



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 10:34 PM UTC

PDB ID : 9R7T / pdb_00009r7t
EMDB ID : EMD-53792
Title : ssRNA-containing helical virus-like particle composed of PVA (isolate B11)
coat protein
Authors : Koritnik, N.; Kezar, A.; Podobnik, M.
Deposited on : 2025-05-15
Resolution : 2.54 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:

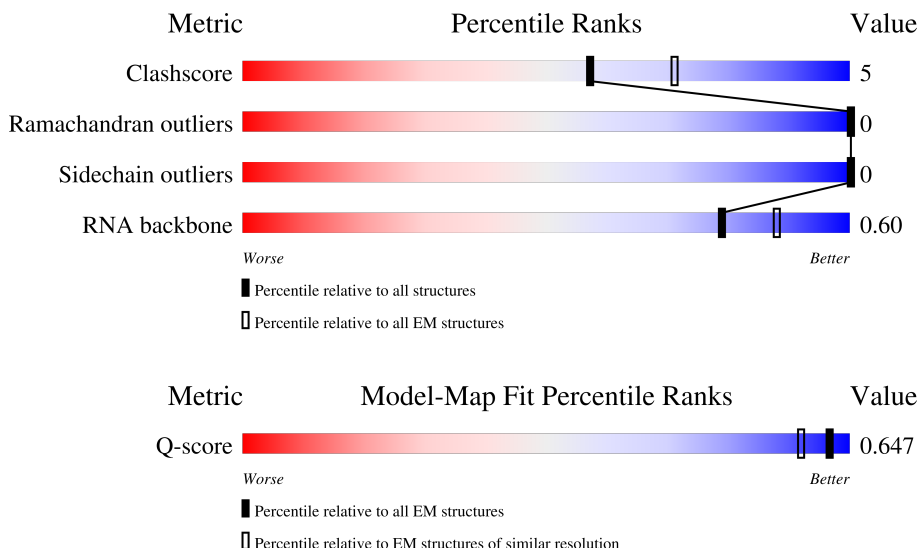
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 2.54 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	7403 (2.04 - 3.04)

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% 76% 8% 16%
1	Ac	269	21% 76% 8% 16%
1	Ae	269	22% 75% 9% 16%

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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	

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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	

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

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 68940 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ac	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ae	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ag	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ai	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ak	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Am	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ao	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Aq	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	As	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Au	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Aw	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ay	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ba	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bc	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Be	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bg	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bi	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bk	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bm	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bo	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bq	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bs	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bu	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Bw	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	By	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ca	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Cc	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ce	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Cg	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ci	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Ck	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Cm	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Co	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Cq	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		
1	Cs	226	Total	C	N	O	S	0	0
			1815	1136	321	343	15		

- 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 100	C 45	N 10	O 40	P 5	0	0
2	Ad	5	Total 100	C 45	N 10	O 40	P 5	0	0
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

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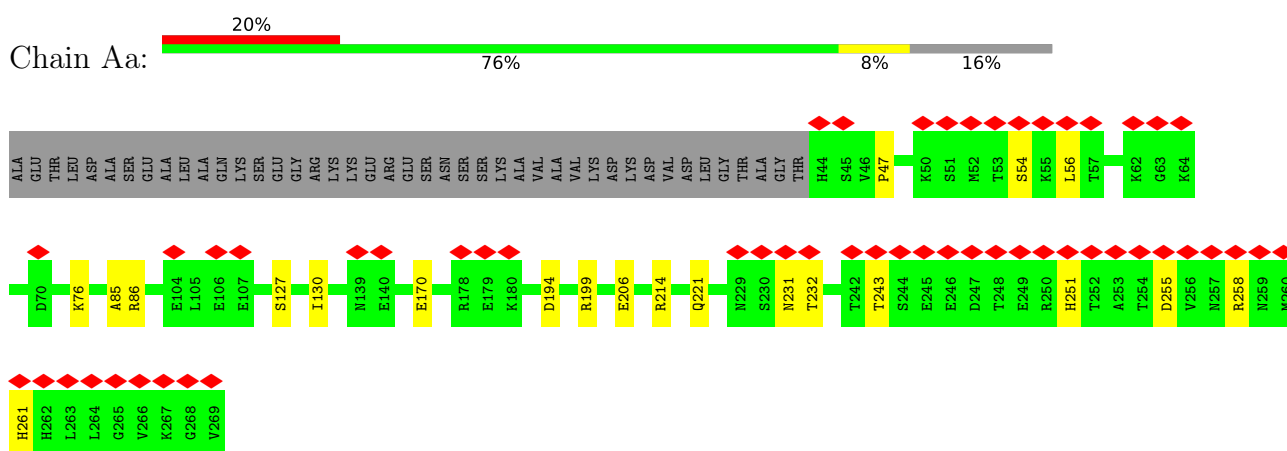
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bt	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bv	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bx	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bz	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cb	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cd	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

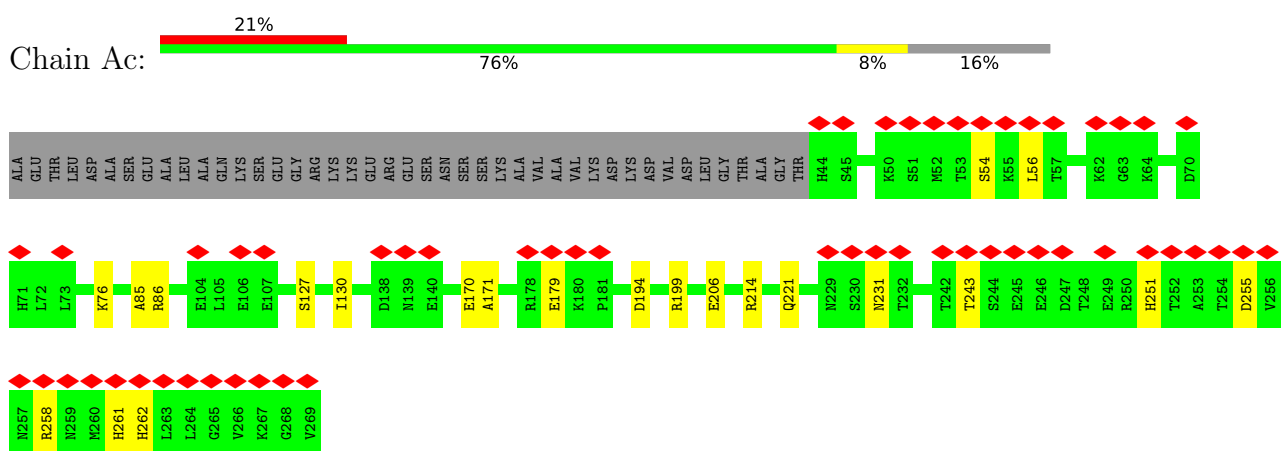
3 Residue-property plots

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.

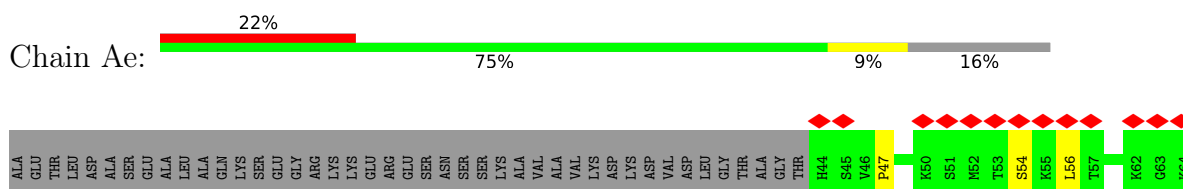
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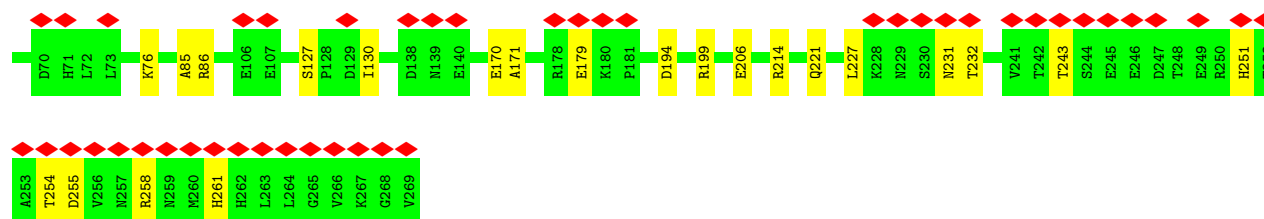


• Molecule 1: Capsid protein

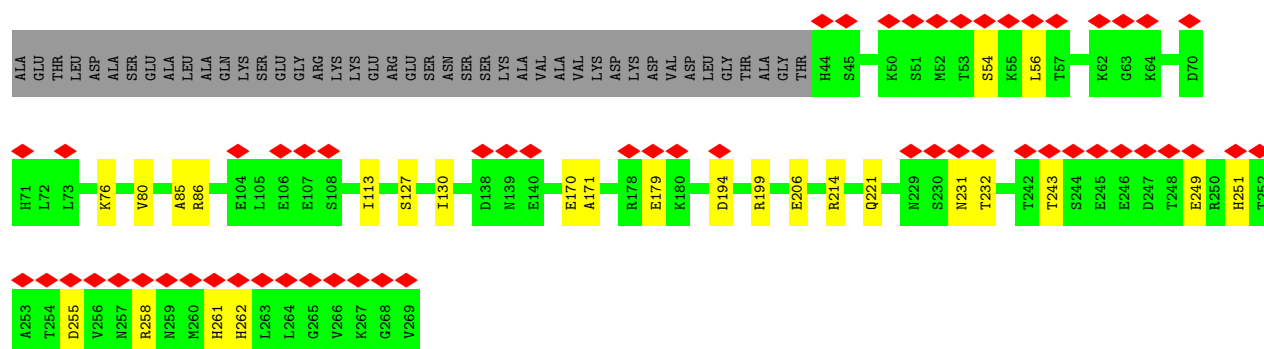
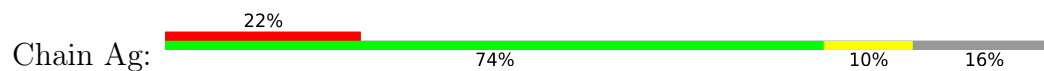


• Molecule 1: Capsid protein

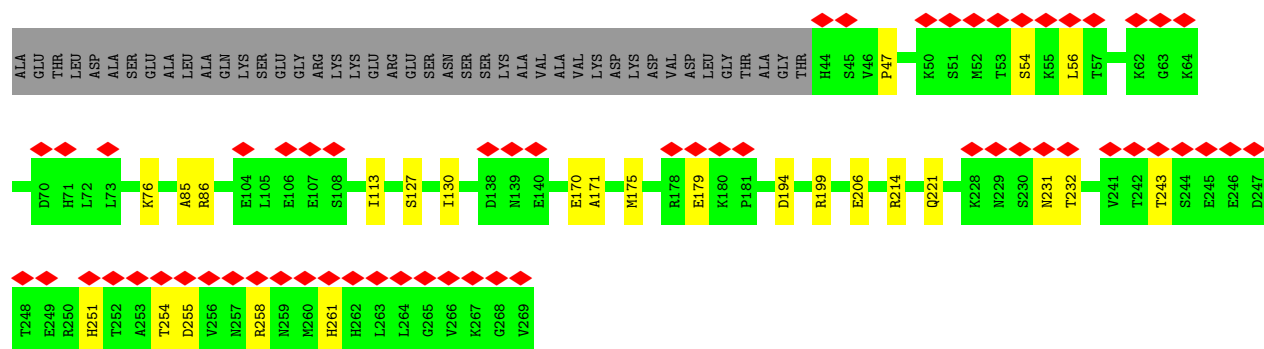
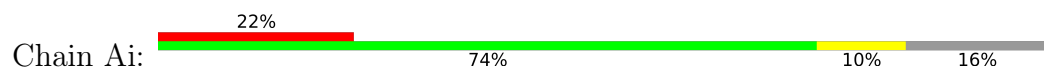




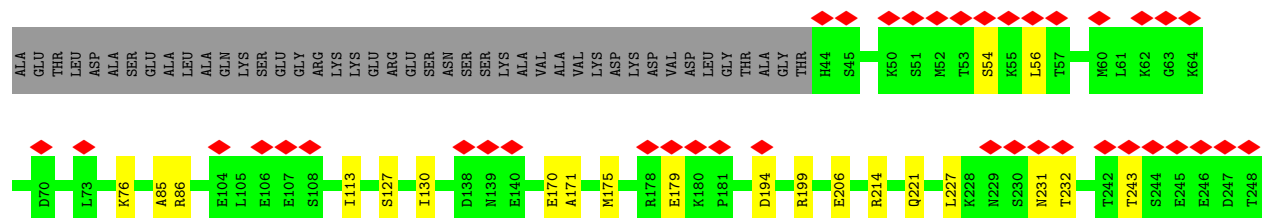
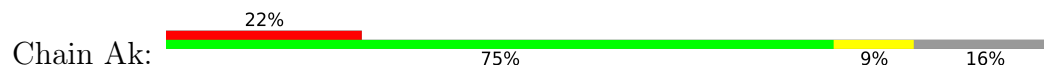
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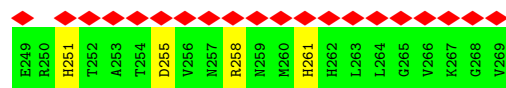


• Molecule 1: Capsid protein

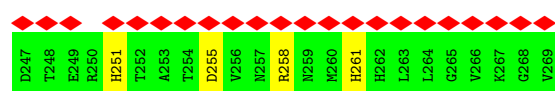
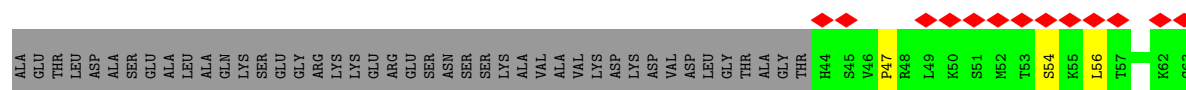
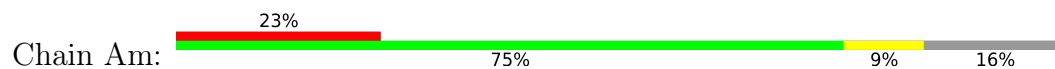


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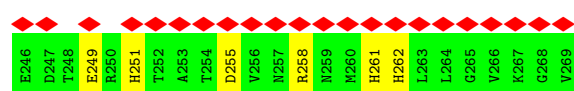
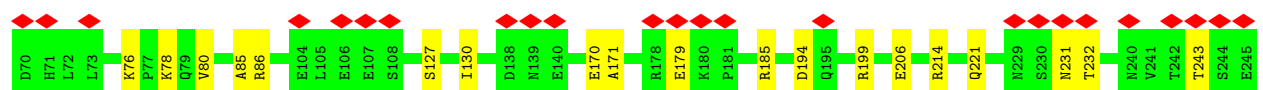
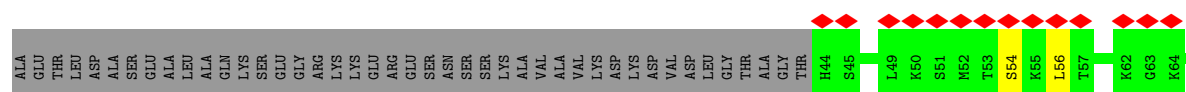
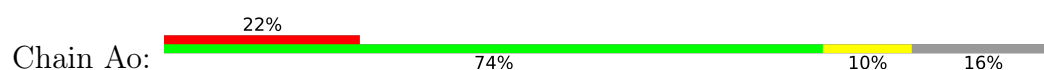




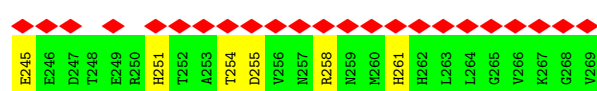
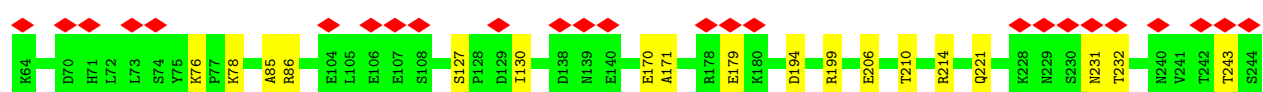
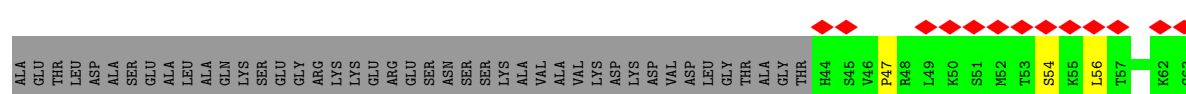
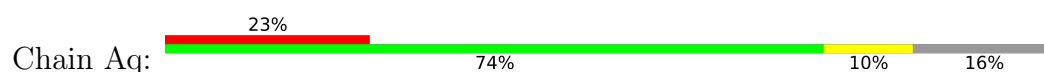
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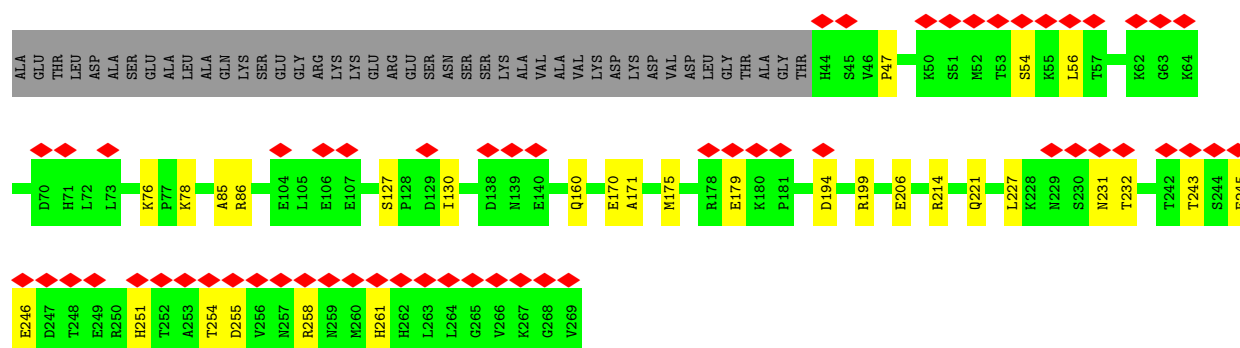
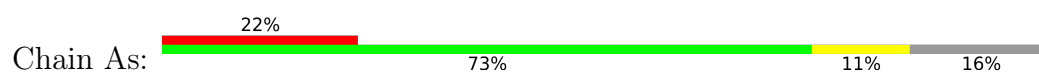
• Molecule 1: Capsid protein



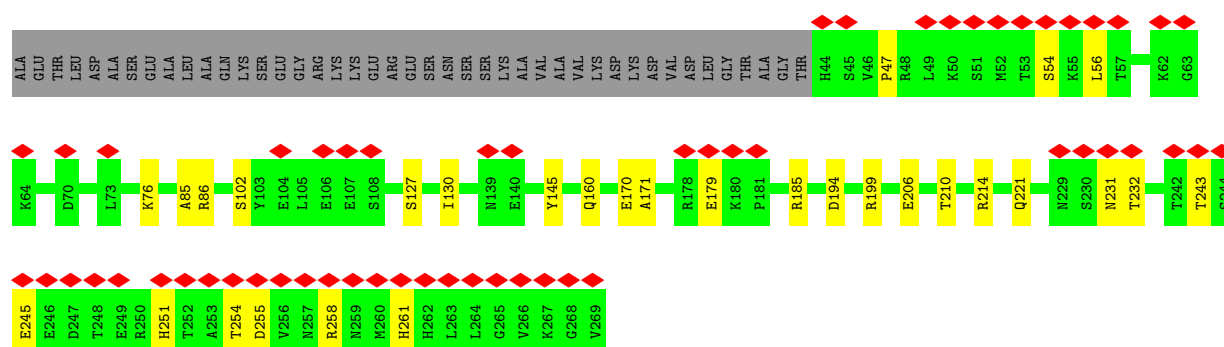
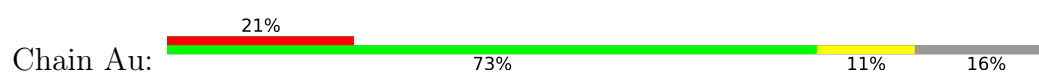
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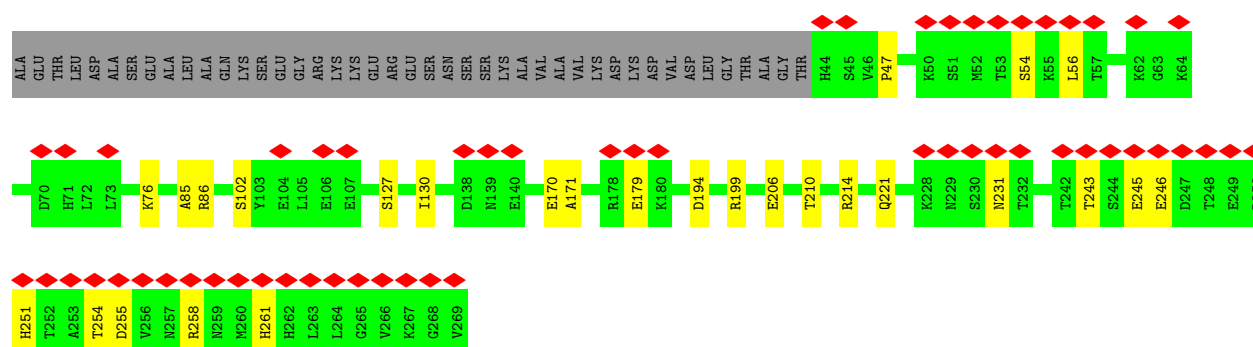
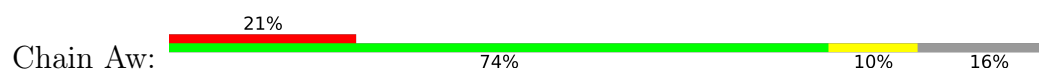
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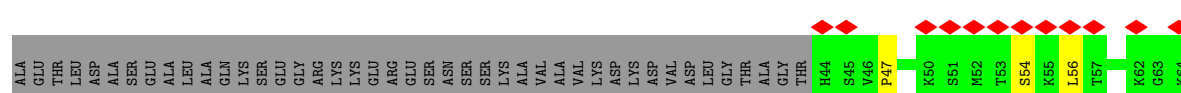
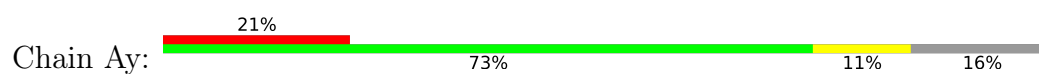
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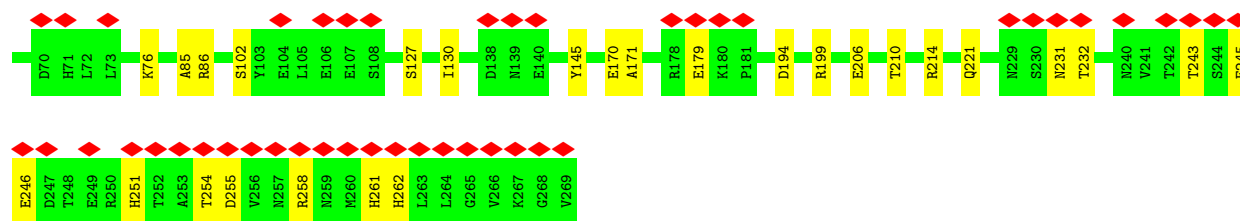


