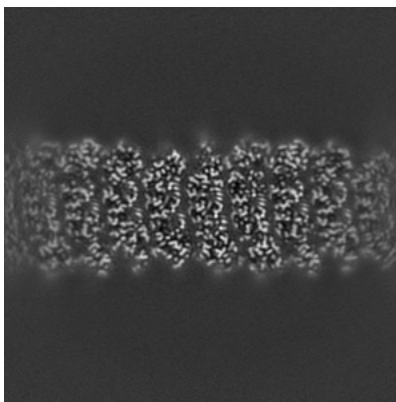


Z Index: 165

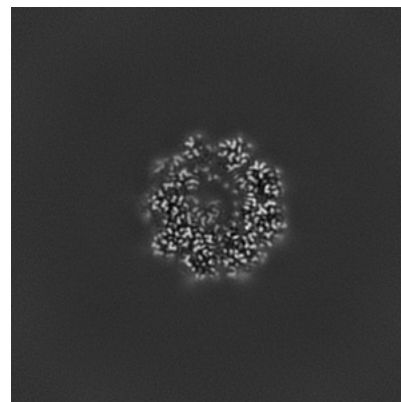
6.3.2 Raw map



X Index: 143



Y Index: 143

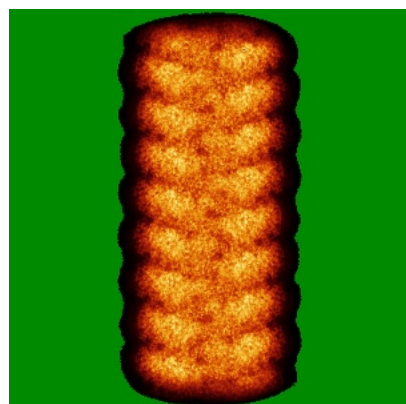


Z Index: 178

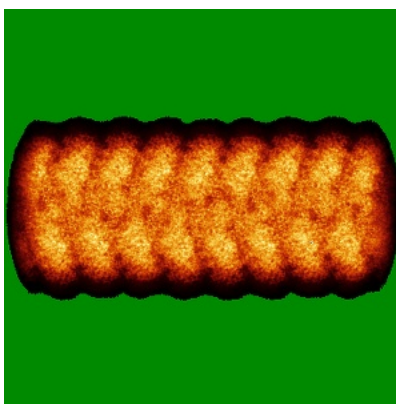
The images above show the largest variance slices of the map in three orthogonal directions.

