



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:07 AM UTC

PDB ID : 9R9Z / pdb_00009r9z
EMDB ID : EMD-53865
Title : ssRNA-containing helical virus-like particle composed of JGMV coat protein
Authors : Koritnik, N.; Kezar, A.; Podobnik, M.
Deposited on : 2025-05-20
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

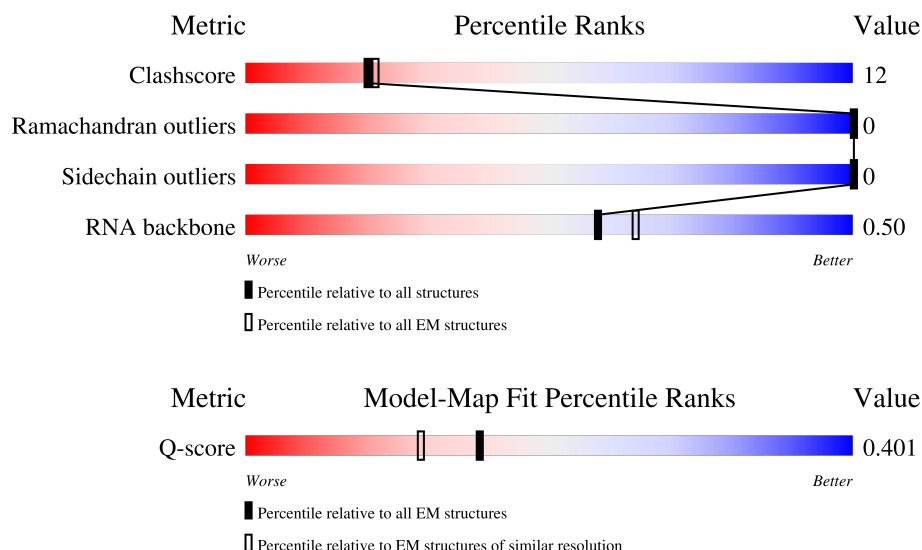
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	303	46% 57% 17% 26%
1	Ac	303	46% 56% 18% 26%
1	Ae	303	44% 56% 17% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ag	303	44% 56%18%26%
1	Ai	303	43% 55%18%26%
1	Ak	303	39% 55%19%26%
1	Am	303	39% 55%18%26%
1	Ao	303	38% 56%18%26%
1	Aq	303	41% 56%18%26%
1	As	303	42% 54%19%26%
1	Au	303	43% 55%19%26%
1	Aw	303	42% 56%18%26%
1	Ay	303	42% 53%20%26%
1	Ba	303	39% 54%19%26%
1	Bc	303	38% 56%18%26%
1	Be	303	34% 54%19%26%
1	Bg	303	35% 54%19%26%
1	Bi	303	39% 54%19%26%
1	Bk	303	42% 54%19%26%
1	Bm	303	41% 55%18%26%
1	Bo	303	39% 55%18%26%
1	Bq	303	37% 56%17%26%
1	Bs	303	37% 53%20%26%
1	Bu	303	36% 54%19%26%
1	Bw	303	34% 54%20%26%
1	By	303	33% 56%18%26%
1	Ca	303	38% 55%18%26%
1	Cc	303	41% 54%19%26%

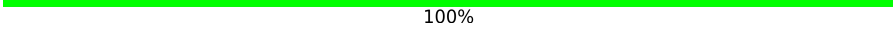
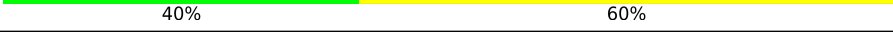
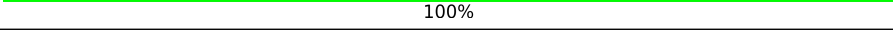
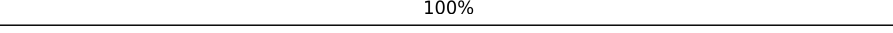
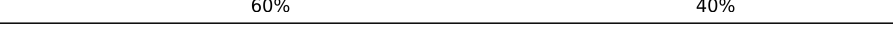
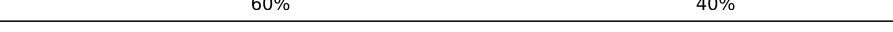
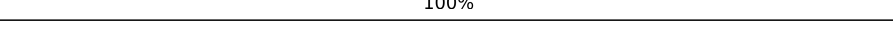
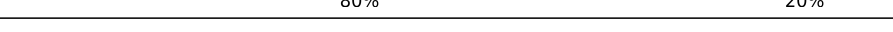
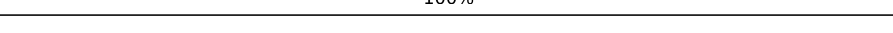
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ce	303	
1	Cg	303	
1	Ci	303	
1	Ck	303	
1	Cm	303	
1	Co	303	
1	Cq	303	
1	Cs	303	
2	Ab	5	
2	Ad	5	
2	Af	5	
2	Ah	5	
2	Aj	5	
2	Al	5	
2	An	5	
2	Ap	5	
2	Ar	5	
2	At	5	
2	Av	5	
2	Ax	5	
2	Az	5	
2	Bb	5	
2	Bd	5	
2	Bf	5	
2	Bh	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Bj	5	 80%20%
2	Bl	5	 60%40%
2	Bn	5	 80%20%
2	Bp	5	 60%40%
2	Br	5	 60%40%
2	Bt	5	 100%
2	Bv	5	 80%20%
2	Bx	5	 40%60%
2	Bz	5	 100%
2	Cb	5	 60%40%
2	Cd	5	 40%60%
2	Cf	5	 100%
2	Ch	5	 60%40%
2	Cj	5	 60%40%
2	Cl	5	 100%
2	Cn	5	 80%20%
2	Cp	5	 40%60%
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 68976 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ac	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ae	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ag	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ai	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ak	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Am	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ao	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Aq	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	As	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Au	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Aw	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ay	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ba	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bc	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Be	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bg	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bi	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bk	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bm	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bo	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bq	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bs	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bu	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Bw	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	By	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ca	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Cc	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ce	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Cg	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ci	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Ck	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Cm	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Co	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Cq	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		
1	Cs	224	Total	C	N	O	S	0	0
			1816	1133	331	338	14		

- 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

Continued on next page...

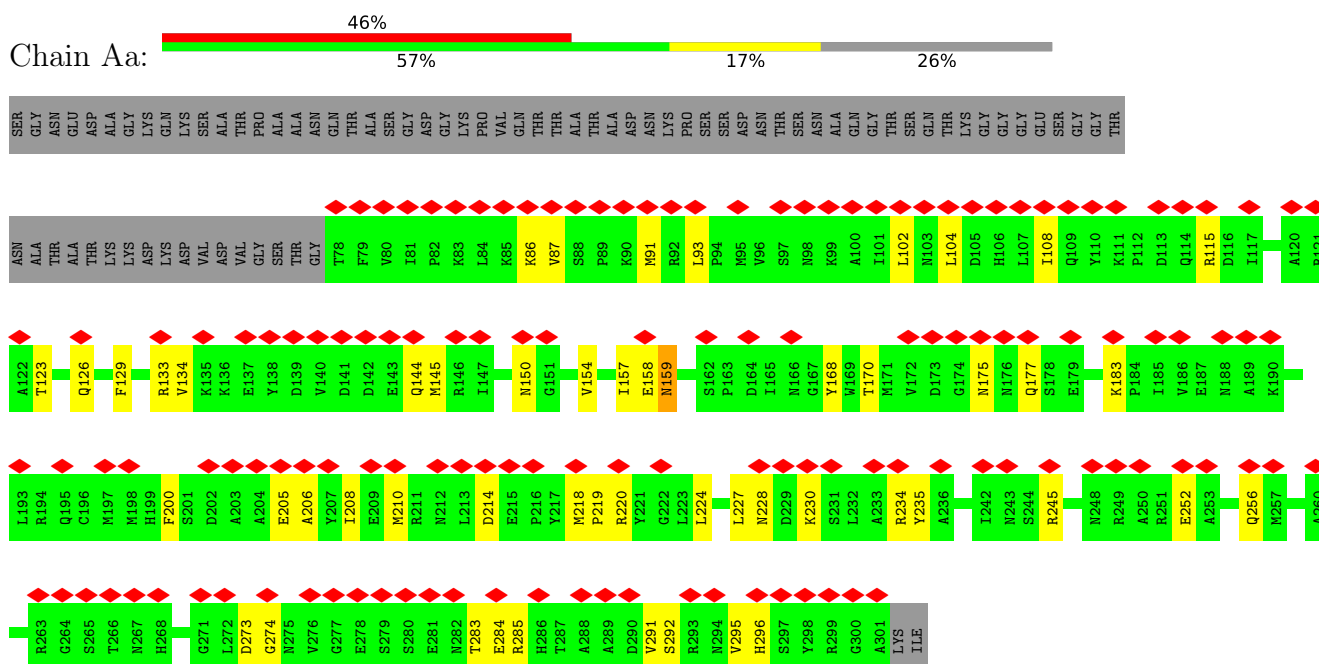
Continued from previous page...

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

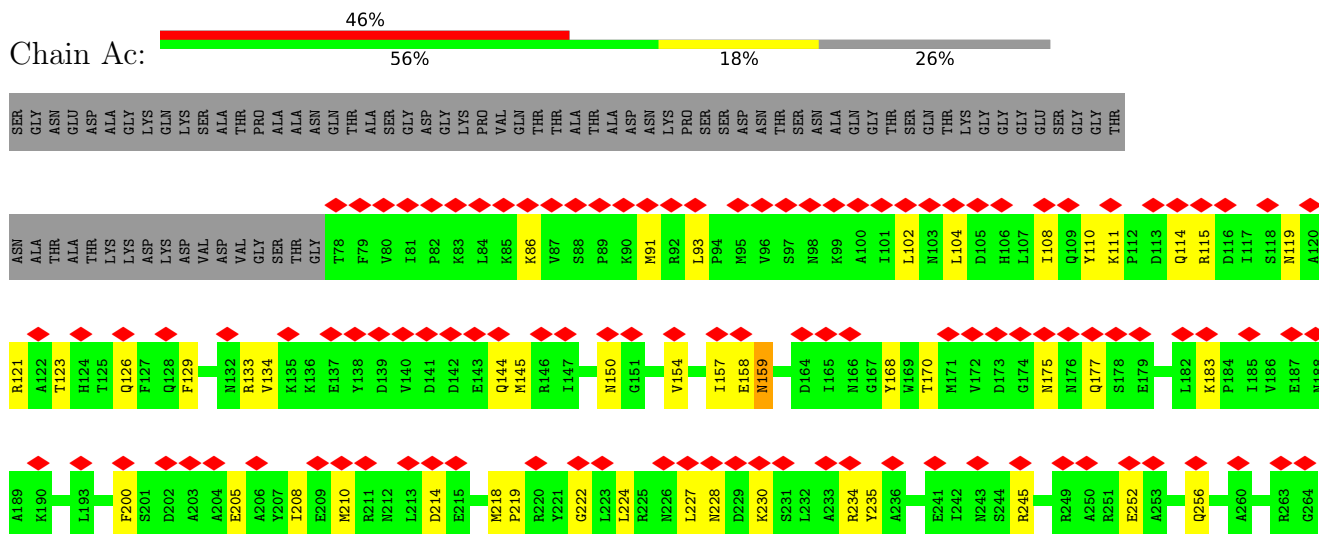
3 Residue-property plots

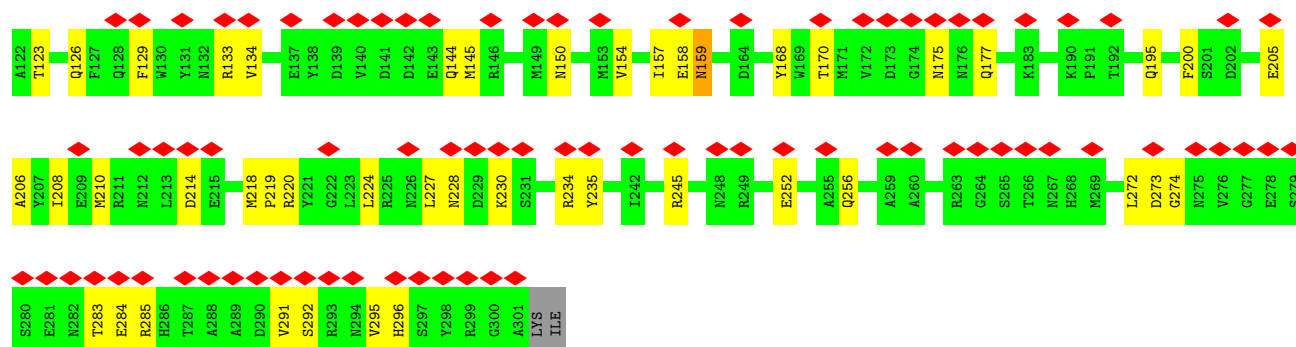
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

• Molecule 1: Genome polyprotein

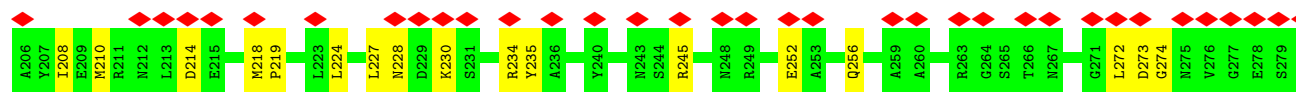
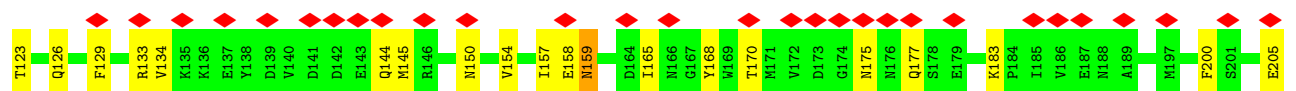
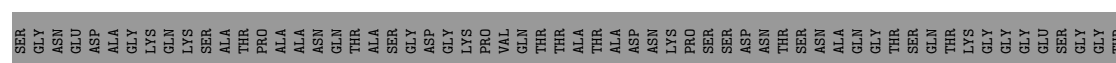
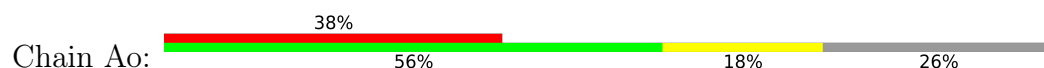


• Molecule 1: Genome polyprotein

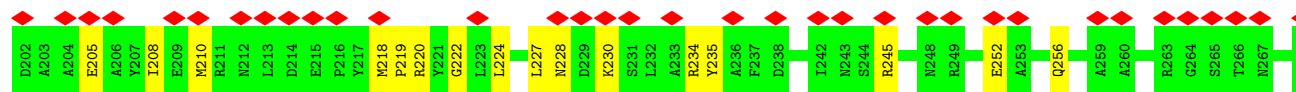
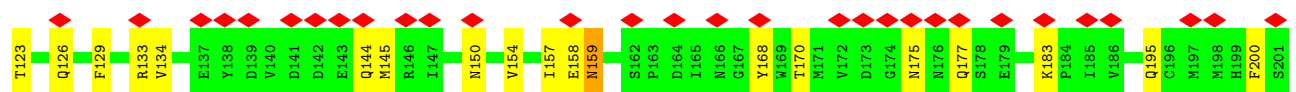
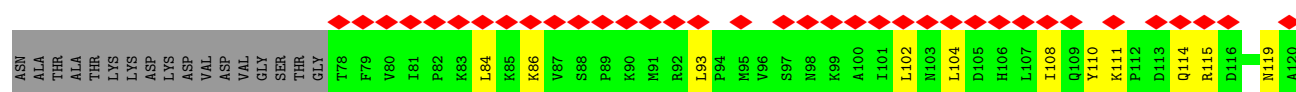
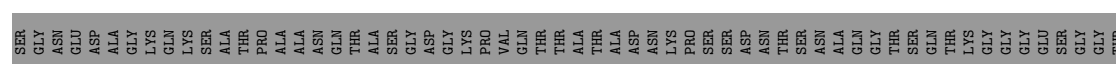
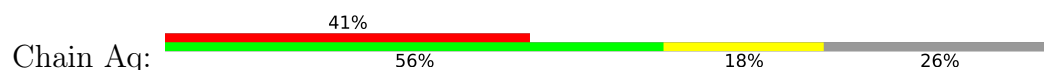