• Molecule 1: Capsid protein

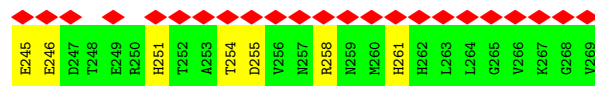
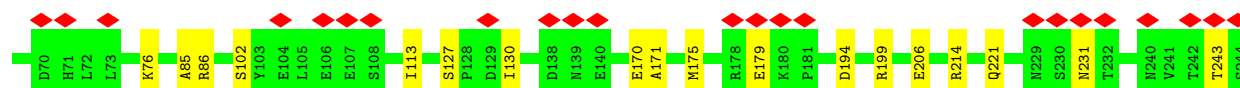
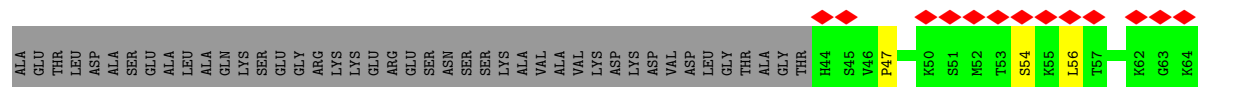
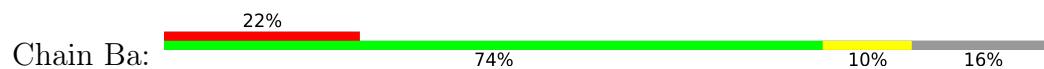


• Molecule 1: Capsid protein

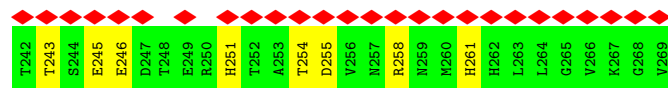
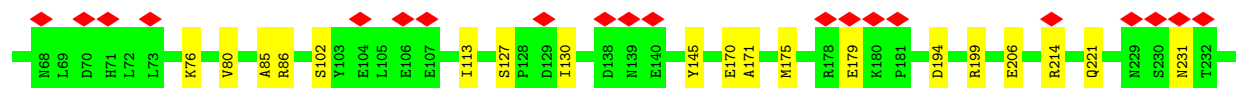
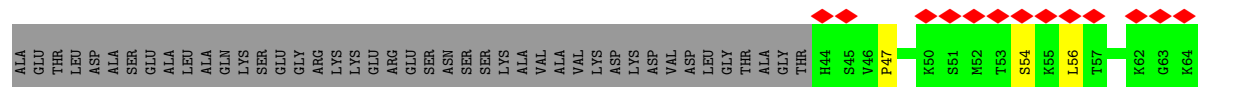
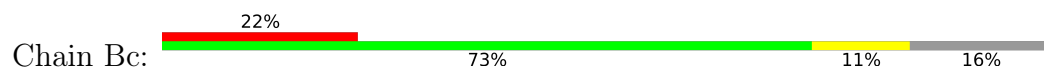




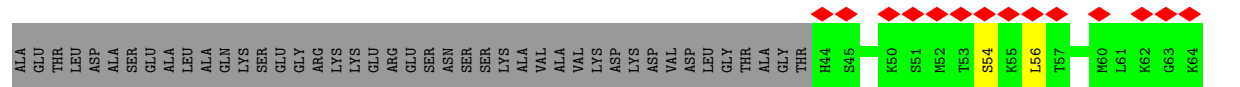
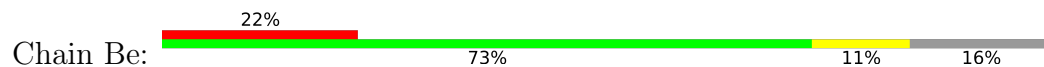
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein

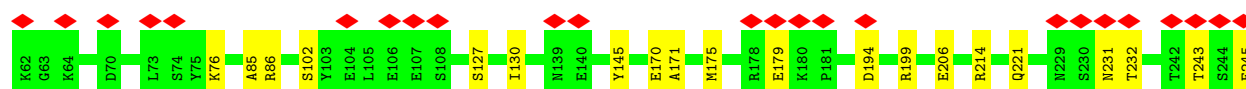
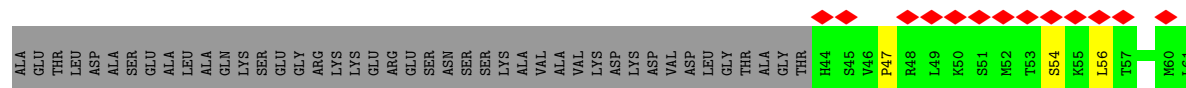
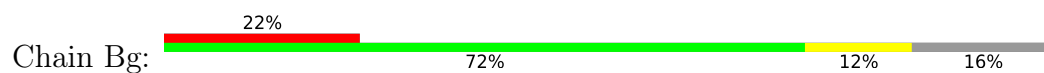


• Molecule 1: Capsid protein

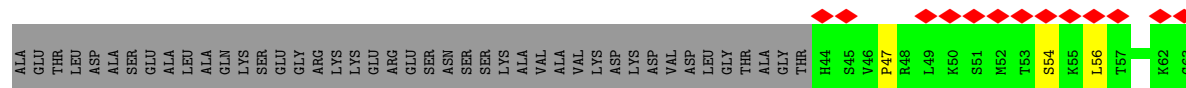
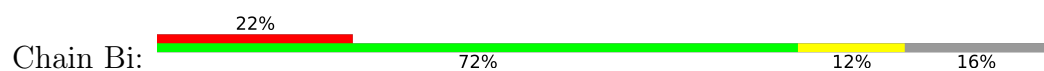




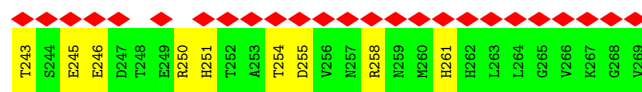
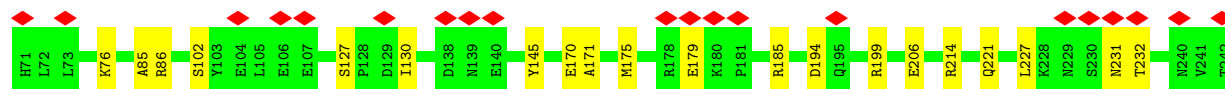
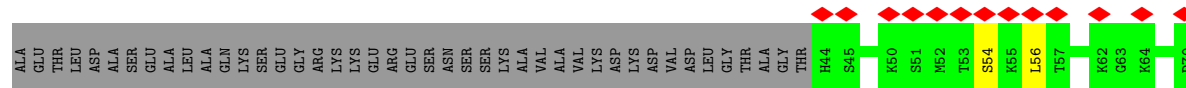
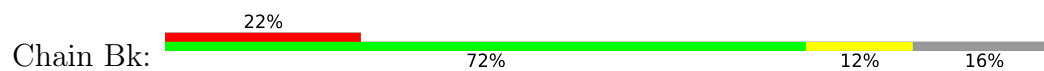
• Molecule 1: Capsid protein



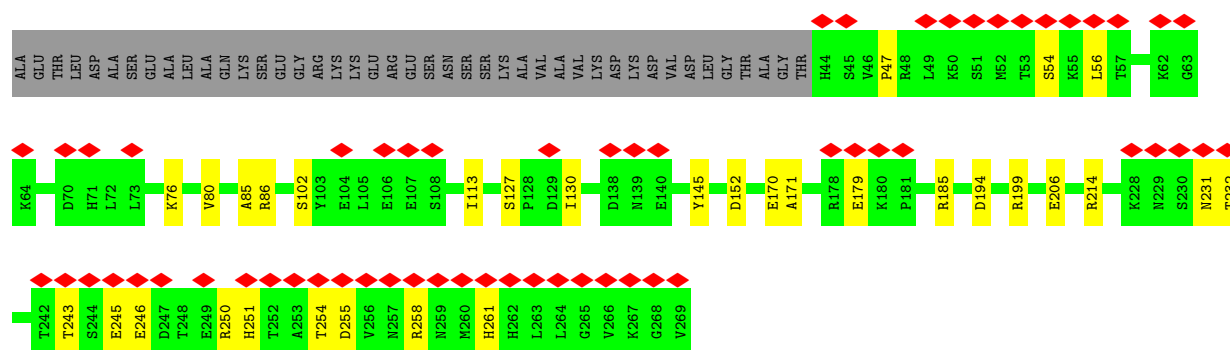
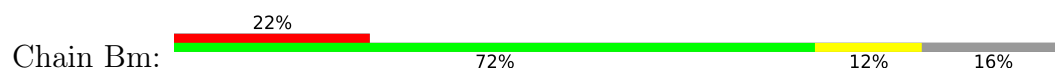
• Molecule 1: Capsid protein



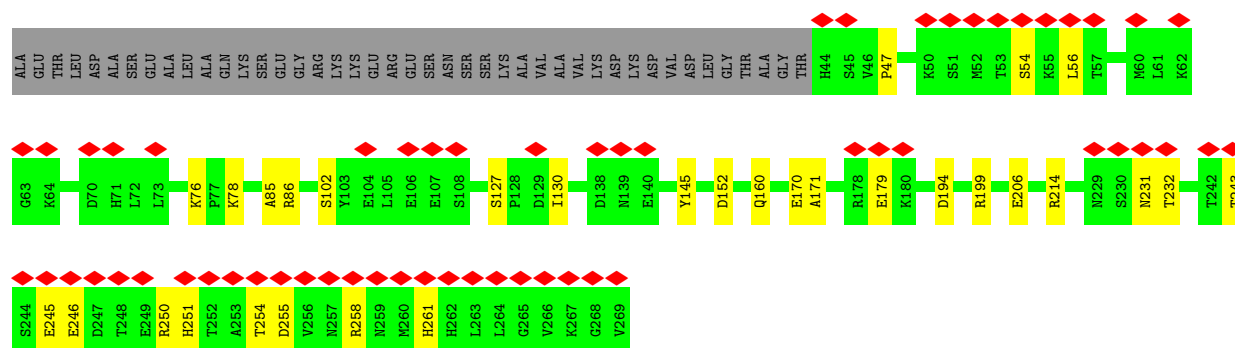
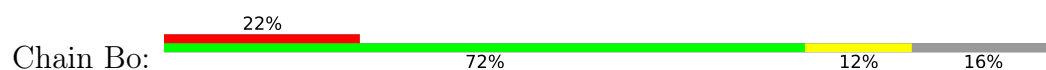
• Molecule 1: Capsid protein



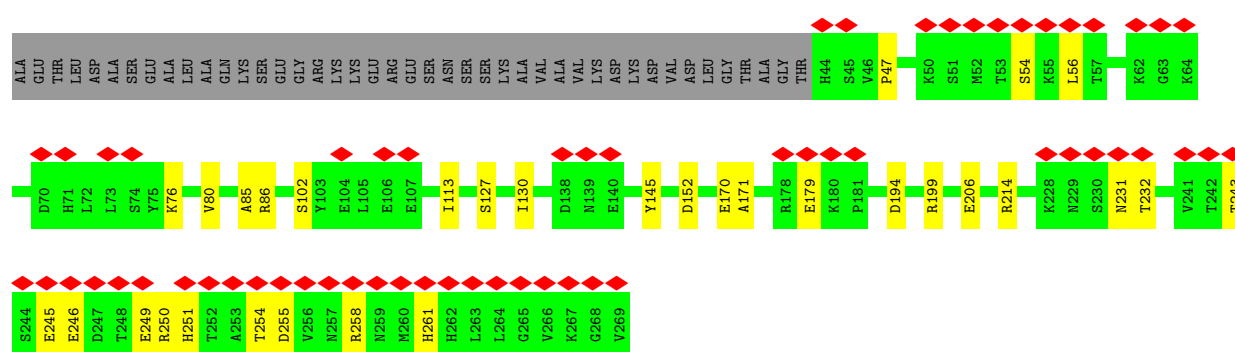
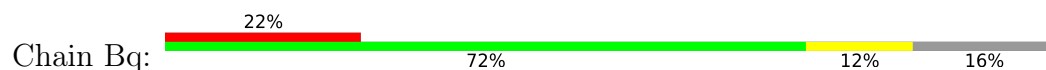
• Molecule 1: Capsid protein



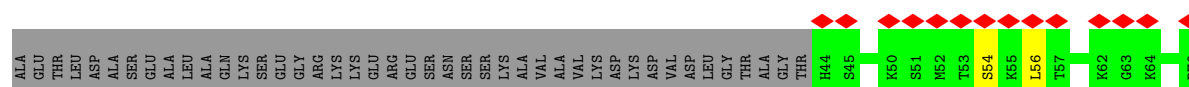
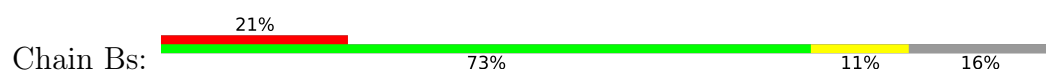
• Molecule 1: Capsid protein

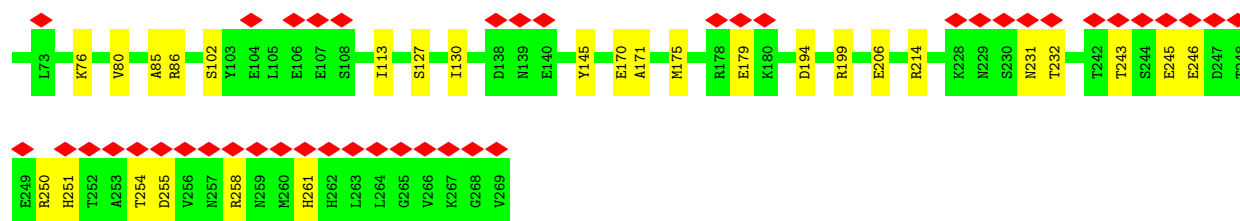


• Molecule 1: Capsid protein

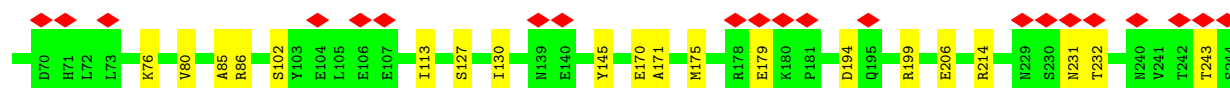
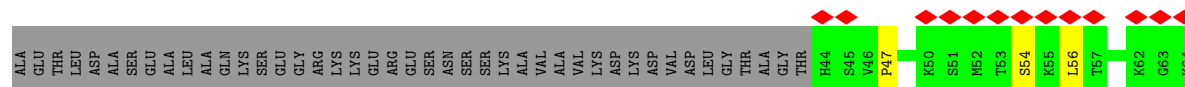
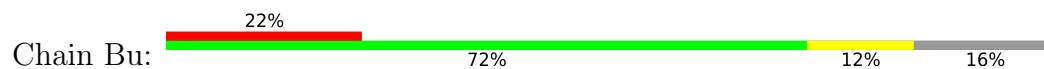


• Molecule 1: Capsid protein

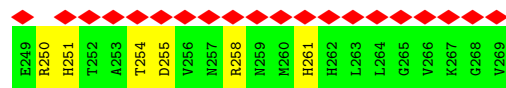
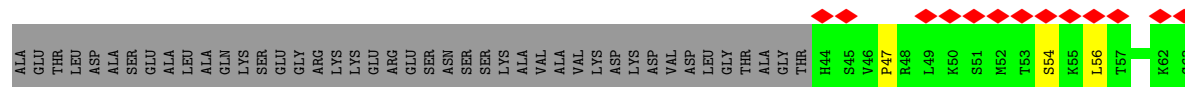
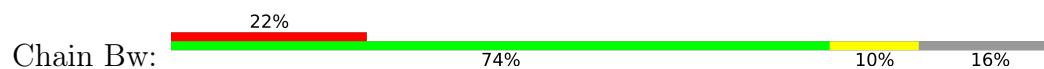




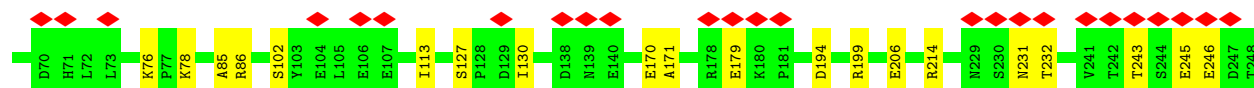
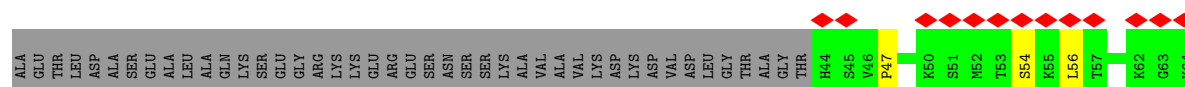
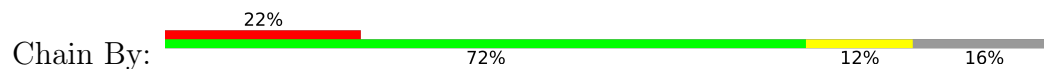
• Molecule 1: Capsid protein

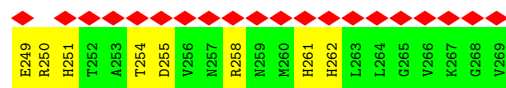


• Molecule 1: Capsid protein

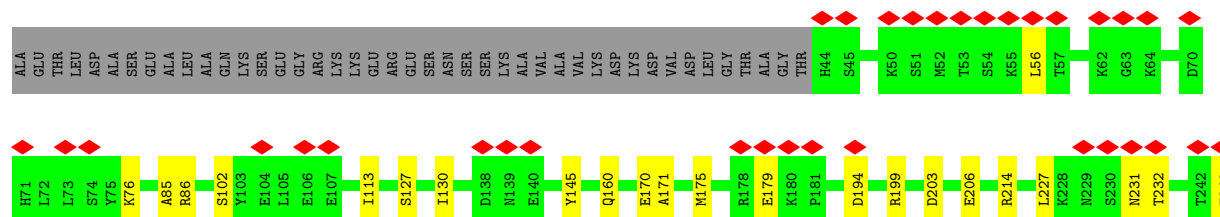
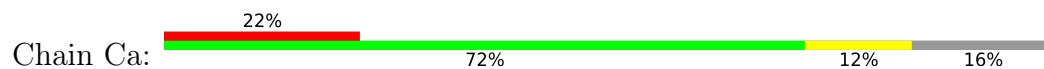


• Molecule 1: Capsid protein

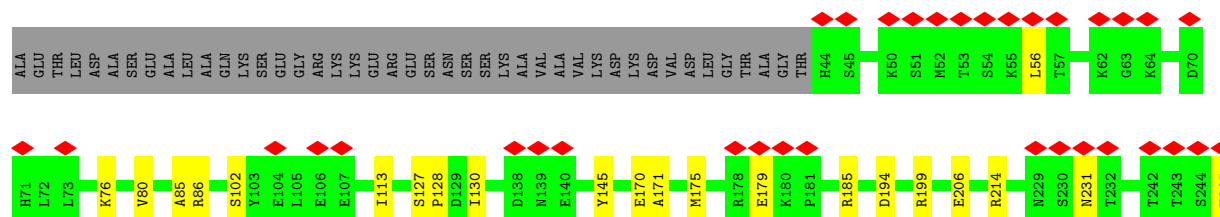
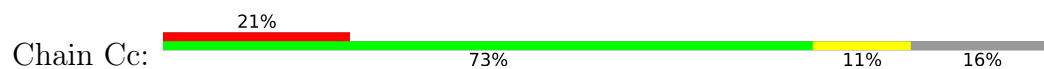