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

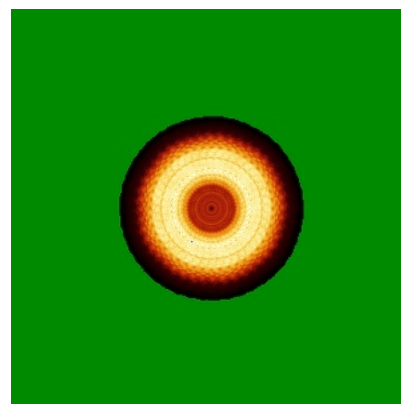
6.4.1 Primary map



X

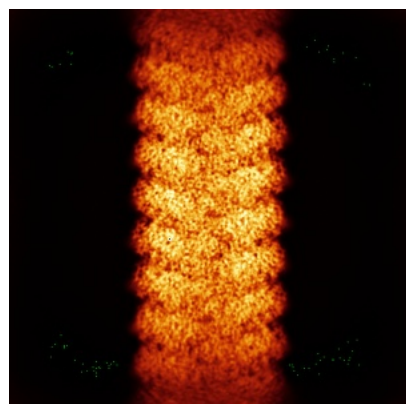


Y

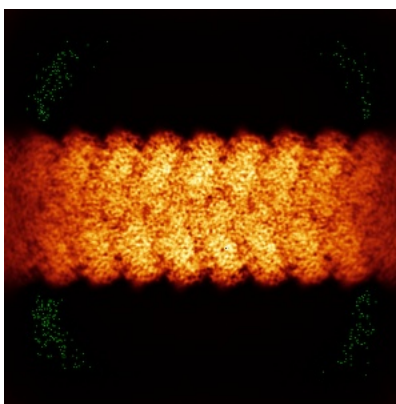


Z

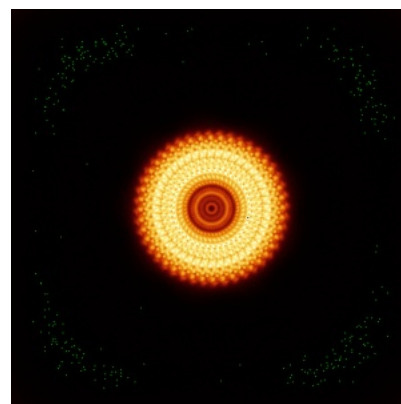
6.4.2 Raw map



X



Y

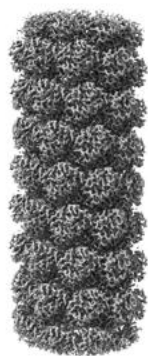


Z

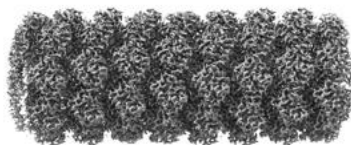
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

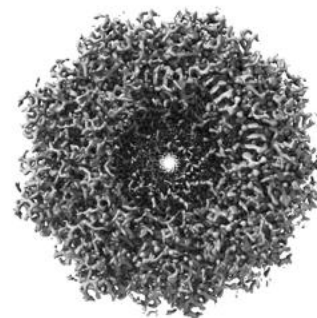
6.5.1 Primary map



X



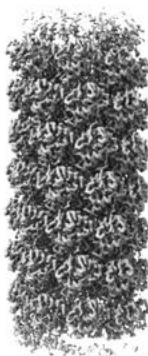
Y



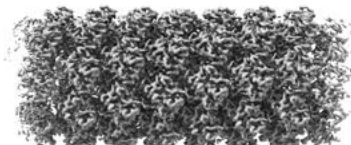
Z

The images above show the 3D surface view of the map at the recommended contour level 2.39. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

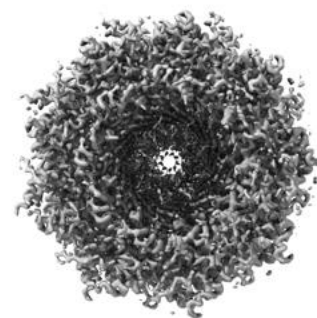
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

