



Full wwPDB EM Validation Report ⓘ

Mar 18, 2026 – 12:06 AM UTC

PDB ID : 9R7S / pdb_00009r7s
EMDB ID : EMD-53791
Title : Potato virus A (PVA) after incubation in solution at 4C for 6 months
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

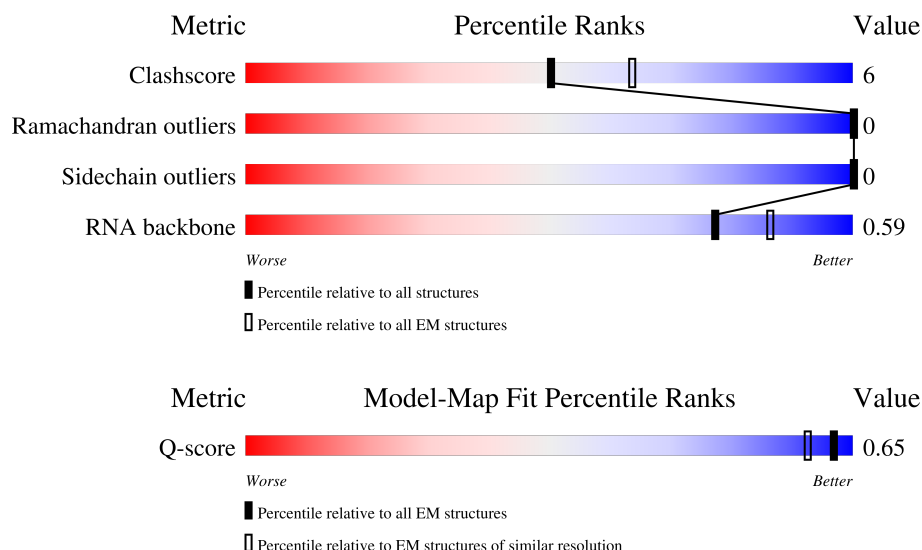
1 Overall quality at a glance i

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	19% 74% 10% 16%
1	Ac	269	18% 71% 13% 16%
1	Ae	269	19% 73% 11% 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	

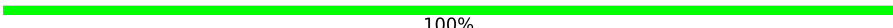
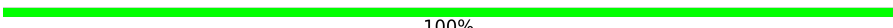
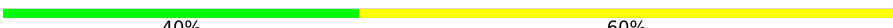
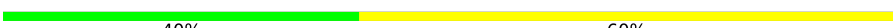
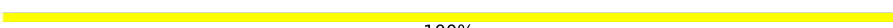
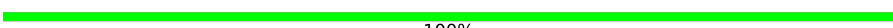
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Mol	Chain	Length	Quality of chain
1	Ce	269	
1	Cg	269	
1	Ci	269	
1	Ck	269	
1	Cm	269	
1	Co	269	
1	Cq	269	
1	Cs	269	
2	Ab	5	
2	Ad	5	
2	Af	5	
2	Ah	5	
2	Aj	5	
2	Al	5	
2	An	5	
2	Ap	5	
2	Ar	5	
2	At	5	
2	Av	5	
2	Ax	5	
2	Az	5	
2	Bb	5	
2	Bd	5	
2	Bf	5	
2	Bh	5	

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

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

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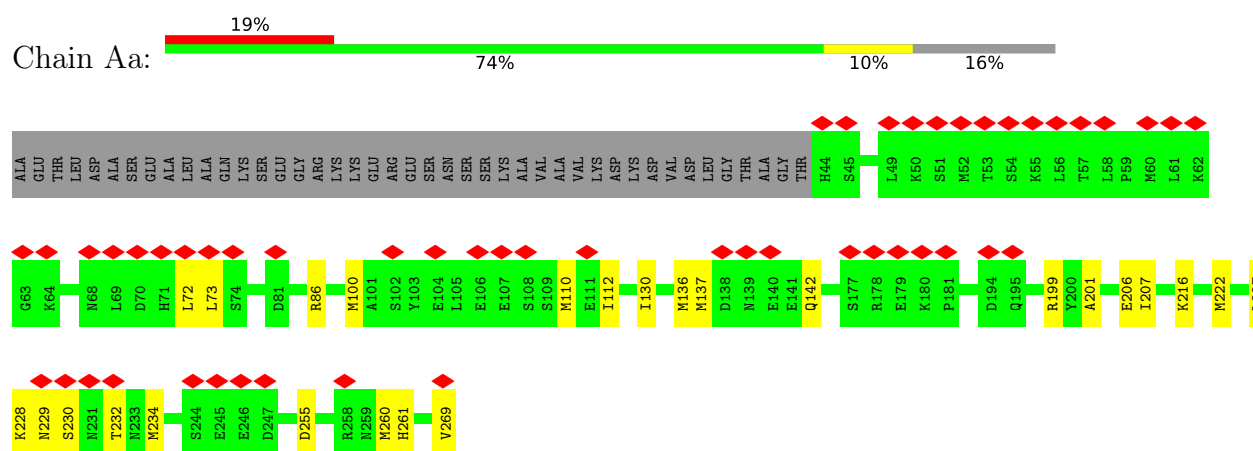
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Bt	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bv	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bx	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Bz	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cb	5	Total 100	C 45	N 10	O 40	P 5	0	0
2	Cd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

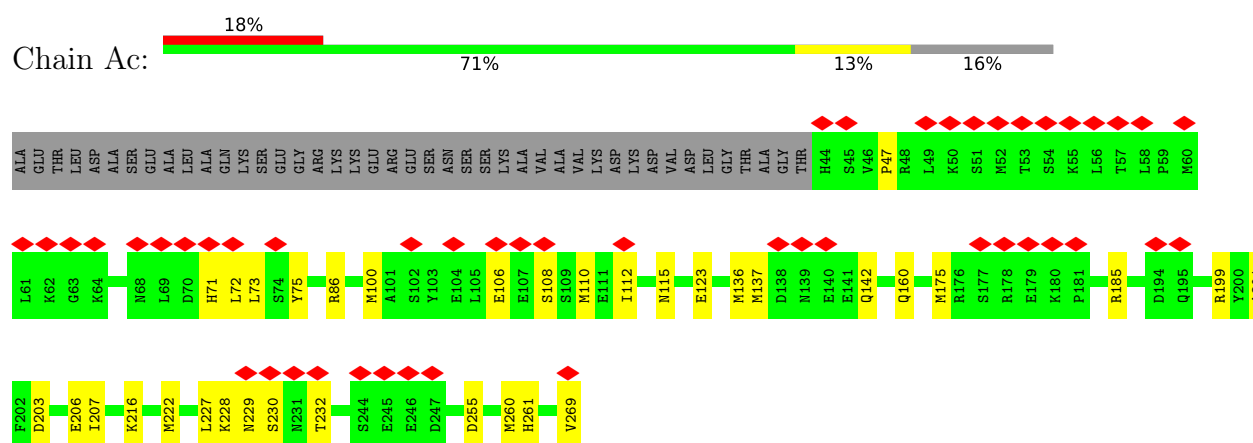
3 Residue-property plots

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.

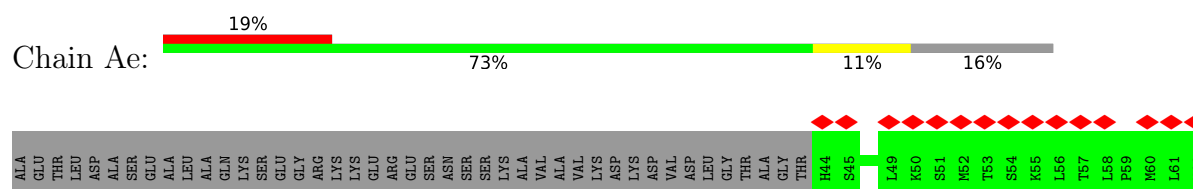
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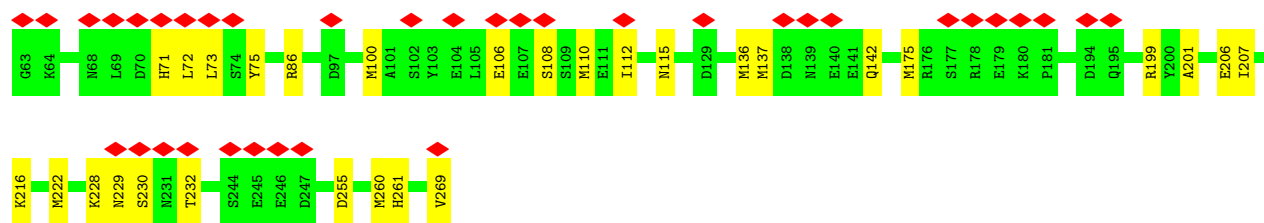


- Molecule 1: Capsid protein

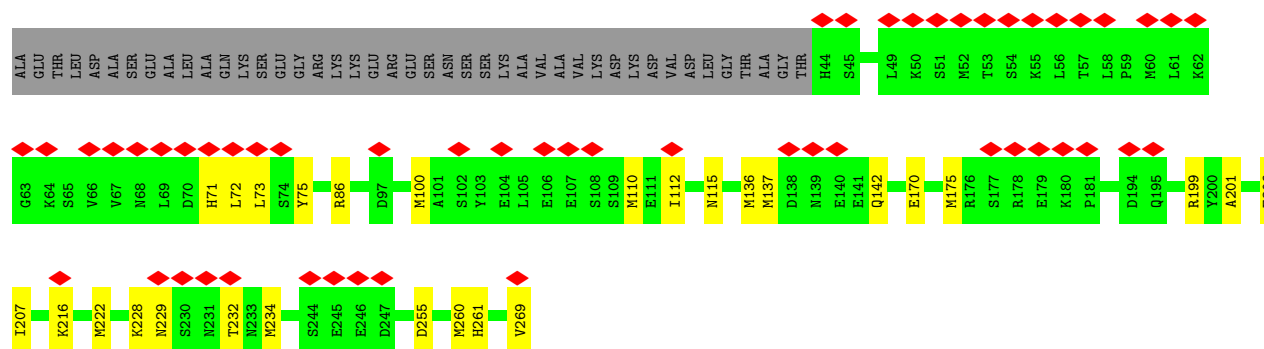
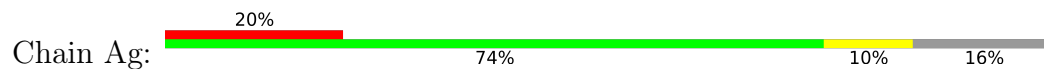


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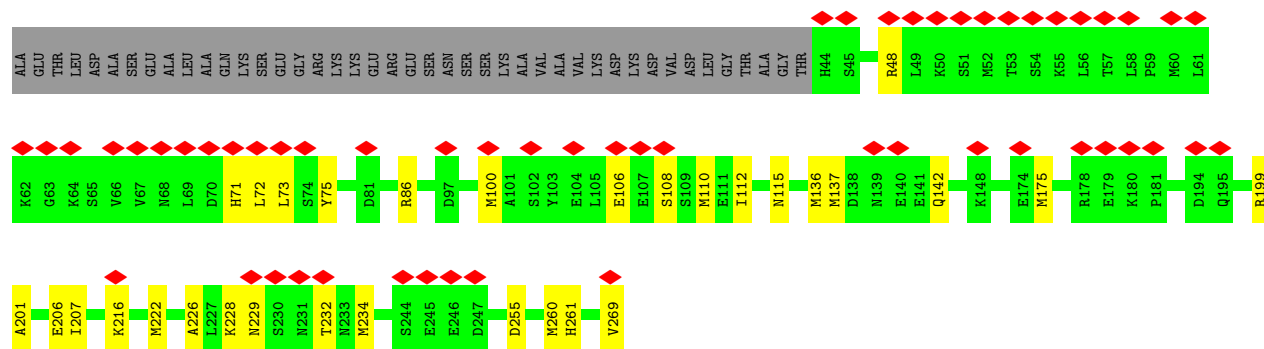
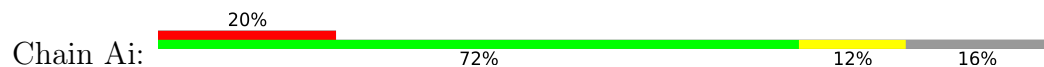




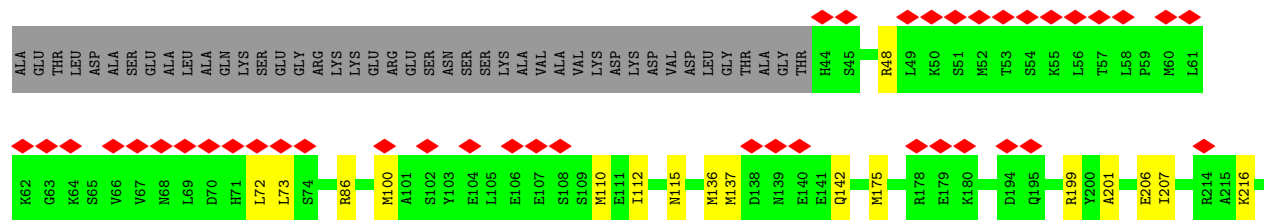
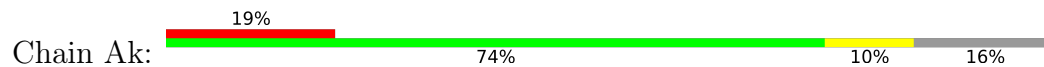
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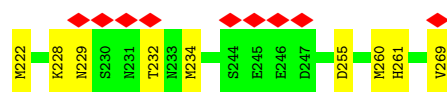


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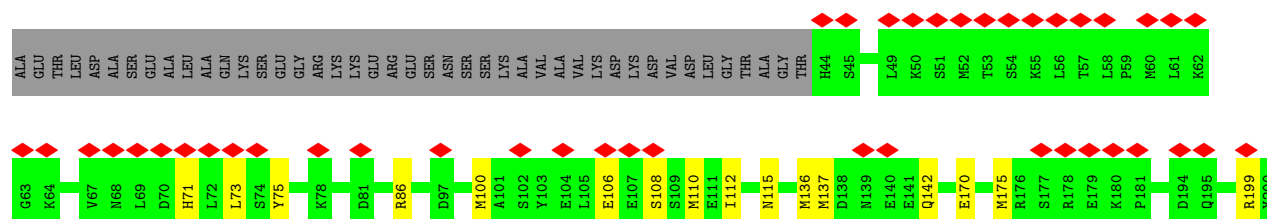
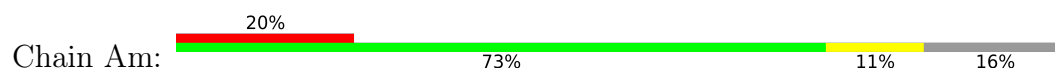


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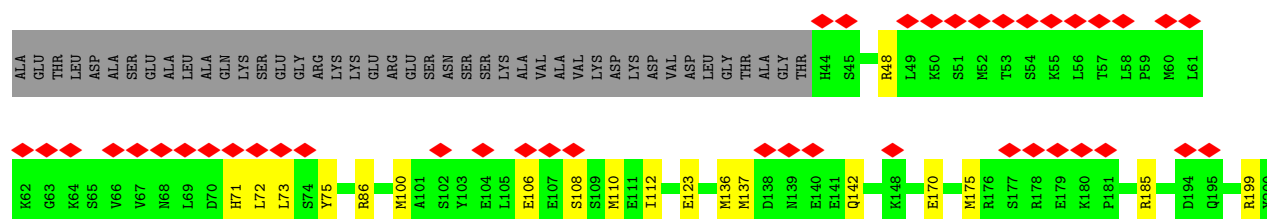
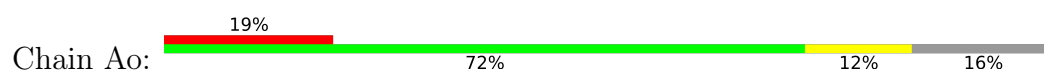




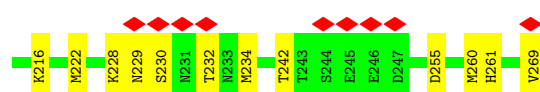
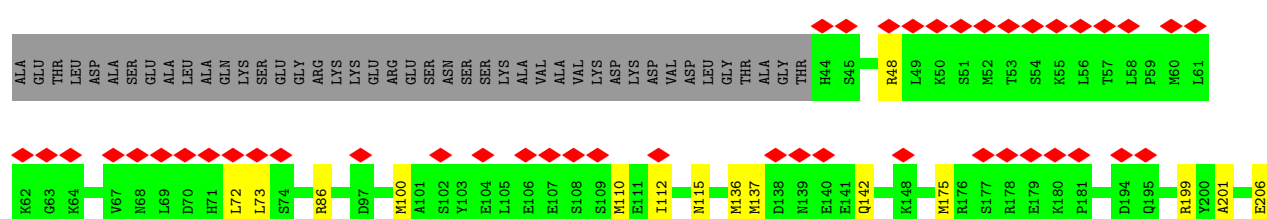
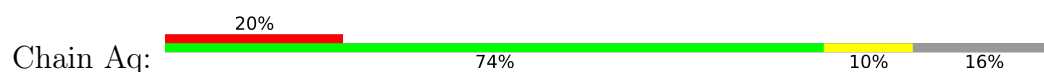
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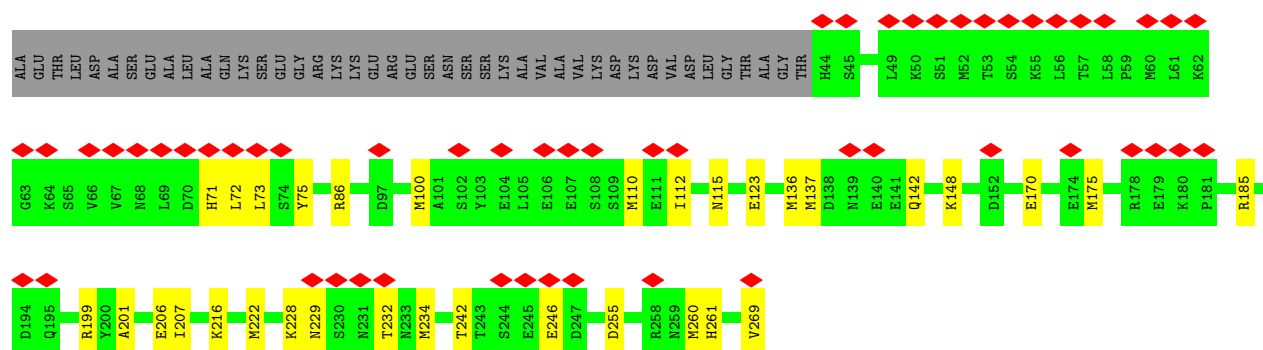
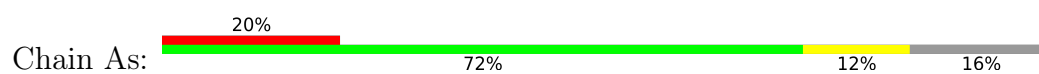
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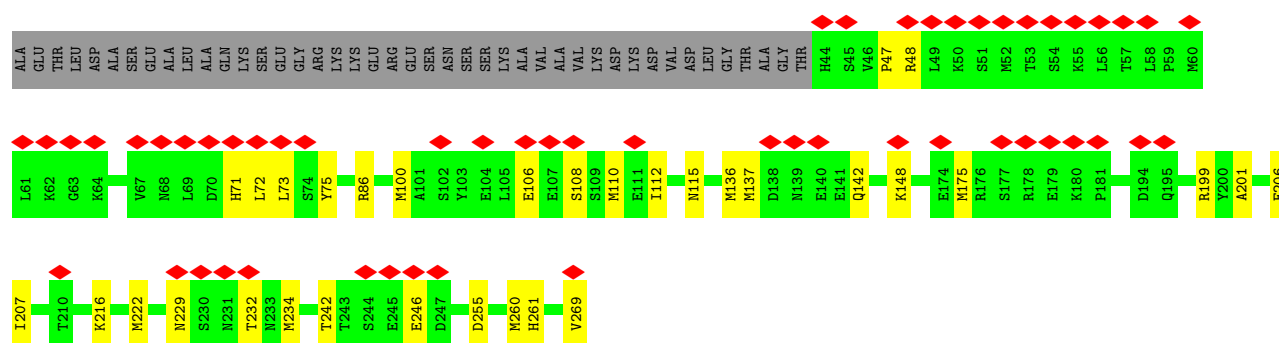
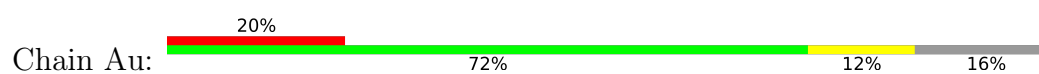
• Molecule 1: Capsid protein



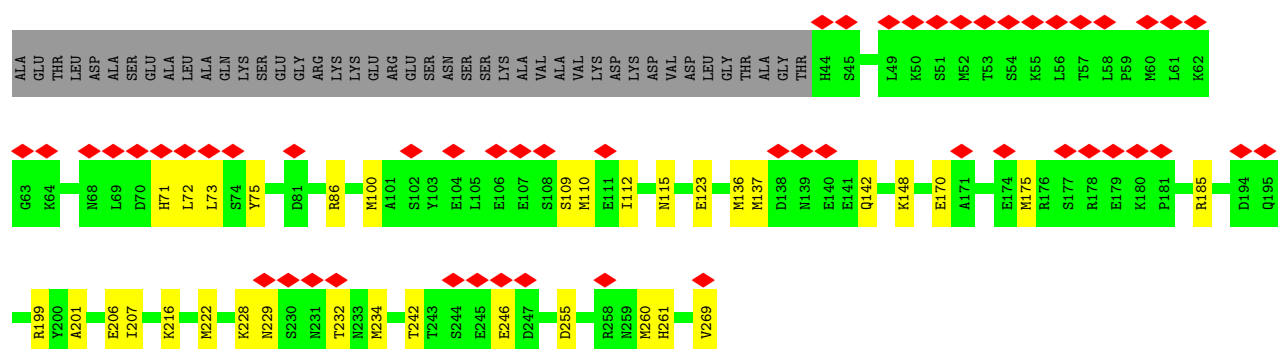
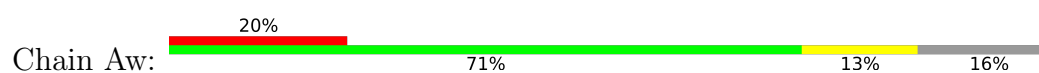
• Molecule 1: Capsid protein