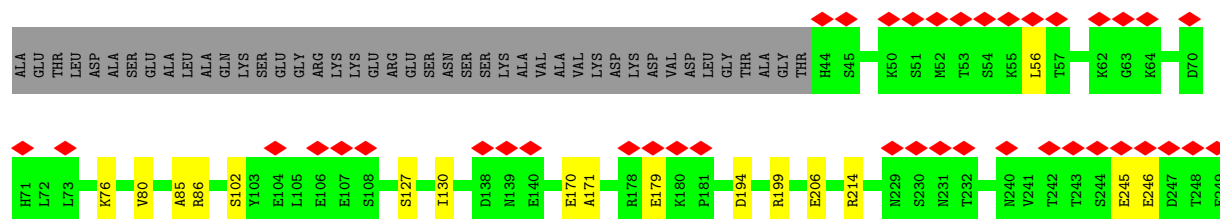
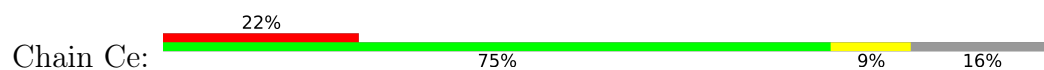
- Molecule 1: Capsid protein



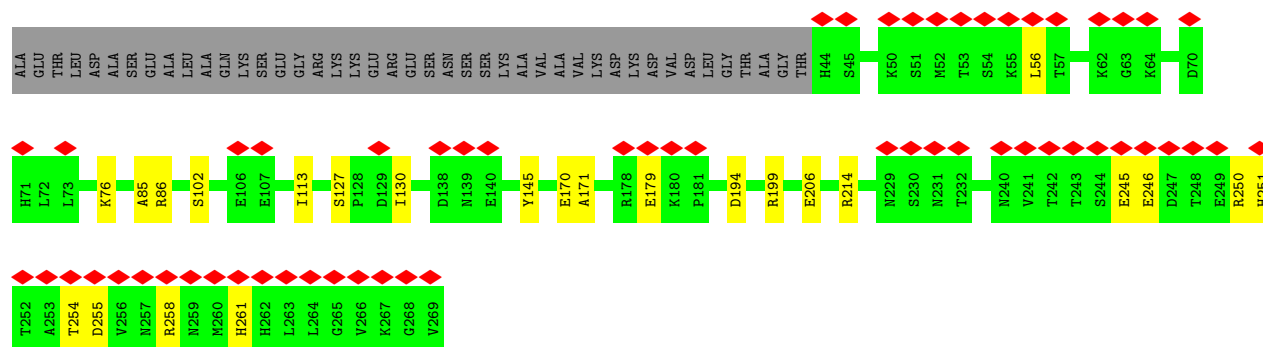
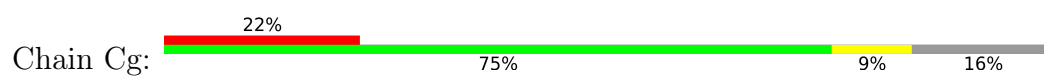
- Molecule 1: Capsid protein



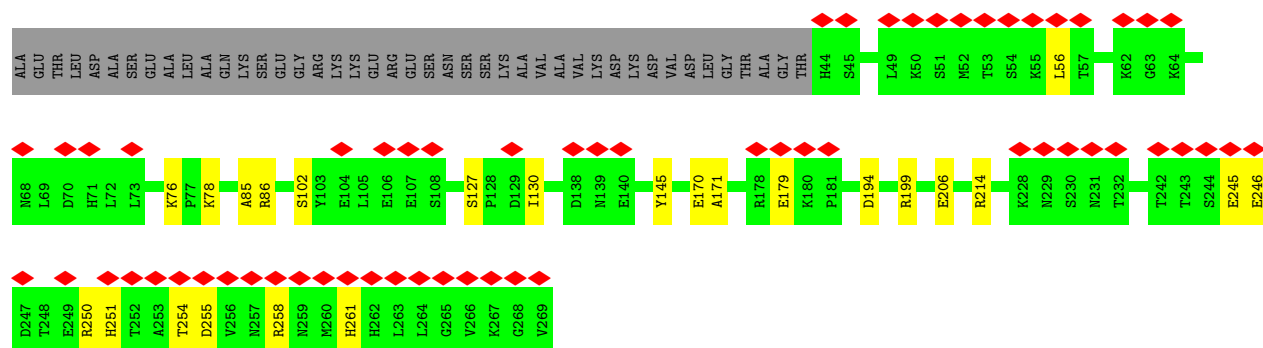
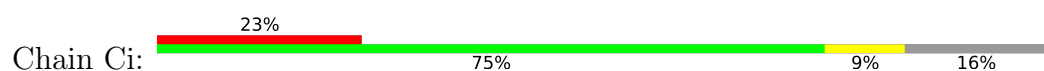
- Molecule 1: Capsid protein



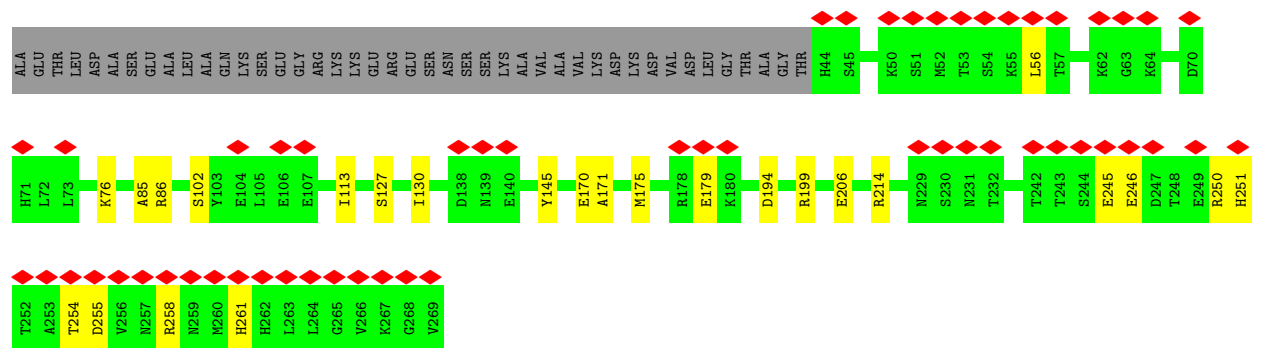
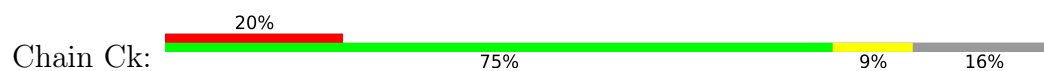
- Molecule 1: Capsid protein



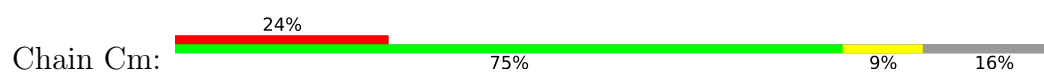
• Molecule 1: Capsid protein

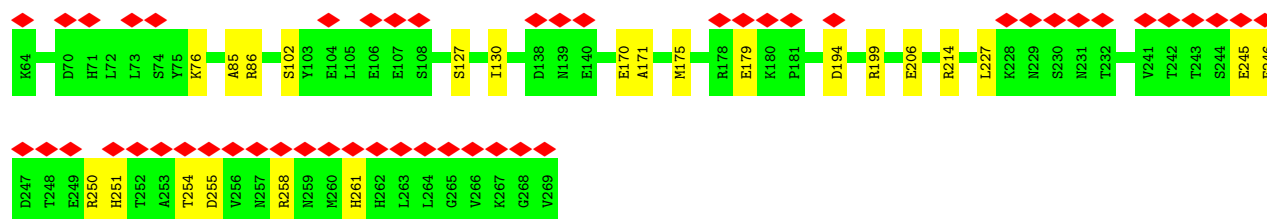


• Molecule 1: Capsid protein

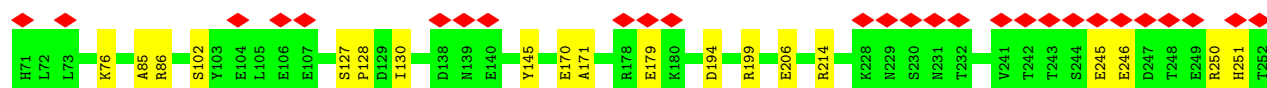
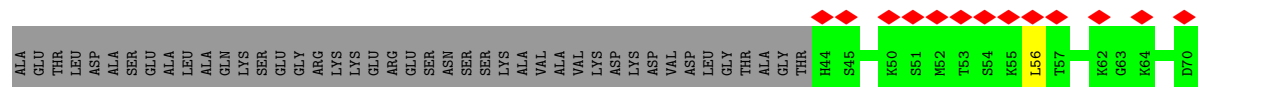
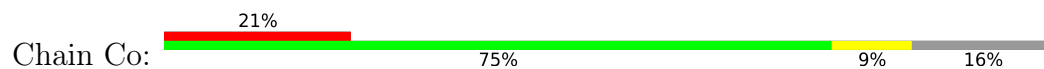


• Molecule 1: Capsid protein

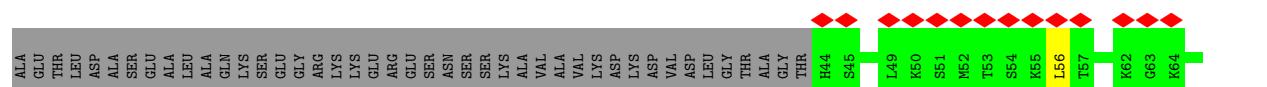
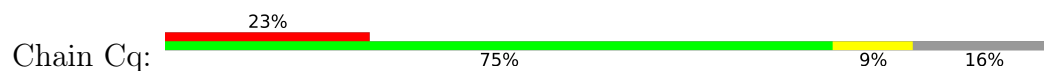




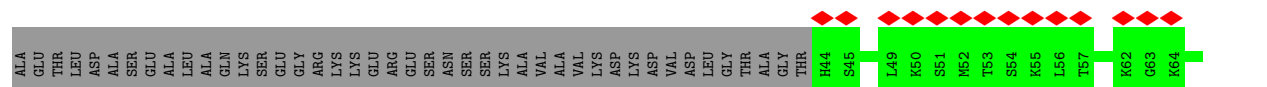
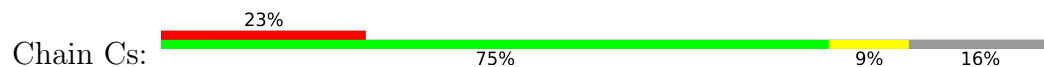
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein





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

Chain Ab: 80% 20%



- 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: 40% 60%



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

Chain Ah: 80% 20%



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

Chain Aj: 60% 40%



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

Chain Al: 60% 40%



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

Chain An: 60% 40%



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

Chain Ap:  80% 20%

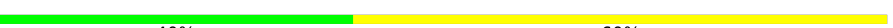


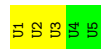
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ar:  80% 20%



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

Chain At:  40% 60%

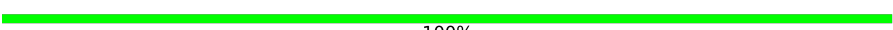


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Av:  60% 40%

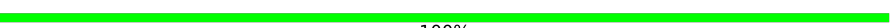


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

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%

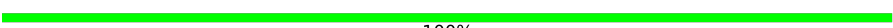
There are no outlier residues recorded for this chain.

- 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:  100%

There are no outlier residues recorded for this chain.

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

Chain Bf:  80% 20%



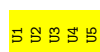
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

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%



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

Chain Bl:  60% 40%



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

Chain Bn:  80% 20%



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

Chain Bp:  80% 20%



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

Chain Br:  80% 20%



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

Chain Bt:  60% 40%



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

Chain Bv:  80% 20%



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

Chain Bx:  60% 40%



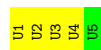
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bz:  80% 20%



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

Chain Cb:  20% 80%



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

Chain Cd:  60% 40%



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

Chain Cf:  100%

There are no outlier residues recorded for this chain.

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

Chain Ch:  80% 20%



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

Chain Cj: 80% 20%



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

Chain Cl: 80% 20%



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

Chain Cn: 80% 20%



- 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: 100%

There are no outlier residues recorded for this chain.

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

Chain Ct: 60% 40%



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	291040	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	12.718	Depositor
Minimum map value	-5.681	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.506	Depositor
Recommended contour level	2.26	Depositor
Map size (Å)	331.45, 331.45, 331.45	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.947, 0.947, 0.947	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	0.44	1/1854 (0.1%)	0.59	0/2503
1	Ac	0.45	1/1854 (0.1%)	0.58	0/2503
1	Ae	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ag	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ai	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ak	0.45	1/1854 (0.1%)	0.59	0/2503
1	Am	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ao	0.45	1/1854 (0.1%)	0.59	0/2503
1	Aq	0.45	1/1854 (0.1%)	0.59	0/2503
1	As	0.45	1/1854 (0.1%)	0.59	0/2503
1	Au	0.45	1/1854 (0.1%)	0.59	0/2503
1	Aw	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ay	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ba	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bc	0.45	1/1854 (0.1%)	0.59	0/2503
1	Be	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bg	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bi	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bk	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bm	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bo	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bq	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bs	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bu	0.45	1/1854 (0.1%)	0.59	0/2503
1	Bw	0.45	1/1854 (0.1%)	0.59	0/2503
1	By	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ca	0.45	1/1854 (0.1%)	0.59	0/2503
1	Cc	0.45	1/1854 (0.1%)	0.58	0/2503
1	Ce	0.45	1/1854 (0.1%)	0.59	0/2503
1	Cg	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ci	0.45	1/1854 (0.1%)	0.59	0/2503
1	Ck	0.45	1/1854 (0.1%)	0.59	0/2503
1	Cm	0.45	1/1854 (0.1%)	0.59	0/2503
1	Co	0.45	1/1854 (0.1%)	0.58	0/2503

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Cq	0.45	1/1854 (0.1%)	0.59	0/2503
1	Cs	0.45	1/1854 (0.1%)	0.59	0/2503
2	Ab	0.29	0/109	0.29	0/166
2	Ad	0.29	0/109	0.29	0/166
2	Af	0.29	0/109	0.29	0/166
2	Ah	0.29	0/109	0.29	0/166
2	Aj	0.29	0/109	0.30	0/166
2	Al	0.29	0/109	0.29	0/166
2	An	0.29	0/109	0.29	0/166
2	Ap	0.29	0/109	0.30	0/166
2	Ar	0.29	0/109	0.30	0/166
2	At	0.29	0/109	0.29	0/166
2	Av	0.29	0/109	0.29	0/166
2	Ax	0.29	0/109	0.29	0/166
2	Az	0.29	0/109	0.29	0/166
2	Bb	0.29	0/109	0.30	0/166
2	Bd	0.29	0/109	0.30	0/166
2	Bf	0.29	0/109	0.30	0/166
2	Bh	0.29	0/109	0.29	0/166
2	Bj	0.29	0/109	0.29	0/166
2	Bl	0.29	0/109	0.29	0/166
2	Bn	0.29	0/109	0.29	0/166
2	Bp	0.29	0/109	0.29	0/166
2	Br	0.29	0/109	0.29	0/166
2	Bt	0.29	0/109	0.30	0/166
2	Bv	0.29	0/109	0.29	0/166
2	Bx	0.29	0/109	0.30	0/166
2	Bz	0.29	0/109	0.29	0/166
2	Cb	0.29	0/109	0.30	0/166
2	Cd	0.29	0/109	0.29	0/166
2	Cf	0.29	0/109	0.29	0/166
2	Ch	0.29	0/109	0.29	0/166
2	Cj	0.29	0/109	0.30	0/166
2	Cl	0.29	0/109	0.30	0/166
2	Cn	0.29	0/109	0.30	0/166
2	Cp	0.29	0/109	0.30	0/166
2	Cr	0.29	0/109	0.30	0/166
2	Ct	0.29	0/109	0.30	0/166
All	All	0.44	36/70668 (0.1%)	0.57	0/96084

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Be	85	ALA	C-N	5.65	1.41	1.33
1	Ck	85	ALA	C-N	5.64	1.41	1.33
1	Am	85	ALA	C-N	5.64	1.40	1.33
1	Aw	85	ALA	C-N	5.64	1.40	1.33
1	Co	85	ALA	C-N	5.64	1.40	1.33
1	Ci	85	ALA	C-N	5.63	1.40	1.33
1	Ae	85	ALA	C-N	5.62	1.40	1.33
1	As	85	ALA	C-N	5.62	1.40	1.33
1	Ag	85	ALA	C-N	5.62	1.40	1.33
1	Bs	85	ALA	C-N	5.62	1.40	1.33
1	Bq	85	ALA	C-N	5.61	1.40	1.33
1	Cs	85	ALA	C-N	5.61	1.40	1.33
1	Bo	85	ALA	C-N	5.61	1.40	1.33
1	Ao	85	ALA	C-N	5.60	1.40	1.33
1	Bu	85	ALA	C-N	5.60	1.40	1.33
1	Bi	85	ALA	C-N	5.60	1.40	1.33
1	Ai	85	ALA	C-N	5.59	1.40	1.33
1	By	85	ALA	C-N	5.59	1.40	1.33
1	Aa	85	ALA	C-N	5.59	1.40	1.33
1	Bw	85	ALA	C-N	5.59	1.40	1.33
1	Bk	85	ALA	C-N	5.59	1.40	1.33
1	Cg	85	ALA	C-N	5.59	1.40	1.33
1	Ce	85	ALA	C-N	5.59	1.40	1.33
1	Aq	85	ALA	C-N	5.58	1.40	1.33
1	Ba	85	ALA	C-N	5.58	1.40	1.33
1	Ak	85	ALA	C-N	5.58	1.40	1.33
1	Ay	85	ALA	C-N	5.58	1.40	1.33
1	Cm	85	ALA	C-N	5.58	1.40	1.33
1	Bm	85	ALA	C-N	5.58	1.40	1.33
1	Ac	85	ALA	C-N	5.57	1.40	1.33
1	Cc	85	ALA	C-N	5.56	1.40	1.33
1	Ca	85	ALA	C-N	5.56	1.40	1.33
1	Cq	85	ALA	C-N	5.55	1.40	1.33
1	Bg	85	ALA	C-N	5.53	1.40	1.33
1	Bc	85	ALA	C-N	5.52	1.40	1.33
1	Au	85	ALA	C-N	5.50	1.40	1.33