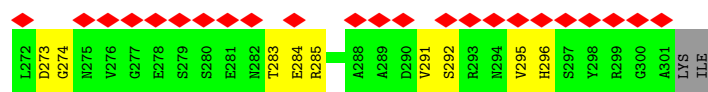


• Molecule 1: Genome polyprotein

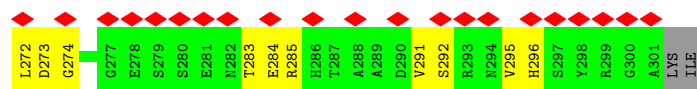
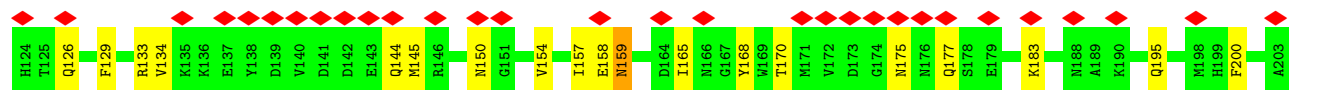
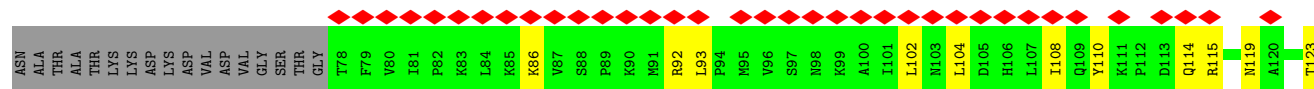
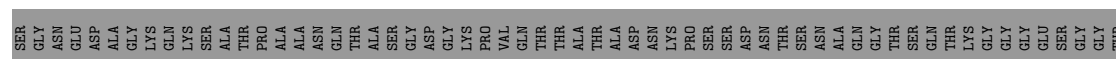
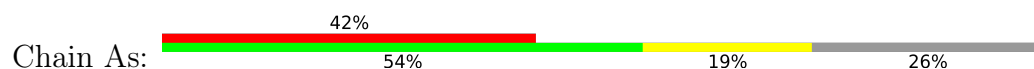


• Molecule 1: Genome polyprotein

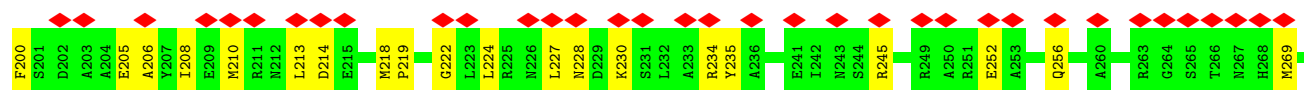
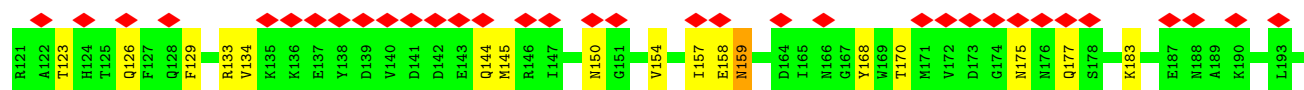
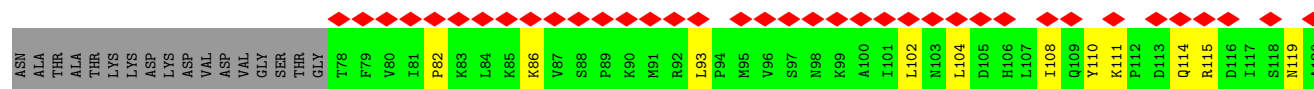
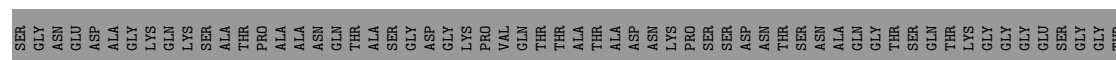




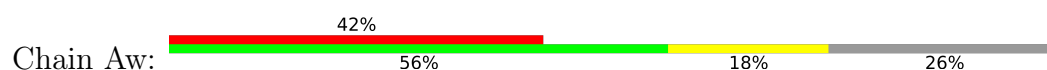
• Molecule 1: Genome polyprotein

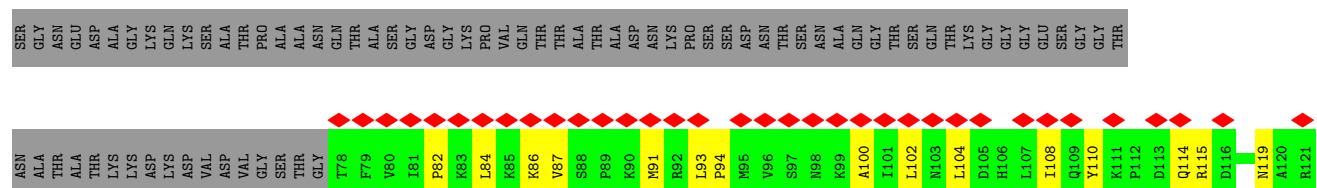


• Molecule 1: Genome polyprotein

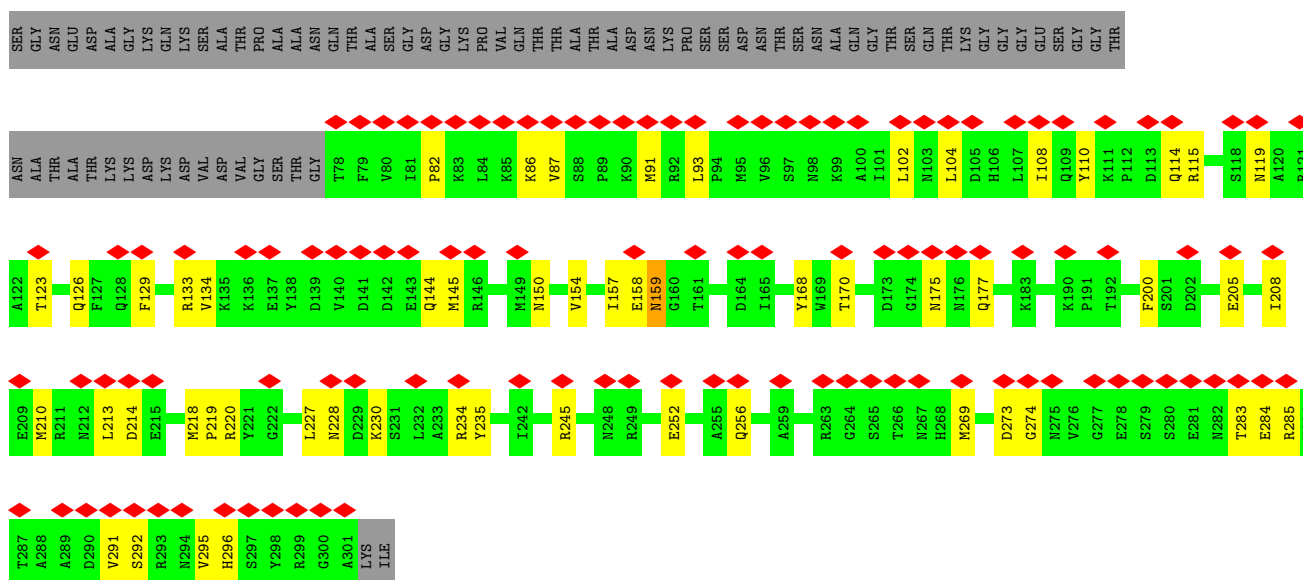


• Molecule 1: Genome polyprotein

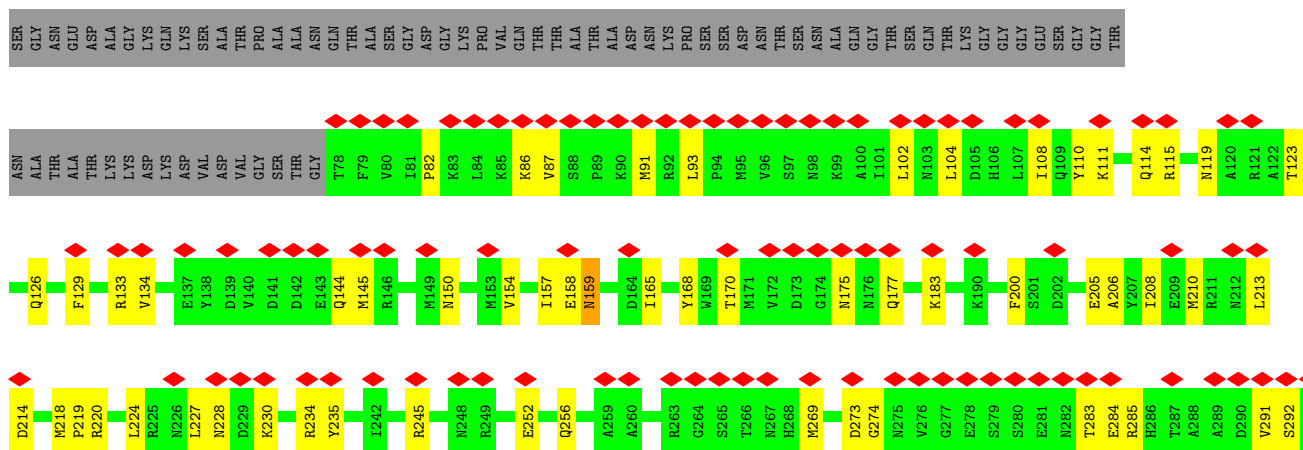




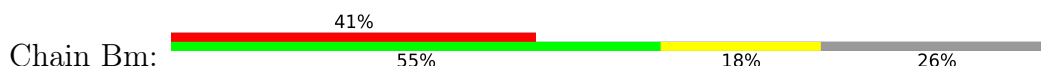
- Molecule 1: Genome polypeptide



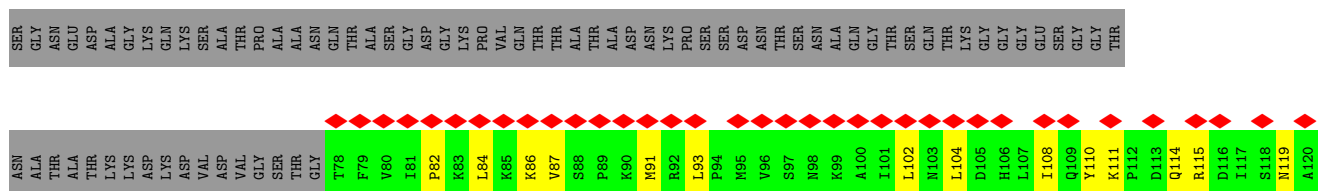
- Molecule 1: Genome polypeptide

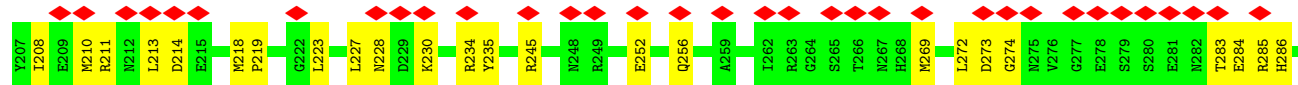


- Molecule 1: Genome polypprotein

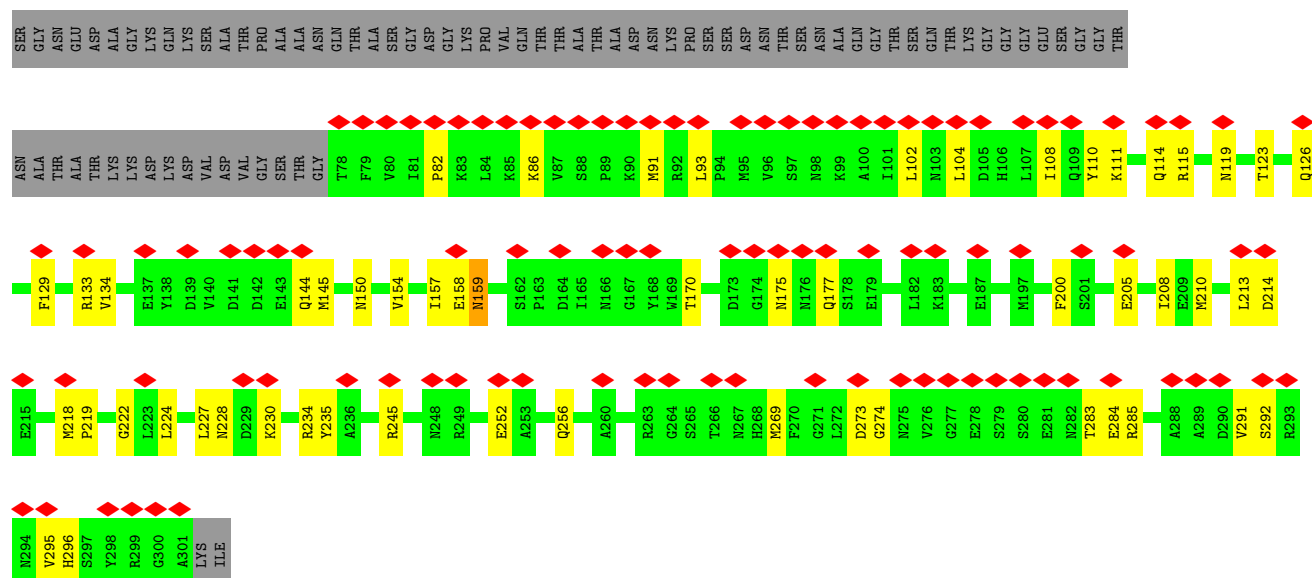


- Molecule 1: Genome polypprotein

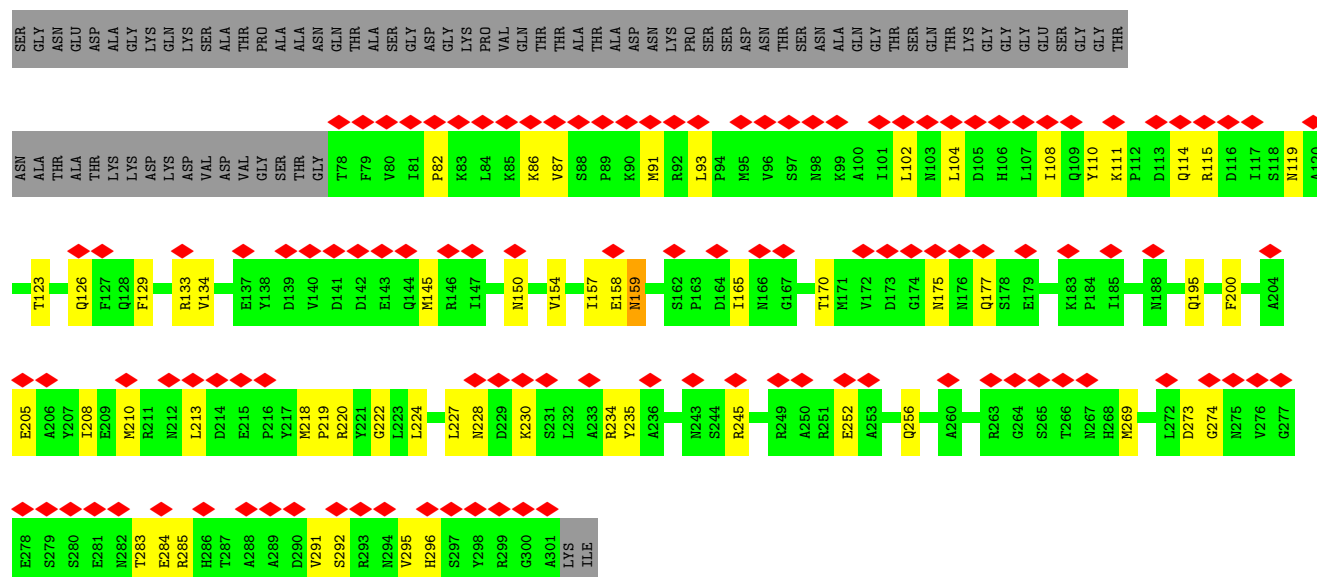
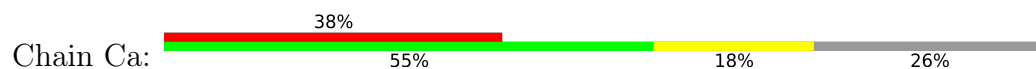