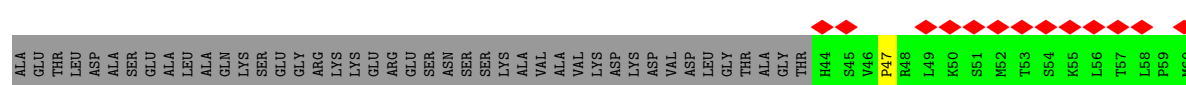
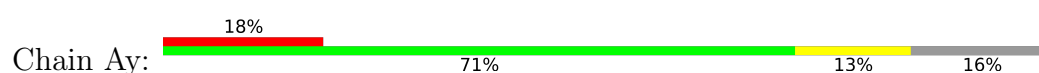
• Molecule 1: Capsid protein

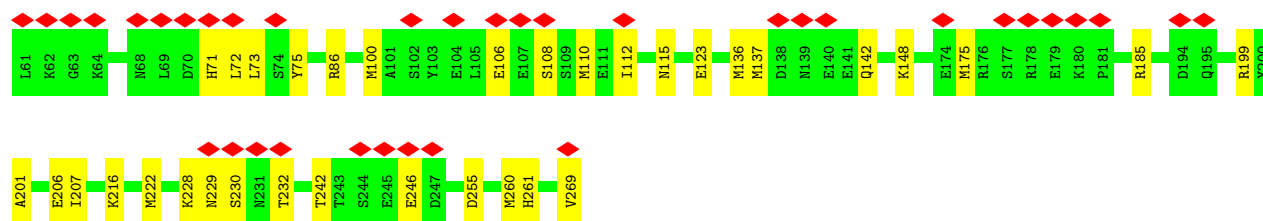


• Molecule 1: Capsid protein

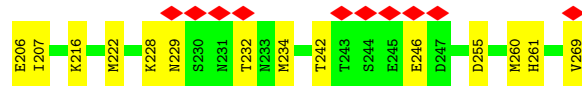
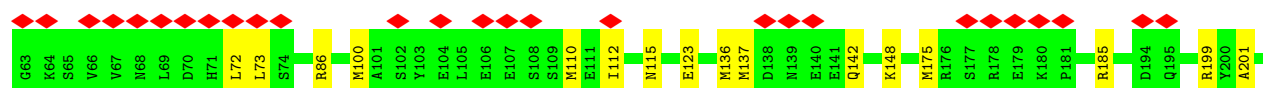
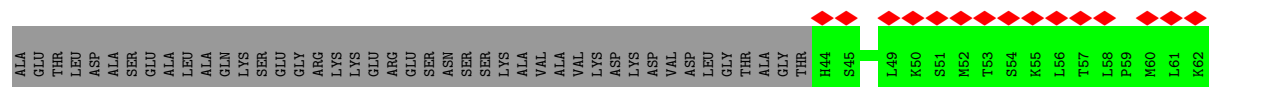
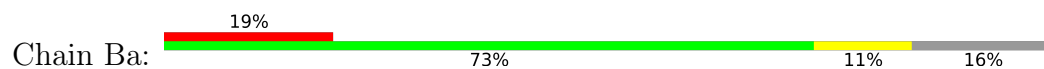


• Molecule 1: Capsid protein

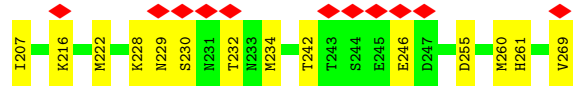
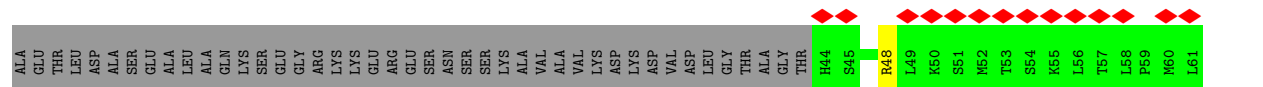
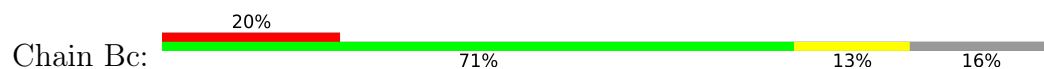




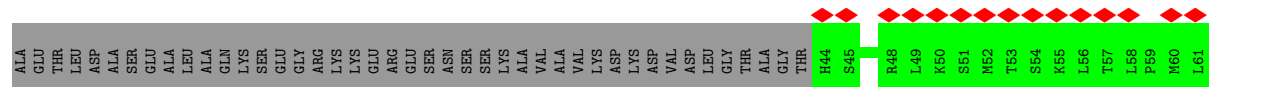
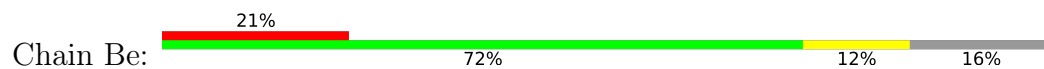
• Molecule 1: Capsid protein

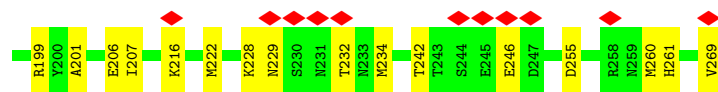


• Molecule 1: Capsid protein

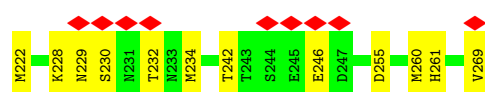
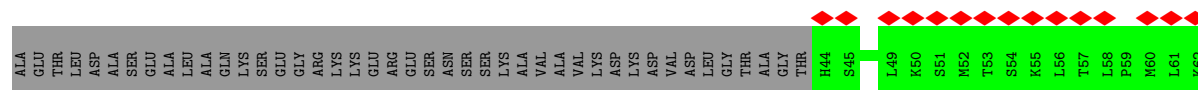
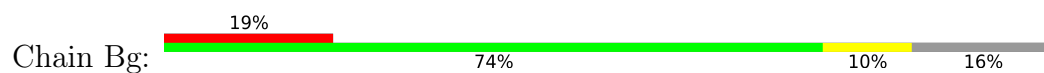


• Molecule 1: Capsid protein

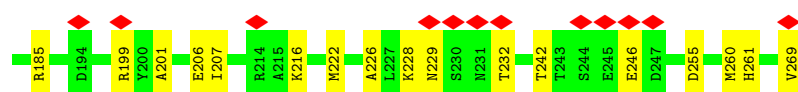
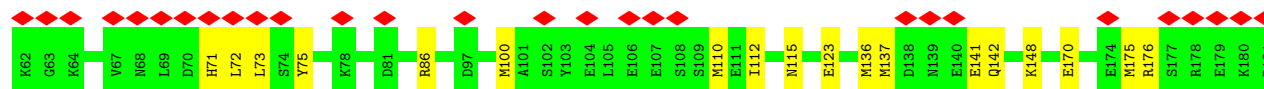
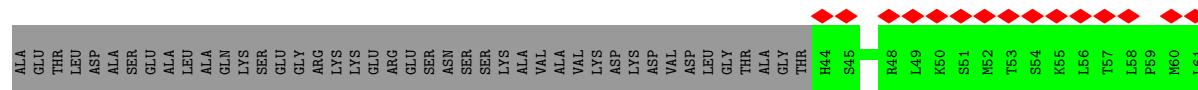




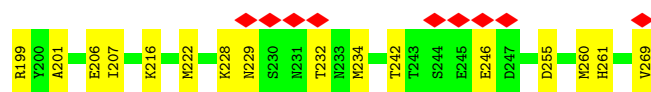
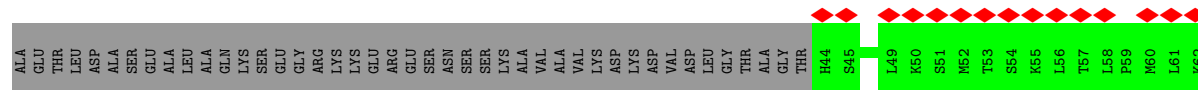
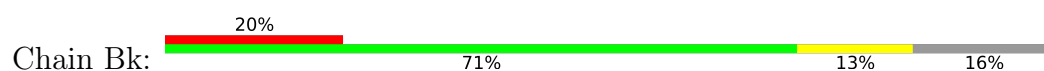
- Molecule 1: Capsid protein



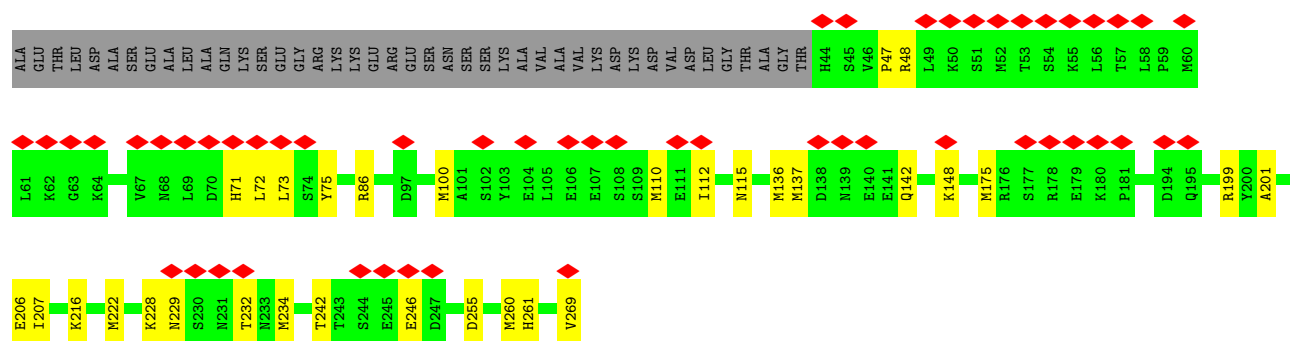
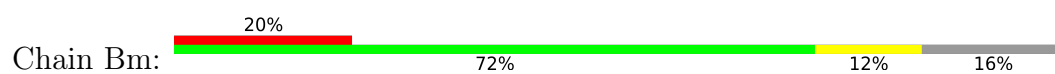
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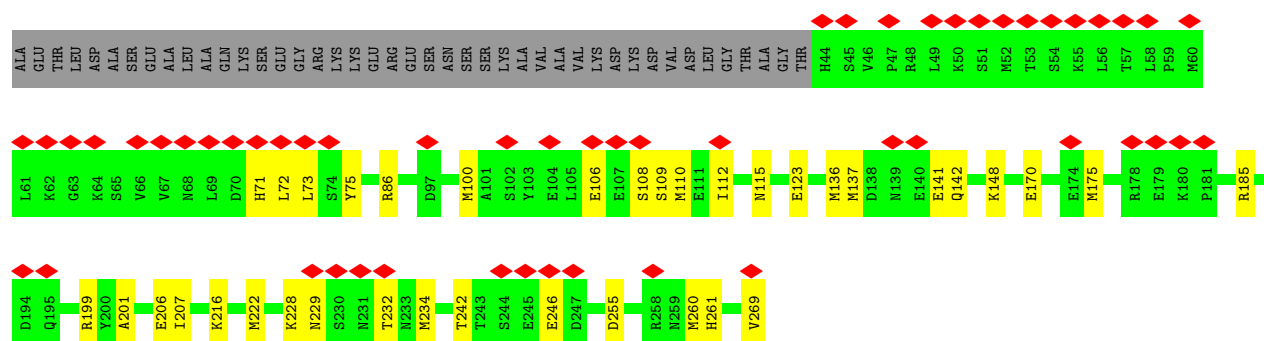
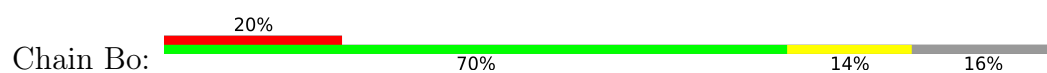
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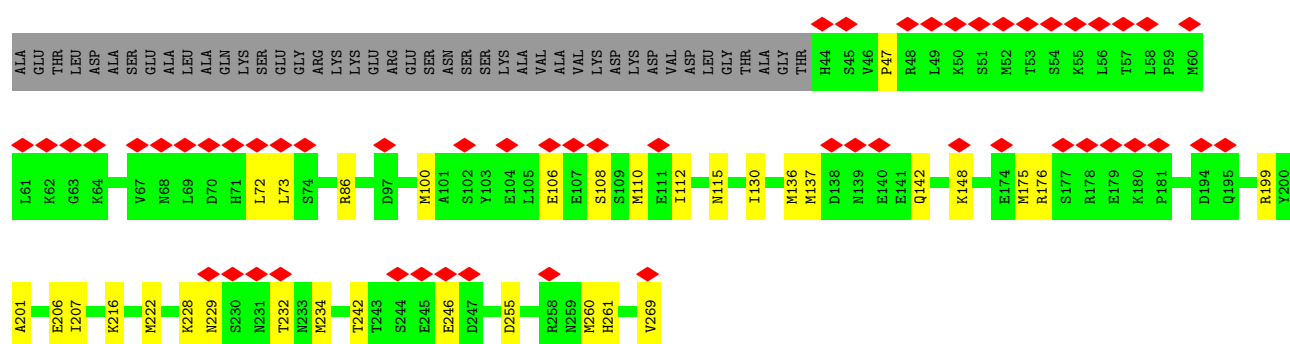
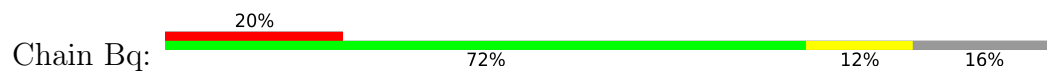
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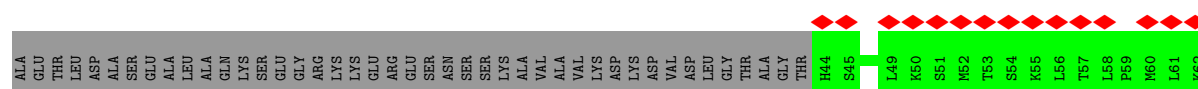
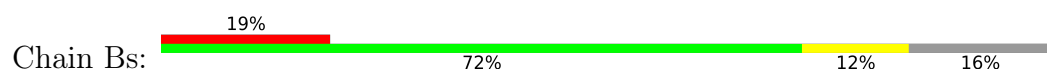
• Molecule 1: Capsid protein

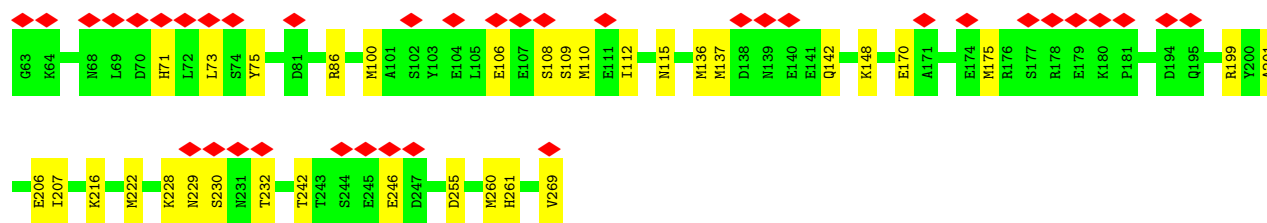


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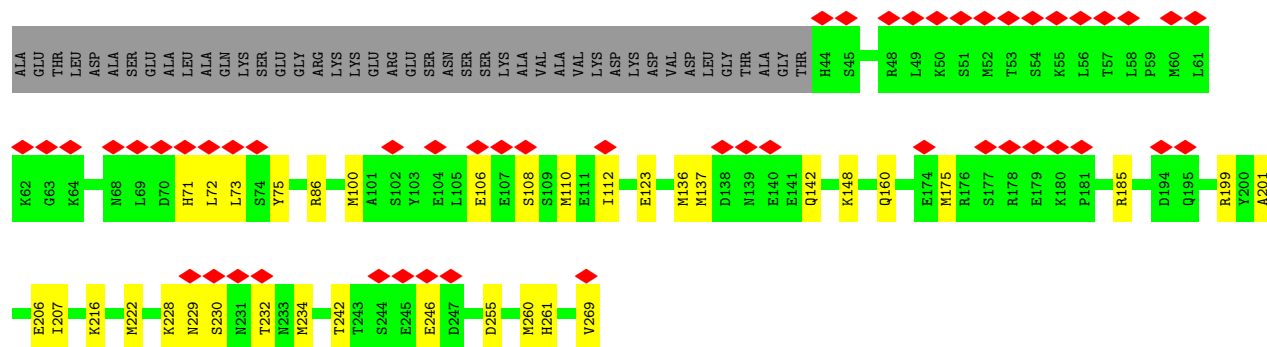
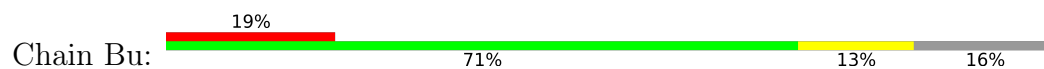


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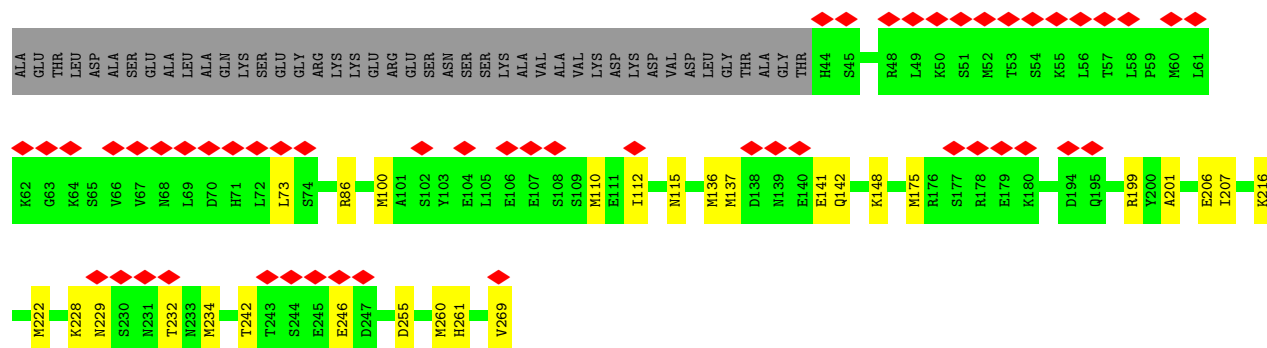
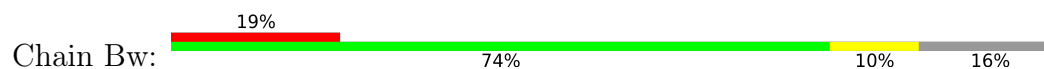




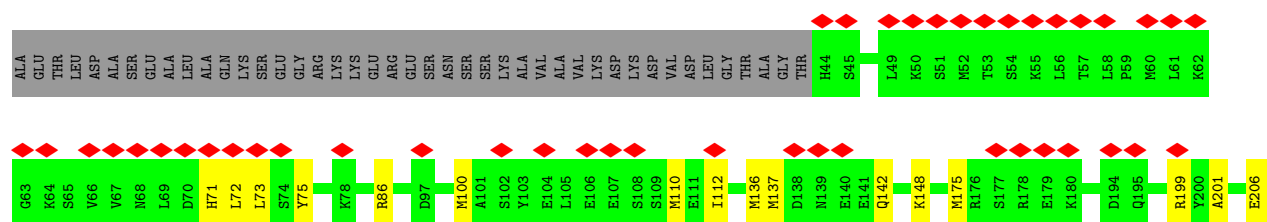
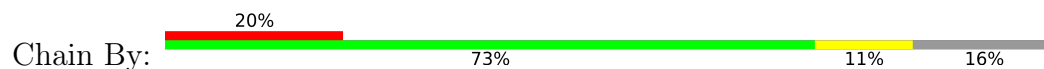
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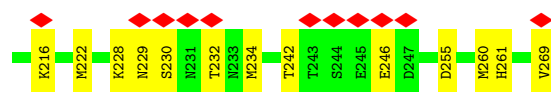


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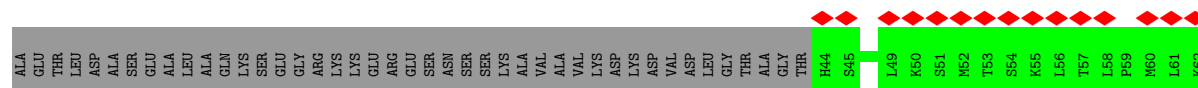
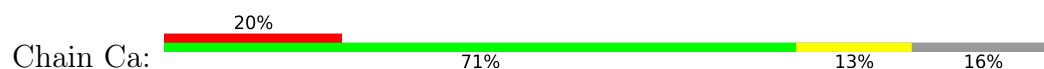


• Molecule 1: Capsid protein

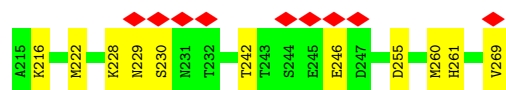
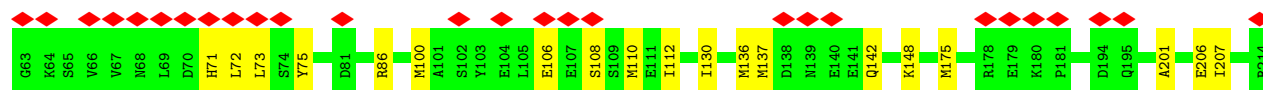
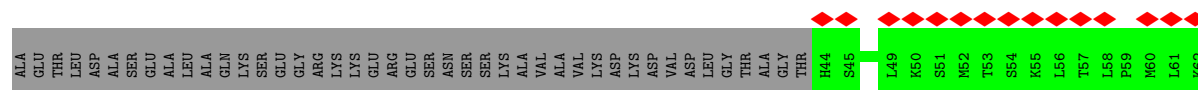
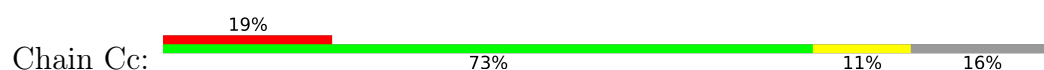




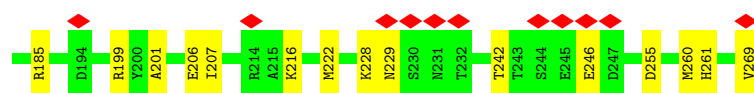
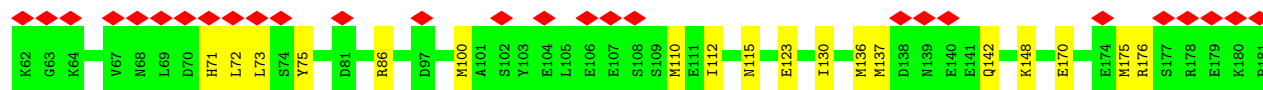
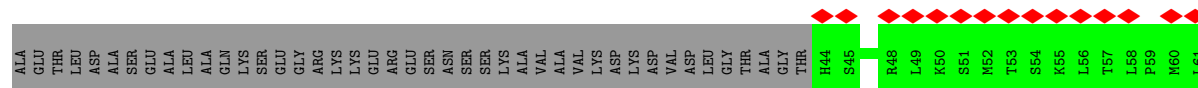
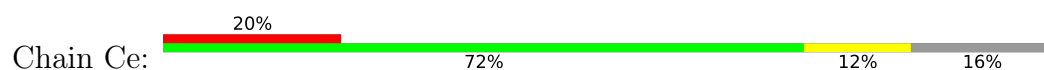
- Molecule 1: Capsid protein