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	1815	0	1785	18	0
1	Ac	1815	0	1785	19	0
1	Ae	1815	0	1785	23	0
1	Ag	1815	0	1785	25	0
1	Ai	1815	0	1785	27	0
1	Ak	1815	0	1785	24	0
1	Am	1815	0	1785	26	0
1	Ao	1815	0	1785	25	0
1	Aq	1815	0	1785	28	0
1	As	1815	0	1785	28	0
1	Au	1815	0	1785	28	0
1	Aw	1815	0	1785	24	0
1	Ay	1815	0	1785	28	0
1	Ba	1815	0	1785	28	0
1	Bc	1815	0	1785	27	0
1	Be	1815	0	1785	27	0
1	Bg	1815	0	1785	28	0
1	Bi	1815	0	1785	37	0
1	Bk	1815	0	1785	30	0
1	Bm	1815	0	1785	30	0
1	Bo	1815	0	1785	27	0
1	Bq	1815	0	1785	31	0
1	Bs	1815	0	1785	30	0
1	Bu	1815	0	1785	29	0
1	Bw	1815	0	1785	27	0
1	By	1815	0	1785	29	0
1	Ca	1815	0	1785	35	0
1	Cc	1815	0	1785	28	0
1	Ce	1815	0	1785	20	0
1	Cg	1815	0	1785	21	0
1	Ci	1815	0	1785	22	0
1	Ck	1815	0	1785	25	0
1	Cm	1815	0	1785	23	0
1	Co	1815	0	1785	23	0
1	Cq	1815	0	1785	21	0
1	Cs	1815	0	1785	23	0
2	Ab	100	0	51	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ad	100	0	51	0	0
2	Af	100	0	51	3	0
2	Ah	100	0	51	2	0
2	Aj	100	0	51	2	0
2	Al	100	0	51	2	0
2	An	100	0	51	5	0
2	Ap	100	0	51	1	0
2	Ar	100	0	51	1	0
2	At	100	0	51	3	0
2	Av	100	0	51	2	0
2	Ax	100	0	51	0	0
2	Az	100	0	51	0	0
2	Bb	100	0	51	1	0
2	Bd	100	0	51	0	0
2	Bf	100	0	51	1	0
2	Bh	100	0	51	0	0
2	Bj	100	0	51	8	0
2	Bl	100	0	51	3	0
2	Bn	100	0	51	1	0
2	Bp	100	0	51	1	0
2	Br	100	0	51	1	0
2	Bt	100	0	51	2	0
2	Bv	100	0	51	1	0
2	Bx	100	0	51	2	0
2	Bz	100	0	51	1	0
2	Cb	100	0	51	7	0
2	Cd	100	0	51	2	0
2	Cf	100	0	51	0	0
2	Ch	100	0	51	1	0
2	Cj	100	0	51	1	0
2	Cl	100	0	51	1	0
2	Cn	100	0	51	1	0
2	Cp	100	0	51	2	0
2	Cr	100	0	51	0	0
2	Ct	100	0	51	3	0
All	All	68940	0	66096	646	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 (646) 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:Am:130:ILE:HG22	2:An:5:U:H1'	1.65	0.79
2:Cb:1:U:P	1:Cc:185:ARG:HH12	2.09	0.74
1:Ae:243:THR:HG22	1:Aw:254:THR:HG23	1.76	0.67
1:Ag:243:THR:HG22	1:Ay:254:THR:HG23	1.76	0.67
1:Bm:243:THR:HG22	1:Ce:254:THR:HG23	1.77	0.67
1:Ac:243:THR:HG22	1:Au:254:THR:HG23	1.77	0.66
1:Ca:227:LEU:CD2	2:Cb:3:U:H2'	2.25	0.66
1:Bo:243:THR:HG22	1:Cg:254:THR:HG23	1.77	0.66
1:Bk:243:THR:HG22	1:Cc:254:THR:HG23	1.77	0.66
1:Bw:243:THR:HG22	1:Co:254:THR:HG23	1.77	0.66
1:Ai:243:THR:HG22	1:Ba:254:THR:HG23	1.77	0.66
1:Am:243:THR:HG22	1:Be:254:THR:HG23	1.77	0.66
1:Ak:243:THR:HG22	1:Bc:254:THR:HG23	1.77	0.66
1:Bu:243:THR:HG22	1:Cm:254:THR:HG23	1.78	0.65
1:Au:243:THR:HG22	1:Bm:254:THR:HG23	1.78	0.65
1:Aw:243:THR:HG22	1:Bo:254:THR:HG23	1.78	0.65
1:Bq:243:THR:HG22	1:Ci:254:THR:HG23	1.78	0.65
1:Ay:243:THR:HG22	1:Bq:254:THR:HG23	1.78	0.65
1:Aa:243:THR:HG22	1:As:254:THR:HG23	1.78	0.65
1:By:243:THR:HG22	1:Cq:254:THR:HG23	1.77	0.65
1:Ao:243:THR:HG22	1:Bg:254:THR:HG23	1.79	0.65
1:Be:243:THR:HG22	1:Bw:254:THR:HG23	1.77	0.65
1:Bg:243:THR:HG22	1:By:254:THR:HG23	1.77	0.65
1:Ca:243:THR:HG22	1:Cs:254:THR:HG23	1.77	0.65
1:As:243:THR:HG22	1:Bk:254:THR:HG23	1.78	0.64
1:Bc:243:THR:HG22	1:Bu:254:THR:HG23	1.77	0.64
1:Bs:243:THR:HG22	1:Ck:254:THR:HG23	1.78	0.64
1:Ba:243:THR:HG22	1:Bs:254:THR:HG23	1.78	0.64
1:Bi:243:THR:HG22	1:Ca:254:THR:HG23	1.78	0.64
1:Aq:243:THR:HG22	1:Bi:254:THR:HG23	1.79	0.63
1:Ao:54:SER:HB2	1:Bi:102:SER:O	2.00	0.62
1:By:54:SER:HB2	1:Cs:102:SER:O	2.00	0.62
1:Bm:54:SER:HB2	1:Cg:102:SER:O	2.00	0.62
1:Ak:54:SER:HB2	1:Be:102:SER:O	2.00	0.61
1:Ag:54:SER:HB2	1:Ba:102:SER:O	1.99	0.61
1:Bg:54:SER:HB2	1:Ca:102:SER:O	2.00	0.61
1:Am:54:SER:HB2	1:Bg:102:SER:O	2.00	0.61
1:Bk:251:HIS:CD2	1:Bk:258:ARG:HG3	2.36	0.61
1:Bo:251:HIS:CD2	1:Bo:258:ARG:HG3	2.36	0.61
1:Bi:251:HIS:CD2	1:Bi:258:ARG:HG3	2.36	0.61
1:Bm:251:HIS:CD2	1:Bm:258:ARG:HG3	2.36	0.61
1:Bq:251:HIS:CD2	1:Bq:258:ARG:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ce:251:HIS:CD2	1:Ce:258:ARG:HG3	2.36	0.61
1:Aa:251:HIS:CD2	1:Aa:258:ARG:HG3	2.36	0.61
1:Ac:251:HIS:CD2	1:Ac:258:ARG:HG3	2.36	0.61
1:Ae:251:HIS:CD2	1:Ae:258:ARG:HG3	2.36	0.61
1:Cs:251:HIS:CD2	1:Cs:258:ARG:HG3	2.36	0.61
1:Ag:251:HIS:CD2	1:Ag:258:ARG:HG3	2.36	0.61
1:Bq:54:SER:HB2	1:Ck:102:SER:O	2.00	0.61
1:Cc:251:HIS:CD2	1:Cc:258:ARG:HG3	2.36	0.61
1:Cq:251:HIS:CD2	1:Cq:258:ARG:HG3	2.36	0.61
1:Ai:251:HIS:CD2	1:Ai:258:ARG:HG3	2.36	0.61
1:As:251:HIS:CD2	1:As:258:ARG:HG3	2.36	0.61
1:Au:251:HIS:CD2	1:Au:258:ARG:HG3	2.36	0.61
1:Bg:251:HIS:CD2	1:Bg:258:ARG:HG3	2.36	0.61
1:Bs:251:HIS:CD2	1:Bs:258:ARG:HG3	2.36	0.61
1:Co:251:HIS:CD2	1:Co:258:ARG:HG3	2.36	0.61
1:Ai:54:SER:HB2	1:Bc:102:SER:O	2.00	0.61
1:Bw:251:HIS:CD2	1:Bw:258:ARG:HG3	2.36	0.61
1:Aq:54:SER:HB2	1:Bk:102:SER:O	2.01	0.60
1:Aw:56:LEU:HD21	1:Ay:171:ALA:CB	2.31	0.60
1:Aw:251:HIS:CD2	1:Aw:258:ARG:HG3	2.36	0.60
1:Bu:251:HIS:CD2	1:Bu:258:ARG:HG3	2.36	0.60
1:Cg:251:HIS:CD2	1:Cg:258:ARG:HG3	2.36	0.60
1:Ak:251:HIS:CD2	1:Ak:258:ARG:HG3	2.36	0.60
1:Am:251:HIS:CD2	1:Am:258:ARG:HG3	2.36	0.60
1:Bo:56:LEU:HD21	1:Bq:171:ALA:CB	2.31	0.60
1:Bs:54:SER:HB2	1:Cm:102:SER:O	2.01	0.60
1:Ay:251:HIS:CD2	1:Ay:258:ARG:HG3	2.36	0.60
1:Be:251:HIS:CD2	1:Be:258:ARG:HG3	2.36	0.60
1:Bc:251:HIS:CD2	1:Bc:258:ARG:HG3	2.36	0.60
1:Cm:251:HIS:CD2	1:Cm:258:ARG:HG3	2.36	0.60
1:Aa:56:LEU:HD21	1:Ac:171:ALA:CB	2.32	0.60
1:Ao:251:HIS:CD2	1:Ao:258:ARG:HG3	2.36	0.60
1:Ca:251:HIS:CD2	1:Ca:258:ARG:HG3	2.36	0.60
1:Ac:54:SER:HB2	1:Aw:102:SER:O	2.01	0.60
1:Aq:251:HIS:CD2	1:Aq:258:ARG:HG3	2.36	0.60
1:As:56:LEU:HD21	1:Au:171:ALA:CB	2.32	0.60
1:Bk:56:LEU:HD21	1:Bm:171:ALA:CB	2.32	0.60
1:Ck:251:HIS:CD2	1:Ck:258:ARG:HG3	2.36	0.60
1:Ai:56:LEU:HD21	1:Ak:171:ALA:CB	2.32	0.60
1:Ak:56:LEU:HD21	1:Am:171:ALA:CB	2.32	0.60
1:Ba:251:HIS:CD2	1:Ba:258:ARG:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:54:SER:HB2	1:Ce:102:SER:O	2.02	0.60
1:Ck:56:LEU:HD21	1:Cm:171:ALA:CB	2.32	0.60
1:Bc:56:LEU:HD21	1:Be:171:ALA:CB	2.32	0.60
1:Bi:54:SER:HB2	1:Cc:102:SER:O	2.01	0.60
1:Cc:56:LEU:HD21	1:Ce:171:ALA:CB	2.32	0.60
1:Cm:56:LEU:HD21	1:Co:171:ALA:CB	2.32	0.60
1:Bu:54:SER:HB2	1:Co:102:SER:O	2.02	0.60
1:Ci:251:HIS:CD2	1:Ci:258:ARG:HG3	2.36	0.60
1:Ay:54:SER:HB2	1:Bs:102:SER:O	2.02	0.60
1:Be:54:SER:HB2	1:By:102:SER:O	2.02	0.60
1:Bw:54:SER:HB2	1:Cq:102:SER:O	2.01	0.60
1:Ae:54:SER:HB2	1:Ay:102:SER:O	2.02	0.59
1:Bs:56:LEU:HD21	1:Bu:171:ALA:CB	2.32	0.59
1:By:251:HIS:CD2	1:By:258:ARG:HG3	2.36	0.59
1:Am:130:ILE:CG2	2:An:5:U:H1'	2.31	0.59
1:Ca:227:LEU:HD22	2:Cb:3:U:H2'	1.84	0.59
1:Cg:56:LEU:HD21	1:Ci:171:ALA:CB	2.31	0.59
1:Be:56:LEU:HD21	1:Bg:171:ALA:CB	2.32	0.59
1:Ae:56:LEU:HD21	1:Ag:171:ALA:CB	2.31	0.59
1:Aq:130:ILE:HG22	2:Ar:5:U:H1'	1.84	0.59
1:Ba:56:LEU:HD21	1:Bc:171:ALA:CB	2.32	0.59
1:Bo:54:SER:HB2	1:Ci:102:SER:O	2.02	0.59
1:As:54:SER:HB2	1:Bm:102:SER:O	2.03	0.59
1:Au:54:SER:HB2	1:Bo:102:SER:O	2.02	0.59
1:Bc:54:SER:HB2	1:Bw:102:SER:O	2.03	0.59
1:Bu:56:LEU:HD21	1:Bw:171:ALA:CB	2.32	0.59
1:Ca:56:LEU:HD21	1:Cc:171:ALA:CB	2.33	0.59
1:Aa:54:SER:HB2	1:Au:102:SER:O	2.03	0.59
1:Aq:56:LEU:HD21	1:As:171:ALA:CB	2.32	0.59
1:Au:56:LEU:HD21	1:Aw:171:ALA:CB	2.33	0.59
1:Bq:56:LEU:HD21	1:Bs:171:ALA:CB	2.33	0.59
1:Am:56:LEU:HD21	1:Ao:171:ALA:CB	2.33	0.58
1:Bw:56:LEU:HD21	1:By:171:ALA:CB	2.32	0.58
1:Co:56:LEU:HD21	1:Cq:171:ALA:CB	2.33	0.58
1:Ao:56:LEU:HD21	1:Aq:171:ALA:CB	2.34	0.58
1:Bg:56:LEU:HD21	1:Bi:171:ALA:CB	2.34	0.58
1:Bi:56:LEU:HD21	1:Bk:171:ALA:CB	2.32	0.58
1:By:56:LEU:HD21	1:Ca:171:ALA:CB	2.34	0.58
1:Ag:56:LEU:HD21	1:Ai:171:ALA:CB	2.33	0.58
1:Ci:56:LEU:HD21	1:Ck:171:ALA:CB	2.33	0.58
1:Cq:56:LEU:HD21	1:Cs:171:ALA:CB	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:54:SER:HB2	1:Bu:102:SER:O	2.03	0.58
1:Ce:56:LEU:HD21	1:Cg:171:ALA:CB	2.33	0.58
1:Ca:160:GLN:HE21	2:Cb:2:U:P	2.26	0.58
1:Ac:56:LEU:HD21	1:Ae:171:ALA:CB	2.33	0.58
1:Bm:56:LEU:HD21	1:Bo:171:ALA:CB	2.33	0.58
1:Ay:56:LEU:HD21	1:Ba:171:ALA:CB	2.33	0.58
1:Aw:54:SER:HB2	1:Bq:102:SER:O	2.04	0.57
1:Cs:130:ILE:HG22	2:Ct:5:U:H1'	1.86	0.57
1:Cg:194:ASP:CG	1:Cg:214:ARG:HH12	2.13	0.57
1:Ag:194:ASP:CG	1:Ag:214:ARG:HH12	2.13	0.57
1:Bs:194:ASP:CG	1:Bs:214:ARG:HH12	2.13	0.57
1:Bu:194:ASP:CG	1:Bu:214:ARG:HH12	2.13	0.57
1:Cm:194:ASP:CG	1:Cm:214:ARG:HH12	2.13	0.57
1:Au:194:ASP:CG	1:Au:214:ARG:HH12	2.13	0.57
1:Aw:194:ASP:CG	1:Aw:214:ARG:HH12	2.13	0.57
1:Bc:194:ASP:CG	1:Bc:214:ARG:HH12	2.13	0.57
1:Ac:194:ASP:CG	1:Ac:214:ARG:HH12	2.13	0.56
1:Ai:194:ASP:CG	1:Ai:214:ARG:HH12	2.13	0.56
1:Bq:194:ASP:CG	1:Bq:214:ARG:HH12	2.13	0.56
1:Ba:194:ASP:CG	1:Ba:214:ARG:HH12	2.13	0.56
1:Cc:130:ILE:HG22	2:Cd:5:U:H1'	1.87	0.56
1:Cc:194:ASP:CG	1:Cc:214:ARG:HH12	2.13	0.56
1:Ae:86:ARG:HD2	1:Ae:206:GLU:OE2	2.06	0.56
1:Ae:194:ASP:CG	1:Ae:214:ARG:HH12	2.13	0.56
1:Aq:86:ARG:HD2	1:Aq:206:GLU:OE2	2.06	0.56
1:Bg:86:ARG:HD2	1:Bg:206:GLU:OE2	2.06	0.56
1:Bi:194:ASP:CG	1:Bi:214:ARG:HH12	2.13	0.56
1:Bk:86:ARG:HD2	1:Bk:206:GLU:OE2	2.06	0.56
1:Bk:194:ASP:CG	1:Bk:214:ARG:HH12	2.13	0.56
1:Bo:194:ASP:CG	1:Bo:214:ARG:HH12	2.13	0.56
1:Bq:86:ARG:HD2	1:Bq:206:GLU:OE2	2.06	0.56
1:Bw:86:ARG:HD2	1:Bw:206:GLU:OE2	2.06	0.56
1:Ca:194:ASP:CG	1:Ca:214:ARG:HH12	2.13	0.56
1:Ce:194:ASP:CG	1:Ce:214:ARG:HH12	2.13	0.56
1:Cg:86:ARG:HD2	1:Cg:206:GLU:OE2	2.06	0.56
1:Ci:194:ASP:CG	1:Ci:214:ARG:HH12	2.13	0.56
1:Cs:86:ARG:HD2	1:Cs:206:GLU:OE2	2.06	0.56
1:Ak:194:ASP:CG	1:Ak:214:ARG:HH12	2.13	0.56
1:Ay:86:ARG:HD2	1:Ay:206:GLU:OE2	2.06	0.56
1:Bm:86:ARG:HD2	1:Bm:206:GLU:OE2	2.06	0.56
1:By:86:ARG:HD2	1:By:206:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Co:86:ARG:HD2	1:Co:206:GLU:OE2	2.06	0.56
1:Aq:76:LYS:HD3	1:As:179:GLU:OE2	2.06	0.56
1:Bm:194:ASP:CG	1:Bm:214:ARG:HH12	2.13	0.56
1:Bo:86:ARG:HD2	1:Bo:206:GLU:OE2	2.06	0.56
1:Ca:76:LYS:HD3	1:Cc:179:GLU:OE2	2.06	0.56
1:Cq:86:ARG:HD2	1:Cq:206:GLU:OE2	2.06	0.56
1:Cs:194:ASP:CG	1:Cs:214:ARG:HH12	2.13	0.56
1:Aa:194:ASP:CG	1:Aa:214:ARG:HH12	2.13	0.56
1:Ac:86:ARG:HD2	1:Ac:206:GLU:OE2	2.06	0.56
1:Ai:86:ARG:HD2	1:Ai:206:GLU:OE2	2.06	0.56
1:Ao:86:ARG:HD2	1:Ao:206:GLU:OE2	2.06	0.56
1:Ao:194:ASP:CG	1:Ao:214:ARG:HH12	2.13	0.56
1:Aq:194:ASP:CG	1:Aq:214:ARG:HH12	2.13	0.56
1:As:86:ARG:HD2	1:As:206:GLU:OE2	2.06	0.56
1:Aw:76:LYS:HD3	1:Ay:179:GLU:OE2	2.06	0.56
1:Ba:86:ARG:HD2	1:Ba:206:GLU:OE2	2.06	0.56
1:Be:194:ASP:CG	1:Be:214:ARG:HH12	2.13	0.56
1:Ce:86:ARG:HD2	1:Ce:206:GLU:OE2	2.06	0.56
1:Co:194:ASP:CG	1:Co:214:ARG:HH12	2.13	0.56
1:Ag:86:ARG:HD2	1:Ag:206:GLU:OE2	2.06	0.56
1:Ay:194:ASP:CG	1:Ay:214:ARG:HH12	2.13	0.56
1:By:194:ASP:CG	1:By:214:ARG:HH12	2.13	0.56
1:Cm:86:ARG:HD2	1:Cm:206:GLU:OE2	2.06	0.56
1:Aa:86:ARG:HD2	1:Aa:206:GLU:OE2	2.06	0.56
1:Ak:86:ARG:HD2	1:Ak:206:GLU:OE2	2.06	0.56
1:Ba:76:LYS:HD3	1:Bc:179:GLU:OE2	2.06	0.56
1:Bi:86:ARG:HD2	1:Bi:206:GLU:OE2	2.06	0.56
1:Cg:76:LYS:HD3	1:Ci:179:GLU:OE2	2.06	0.56
1:Ci:86:ARG:HD2	1:Ci:206:GLU:OE2	2.06	0.56
1:Am:194:ASP:CG	1:Am:214:ARG:HH12	2.13	0.56
1:Aw:86:ARG:HD2	1:Aw:206:GLU:OE2	2.06	0.56
1:Bi:76:LYS:HD3	1:Bk:179:GLU:OE2	2.06	0.56
1:As:194:ASP:CG	1:As:214:ARG:HH12	2.13	0.56
1:Be:86:ARG:HD2	1:Be:206:GLU:OE2	2.06	0.56
1:Ck:194:ASP:CG	1:Ck:214:ARG:HH12	2.13	0.56
1:Ay:76:LYS:HD3	1:Ba:179:GLU:OE2	2.07	0.55
1:Bg:194:ASP:CG	1:Bg:214:ARG:HH12	2.13	0.55
1:Bu:76:LYS:HD3	1:Bw:179:GLU:OE2	2.06	0.55
1:Bu:86:ARG:HD2	1:Bu:206:GLU:OE2	2.06	0.55
1:Ca:86:ARG:HD2	1:Ca:206:GLU:OE2	2.06	0.55
1:Ae:76:LYS:HD3	1:Ag:179:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:As:76:LYS:HD3	1:Au:179:GLU:OE2	2.07	0.55
1:Bc:86:ARG:HD2	1:Bc:206:GLU:OE2	2.06	0.55
1:Ci:76:LYS:HD3	1:Ck:179:GLU:OE2	2.06	0.55
1:Ak:76:LYS:HD3	1:Am:179:GLU:OE2	2.06	0.55
1:Bs:86:ARG:HD2	1:Bs:206:GLU:OE2	2.06	0.55
1:Bs:76:LYS:HD3	1:Bu:179:GLU:OE2	2.06	0.55
1:Am:86:ARG:HD2	1:Am:206:GLU:OE2	2.06	0.55
1:Bo:76:LYS:HD3	1:Bq:179:GLU:OE2	2.06	0.55
1:Bw:194:ASP:CG	1:Bw:214:ARG:HH12	2.13	0.55
1:Cc:86:ARG:HD2	1:Cc:206:GLU:OE2	2.06	0.55
1:Cq:194:ASP:CG	1:Cq:214:ARG:HH12	2.13	0.55
1:Au:86:ARG:HD2	1:Au:206:GLU:OE2	2.06	0.55
1:Bc:76:LYS:HD3	1:Be:179:GLU:OE2	2.06	0.55
1:Cc:76:LYS:HD3	1:Ce:179:GLU:OE2	2.06	0.55
1:Ck:76:LYS:HD3	1:Cm:179:GLU:OE2	2.06	0.55
1:Bk:76:LYS:HD3	1:Bm:179:GLU:OE2	2.06	0.55
1:Ck:86:ARG:HD2	1:Ck:206:GLU:OE2	2.06	0.55
1:Ag:76:LYS:HD3	1:Ai:179:GLU:OE2	2.07	0.55
1:Bw:76:LYS:HD3	1:By:179:GLU:OE2	2.07	0.54
1:Ao:76:LYS:HD3	1:Aq:179:GLU:OE2	2.07	0.54
1:Au:76:LYS:HD3	1:Aw:179:GLU:OE2	2.07	0.54
1:Bq:76:LYS:HD3	1:Bs:179:GLU:OE2	2.07	0.54
1:By:76:LYS:HD3	1:Ca:179:GLU:OE2	2.07	0.54
1:Cm:76:LYS:HD3	1:Co:179:GLU:OE2	2.06	0.54
1:Be:76:LYS:HD3	1:Bg:179:GLU:OE2	2.07	0.54
1:Am:76:LYS:HD3	1:Ao:179:GLU:OE2	2.07	0.54
1:Co:76:LYS:HD3	1:Cq:179:GLU:OE2	2.07	0.54
1:Cq:76:LYS:HD3	1:Cs:179:GLU:OE2	2.07	0.54
1:Ai:76:LYS:HD3	1:Ak:179:GLU:OE2	2.06	0.54
1:Ce:76:LYS:HD3	1:Cg:179:GLU:OE2	2.08	0.54
1:Aa:76:LYS:HD3	1:Ac:179:GLU:OE2	2.07	0.54
1:Bi:160:GLN:HE21	2:Bj:2:U:P	2.30	0.54
1:Ac:76:LYS:HD3	1:Ae:179:GLU:OE2	2.08	0.54
1:Bm:130:ILE:HG22	2:Bn:5:U:H1'	1.89	0.54
1:Bm:76:LYS:HD3	1:Bo:179:GLU:OE2	2.08	0.53
1:Bg:76:LYS:HD3	1:Bi:179:GLU:OE2	2.07	0.53
1:Ac:251:HIS:CE1	1:Ac:258:ARG:HA	2.44	0.53
1:Bm:251:HIS:CE1	1:Bm:258:ARG:HA	2.44	0.53
1:Bs:251:HIS:CE1	1:Bs:258:ARG:HA	2.44	0.53
1:By:251:HIS:CE1	1:By:258:ARG:HA	2.44	0.53
1:Cc:231:ASN:HB2	1:Cs:245:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aa:231:ASN:HB2	1:Aq:245:GLU:OE2	2.09	0.52
1:Ag:251:HIS:CE1	1:Ag:258:ARG:HA	2.44	0.52
1:As:251:HIS:CE1	1:As:258:ARG:HA	2.45	0.52
1:Bc:251:HIS:CE1	1:Bc:258:ARG:HA	2.45	0.52
1:Bi:227:LEU:CD2	2:Bj:3:U:H2'	2.39	0.52
2:Bl:1:U:P	1:Bm:185:ARG:HH12	2.31	0.52
1:Cc:251:HIS:CE1	1:Cc:258:ARG:HA	2.45	0.52
1:Ck:251:HIS:CE1	1:Ck:258:ARG:HA	2.45	0.52
1:Am:251:HIS:CE1	1:Am:258:ARG:HA	2.44	0.52
1:Aw:251:HIS:CE1	1:Aw:258:ARG:HA	2.45	0.52
1:Bi:251:HIS:CE1	1:Bi:258:ARG:HA	2.45	0.52
1:Bq:251:HIS:CE1	1:Bq:258:ARG:HA	2.44	0.52
1:Cg:251:HIS:CE1	1:Cg:258:ARG:HA	2.44	0.52
1:Cq:251:HIS:CE1	1:Cq:258:ARG:HA	2.45	0.52
1:Cs:251:HIS:CE1	1:Cs:258:ARG:HA	2.45	0.52
1:Ci:251:HIS:CE1	1:Ci:258:ARG:HA	2.44	0.52
1:Co:251:HIS:CE1	1:Co:258:ARG:HA	2.44	0.52
1:Aq:231:ASN:HB2	1:Bg:245:GLU:OE2	2.10	0.52
1:Ay:251:HIS:CE1	1:Ay:258:ARG:HA	2.44	0.52
1:Bo:251:HIS:CE1	1:Bo:258:ARG:HA	2.44	0.52
1:Ca:203:ASP:HB2	2:Cb:4:U:C2	2.44	0.52
1:Aq:251:HIS:CE1	1:Aq:258:ARG:HA	2.45	0.52
1:As:231:ASN:HB2	1:Bi:245:GLU:OE2	2.09	0.52
1:Ak:251:HIS:CE1	1:Ak:258:ARG:HA	2.45	0.52
1:Ao:251:HIS:CE1	1:Ao:258:ARG:HA	2.44	0.52
1:Ba:251:HIS:CE1	1:Ba:258:ARG:HA	2.45	0.52
1:Bg:251:HIS:CE1	1:Bg:258:ARG:HA	2.44	0.52
1:Bk:231:ASN:HB2	1:Ca:245:GLU:OE2	2.09	0.52
1:Bu:251:HIS:CE1	1:Bu:258:ARG:HA	2.45	0.52
1:Ce:251:HIS:CE1	1:Ce:258:ARG:HA	2.44	0.52
1:Ae:251:HIS:CE1	1:Ae:258:ARG:HA	2.44	0.52
1:Ai:251:HIS:CE1	1:Ai:258:ARG:HA	2.44	0.52
1:Ca:251:HIS:CE1	1:Ca:258:ARG:HA	2.45	0.52
1:Aa:251:HIS:CE1	1:Aa:258:ARG:HA	2.44	0.52
1:Ba:231:ASN:HB2	1:Bq:245:GLU:OE2	2.09	0.52
1:Be:251:HIS:CE1	1:Be:258:ARG:HA	2.45	0.52
1:As:160:GLN:HE21	2:At:2:U:P	2.32	0.52
1:Bs:231:ASN:HB2	1:Ci:245:GLU:OE2	2.10	0.52
1:Au:251:HIS:CE1	1:Au:258:ARG:HA	2.45	0.51
1:Bk:251:HIS:CE1	1:Bk:258:ARG:HA	2.45	0.51
1:Bc:231:ASN:HB2	1:Bs:245:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bw:251:HIS:CE1	1:Bw:258:ARG:HA	2.44	0.51
1:Ac:231:ASN:HB2	1:As:245:GLU:OE2	2.11	0.51
1:Be:231:ASN:HB2	1:Bu:245:GLU:OE2	2.11	0.51
1:Cm:251:HIS:CE1	1:Cm:258:ARG:HA	2.45	0.51
1:Bi:231:ASN:HB2	1:By:245:GLU:OE2	2.11	0.51
1:Ca:231:ASN:HB2	1:Cq:245:GLU:OE2	2.11	0.51
1:Bu:231:ASN:HB2	1:Ck:245:GLU:OE2	2.11	0.51
1:Bi:203:ASP:HB2	2:Bj:4:U:C2	2.46	0.50
1:Bw:231:ASN:HB2	1:Cm:245:GLU:OE2	2.11	0.50
1:Au:231:ASN:HB2	1:Bk:245:GLU:OE2	2.11	0.50
1:Ay:231:ASN:HB2	1:Bo:245:GLU:OE2	2.11	0.50
1:Ai:231:ASN:HB2	1:Ay:245:GLU:OE2	2.11	0.50
1:Ae:231:ASN:HB2	1:Au:245:GLU:OE2	2.12	0.50
1:Aw:231:ASN:HB2	1:Bm:245:GLU:OE2	2.11	0.50
1:Bi:214:ARG:HH21	1:Cq:246:GLU:CD	2.20	0.50
1:Bm:231:ASN:HB2	1:Cc:245:GLU:OE2	2.12	0.50
1:Bq:231:ASN:HB2	1:Cg:245:GLU:OE2	2.12	0.50
1:Ae:214:ARG:HH21	1:Bm:246:GLU:CD	2.20	0.50
1:Ak:227:LEU:CD2	2:Al:3:U:H2'	2.42	0.49
1:Am:231:ASN:HB2	1:Bc:245:GLU:OE2	2.12	0.49
1:Bo:231:ASN:HB2	1:Ce:245:GLU:OE2	2.12	0.49
1:By:231:ASN:HB2	1:Co:245:GLU:OE2	2.13	0.49
1:Ag:231:ASN:HB2	1:Aw:245:GLU:OE2	2.13	0.49
1:Ao:231:ASN:HB2	1:Be:245:GLU:OE2	2.13	0.49
1:Aq:214:ARG:HH21	1:By:246:GLU:CD	2.21	0.49
1:Bg:231:ASN:HB2	1:Bw:245:GLU:OE2	2.13	0.49
1:Ai:214:ARG:HH21	1:Bq:246:GLU:CD	2.21	0.49
1:Ba:130:ILE:HG22	2:Bb:5:U:H1'	1.95	0.48
1:Bg:214:ARG:HH21	1:Co:246:GLU:CD	2.21	0.48
1:Ag:214:ARG:HH21	1:Bo:246:GLU:CD	2.21	0.48
1:Ak:231:ASN:HB2	1:Ba:245:GLU:OE2	2.12	0.48
1:Be:221:GLN:OE1	1:Cm:250:ARG:HD3	2.13	0.48
1:Be:214:ARG:HH21	1:Cm:246:GLU:CD	2.22	0.48
1:Bk:221:GLN:OE1	1:Cs:250:ARG:HD3	2.14	0.48
1:Am:221:GLN:OE1	1:Bu:250:ARG:HD3	2.14	0.48
1:Aw:214:ARG:HH21	1:Ce:246:GLU:CD	2.21	0.47
1:Ac:221:GLN:OE1	1:Bk:250:ARG:HD3	2.14	0.47
1:Au:221:GLN:OE1	1:Cc:250:ARG:HD3	2.14	0.47
1:Ay:221:GLN:OE1	1:Cg:250:ARG:HD3	2.14	0.47
1:Ba:214:ARG:HH21	1:Ci:246:GLU:CD	2.22	0.47
1:Bc:221:GLN:OE1	1:Ck:250:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:221:GLN:OE1	1:Bq:250:ARG:HD3	2.15	0.47
1:Ba:47:PRO:O	1:Bu:145:TYR:OH	2.31	0.47
1:As:221:GLN:OE1	1:Ca:250:ARG:HD3	2.14	0.47
1:Ba:221:GLN:OE1	1:Ci:250:ARG:HD3	2.14	0.47
1:Bc:214:ARG:HH21	1:Ck:246:GLU:CD	2.23	0.47
1:Bk:227:LEU:CD2	2:Bl:3:U:H2'	2.45	0.47
1:Cm:227:LEU:CD2	2:Cn:3:U:H2'	2.45	0.47
1:Aa:221:GLN:OE1	1:Bi:250:ARG:HD3	2.14	0.47
1:Bi:47:PRO:O	1:Cc:145:TYR:OH	2.31	0.47
1:Ak:214:ARG:HH21	1:Bs:246:GLU:CD	2.23	0.47
1:Ae:76:LYS:CE	1:Ag:179:GLU:OE2	2.64	0.46
1:Ag:221:GLN:OE1	1:Bo:250:ARG:HD3	2.14	0.46
1:Bi:130:ILE:HG22	2:Bj:5:U:H1'	1.96	0.46
1:Ac:214:ARG:HH21	1:Bk:246:GLU:CD	2.23	0.46
1:Ae:47:PRO:O	1:Ay:145:TYR:OH	2.30	0.46
1:Ao:130:ILE:HG22	2:Ap:5:U:H1'	1.97	0.46