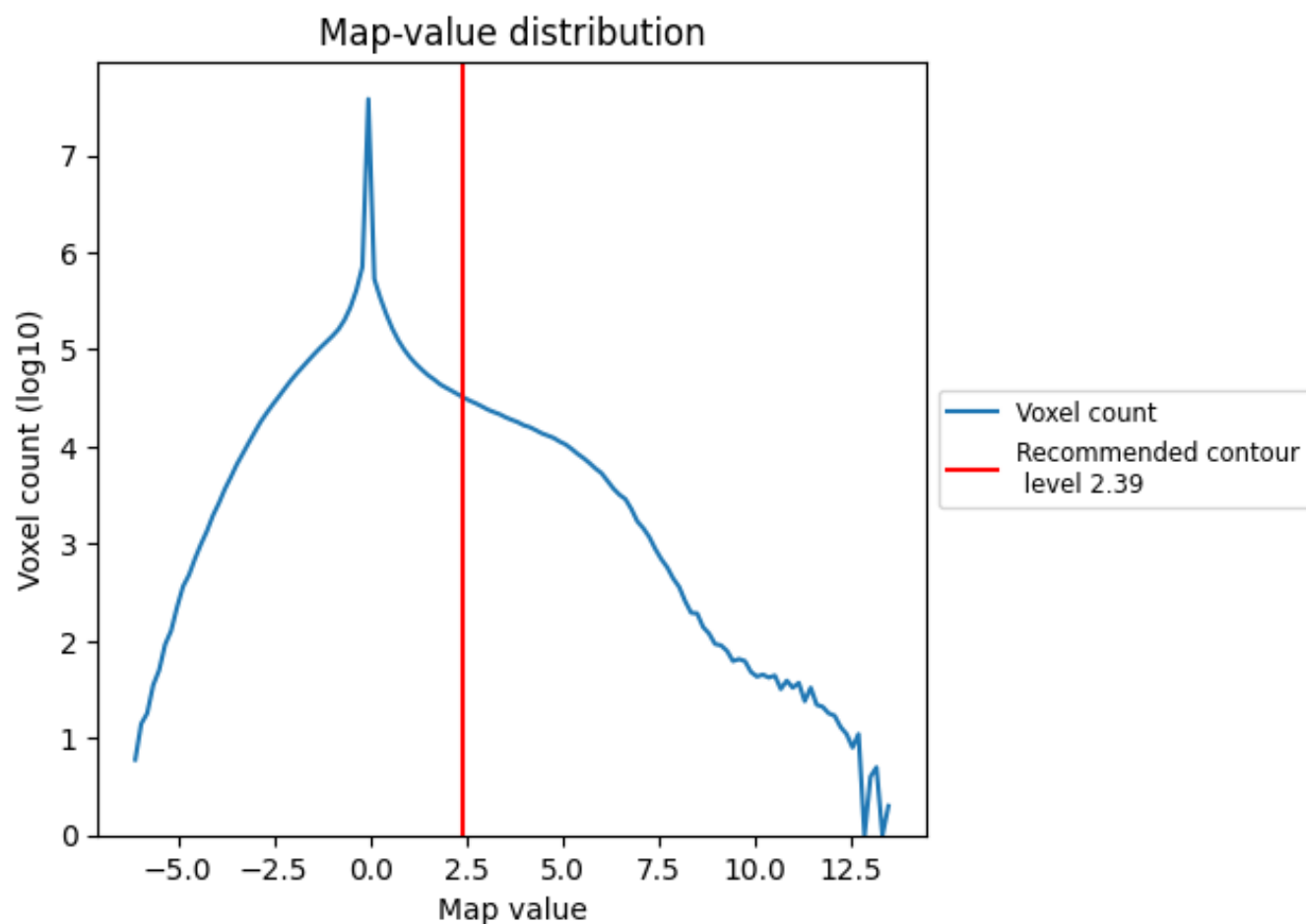
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