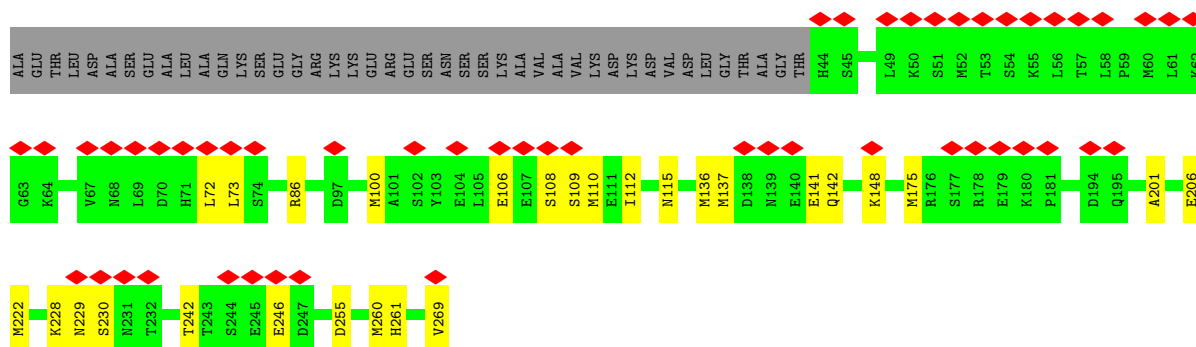
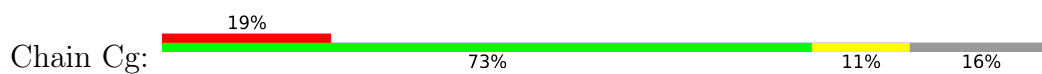
- Molecule 1: Capsid protein



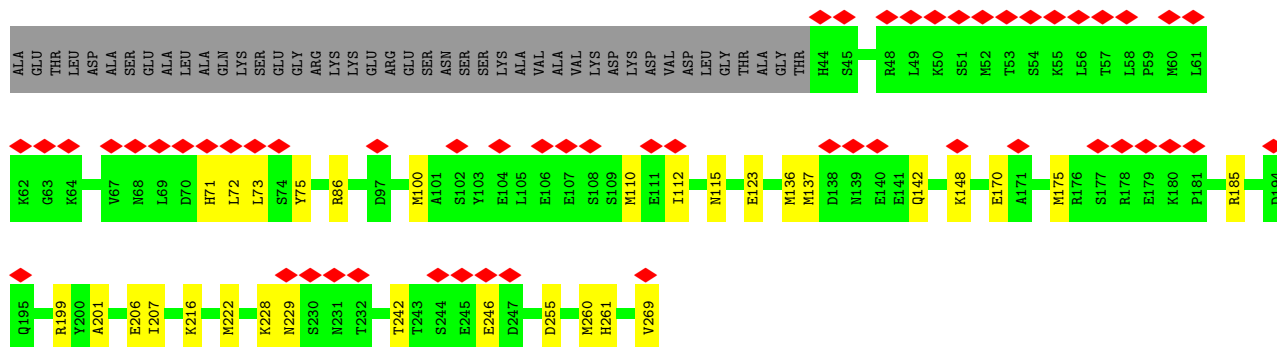
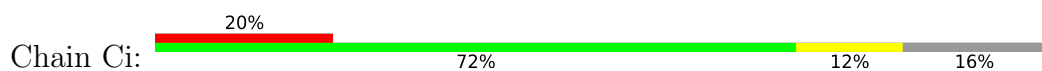
- Molecule 1: Capsid protein



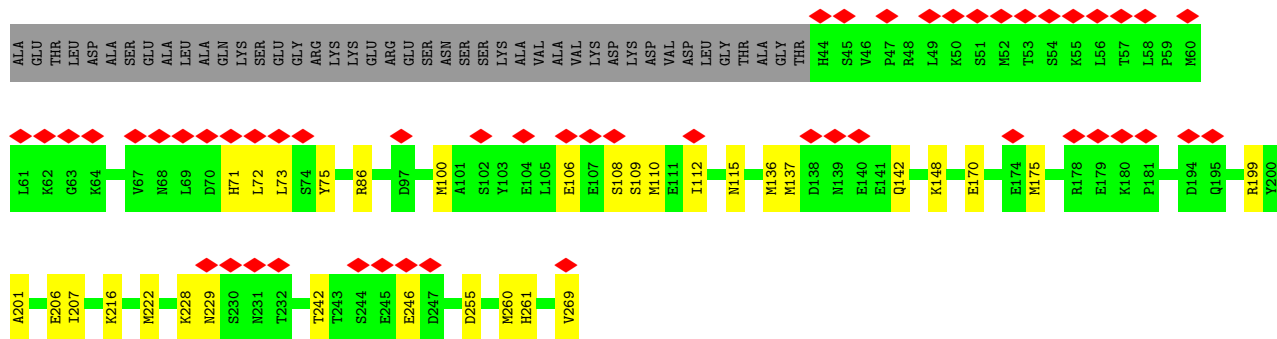
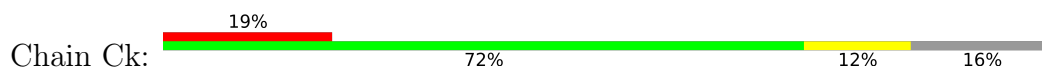
- Molecule 1: Capsid protein



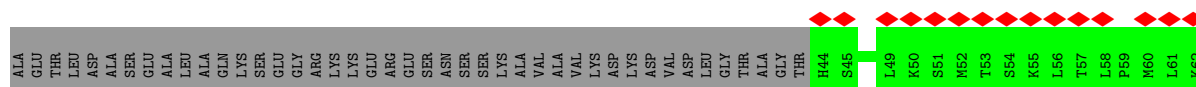
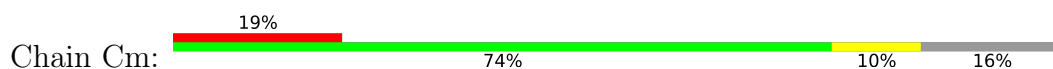
• Molecule 1: Capsid protein

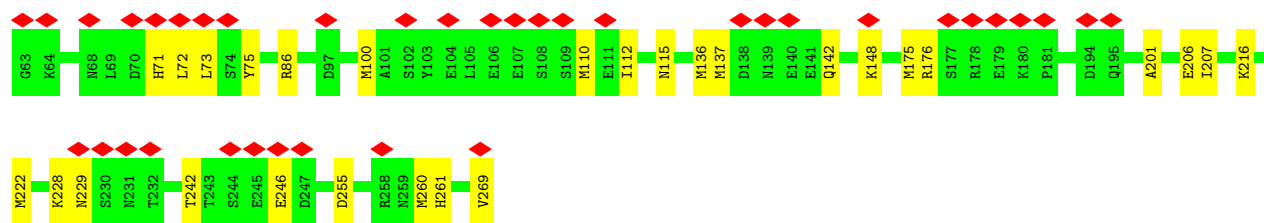


• Molecule 1: Capsid protein

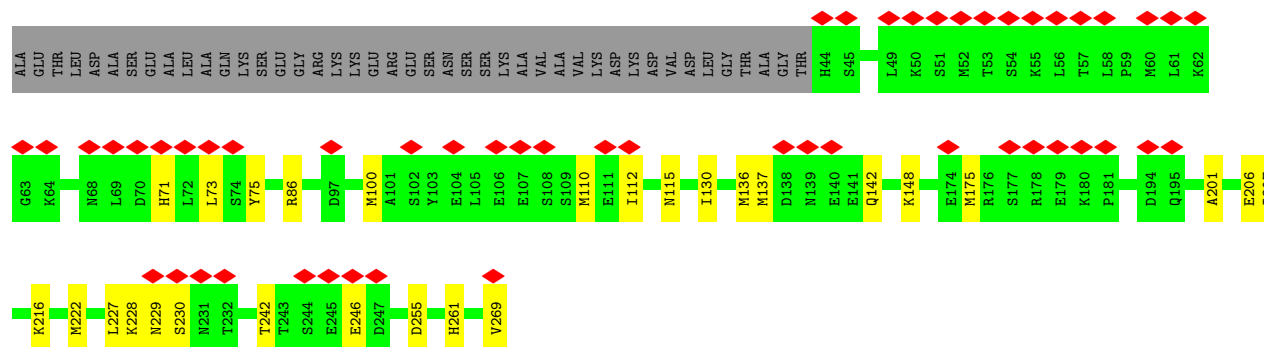
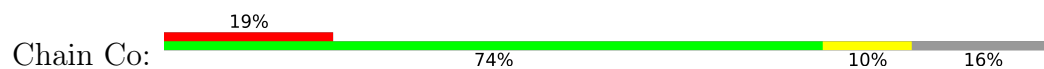


• Molecule 1: Capsid protein

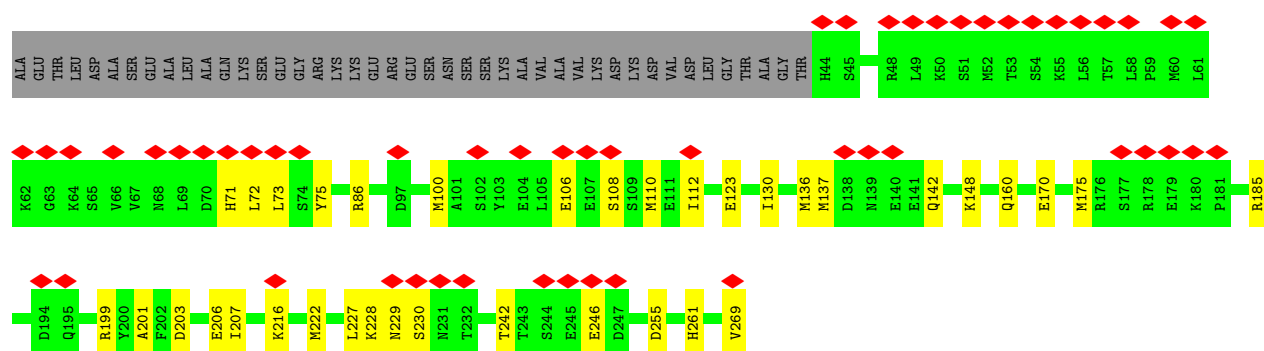
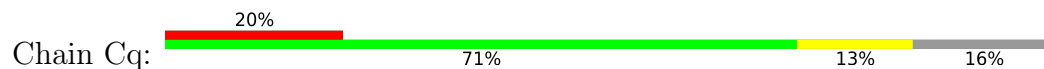




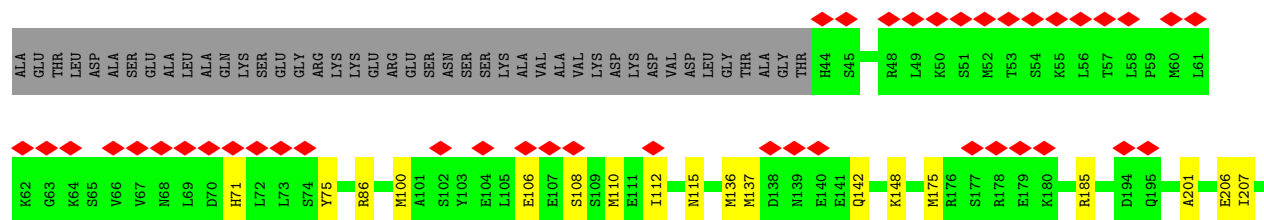
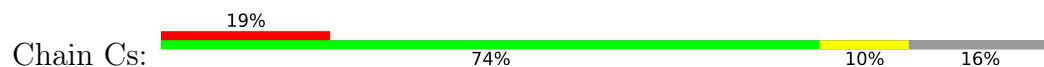
• Molecule 1: Capsid protein

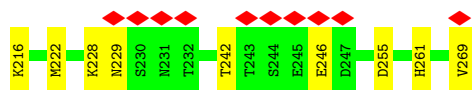


• Molecule 1: Capsid protein



• Molecule 1: Capsid protein





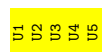
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ab: 40% 60%



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

Chain Ad: 100%



- 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: 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: 80% 20%



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

Chain An: 40% 60%



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

Chain Ap:  60% 40%



- 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:  80% 20%



- 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:  60% 40%



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

Chain Az:  40% 60%



- 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:  60% 40%



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

Chain Bj:  60% 40%



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

Chain Bl:  80% 20%



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

Chain Bn:  60% 40%



- 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: 100%

There are no outlier residues recorded for this chain.

- 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: 100%

There are no outlier residues recorded for this chain.

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

Chain Cb: 80% 20%



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

Chain Cd: 40% 60%



- 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:  60% 40%



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

Chain Cl:  60% 40%



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

Chain Cn:  60% 40%



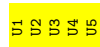
- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Cp:  40% 60%



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

Chain Cr:  100%



- 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=-40.90°, rise=3.89 Å, axial sym=C1	Depositor
Number of segments used	629681	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	10.928	Depositor
Minimum map value	-6.443	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.448	Depositor
Recommended contour level	2.01	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	0.40	0/1854	0.56	0/2503
1	Ac	0.40	0/1854	0.56	0/2503
1	Ae	0.40	0/1854	0.56	0/2503
1	Ag	0.40	0/1854	0.56	0/2503
1	Ai	0.40	0/1854	0.56	0/2503
1	Ak	0.40	0/1854	0.56	0/2503
1	Am	0.40	0/1854	0.56	0/2503
1	Ao	0.40	0/1854	0.56	0/2503
1	Aq	0.40	0/1854	0.56	0/2503
1	As	0.40	0/1854	0.56	0/2503
1	Au	0.40	0/1854	0.56	0/2503
1	Aw	0.40	0/1854	0.56	0/2503
1	Ay	0.40	0/1854	0.56	0/2503
1	Ba	0.40	0/1854	0.56	0/2503
1	Bc	0.40	0/1854	0.56	0/2503
1	Be	0.40	0/1854	0.56	0/2503
1	Bg	0.40	0/1854	0.56	0/2503
1	Bi	0.40	0/1854	0.56	0/2503
1	Bk	0.40	0/1854	0.56	0/2503
1	Bm	0.40	0/1854	0.56	0/2503
1	Bo	0.40	0/1854	0.56	0/2503
1	Bq	0.40	0/1854	0.56	0/2503
1	Bs	0.40	0/1854	0.56	0/2503
1	Bu	0.40	0/1854	0.56	0/2503
1	Bw	0.40	0/1854	0.56	0/2503
1	By	0.40	0/1854	0.56	0/2503
1	Ca	0.40	0/1854	0.56	0/2503
1	Cc	0.40	0/1854	0.56	0/2503
1	Ce	0.40	0/1854	0.56	0/2503
1	Cg	0.40	0/1854	0.56	0/2503
1	Ci	0.40	0/1854	0.56	0/2503
1	Ck	0.40	0/1854	0.56	0/2503
1	Cm	0.40	0/1854	0.56	0/2503
1	Co	0.40	0/1854	0.56	0/2503

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Cq	0.40	0/1854	0.56	0/2503
1	Cs	0.40	0/1854	0.56	0/2503
2	Ab	0.33	0/109	0.33	0/166
2	Ad	0.33	0/109	0.33	0/166
2	Af	0.33	0/109	0.33	0/166
2	Ah	0.33	0/109	0.34	0/166
2	Aj	0.33	0/109	0.33	0/166
2	Al	0.32	0/109	0.34	0/166
2	An	0.32	0/109	0.34	0/166
2	Ap	0.32	0/109	0.34	0/166
2	Ar	0.33	0/109	0.33	0/166
2	At	0.32	0/109	0.33	0/166
2	Av	0.33	0/109	0.33	0/166
2	Ax	0.33	0/109	0.33	0/166
2	Az	0.32	0/109	0.34	0/166
2	Bb	0.33	0/109	0.34	0/166
2	Bd	0.32	0/109	0.34	0/166
2	Bf	0.32	0/109	0.34	0/166
2	Bh	0.32	0/109	0.34	0/166
2	Bj	0.33	0/109	0.34	0/166
2	Bl	0.33	0/109	0.34	0/166
2	Bn	0.32	0/109	0.34	0/166
2	Bp	0.33	0/109	0.34	0/166
2	Br	0.33	0/109	0.34	0/166
2	Bt	0.32	0/109	0.33	0/166
2	Bv	0.32	0/109	0.33	0/166
2	Bx	0.33	0/109	0.34	0/166
2	Bz	0.32	0/109	0.34	0/166
2	Cb	0.32	0/109	0.34	0/166
2	Cd	0.33	0/109	0.33	0/166
2	Cf	0.33	0/109	0.33	0/166
2	Ch	0.33	0/109	0.33	0/166
2	Cj	0.32	0/109	0.34	0/166
2	Cl	0.33	0/109	0.34	0/166
2	Cn	0.32	0/109	0.34	0/166
2	Cp	0.32	0/109	0.34	0/166
2	Cr	0.32	0/109	0.34	0/166
2	Ct	0.33	0/109	0.34	0/166
All	All	0.40	0/70668	0.55	0/96084

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	1815	0	1785	22	0
1	Ac	1815	0	1785	32	0
1	Ae	1815	0	1785	24	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	28	0
1	Aq	1815	0	1785	26	0
1	As	1815	0	1785	30	0
1	Au	1815	0	1785	29	0
1	Aw	1815	0	1785	30	0
1	Ay	1815	0	1785	31	0
1	Ba	1815	0	1785	28	0
1	Bc	1815	0	1785	32	0
1	Be	1815	0	1785	30	0
1	Bg	1815	0	1785	27	0
1	Bi	1815	0	1785	32	0
1	Bk	1815	0	1785	31	0
1	Bm	1815	0	1785	30	0
1	Bo	1815	0	1785	33	0
1	Bq	1815	0	1785	30	0
1	Bs	1815	0	1785	30	0
1	Bu	1815	0	1785	31	0
1	Bw	1815	0	1785	27	0
1	By	1815	0	1785	28	0
1	Ca	1815	0	1785	30	0
1	Cc	1815	0	1785	27	0
1	Ce	1815	0	1785	28	0
1	Cg	1815	0	1785	27	0
1	Ci	1815	0	1785	26	0
1	Ck	1815	0	1785	26	0
1	Cm	1815	0	1785	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Co	1815	0	1785	26	0
1	Cq	1815	0	1785	34	0
1	Cs	1815	0	1785	21	0
2	Ab	100	0	51	5	0
2	Ad	100	0	51	8	0
2	Af	100	0	51	1	0
2	Ah	100	0	51	1	0
2	Aj	100	0	51	2	0
2	Al	100	0	51	1	0
2	An	100	0	51	4	0
2	Ap	100	0	51	3	0
2	Ar	100	0	51	1	0
2	At	100	0	51	1	0
2	Av	100	0	51	2	0
2	Ax	100	0	51	2	0
2	Az	100	0	51	3	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	2	0
2	Bj	100	0	51	2	0
2	Bl	100	0	51	1	0
2	Bn	100	0	51	2	0
2	Bp	100	0	51	1	0
2	Br	100	0	51	1	0
2	Bt	100	0	51	0	0
2	Bv	100	0	51	2	0
2	Bx	100	0	51	1	0
2	Bz	100	0	51	0	0
2	Cb	100	0	51	1	0
2	Cd	100	0	51	3	0
2	Cf	100	0	51	2	0
2	Ch	100	0	51	3	0
2	Cj	100	0	51	3	0
2	Cl	100	0	51	2	0
2	Cn	100	0	51	2	0
2	Cp	100	0	51	5	0
2	Cr	100	0	51	8	0
2	Ct	100	0	51	0	0
All	All	68940	0	66096	752	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 6.