1:Aw:76:LYS:CE	1:Ay:179:GLU:OE2	2.64	0.46
1:Bi:221:GLN:OE1	1:Cq:250:ARG:HD3	2.15	0.46
1:By:262:HIS:NE2	1:Ca:254:THR:O	2.44	0.46
1:Ae:221:GLN:OE1	1:Bm:250:ARG:HD3	2.16	0.46
1:Ao:214:ARG:HH21	1:Bw:246:GLU:CD	2.23	0.46
1:Bo:76:LYS:CE	1:Bq:179:GLU:OE2	2.64	0.46
1:Cc:128:PRO:HG3	2:Cd:3:U:H5''	1.97	0.46
1:Ck:170:GLU:HG2	1:Ck:199:ARG:HE	1.81	0.46
1:Cq:170:GLU:HG2	1:Cq:199:ARG:HE	1.81	0.46
1:Ao:170:GLU:HG2	1:Ao:199:ARG:HE	1.81	0.46
1:Be:170:GLU:HG2	1:Be:199:ARG:HE	1.81	0.46
1:Bu:170:GLU:HG2	1:Bu:199:ARG:HE	1.81	0.46
1:Ca:170:GLU:HG2	1:Ca:199:ARG:HE	1.81	0.46
1:Cg:76:LYS:CE	1:Ci:179:GLU:OE2	2.64	0.46
1:Ag:170:GLU:HG2	1:Ag:199:ARG:HE	1.81	0.46
1:Am:214:ARG:HH21	1:Bu:246:GLU:CD	2.23	0.46
1:As:170:GLU:HG2	1:As:199:ARG:HE	1.81	0.46
1:Aw:170:GLU:HG2	1:Aw:199:ARG:HE	1.81	0.46
1:Ce:170:GLU:HG2	1:Ce:199:ARG:HE	1.81	0.46
1:Ae:227:LEU:CD2	2:Af:3:U:H2'	2.46	0.46
1:Ak:76:LYS:CE	1:Am:179:GLU:OE2	2.64	0.46
1:Au:214:ARG:HH21	1:Cc:246:GLU:CD	2.24	0.46
1:Ac:170:GLU:HG2	1:Ac:199:ARG:HE	1.81	0.46
1:Ai:170:GLU:HG2	1:Ai:199:ARG:HE	1.81	0.46
1:Ao:221:GLN:OE1	1:Bw:250:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:170:GLU:HG2	1:Bi:199:ARG:HE	1.81	0.46
1:Bk:76:LYS:CE	1:Bm:179:GLU:OE2	2.64	0.46
1:Bm:170:GLU:HG2	1:Bm:199:ARG:HE	1.81	0.46
1:Aa:76:LYS:CE	1:Ac:179:GLU:OE2	2.64	0.46
1:As:76:LYS:CE	1:Au:179:GLU:OE2	2.64	0.46
1:Ay:170:GLU:HG2	1:Ay:199:ARG:HE	1.81	0.46
1:Ba:76:LYS:CE	1:Bc:179:GLU:OE2	2.64	0.46
1:Bo:170:GLU:HG2	1:Bo:199:ARG:HE	1.81	0.46
1:Bq:130:ILE:HG22	2:Br:5:U:H1'	1.98	0.46
1:Aa:130:ILE:HG22	2:Ab:5:U:H1'	1.98	0.46
1:Ag:130:ILE:HG22	2:Ah:5:U:H1'	1.98	0.46
1:Ak:221:GLN:OE1	1:Bs:250:ARG:HD3	2.15	0.46
1:Am:170:GLU:HG2	1:Am:199:ARG:HE	1.81	0.46
1:Bc:170:GLU:HG2	1:Bc:199:ARG:HE	1.81	0.46
1:Bs:170:GLU:HG2	1:Bs:199:ARG:HE	1.81	0.46
1:Cc:76:LYS:CE	1:Ce:179:GLU:OE2	2.64	0.46
1:Ci:170:GLU:HG2	1:Ci:199:ARG:HE	1.81	0.46
1:Cm:76:LYS:CE	1:Co:179:GLU:OE2	2.64	0.46
1:Cm:170:GLU:HG2	1:Cm:199:ARG:HE	1.81	0.46
1:Ay:214:ARG:HH21	1:Cg:246:GLU:CD	2.23	0.45
1:Bc:76:LYS:CE	1:Be:179:GLU:OE2	2.64	0.45
1:Bg:221:GLN:OE1	1:Co:250:ARG:HD3	2.15	0.45
1:Bs:76:LYS:CE	1:Bu:179:GLU:OE2	2.64	0.45
1:Bu:47:PRO:O	1:Co:145:TYR:OH	2.31	0.45
1:Bu:76:LYS:CE	1:Bw:179:GLU:OE2	2.64	0.45
2:Bj:1:U:P	1:Bk:185:ARG:HH12	2.39	0.45
1:Bw:170:GLU:HG2	1:Bw:199:ARG:HE	1.81	0.45
1:Ai:76:LYS:CE	1:Ak:179:GLU:OE2	2.64	0.45
1:Bk:214:ARG:HH21	1:Cs:246:GLU:CD	2.24	0.45
1:By:170:GLU:HG2	1:By:199:ARG:HE	1.81	0.45
1:Ck:130:ILE:HG22	2:Cl:5:U:H1'	1.98	0.45
1:Aa:170:GLU:HG2	1:Aa:199:ARG:HE	1.81	0.45
1:Aq:76:LYS:CE	1:As:179:GLU:OE2	2.64	0.45
1:Aw:221:GLN:OE1	1:Ce:250:ARG:HD3	2.16	0.45
1:Bk:170:GLU:HG2	1:Bk:199:ARG:HE	1.81	0.45
1:Bg:170:GLU:HG2	1:Bg:199:ARG:HE	1.81	0.45
1:Bi:76:LYS:CE	1:Bk:179:GLU:OE2	2.64	0.45
1:Ae:130:ILE:HG22	2:Af:5:U:H1'	1.99	0.45
1:Ae:170:GLU:HG2	1:Ae:199:ARG:HE	1.81	0.45
1:Aq:221:GLN:OE1	1:By:250:ARG:HD3	2.16	0.45
1:Aa:214:ARG:HH21	1:Bi:246:GLU:CD	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cc:170:GLU:HG2	1:Cc:199:ARG:HE	1.81	0.45
1:Ck:76:LYS:CE	1:Cm:179:GLU:OE2	2.64	0.45
1:Aq:47:PRO:O	1:Bk:145:TYR:OH	2.31	0.45
1:Ca:76:LYS:CE	1:Cc:179:GLU:OE2	2.64	0.45
1:Ci:76:LYS:CE	1:Ck:179:GLU:OE2	2.65	0.45
1:Co:170:GLU:HG2	1:Co:199:ARG:HE	1.81	0.45
1:Cs:130:ILE:CG2	2:Ct:5:U:H1'	2.47	0.45
1:Ak:170:GLU:HG2	1:Ak:199:ARG:HE	1.81	0.45
1:As:214:ARG:HH21	1:Ca:246:GLU:CD	2.25	0.45
1:Bq:76:LYS:CE	1:Bs:179:GLU:OE2	2.65	0.45
1:Cg:170:GLU:HG2	1:Cg:199:ARG:HE	1.81	0.45
1:Cs:170:GLU:HG2	1:Cs:199:ARG:HE	1.81	0.45
1:Ba:170:GLU:HG2	1:Ba:199:ARG:HE	1.81	0.44
1:Bg:76:LYS:CE	1:Bi:179:GLU:OE2	2.66	0.44
1:Bq:170:GLU:HG2	1:Bq:199:ARG:HE	1.81	0.44
1:Ao:76:LYS:CE	1:Aq:179:GLU:OE2	2.66	0.44
1:By:76:LYS:CE	1:Ca:179:GLU:OE2	2.66	0.44
1:Ai:47:PRO:O	1:Bc:145:TYR:OH	2.31	0.44
1:Aq:170:GLU:HG2	1:Aq:199:ARG:HE	1.81	0.44
1:Au:160:GLN:HE21	2:Av:2:U:P	2.40	0.44
1:Au:170:GLU:HG2	1:Au:199:ARG:HE	1.81	0.44
1:Cq:76:LYS:CE	1:Cs:179:GLU:OE2	2.66	0.44
1:Bs:130:ILE:HG22	2:Bt:5:U:H1'	1.98	0.44
1:Co:130:ILE:HG22	2:Cp:5:U:H1'	1.99	0.44
1:As:47:PRO:O	1:Bm:145:TYR:OH	2.32	0.44
1:Ay:76:LYS:CE	1:Ba:179:GLU:OE2	2.65	0.44
1:Bw:76:LYS:CE	1:By:179:GLU:OE2	2.65	0.44
1:Co:76:LYS:CE	1:Cq:179:GLU:OE2	2.65	0.44
1:Am:76:LYS:CE	1:Ao:179:GLU:OE2	2.65	0.44
1:Ag:76:LYS:CE	1:Ai:179:GLU:OE2	2.65	0.44
1:Au:76:LYS:CE	1:Aw:179:GLU:OE2	2.66	0.44
1:Be:76:LYS:CE	1:Bg:179:GLU:OE2	2.65	0.43
1:Bq:47:PRO:O	1:Ck:145:TYR:OH	2.32	0.43
1:Ac:76:LYS:CE	1:Ae:179:GLU:OE2	2.66	0.43
1:Ai:127:SER:O	1:Ai:130:ILE:HG12	2.19	0.43
1:Bc:47:PRO:O	1:Bw:145:TYR:OH	2.31	0.43
1:Bm:76:LYS:CE	1:Bo:179:GLU:OE2	2.66	0.43
1:Ca:127:SER:O	1:Ca:130:ILE:HG12	2.19	0.43
1:Ce:76:LYS:CE	1:Cg:179:GLU:OE2	2.66	0.43
1:Am:127:SER:O	1:Am:130:ILE:HG12	2.19	0.43
1:Au:127:SER:O	1:Au:130:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:130:ILE:HG22	2:Av:5:U:H1'	2.01	0.43
1:Aw:127:SER:O	1:Aw:130:ILE:HG12	2.19	0.43
1:Bc:127:SER:O	1:Bc:130:ILE:HG12	2.19	0.43
1:Bg:262:HIS:NE2	1:Bi:254:THR:O	2.44	0.43
1:Bk:127:SER:O	1:Bk:130:ILE:HG12	2.19	0.43
1:Bq:127:SER:O	1:Bq:130:ILE:HG12	2.19	0.43
1:Bu:127:SER:O	1:Bu:130:ILE:HG12	2.19	0.43
1:Cc:127:SER:O	1:Cc:130:ILE:HG12	2.19	0.43
1:Ck:127:SER:O	1:Ck:130:ILE:HG12	2.19	0.43
1:Cs:159:ARG:NH2	2:Ct:4:U:H2'	2.34	0.43
1:As:127:SER:O	1:As:130:ILE:HG12	2.19	0.43
1:Bm:47:PRO:O	1:Cg:145:TYR:OH	2.33	0.43
1:Bo:127:SER:O	1:Bo:130:ILE:HG12	2.19	0.43
1:Bs:127:SER:O	1:Bs:130:ILE:HG12	2.19	0.43
1:Ck:113:ILE:HD13	1:Ck:113:ILE:HA	1.81	0.43
1:Aa:127:SER:O	1:Aa:130:ILE:HG12	2.19	0.43
2:Af:1:U:P	2:Ah:5:U:O3'	2.77	0.43
1:Ak:127:SER:O	1:Ak:130:ILE:HG12	2.19	0.43
1:Be:127:SER:O	1:Be:130:ILE:HG12	2.19	0.43
1:Cq:127:SER:O	1:Cq:130:ILE:HG12	2.19	0.43
1:Cs:127:SER:O	1:Cs:130:ILE:HG12	2.19	0.43
1:Bi:127:SER:O	1:Bi:130:ILE:HG12	2.19	0.43
1:Bo:47:PRO:O	1:Ci:145:TYR:OH	2.31	0.43
1:Ac:127:SER:O	1:Ac:130:ILE:HG12	2.19	0.43
1:Ae:127:SER:O	1:Ae:130:ILE:HG12	2.19	0.43
1:Ag:127:SER:O	1:Ag:130:ILE:HG12	2.19	0.43
1:Am:47:PRO:O	1:Bg:145:TYR:OH	2.34	0.43
1:Bi:203:ASP:HB2	2:Bj:4:U:O2	2.19	0.43
2:Bx:1:U:P	2:Bz:5:U:O3'	2.76	0.43
1:Ce:127:SER:O	1:Ce:130:ILE:HG12	2.19	0.43
1:Ci:127:SER:O	1:Ci:130:ILE:HG12	2.19	0.43
1:Cm:127:SER:O	1:Cm:130:ILE:HG12	2.19	0.43
1:Ao:127:SER:O	1:Ao:130:ILE:HG12	2.19	0.43
1:Ao:262:HIS:NE2	1:Aq:254:THR:O	2.44	0.43
1:Bg:127:SER:O	1:Bg:130:ILE:HG12	2.19	0.43
1:Bm:127:SER:O	1:Bm:130:ILE:HG12	2.19	0.43
1:Bw:130:ILE:HG22	2:Bx:5:U:H1'	2.00	0.43
1:Ca:160:GLN:NE2	2:Cb:1:U:O3'	2.51	0.42
1:Ai:255:ASP:OD1	1:Ai:261:HIS:ND1	2.53	0.42
1:Ba:113:ILE:HD13	1:Ba:113:ILE:HA	1.82	0.42
1:Bq:255:ASP:OD1	1:Bq:261:HIS:ND1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:By:127:SER:O	1:By:130:ILE:HG12	2.19	0.42
1:Cc:113:ILE:HD13	1:Cc:113:ILE:HA	1.81	0.42
1:Cg:255:ASP:OD1	1:Cg:261:HIS:ND1	2.52	0.42
1:Aa:47:PRO:O	1:Au:145:TYR:OH	2.31	0.42
1:Ay:127:SER:O	1:Ay:130:ILE:HG12	2.19	0.42
1:Ba:127:SER:O	1:Ba:130:ILE:HG12	2.19	0.42
1:Ba:255:ASP:OD1	1:Ba:261:HIS:ND1	2.53	0.42
1:Bg:255:ASP:OD1	1:Bg:261:HIS:ND1	2.53	0.42
1:Ca:255:ASP:OD1	1:Ca:261:HIS:ND1	2.53	0.42
1:Co:127:SER:O	1:Co:130:ILE:HG12	2.19	0.42
1:Ae:255:ASP:OD1	1:Ae:261:HIS:ND1	2.53	0.42
1:As:255:ASP:OD1	1:As:261:HIS:ND1	2.53	0.42
1:Ay:255:ASP:OD1	1:Ay:261:HIS:ND1	2.53	0.42
1:Cs:255:ASP:OD1	1:Cs:261:HIS:ND1	2.53	0.42
2:An:1:U:P	1:Ao:185:ARG:HH12	2.42	0.42
1:Ao:255:ASP:OD1	1:Ao:261:HIS:ND1	2.53	0.42
1:Bq:113:ILE:HD13	1:Bq:113:ILE:HA	1.82	0.42
1:Co:255:ASP:OD1	1:Co:261:HIS:ND1	2.53	0.42
1:Bk:227:LEU:HD22	2:Bl:3:U:H2'	2.00	0.42
1:Bk:255:ASP:OD1	1:Bk:261:HIS:ND1	2.53	0.42
1:Bu:255:ASP:OD1	1:Bu:261:HIS:ND1	2.53	0.42
1:Bw:127:SER:O	1:Bw:130:ILE:HG12	2.19	0.42
1:Ca:76:LYS:NZ	1:Cc:175:MET:HE3	2.35	0.42
1:Cg:127:SER:O	1:Cg:130:ILE:HG12	2.19	0.42
1:Ci:78:LYS:HB3	1:Ci:78:LYS:HE2	1.95	0.42
2:Aj:1:U:C4	2:Al:5:U:C4	3.08	0.42
1:Aq:127:SER:O	1:Aq:130:ILE:HG12	2.19	0.42
1:Au:255:ASP:OD1	1:Au:261:HIS:ND1	2.53	0.42
1:Bc:113:ILE:HD13	1:Bc:113:ILE:HA	1.82	0.42
1:Bk:232:THR:HG23	1:Cc:246:GLU:HG3	2.02	0.42
1:Bw:255:ASP:OD1	1:Bw:261:HIS:ND1	2.53	0.42
1:Ci:255:ASP:OD1	1:Ci:261:HIS:ND1	2.53	0.42
1:Ac:255:ASP:OD1	1:Ac:261:HIS:ND1	2.53	0.42
1:Ak:232:THR:HG23	1:Bc:246:GLU:HG3	2.02	0.42
1:Aq:255:ASP:OD1	1:Aq:261:HIS:ND1	2.53	0.42
1:Ck:255:ASP:OD1	1:Ck:261:HIS:ND1	2.52	0.42
1:Bi:255:ASP:OD1	1:Bi:261:HIS:ND1	2.53	0.42
1:Bo:160:GLN:HE21	2:Bp:2:U:P	2.42	0.42
1:Bo:255:ASP:OD1	1:Bo:261:HIS:ND1	2.53	0.42
1:By:255:ASP:OD1	1:By:261:HIS:ND1	2.53	0.42
1:Cq:255:ASP:OD1	1:Cq:261:HIS:ND1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:255:ASP:OD1	1:Am:261:HIS:ND1	2.53	0.42
1:Bu:113:ILE:HD13	1:Bu:113:ILE:HA	1.82	0.42
1:Ca:232:THR:HG23	1:Cs:246:GLU:HG3	2.02	0.42
1:Aa:255:ASP:OD1	1:Aa:261:HIS:ND1	2.53	0.41
1:Aw:47:PRO:O	1:Bq:145:TYR:OH	2.31	0.41
1:Bo:78:LYS:HB3	1:Bo:78:LYS:HE2	1.95	0.41
2:Bt:1:U:P	2:Bv:5:U:O3'	2.78	0.41
1:Ce:255:ASP:OD1	1:Ce:261:HIS:ND1	2.53	0.41
1:Ak:113:ILE:HD13	1:Ak:113:ILE:HA	1.82	0.41
1:Au:47:PRO:O	1:Bo:145:TYR:OH	2.33	0.41
1:Bg:47:PRO:O	1:Ca:145:TYR:OH	2.33	0.41
1:By:113:ILE:HD13	1:By:113:ILE:HA	1.81	0.41
1:Ag:255:ASP:OD1	1:Ag:261:HIS:ND1	2.53	0.41
1:Ao:249:GLU:CD	1:Aq:251:HIS:HE2	2.28	0.41
1:Bc:255:ASP:OD1	1:Bc:261:HIS:ND1	2.53	0.41
1:Ca:113:ILE:HD13	1:Ca:113:ILE:HA	1.82	0.41
1:Cg:113:ILE:HD13	1:Cg:113:ILE:HA	1.81	0.41
1:Co:128:PRO:HG3	2:Cp:3:U:H5''	2.01	0.41
1:Aw:255:ASP:OD1	1:Aw:261:HIS:ND1	2.52	0.41
1:Bi:232:THR:HG23	1:Ca:246:GLU:HG3	2.02	0.41
1:Bm:255:ASP:OD1	1:Bm:261:HIS:ND1	2.53	0.41
1:Bo:232:THR:HG23	1:Cg:246:GLU:HG3	2.03	0.41
1:Cq:249:GLU:CD	1:Cs:251:HIS:HE2	2.27	0.41
1:Cs:78:LYS:HB3	1:Cs:78:LYS:HE2	1.95	0.41
1:Ak:255:ASP:OD1	1:Ak:261:HIS:ND1	2.53	0.41
1:Am:232:THR:HG23	1:Be:246:GLU:HG3	2.02	0.41
1:Ay:47:PRO:O	1:Bs:145:TYR:OH	2.32	0.41
1:Be:255:ASP:OD1	1:Be:261:HIS:ND1	2.53	0.41
1:Ca:203:ASP:HB2	2:Cb:4:U:O2	2.19	0.41
1:Cc:255:ASP:OD1	1:Cc:261:HIS:ND1	2.53	0.41
1:As:232:THR:HG23	1:Bk:246:GLU:HG3	2.02	0.41
1:Be:232:THR:HG23	1:Bw:246:GLU:HG3	2.03	0.41
1:Bq:76:LYS:NZ	1:Bs:175:MET:HE3	2.36	0.41
1:By:249:GLU:CD	1:Ca:251:HIS:HE2	2.28	0.41
1:Aq:232:THR:HG23	1:Bi:246:GLU:HG3	2.03	0.41
1:Ay:76:LYS:NZ	1:Ba:175:MET:HE3	2.36	0.41
1:Bi:76:LYS:NZ	1:Bk:175:MET:HE3	2.36	0.41
1:Bs:255:ASP:OD1	1:Bs:261:HIS:ND1	2.53	0.41
1:Bu:232:THR:HG23	1:Cm:246:GLU:HG3	2.03	0.41
1:Cm:255:ASP:OD1	1:Cm:261:HIS:ND1	2.53	0.41
1:Ai:232:THR:HG23	1:Ba:246:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:232:THR:HG23	1:Bg:246:GLU:HG3	2.03	0.41
1:Au:232:THR:HG23	1:Bm:246:GLU:HG3	2.03	0.41
1:Bg:249:GLU:CD	1:Bi:251:HIS:HE2	2.28	0.41
1:Bi:227:LEU:HD22	2:Bj:3:U:H2'	2.03	0.41
1:Bs:76:LYS:NZ	1:Bu:175:MET:HE3	2.36	0.41
1:Aa:232:THR:HG23	1:As:246:GLU:HG3	2.03	0.41
1:Ag:76:LYS:NZ	1:Ai:175:MET:HE3	2.36	0.41
1:Ag:113:ILE:HD13	1:Ag:113:ILE:HA	1.82	0.41
1:Aq:76:LYS:NZ	1:As:175:MET:HE3	2.36	0.41
1:Aq:210:THR:HB	1:Bi:152:ASP:OD1	2.21	0.41
1:Be:128:PRO:HG3	2:Bf:3:U:H5''	2.02	0.41
1:Bi:159:ARG:NH2	2:Bj:4:U:H2'	2.36	0.41
1:By:47:PRO:O	1:Cs:145:TYR:OH	2.33	0.41
1:By:78:LYS:HB3	1:By:78:LYS:HE2	1.95	0.41
1:Ck:76:LYS:NZ	1:Cm:175:MET:HE3	2.36	0.41
1:Ag:232:THR:HG23	1:Ay:246:GLU:HG3	2.03	0.41
1:Bm:232:THR:HG23	1:Ce:246:GLU:HG3	2.02	0.41
1:Bq:232:THR:HG23	1:Ci:246:GLU:HG3	2.02	0.41
1:Bw:232:THR:HG23	1:Co:246:GLU:HG3	2.03	0.41
1:Ci:76:LYS:NZ	1:Ck:175:MET:HE3	2.36	0.41
1:Ag:249:GLU:CD	1:Ai:251:HIS:HE2	2.29	0.40
1:Ai:113:ILE:HA	1:Ai:113:ILE:HD13	1.81	0.40
1:Am:80:VAL:HB	1:Am:86:ARG:NH1	2.37	0.40
1:As:227:LEU:CD2	2:At:3:U:H2'	2.51	0.40
1:Ba:76:LYS:NZ	1:Bc:175:MET:HE3	2.36	0.40
1:Bq:249:GLU:CD	1:Bs:251:HIS:HE2	2.29	0.40
1:Ac:262:HIS:NE2	1:Ae:254:THR:O	2.48	0.40
1:Ak:76:LYS:CD	1:Am:179:GLU:OE2	2.70	0.40
1:Am:129:ASP:HB2	2:An:5:U:C4	2.56	0.40
1:Ao:78:LYS:HB3	1:Ao:78:LYS:HE2	1.95	0.40
1:Aw:210:THR:HB	1:Bo:152:ASP:OD1	2.22	0.40
1:Ay:262:HIS:NE2	1:Ba:254:THR:O	2.46	0.40
1:Bc:80:VAL:HB	1:Bc:86:ARG:NH1	2.37	0.40
1:Bs:232:THR:HG23	1:Ck:246:GLU:HG3	2.03	0.40
1:Bu:76:LYS:CD	1:Bw:179:GLU:OE2	2.70	0.40
1:By:232:THR:HG23	1:Cq:246:GLU:HG3	2.03	0.40
1:Ae:232:THR:HG23	1:Aw:246:GLU:HG3	2.04	0.40
1:Ai:130:ILE:HG22	2:Aj:5:U:H1'	2.02	0.40
1:Am:130:ILE:HA	2:An:5:U:O2	2.22	0.40
1:Aq:56:LEU:HD21	1:As:171:ALA:HB2	2.04	0.40
1:Be:78:LYS:HB3	1:Be:78:LYS:HE2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:80:VAL:HB	1:Be:86:ARG:NH1	2.37	0.40
1:Bm:113:ILE:HA	1:Bm:113:ILE:HD13	1.82	0.40
1:Bs:113:ILE:HA	1:Bs:113:ILE:HD13	1.81	0.40
1:Bw:47:PRO:O	1:Cq:145:TYR:OH	2.32	0.40
1:Cc:80:VAL:HB	1:Cc:86:ARG:NH1	2.37	0.40
2:Ch:1:U:P	2:Cj:5:U:O3'	2.80	0.40
1:Cs:80:VAL:HB	1:Cs:86:ARG:NH1	2.37	0.40
1:Ag:80:VAL:HB	1:Ag:86:ARG:NH1	2.37	0.40
1:Ai:76:LYS:NZ	1:Ak:175:MET:HE3	2.36	0.40
1:Ai:76:LYS:CD	1:Ak:179:GLU:OE2	2.70	0.40
2:At:1:U:P	1:Au:185:ARG:HH12	2.43	0.40
1:Bm:80:VAL:HB	1:Bm:86:ARG:NH1	2.37	0.40
1:Bq:80:VAL:HB	1:Bq:86:ARG:NH1	2.36	0.40
1:Bs:76:LYS:CD	1:Bu:179:GLU:OE2	2.70	0.40
1:Ce:80:VAL:HB	1:Ce:86:ARG:NH1	2.37	0.40
1:Ag:262:HIS:NE2	1:Ai:254:THR:O	2.46	0.40
1:Ao:80:VAL:HB	1:Ao:86:ARG:NH1	2.37	0.40
1:Aq:78:LYS:HB3	1:Aq:78:LYS:HE2	1.95	0.40
1:As:78:LYS:HB3	1:As:78:LYS:HE2	1.95	0.40
1:Au:210:THR:HB	1:Bm:152:ASP:OD1	2.22	0.40
1:Ay:210:THR:HB	1:Bq:152:ASP:OD1	2.22	0.40
1:Ay:232:THR:HG23	1:Bq:246:GLU:HG3	2.03	0.40
1:Be:76:LYS:NZ	1:Bg:175:MET:HE3	2.37	0.40
1:Bg:232:THR:HG23	1:By:246:GLU:HG3	2.03	0.40
1:Bs:80:VAL:HB	1:Bs:86:ARG:NH1	2.36	0.40
1:Bu:80:VAL:HB	1:Bu:86:ARG:NH1	2.37	0.40
1:By:76:LYS:NZ	1:Ca:175:MET:HE3	2.37	0.40
1:Ca:262:HIS:NE2	1:Cc:254:THR:O	2.47	0.40
1:Ck:76:LYS:CD	1:Cm:179:GLU:OE2	2.70	0.40
1:Cm:76:LYS:CD	1:Co:179:GLU:OE2	2.70	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%)	218 (97%)	6 (3%)	0	100	100
1	Ac	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ae	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ag	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ai	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ak	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Am	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ao	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Aq	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	As	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Au	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Aw	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ay	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ba	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bc	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Be	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bg	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bi	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bk	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bm	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bo	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bq	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bs	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bu	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Bw	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	By	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ca	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Cc	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ce	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Cg	224/269 (83%)	218 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Ci	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Ck	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Cm	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Co	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Cq	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
1	Cs	224/269 (83%)	218 (97%)	6 (3%)	0	100	100
All	All	8064/9684 (83%)	7848 (97%)	216 (3%)	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%)	200 (100%)	0	100	100
1	Ac	200/233 (86%)	200 (100%)	0	100	100
1	Ae	200/233 (86%)	200 (100%)	0	100	100
1	Ag	200/233 (86%)	200 (100%)	0	100	100
1	Ai	200/233 (86%)	200 (100%)	0	100	100
1	Ak	200/233 (86%)	200 (100%)	0	100	100
1	Am	200/233 (86%)	200 (100%)	0	100	100
1	Ao	200/233 (86%)	200 (100%)	0	100	100
1	Aq	200/233 (86%)	200 (100%)	0	100	100
1	As	200/233 (86%)	200 (100%)	0	100	100
1	Au	200/233 (86%)	200 (100%)	0	100	100
1	Aw	200/233 (86%)	200 (100%)	0	100	100
1	Ay	200/233 (86%)	200 (100%)	0	100	100
1	Ba	200/233 (86%)	200 (100%)	0	100	100
1	Bc	200/233 (86%)	200 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Be	200/233 (86%)	200 (100%)	0	100	100
1	Bg	200/233 (86%)	200 (100%)	0	100	100
1	Bi	200/233 (86%)	200 (100%)	0	100	100
1	Bk	200/233 (86%)	200 (100%)	0	100	100
1	Bm	200/233 (86%)	200 (100%)	0	100	100
1	Bo	200/233 (86%)	200 (100%)	0	100	100
1	Bq	200/233 (86%)	200 (100%)	0	100	100
1	Bs	200/233 (86%)	200 (100%)	0	100	100
1	Bu	200/233 (86%)	200 (100%)	0	100	100
1	Bw	200/233 (86%)	200 (100%)	0	100	100
1	By	200/233 (86%)	200 (100%)	0	100	100
1	Ca	200/233 (86%)	200 (100%)	0	100	100
1	Cc	200/233 (86%)	200 (100%)	0	100	100
1	Ce	200/233 (86%)	200 (100%)	0	100	100
1	Cg	200/233 (86%)	200 (100%)	0	100	100
1	Ci	200/233 (86%)	200 (100%)	0	100	100
1	Ck	200/233 (86%)	200 (100%)	0	100	100
1	Cm	200/233 (86%)	200 (100%)	0	100	100
1	Co	200/233 (86%)	200 (100%)	0	100	100
1	Cq	200/233 (86%)	200 (100%)	0	100	100
1	Cs	200/233 (86%)	200 (100%)	0	100	100
All	All	7200/8388 (86%)	7200 (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 (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	153	HIS
1	Aa	229	ASN
1	Aa	251	HIS
1	Ac	153	HIS
1	Ac	229	ASN
1	Ae	153	HIS