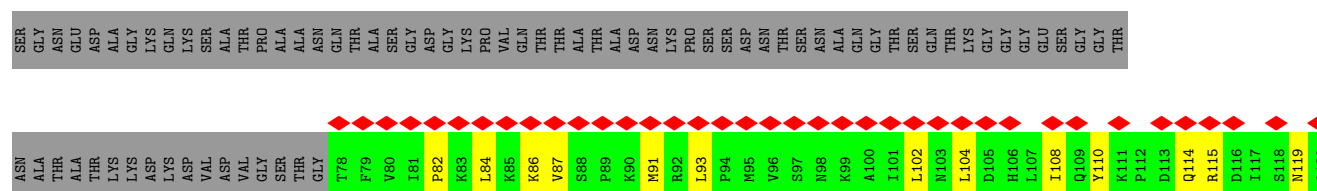
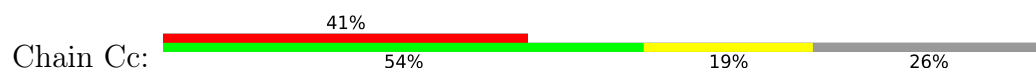




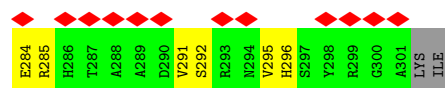
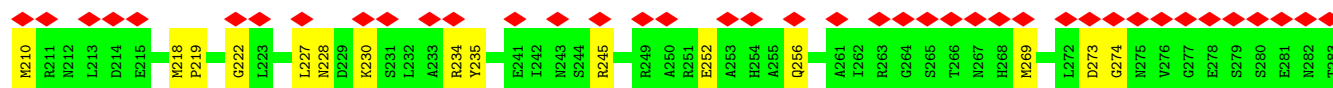
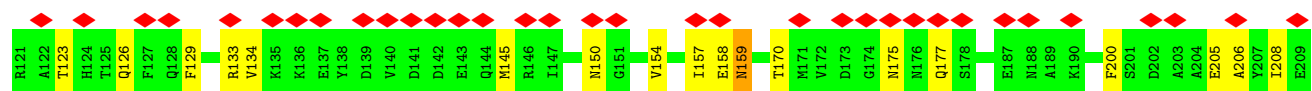
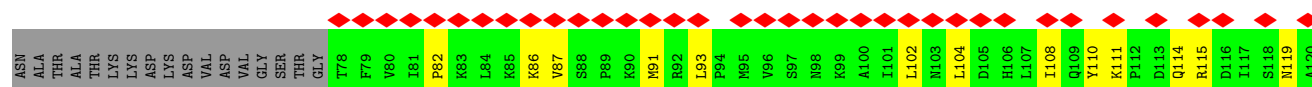
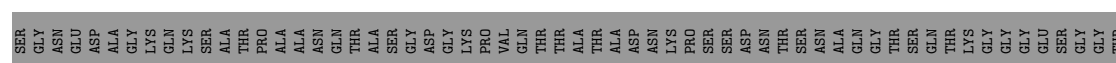
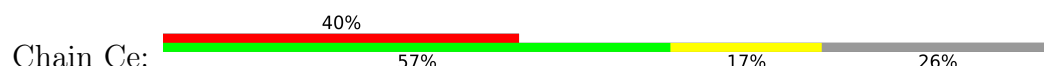
• Molecule 1: Genome polypeptide



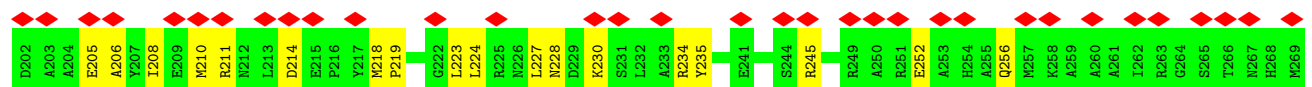
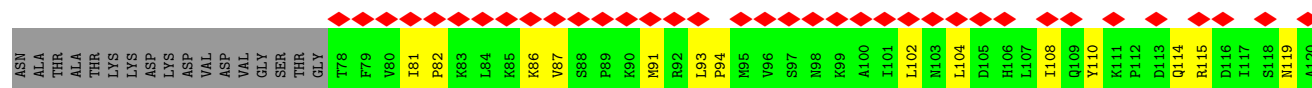
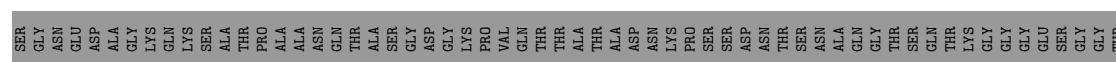
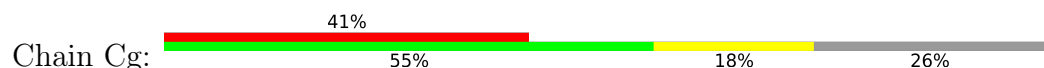
• Molecule 1: Genome polypeptide



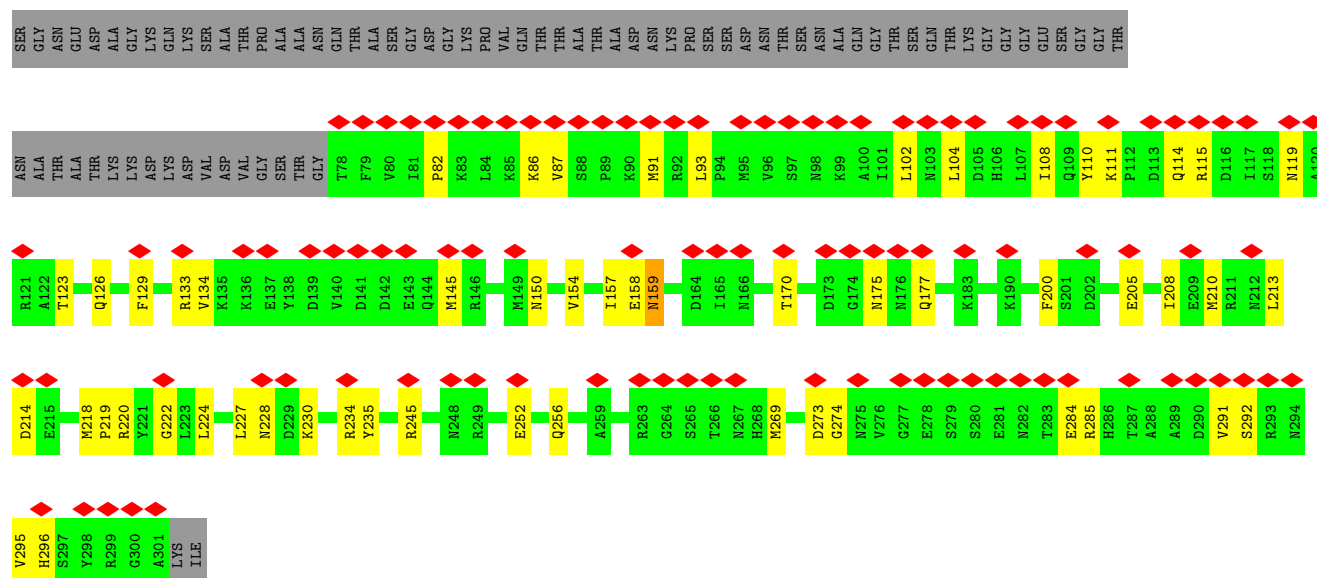
- Molecule 1: Genome polyprotein



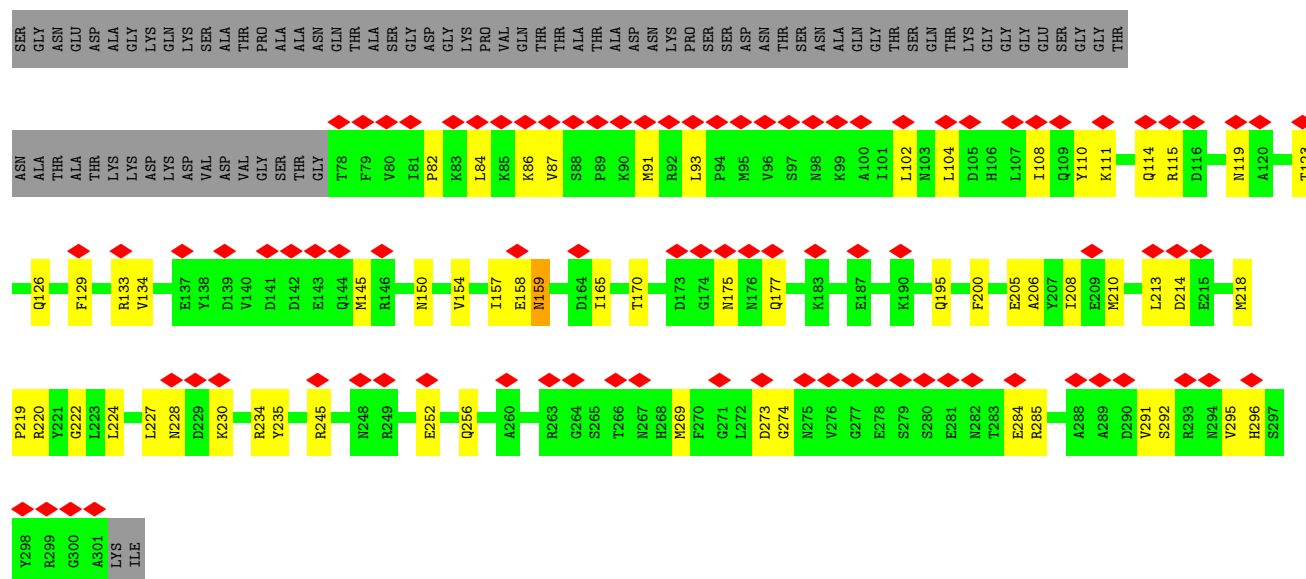
- Molecule 1: Genome polyprotein



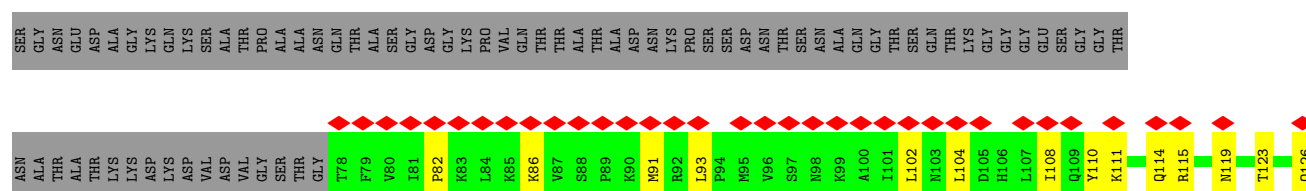


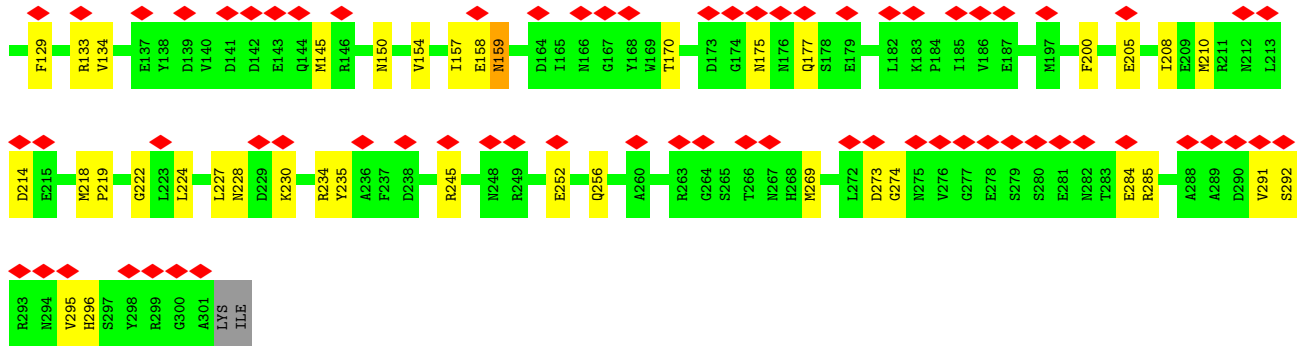


• Molecule 1: Genome polyprotein

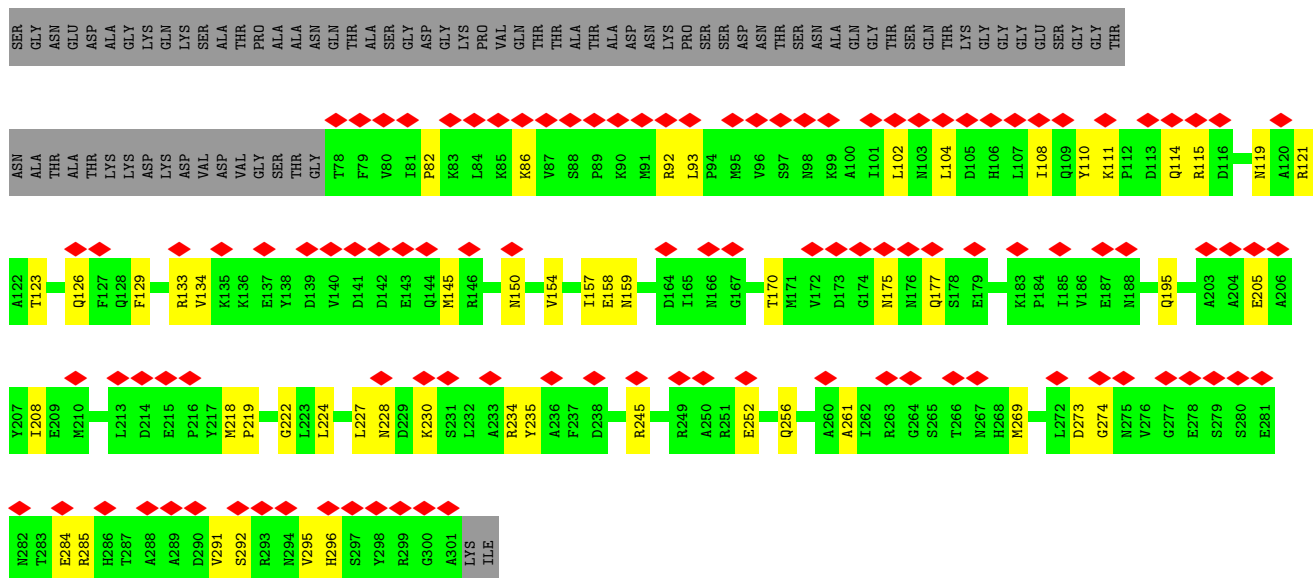


• Molecule 1: Genome polyprotein

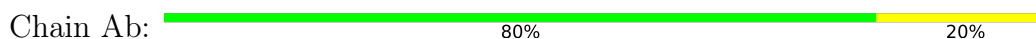




- Molecule 1: Genome polyprotein



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



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



There are no outlier residues recorded for this chain.

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



There are no outlier residues recorded for this chain.

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

Chain Ah:  60% 40%



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

Chain Aj:  80% 20%



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

Chain Al:  100%

There are no outlier residues recorded for this chain.