All (752) 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:Ac:230:SER:HB2	2:Ad:3:U:O2'	1.93	0.69
2:Cr:1:U:P	1:Cs:185:ARG:HH12	2.16	0.68
1:Ca:229:ASN:ND2	1:Cq:242:THR:O	2.33	0.61
1:Ak:229:ASN:ND2	1:Ba:242:THR:O	2.34	0.61
1:Am:229:ASN:ND2	1:Bc:242:THR:O	2.33	0.61
1:Be:229:ASN:ND2	1:Bu:242:THR:O	2.34	0.61
1:Bi:229:ASN:ND2	1:By:242:THR:O	2.34	0.61
1:Ai:229:ASN:ND2	1:Ay:242:THR:O	2.33	0.60
1:Bk:229:ASN:ND2	1:Ca:242:THR:O	2.34	0.60
1:Bm:229:ASN:ND2	1:Cc:242:THR:O	2.34	0.60
1:Bo:229:ASN:ND2	1:Ce:242:THR:O	2.35	0.60
1:Aa:229:ASN:ND2	1:Aq:242:THR:O	2.34	0.60
1:Aw:229:ASN:ND2	1:Bm:242:THR:O	2.35	0.60
1:Ba:229:ASN:ND2	1:Bq:242:THR:O	2.34	0.60
1:Ca:130:ILE:HG22	2:Cb:5:U:H1'	1.83	0.60
1:As:229:ASN:ND2	1:Bi:242:THR:O	2.34	0.60
1:Bw:229:ASN:ND2	1:Cm:242:THR:O	2.34	0.60
1:Aq:229:ASN:ND2	1:Bg:242:THR:O	2.34	0.60
1:Ac:229:ASN:ND2	1:As:242:THR:O	2.35	0.60
1:Ao:229:ASN:ND2	1:Be:242:THR:O	2.35	0.60
1:Cc:229:ASN:ND2	1:Cs:242:THR:O	2.34	0.60
1:Au:229:ASN:ND2	1:Bk:242:THR:O	2.35	0.60
1:Ag:229:ASN:ND2	1:Aw:242:THR:O	2.35	0.59
1:Ae:229:ASN:ND2	1:Au:242:THR:O	2.35	0.59
1:Ac:160:GLN:HE21	2:Ad:2:U:P	2.24	0.59
1:By:229:ASN:ND2	1:Co:242:THR:O	2.35	0.59
1:Bc:229:ASN:ND2	1:Bs:242:THR:O	2.35	0.59
1:Bs:229:ASN:ND2	1:Ci:242:THR:O	2.35	0.59
1:Bu:229:ASN:ND2	1:Ck:242:THR:O	2.35	0.59
1:Bg:229:ASN:ND2	1:Bw:242:THR:O	2.36	0.59
1:Cq:160:GLN:HE21	2:Cr:2:U:P	2.26	0.59
1:Au:73:LEU:HD12	1:Aw:175:MET:SD	2.43	0.58
1:Ay:229:ASN:ND2	1:Bo:242:THR:O	2.36	0.58
1:Ca:73:LEU:HD12	1:Cc:175:MET:SD	2.43	0.58
1:Bm:73:LEU:HD12	1:Bo:175:MET:SD	2.44	0.58
1:Bi:73:LEU:HD12	1:Bk:175:MET:SD	2.44	0.58
1:Bu:73:LEU:HD12	1:Bw:175:MET:SD	2.43	0.58
1:Bq:229:ASN:ND2	1:Cg:242:THR:O	2.37	0.57
1:Ce:73:LEU:HD12	1:Cg:175:MET:SD	2.43	0.57
1:Cm:73:LEU:HD12	1:Co:175:MET:SD	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:73:LEU:HD12	1:Am:175:MET:SD	2.43	0.57
1:Bc:73:LEU:HD12	1:Be:175:MET:SD	2.43	0.57
1:Ac:73:LEU:HD12	1:Ae:175:MET:SD	2.43	0.57
1:Ag:73:LEU:HD12	1:Ai:175:MET:SD	2.45	0.57
1:Cc:73:LEU:HD12	1:Ce:175:MET:SD	2.45	0.57
1:Aq:73:LEU:HD12	1:As:175:MET:SD	2.44	0.57
1:As:73:LEU:HD12	1:Au:175:MET:SD	2.45	0.57
1:Aa:73:LEU:HD12	1:Ac:175:MET:SD	2.45	0.57
1:Ci:73:LEU:HD12	1:Ck:175:MET:SD	2.45	0.57
1:Cq:73:LEU:HD12	1:Cs:175:MET:SD	2.45	0.57
1:Ay:73:LEU:HD12	1:Ba:175:MET:SD	2.45	0.57
1:Bg:73:LEU:HD12	1:Bi:175:MET:SD	2.45	0.57
1:Ao:73:LEU:HD12	1:Aq:175:MET:SD	2.45	0.56
1:Bo:73:LEU:HD12	1:Bq:175:MET:SD	2.45	0.56
1:Ba:73:LEU:HD12	1:Bc:175:MET:SD	2.45	0.56
1:Ae:73:LEU:HD12	1:Ag:175:MET:SD	2.45	0.56
1:By:73:LEU:HD12	1:Ca:175:MET:SD	2.45	0.56
1:Bq:73:LEU:HD12	1:Bs:175:MET:SD	2.45	0.56
1:Cg:73:LEU:HD12	1:Ci:175:MET:SD	2.45	0.56
1:Bk:73:LEU:HD12	1:Bm:175:MET:SD	2.45	0.56
1:Ai:73:LEU:HD12	1:Ak:175:MET:SD	2.45	0.56
2:Ap:1:U:P	2:Ar:5:U:O3'	2.64	0.56
1:Bs:73:LEU:HD12	1:Bu:175:MET:SD	2.45	0.56
1:Ck:73:LEU:HD12	1:Cm:175:MET:SD	2.45	0.56
1:Aw:73:LEU:HD12	1:Ay:175:MET:SD	2.45	0.56
1:Am:73:LEU:HD12	1:Ao:175:MET:SD	2.46	0.55
1:Be:73:LEU:HD12	1:Bg:175:MET:SD	2.46	0.55
1:Co:73:LEU:HD12	1:Cq:175:MET:SD	2.46	0.55
1:Bw:73:LEU:HD12	1:By:175:MET:SD	2.46	0.55
1:Ai:255:ASP:OD2	1:Ai:261:HIS:ND1	2.41	0.54
1:Cq:160:GLN:NE2	2:Cr:1:U:O3'	2.41	0.54
1:Ay:255:ASP:OD2	1:Ay:261:HIS:ND1	2.42	0.54
1:Bo:255:ASP:OD2	1:Bo:261:HIS:ND1	2.41	0.54
1:Ak:255:ASP:OD2	1:Ak:261:HIS:ND1	2.41	0.53
1:Ba:255:ASP:OD2	1:Ba:261:HIS:ND1	2.41	0.53
1:Cm:255:ASP:OD2	1:Cm:261:HIS:ND1	2.41	0.53
1:Ce:255:ASP:OD2	1:Ce:261:HIS:ND1	2.41	0.53
1:Ag:255:ASP:OD2	1:Ag:261:HIS:ND1	2.41	0.53
1:Bq:255:ASP:OD2	1:Bq:261:HIS:ND1	2.41	0.53
1:Cg:255:ASP:OD2	1:Cg:261:HIS:ND1	2.41	0.53
1:Aw:255:ASP:OD2	1:Aw:261:HIS:ND1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ck:255:ASP:OD2	1:Ck:261:HIS:ND1	2.41	0.53
1:Ac:227:LEU:CD2	2:Ad:3:U:H2'	2.39	0.53
1:Bm:255:ASP:OD2	1:Bm:261:HIS:ND1	2.41	0.53
1:Bw:255:ASP:OD2	1:Bw:261:HIS:ND1	2.42	0.53
1:Bu:255:ASP:OD2	1:Bu:261:HIS:ND1	2.41	0.53
1:Co:255:ASP:OD2	1:Co:261:HIS:ND1	2.41	0.53
1:Ac:255:ASP:OD2	1:Ac:261:HIS:ND1	2.41	0.53
1:Bg:255:ASP:OD2	1:Bg:261:HIS:ND1	2.41	0.53
2:Ab:1:U:P	1:Ac:185:ARG:HH12	2.32	0.53
1:Aa:255:ASP:OD2	1:Aa:261:HIS:ND1	2.41	0.53
1:Aq:255:ASP:OD2	1:Aq:261:HIS:ND1	2.41	0.53
1:Bc:255:ASP:OD2	1:Bc:261:HIS:ND1	2.41	0.53
1:Be:255:ASP:OD2	1:Be:261:HIS:ND1	2.41	0.53
1:Bs:255:ASP:OD2	1:Bs:261:HIS:ND1	2.41	0.53
1:By:255:ASP:OD2	1:By:261:HIS:ND1	2.41	0.53
1:Cc:255:ASP:OD2	1:Cc:261:HIS:ND1	2.41	0.53
1:Am:255:ASP:OD2	1:Am:261:HIS:ND1	2.41	0.52
1:Bi:255:ASP:OD2	1:Bi:261:HIS:ND1	2.41	0.52
1:Ao:255:ASP:OD2	1:Ao:261:HIS:ND1	2.41	0.52
1:As:255:ASP:OD2	1:As:261:HIS:ND1	2.42	0.52
1:Ci:255:ASP:OD2	1:Ci:261:HIS:ND1	2.41	0.52
1:Cs:255:ASP:OD2	1:Cs:261:HIS:ND1	2.41	0.52
1:Ae:255:ASP:OD2	1:Ae:261:HIS:ND1	2.41	0.52
1:Cq:227:LEU:CD2	2:Cr:3:U:H2'	2.40	0.52
2:Ad:1:U:OP1	2:Af:5:U:O3'	2.28	0.52
1:Au:255:ASP:OD2	1:Au:261:HIS:ND1	2.41	0.52
1:Cq:255:ASP:OD2	1:Cq:261:HIS:ND1	2.41	0.51
1:Bk:255:ASP:OD2	1:Bk:261:HIS:ND1	2.41	0.51
1:Ca:255:ASP:OD2	1:Ca:261:HIS:ND1	2.41	0.51
1:Ce:130:ILE:HG22	2:Cf:5:U:H1'	1.93	0.50
1:Aa:230:SER:HB2	2:Ab:3:U:O2'	2.11	0.50
1:Ac:86:ARG:NH1	1:Ac:206:GLU:OE1	2.44	0.50
1:Ac:160:GLN:NE2	2:Ad:1:U:O3'	2.45	0.50
1:Ag:86:ARG:NH1	1:Ag:206:GLU:OE1	2.44	0.50
1:Bo:86:ARG:NH1	1:Bo:206:GLU:OE1	2.44	0.50
1:Ce:86:ARG:NH1	1:Ce:206:GLU:OE1	2.44	0.50
1:Ac:203:ASP:OD1	2:Ad:4:U:C2	2.65	0.50
1:Aw:86:ARG:NH1	1:Aw:206:GLU:OE1	2.44	0.49
1:Bm:86:ARG:NH1	1:Bm:206:GLU:OE1	2.44	0.49
1:Ay:230:SER:HB2	2:Az:3:U:O2'	2.12	0.49
1:Ca:260:MET:HE1	1:Cg:269:VAL:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cc:86:ARG:NH1	1:Cc:206:GLU:OE1	2.44	0.49
1:Ao:260:MET:HE1	1:Au:269:VAL:HB	1.94	0.48
1:Bq:86:ARG:NH1	1:Bq:206:GLU:OE1	2.44	0.48
1:Ae:86:ARG:NH1	1:Ae:206:GLU:OE1	2.44	0.48
1:Am:260:MET:HE1	1:As:269:VAL:HB	1.95	0.48
1:Bi:260:MET:HE1	1:Bo:269:VAL:HB	1.95	0.48
1:Cs:86:ARG:NH1	1:Cs:206:GLU:OE1	2.44	0.48
1:Aq:260:MET:HE1	1:Aw:269:VAL:HB	1.95	0.48
1:Ai:86:ARG:NH1	1:Ai:206:GLU:OE1	2.44	0.48
1:Bg:260:MET:HE1	1:Bm:269:VAL:HB	1.95	0.48
1:Au:86:ARG:NH1	1:Au:206:GLU:OE1	2.44	0.47
1:Au:260:MET:HE1	1:Ba:269:VAL:HB	1.96	0.47
1:Bm:260:MET:HE1	1:Bs:269:VAL:HB	1.96	0.47
1:Be:112:ILE:HG22	1:Be:136:MET:HE1	1.97	0.47
1:Cc:260:MET:HE1	1:Ci:269:VAL:HB	1.96	0.47
1:Cm:112:ILE:HG22	1:Cm:136:MET:HE1	1.97	0.47
1:Co:112:ILE:HG22	1:Co:136:MET:HE1	1.97	0.47
1:Ac:199:ARG:NH2	1:Au:148:LYS:HD2	2.30	0.47
1:As:260:MET:HE1	1:Ay:269:VAL:HB	1.96	0.47
1:Bg:112:ILE:HG22	1:Bg:136:MET:HE1	1.97	0.47
1:Cg:86:ARG:NH1	1:Cg:206:GLU:OE1	2.44	0.47
1:Ck:86:ARG:NH1	1:Ck:206:GLU:OE1	2.44	0.47
1:Aa:260:MET:HE1	1:Ag:269:VAL:HB	1.96	0.47
1:Ac:260:MET:HE1	1:Ai:269:VAL:HB	1.96	0.47
1:Ai:112:ILE:HG22	1:Ai:136:MET:HE1	1.97	0.47
1:Ak:112:ILE:HG22	1:Ak:136:MET:HE1	1.97	0.47
1:Ce:260:MET:HE1	1:Ck:269:VAL:HB	1.96	0.47
1:Ck:112:ILE:HG22	1:Ck:136:MET:HE1	1.97	0.47
1:Am:112:ILE:HG22	1:Am:136:MET:HE1	1.97	0.47
1:Bc:112:ILE:HG22	1:Bc:136:MET:HE1	1.97	0.47
1:Bk:260:MET:HE1	1:Bq:269:VAL:HB	1.96	0.47
1:Bs:112:ILE:HG22	1:Bs:136:MET:HE1	1.97	0.47
1:Aa:199:ARG:NH2	1:As:148:LYS:HD2	2.30	0.47
1:Bk:86:ARG:NH1	1:Bk:206:GLU:OE1	2.44	0.47
1:Bq:199:ARG:NH2	1:Ci:148:LYS:HD2	2.30	0.47
1:Bu:260:MET:HE1	1:Ca:269:VAL:HB	1.97	0.47
1:By:260:MET:HE1	1:Ce:269:VAL:HB	1.95	0.47
1:Ca:73:LEU:CD1	1:Cc:175:MET:SD	3.03	0.47
2:Bh:1:U:P	2:Bj:5:U:O3'	2.73	0.47
1:Bq:112:ILE:HG22	1:Bq:136:MET:HE1	1.97	0.47
1:Cq:112:ILE:HG22	1:Cq:136:MET:HE1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:73:LEU:CD1	1:Am:175:MET:SD	3.03	0.46
1:Aq:73:LEU:CD1	1:As:175:MET:SD	3.03	0.46
1:Au:199:ARG:NH2	1:Bm:148:LYS:HD2	2.30	0.46
1:Bc:73:LEU:CD1	1:Be:175:MET:SD	3.03	0.46
1:Bi:199:ARG:NH2	1:Ca:148:LYS:HD2	2.30	0.46
1:Bu:73:LEU:CD1	1:Bw:175:MET:SD	3.03	0.46
1:Cm:73:LEU:CD1	1:Co:175:MET:SD	3.03	0.46
1:Aq:199:ARG:NH2	1:Bi:148:LYS:HD2	2.30	0.46
1:Aw:199:ARG:NH2	1:Bo:148:LYS:HD2	2.31	0.46
1:Ay:199:ARG:NH2	1:Bq:148:LYS:HD2	2.30	0.46
1:Be:86:ARG:NH1	1:Be:206:GLU:OE1	2.44	0.46
1:Bg:199:ARG:NH2	1:By:148:LYS:HD2	2.31	0.46
1:Bi:112:ILE:HG22	1:Bi:136:MET:HE1	1.97	0.46
1:Bs:199:ARG:NH2	1:Ck:148:LYS:HD2	2.30	0.46
1:Ca:112:ILE:HG22	1:Ca:136:MET:HE1	1.97	0.46
1:Ci:260:MET:HE1	1:Co:269:VAL:HB	1.97	0.46
1:Aa:112:ILE:HG22	1:Aa:136:MET:HE1	1.97	0.46
1:Ay:260:MET:HE1	1:Be:269:VAL:HB	1.97	0.46
1:Bu:112:ILE:HG22	1:Bu:136:MET:HE1	1.97	0.46
1:By:112:ILE:HG22	1:By:136:MET:HE1	1.97	0.46
1:Ce:73:LEU:CD1	1:Cg:175:MET:SD	3.03	0.46
1:Ag:112:ILE:HG22	1:Ag:136:MET:HE1	1.97	0.46
1:Ak:260:MET:HE1	1:Aq:269:VAL:HB	1.97	0.46
1:Am:86:ARG:NH1	1:Am:206:GLU:OE1	2.44	0.46
1:Ba:112:ILE:HG22	1:Ba:136:MET:HE1	1.97	0.46
1:Bc:86:ARG:NH1	1:Bc:206:GLU:OE1	2.44	0.46
1:Cg:230:SER:HB2	2:Ch:3:U:O2'	2.16	0.46
1:Ci:112:ILE:HG22	1:Ci:136:MET:HE1	1.97	0.46
1:Ac:73:LEU:CD1	1:Ae:175:MET:SD	3.03	0.46
1:Ao:86:ARG:NH1	1:Ao:206:GLU:OE1	2.44	0.46
1:Ao:112:ILE:HG22	1:Ao:136:MET:HE1	1.97	0.46
1:Aq:232:THR:HG22	1:Bi:246:GLU:HG3	1.98	0.46
1:Au:73:LEU:CD1	1:Aw:175:MET:SD	3.03	0.46
1:Ay:86:ARG:NH1	1:Ay:206:GLU:OE1	2.44	0.46
1:Ba:260:MET:HE1	1:Bg:269:VAL:HB	1.97	0.46
1:Bm:73:LEU:CD1	1:Bo:175:MET:SD	3.03	0.46
1:Cc:112:ILE:HG22	1:Cc:136:MET:HE1	1.97	0.46
1:As:112:ILE:HG22	1:As:136:MET:HE1	1.97	0.46
1:Bi:73:LEU:CD1	1:Bk:175:MET:SD	3.04	0.46
1:Bo:112:ILE:HG22	1:Bo:136:MET:HE1	1.97	0.46
1:Bu:86:ARG:NH1	1:Bu:206:GLU:OE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:227:LEU:HD22	2:Ad:3:U:H2'	1.98	0.46
1:As:199:ARG:NH2	1:Bk:148:LYS:HD2	2.31	0.46
1:Au:112:ILE:HG22	1:Au:136:MET:HE1	1.97	0.46
1:Cm:260:MET:HE1	1:Cs:269:VAL:HB	1.97	0.46
1:Ae:199:ARG:NH2	1:Aw:148:LYS:HD2	2.31	0.46
2:An:1:U:P	2:Ap:5:U:O3'	2.74	0.46
1:Bc:260:MET:HE1	1:Bi:269:VAL:HB	1.97	0.46
1:Bs:260:MET:HE1	1:By:269:VAL:HB	1.98	0.46
1:Bw:86:ARG:NH1	1:Bw:206:GLU:OE1	2.44	0.46
1:Bw:112:ILE:HG22	1:Bw:136:MET:HE1	1.97	0.46
1:Co:86:ARG:NH1	1:Co:206:GLU:OE1	2.44	0.46
2:Cp:1:U:P	1:Cq:185:ARG:HH12	2.39	0.46
1:Aw:112:ILE:HG22	1:Aw:136:MET:HE1	1.97	0.46
1:Ba:199:ARG:NH2	1:Bs:148:LYS:HD2	2.31	0.46
1:Be:199:ARG:NH2	1:Bw:148:LYS:HD2	2.31	0.46
1:Be:260:MET:HE1	1:Bk:269:VAL:HB	1.96	0.46
1:Bu:199:ARG:NH2	1:Cm:148:LYS:HD2	2.31	0.46
1:Bw:260:MET:HE1	1:Cc:269:VAL:HB	1.98	0.46
1:Cm:86:ARG:NH1	1:Cm:206:GLU:OE1	2.44	0.46
1:Ag:260:MET:HE1	1:Am:269:VAL:HB	1.97	0.46
1:Aq:112:ILE:HG22	1:Aq:136:MET:HE1	1.97	0.46
1:Aw:269:VAL:HA	1:Ay:269:VAL:HG22	1.98	0.46
1:Bm:112:ILE:HG22	1:Bm:136:MET:HE1	1.97	0.46
1:Cq:86:ARG:NH1	1:Cq:206:GLU:OE1	2.44	0.46
1:Ae:260:MET:HE1	1:Ak:269:VAL:HB	1.97	0.45
1:Am:269:VAL:HA	1:Ao:269:VAL:HG22	1.98	0.45
1:Bm:199:ARG:NH2	1:Ce:148:LYS:HD2	2.31	0.45
1:Bq:130:ILE:HG22	2:Br:5:U:H1'	1.97	0.45
1:Co:227:LEU:CD2	2:Cp:3:U:H2'	2.46	0.45
1:Ao:73:LEU:CD1	1:Aq:175:MET:SD	3.05	0.45
1:Bo:199:ARG:NH2	1:Cg:148:LYS:HD2	2.31	0.45
1:Bs:269:VAL:HA	1:Bu:269:VAL:HG22	1.99	0.45
1:By:86:ARG:NH1	1:By:206:GLU:OE1	2.44	0.45
1:Ca:86:ARG:NH1	1:Ca:206:GLU:OE1	2.44	0.45
1:Cc:73:LEU:CD1	1:Ce:175:MET:SD	3.05	0.45
1:Aa:130:ILE:HG22	2:Ab:5:U:H1'	1.98	0.45
1:Ac:86:ARG:HD2	1:Ac:206:GLU:OE2	2.17	0.45
1:Ae:230:SER:O	1:Ae:230:SER:OG	2.35	0.45
1:Ay:73:LEU:CD1	1:Ba:175:MET:SD	3.05	0.45
1:Ba:86:ARG:HD2	1:Ba:206:GLU:OE2	2.17	0.45
1:Bc:86:ARG:HD2	1:Bc:206:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:73:LEU:CD1	1:Bi:175:MET:SD	3.05	0.45
1:Bk:73:LEU:CD1	1:Bm:175:MET:SD	3.05	0.45
1:Bk:86:ARG:HD2	1:Bk:206:GLU:OE2	2.17	0.45
1:Bk:112:ILE:HG22	1:Bk:136:MET:HE1	1.97	0.45
1:By:73:LEU:CD1	1:Ca:175:MET:SD	3.05	0.45
1:Ce:112:ILE:HG22	1:Ce:136:MET:HE1	1.97	0.45
1:Cg:269:VAL:HA	1:Ci:269:VAL:HG22	1.98	0.45
1:Cq:73:LEU:CD1	1:Cs:175:MET:SD	3.05	0.45
1:Ac:112:ILE:HG22	1:Ac:136:MET:HE1	1.97	0.45
1:Ag:73:LEU:CD1	1:Ai:175:MET:SD	3.05	0.45
1:Ao:199:ARG:NH2	1:Bg:148:LYS:HD2	2.31	0.45
1:As:73:LEU:CD1	1:Au:175:MET:SD	3.05	0.45
1:Ay:112:ILE:HG22	1:Ay:136:MET:HE1	1.97	0.45
1:Bg:86:ARG:NH1	1:Bg:206:GLU:OE1	2.44	0.45
1:Bq:73:LEU:CD1	1:Bs:175:MET:SD	3.05	0.45
1:Bq:260:MET:HE1	1:Bw:269:VAL:HB	1.97	0.45
1:Cg:260:MET:HE1	1:Cm:269:VAL:HB	1.97	0.45
1:Ci:73:LEU:CD1	1:Ck:175:MET:SD	3.05	0.45
1:Co:269:VAL:HA	1:Cq:269:VAL:HG22	1.99	0.45
1:Ae:112:ILE:HG22	1:Ae:136:MET:HE1	1.97	0.45
1:Ai:73:LEU:CD1	1:Ak:175:MET:SD	3.05	0.45
1:Au:86:ARG:HD2	1:Au:206:GLU:OE2	2.17	0.45
1:Bw:86:ARG:HD2	1:Bw:206:GLU:OE2	2.17	0.45
1:Ca:86:ARG:HD2	1:Ca:206:GLU:OE2	2.17	0.45
1:Ca:199:ARG:NH2	1:Cs:148:LYS:HD2	2.31	0.45
1:Ck:260:MET:HE1	1:Cq:269:VAL:HB	1.97	0.45
1:Cs:112:ILE:HG22	1:Cs:136:MET:HE1	1.97	0.45
1:Aa:232:THR:HG22	1:As:246:GLU:HG3	1.99	0.45
1:Ai:226:ALA:HB1	2:Aj:4:U:H1'	1.98	0.45
1:Ao:232:THR:HG22	1:Bg:246:GLU:HG3	1.99	0.45
1:Aw:260:MET:HE1	1:Bc:269:VAL:HB	1.97	0.45
1:Ba:73:LEU:CD1	1:Bc:175:MET:SD	3.05	0.45
1:Bu:86:ARG:HD2	1:Bu:206:GLU:OE2	2.17	0.45
1:Bw:269:VAL:HA	1:By:269:VAL:HG22	1.98	0.45
1:Ce:86:ARG:HD2	1:Ce:206:GLU:OE2	2.17	0.45
1:Ci:86:ARG:HD2	1:Ci:206:GLU:OE2	2.17	0.45
1:Ck:86:ARG:HD2	1:Ck:206:GLU:OE2	2.17	0.45
1:Aa:73:LEU:CD1	1:Ac:175:MET:SD	3.05	0.45
1:Ac:232:THR:HG22	1:Au:246:GLU:HG3	1.99	0.45
1:As:86:ARG:HD2	1:As:206:GLU:OE2	2.17	0.45
1:Ay:86:ARG:HD2	1:Ay:206:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:199:ARG:NH2	1:Bu:148:LYS:HD2	2.31	0.45
1:Bg:232:THR:HG22	1:By:246:GLU:HG3	1.99	0.45
1:Bk:199:ARG:NH2	1:Cc:148:LYS:HD2	2.32	0.45
1:Bo:260:MET:HE1	1:Bu:269:VAL:HB	1.97	0.45
1:Bs:73:LEU:CD1	1:Bu:175:MET:SD	3.05	0.45
1:Bw:100:MET:HG3	1:Bw:110:MET:HG3	1.99	0.45
1:Cg:112:ILE:HG22	1:Cg:136:MET:HE1	1.97	0.45
1:Ck:73:LEU:CD1	1:Cm:175:MET:SD	3.05	0.45
1:Cs:86:ARG:HD2	1:Cs:206:GLU:OE2	2.17	0.45
2:Ab:1:U:C4	2:Ad:5:U:C4	3.05	0.45
1:Ag:199:ARG:NH2	1:Ay:148:LYS:HD2	2.31	0.45
1:Be:100:MET:HG3	1:Be:110:MET:HG3	1.99	0.45
1:Bg:230:SER:O	1:Bg:230:SER:OG	2.35	0.45
1:Bi:232:THR:HG22	1:Ca:246:GLU:HG3	1.99	0.45
1:Bo:73:LEU:CD1	1:Bq:175:MET:SD	3.05	0.45
1:Bo:86:ARG:HD2	1:Bo:206:GLU:OE2	2.17	0.45
1:Bs:100:MET:HG3	1:Bs:110:MET:HG3	1.99	0.45
1:Cg:73:LEU:CD1	1:Ci:175:MET:SD	3.05	0.45
1:Ck:100:MET:HG3	1:Ck:110:MET:HG3	1.99	0.45
1:Co:100:MET:HG3	1:Co:110:MET:HG3	1.99	0.45
1:Ae:73:LEU:CD1	1:Ag:175:MET:SD	3.05	0.45
1:Ae:269:VAL:HA	1:Ag:269:VAL:HG22	1.98	0.45
1:Ao:86:ARG:HD2	1:Ao:206:GLU:OE2	2.17	0.45
1:As:232:THR:HG22	1:Bk:246:GLU:HG3	1.99	0.45
1:Au:232:THR:HG22	1:Bm:246:GLU:HG3	1.98	0.45
1:Aw:73:LEU:CD1	1:Ay:175:MET:SD	3.05	0.45
1:Ba:100:MET:HG3	1:Ba:110:MET:HG3	1.99	0.45
1:Ba:269:VAL:HA	1:Bc:269:VAL:HG22	1.99	0.45
1:Be:86:ARG:HD2	1:Be:206:GLU:OE2	2.17	0.45
1:Bm:232:THR:HG22	1:Ce:246:GLU:HG3	1.98	0.45
1:Bo:269:VAL:HA	1:Bq:269:VAL:HG22	1.98	0.45
1:By:86:ARG:HD2	1:By:206:GLU:OE2	2.17	0.45
1:Co:230:SER:O	1:Co:230:SER:OG	2.35	0.45
1:Ai:269:VAL:HA	1:Ak:269:VAL:HG22	1.99	0.45
1:Ak:100:MET:HG3	1:Ak:110:MET:HG3	1.99	0.45
1:Am:86:ARG:HD2	1:Am:206:GLU:OE2	2.17	0.45
1:Am:100:MET:HG3	1:Am:110:MET:HG3	1.99	0.45
1:Aq:100:MET:HG3	1:Aq:110:MET:HG3	1.99	0.45
1:Bq:232:THR:HG22	1:Ci:246:GLU:HG3	1.98	0.45
1:Bw:199:ARG:NH2	1:Co:148:LYS:HD2	2.31	0.45
1:Cc:86:ARG:HD2	1:Cc:206:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cg:86:ARG:HD2	1:Cg:206:GLU:OE2	2.17	0.45
1:Ae:86:ARG:HD2	1:Ae:206:GLU:OE2	2.17	0.44
1:Ag:86:ARG:HD2	1:Ag:206:GLU:OE2	2.17	0.44
1:Bi:100:MET:HG3	1:Bi:110:MET:HG3	1.99	0.44
1:Bo:232:THR:HG22	1:Cg:246:GLU:HG3	1.98	0.44
1:Bs:86:ARG:HD2	1:Bs:206:GLU:OE2	2.17	0.44
1:By:199:ARG:NH2	1:Cq:148:LYS:HD2	2.31	0.44
1:Ac:201:ALA:HA	1:Ac:222:MET:HE1	2.00	0.44
1:Ai:260:MET:HE1	1:Ao:269:VAL:HB	1.98	0.44
1:Ak:86:ARG:NH1	1:Ak:206:GLU:OE1	2.44	0.44
1:Aw:201:ALA:HA	1:Aw:222:MET:HE1	2.00	0.44
1:Ay:100:MET:HG3	1:Ay:110:MET:HG3	1.99	0.44
1:Ay:201:ALA:HA	1:Ay:222:MET:HE1	2.00	0.44
1:Be:269:VAL:HA	1:Bg:269:VAL:HG22	1.98	0.44
1:Ca:232:THR:HG22	1:Cs:246:GLU:HG3	2.00	0.44
1:Cg:201:ALA:HA	1:Cg:222:MET:HE1	2.00	0.44
1:Cm:86:ARG:HD2	1:Cm:206:GLU:OE2	2.17	0.44
1:Ag:100:MET:HG3	1:Ag:110:MET:HG3	1.99	0.44
1:Ai:86:ARG:HD2	1:Ai:206:GLU:OE2	2.17	0.44
1:Am:199:ARG:NH2	1:Be:148:LYS:HD2	2.33	0.44
1:Am:232:THR:HG22	1:Be:246:GLU:HG3	2.00	0.44
1:Ao:100:MET:HG3	1:Ao:110:MET:HG3	1.99	0.44
1:Ay:269:VAL:HA	1:Ba:269:VAL:HG22	2.00	0.44
1:Bc:100:MET:HG3	1:Bc:110:MET:HG3	1.99	0.44
1:Be:232:THR:HG22	1:Bw:246:GLU:HG3	2.00	0.44
1:Bi:86:ARG:NH1	1:Bi:206:GLU:OE1	2.44	0.44
1:Bk:201:ALA:HA	1:Bk:222:MET:HE1	2.00	0.44
1:Bs:86:ARG:NH1	1:Bs:206:GLU:OE1	2.44	0.44
1:Bs:201:ALA:HA	1:Bs:222:MET:HE1	2.00	0.44
1:Ca:269:VAL:HA	1:Cc:269:VAL:HG22	1.99	0.44
1:Ce:201:ALA:HA	1:Ce:222:MET:HE1	2.00	0.44
1:Cq:86:ARG:HD2	1:Cq:206:GLU:OE2	2.17	0.44
1:Aa:86:ARG:HD2	1:Aa:206:GLU:OE2	2.17	0.44
1:Ae:201:ALA:HA	1:Ae:222:MET:HE1	2.00	0.44
1:Ai:207:ILE:HD13	1:Ai:216:LYS:HG2	2.00	0.44
1:Aq:86:ARG:HD2	1:Aq:206:GLU:OE2	2.17	0.44
1:Au:269:VAL:HA	1:Aw:269:VAL:HG22	2.00	0.44
2:Ax:1:U:P	2:Az:5:U:O3'	2.76	0.44
1:Bi:86:ARG:HD2	1:Bi:206:GLU:OE2	2.17	0.44
1:Bm:86:ARG:HD2	1:Bm:206:GLU:OE2	2.17	0.44
1:Bq:269:VAL:HA	1:Bs:269:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ca:100:MET:HG3	1:Ca:110:MET:HG3	1.99	0.44
2:Cd:1:U:P	2:Cf:5:U:O3'	2.75	0.44
1:Cq:130:ILE:HG22	2:Cr:5:U:H1'	1.99	0.44
1:Aa:201:ALA:HA	1:Aa:222:MET:HE1	2.00	0.44
1:Aa:207:ILE:HD13	1:Aa:216:LYS:HG2	2.00	0.44
1:Ai:100:MET:HG3	1:Ai:110:MET:HG3	1.99	0.44
1:Aw:86:ARG:HD2	1:Aw:206:GLU:OE2	2.17	0.44
1:Bg:86:ARG:HD2	1:Bg:206:GLU:OE2	2.17	0.44
1:Bk:232:THR:HG22	1:Cc:246:GLU:HG3	2.00	0.44
1:Bq:100:MET:HG3	1:Bq:110:MET:HG3	1.99	0.44
1:Bs:232:THR:HG22	1:Ck:246:GLU:HG3	1.99	0.44
1:Cc:207:ILE:HD13	1:Cc:216:LYS:HG2	2.00	0.44
1:Ck:207:ILE:HD13	1:Ck:216:LYS:HG2	2.00	0.44
1:Ck:269:VAL:HA	1:Cm:269:VAL:HG22	1.99	0.44
1:Cq:100:MET:HG3	1:Cq:110:MET:HG3	1.99	0.44
1:Ac:207:ILE:HD13	1:Ac:216:LYS:HG2	2.00	0.44
1:Ak:86:ARG:HD2	1:Ak:206:GLU:OE2	2.17	0.44
1:As:207:ILE:HD13	1:As:216:LYS:HG2	2.00	0.44
1:Ba:207:ILE:HD13	1:Ba:216:LYS:HG2	2.00	0.44
1:Bc:232:THR:HG22	1:Bu:246:GLU:HG3	2.00	0.44
1:Bi:201:ALA:HA	1:Bi:222:MET:HE1	2.00	0.44
1:Bm:201:ALA:HA	1:Bm:222:MET:HE1	2.00	0.44
1:Bq:201:ALA:HA	1:Bq:222:MET:HE1	2.00	0.44