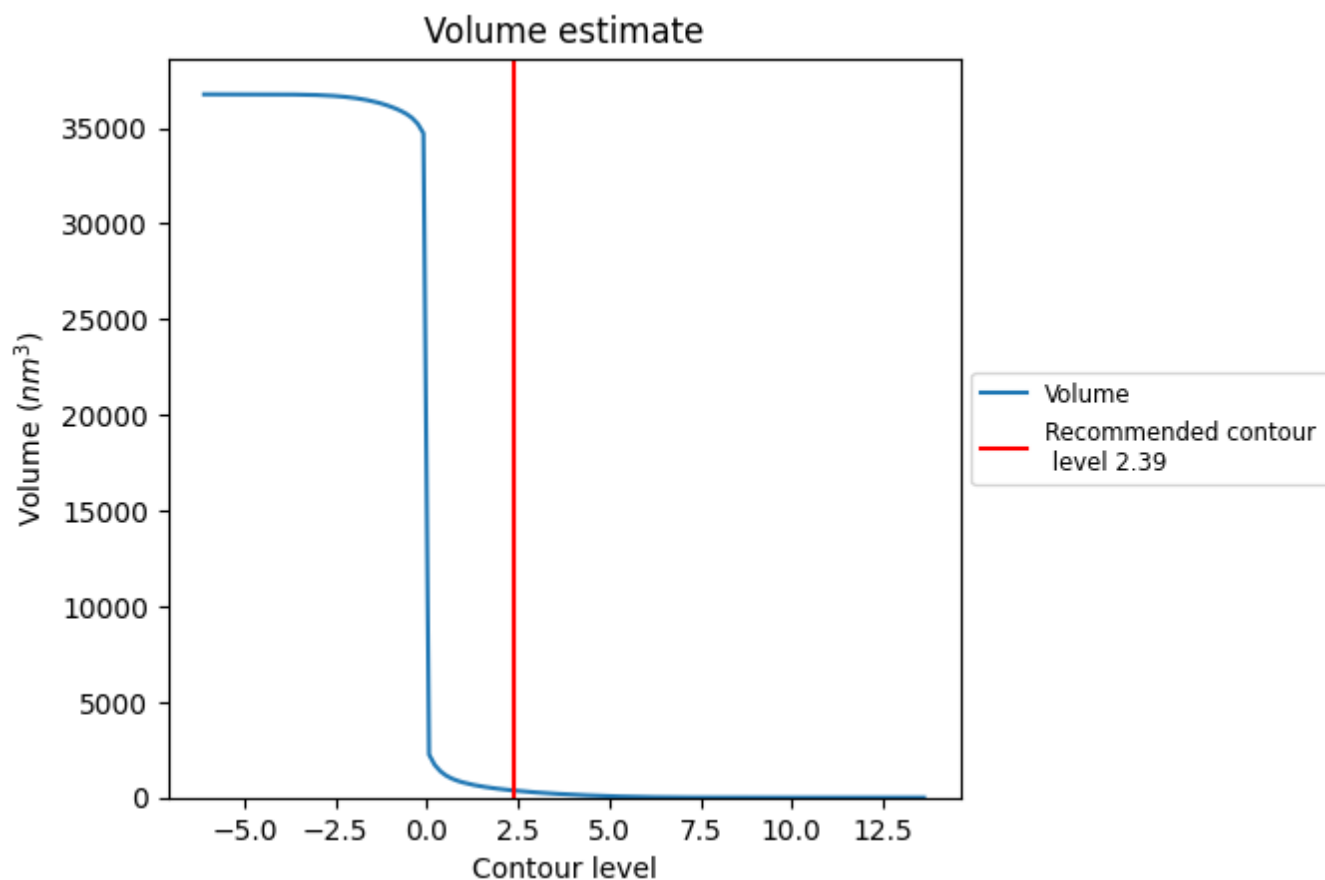
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