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

Chain An:  60% 40%



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

Chain Ap:  20% 60% 40%

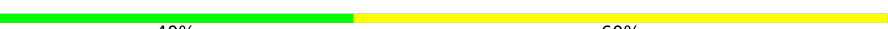


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Ar:  40% 60%



- 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:  100%

There are no outlier residues recorded for this chain.

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

Chain Ax:  80% 20%



- 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:  100%

There are no outlier residues recorded for this chain.

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

Chain Bd:  80% 20%



- 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')

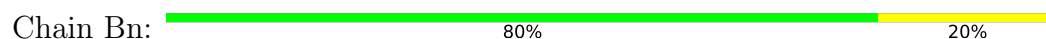
Chain Bj:  80% 20%



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



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



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



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

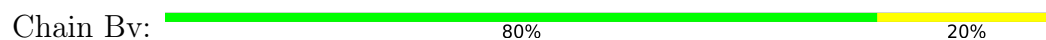


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')



There are no outlier residues recorded for this chain.

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



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





- 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: 60% 40%



- 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: 100%

There are no outlier residues recorded for this chain.

- 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: 100%

There are no outlier residues recorded for this chain.

- 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:  40% 60%



- 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=4.03 Å, axial sym=C1	Depositor
Number of segments used	31352	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	3.277	Depositor
Minimum map value	-1.360	Depositor
Average map value	0.060	Depositor
Map value standard deviation	0.239	Depositor
Recommended contour level	1.34	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 ⓘ

5.1 Standard geometry ⓘ

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	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ac	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ae	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ag	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ai	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ak	0.51	0/1857	0.63	3/2508 (0.1%)
1	Am	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ao	0.51	0/1857	0.63	3/2508 (0.1%)
1	Aq	0.51	0/1857	0.63	3/2508 (0.1%)
1	As	0.51	0/1857	0.63	3/2508 (0.1%)
1	Au	0.51	0/1857	0.63	3/2508 (0.1%)
1	Aw	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ay	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ba	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bc	0.51	0/1857	0.63	3/2508 (0.1%)
1	Be	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bg	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bi	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bk	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bm	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bo	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bq	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bs	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bu	0.51	0/1857	0.63	3/2508 (0.1%)
1	Bw	0.51	0/1857	0.63	3/2508 (0.1%)
1	By	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ca	0.51	0/1857	0.63	3/2508 (0.1%)
1	Cc	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ce	0.51	0/1857	0.63	3/2508 (0.1%)
1	Cg	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ci	0.51	0/1857	0.63	3/2508 (0.1%)
1	Ck	0.51	0/1857	0.63	3/2508 (0.1%)
1	Cm	0.51	0/1857	0.63	3/2508 (0.1%)
1	Co	0.51	0/1857	0.63	3/2508 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Cq	0.51	0/1857	0.63	3/2508 (0.1%)
1	Cs	0.51	0/1857	0.63	3/2508 (0.1%)
2	Ab	0.32	0/109	0.27	0/166
2	Ad	0.32	0/109	0.27	0/166
2	Af	0.32	0/109	0.27	0/166
2	Ah	0.32	0/109	0.27	0/166
2	Aj	0.32	0/109	0.27	0/166
2	Al	0.32	0/109	0.27	0/166
2	An	0.32	0/109	0.27	0/166
2	Ap	0.32	0/109	0.27	0/166
2	Ar	0.32	0/109	0.27	0/166
2	At	0.32	0/109	0.27	0/166
2	Av	0.32	0/109	0.27	0/166
2	Ax	0.32	0/109	0.27	0/166
2	Az	0.32	0/109	0.27	0/166
2	Bb	0.32	0/109	0.27	0/166
2	Bd	0.32	0/109	0.27	0/166
2	Bf	0.32	0/109	0.27	0/166
2	Bh	0.32	0/109	0.27	0/166
2	Bj	0.32	0/109	0.27	0/166
2	Bl	0.32	0/109	0.27	0/166
2	Bn	0.32	0/109	0.27	0/166
2	Bp	0.32	0/109	0.27	0/166
2	Br	0.32	0/109	0.27	0/166
2	Bt	0.32	0/109	0.27	0/166
2	Bv	0.32	0/109	0.27	0/166
2	Bx	0.32	0/109	0.27	0/166
2	Bz	0.32	0/109	0.27	0/166
2	Cb	0.32	0/109	0.27	0/166
2	Cd	0.32	0/109	0.28	0/166
2	Cf	0.32	0/109	0.27	0/166
2	Ch	0.32	0/109	0.28	0/166
2	Cj	0.32	0/109	0.27	0/166
2	Cl	0.32	0/109	0.27	0/166
2	Cn	0.32	0/109	0.27	0/166
2	Cp	0.32	0/109	0.27	0/166
2	Cr	0.32	0/109	0.27	0/166
2	Ct	0.32	0/109	0.27	0/166
All	All	0.50	0/70776	0.62	108/96264 (0.1%)

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bu	175	ASN	CA-C-N	-6.46	114.01	123.05
1	Bu	175	ASN	C-N-CA	-6.46	114.01	123.05
1	Cg	175	ASN	CA-C-N	-6.46	114.01	123.05
1	Cg	175	ASN	C-N-CA	-6.46	114.01	123.05
1	Ak	175	ASN	CA-C-N	-6.43	114.04	123.05
1	Ak	175	ASN	C-N-CA	-6.43	114.04	123.05
1	Ba	175	ASN	CA-C-N	-6.43	114.05	123.05
1	Ba	175	ASN	C-N-CA	-6.43	114.05	123.05
1	Bm	175	ASN	CA-C-N	-6.43	114.05	123.05
1	Bm	175	ASN	C-N-CA	-6.43	114.05	123.05
1	Cs	175	ASN	CA-C-N	-6.43	114.05	123.05
1	Cs	175	ASN	C-N-CA	-6.43	114.05	123.05
1	Bo	175	ASN	CA-C-N	-6.43	114.05	123.05
1	Bo	175	ASN	C-N-CA	-6.43	114.05	123.05
1	Be	175	ASN	CA-C-N	-6.43	114.05	123.05
1	Be	175	ASN	C-N-CA	-6.43	114.05	123.05
1	Au	175	ASN	CA-C-N	-6.42	114.06	123.05
1	Au	175	ASN	C-N-CA	-6.42	114.06	123.05
1	Ae	175	ASN	CA-C-N	-6.42	114.06	123.05
1	Ae	175	ASN	C-N-CA	-6.42	114.06	123.05
1	Cc	175	ASN	CA-C-N	-6.42	114.06	123.05
1	Cc	175	ASN	C-N-CA	-6.42	114.06	123.05
1	Am	175	ASN	CA-C-N	-6.42	114.06	123.05
1	Am	175	ASN	C-N-CA	-6.42	114.06	123.05
1	Ac	175	ASN	CA-C-N	-6.41	114.07	123.05
1	Ac	175	ASN	C-N-CA	-6.41	114.07	123.05
1	Bc	175	ASN	CA-C-N	-6.41	114.08	123.05
1	Bc	175	ASN	C-N-CA	-6.41	114.08	123.05
1	Bk	175	ASN	CA-C-N	-6.41	114.08	123.05
1	Bk	175	ASN	C-N-CA	-6.41	114.08	123.05
1	Co	175	ASN	CA-C-N	-6.41	114.08	123.05
1	Co	175	ASN	C-N-CA	-6.41	114.08	123.05
1	Cq	175	ASN	CA-C-N	-6.41	114.08	123.05
1	Cq	175	ASN	C-N-CA	-6.41	114.08	123.05
1	Bw	175	ASN	CA-C-N	-6.40	114.08	123.05
1	Bw	175	ASN	C-N-CA	-6.40	114.08	123.05
1	Aw	175	ASN	CA-C-N	-6.40	114.09	123.05
1	Aw	175	ASN	C-N-CA	-6.40	114.09	123.05
1	Aq	175	ASN	CA-C-N	-6.40	114.09	123.05
1	Aq	175	ASN	C-N-CA	-6.40	114.09	123.05
1	Ce	175	ASN	CA-C-N	-6.40	114.09	123.05
1	Ce	175	ASN	C-N-CA	-6.40	114.09	123.05
1	Cm	175	ASN	CA-C-N	-6.40	114.09	123.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Cm	175	ASN	C-N-CA	-6.40	114.09	123.05
1	Ck	175	ASN	CA-C-N	-6.40	114.10	123.05
1	Ck	175	ASN	C-N-CA	-6.40	114.10	123.05
1	Bi	175	ASN	CA-C-N	-6.39	114.10	123.05
1	Bi	175	ASN	C-N-CA	-6.39	114.10	123.05
1	Ca	175	ASN	CA-C-N	-6.39	114.10	123.05
1	Ca	175	ASN	C-N-CA	-6.39	114.10	123.05
1	Ci	175	ASN	CA-C-N	-6.39	114.10	123.05
1	Ci	175	ASN	C-N-CA	-6.39	114.10	123.05
1	Ao	175	ASN	CA-C-N	-6.39	114.10	123.05
1	Ao	175	ASN	C-N-CA	-6.39	114.10	123.05
1	Bs	175	ASN	CA-C-N	-6.39	114.10	123.05
1	Bs	175	ASN	C-N-CA	-6.39	114.10	123.05
1	Ai	175	ASN	CA-C-N	-6.39	114.10	123.05
1	Ai	175	ASN	C-N-CA	-6.39	114.10	123.05
1	As	175	ASN	CA-C-N	-6.39	114.10	123.05
1	As	175	ASN	C-N-CA	-6.39	114.10	123.05
1	Aa	175	ASN	CA-C-N	-6.39	114.11	123.05
1	Aa	175	ASN	C-N-CA	-6.39	114.11	123.05
1	By	175	ASN	CA-C-N	-6.39	114.11	123.05
1	By	175	ASN	C-N-CA	-6.39	114.11	123.05
1	Bq	175	ASN	CA-C-N	-6.38	114.11	123.05
1	Bq	175	ASN	C-N-CA	-6.38	114.11	123.05
1	Ag	175	ASN	CA-C-N	-6.38	114.12	123.05
1	Ag	175	ASN	C-N-CA	-6.38	114.12	123.05
1	Bg	175	ASN	CA-C-N	-6.38	114.11	123.05
1	Bg	175	ASN	C-N-CA	-6.38	114.11	123.05
1	Ay	175	ASN	CA-C-N	-6.36	114.14	123.05
1	Ay	175	ASN	C-N-CA	-6.36	114.14	123.05
1	Ae	159	ASN	CA-C-O	-5.71	115.42	121.88
1	Ao	159	ASN	CA-C-O	-5.71	115.42	121.88
1	Aw	159	ASN	CA-C-O	-5.71	115.43	121.88
1	Cc	159	ASN	CA-C-O	-5.71	115.43	121.88
1	By	159	ASN	CA-C-O	-5.71	115.43	121.88
1	Bo	159	ASN	CA-C-O	-5.70	115.43	121.88
1	Bs	159	ASN	CA-C-O	-5.70	115.44	121.88
1	Bg	159	ASN	CA-C-O	-5.70	115.44	121.88
1	Aa	159	ASN	CA-C-O	-5.70	115.44	121.88
1	As	159	ASN	CA-C-O	-5.70	115.44	121.88
1	Co	159	ASN	CA-C-O	-5.70	115.44	121.88
1	Bk	159	ASN	CA-C-O	-5.69	115.45	121.88
1	Cq	159	ASN	CA-C-O	-5.68	115.46	121.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Bc	159	ASN	CA-C-O	-5.68	115.46	121.88
1	Cg	159	ASN	CA-C-O	-5.68	115.46	121.88
1	Bq	159	ASN	CA-C-O	-5.67	115.48	121.88
1	Bm	159	ASN	CA-C-O	-5.66	115.48	121.88
1	Am	159	ASN	CA-C-O	-5.66	115.49	121.88
1	Be	159	ASN	CA-C-O	-5.65	115.49	121.88
1	Ac	159	ASN	CA-C-O	-5.65	115.49	121.88
1	Ai	159	ASN	CA-C-O	-5.65	115.50	121.88
1	Au	159	ASN	CA-C-O	-5.65	115.49	121.88
1	Ag	159	ASN	CA-C-O	-5.65	115.50	121.88
1	Bw	159	ASN	CA-C-O	-5.65	115.50	121.88
1	Ak	159	ASN	CA-C-O	-5.64	115.50	121.88
1	Bu	159	ASN	CA-C-O	-5.64	115.50	121.88
1	Cm	159	ASN	CA-C-O	-5.64	115.50	121.88
1	Bi	159	ASN	CA-C-O	-5.64	115.51	121.88
1	Ay	159	ASN	CA-C-O	-5.64	115.51	121.88
1	Ba	159	ASN	CA-C-O	-5.63	115.52	121.88
1	Ca	159	ASN	CA-C-O	-5.63	115.51	121.88
1	Aq	159	ASN	CA-C-O	-5.63	115.52	121.88
1	Ce	159	ASN	CA-C-O	-5.62	115.53	121.88
1	Cs	159	ASN	CA-C-O	-5.62	115.53	121.88
1	Ci	159	ASN	CA-C-O	-5.62	115.53	121.88
1	Ck	159	ASN	CA-C-O	-5.60	115.56	121.88