1:Cc:201:ALA:HA	1:Cc:222:MET:HE1	2.00	0.44
1:Ce:207:ILE:HD13	1:Ce:216:LYS:HG2	2.00	0.44
1:Ce:269:VAL:HA	1:Cg:269:VAL:HG22	2.00	0.44
1:Cs:201:ALA:HA	1:Cs:222:MET:HE1	2.00	0.44
1:Cs:207:ILE:HD13	1:Cs:216:LYS:HG2	2.00	0.44
1:Ae:207:ILE:HD13	1:Ae:216:LYS:HG2	2.00	0.44
1:Ag:207:ILE:HD13	1:Ag:216:LYS:HG2	2.00	0.44
1:Ai:199:ARG:NH2	1:Ba:148:LYS:HD2	2.33	0.44
1:Aq:86:ARG:NH1	1:Aq:206:GLU:OE1	2.44	0.44
1:As:86:ARG:NH1	1:As:206:GLU:OE1	2.44	0.44
1:Bk:207:ILE:HD13	1:Bk:216:LYS:HG2	2.00	0.44
1:Bu:232:THR:HG22	1:Cm:246:GLU:HG3	2.00	0.44
1:Ca:207:ILE:HD13	1:Ca:216:LYS:HG2	2.00	0.44
1:Cg:100:MET:HG3	1:Cg:110:MET:HG3	1.99	0.44
1:Cg:207:ILE:HD13	1:Cg:216:LYS:HG2	2.00	0.44
1:Ci:207:ILE:HD13	1:Ci:216:LYS:HG2	2.00	0.44
1:Co:73:LEU:CD1	1:Cq:175:MET:SD	3.06	0.44
1:Ak:201:ALA:HA	1:Ak:222:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:207:ILE:HD13	1:Ak:216:LYS:HG2	2.00	0.44
1:Ak:269:VAL:HA	1:Am:269:VAL:HG22	2.00	0.44
1:Am:73:LEU:CD1	1:Ao:175:MET:SD	3.06	0.44
1:Aq:207:ILE:HD13	1:Aq:216:LYS:HG2	2.00	0.44
1:Aw:207:ILE:HD13	1:Aw:216:LYS:HG2	2.00	0.44
1:Aw:232:THR:HG22	1:Bo:246:GLU:HG3	1.99	0.44
1:Ay:207:ILE:HD13	1:Ay:216:LYS:HG2	2.00	0.44
1:Be:73:LEU:CD1	1:Bg:175:MET:SD	3.06	0.44
1:Bg:100:MET:HG3	1:Bg:110:MET:HG3	1.99	0.44
1:Bs:207:ILE:HD13	1:Bs:216:LYS:HG2	2.00	0.44
1:Bu:207:ILE:HD13	1:Bu:216:LYS:HG2	2.00	0.44
1:Bu:269:VAL:HA	1:Bw:269:VAL:HG22	2.00	0.44
1:Bw:73:LEU:CD1	1:By:175:MET:SD	3.06	0.44
1:Co:86:ARG:HD2	1:Co:206:GLU:OE2	2.17	0.44
1:Ak:199:ARG:NH2	1:Bc:148:LYS:HD2	2.33	0.44
1:Am:230:SER:HB2	2:An:3:U:O2'	2.17	0.44
1:Au:207:ILE:HD13	1:Au:216:LYS:HG2	2.00	0.44
1:Be:207:ILE:HD13	1:Be:216:LYS:HG2	2.00	0.44
1:Bk:100:MET:HG3	1:Bk:110:MET:HG3	1.99	0.44
1:Bm:207:ILE:HD13	1:Bm:216:LYS:HG2	2.00	0.44
1:Bu:100:MET:HG3	1:Bu:110:MET:HG3	1.99	0.44
1:Bu:201:ALA:HA	1:Bu:222:MET:HE1	2.00	0.44
1:Bw:207:ILE:HD13	1:Bw:216:LYS:HG2	2.00	0.44
1:By:100:MET:HG3	1:By:110:MET:HG3	1.99	0.44
1:By:230:SER:O	1:By:230:SER:OG	2.35	0.44
1:By:232:THR:HG22	1:Cq:246:GLU:HG3	2.00	0.44
1:Cc:100:MET:HG3	1:Cc:110:MET:HG3	1.99	0.44
1:Ce:100:MET:HG3	1:Ce:110:MET:HG3	1.99	0.44
1:Cm:207:ILE:HD13	1:Cm:216:LYS:HG2	2.00	0.44
1:Cq:201:ALA:HA	1:Cq:222:MET:HE1	2.00	0.44
1:Cs:100:MET:HG3	1:Cs:110:MET:HG3	1.99	0.44
1:Ac:269:VAL:HA	1:Ae:269:VAL:HG22	2.00	0.43
1:Ae:100:MET:HG3	1:Ae:110:MET:HG3	1.99	0.43
1:Ai:201:ALA:HA	1:Ai:222:MET:HE1	2.00	0.43
1:Am:201:ALA:HA	1:Am:222:MET:HE1	2.00	0.43
1:Ao:207:ILE:HD13	1:Ao:216:LYS:HG2	2.00	0.43
1:Au:201:ALA:HA	1:Au:222:MET:HE1	2.00	0.43
1:Ba:201:ALA:HA	1:Ba:222:MET:HE1	2.00	0.43
1:Bg:207:ILE:HD13	1:Bg:216:LYS:HG2	2.00	0.43
1:Bo:100:MET:HG3	1:Bo:110:MET:HG3	1.99	0.43
1:Bo:207:ILE:HD13	1:Bo:216:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bq:86:ARG:HD2	1:Bq:206:GLU:OE2	2.16	0.43
1:Cc:269:VAL:HA	1:Cc:269:VAL:HG22	2.00	0.43
1:Ci:100:MET:HG3	1:Ci:110:MET:HG3	1.99	0.43
1:Ci:201:ALA:HA	1:Ci:222:MET:HE1	2.00	0.43
1:Cm:100:MET:HG3	1:Cm:110:MET:HG3	1.99	0.43
1:Cq:207:ILE:HD13	1:Cq:216:LYS:HG2	2.00	0.43
1:As:100:MET:HG3	1:As:110:MET:HG3	1.99	0.43
1:Ay:232:THR:HG22	1:Bq:246:GLU:HG3	1.99	0.43
1:Ba:232:THR:HG22	1:Bs:246:GLU:HG3	2.00	0.43
1:Bc:207:ILE:HD13	1:Bc:216:LYS:HG2	2.00	0.43
1:Bi:207:ILE:HD13	1:Bi:216:LYS:HG2	2.00	0.43
1:Bq:207:ILE:HD13	1:Bq:216:LYS:HG2	2.00	0.43
1:Co:201:ALA:HA	1:Co:222:MET:HE1	2.00	0.43
1:Aa:269:VAL:HA	1:Ac:269:VAL:HG22	2.00	0.43
1:Ao:201:ALA:HA	1:Ao:222:MET:HE1	2.00	0.43
1:Aq:201:ALA:HA	1:Aq:222:MET:HE1	2.00	0.43
1:Bm:100:MET:HG3	1:Bm:110:MET:HG3	1.99	0.43
1:Bw:232:THR:HG22	1:Co:246:GLU:HG3	2.00	0.43
1:By:207:ILE:HD13	1:By:216:LYS:HG2	2.00	0.43
1:Cc:230:SER:HB2	2:Cd:3:U:O2'	2.19	0.43
1:Am:207:ILE:HD13	1:Am:216:LYS:HG2	2.00	0.43
1:Bg:201:ALA:HA	1:Bg:222:MET:HE1	2.00	0.43
1:Ci:71:HIS:O	1:Ci:75:TYR:N	2.51	0.43
1:Aw:100:MET:HG3	1:Aw:110:MET:HG3	1.99	0.43
1:Ba:86:ARG:NH1	1:Ba:206:GLU:OE1	2.44	0.43
1:Bi:269:VAL:HA	1:Bk:269:VAL:HG22	2.00	0.43
1:Bs:71:HIS:O	1:Bs:75:TYR:N	2.51	0.43
1:Cm:269:VAL:HA	1:Co:269:VAL:HG22	2.00	0.43
1:Co:207:ILE:HD13	1:Co:216:LYS:HG2	2.00	0.43
1:Ac:100:MET:HG3	1:Ac:110:MET:HG3	1.99	0.43
1:Ag:201:ALA:HA	1:Ag:222:MET:HE1	2.00	0.43
1:Ci:269:VAL:HA	1:Ck:269:VAL:HG22	2.00	0.43
1:Aa:100:MET:HG3	1:Aa:110:MET:HG3	1.99	0.43
1:Bk:269:VAL:HA	1:Bm:269:VAL:HG22	2.00	0.43
1:Bm:72:LEU:HB2	1:Bo:115:ASN:ND2	2.34	0.43
1:Bw:201:ALA:HA	1:Bw:222:MET:HE1	2.00	0.43
1:Cm:201:ALA:HA	1:Cm:222:MET:HE1	2.00	0.43
1:Ae:232:THR:HG22	1:Aw:246:GLU:HG3	2.00	0.43
2:An:1:U:OP1	2:Ap:5:U:H3'	2.19	0.43
1:As:201:ALA:HA	1:As:222:MET:HE1	2.00	0.43
1:As:269:VAL:HA	1:Au:269:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:100:MET:HG3	1:Au:110:MET:HG3	1.99	0.43
1:Bo:201:ALA:HA	1:Bo:222:MET:HE1	2.00	0.43
1:Ae:71:HIS:O	1:Ae:75:TYR:N	2.51	0.43
1:Ag:269:VAL:HA	1:Ai:269:VAL:HG22	2.00	0.43
1:Bc:71:HIS:O	1:Bc:75:TYR:N	2.51	0.43
1:Bg:269:VAL:HA	1:Bi:269:VAL:HG22	2.01	0.43
1:Ck:201:ALA:HA	1:Ck:222:MET:HE1	2.00	0.43
1:Ag:71:HIS:O	1:Ag:75:TYR:N	2.51	0.43
1:Ak:232:THR:HG22	1:Bc:246:GLU:HG3	2.01	0.43
1:Bm:269:VAL:HA	1:Bo:269:VAL:HG22	2.00	0.43
1:Ci:86:ARG:NH1	1:Ci:206:GLU:OE1	2.44	0.43
1:Bc:269:VAL:HA	1:Be:269:VAL:HG22	2.00	0.42
1:By:201:ALA:HA	1:By:222:MET:HE1	2.00	0.42
1:Ca:201:ALA:HA	1:Ca:222:MET:HE1	2.00	0.42
2:Ch:1:U:P	2:Cj:5:U:O3'	2.77	0.42
1:Cq:269:VAL:HA	1:Cs:269:VAL:HG22	2.01	0.42
1:Ac:72:LEU:HB2	1:Ae:115:ASN:ND2	2.34	0.42
1:Ao:269:VAL:HA	1:Aq:269:VAL:HG22	2.01	0.42
1:Bc:201:ALA:HA	1:Bc:222:MET:HE1	2.00	0.42
1:Aa:86:ARG:NH1	1:Aa:206:GLU:OE1	2.44	0.42
2:Al:1:U:P	2:An:5:U:O3'	2.77	0.42
2:At:1:U:P	2:Av:5:U:O3'	2.77	0.42
1:Aw:71:HIS:O	1:Aw:75:TYR:N	2.52	0.42
1:Be:201:ALA:HA	1:Be:222:MET:HE1	2.00	0.42
1:Ck:71:HIS:O	1:Ck:75:TYR:N	2.51	0.42
1:Am:71:HIS:O	1:Am:75:TYR:N	2.52	0.42
2:Bl:1:U:P	2:Bn:5:U:O3'	2.78	0.42
1:Au:72:LEU:HB2	1:Aw:115:ASN:ND2	2.34	0.42
1:Ce:72:LEU:HB2	1:Cg:115:ASN:ND2	2.34	0.42
1:Ag:232:THR:HG22	1:Ay:246:GLU:HG3	2.00	0.42
1:Am:230:SER:O	1:Am:230:SER:OG	2.35	0.42
1:Au:71:HIS:O	1:Au:75:TYR:N	2.52	0.42
1:Bc:230:SER:O	1:Bc:230:SER:OG	2.35	0.42
1:Ai:232:THR:HG22	1:Ba:246:GLU:HG3	2.01	0.42
1:Ao:230:SER:O	1:Ao:230:SER:OG	2.35	0.42
1:Co:71:HIS:O	1:Co:75:TYR:N	2.52	0.42
1:Aa:227:LEU:CD2	2:Ab:3:U:H2'	2.50	0.42
1:Ag:72:LEU:HB2	1:Ai:115:ASN:ND2	2.35	0.42
1:Am:234:MET:HE3	1:Be:246:GLU:OE2	2.20	0.42
1:Aq:230:SER:O	1:Aq:230:SER:OG	2.35	0.42
1:Bu:71:HIS:O	1:Bu:75:TYR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ci:72:LEU:HB2	1:Ck:115:ASN:ND2	2.35	0.42
2:Cj:1:U:P	2:Cl:5:U:O3'	2.77	0.42
1:Co:130:ILE:HG22	2:Cp:5:U:H1'	2.02	0.42
1:Aq:228:LYS:HG3	1:Aq:229:ASN:N	2.35	0.42
1:As:71:HIS:O	1:As:75:TYR:N	2.51	0.42
1:Be:137:MET:SD	1:Be:142:GLN:HG3	2.60	0.42
1:Bm:71:HIS:O	1:Bm:75:TYR:N	2.52	0.42
1:Ca:228:LYS:HG3	1:Ca:229:ASN:N	2.35	0.42
1:Ak:234:MET:HE3	1:Bc:246:GLU:OE2	2.20	0.42
1:Ba:228:LYS:HG3	1:Ba:229:ASN:N	2.35	0.42
1:Bc:228:LYS:HG3	1:Bc:229:ASN:N	2.35	0.42
1:Cm:137:MET:SD	1:Cm:142:GLN:HG3	2.60	0.42
1:Cq:71:HIS:O	1:Cq:75:TYR:N	2.51	0.42
1:Ac:137:MET:SD	1:Ac:142:GLN:HG3	2.60	0.41
1:As:228:LYS:HG3	1:As:229:ASN:N	2.35	0.41
1:Bg:72:LEU:HB2	1:Bi:115:ASN:ND2	2.35	0.41
1:Bi:228:LYS:HG3	1:Bi:229:ASN:N	2.35	0.41
1:Bk:234:MET:HE3	1:Cc:246:GLU:OE2	2.20	0.41
1:Bu:160:GLN:HE21	2:Bv:2:U:P	2.43	0.41
1:By:137:MET:SD	1:By:142:GLN:HG3	2.60	0.41
1:Cc:130:ILE:HG22	2:Cd:5:U:H1'	2.02	0.41
1:Cc:228:LYS:HG3	1:Cc:229:ASN:N	2.35	0.41
1:Cq:228:LYS:HG3	1:Cq:229:ASN:N	2.35	0.41
1:Ac:228:LYS:HG3	1:Ac:229:ASN:N	2.35	0.41
1:Ao:234:MET:HE3	1:Bg:246:GLU:OE2	2.20	0.41
1:Ay:71:HIS:O	1:Ay:75:TYR:N	2.51	0.41
2:Bf:1:U:P	2:Bh:5:U:O3'	2.78	0.41
1:Bi:72:LEU:HB2	1:Bk:115:ASN:ND2	2.35	0.41
1:Bq:47:PRO:HG3	1:Ck:109:SER:HB2	2.02	0.41
1:Bq:228:LYS:HG3	1:Bq:229:ASN:N	2.35	0.41
1:Bs:228:LYS:HG3	1:Bs:229:ASN:N	2.35	0.41
1:Bu:137:MET:SD	1:Bu:142:GLN:HG3	2.60	0.41
1:Ce:137:MET:SD	1:Ce:142:GLN:HG3	2.60	0.41
1:Cg:137:MET:SD	1:Cg:142:GLN:HG3	2.60	0.41
1:Aa:228:LYS:HG3	1:Aa:229:ASN:N	2.35	0.41
1:Ai:71:HIS:O	1:Ai:75:TYR:N	2.51	0.41
1:Ak:137:MET:SD	1:Ak:142:GLN:HG3	2.60	0.41
1:Ay:72:LEU:HB2	1:Ba:115:ASN:ND2	2.35	0.41
1:Bg:228:LYS:HG3	1:Bg:229:ASN:N	2.35	0.41
1:Bk:71:HIS:O	1:Bk:75:TYR:N	2.52	0.41
1:Bk:72:LEU:HB2	1:Bm:115:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:228:LYS:HG3	1:Bk:229:ASN:N	2.35	0.41
1:Bo:71:HIS:O	1:Bo:75:TYR:N	2.51	0.41
1:Bq:137:MET:SD	1:Bq:142:GLN:HG3	2.60	0.41
1:Bu:230:SER:O	1:Bu:230:SER:OG	2.35	0.41
1:By:234:MET:HE3	1:Cq:246:GLU:OE2	2.21	0.41
1:Ca:234:MET:HE3	1:Cs:246:GLU:OE2	2.20	0.41
1:Cq:137:MET:SD	1:Cq:142:GLN:HG3	2.60	0.41
1:Am:137:MET:SD	1:Am:142:GLN:HG3	2.60	0.41
1:Ao:137:MET:SD	1:Ao:142:GLN:HG3	2.60	0.41
1:As:137:MET:SD	1:As:142:GLN:HG3	2.60	0.41
1:Ay:228:LYS:HG3	1:Ay:229:ASN:N	2.35	0.41
1:Bi:137:MET:SD	1:Bi:142:GLN:HG3	2.60	0.41
1:Bo:137:MET:SD	1:Bo:142:GLN:HG3	2.60	0.41
1:Bu:228:LYS:HG3	1:Bu:229:ASN:N	2.35	0.41
1:By:71:HIS:O	1:By:75:TYR:N	2.51	0.41
1:By:269:VAL:HA	1:Ca:269:VAL:HG22	2.01	0.41
2:Cl:1:U:P	2:Cn:5:U:O3'	2.78	0.41
1:Co:230:SER:HB2	2:Cp:3:U:O2'	2.20	0.41
1:Cs:228:LYS:HG3	1:Cs:229:ASN:N	2.35	0.41
1:Ae:72:LEU:HB2	1:Ag:115:ASN:ND2	2.36	0.41
1:Ae:137:MET:SD	1:Ae:142:GLN:HG3	2.60	0.41
1:Ak:228:LYS:HG3	1:Ak:229:ASN:N	2.35	0.41
1:Au:137:MET:SD	1:Au:142:GLN:HG3	2.60	0.41
2:Av:1:U:P	2:Ax:5:U:O3'	2.79	0.41
1:Ay:137:MET:SD	1:Ay:142:GLN:HG3	2.60	0.41
1:Ba:137:MET:SD	1:Ba:142:GLN:HG3	2.60	0.41
1:Be:71:HIS:O	1:Be:75:TYR:N	2.51	0.41
1:Bm:228:LYS:HG3	1:Bm:229:ASN:N	2.35	0.41
1:Bo:72:LEU:HB2	1:Bq:115:ASN:ND2	2.36	0.41
1:Bo:234:MET:HE3	1:Cg:246:GLU:OE2	2.21	0.41
1:Bq:72:LEU:HB2	1:Bs:115:ASN:ND2	2.35	0.41
2:Ch:1:U:OP1	2:Cj:5:U:H3'	2.21	0.41
1:Ck:228:LYS:HG3	1:Ck:229:ASN:N	2.35	0.41
1:Cq:72:LEU:HB2	1:Cs:115:ASN:ND2	2.35	0.41
1:Cq:230:SER:HB2	2:Cr:3:U:O2'	2.20	0.41
1:Aa:137:MET:SD	1:Aa:142:GLN:HG3	2.60	0.41
1:Ai:234:MET:HE3	1:Ba:246:GLU:OE2	2.20	0.41
1:As:72:LEU:HB2	1:Au:115:ASN:ND2	2.35	0.41
1:Ba:72:LEU:HB2	1:Be:115:ASN:ND2	2.36	0.41
1:Be:228:LYS:HG3	1:Be:229:ASN:N	2.35	0.41
1:Bi:71:HIS:O	1:Bi:75:TYR:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:226:ALA:HB1	2:Bj:4:U:H1'	2.01	0.41
1:Bm:48:ARG:NH2	1:Cg:141:GLU:OE2	2.54	0.41
2:Bn:1:U:P	2:Bp:5:U:O3'	2.79	0.41
1:By:72:LEU:HB2	1:Ca:115:ASN:ND2	2.35	0.41
1:Ca:71:HIS:O	1:Ca:75:TYR:N	2.51	0.41
1:Cc:71:HIS:O	1:Cc:75:TYR:N	2.52	0.41
1:Cg:72:LEU:HB2	1:Ci:115:ASN:ND2	2.36	0.41
1:Ai:72:LEU:HB2	1:Ak:115:ASN:ND2	2.36	0.41
1:Ak:48:ARG:NH2	1:Be:141:GLU:OE2	2.52	0.41
1:Bm:234:MET:HE3	1:Ce:246:GLU:OE2	2.21	0.41
1:Bo:228:LYS:HG3	1:Bo:229:ASN:N	2.35	0.41
1:Bw:137:MET:SD	1:Bw:142:GLN:HG3	2.60	0.41
1:Bw:234:MET:HE3	1:Co:246:GLU:OE2	2.21	0.41
1:Ci:137:MET:SD	1:Ci:142:GLN:HG3	2.60	0.41
1:Ck:72:LEU:HB2	1:Cm:115:ASN:ND2	2.36	0.41
1:Cm:176:ARG:HE	1:Cm:176:ARG:HB3	1.80	0.41
1:Cm:228:LYS:HG3	1:Cm:229:ASN:N	2.35	0.41
2:Cn:1:U:P	2:Cp:5:U:O3'	2.78	0.41
1:Co:137:MET:SD	1:Co:142:GLN:HG3	2.60	0.41
1:Cq:230:SER:O	1:Cq:230:SER:OG	2.35	0.41
1:Aa:230:SER:O	1:Aa:230:SER:OG	2.35	0.41
1:Ai:137:MET:SD	1:Ai:142:GLN:HG3	2.60	0.41
1:Aq:137:MET:SD	1:Aq:142:GLN:HG3	2.60	0.41
1:Aq:269:VAL:HA	1:As:269:VAL:HG22	2.01	0.41
1:Bk:137:MET:SD	1:Bk:142:GLN:HG3	2.60	0.41
1:Bm:137:MET:SD	1:Bm:142:GLN:HG3	2.60	0.41
1:Ce:71:HIS:O	1:Ce:75:TYR:N	2.51	0.41
1:Ac:123:GLU:O	1:Ac:185:ARG:HB3	2.21	0.41
1:Ag:228:LYS:HG3	1:Ag:229:ASN:N	2.35	0.41
2:Ah:1:U:P	2:Aj:5:U:O3'	2.79	0.41
1:Ai:228:LYS:HG3	1:Ai:229:ASN:N	2.35	0.41
1:Ao:71:HIS:O	1:Ao:75:TYR:N	2.51	0.41
1:Aq:234:MET:HE3	1:Bi:246:GLU:OE2	2.21	0.41
1:Au:106:GLU:HG2	1:Au:108:SER:H	1.86	0.41
1:Aw:137:MET:SD	1:Aw:142:GLN:HG3	2.60	0.41
1:Aw:228:LYS:HG3	1:Aw:229:ASN:N	2.35	0.41
1:Bc:234:MET:HE3	1:Bu:246:GLU:OE2	2.20	0.41
1:Be:234:MET:HE3	1:Bw:246:GLU:OE2	2.21	0.41
1:Bi:176:ARG:HE	1:Bi:176:ARG:HB3	1.80	0.41
1:Bs:230:SER:O	1:Bs:230:SER:OG	2.35	0.41
1:By:228:LYS:HG3	1:By:229:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ca:106:GLU:HG2	1:Ca:108:SER:H	1.86	0.41
1:Ca:137:MET:SD	1:Ca:142:GLN:HG3	2.60	0.41
1:Cg:106:GLU:HG2	1:Cg:108:SER:H	1.86	0.41
1:Ci:228:LYS:HG3	1:Ci:229:ASN:N	2.35	0.41
1:Ck:106:GLU:HG2	1:Ck:108:SER:H	1.86	0.41
1:Cq:106:GLU:HG2	1:Cq:108:SER:H	1.86	0.41
1:Cq:203:ASP:OD1	2:Cr:4:U:C2	2.74	0.41
1:Aa:72:LEU:HB2	1:Ac:115:ASN:ND2	2.35	0.41
1:Ae:106:GLU:HG2	1:Ae:108:SER:H	1.86	0.41
1:Ao:72:LEU:HB2	1:Aq:115:ASN:ND2	2.35	0.41
1:Ao:106:GLU:HG2	1:Ao:108:SER:H	1.86	0.41
1:Aq:72:LEU:HB2	1:As:115:ASN:ND2	2.35	0.41
1:As:123:GLU:O	1:As:185:ARG:HB3	2.21	0.41
1:As:234:MET:HE3	1:Bk:246:GLU:OE2	2.21	0.41
1:Aw:72:LEU:HB2	1:Ay:115:ASN:ND2	2.36	0.41
1:Ay:106:GLU:HG2	1:Ay:108:SER:H	1.86	0.41
2:Az:1:U:P	2:Bb:5:U:O3'	2.79	0.41
1:Bc:72:LEU:HB2	1:Be:115:ASN:ND2	2.36	0.41
1:Bk:106:GLU:HG2	1:Bk:108:SER:H	1.86	0.41
1:Bu:106:GLU:HG2	1:Bu:108:SER:H	1.86	0.41
1:Cc:137:MET:SD	1:Cc:142:GLN:HG3	2.60	0.41
1:Ce:123:GLU:O	1:Ce:185:ARG:HB3	2.21	0.41
1:Ce:176:ARG:HE	1:Ce:176:ARG:HB3	1.80	0.41
1:Cs:106:GLU:HG2	1:Cs:108:SER:H	1.86	0.41
1:Ac:71:HIS:O	1:Ac:75:TYR:N	2.51	0.40
1:Ae:228:LYS:HG3	1:Ae:229:ASN:N	2.35	0.40
1:Ai:106:GLU:HG2	1:Ai:108:SER:H	1.86	0.40
1:Am:106:GLU:HG2	1:Am:108:SER:H	1.86	0.40
1:Aw:234:MET:HE3	1:Bo:246:GLU:OE2	2.21	0.40
1:Ay:47:PRO:HG3	1:Bs:109:SER:HB2	2.03	0.40
1:Bc:106:GLU:HG2	1:Bc:108:SER:H	1.86	0.40
1:Be:106:GLU:HG2	1:Be:108:SER:H	1.86	0.40
1:Bg:137:MET:SD	1:Bg:142:GLN:HG3	2.60	0.40
1:Bs:137:MET:SD	1:Bs:142:GLN:HG3	2.60	0.40
1:Bu:72:LEU:HB2	1:Bw:115:ASN:ND2	2.36	0.40
1:Ca:123:GLU:O	1:Ca:185:ARG:HB3	2.21	0.40
1:Cc:106:GLU:HG2	1:Cc:108:SER:H	1.86	0.40
1:Ck:137:MET:SD	1:Ck:142:GLN:HG3	2.60	0.40
1:Cq:123:GLU:O	1:Cq:185:ARG:HB3	2.21	0.40
1:Cq:170:GLU:HG2	1:Cq:199:ARG:HE	1.87	0.40
1:Cs:71:HIS:O	1:Cs:75:TYR:N	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:137:MET:SD	1:Ag:142:GLN:HG3	2.60	0.40
1:Ag:170:GLU:HG2	1:Ag:199:ARG:HE	1.87	0.40
1:Aw:170:GLU:HG2	1:Aw:199:ARG:HE	1.87	0.40
1:Bi:123:GLU:O	1:Bi:185:ARG:HB3	2.21	0.40
1:Bu:234:MET:HE3	1:Cm:246:GLU:OE2	2.21	0.40
1:Cc:72:LEU:HB2	1:Ce:115:ASN:ND2	2.35	0.40
1:Cq:227:LEU:HD22	2:Cr:3:U:H2'	2.03	0.40
1:Ac:106:GLU:HG2	1:Ac:108:SER:H	1.86	0.40
1:Ag:234:MET:HE3	1:Ay:246:GLU:OE2	2.21	0.40
1:Ak:72:LEU:HB2	1:Am:115:ASN:ND2	2.36	0.40
1:Ao:228:LYS:HG3	1:Ao:229:ASN:N	2.35	0.40
1:Au:48:ARG:NH2	1:Bo:141:GLU:OE2	2.55	0.40
1:Bc:137:MET:SD	1:Bc:142:GLN:HG3	2.60	0.40
1:Bk:123:GLU:O	1:Bk:185:ARG:HB3	2.21	0.40
1:Bo:123:GLU:O	1:Bo:185:ARG:HB3	2.21	0.40
1:Bq:176:ARG:HE	1:Bq:176:ARG:HB3	1.80	0.40
2:Bv:1:U:P	2:Bx:5:U:O3'	2.78	0.40
1:Bw:228:LYS:HG3	1:Bw:229:ASN:N	2.35	0.40
1:Cg:228:LYS:HG3	1:Cg:229:ASN:N	2.35	0.40
1:Cm:72:LEU:HB2	1:Co:115:ASN:ND2	2.36	0.40
1:Cs:137:MET:SD	1:Cs:142:GLN:HG3	2.60	0.40
1:Am:170:GLU:HG2	1:Am:199:ARG:HE	1.87	0.40
1:Ao:48:ARG:NH2	1:Bi:141:GLU:OE2	2.55	0.40
1:Ao:123:GLU:O	1:Ao:185:ARG:HB3	2.21	0.40
1:Ao:170:GLU:HG2	1:Ao:199:ARG:HE	1.87	0.40
1:Aq:48:ARG:NH2	1:Bk:141:GLU:OE2	2.55	0.40
1:As:170:GLU:HG2	1:As:199:ARG:HE	1.87	0.40
1:Au:47:PRO:HG3	1:Bo:109:SER:HB2	2.04	0.40
1:Ba:123:GLU:O	1:Ba:185:ARG:HB3	2.21	0.40
1:Be:170:GLU:HG2	1:Be:199:ARG:HE	1.87	0.40
1:Bm:47:PRO:HG3	1:Cg:109:SER:HB2	2.03	0.40
1:Bq:106:GLU:HG2	1:Bq:108:SER:H	1.86	0.40
1:Bq:234:MET:HE3	1:Ci:246:GLU:OE2	2.22	0.40
1:Bs:170:GLU:HG2	1:Bs:199:ARG:HE	1.87	0.40
1:Bu:123:GLU:O	1:Bu:185:ARG:HB3	2.21	0.40
1:Ce:228:LYS:HG3	1:Ce:229:ASN:N	2.35	0.40
1:Ci:170:GLU:HG2	1:Ci:199:ARG:HE	1.87	0.40
1:Ck:170:GLU:HG2	1:Ck:199:ARG:HE	1.87	0.40
1:Cm:71:HIS:O	1:Cm:75:TYR:N	2.51	0.40
1:Co:228:LYS:HG3	1:Co:229:ASN:N	2.35	0.40
1:Aa:234:MET:HE3	1:As:246:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:47:PRO:HG3	1:Aw:109:SER:HB2	2.04	0.40
1:Ai:48:ARG:NH2	1:Bc:141:GLU:OE2	2.54	0.40
1:Au:234:MET:HE3	1:Bm:246:GLU:OE2	2.22	0.40
1:Aw:123:GLU:O	1:Aw:185:ARG:HB3	2.21	0.40
1:Ay:123:GLU:O	1:Ay:185:ARG:HB3	2.21	0.40
1:Ba:234:MET:HE3	1:Bs:246:GLU:OE2	2.21	0.40
1:Bc:48:ARG:NH2	1:Bw:141:GLU:OE2	2.54	0.40
1:Bg:234:MET:HE3	1:By:246:GLU:OE2	2.21	0.40
1:Bi:170:GLU:HG2	1:Bi:199:ARG:HE	1.87	0.40
1:Bo:106:GLU:HG2	1:Bo:108:SER:H	1.86	0.40
1:Bo:170:GLU:HG2	1:Bo:199:ARG:HE	1.87	0.40
1:Bs:106:GLU:HG2	1:Bs:108:SER:H	1.86	0.40
1:Ca:170:GLU:HG2	1:Ca:199:ARG:HE	1.87	0.40
1:Ce:170:GLU:HG2	1:Ce:199:ARG:HE	1.87	0.40
1:Ci:123:GLU:O	1:Ci:185:ARG:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Aa	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
1	Ag	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ai	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ak	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Am	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ao	224/269 (83%)	221 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	221 (99%)	3 (1%)	0	100	100
1	Bc	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Be	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bg	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Bi	224/269 (83%)	221 (99%)	3 (1%)	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%)	221 (99%)	3 (1%)	0	100	100
1	Bw	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	By	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Ca	224/269 (83%)	221 (99%)	3 (1%)	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%)	221 (99%)	3 (1%)	0	100	100
1	Cm	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Co	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Cq	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
1	Cs	224/269 (83%)	221 (99%)	3 (1%)	0	100	100
All	All	8064/9684 (83%)	7956 (99%)	108 (1%)	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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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 (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	79	GLN
1	Aa	131	ASN
1	Aa	240	ASN
1	Aa	251	HIS
1	Ac	79	GLN
1	Ac	131	ASN
1	Ac	240	ASN
1	Ae	79	GLN
1	Ae	131	ASN
1	Ae	240	ASN
1	Ag	79	GLN
1	Ag	131	ASN
1	Ag	240	ASN
1	Ai	79	GLN
1	Ai	131	ASN
1	Ai	240	ASN
1	Ak	79	GLN
1	Ak	131	ASN
1	Ak	240	ASN
1	Am	79	GLN
1	Am	131	ASN