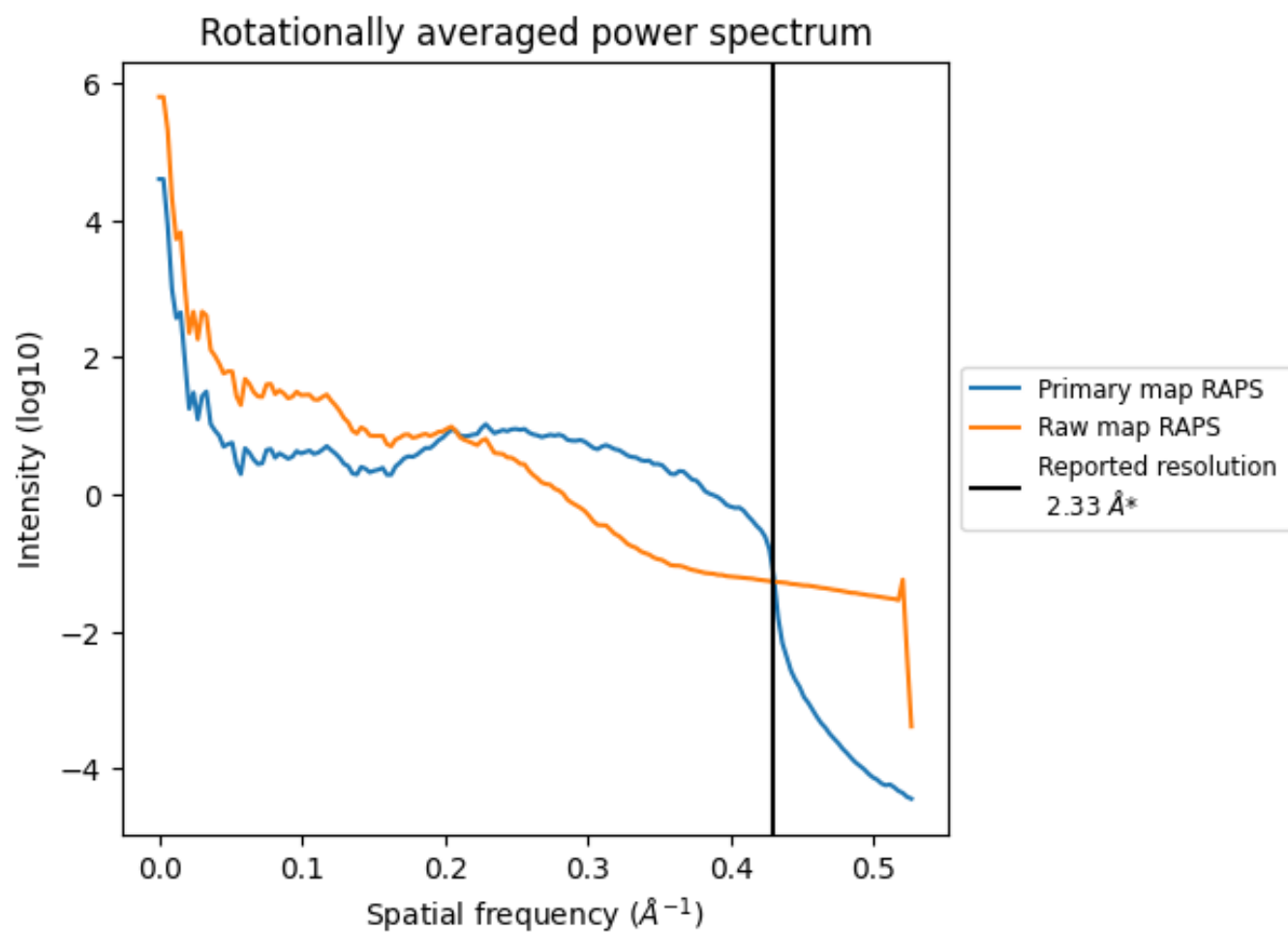
7.2 Volume estimate [i](#)