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Mol	Chain	Res	Type
1	Ae	229	ASN
1	Ag	153	HIS
1	Ag	229	ASN
1	Ai	153	HIS
1	Ai	229	ASN
1	Ak	153	HIS
1	Ak	229	ASN
1	Am	153	HIS
1	Am	229	ASN
1	Ao	153	HIS
1	Ao	229	ASN
1	Aq	153	HIS
1	Aq	229	ASN
1	As	153	HIS
1	As	229	ASN
1	Au	153	HIS
1	Au	229	ASN
1	Aw	153	HIS
1	Aw	229	ASN
1	Ay	153	HIS
1	Ay	229	ASN
1	Ba	153	HIS
1	Ba	229	ASN
1	Bc	153	HIS
1	Bc	229	ASN
1	Be	153	HIS
1	Be	229	ASN
1	Bg	153	HIS
1	Bg	229	ASN
1	Bi	153	HIS
1	Bi	229	ASN
1	Bk	153	HIS
1	Bk	229	ASN
1	Bm	153	HIS
1	Bm	229	ASN
1	Bo	153	HIS
1	Bo	229	ASN
1	Bq	153	HIS
1	Bq	229	ASN
1	Bs	153	HIS
1	Bs	229	ASN
1	Bu	153	HIS

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Mol	Chain	Res	Type
1	Bu	229	ASN
1	Bw	153	HIS
1	Bw	229	ASN
1	By	153	HIS
1	By	229	ASN
1	Ca	153	HIS
1	Ca	229	ASN
1	Cc	153	HIS
1	Cc	229	ASN
1	Ce	153	HIS
1	Cg	153	HIS
1	Ci	153	HIS
1	Ck	153	HIS
1	Cm	153	HIS
1	Co	153	HIS
1	Cq	153	HIS
1	Cs	153	HIS

5.3.3 RNA ⓘ

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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
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 ⓘ

There are no chain breaks in this entry.