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Mol	Chain	Res	Type
1	Am	240	ASN
1	Ao	79	GLN
1	Ao	94	ASN
1	Ao	131	ASN
1	Ao	240	ASN
1	Aq	131	ASN
1	Aq	240	ASN
1	As	79	GLN
1	As	240	ASN
1	Au	79	GLN
1	Au	240	ASN
1	Aw	79	GLN
1	Aw	240	ASN
1	Ay	79	GLN
1	Ay	240	ASN
1	Ba	79	GLN
1	Ba	115	ASN
1	Ba	240	ASN
1	Bc	79	GLN
1	Bc	240	ASN
1	Be	79	GLN
1	Be	240	ASN
1	Bg	240	ASN
1	Bi	79	GLN
1	Bi	94	ASN
1	Bi	240	ASN
1	Bk	79	GLN
1	Bk	240	ASN
1	Bm	240	ASN
1	Bo	79	GLN
1	Bo	240	ASN
1	Bq	79	GLN
1	Bq	240	ASN
1	Bs	79	GLN
1	Bs	240	ASN
1	Bu	79	GLN
1	Bu	240	ASN
1	Bw	79	GLN
1	Bw	240	ASN
1	By	79	GLN
1	By	240	ASN
1	Ca	240	ASN

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Mol	Chain	Res	Type
1	Cc	79	GLN
1	Cc	240	ASN
1	Ce	115	ASN
1	Ce	191	ASN
1	Ce	240	ASN
1	Cg	79	GLN
1	Cg	240	ASN
1	Ci	79	GLN
1	Ci	115	ASN
1	Ci	240	ASN
1	Ck	79	GLN
1	Ck	240	ASN
1	Cm	79	GLN
1	Cm	191	ASN
1	Cm	240	ASN
1	Co	79	GLN
1	Co	240	ASN
1	Cq	240	ASN
1	Cs	240	ASN

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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
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.