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

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

7.3 Rotationally averaged power spectrum ⓘ

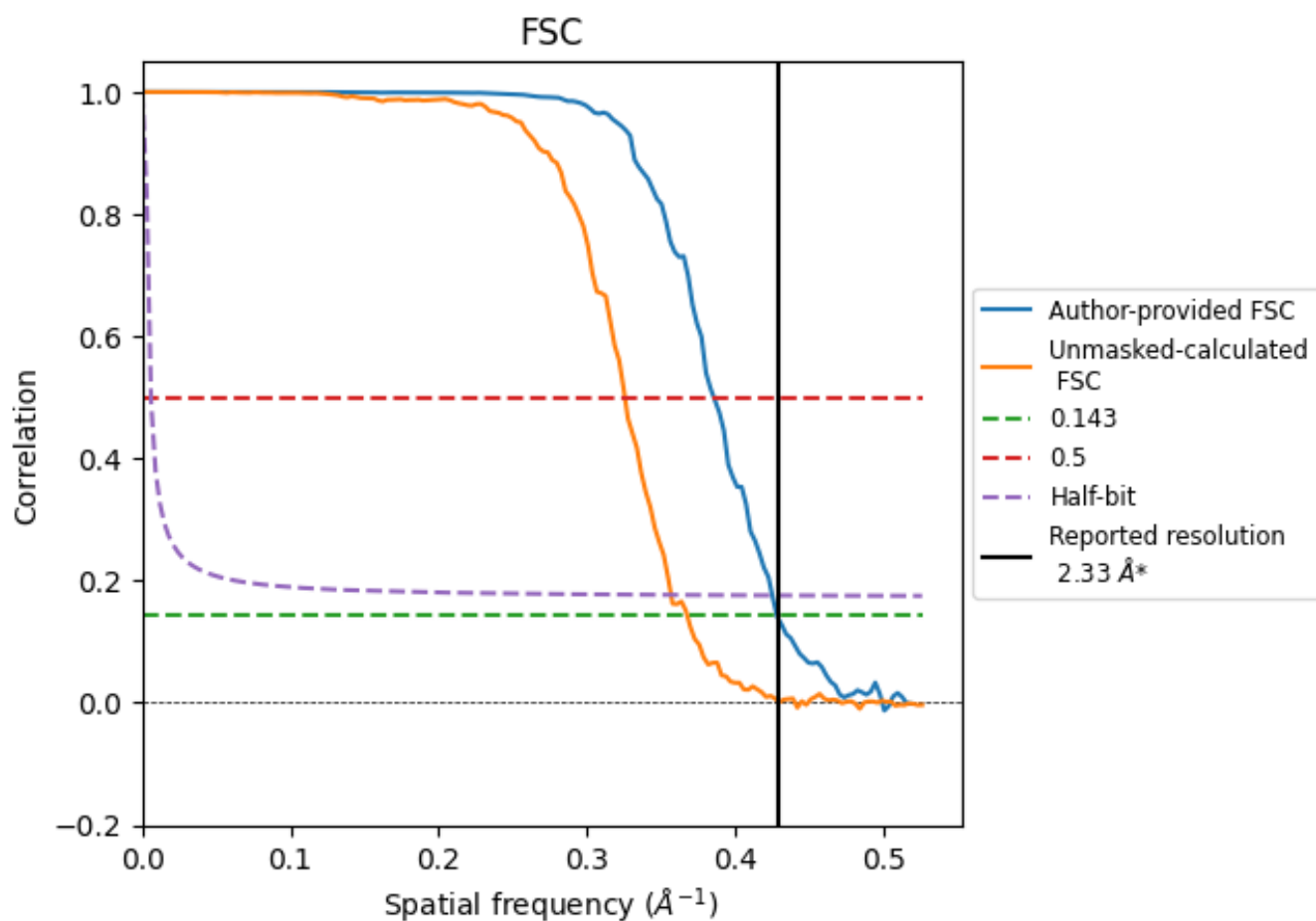


*Reported resolution corresponds to spatial frequency of 0.429 Å⁻¹

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 0.429 $\text{\AA}^{-1}$

8.2 Resolution estimates

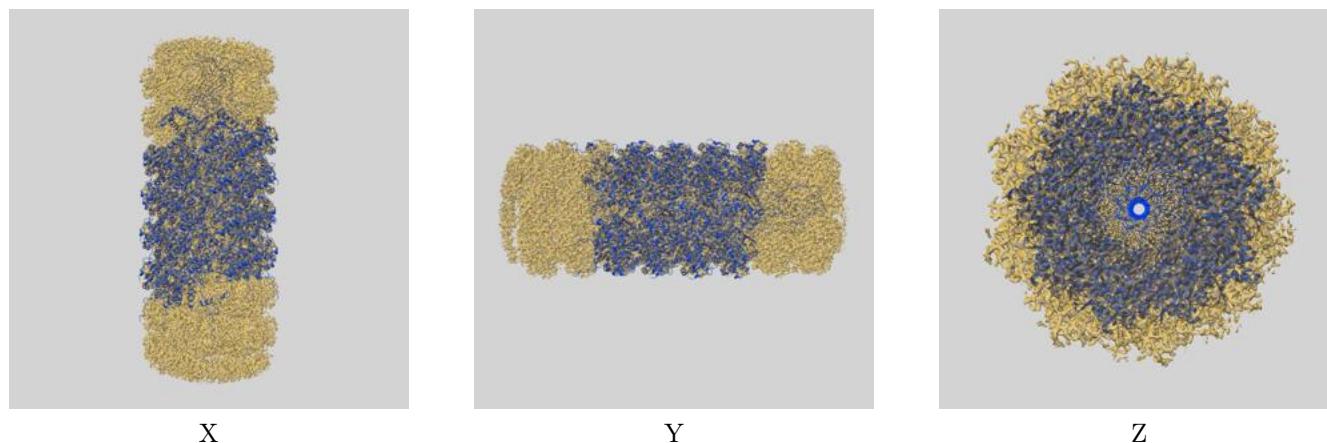
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.33	2.59	2.35
Unmasked-calculated*	2.72	3.07	2.80

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.72 differs from the reported value 2.33 by more than 10 %