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	1816	0	1764	49	0
1	Ac	1816	0	1764	55	0
1	Ae	1816	0	1764	55	0
1	Ag	1816	0	1764	59	0
1	Ai	1816	0	1764	57	0
1	Ak	1816	0	1764	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Am	1816	0	1764	59	0
1	Ao	1816	0	1764	60	0
1	Aq	1816	0	1764	56	0
1	As	1816	0	1764	64	0
1	Au	1816	0	1764	59	0
1	Aw	1816	0	1764	55	0
1	Ay	1816	0	1764	66	0
1	Ba	1816	0	1764	61	0
1	Bc	1816	0	1764	55	0
1	Be	1816	0	1764	61	0
1	Bg	1816	0	1764	64	0
1	Bi	1816	0	1764	65	0
1	Bk	1816	0	1764	66	0
1	Bm	1816	0	1764	59	0
1	Bo	1816	0	1764	58	0
1	Bq	1816	0	1764	55	0
1	Bs	1816	0	1764	63	0
1	Bu	1816	0	1764	66	0
1	Bw	1816	0	1764	67	0
1	By	1816	0	1764	59	0
1	Ca	1816	0	1764	60	0
1	Cc	1816	0	1764	62	0
1	Ce	1816	0	1764	52	0
1	Cg	1816	0	1764	56	0
1	Ci	1816	0	1764	56	0
1	Ck	1816	0	1764	55	0
1	Cm	1816	0	1764	59	0
1	Co	1816	0	1764	61	0
1	Cq	1816	0	1764	55	0
1	Cs	1816	0	1764	47	0
2	Ab	100	0	51	1	0
2	Ad	100	0	51	0	0
2	Af	100	0	51	0	0
2	Ah	100	0	51	2	0
2	Aj	100	0	51	1	0
2	Al	100	0	51	0	0
2	An	100	0	51	2	0
2	Ap	100	0	51	3	0
2	Ar	100	0	51	4	0
2	At	100	0	51	6	0
2	Av	100	0	51	0	0
2	Ax	100	0	51	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Az	100	0	51	3	0
2	Bb	100	0	51	0	0
2	Bd	100	0	51	1	0
2	Bf	100	0	51	2	0
2	Bh	100	0	51	2	0
2	Bj	100	0	51	1	0
2	Bl	100	0	51	2	0
2	Bn	100	0	51	3	0
2	Bp	100	0	51	4	0
2	Br	100	0	51	4	0
2	Bt	100	0	51	0	0
2	Bv	100	0	51	1	0
2	Bx	100	0	51	6	0
2	Bz	100	0	51	0	0
2	Cb	100	0	51	3	0
2	Cd	100	0	51	4	0
2	Cf	100	0	51	0	0
2	Ch	100	0	51	2	0
2	Cj	100	0	51	3	0
2	Cl	100	0	51	0	0
2	Cn	100	0	51	1	0
2	Cp	100	0	51	4	0
2	Cr	100	0	51	0	0
2	Ct	100	0	51	3	0
All	All	68976	0	65340	1649	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1649) 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:Cg:154:VAL:HG11	1:Ci:110:TYR:CE2	2.23	0.73
1:Ak:283:THR:O	1:Bs:256:GLN:NE2	2.23	0.72
1:Aw:283:THR:O	1:Ce:256:GLN:NE2	2.23	0.72
1:Am:283:THR:O	1:Bu:256:GLN:NE2	2.23	0.72
1:Bg:283:THR:O	1:Co:256:GLN:NE2	2.23	0.72
1:Aa:283:THR:O	1:Bi:256:GLN:NE2	2.23	0.71
1:Bc:283:THR:O	1:Ck:256:GLN:NE2	2.24	0.71
1:Ag:283:THR:O	1:Bo:256:GLN:NE2	2.24	0.71
1:Be:283:THR:O	1:Cm:256:GLN:NE2	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:283:THR:O	1:Cq:256:GLN:NE2	2.24	0.71
1:Aq:283:THR:O	1:By:256:GLN:NE2	2.24	0.71
1:Ao:283:THR:O	1:Bw:256:GLN:NE2	2.23	0.70
1:Am:150:ASN:O	1:Am:154:VAL:HG12	1.92	0.70
1:Bc:150:ASN:O	1:Bc:154:VAL:HG12	1.92	0.70
1:Ai:283:THR:O	1:Bq:256:GLN:NE2	2.24	0.70
1:Be:150:ASN:O	1:Be:154:VAL:HG12	1.92	0.70
1:Bs:150:ASN:O	1:Bs:154:VAL:HG12	1.92	0.70
1:Cg:150:ASN:O	1:Cg:154:VAL:HG12	1.92	0.70
1:As:283:THR:O	1:Ca:256:GLN:NE2	2.25	0.70
1:Ba:150:ASN:O	1:Ba:154:VAL:HG12	1.92	0.70
1:Bq:150:ASN:O	1:Bq:154:VAL:HG12	1.92	0.70
1:Bu:150:ASN:O	1:Bu:154:VAL:HG12	1.92	0.70
1:Ci:150:ASN:O	1:Ci:154:VAL:HG12	1.92	0.70
1:Ag:150:ASN:O	1:Ag:154:VAL:HG12	1.92	0.70
1:Co:150:ASN:O	1:Co:154:VAL:HG12	1.92	0.70
1:Ao:150:ASN:O	1:Ao:154:VAL:HG12	1.92	0.70
1:Ay:150:ASN:O	1:Ay:154:VAL:HG12	1.92	0.70
1:Ck:150:ASN:O	1:Ck:154:VAL:HG12	1.92	0.70
1:Cm:150:ASN:O	1:Cm:154:VAL:HG12	1.92	0.70
1:Bo:150:ASN:O	1:Bo:154:VAL:HG12	1.92	0.69
1:Ae:150:ASN:O	1:Ae:154:VAL:HG12	1.92	0.69
1:Bg:150:ASN:O	1:Bg:154:VAL:HG12	1.92	0.69
1:Ak:150:ASN:O	1:Ak:154:VAL:HG12	1.92	0.69
1:Aw:154:VAL:HG11	1:Ay:110:TYR:CE2	2.28	0.69
1:Bm:150:ASN:O	1:Bm:154:VAL:HG12	1.92	0.69
1:Bw:150:ASN:O	1:Bw:154:VAL:HG12	1.92	0.69
1:Au:283:THR:O	1:Cc:256:GLN:NE2	2.26	0.69
1:As:165:ILE:HG22	2:At:5:U:O2	1.91	0.69
1:Ce:150:ASN:O	1:Ce:154:VAL:HG12	1.92	0.69
1:Ca:150:ASN:O	1:Ca:154:VAL:HG12	1.92	0.69
1:Ai:150:ASN:O	1:Ai:154:VAL:HG12	1.92	0.69
1:Aq:150:ASN:O	1:Aq:154:VAL:HG12	1.92	0.69
1:As:150:ASN:O	1:As:154:VAL:HG12	1.92	0.69
1:Au:150:ASN:O	1:Au:154:VAL:HG12	1.92	0.69
1:Ay:283:THR:O	1:Cg:256:GLN:NE2	2.25	0.69
1:Bw:165:ILE:HG22	2:Bx:5:U:O2	1.91	0.69
1:By:150:ASN:O	1:By:154:VAL:HG12	1.92	0.69
1:Aa:150:ASN:O	1:Aa:154:VAL:HG12	1.92	0.69
1:Ac:150:ASN:O	1:Ac:154:VAL:HG12	1.92	0.69
1:Bi:150:ASN:O	1:Bi:154:VAL:HG12	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bs:154:VAL:HG11	1:Bu:110:TYR:CE2	2.29	0.68
1:Cc:150:ASN:O	1:Cc:154:VAL:HG12	1.92	0.68
1:Cs:150:ASN:O	1:Cs:154:VAL:HG12	1.92	0.68
1:Aw:150:ASN:O	1:Aw:154:VAL:HG12	1.92	0.68
1:Cq:150:ASN:O	1:Cq:154:VAL:HG12	1.92	0.68
1:Ba:154:VAL:HG11	1:Bc:110:TYR:CE2	2.29	0.68
1:Bk:150:ASN:O	1:Bk:154:VAL:HG12	1.92	0.68
1:Be:220:ARG:NH2	2:Bf:5:U:O3'	2.26	0.67
1:Bq:144:GLN:HB3	1:Ck:82:PRO:HG3	1.77	0.67
1:Ba:144:GLN:HB3	1:Bu:82:PRO:HG3	1.77	0.66
1:Bk:283:THR:O	1:Cs:256:GLN:NE2	2.30	0.65
1:Cg:158:GLU:OE1	1:Ci:114:GLN:HG3	1.96	0.65
1:Ae:283:THR:O	1:Bm:256:GLN:NE2	2.30	0.65
1:Ac:283:THR:O	1:Bk:256:GLN:NE2	2.29	0.65
1:Bs:210:MET:HE2	1:Bu:108:ILE:HA	1.78	0.64
1:Bk:154:VAL:HG11	1:Bm:110:TYR:CE2	2.32	0.64
2:Bn:5:U:O3'	2:Bp:1:U:H5'	1.98	0.64
1:Ai:154:VAL:HG11	1:Ak:110:TYR:CE2	2.33	0.63
1:Am:220:ARG:NH2	2:An:5:U:O3'	2.32	0.63
1:Bs:291:VAL:O	1:Bu:296:HIS:CD2	2.53	0.62
1:Au:154:VAL:HG11	1:Aw:110:TYR:CE2	2.35	0.62
1:Cc:154:VAL:HG11	1:Ce:110:TYR:CE2	2.35	0.62
1:Ag:195:GLN:HE21	2:Ah:2:U:H5'	1.63	0.61
1:Bu:154:VAL:HG11	1:Bw:110:TYR:CE2	2.36	0.61
1:Aa:154:VAL:HG11	1:Ac:110:TYR:CE2	2.36	0.61
1:Ac:154:VAL:HG11	1:Ae:110:TYR:CE2	2.35	0.61
1:Ci:154:VAL:HG11	1:Ck:110:TYR:CE2	2.35	0.61
1:Cm:154:VAL:HG11	1:Co:110:TYR:CE2	2.36	0.61
1:Am:195:GLN:HE21	2:An:2:U:H5'	1.66	0.61
1:Bc:154:VAL:HG11	1:Be:110:TYR:CE2	2.36	0.61
1:Bg:154:VAL:HG11	1:Bi:110:TYR:CE2	2.35	0.61
1:Cq:154:VAL:HG11	1:Cs:110:TYR:CE2	2.35	0.61
1:Bo:154:VAL:HG11	1:Bq:110:TYR:CE2	2.35	0.61
1:Am:154:VAL:HG11	1:Ao:110:TYR:CE2	2.36	0.61
1:By:154:VAL:HG11	1:Ca:110:TYR:CE2	2.35	0.61
1:Ag:144:GLN:HB3	1:Ba:82:PRO:HG3	1.82	0.61
1:Ak:154:VAL:HG11	1:Am:110:TYR:CE2	2.36	0.61
1:As:154:VAL:HG11	1:Au:110:TYR:CE2	2.36	0.61
1:Ae:154:VAL:HG11	1:Ag:110:TYR:CE2	2.35	0.61
1:Be:154:VAL:HG11	1:Bg:110:TYR:CE2	2.36	0.61
1:Ck:154:VAL:HG11	1:Cm:110:TYR:CE2	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:154:VAL:HG11	1:Aq:110:TYR:CE2	2.35	0.61
1:Bw:154:VAL:HG11	1:By:110:TYR:CE2	2.36	0.61
1:Bw:220:ARG:NH2	2:Bx:5:U:O3'	2.34	0.61
1:Co:154:VAL:HG11	1:Cq:110:TYR:CE2	2.36	0.61
1:Aq:144:GLN:HB3	1:Bk:82:PRO:HG3	1.81	0.61
1:Bi:144:GLN:HB3	1:Cc:82:PRO:HG3	1.82	0.61
1:Bm:154:VAL:HG11	1:Bo:110:TYR:CE2	2.35	0.61
1:Ae:144:GLN:HB3	1:Ay:82:PRO:HG3	1.83	0.60
1:Bq:195:GLN:HE21	2:Br:2:U:H5'	1.65	0.60
1:Aq:154:VAL:HG11	1:As:110:TYR:CE2	2.36	0.60
1:Ac:170:THR:HG21	1:Ac:177:GLN:HE21	1.67	0.60
1:As:195:GLN:HE21	2:At:2:U:H5'	1.65	0.60
1:Aa:170:THR:HG21	1:Aa:177:GLN:HE21	1.67	0.60
1:Ca:170:THR:HG21	1:Ca:177:GLN:HE21	1.67	0.60
1:Cc:170:THR:HG21	1:Cc:177:GLN:HE21	1.67	0.60
1:Ae:170:THR:HG21	1:Ae:177:GLN:HE21	1.67	0.60
1:Ce:170:THR:HG21	1:Ce:177:GLN:HE21	1.67	0.60
1:Cm:220:ARG:NH2	2:Cn:5:U:O3'	2.35	0.60
1:Bo:170:THR:HG21	1:Bo:177:GLN:HE21	1.67	0.60
1:Aq:170:THR:HG21	1:Aq:177:GLN:HE21	1.67	0.60
1:Ca:165:ILE:HG22	2:Cb:5:U:O2	2.01	0.60
1:Ag:154:VAL:HG11	1:Ai:110:TYR:CE2	2.36	0.59
1:Ay:291:VAL:O	1:Ba:296:HIS:CD2	2.54	0.59
1:Bs:283:THR:OG1	1:Ck:269:MET:HE3	2.02	0.59
1:Ao:170:THR:HG21	1:Ao:177:GLN:HE21	1.67	0.59
1:Bm:170:THR:HG21	1:Bm:177:GLN:HE21	1.67	0.59
1:By:170:THR:HG21	1:By:177:GLN:HE21	1.67	0.59
1:Cs:261:ALA:HB1	2:Ct:4:U:H1'	1.82	0.59
1:As:170:THR:HG21	1:As:177:GLN:HE21	1.67	0.59
1:Bk:170:THR:HG21	1:Bk:177:GLN:HE21	1.67	0.59
1:Bq:170:THR:HG21	1:Bq:177:GLN:HE21	1.67	0.59
1:Au:170:THR:HG21	1:Au:177:GLN:HE21	1.67	0.59
1:Co:170:THR:HG21	1:Co:177:GLN:HE21	1.67	0.59
1:Cq:170:THR:HG21	1:Cq:177:GLN:HE21	1.67	0.59
1:Ag:170:THR:HG21	1:Ag:177:GLN:HE21	1.67	0.59
1:Bs:170:THR:HG21	1:Bs:177:GLN:HE21	1.67	0.59
1:Cg:154:VAL:HG11	1:Ci:110:TYR:HE2	1.67	0.59
1:Cg:170:THR:HG21	1:Cg:177:GLN:HE21	1.67	0.59
1:Ai:170:THR:HG21	1:Ai:177:GLN:HE21	1.67	0.59
1:Be:170:THR:HG21	1:Be:177:GLN:HE21	1.67	0.59
1:Bc:170:THR:HG21	1:Bc:177:GLN:HE21	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:170:THR:HG21	1:Bu:177:GLN:HE21	1.67	0.59
1:Ci:170:THR:HG21	1:Ci:177:GLN:HE21	1.67	0.59
1:Am:170:THR:HG21	1:Am:177:GLN:HE21	1.67	0.58
1:Ck:170:THR:HG21	1:Ck:177:GLN:HE21	1.67	0.58
1:Cs:170:THR:HG21	1:Cs:177:GLN:HE21	1.67	0.58
1:Ak:170:THR:HG21	1:Ak:177:GLN:HE21	1.67	0.58
1:Ay:170:THR:HG21	1:Ay:177:GLN:HE21	1.67	0.58
1:Ca:154:VAL:HG11	1:Cc:110:TYR:CE2	2.39	0.58