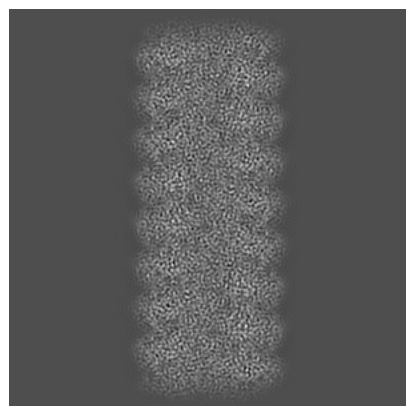
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53792. These allow visual inspection of the internal detail of the map and identification of artifacts.

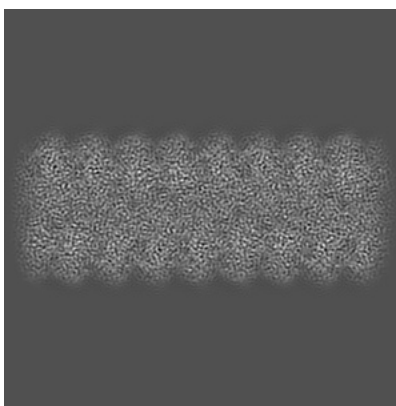
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

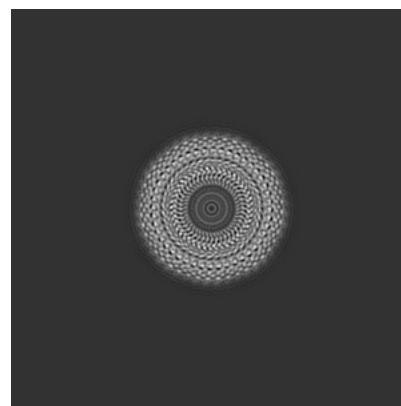
6.1.1 Primary map



X

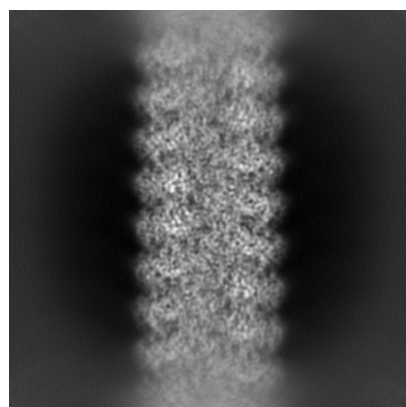


Y

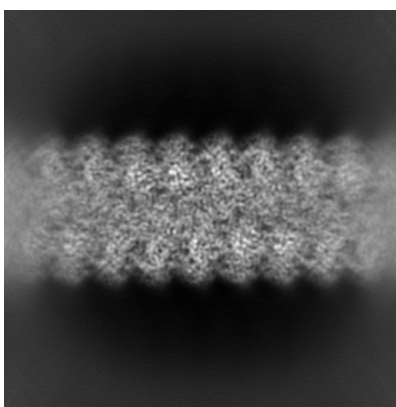


Z

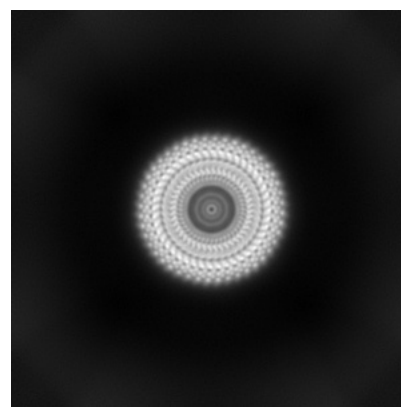
6.1.2 Raw map



X



Y

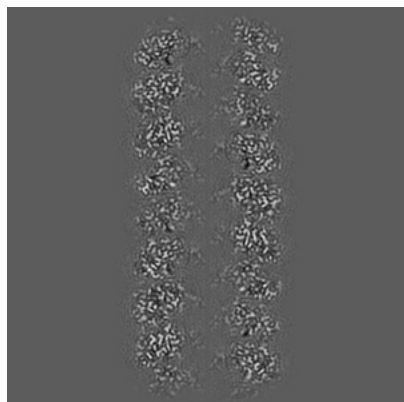


Z

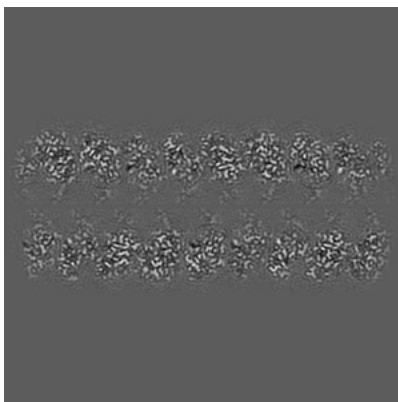
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

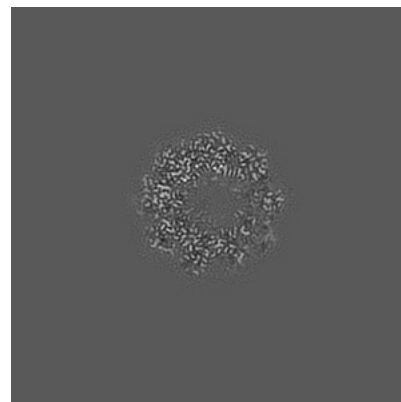
6.2.1 Primary map



X Index: 175

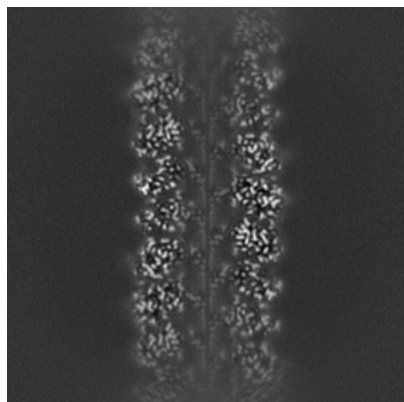


Y Index: 175

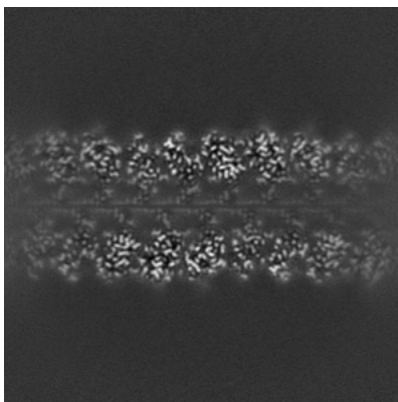


Z Index: 175

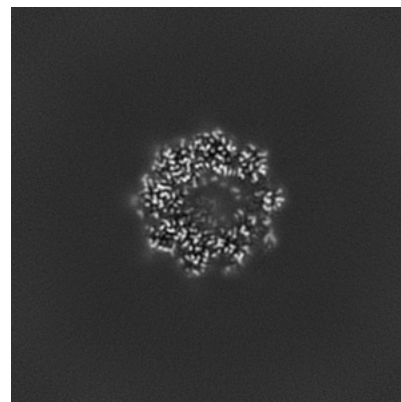
6.2.2 Raw map



X Index: 175



Y Index: 175

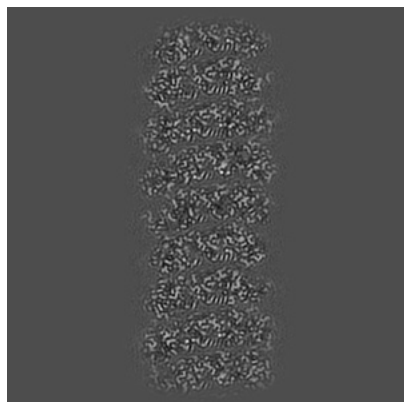


Z Index: 175

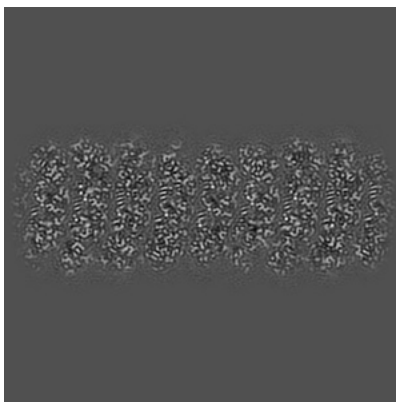
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

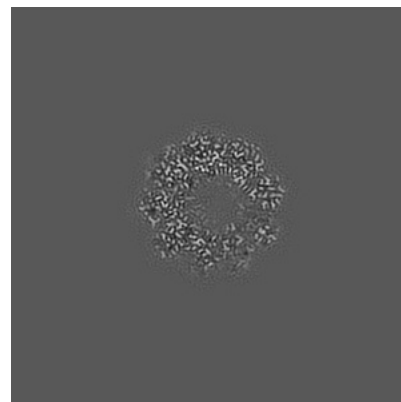
6.3.1 Primary map



X Index: 144

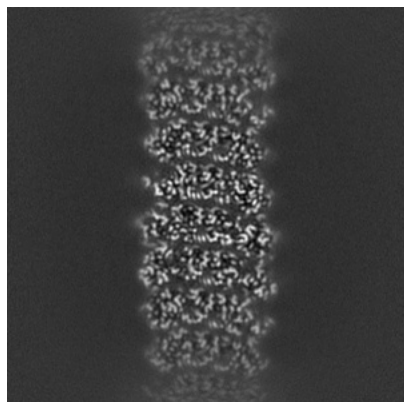


Y Index: 207

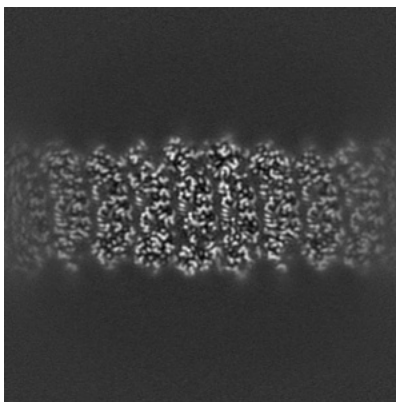


Z Index: 141

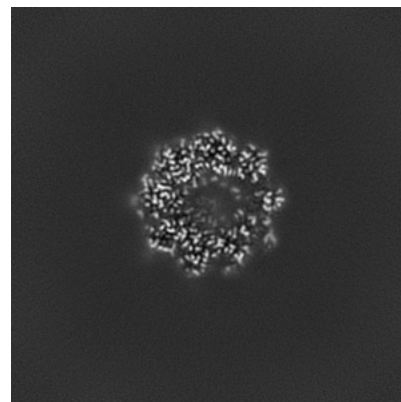
6.3.2 Raw map



X Index: 207



Y Index: 143

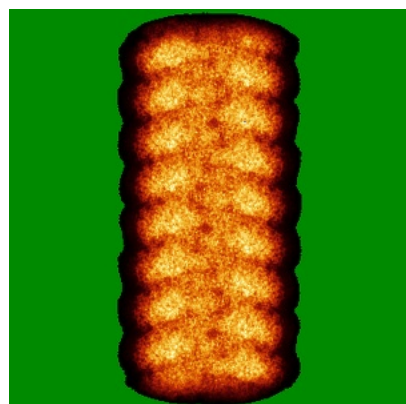


Z Index: 175

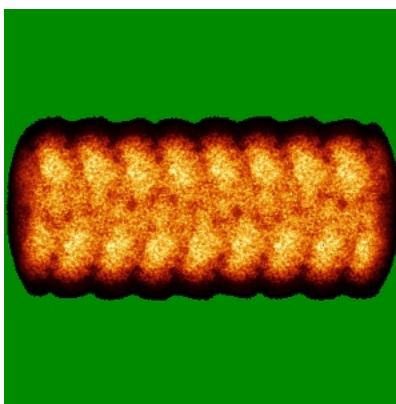
The images above show the largest variance slices of the map in three orthogonal directions.

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

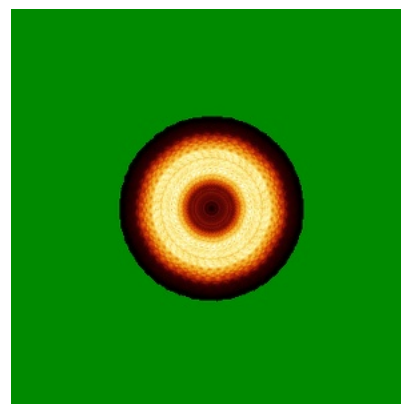
6.4.1 Primary map



X

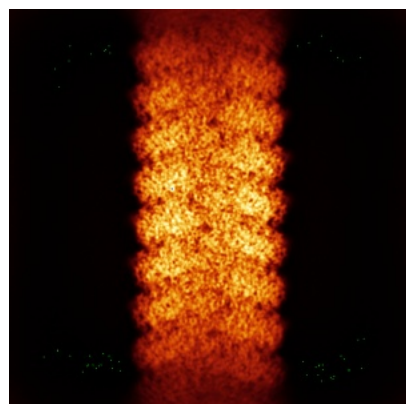


Y

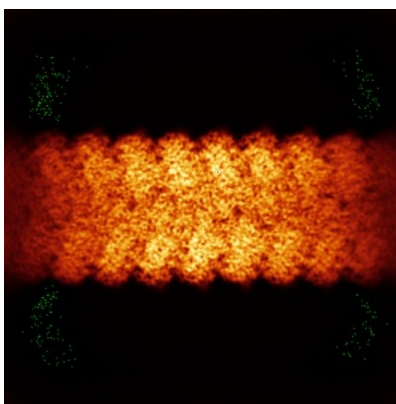


Z

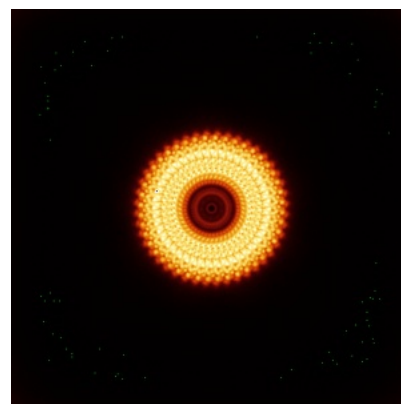
6.4.2 Raw map



X



Y

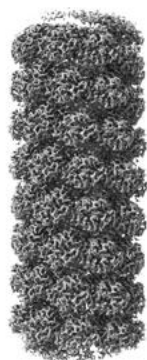


Z

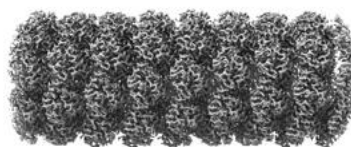
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

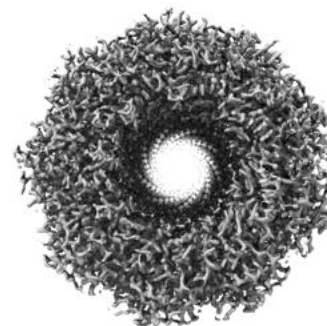
6.5.1 Primary map



X



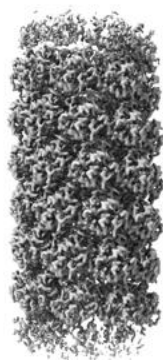
Y



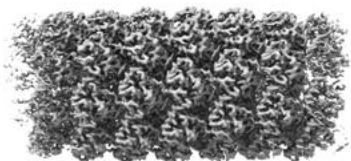
Z

The images above show the 3D surface view of the map at the recommended contour level 2.26. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

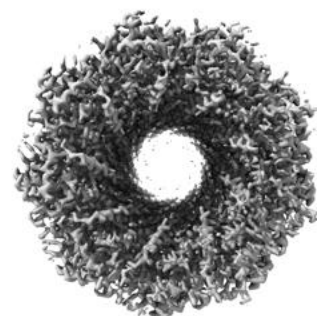
6.5.2 Raw map



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.

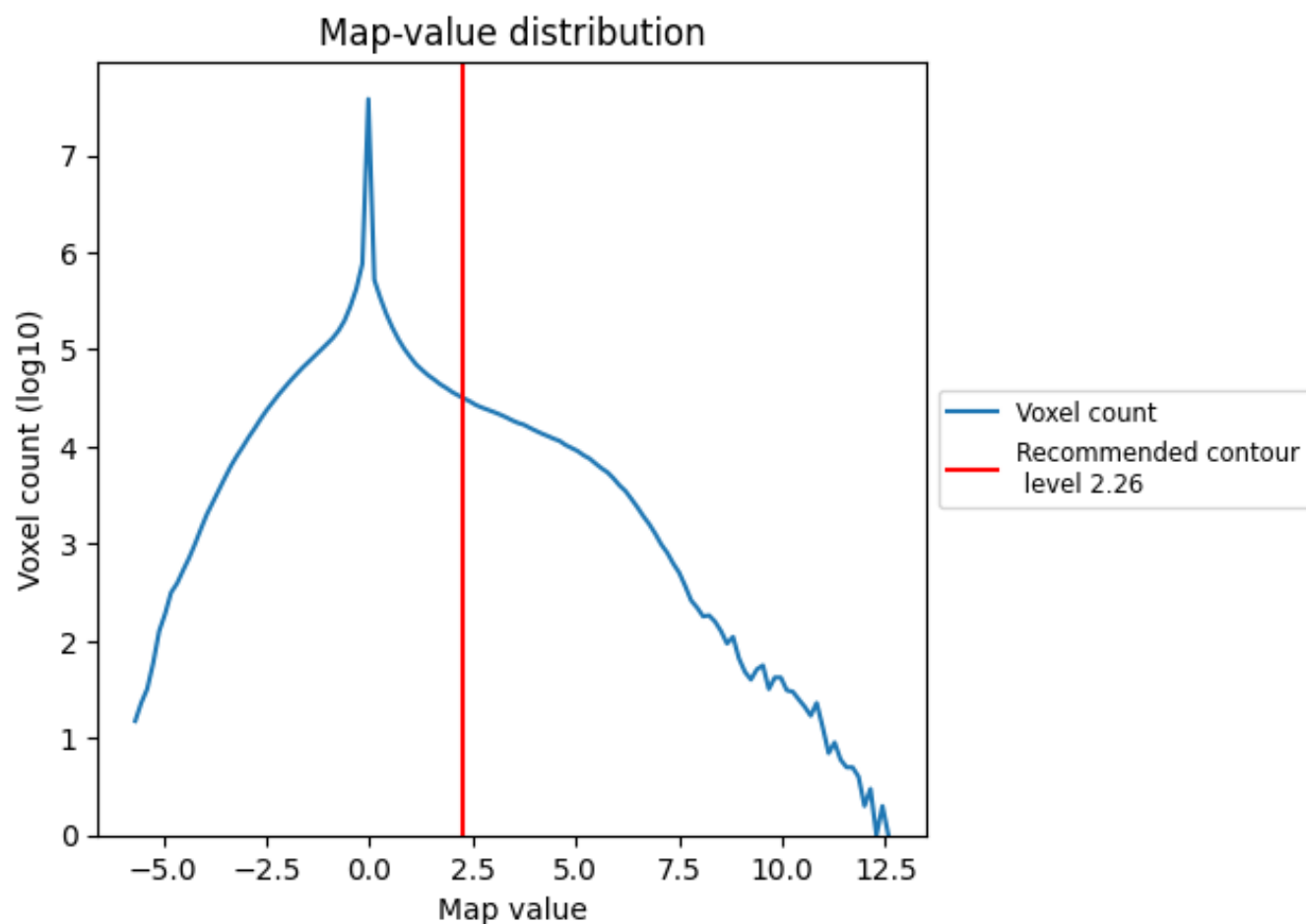
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

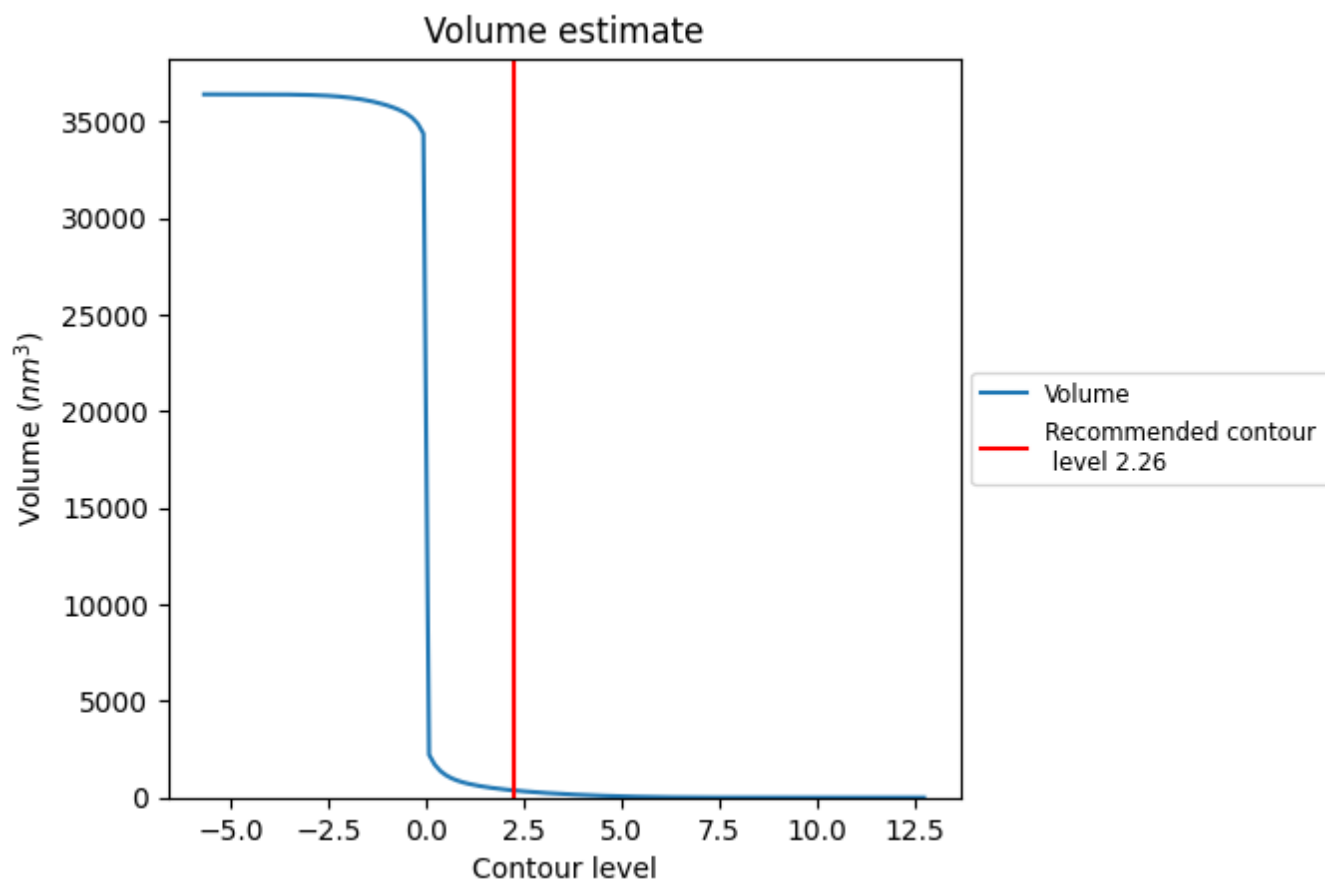
This section contains the results of statistical analysis of the map.