9 Map-model fit [i](#)

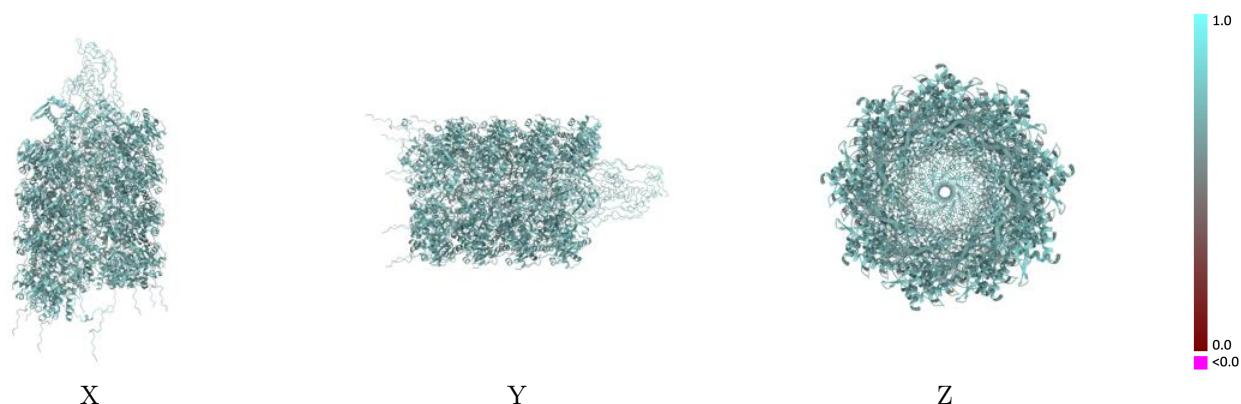
This section contains information regarding the fit between EMDB map EMD-53802 and PDB model 9R81. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.39 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](#)