1:Ba:170:THR:HG21	1:Ba:177:GLN:HE21	1.67	0.58
1:Cm:170:THR:HG21	1:Cm:177:GLN:HE21	1.67	0.58
1:Co:220:ARG:NH2	2:Cp:5:U:O3'	2.37	0.58
1:Bi:170:THR:HG21	1:Bi:177:GLN:HE21	1.67	0.58
1:Co:165:ILE:HG22	2:Cp:5:U:O2	2.03	0.58
1:Ba:158:GLU:OE1	1:Bc:114:GLN:HG3	2.03	0.58
1:Aw:170:THR:HG21	1:Aw:177:GLN:HE21	1.67	0.58
1:Bs:158:GLU:OE1	1:Bu:114:GLN:HG3	2.04	0.58
1:Bw:170:THR:HG21	1:Bw:177:GLN:HE21	1.67	0.58
1:Bw:195:GLN:HE21	2:Bx:2:U:H5'	1.68	0.58
1:Aa:144:GLN:HB3	1:Au:82:PRO:HG3	1.86	0.58
1:Bg:170:THR:HG21	1:Bg:177:GLN:HE21	1.67	0.57
1:Ag:134:VAL:HG12	1:Ag:145:MET:HE1	1.87	0.57
1:Bc:144:GLN:HB3	1:Bw:82:PRO:HG3	1.86	0.57
1:Bm:134:VAL:HG12	1:Bm:145:MET:HE1	1.87	0.57
1:Ci:134:VAL:HG12	1:Ci:145:MET:HE1	1.87	0.57
1:Ck:134:VAL:HG12	1:Ck:145:MET:HE1	1.87	0.57
1:Ai:134:VAL:HG12	1:Ai:145:MET:HE1	1.87	0.57
1:Bo:134:VAL:HG12	1:Bo:145:MET:HE1	1.87	0.57
1:Bc:134:VAL:HG12	1:Bc:145:MET:HE1	1.87	0.57
1:Ae:134:VAL:HG12	1:Ae:145:MET:HE1	1.87	0.57
1:Ba:154:VAL:HG11	1:Bc:110:TYR:HE2	1.69	0.57
1:Ci:291:VAL:O	1:Ck:296:HIS:CD2	2.57	0.57
1:Ba:134:VAL:HG12	1:Ba:145:MET:HE1	1.87	0.57
1:Ba:283:THR:O	1:Ci:256:GLN:NE2	2.38	0.57
1:Cg:134:VAL:HG12	1:Cg:145:MET:HE1	1.87	0.57
1:Ac:144:GLN:HB3	1:Aw:82:PRO:HG3	1.86	0.57
1:Ck:210:MET:HE2	1:Cm:108:ILE:HA	1.86	0.57
1:Cs:134:VAL:HG12	1:Cs:145:MET:HE1	1.86	0.57
1:Ak:134:VAL:HG12	1:Ak:145:MET:HE1	1.87	0.57
1:As:134:VAL:HG12	1:As:145:MET:HE1	1.87	0.57
1:Bg:144:GLN:HB3	1:Ca:82:PRO:HG3	1.87	0.57
1:Bq:134:VAL:HG12	1:Bq:145:MET:HE1	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aw:291:VAL:O	1:Ay:296:HIS:CD2	2.58	0.57
1:Be:134:VAL:HG12	1:Be:145:MET:HE1	1.87	0.57
1:Bk:134:VAL:HG12	1:Bk:145:MET:HE1	1.87	0.57
1:Au:134:VAL:HG12	1:Au:145:MET:HE1	1.87	0.57
1:Cm:134:VAL:HG12	1:Cm:145:MET:HE1	1.87	0.57
1:Ac:134:VAL:HG12	1:Ac:145:MET:HE1	1.87	0.56
1:Ac:159:ASN:CG	1:Ae:119:ASN:HB2	2.30	0.56
1:Ai:291:VAL:O	1:Ak:296:HIS:CD2	2.58	0.56
1:Aq:134:VAL:HG12	1:Aq:145:MET:HE1	1.87	0.56
1:By:134:VAL:HG12	1:By:145:MET:HE1	1.86	0.56
1:Ce:134:VAL:HG12	1:Ce:145:MET:HE1	1.87	0.56
1:Bw:134:VAL:HG12	1:Bw:145:MET:HE1	1.87	0.56
1:As:144:GLN:HB3	1:Bm:82:PRO:HG3	1.87	0.56
1:Ay:134:VAL:HG12	1:Ay:145:MET:HE1	1.87	0.56
1:Bk:144:GLN:HB3	1:Ce:82:PRO:HG3	1.86	0.56
1:Bk:283:THR:OG1	1:Cc:269:MET:HE3	2.04	0.56
1:Bs:134:VAL:HG12	1:Bs:145:MET:HE1	1.87	0.56
1:Ca:134:VAL:HG12	1:Ca:145:MET:HE1	1.87	0.56
1:Ao:144:GLN:HB3	1:Bi:82:PRO:HG3	1.87	0.56
1:Aw:158:GLU:OE1	1:Ay:114:GLN:HG3	2.04	0.56
1:Bu:134:VAL:HG12	1:Bu:145:MET:HE1	1.86	0.56
1:Be:144:GLN:HB3	1:By:82:PRO:HG3	1.88	0.56
1:Bo:144:GLN:HB3	1:Ci:82:PRO:HG3	1.88	0.56
1:Cq:134:VAL:HG12	1:Cq:145:MET:HE1	1.86	0.56
1:Ao:134:VAL:HG12	1:Ao:145:MET:HE1	1.86	0.56
1:Ay:154:VAL:HG11	1:Ba:110:TYR:CE2	2.40	0.56
1:Au:144:GLN:HB3	1:Bo:82:PRO:HG3	1.88	0.56
1:Aw:134:VAL:HG12	1:Aw:145:MET:HE1	1.87	0.56
1:Bg:134:VAL:HG12	1:Bg:145:MET:HE1	1.86	0.56
1:Cc:134:VAL:HG12	1:Cc:145:MET:HE1	1.87	0.56
1:Bi:154:VAL:HG11	1:Bk:110:TYR:CE2	2.41	0.56
1:Cg:210:MET:HE2	1:Ci:108:ILE:HA	1.87	0.56
1:Aa:134:VAL:HG12	1:Aa:145:MET:HE1	1.87	0.55
1:Am:134:VAL:HG12	1:Am:145:MET:HE1	1.87	0.55
1:Bg:158:GLU:OE1	1:Bi:114:GLN:HG3	2.07	0.55
1:Bi:134:VAL:HG12	1:Bi:145:MET:HE1	1.87	0.55
1:Bu:144:GLN:HB3	1:Co:82:PRO:HG3	1.87	0.55
1:Am:158:GLU:OE1	1:Ao:114:GLN:HG3	2.07	0.55
1:Bw:158:GLU:OE1	1:By:114:GLN:HG3	2.07	0.55
1:Ak:158:GLU:OE1	1:Am:114:GLN:HG3	2.07	0.55
1:Ao:158:GLU:OE1	1:Aq:114:GLN:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Aw:144:GLN:HB3	1:Bq:82:PRO:HG3	1.89	0.55
1:Bu:158:GLU:OE1	1:Bw:114:GLN:HG3	2.07	0.55
1:Cm:158:GLU:OE1	1:Co:114:GLN:HG3	2.07	0.55
1:Co:134:VAL:HG12	1:Co:145:MET:HE1	1.87	0.55
1:Co:158:GLU:OE1	1:Cq:114:GLN:HG3	2.07	0.55
1:Be:158:GLU:OE1	1:Bg:114:GLN:HG3	2.07	0.55
1:By:158:GLU:OE1	1:Ca:114:GLN:HG3	2.07	0.55
1:Cq:158:GLU:OE1	1:Cs:114:GLN:HG3	2.07	0.55
1:Aa:158:GLU:OE1	1:Ac:114:GLN:HG3	2.07	0.55
1:Ac:158:GLU:OE1	1:Ae:114:GLN:HG3	2.06	0.55
1:Ai:144:GLN:HB3	1:Bc:82:PRO:HG3	1.89	0.55
1:As:158:GLU:OE1	1:Au:114:GLN:HG3	2.07	0.55
1:Bc:158:GLU:OE1	1:Be:114:GLN:HG3	2.07	0.55
1:Bo:158:GLU:OE1	1:Bq:114:GLN:HG3	2.06	0.55
1:By:144:GLN:HB3	1:Cs:82:PRO:HG3	1.89	0.54
1:Ag:158:GLU:OE1	1:Ai:114:GLN:HG3	2.07	0.54
1:Aw:154:VAL:HG11	1:Ay:110:TYR:HE2	1.70	0.54
1:Am:144:GLN:HB3	1:Bg:82:PRO:HG3	1.88	0.54
1:Bq:159:ASN:CG	1:Bs:119:ASN:HB2	2.32	0.54
1:Aq:158:GLU:OE1	1:As:114:GLN:HG3	2.07	0.54
1:Bm:158:GLU:OE1	1:Bo:114:GLN:HG3	2.07	0.54
1:Bs:200:PHE:HE1	1:Bu:102:LEU:HD21	1.72	0.54
1:Au:158:GLU:OE1	1:Aw:114:GLN:HG3	2.07	0.54
1:Ae:210:MET:HE2	1:Ag:108:ILE:HA	1.90	0.54
1:Ai:158:GLU:OE1	1:Ak:114:GLN:HG3	2.07	0.54
1:Ak:144:GLN:HB3	1:Be:82:PRO:HG3	1.90	0.54
2:Bn:5:U:H2'	2:Bp:1:U:O4'	2.08	0.54
1:Bs:206:ALA:HB2	1:Bu:91:MET:HE2	1.90	0.54
1:Bw:144:GLN:HB3	1:Cq:82:PRO:HG3	1.90	0.54
1:Cg:200:PHE:HE1	1:Ci:102:LEU:HD21	1.73	0.54
1:Ci:158:GLU:OE1	1:Ck:114:GLN:HG3	2.08	0.54
1:Bc:159:ASN:CG	1:Be:119:ASN:HB2	2.33	0.53
1:Cm:159:ASN:CG	1:Co:119:ASN:HB2	2.33	0.53
1:Aa:159:ASN:CG	1:Ac:119:ASN:HB2	2.34	0.53
1:Ay:272:LEU:N	1:Bq:252:GLU:OE1	2.39	0.53
1:Bo:159:ASN:CG	1:Bq:119:ASN:HB2	2.34	0.53
1:Ca:291:VAL:O	1:Cc:296:HIS:CD2	2.61	0.53
1:Ck:158:GLU:OE1	1:Cm:114:GLN:HG3	2.08	0.53
1:Ag:283:THR:OG1	1:Ay:269:MET:HE3	2.09	0.53
1:By:159:ASN:CG	1:Ca:119:ASN:HB2	2.34	0.53
1:Ci:159:ASN:CG	1:Ck:119:ASN:HB2	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cq:159:ASN:CG	1:Cs:119:ASN:HB2	2.34	0.53
1:Aq:159:ASN:CG	1:As:119:ASN:HB2	2.34	0.53
1:As:159:ASN:CG	1:Au:119:ASN:HB2	2.34	0.53
1:Bg:159:ASN:CG	1:Bi:119:ASN:HB2	2.34	0.53
1:Bi:159:ASN:CG	1:Bk:119:ASN:HB2	2.34	0.53
1:Ao:159:ASN:CG	1:Aq:119:ASN:HB2	2.34	0.53
1:As:220:ARG:NH2	2:At:5:U:O3'	2.41	0.53
1:Aw:200:PHE:HE1	1:Ay:102:LEU:HD21	1.74	0.53
1:Bk:158:GLU:OE1	1:Bm:114:GLN:HG3	2.08	0.53
1:Ac:291:VAL:O	1:Ae:296:HIS:CD2	2.62	0.52
1:Au:159:ASN:CG	1:Aw:119:ASN:HB2	2.35	0.52
1:Ca:220:ARG:NH2	2:Cb:5:U:O3'	2.42	0.52
1:Cc:158:GLU:OE1	1:Ce:114:GLN:HG3	2.08	0.52
1:Ag:159:ASN:CG	1:Ai:119:ASN:HB2	2.33	0.52
1:Bw:159:ASN:CG	1:By:119:ASN:HB2	2.35	0.52
1:Am:86:LYS:HD2	1:Am:86:LYS:N	2.25	0.52
1:Bk:154:VAL:HG11	1:Bm:110:TYR:HE2	1.73	0.52
1:Am:159:ASN:CG	1:Ao:119:ASN:HB2	2.35	0.52
1:Bu:86:LYS:HD2	1:Bu:86:LYS:N	2.25	0.52
1:Bu:159:ASN:CG	1:Bw:119:ASN:HB2	2.34	0.52
1:Au:283:THR:OG1	1:Bm:269:MET:HE3	2.10	0.52
1:Bc:86:LYS:N	1:Bc:86:LYS:HD2	2.25	0.52
1:By:86:LYS:HD2	1:By:86:LYS:N	2.25	0.52
1:Ak:210:MET:HE2	1:Am:108:ILE:HA	1.91	0.52
1:Be:159:ASN:CG	1:Bg:119:ASN:HB2	2.35	0.52
1:Cg:291:VAL:O	1:Ci:296:HIS:CD2	2.62	0.52
1:Ak:252:GLU:OE2	1:Ak:256:GLN:NE2	2.43	0.52
1:Aw:283:THR:OG1	1:Bo:269:MET:HE3	2.10	0.52
1:Ba:252:GLU:OE2	1:Ba:256:GLN:NE2	2.43	0.52
1:Be:165:ILE:HG22	2:Bf:5:U:O2	2.09	0.52
1:Bi:86:LYS:HD2	1:Bi:86:LYS:N	2.25	0.52
1:Ck:86:LYS:HD2	1:Ck:86:LYS:N	2.25	0.52
1:Co:86:LYS:HD2	1:Co:86:LYS:N	2.25	0.52
1:Be:86:LYS:HD2	1:Be:86:LYS:N	2.25	0.52
1:Bm:159:ASN:CG	1:Bo:119:ASN:HB2	2.35	0.52
1:Bq:252:GLU:OE2	1:Bq:256:GLN:NE2	2.43	0.52
1:Co:159:ASN:CG	1:Cq:119:ASN:HB2	2.35	0.52
1:Co:252:GLU:OE2	1:Co:256:GLN:NE2	2.43	0.52
1:Cq:86:LYS:N	1:Cq:86:LYS:HD2	2.25	0.52
1:Aq:86:LYS:HD2	1:Aq:86:LYS:N	2.25	0.52
1:Bc:252:GLU:OE2	1:Bc:256:GLN:NE2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bw:252:GLU:OE2	1:Bw:256:GLN:NE2	2.43	0.52
1:Ci:252:GLU:OE2	1:Ci:256:GLN:NE2	2.43	0.52
1:Ai:252:GLU:OE2	1:Ai:256:GLN:NE2	2.43	0.51
1:Aq:129:PHE:HE2	1:Aq:133:ARG:HE	1.59	0.51
1:Be:252:GLU:OE2	1:Be:256:GLN:NE2	2.43	0.51
1:Bu:252:GLU:OE2	1:Bu:256:GLN:NE2	2.43	0.51
1:Bw:129:PHE:HE2	1:Bw:133:ARG:HE	1.58	0.51
1:Cg:252:GLU:OE2	1:Cg:256:GLN:NE2	2.43	0.51
1:Cm:252:GLU:OE2	1:Cm:256:GLN:NE2	2.43	0.51
1:Aa:86:LYS:HD2	1:Aa:86:LYS:N	2.25	0.51
1:Aa:129:PHE:HE2	1:Aa:133:ARG:HE	1.59	0.51
1:Bg:129:PHE:HE2	1:Bg:133:ARG:HE	1.59	0.51
1:Bg:252:GLU:OE2	1:Bg:256:GLN:NE2	2.43	0.51
1:Bi:158:GLU:OE1	1:Bk:114:GLN:HG3	2.10	0.51
1:Bs:252:GLU:OE2	1:Bs:256:GLN:NE2	2.43	0.51
1:Cm:129:PHE:HE2	1:Cm:133:ARG:HE	1.59	0.51
1:Ai:86:LYS:HD2	1:Ai:86:LYS:N	2.25	0.51
1:Ay:252:GLU:OE2	1:Ay:256:GLN:NE2	2.43	0.51
1:Ba:129:PHE:HE2	1:Ba:133:ARG:HE	1.59	0.51
1:By:252:GLU:OE2	1:By:256:GLN:NE2	2.43	0.51
1:Ae:158:GLU:OE1	1:Ag:114:GLN:HG3	2.10	0.51
1:Ai:129:PHE:HE2	1:Ai:133:ARG:HE	1.59	0.51
1:Ai:159:ASN:CG	1:Ak:119:ASN:HB2	2.36	0.51
1:Ak:129:PHE:HE2	1:Ak:133:ARG:HE	1.59	0.51