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.

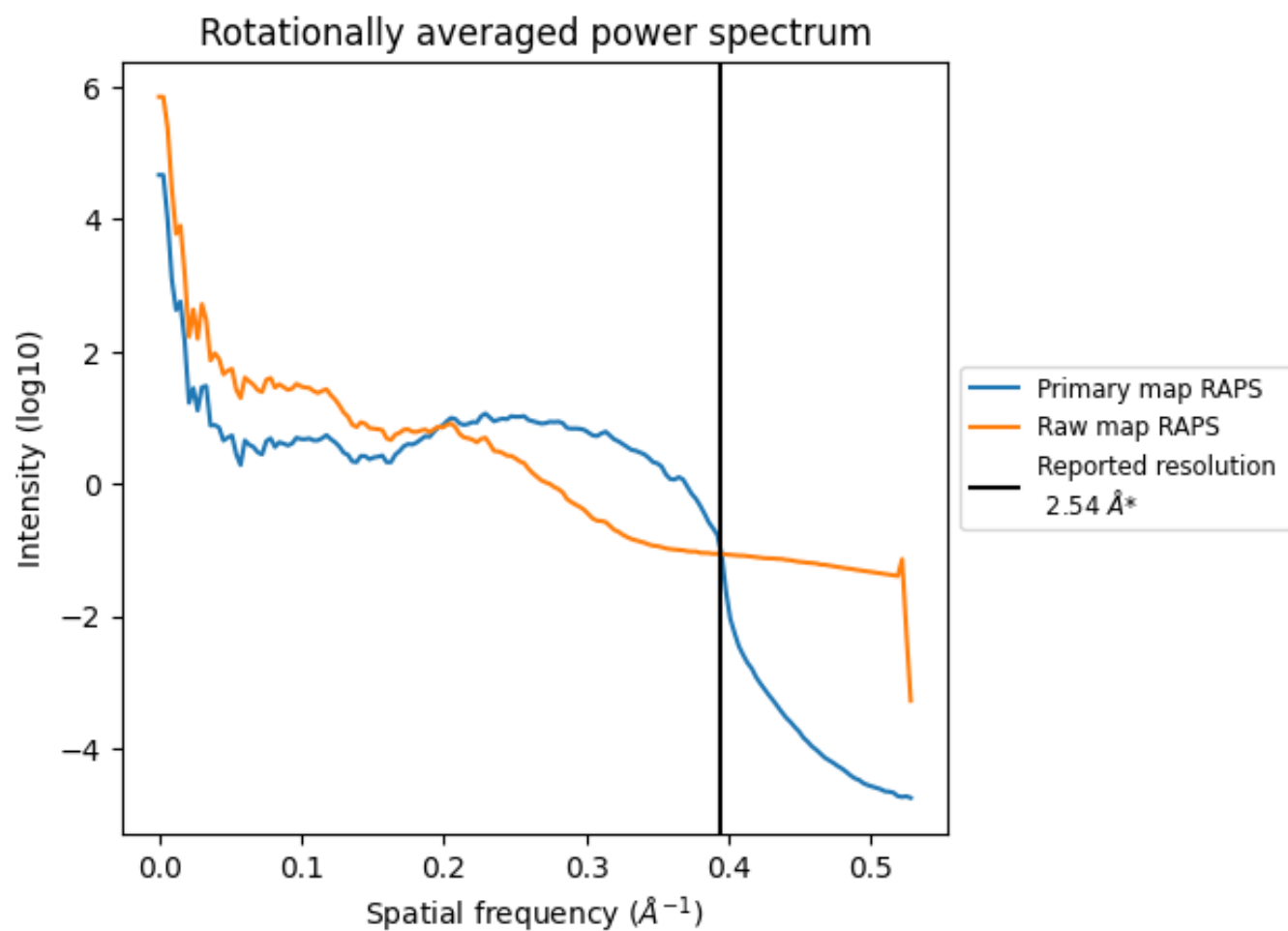
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 366 nm³; this corresponds to an approximate mass of 330 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 ⓘ

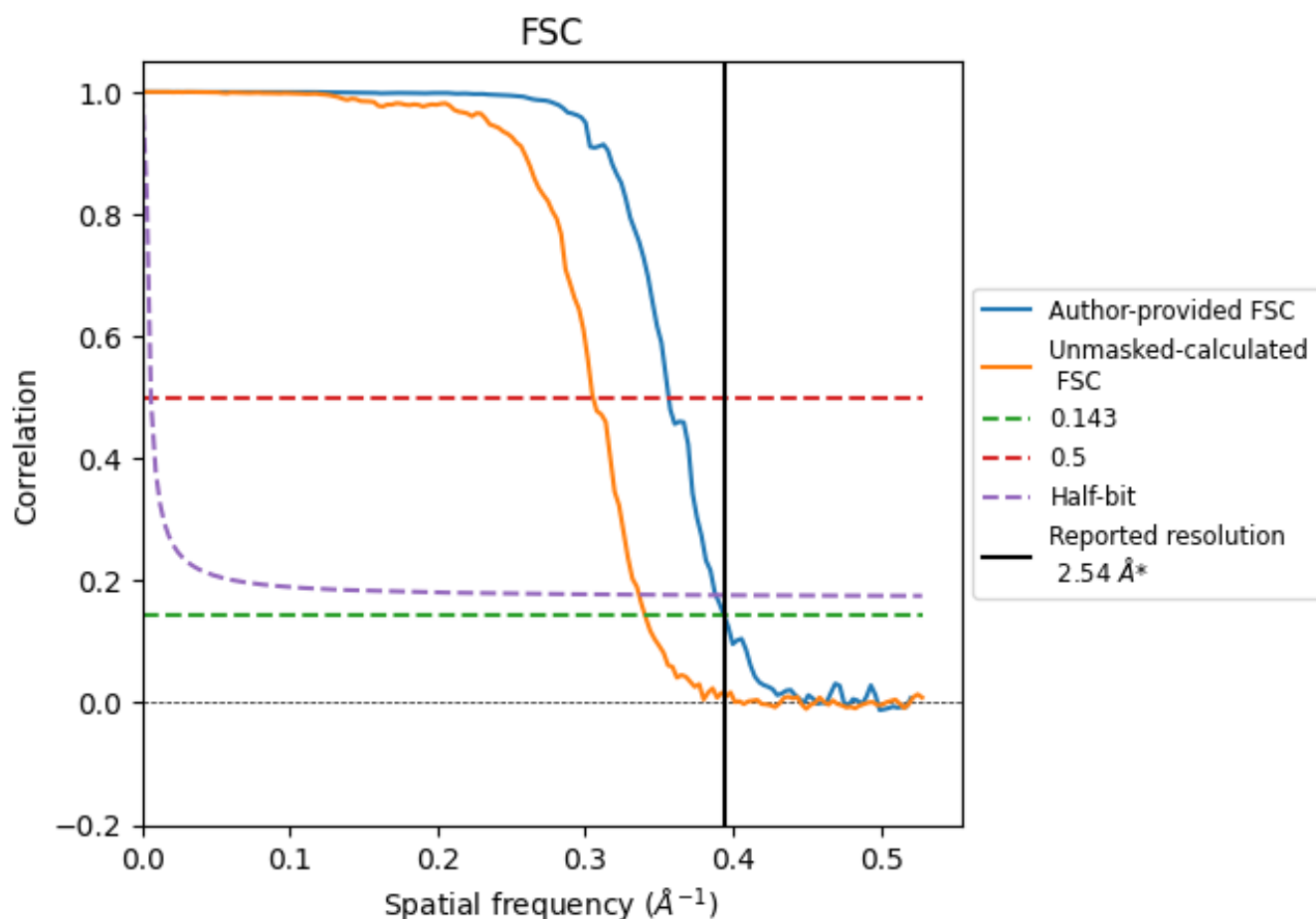


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

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 0.394 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

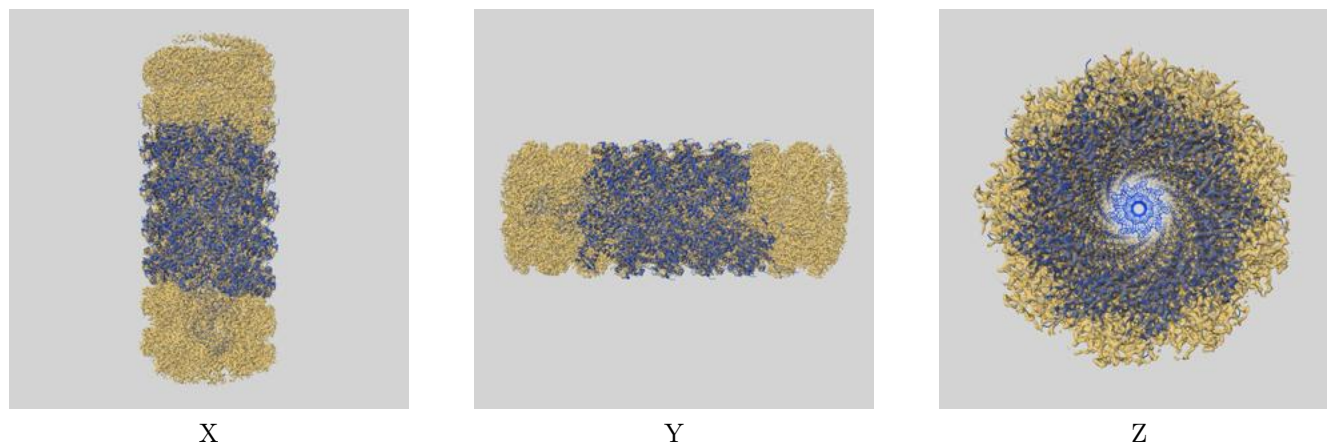
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.81	2.58
Unmasked-calculated*	2.94	3.28	2.97

*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 2.94 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

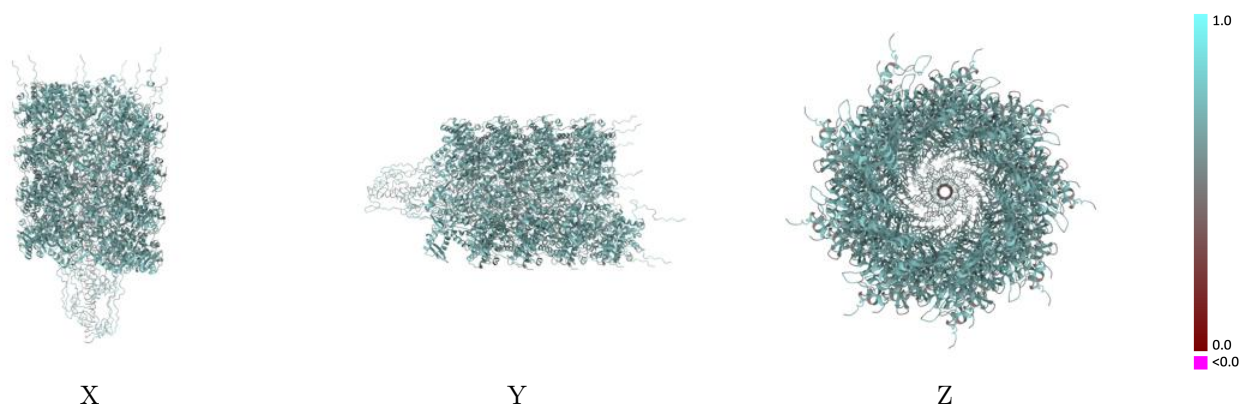
This section contains information regarding the fit between EMDB map EMD-53792 and PDB model 9R7T. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



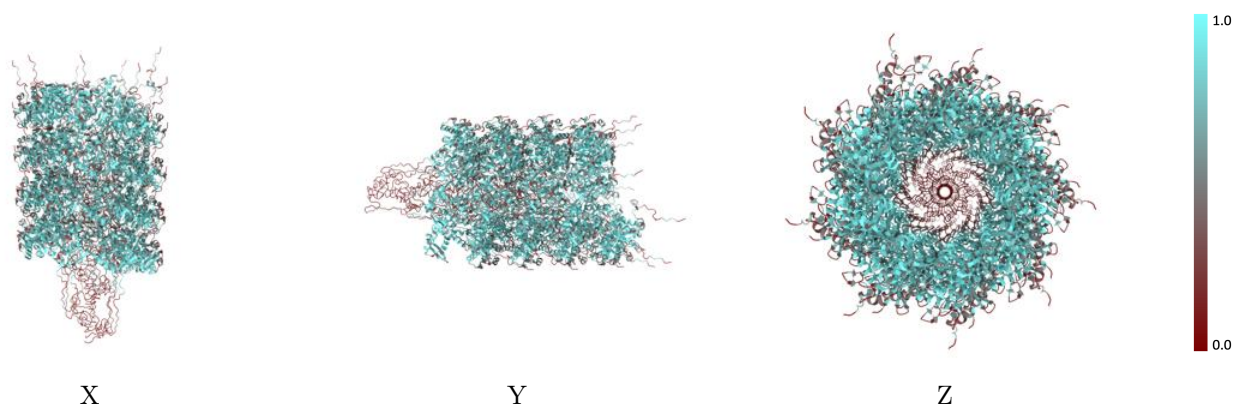
The images above show the 3D surface view of the map at the recommended contour level 2.26 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



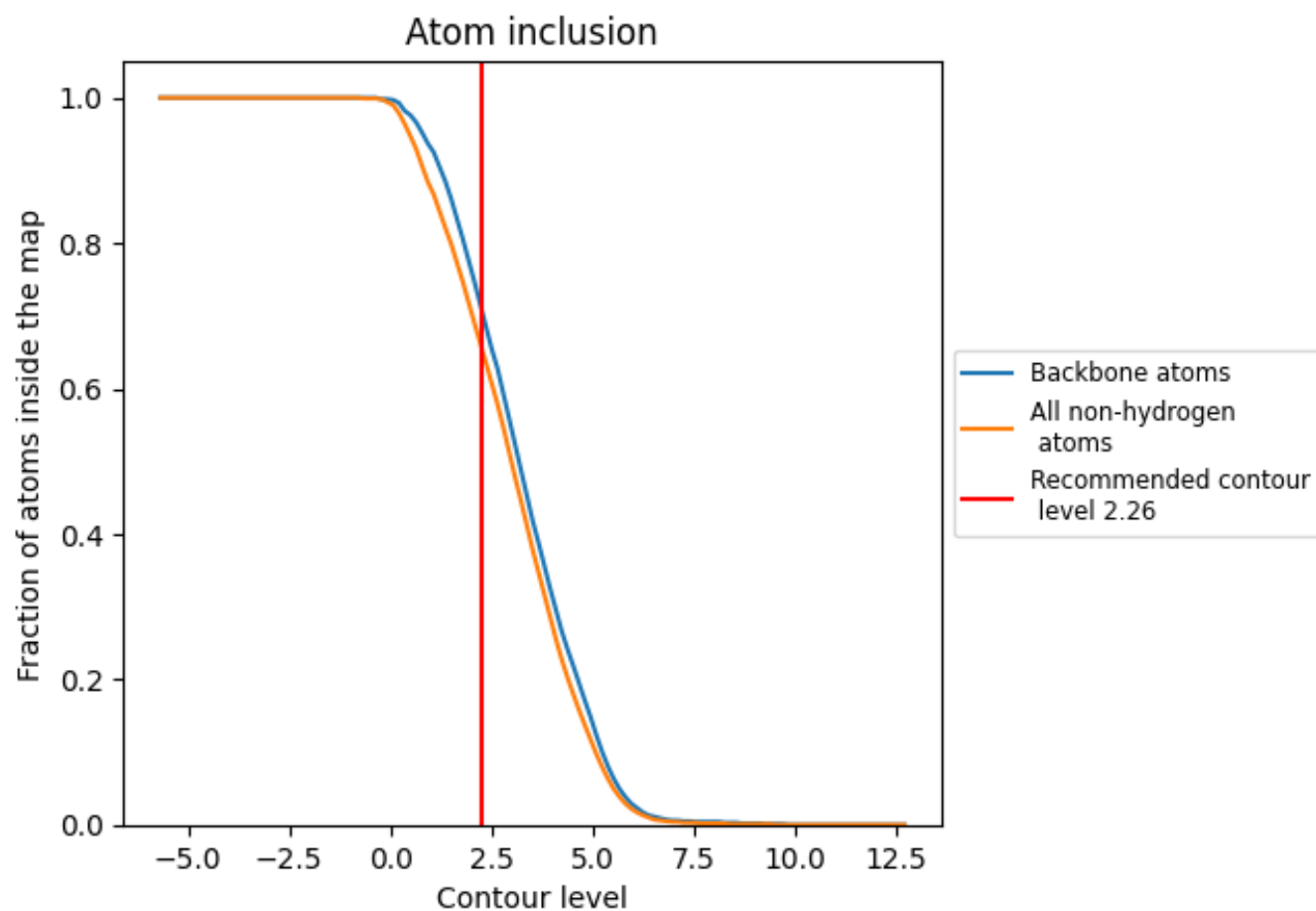
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.26).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% 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 (2.26) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.6470
Aa	 0.6480	 0.6480
Ab	 0.8800	 0.6440
Ac	 0.6500	 0.6480
Ad	 0.9000	 0.6490
Ae	 0.6430	 0.6470
Af	 0.8700	 0.6450
Ag	 0.6400	 0.6470
Ah	 0.8700	 0.6460
Ai	 0.6440	 0.6460
Aj	 0.9000	 0.6450
Ak	 0.6480	 0.6470
Al	 0.8600	 0.6380
Am	 0.6430	 0.6470
An	 0.8700	 0.6190
Ao	 0.6450	 0.6480
Ap	 0.8900	 0.6500
Aq	 0.6410	 0.6480
Ar	 0.8400	 0.6430
As	 0.6400	 0.6470
At	 0.8100	 0.6250
Au	 0.6440	 0.6470
Av	 0.8500	 0.6330
Aw	 0.6450	 0.6470
Ax	 0.9300	 0.6460
Ay	 0.6530	 0.6470
Az	 0.9300	 0.6480
Ba	 0.6430	 0.6470
Bb	 0.8600	 0.6500
Bc	 0.6410	 0.6470
Bd	 0.8600	 0.6490
Be	 0.6390	 0.6460
Bf	 0.8600	 0.6320
Bg	 0.6400	 0.6470
Bh	 0.9300	 0.6510



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Chain	Atom inclusion	Q-score
Bi	 0.6450	 0.6470
Bj	 0.8300	 0.6180
Bk	 0.6410	 0.6470
Bl	 0.8500	 0.6360
Bm	 0.6410	 0.6480
Bn	 0.8600	 0.6350
Bo	 0.6410	 0.6470
Bp	 0.8500	 0.6330
Bq	 0.6400	 0.6450
Br	 0.8900	 0.6460
Bs	 0.6460	 0.6460
Bt	 0.8800	 0.6440
Bu	 0.6470	 0.6470
Bv	 0.9100	 0.6420
Bw	 0.6430	 0.6470
Bx	 0.8500	 0.6530
By	 0.6460	 0.6480
Bz	 0.8900	 0.6540
Ca	 0.6410	 0.6470
Cb	 0.8200	 0.6160
Cc	 0.6400	 0.6470
Cd	 0.8600	 0.6450
Ce	 0.6440	 0.6480
Cf	 0.9200	 0.6480
Cg	 0.6480	 0.6470
Ch	 0.9200	 0.6500
Ci	 0.6390	 0.6480
Cj	 0.9300	 0.6470
Ck	 0.6440	 0.6480
Cl	 0.8900	 0.6460
Cm	 0.6400	 0.6460
Cn	 0.8900	 0.6390
Co	 0.6480	 0.6470
Cp	 0.8800	 0.6240
Cq	 0.6440	 0.6470
Cr	 0.8900	 0.6440
Cs	 0.6440	 0.6480
Ct	 0.8200	 0.6370