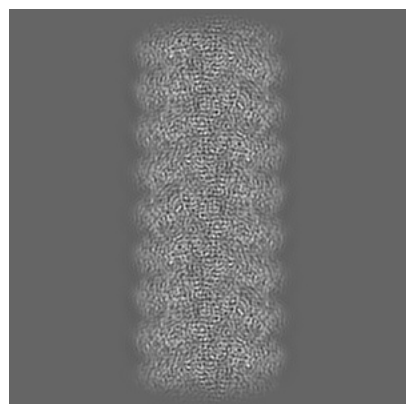
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53791. These allow visual inspection of the internal detail of the map and identification of artifacts.

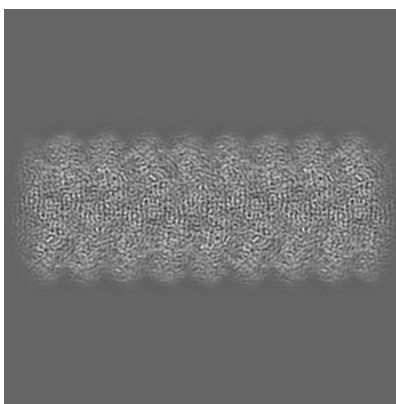
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

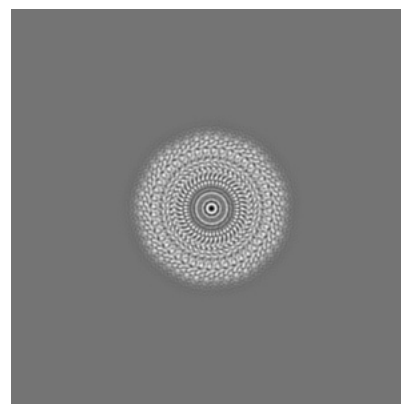
6.1.1 Primary map



X

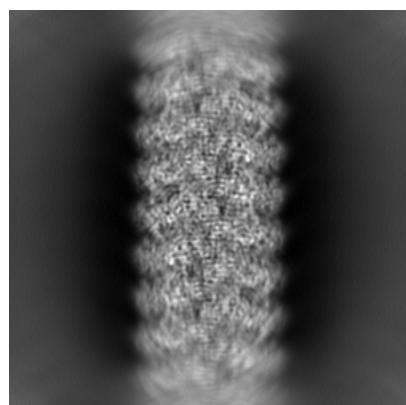


Y

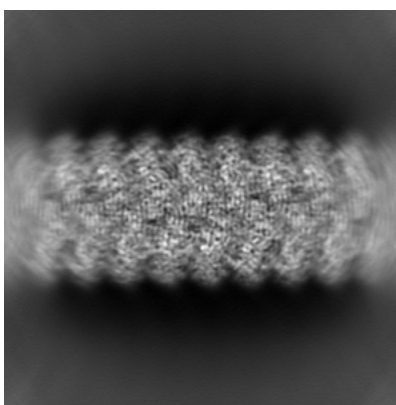


Z

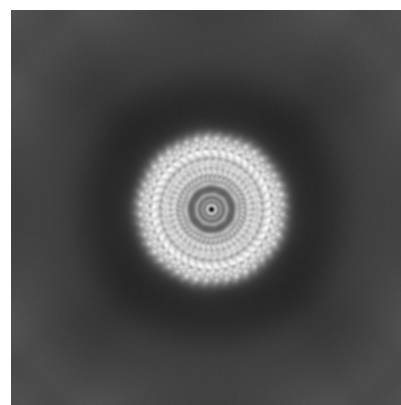
6.1.2 Raw map



X



Y

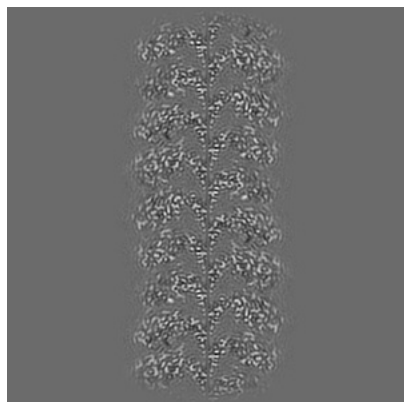


Z

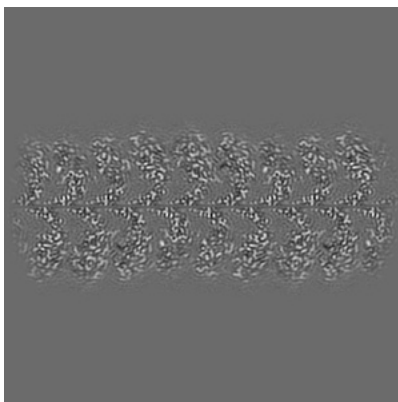
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

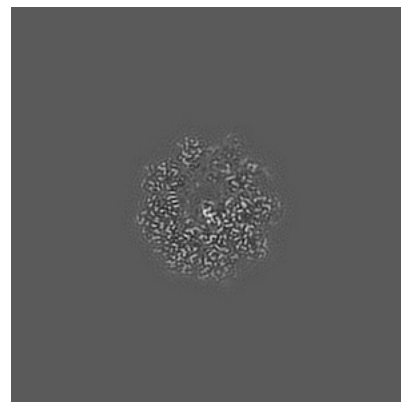
6.2.1 Primary map



X Index: 175

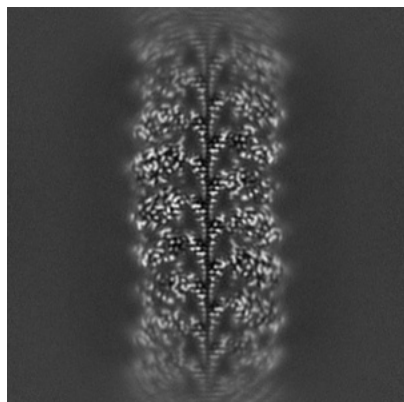


Y Index: 175

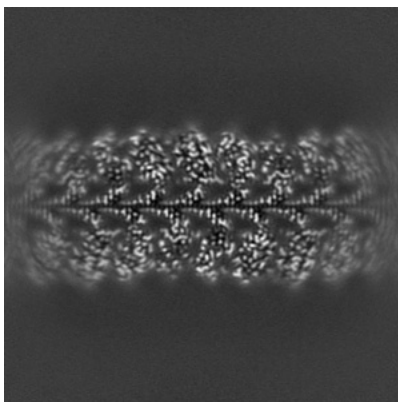


Z Index: 175

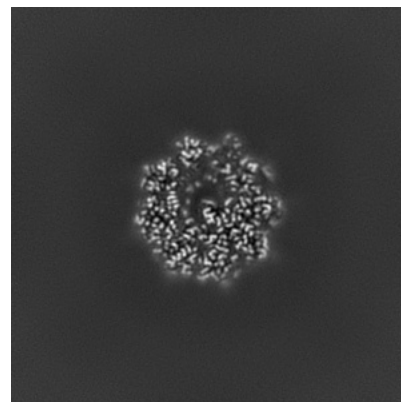
6.2.2 Raw map



X Index: 175



Y Index: 175

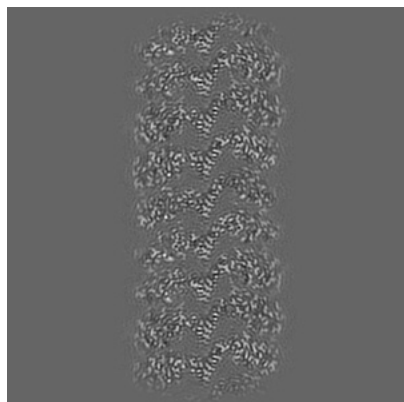


Z Index: 175

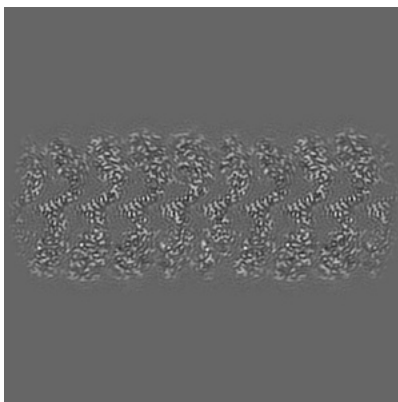
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

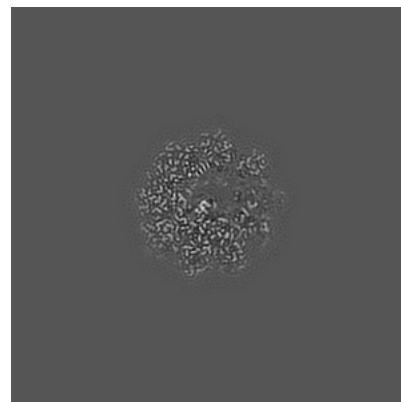
6.3.1 Primary map



X Index: 171

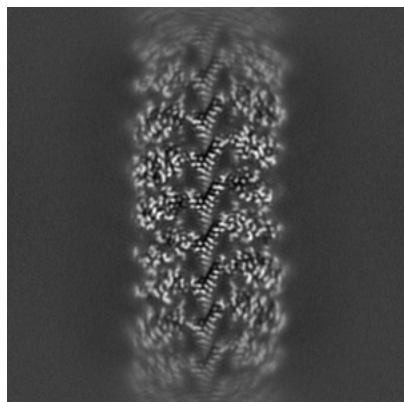


Y Index: 179

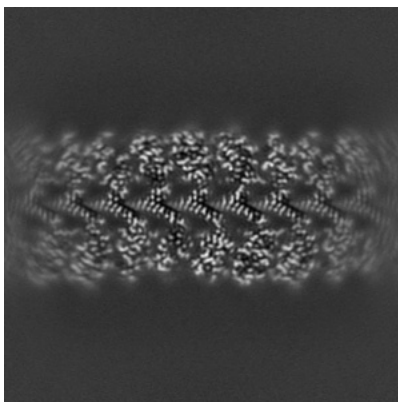


Z Index: 109

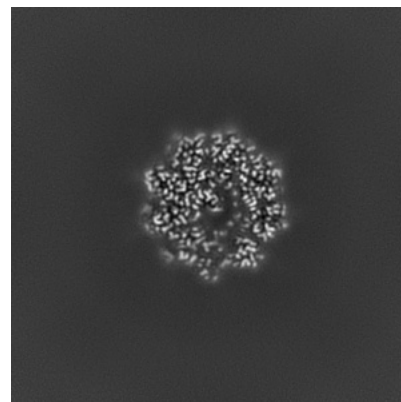
6.3.2 Raw map



X Index: 172



Y Index: 172

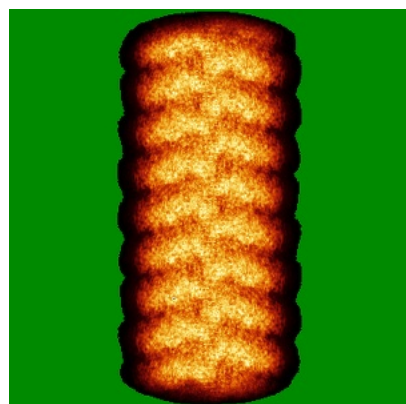


Z Index: 192

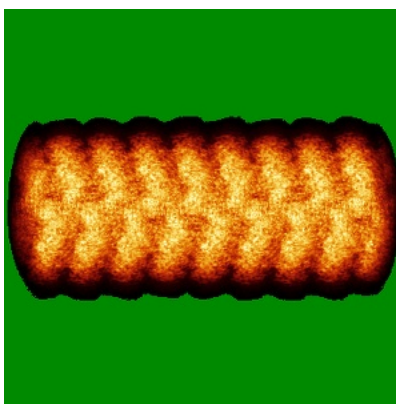
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

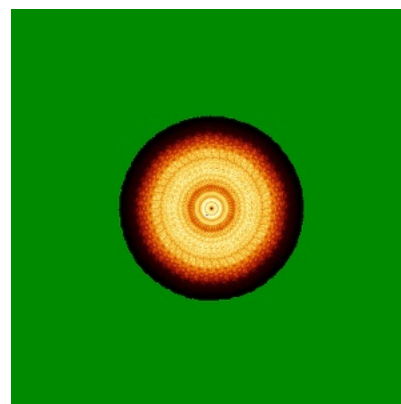
6.4.1 Primary map



X

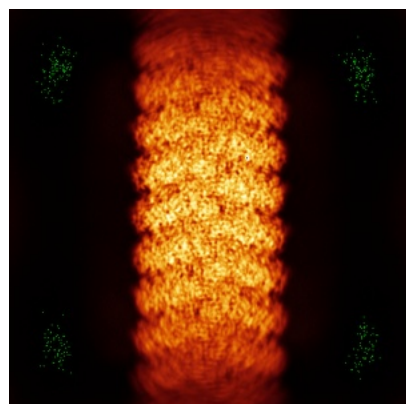


Y

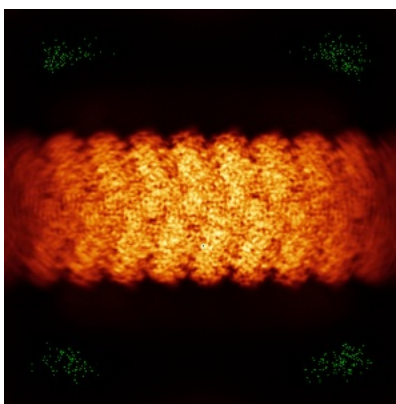


Z

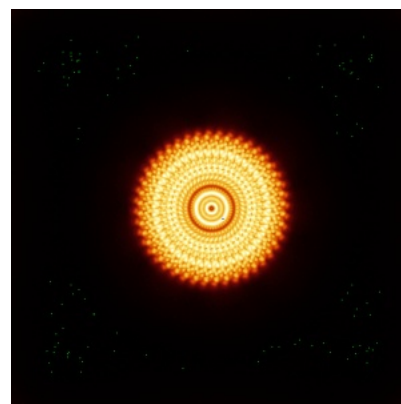
6.4.2 Raw map



X



Y

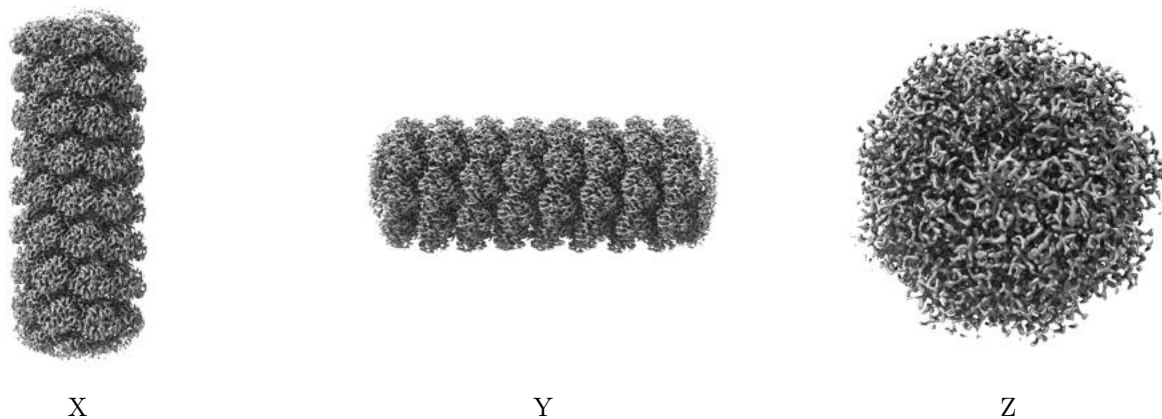


Z

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

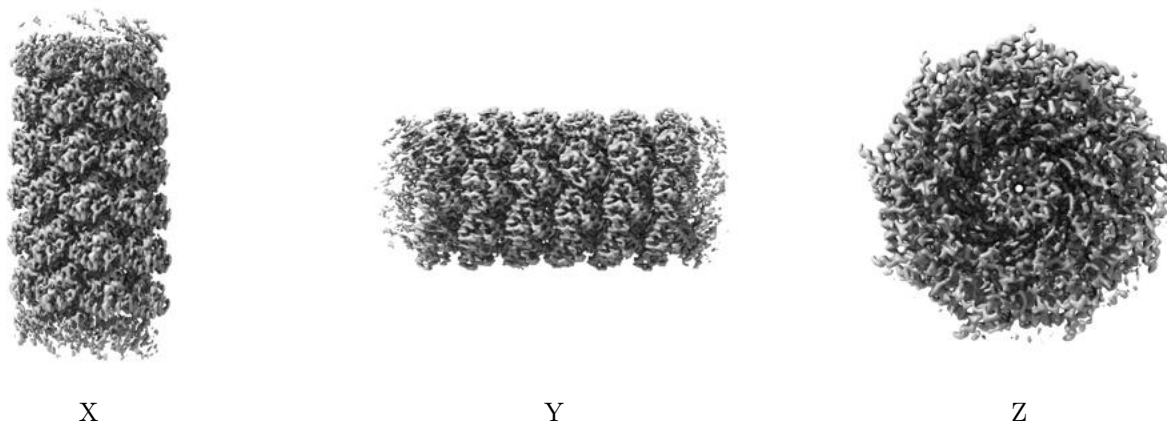
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

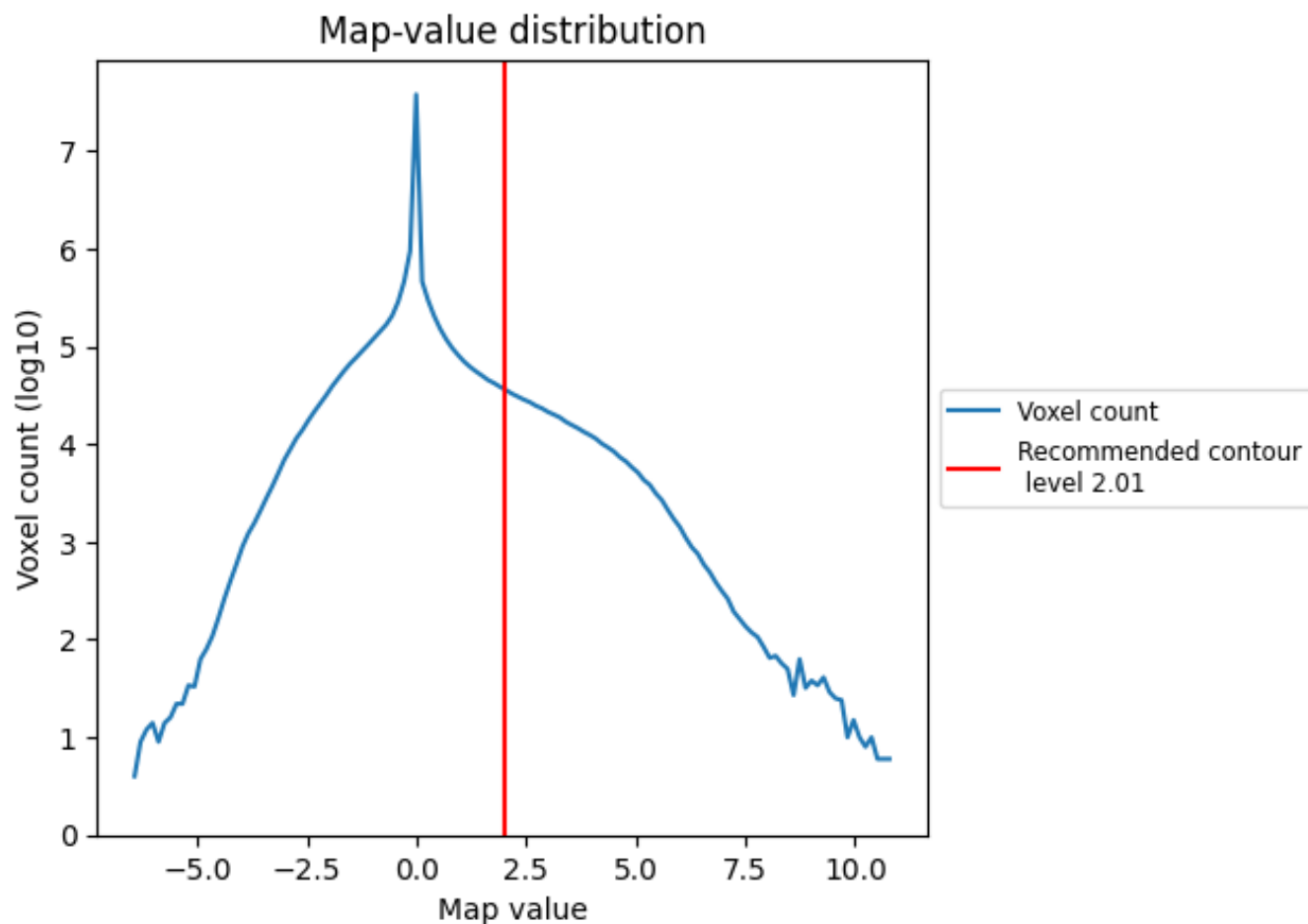
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