1:Am:252:GLU:OE2	1:Am:256:GLN:NE2	2.43	0.51
1:Ba:159:ASN:CG	1:Bc:119:ASN:HB2	2.35	0.51
1:Bg:86:LYS:HD2	1:Bg:86:LYS:N	2.25	0.51
1:Cm:86:LYS:N	1:Cm:86:LYS:HD2	2.25	0.51
1:Cs:129:PHE:HE2	1:Cs:133:ARG:HE	1.59	0.51
1:Ag:252:GLU:OE2	1:Ag:256:GLN:NE2	2.43	0.51
1:Ak:86:LYS:HD2	1:Ak:86:LYS:N	2.25	0.51
1:Am:283:THR:OG1	1:Be:269:MET:HE3	2.10	0.51
1:Aq:252:GLU:OE2	1:Aq:256:GLN:NE2	2.43	0.51
1:Bq:129:PHE:HE2	1:Bq:133:ARG:HE	1.59	0.51
1:Bs:86:LYS:N	1:Bs:86:LYS:HD2	2.25	0.51
1:Ca:159:ASN:CG	1:Cc:119:ASN:HB2	2.36	0.51
1:Cc:129:PHE:HE2	1:Cc:133:ARG:HE	1.59	0.51
1:Ck:252:GLU:OE2	1:Ck:256:GLN:NE2	2.43	0.51
1:Co:129:PHE:HE2	1:Co:133:ARG:HE	1.58	0.51
1:Ay:210:MET:HE2	1:Ba:108:ILE:HA	1.93	0.51
1:Bi:129:PHE:HE2	1:Bi:133:ARG:HE	1.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:252:GLU:OE2	1:Bi:256:GLN:NE2	2.43	0.51
1:Bm:129:PHE:HE2	1:Bm:133:ARG:HE	1.59	0.51
1:Bo:252:GLU:OE2	1:Bo:256:GLN:NE2	2.43	0.51
1:By:129:PHE:HE2	1:By:133:ARG:HE	1.59	0.51
1:Ae:129:PHE:HE2	1:Ae:133:ARG:HE	1.59	0.51
1:Ae:252:GLU:OE2	1:Ae:256:GLN:NE2	2.43	0.51
1:Ao:86:LYS:HD2	1:Ao:86:LYS:N	2.25	0.51
1:Ao:252:GLU:OE2	1:Ao:256:GLN:NE2	2.43	0.51
1:As:252:GLU:OE2	1:As:256:GLN:NE2	2.43	0.51
1:Bk:220:ARG:NH2	2:Bl:5:U:O3'	2.44	0.51
1:Bk:252:GLU:OE2	1:Bk:256:GLN:NE2	2.43	0.51
1:Ca:158:GLU:OE1	1:Cc:114:GLN:HG3	2.10	0.51
1:Cq:252:GLU:OE2	1:Cq:256:GLN:NE2	2.43	0.51
1:Au:157:ILE:HG22	1:Au:158:GLU:OE2	2.11	0.51
1:Au:252:GLU:OE2	1:Au:256:GLN:NE2	2.43	0.51
1:Bi:157:ILE:HG22	1:Bi:158:GLU:OE2	2.11	0.51
1:Bo:157:ILE:HG22	1:Bo:158:GLU:OE2	2.11	0.51
1:Bu:129:PHE:HE2	1:Bu:133:ARG:HE	1.59	0.51
1:Ca:86:LYS:N	1:Ca:86:LYS:HD2	2.25	0.51
1:Cc:86:LYS:HD2	1:Cc:86:LYS:N	2.25	0.51
1:Cc:252:GLU:OE2	1:Cc:256:GLN:NE2	2.43	0.51
1:Aa:157:ILE:HG22	1:Aa:158:GLU:OE2	2.11	0.51
1:Aa:252:GLU:OE2	1:Aa:256:GLN:NE2	2.43	0.51
1:Ac:252:GLU:OE2	1:Ac:256:GLN:NE2	2.43	0.51
1:Aq:157:ILE:HG22	1:Aq:158:GLU:OE2	2.11	0.51
1:Ay:86:LYS:HD2	1:Ay:86:LYS:N	2.25	0.51
1:Be:129:PHE:HE2	1:Be:133:ARG:HE	1.59	0.51
1:Bm:252:GLU:OE2	1:Bm:256:GLN:NE2	2.43	0.51
1:Bq:86:LYS:HD2	1:Bq:86:LYS:N	2.25	0.51
1:Ca:252:GLU:OE2	1:Ca:256:GLN:NE2	2.43	0.51
1:Cc:157:ILE:HG22	1:Cc:158:GLU:OE2	2.11	0.51
1:Cc:159:ASN:CG	1:Ce:119:ASN:HB2	2.35	0.51
1:Cg:129:PHE:HE2	1:Cg:133:ARG:HE	1.59	0.51
1:Cg:157:ILE:HG22	1:Cg:158:GLU:OE2	2.11	0.51
1:Ci:154:VAL:HG11	1:Ck:110:TYR:HE2	1.74	0.51
1:Ck:129:PHE:HE2	1:Ck:133:ARG:HE	1.59	0.51
1:Ag:157:ILE:HG22	1:Ag:158:GLU:OE2	2.11	0.51
1:Ao:129:PHE:HE2	1:Ao:133:ARG:HE	1.59	0.51
1:Ao:157:ILE:HG22	1:Ao:158:GLU:OE2	2.11	0.51
1:As:86:LYS:HD2	1:As:86:LYS:N	2.25	0.51
1:As:129:PHE:HE2	1:As:133:ARG:HE	1.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:129:PHE:HE2	1:Au:133:ARG:HE	1.59	0.51
1:Ce:154:VAL:HG11	1:Cg:110:TYR:CE2	2.46	0.51
1:Cg:159:ASN:CG	1:Ci:119:ASN:HB2	2.36	0.51
1:Co:157:ILE:HG22	1:Co:158:GLU:OE2	2.11	0.51
1:Cq:157:ILE:HG22	1:Cq:158:GLU:OE2	2.11	0.51
1:Ac:86:LYS:HD2	1:Ac:86:LYS:N	2.25	0.50
1:Am:86:LYS:HA	1:Am:86:LYS:HE3	1.94	0.50
1:Ay:129:PHE:HE2	1:Ay:133:ARG:HE	1.59	0.50
1:Ba:157:ILE:HG22	1:Ba:158:GLU:OE2	2.11	0.50
1:Bg:157:ILE:HG22	1:Bg:158:GLU:OE2	2.11	0.50
1:Bs:86:LYS:HE3	1:Bs:86:LYS:HA	1.94	0.50
1:Bw:86:LYS:N	1:Bw:86:LYS:HD2	2.25	0.50
1:Ca:157:ILE:HG22	1:Ca:158:GLU:OE2	2.11	0.50
1:Ce:157:ILE:HG22	1:Ce:158:GLU:OE2	2.11	0.50
1:Ce:252:GLU:OE2	1:Ce:256:GLN:NE2	2.43	0.50
1:Cg:86:LYS:HD2	1:Cg:86:LYS:N	2.25	0.50
1:Ci:129:PHE:HE2	1:Ci:133:ARG:HE	1.59	0.50
1:Ci:157:ILE:HG22	1:Ci:158:GLU:OE2	2.11	0.50
1:Co:86:LYS:HE3	1:Co:86:LYS:HA	1.94	0.50
1:Ak:273:ASP:OD2	1:Ak:274:GLY:N	2.45	0.50
1:Am:157:ILE:HG22	1:Am:158:GLU:OE2	2.11	0.50
1:Aw:129:PHE:HE2	1:Aw:133:ARG:HE	1.59	0.50
1:Ba:273:ASP:OD2	1:Ba:274:GLY:N	2.45	0.50
1:Bg:86:LYS:HA	1:Bg:86:LYS:HE3	1.94	0.50
1:Bi:273:ASP:OD2	1:Bi:274:GLY:N	2.45	0.50
1:Bi:283:THR:OG1	1:Ca:269:MET:HE3	2.11	0.50
1:Bq:157:ILE:HG22	1:Bq:158:GLU:OE2	2.11	0.50
1:Co:273:ASP:OD2	1:Co:274:GLY:N	2.45	0.50
1:Cq:273:ASP:OD2	1:Cq:274:GLY:N	2.45	0.50
1:Cs:252:GLU:OE2	1:Cs:256:GLN:NE2	2.43	0.50
1:Ac:157:ILE:HG22	1:Ac:158:GLU:OE2	2.11	0.50
1:Ai:157:ILE:HG22	1:Ai:158:GLU:OE2	2.11	0.50
1:Ak:86:LYS:HE3	1:Ak:86:LYS:HA	1.93	0.50
1:Ak:159:ASN:CG	1:Am:119:ASN:HB2	2.36	0.50
1:As:157:ILE:HG22	1:As:158:GLU:OE2	2.11	0.50
1:Aw:252:GLU:OE2	1:Aw:256:GLN:NE2	2.43	0.50
1:Ay:86:LYS:HA	1:Ay:86:LYS:HE3	1.94	0.50
1:Bc:154:VAL:HG11	1:Be:110:TYR:HE2	1.76	0.50
1:Bi:86:LYS:HE3	1:Bi:86:LYS:HA	1.94	0.50
1:Bk:273:ASP:OD2	1:Bk:274:GLY:N	2.45	0.50
1:Bo:86:LYS:N	1:Bo:86:LYS:HD2	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bq:283:THR:OG1	1:Ci:269:MET:HE3	2.12	0.50
1:Bu:157:ILE:HG22	1:Bu:158:GLU:OE2	2.11	0.50
1:By:273:ASP:OD2	1:By:274:GLY:N	2.45	0.50
1:Cc:273:ASP:OD2	1:Cc:274:GLY:N	2.45	0.50
1:Ce:86:LYS:N	1:Ce:86:LYS:HD2	2.25	0.50
1:Ci:273:ASP:OD2	1:Ci:274:GLY:N	2.45	0.50
1:Cm:86:LYS:HE3	1:Cm:86:LYS:HA	1.94	0.50
1:Cs:86:LYS:HD2	1:Cs:86:LYS:N	2.25	0.50
1:Cs:157:ILE:HG22	1:Cs:158:GLU:OE2	2.11	0.50
1:Aa:86:LYS:HA	1:Aa:86:LYS:HE3	1.94	0.50
1:Ac:283:THR:OG1	1:Au:269:MET:HE3	2.12	0.50
1:Am:273:ASP:OD2	1:Am:274:GLY:N	2.45	0.50
1:Au:86:LYS:HD2	1:Au:86:LYS:N	2.25	0.50
1:Aw:157:ILE:HG22	1:Aw:158:GLU:OE2	2.11	0.50
1:Bc:273:ASP:OD2	1:Bc:274:GLY:N	2.45	0.50
1:Bg:273:ASP:OD2	1:Bg:274:GLY:N	2.45	0.50
1:Bk:129:PHE:HE2	1:Bk:133:ARG:HE	1.59	0.50
1:Bm:86:LYS:HD2	1:Bm:86:LYS:N	2.25	0.50
1:Bs:129:PHE:HE2	1:Bs:133:ARG:HE	1.59	0.50
1:Bu:86:LYS:HE3	1:Bu:86:LYS:HA	1.94	0.50
1:Bw:157:ILE:HG22	1:Bw:158:GLU:OE2	2.11	0.50
1:Ca:273:ASP:OD2	1:Ca:274:GLY:N	2.45	0.50
1:Cq:86:LYS:HE3	1:Cq:86:LYS:HA	1.93	0.50
1:Ae:86:LYS:HD2	1:Ae:86:LYS:N	2.25	0.50
1:Ai:154:VAL:HG11	1:Ak:110:TYR:HE2	1.75	0.50
1:Ao:86:LYS:HE3	1:Ao:86:LYS:HA	1.94	0.50
1:Ao:273:ASP:OD2	1:Ao:274:GLY:N	2.45	0.50
1:Aq:273:ASP:OD2	1:Aq:274:GLY:N	2.45	0.50
1:Aw:159:ASN:CG	1:Ay:119:ASN:HB2	2.36	0.50
1:Ba:86:LYS:HD2	1:Ba:86:LYS:N	2.25	0.50
1:Ba:86:LYS:HE3	1:Ba:86:LYS:HA	1.94	0.50
1:Bc:157:ILE:HG22	1:Bc:158:GLU:OE2	2.11	0.50
1:Be:157:ILE:HG22	1:Be:158:GLU:OE2	2.11	0.50
1:Bk:159:ASN:CG	1:Bm:119:ASN:HB2	2.37	0.50
1:Bq:273:ASP:OD2	1:Bq:274:GLY:N	2.45	0.50
1:Bs:273:ASP:OD2	1:Bs:274:GLY:N	2.45	0.50
1:Cc:165:ILE:HG22	2:Cd:5:U:O2	2.11	0.50
1:Cg:273:ASP:OD2	1:Cg:274:GLY:N	2.45	0.50
1:Cs:273:ASP:OD2	1:Cs:274:GLY:N	2.45	0.50
1:Aa:283:THR:OG1	1:As:269:MET:HE3	2.12	0.50
1:Ae:283:THR:OG1	1:Aw:269:MET:HE3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:210:MET:HE2	1:Ak:108:ILE:HA	1.94	0.50
1:Ai:273:ASP:OD2	1:Ai:274:GLY:N	2.45	0.50
1:Ai:283:THR:OG1	1:Ba:269:MET:HE3	2.12	0.50
1:As:273:ASP:OD2	1:As:274:GLY:N	2.45	0.50
1:Aw:86:LYS:HE3	1:Aw:86:LYS:HA	1.93	0.50
1:Ay:157:ILE:HG22	1:Ay:158:GLU:OE2	2.11	0.50
1:Be:86:LYS:HE3	1:Be:86:LYS:HA	1.93	0.50
1:Bm:157:ILE:HG22	1:Bm:158:GLU:OE2	2.11	0.50
1:Bs:157:ILE:HG22	1:Bs:158:GLU:OE2	2.11	0.50
1:Ca:86:LYS:HE3	1:Ca:86:LYS:HA	1.94	0.50
1:Cc:86:LYS:HE3	1:Cc:86:LYS:HA	1.94	0.50
1:Ce:273:ASP:OD2	1:Ce:274:GLY:N	2.45	0.50
1:Ck:157:ILE:HG22	1:Ck:158:GLU:OE2	2.11	0.50
1:Ck:206:ALA:HB2	1:Cm:91:MET:HE2	1.94	0.50
1:Ck:273:ASP:OD2	1:Ck:274:GLY:N	2.45	0.50
1:Ao:283:THR:OG1	1:Bg:269:MET:HE3	2.11	0.50
1:Bc:129:PHE:HE2	1:Bc:133:ARG:HE	1.59	0.50
1:Bg:154:VAL:HG11	1:Bi:110:TYR:HE2	1.77	0.50
1:Ce:129:PHE:HE2	1:Ce:133:ARG:HE	1.59	0.50
1:Ce:206:ALA:CB	1:Cg:91:MET:HE2	2.42	0.50
1:Ac:86:LYS:HE3	1:Ac:86:LYS:HA	1.94	0.50
1:Ag:86:LYS:HD2	1:Ag:86:LYS:N	2.25	0.50
1:Am:129:PHE:HE2	1:Am:133:ARG:HE	1.59	0.50
1:Be:273:ASP:OD2	1:Be:274:GLY:N	2.45	0.50
1:Bk:86:LYS:HD2	1:Bk:86:LYS:N	2.25	0.50
1:Bm:273:ASP:OD2	1:Bm:274:GLY:N	2.45	0.50
1:Cc:210:MET:HE2	1:Cc:108:ILE:HA	1.92	0.50
1:Ac:273:ASP:OD2	1:Ac:274:GLY:N	2.45	0.50
1:Ae:157:ILE:HG22	1:Ae:158:GLU:OE2	2.11	0.50
1:Ag:129:PHE:HE2	1:Ag:133:ARG:HE	1.59	0.50
1:Ay:273:ASP:OD2	1:Ay:274:GLY:N	2.45	0.50
1:Bk:157:ILE:HG22	1:Bk:158:GLU:OE2	2.11	0.50
1:Bq:86:LYS:HE3	1:Bq:86:LYS:HA	1.94	0.50
1:Bq:154:VAL:HG11	1:Bs:110:TYR:CE2	2.47	0.50
1:Bw:273:ASP:OD2	1:Bw:274:GLY:N	2.45	0.50
1:By:283:THR:OG1	1:Cq:269:MET:HE3	2.11	0.50
1:Ce:86:LYS:HE3	1:Ce:86:LYS:HA	1.94	0.50
1:Cg:86:LYS:HE3	1:Cg:86:LYS:HA	1.94	0.50
1:Cm:273:ASP:OD2	1:Cm:274:GLY:N	2.45	0.50
1:Cq:154:VAL:HG11	1:Cs:110:TYR:HE2	1.76	0.50
1:Aa:273:ASP:OD2	1:Aa:274:GLY:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:129:PHE:HE2	1:Ac:133:ARG:HE	1.59	0.49