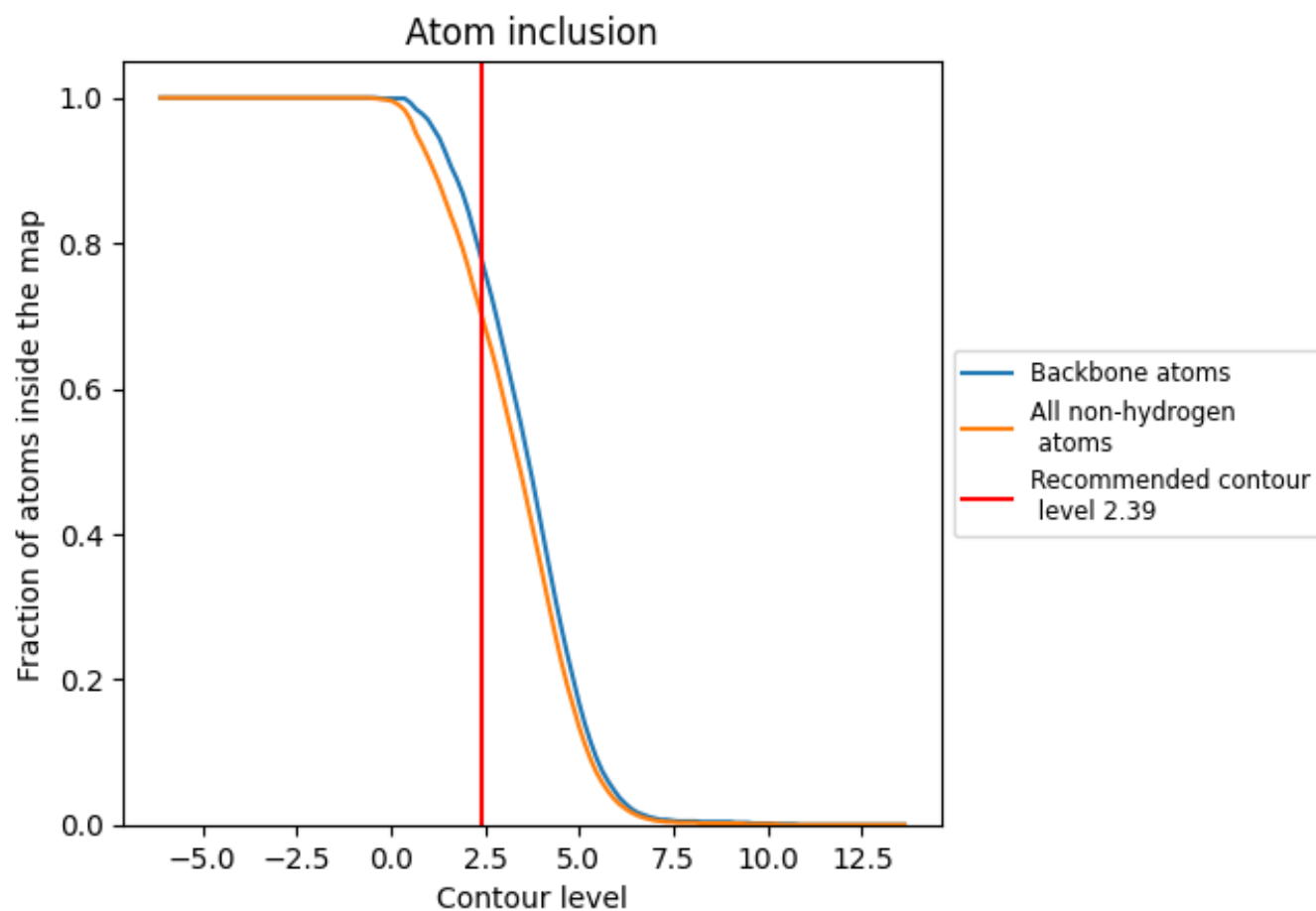


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (2.39) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7040	 0.6830
Aa	 0.6980	 0.6850
Ab	 0.8800	 0.6670
Ac	 0.6960	 0.6840
Ad	 0.9200	 0.6660
Ae	 0.6960	 0.6830
Af	 0.9000	 0.6360
Ag	 0.6900	 0.6820
Ah	 0.9200	 0.6660
Ai	 0.6920	 0.6840
Aj	 0.9300	 0.6660
Ak	 0.6910	 0.6830
Al	 0.9400	 0.6730
Am	 0.6920	 0.6850
An	 0.9000	 0.6690
Ao	 0.6850	 0.6840
Ap	 0.8900	 0.6730
Aq	 0.6910	 0.6830
Ar	 0.9000	 0.6740
As	 0.6930	 0.6820
At	 0.8900	 0.6710
Au	 0.6950	 0.6830
Av	 0.9400	 0.6720
Aw	 0.6920	 0.6840
Ax	 0.9200	 0.6800
Ay	 0.6930	 0.6850
Az	 0.9200	 0.6760
Ba	 0.6960	 0.6830
Bb	 0.8900	 0.6690
Bc	 0.6910	 0.6830
Bd	 0.9200	 0.6730
Be	 0.6900	 0.6830
Bf	 0.9200	 0.6780
Bg	 0.6880	 0.6820
Bh	 0.9300	 0.6760



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bi	 0.6990	 0.6840
Bj	 0.9000	 0.6730
Bk	 0.6960	 0.6840
Bl	 0.9000	 0.6760
Bm	 0.6940	 0.6850
Bn	 0.8800	 0.6690
Bo	 0.6860	 0.6830
Bp	 0.9000	 0.6640
Bq	 0.6900	 0.6840
Br	 0.9200	 0.6660
Bs	 0.6910	 0.6830
Bt	 0.9400	 0.6760
Bu	 0.6910	 0.6850
Bv	 0.9000	 0.6740
Bw	 0.6910	 0.6840
Bx	 0.9300	 0.6780
By	 0.6930	 0.6840
Bz	 0.8800	 0.6700
Ca	 0.6890	 0.6830
Cb	 0.9200	 0.6810
Cc	 0.6900	 0.6820
Cd	 0.9300	 0.6820
Ce	 0.6930	 0.6830
Cf	 0.9600	 0.6810
Cg	 0.6920	 0.6830
Ch	 0.9000	 0.6550
Ci	 0.6980	 0.6850
Cj	 0.8800	 0.6650
Ck	 0.6900	 0.6840
Cl	 0.8900	 0.6660
Cm	 0.6870	 0.6830
Cn	 0.9000	 0.6670
Co	 0.6910	 0.6830
Cp	 0.9500	 0.6790
Cq	 0.6900	 0.6820
Cr	 0.9300	 0.6810
Cs	 0.6910	 0.6830
Ct	 0.9300	 0.6830