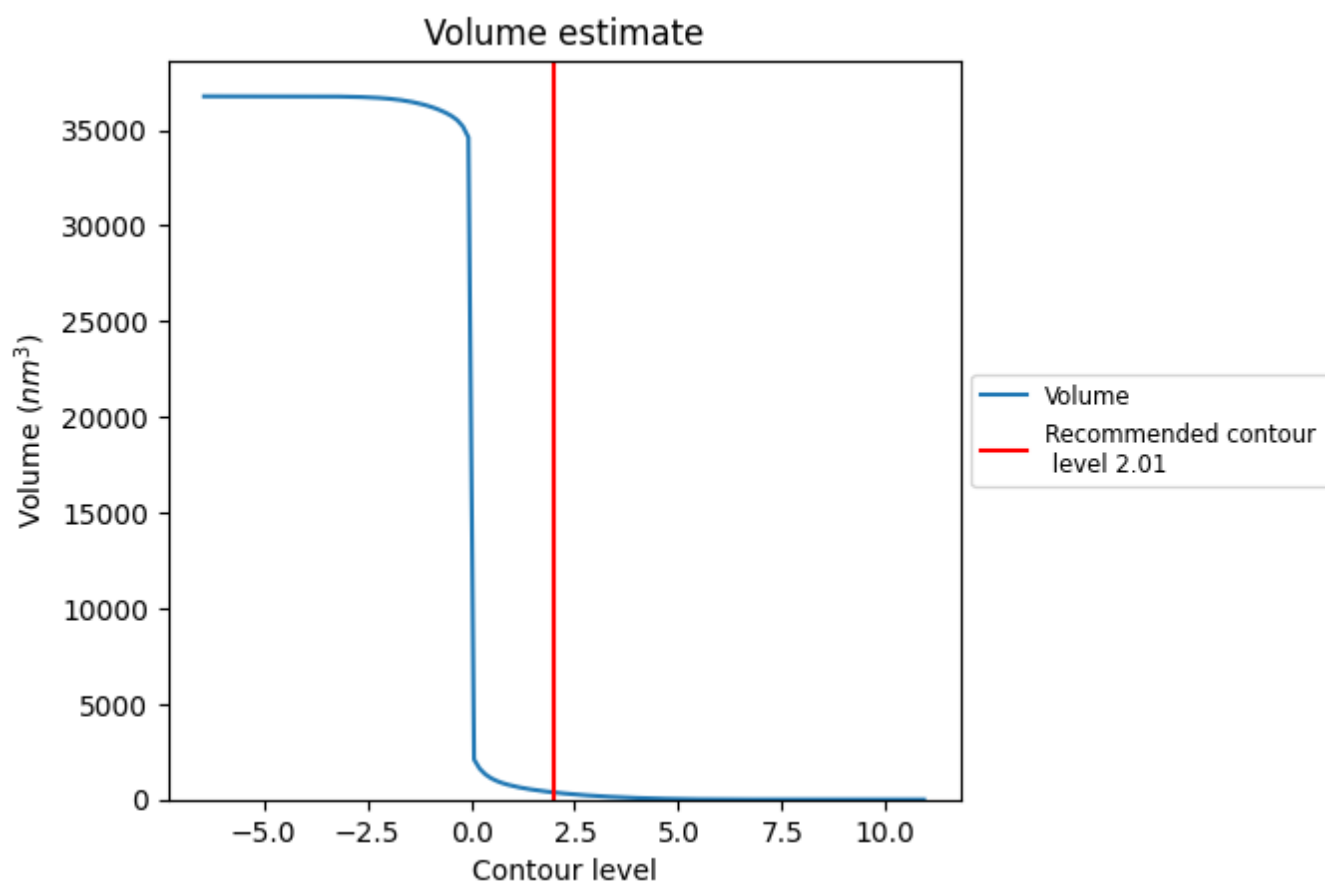
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

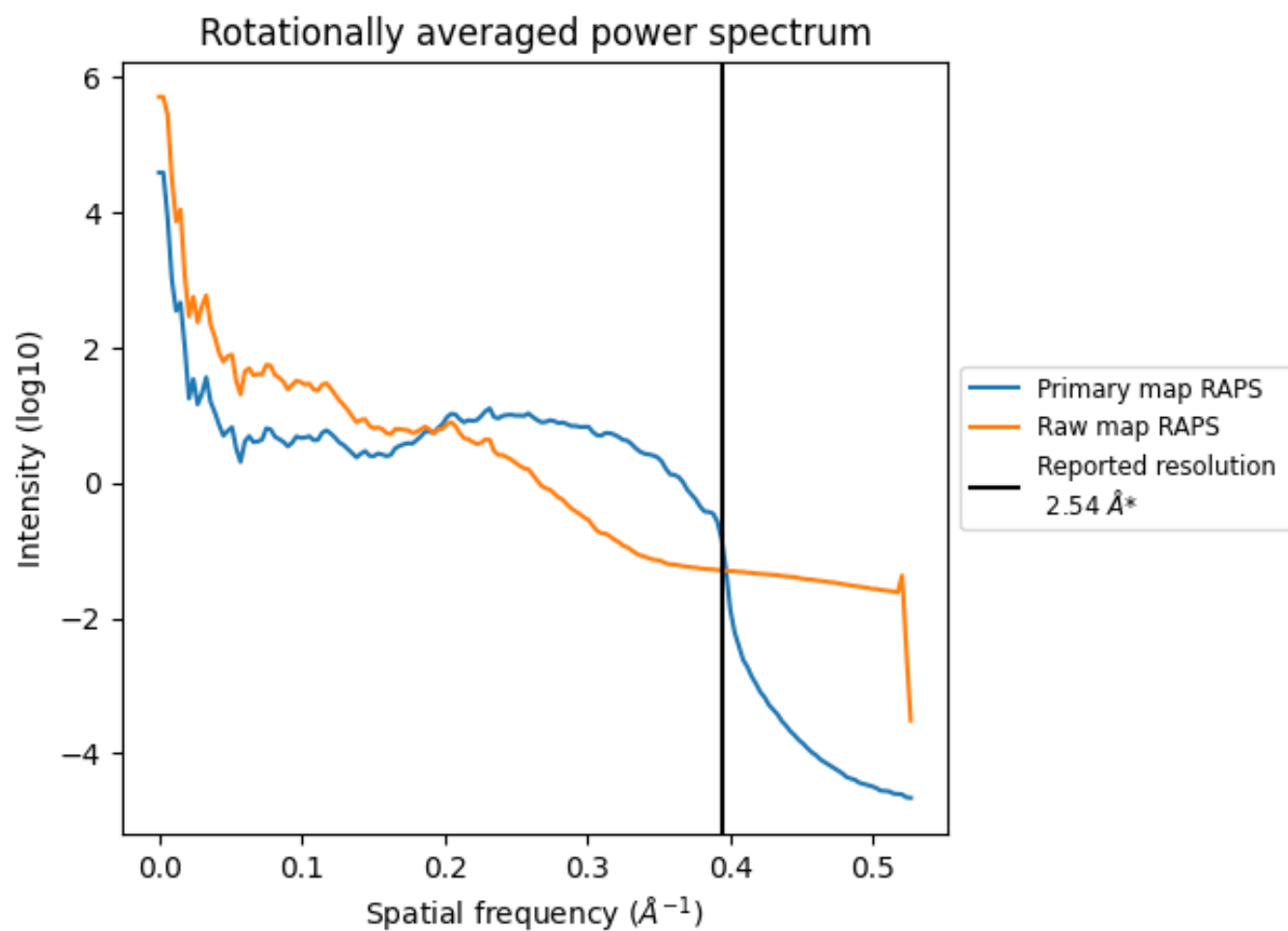
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 370 nm³; this corresponds to an approximate mass of 335 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 ⓘ

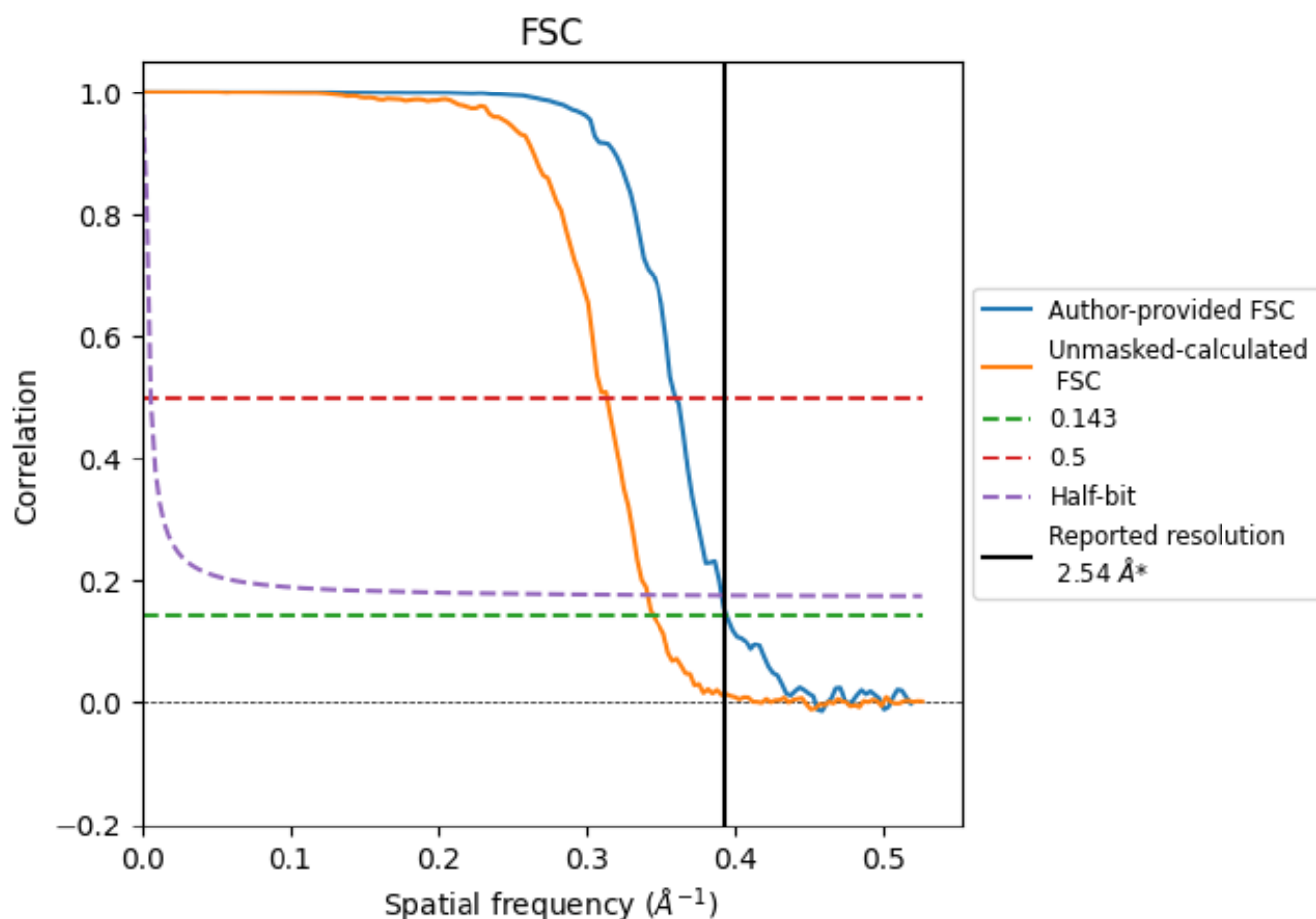


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

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](#)

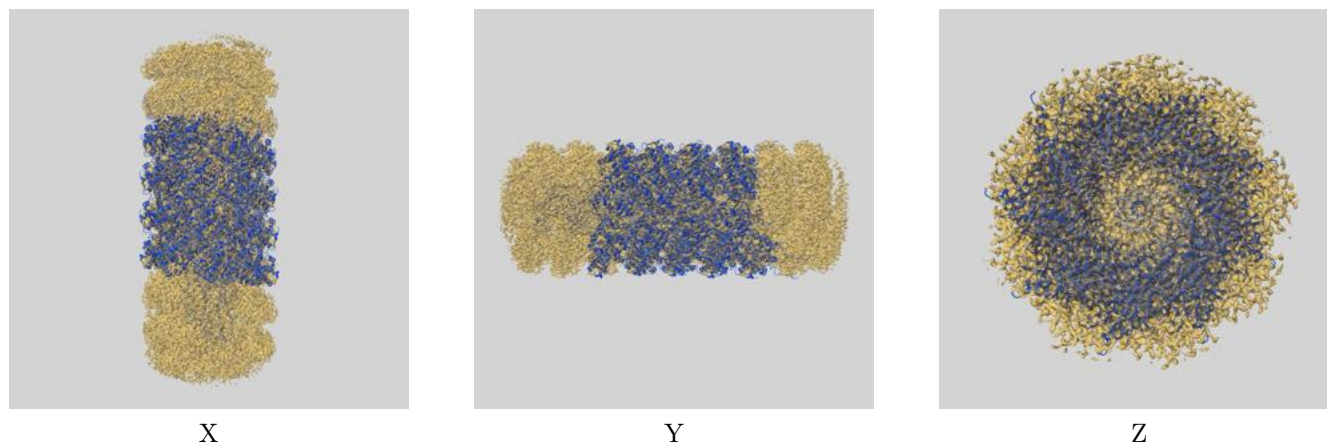
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.53	2.78	2.56
Unmasked-calculated*	2.90	3.19	2.93

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

9 Map-model fit [i](#)

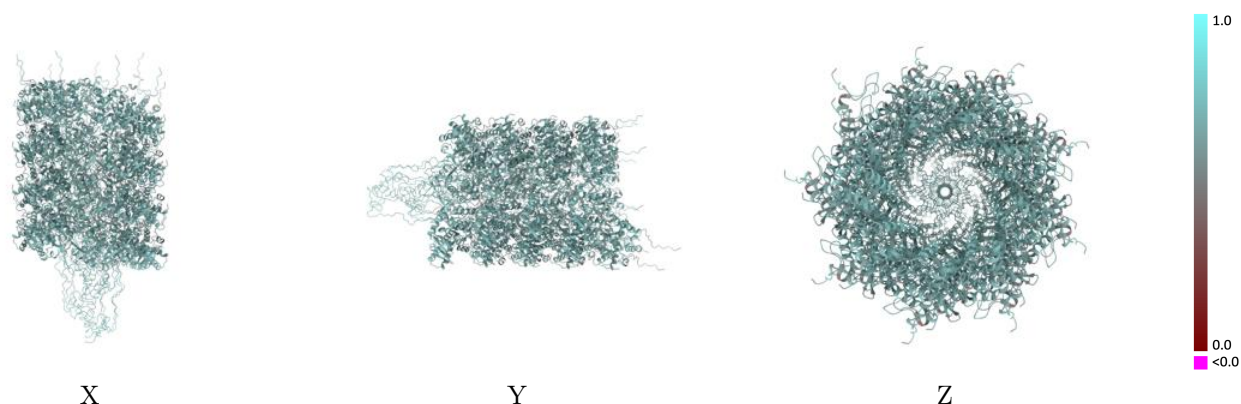
This section contains information regarding the fit between EMDB map EMD-53791 and PDB model 9R7S. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



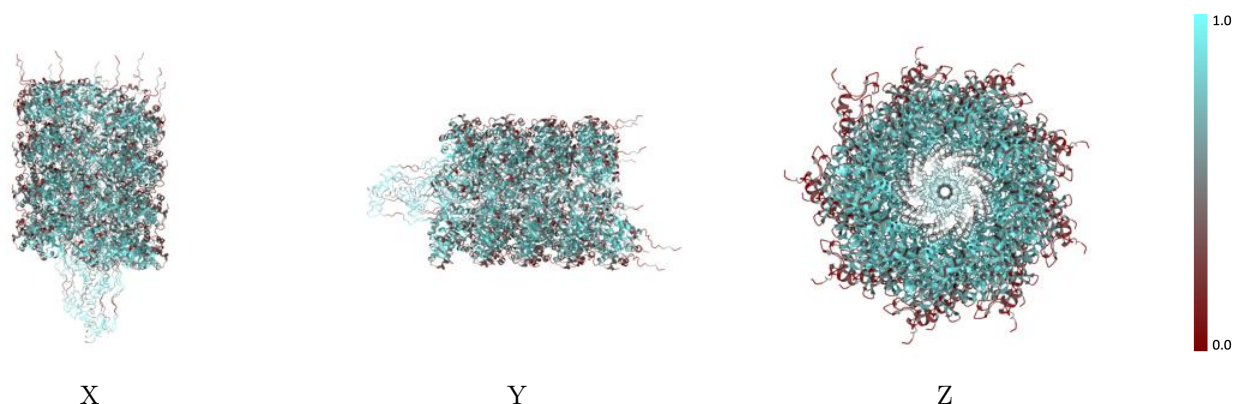
The images above show the 3D surface view of the map at the recommended contour level 2.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



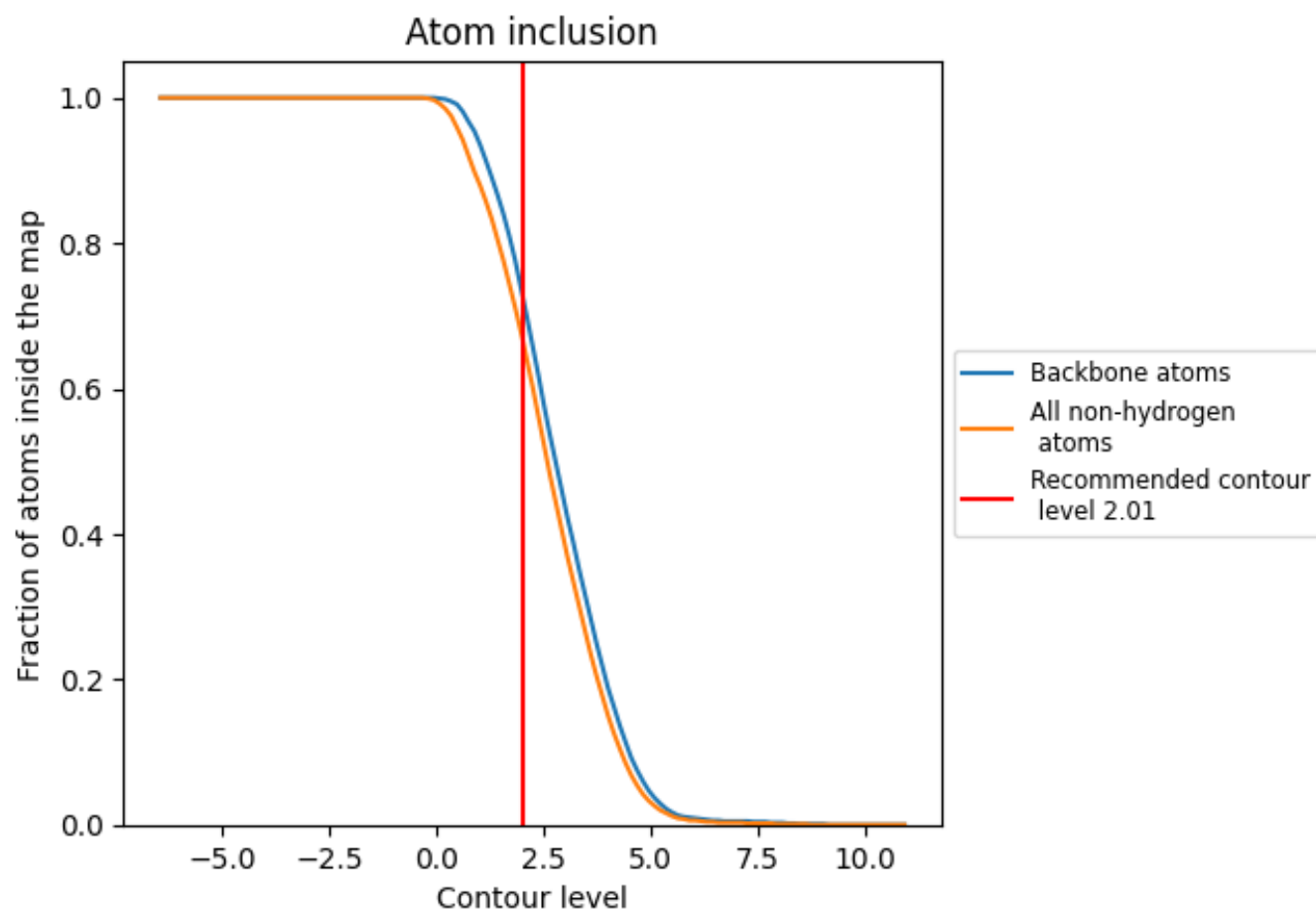
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 67% 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 (2.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.6500
Aa	 0.6620	 0.6510
Ab	 0.8600	 0.6440
Ac	 0.6580	 0.6490
Ad	 0.8400	 0.6110
Ae	 0.6590	 0.6500
Af	 0.9000	 0.6550
Ag	 0.6540	 0.6490
Ah	 0.8900	 0.6600
Ai	 0.6540	 0.6500
Aj	 0.8800	 0.6380
Ak	 0.6590	 0.6490
Al	 0.9200	 0.6510
Am	 0.6510	 0.6490
An	 0.9200	 0.6480
Ao	 0.6610	 0.6500
Ap	 0.9200	 0.6540
Aq	 0.6520	 0.6510
Ar	 0.8700	 0.6460
As	 0.6540	 0.6510
At	 0.8700	 0.6510
Au	 0.6570	 0.6500
Av	 0.9000	 0.6520
Aw	 0.6540	 0.6510
Ax	 0.9300	 0.6580
Ay	 0.6600	 0.6500
Az	 0.8900	 0.6500
Ba	 0.6590	 0.6510
Bb	 0.8800	 0.6470
Bc	 0.6580	 0.6490
Bd	 0.9000	 0.6440
Be	 0.6440	 0.6490
Bf	 0.8700	 0.6530
Bg	 0.6600	 0.6500
Bh	 0.9100	 0.6580



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Chain	Atom inclusion	Q-score
Bi	 0.6490	 0.6490
Bj	 0.8500	 0.6440
Bk	 0.6590	 0.6510
Bl	 0.9100	 0.6570
Bm	 0.6540	 0.6500
Bn	 0.9100	 0.6480
Bo	 0.6550	 0.6520
Bp	 0.8800	 0.6520
Bq	 0.6590	 0.6500
Br	 0.9100	 0.6530
Bs	 0.6570	 0.6510
Bt	 0.9300	 0.6550
Bu	 0.6580	 0.6500
Bv	 0.8400	 0.6510
Bw	 0.6530	 0.6490
Bx	 0.8900	 0.6570
By	 0.6560	 0.6490
Bz	 0.9100	 0.6590
Ca	 0.6470	 0.6490
Cb	 0.8700	 0.6480
Cc	 0.6550	 0.6500
Cd	 0.8400	 0.6500
Ce	 0.6530	 0.6500
Cf	 0.8700	 0.6440
Cg	 0.6580	 0.6510
Ch	 0.9100	 0.6500
Ci	 0.6520	 0.6510
Cj	 0.9100	 0.6480
Ck	 0.6520	 0.6520
Cl	 0.8900	 0.6500
Cm	 0.6550	 0.6500
Cn	 0.9100	 0.6540
Co	 0.6530	 0.6500
Cp	 0.9200	 0.6560
Cq	 0.6540	 0.6500
Cr	 0.8500	 0.6410
Cs	 0.6540	 0.6480
Ct	 0.9100	 0.6590