1:Ak:157:ILE:HG22	1:Ak:158:GLU:OE2	2.11	0.49
1:Ay:195:GLN:HE21	2:Az:2:U:H5'	1.77	0.49
1:Be:154:VAL:HG11	1:Bg:110:TYR:HE2	1.77	0.49
1:Bk:291:VAL:O	1:Bm:296:HIS:CD2	2.64	0.49
1:Bo:273:ASP:OD2	1:Bo:274:GLY:N	2.45	0.49
1:By:157:ILE:HG22	1:By:158:GLU:OE2	2.11	0.49
1:Ca:129:PHE:HE2	1:Ca:133:ARG:HE	1.59	0.49
1:Ci:86:LYS:N	1:Ci:86:LYS:HD2	2.25	0.49
1:Au:273:ASP:OD2	1:Au:274:GLY:N	2.45	0.49
1:Bu:154:VAL:HG11	1:Bw:110:TYR:HE2	1.77	0.49
1:Bu:273:ASP:OD2	1:Bu:274:GLY:N	2.45	0.49
1:Bw:86:LYS:HA	1:Bw:86:LYS:HE3	1.94	0.49
1:By:86:LYS:HE3	1:By:86:LYS:HA	1.94	0.49
1:Ca:283:THR:OG1	1:Cs:269:MET:HE3	2.12	0.49
1:Ag:273:ASP:OD2	1:Ag:274:GLY:N	2.45	0.49
1:Ai:86:LYS:HA	1:Ai:86:LYS:HE3	1.94	0.49
1:Au:86:LYS:HA	1:Au:86:LYS:HE3	1.94	0.49
1:Bk:86:LYS:HA	1:Bk:86:LYS:HE3	1.94	0.49
1:Bo:129:PHE:HE2	1:Bo:133:ARG:HE	1.59	0.49
1:Cq:129:PHE:HE2	1:Cq:133:ARG:HE	1.59	0.49
1:Ae:86:LYS:HA	1:Ae:86:LYS:HE3	1.94	0.49
1:Ae:273:ASP:OD2	1:Ae:274:GLY:N	2.45	0.49
1:Ay:173:ASP:HB2	1:Bs:81:ILE:HG13	1.94	0.49
1:Bc:283:THR:HG23	1:Ck:256:GLN:HE22	1.77	0.49
1:Bk:195:GLN:HE21	2:Bl:2:U:H5'	1.77	0.49
1:Bw:283:THR:OG1	1:Co:269:MET:HE3	2.11	0.49
1:Ci:291:VAL:CG2	1:Ci:295:VAL:HG23	2.43	0.49
1:Cm:157:ILE:HG22	1:Cm:158:GLU:OE2	2.11	0.49
1:Aw:86:LYS:HD2	1:Aw:86:LYS:N	2.25	0.49
1:Ay:158:GLU:OE1	1:Ba:114:GLN:HG3	2.12	0.49
1:Bc:291:VAL:CG2	1:Bc:295:VAL:HG23	2.43	0.49
1:Bg:283:THR:OG1	1:By:269:MET:HE3	2.12	0.49
1:Bs:206:ALA:CB	1:Bu:91:MET:CE	2.91	0.49
1:Bs:291:VAL:CG2	1:Bs:295:VAL:HG23	2.43	0.49
1:Ck:86:LYS:HE3	1:Ck:86:LYS:HA	1.94	0.49
1:Ck:291:VAL:CG2	1:Ck:295:VAL:HG23	2.43	0.49
1:Ae:154:VAL:HG11	1:Ag:110:TYR:HE2	1.77	0.49
1:Ag:291:VAL:CG2	1:Ag:295:VAL:HG23	2.43	0.49
1:Am:291:VAL:CG2	1:Am:295:VAL:HG23	2.43	0.49
1:As:86:LYS:HE3	1:As:86:LYS:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:144:GLN:HB3	1:Bs:82:PRO:HG3	1.95	0.49
1:Bs:286:HIS:HD2	1:Ck:270:PHE:O	1.95	0.49
1:Bu:291:VAL:CG2	1:Bu:295:VAL:HG23	2.43	0.49
1:Ci:86:LYS:HE3	1:Ci:86:LYS:HA	1.94	0.49
1:Aw:273:ASP:OD2	1:Aw:274:GLY:N	2.45	0.49
1:Be:291:VAL:CG2	1:Be:295:VAL:HG23	2.43	0.49
1:Bi:291:VAL:CG2	1:Bi:295:VAL:HG23	2.43	0.49
1:Bu:210:MET:HE2	1:Bw:108:ILE:HA	1.93	0.49
1:Aa:291:VAL:CG2	1:Aa:295:VAL:HG23	2.43	0.49
1:Ac:154:VAL:HG11	1:Ae:110:TYR:HE2	1.76	0.49
1:Aq:86:LYS:HA	1:Aq:86:LYS:HE3	1.94	0.49
1:Aq:283:THR:OG1	1:Bi:269:MET:HE3	2.11	0.49
1:As:291:VAL:CG2	1:As:295:VAL:HG23	2.43	0.49
1:Au:283:THR:HG23	1:Cc:256:GLN:HE22	1.77	0.49
1:Aw:291:VAL:CG2	1:Aw:295:VAL:HG23	2.43	0.49
1:Ba:291:VAL:CG2	1:Ba:295:VAL:HG23	2.43	0.49
1:Bc:86:LYS:HA	1:Bc:86:LYS:HE3	1.94	0.49
1:Bo:86:LYS:HE3	1:Bo:86:LYS:HA	1.93	0.49
1:Bo:93:LEU:HD23	1:Bo:102:LEU:HB2	1.95	0.49
1:Ce:210:MET:HE2	1:Cg:108:ILE:HA	1.94	0.49
1:Cs:86:LYS:HE3	1:Cs:86:LYS:HA	1.94	0.49
1:Ae:93:LEU:HD23	1:Ae:102:LEU:HB2	1.95	0.49
1:Ag:86:LYS:HE3	1:Ag:86:LYS:HA	1.94	0.49
1:As:195:GLN:NE2	2:At:2:U:H5'	2.28	0.49
1:Bk:283:THR:HG23	1:Cs:256:GLN:HE22	1.78	0.49
1:Bm:291:VAL:CG2	1:Bm:295:VAL:HG23	2.43	0.49
1:Bo:210:MET:HE2	1:Bq:108:ILE:HA	1.95	0.49
1:Bs:272:LEU:N	1:Ck:252:GLU:OE1	2.39	0.49
1:Cc:220:ARG:NH2	2:Cd:5:U:O3'	2.46	0.49
1:Ce:93:LEU:HD23	1:Ce:102:LEU:HB2	1.95	0.49
1:Cq:291:VAL:CG2	1:Cq:295:VAL:HG23	2.43	0.49
1:Ae:291:VAL:CG2	1:Ae:295:VAL:HG23	2.43	0.49
1:Au:93:LEU:HD23	1:Au:102:LEU:HB2	1.95	0.49
1:Bq:291:VAL:CG2	1:Bq:295:VAL:HG23	2.43	0.49
1:Cc:291:VAL:CG2	1:Cc:295:VAL:HG23	2.43	0.49
1:Am:283:THR:HG23	1:Bu:256:GLN:HE22	1.77	0.48
1:Ao:291:VAL:CG2	1:Ao:295:VAL:HG23	2.43	0.48
1:Aw:210:MET:HE2	1:Ay:108:ILE:HA	1.95	0.48
1:Ay:93:LEU:HD23	1:Ay:102:LEU:HB2	1.95	0.48
1:Be:210:MET:HE2	1:Bg:108:ILE:HA	1.94	0.48
1:Bm:210:MET:HE2	1:Bo:108:ILE:HA	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:283:THR:OG1	1:Ce:269:MET:HE3	2.13	0.48
1:Bw:154:VAL:HG11	1:By:110:TYR:HE2	1.77	0.48
1:Bw:210:MET:HE2	1:By:108:ILE:HA	1.94	0.48
1:Ca:291:VAL:CG2	1:Ca:295:VAL:HG23	2.43	0.48
1:Co:291:VAL:CG2	1:Co:295:VAL:HG23	2.43	0.48
1:Ak:291:VAL:CG2	1:Ak:295:VAL:HG23	2.43	0.48
1:Ba:168:TYR:CZ	1:Bs:213:LEU:HD21	2.48	0.48
1:Bm:86:LYS:HE3	1:Bm:86:LYS:HA	1.94	0.48
1:Bs:206:ALA:CB	1:Bu:91:MET:HE2	2.42	0.48
1:By:291:VAL:CG2	1:By:295:VAL:HG23	2.43	0.48
1:Cg:291:VAL:CG2	1:Cg:295:VAL:HG23	2.43	0.48
1:Co:210:MET:HE2	1:Cq:108:ILE:HA	1.94	0.48
1:Cs:195:GLN:HE21	2:Ct:2:U:H5'	1.77	0.48
1:Ai:291:VAL:CG2	1:Ai:295:VAL:HG23	2.43	0.48
1:Aq:154:VAL:HG11	1:As:110:TYR:HE2	1.77	0.48
1:Au:210:MET:HE2	1:Aw:108:ILE:HA	1.94	0.48
1:Bk:93:LEU:HD23	1:Bk:102:LEU:HB2	1.95	0.48
1:Cm:291:VAL:CG2	1:Cm:295:VAL:HG23	2.43	0.48
1:Ay:291:VAL:CG2	1:Ay:295:VAL:HG23	2.43	0.48
1:Bo:291:VAL:CG2	1:Bo:295:VAL:HG23	2.43	0.48
1:Ag:154:VAL:HG11	1:Ai:110:TYR:HE2	1.77	0.48
1:As:154:VAL:HG11	1:Au:110:TYR:HE2	1.77	0.48
1:Bo:154:VAL:HG11	1:Bq:110:TYR:HE2	1.76	0.48
1:Bs:148:LEU:HD21	1:Cm:82:PRO:HG2	1.94	0.48
1:Ce:291:VAL:CG2	1:Ce:295:VAL:HG23	2.43	0.48
1:Ci:93:LEU:HD23	1:Ci:102:LEU:HB2	1.95	0.48
1:Ai:93:LEU:HD23	1:Ai:102:LEU:HB2	1.95	0.48
1:As:284:GLU:OE2	1:As:296:HIS:NE2	2.44	0.48
1:Au:291:VAL:CG2	1:Au:295:VAL:HG23	2.43	0.48
1:Ay:283:THR:OG1	1:Bq:269:MET:HE3	2.14	0.48
1:Bg:283:THR:HG23	1:Co:256:GLN:HE22	1.79	0.48
1:Bw:291:VAL:CG2	1:Bw:295:VAL:HG23	2.43	0.48
1:Cs:284:GLU:OE2	1:Cs:296:HIS:NE2	2.44	0.48
1:Aa:93:LEU:HD23	1:Aa:102:LEU:HB2	1.95	0.48
1:Ac:291:VAL:CG2	1:Ac:295:VAL:HG23	2.43	0.48
1:Am:93:LEU:HD23	1:Am:102:LEU:HB2	1.95	0.48
1:Au:154:VAL:HG11	1:Aw:110:TYR:HE2	1.77	0.48
1:Bc:283:THR:OG1	1:Bu:269:MET:HE3	2.12	0.48
1:Bk:284:GLU:OE2	1:Bk:296:HIS:NE2	2.44	0.48
1:Ca:93:LEU:HD23	1:Ca:102:LEU:HB2	1.95	0.48
1:Ac:93:LEU:HD23	1:Ac:102:LEU:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:210:MET:HE2	1:Ao:108:ILE:HA	1.94	0.48
1:Ao:93:LEU:HD23	1:Ao:102:LEU:HB2	1.95	0.48
1:Aq:291:VAL:CG2	1:Aq:295:VAL:HG23	2.43	0.48
1:Be:93:LEU:HD23	1:Be:102:LEU:HB2	1.95	0.48
1:Bg:93:LEU:HD23	1:Bg:102:LEU:HB2	1.95	0.48
1:Bu:93:LEU:HD23	1:Bu:102:LEU:HB2	1.95	0.48
1:Cm:93:LEU:HD23	1:Cm:102:LEU:HB2	1.95	0.48
1:Aa:210:MET:HE2	1:Ac:108:ILE:HA	1.95	0.48
1:Ao:154:VAL:HG11	1:Aq:110:TYR:HE2	1.77	0.48
1:As:93:LEU:HD23	1:As:102:LEU:HB2	1.95	0.48
1:Bc:93:LEU:HD23	1:Bc:102:LEU:HB2	1.95	0.48
1:Be:283:THR:OG1	1:Bw:269:MET:HE3	2.13	0.48
1:Bk:200:PHE:HE1	1:Bm:102:LEU:HD21	1.79	0.48
1:Bm:284:GLU:OE2	1:Bm:296:HIS:NE2	2.43	0.48
1:Bw:93:LEU:HD23	1:Bw:102:LEU:HB2	1.95	0.48
1:By:93:LEU:HD23	1:By:102:LEU:HB2	1.95	0.48
1:Co:93:LEU:HD23	1:Co:102:LEU:HB2	1.95	0.48
1:Cs:291:VAL:CG2	1:Cs:295:VAL:HG23	2.43	0.48
1:Ag:168:TYR:CZ	1:Ay:213:LEU:HD21	2.49	0.48
1:Ao:283:THR:HG23	1:Bw:256:GLN:HE22	1.79	0.48
1:As:283:THR:HG23	1:Ca:256:GLN:HE22	1.79	0.48
1:Bs:93:LEU:HD23	1:Bs:102:LEU:HB2	1.95	0.48
1:By:154:VAL:HG11	1:Ca:110:TYR:HE2	1.77	0.48
2:Ch:5:U:O3'	2:Cj:1:U:H5'	2.14	0.48
1:Ak:93:LEU:HD23	1:Ak:102:LEU:HB2	1.95	0.47
1:Aq:284:GLU:OE2	1:Aq:296:HIS:NE2	2.44	0.47
1:As:210:MET:HE2	1:Au:108:ILE:HA	1.95	0.47
1:Ba:210:MET:HE2	1:Bc:108:ILE:HA	1.96	0.47
1:Bg:291:VAL:CG2	1:Bg:295:VAL:HG23	2.43	0.47
1:Bm:93:LEU:HD23	1:Bm:102:LEU:HB2	1.95	0.47
1:Au:284:GLU:OE2	1:Au:296:HIS:NE2	2.44	0.47
1:Cc:93:LEU:HD23	1:Cc:102:LEU:HB2	1.95	0.47
1:Cc:154:VAL:HG11	1:Ce:110:TYR:HE2	1.77	0.47
1:Cq:93:LEU:HD23	1:Cq:102:LEU:HB2	1.95	0.47
1:Ac:284:GLU:OE2	1:Ac:296:HIS:NE2	2.43	0.47
1:Ak:154:VAL:HG11	1:Am:110:TYR:HE2	1.78	0.47
1:Aq:93:LEU:HD23	1:Aq:102:LEU:HB2	1.95	0.47
1:Aw:93:LEU:HD23	1:Aw:102:LEU:HB2	1.95	0.47
1:Ba:200:PHE:HE1	1:Bc:102:LEU:HD21	1.79	0.47
1:Bk:210:MET:HE2	1:Bm:108:ILE:HA	1.95	0.47
1:Bk:291:VAL:CG2	1:Bk:295:VAL:HG23	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ca:284:GLU:OE2	1:Ca:296:HIS:NE2	2.44	0.47
1:Ck:159:ASN:CG	1:Cm:119:ASN:HB2	2.39	0.47
1:Cm:224:LEU:HD11	2:Cp:1:U:OP2	2.15	0.47
1:Cm:284:GLU:HG3	1:Cm:285:ARG:H	1.80	0.47
1:Cq:210:MET:HE2	1:Cs:108:ILE:HA	1.95	0.47
1:Ak:284:GLU:HG3	1:Ak:285:ARG:H	1.80	0.47
1:Bg:210:MET:HE2	1:Bi:108:ILE:HA	1.95	0.47
1:Cg:93:LEU:HD23	1:Cg:102:LEU:HB2	1.95	0.47
1:Aa:283:THR:HG23	1:Bi:256:GLN:HE22	1.80	0.47
1:Ai:283:THR:HG23	1:Bq:256:GLN:HE22	1.79	0.47
1:Aw:284:GLU:HG3	1:Aw:285:ARG:H	1.80	0.47
1:Bc:284:GLU:HG3	1:Bc:285:ARG:H	1.80	0.47
1:Bi:283:THR:HG23	1:Cq:256:GLN:HE22	1.79	0.47
1:Bm:144:GLN:HB3	1:Cg:82:PRO:HG3	1.95	0.47
1:Bs:200:PHE:CD1	1:Bu:94:PRO:HG3	2.49	0.47
1:By:210:MET:HE2	1:Ca:108:ILE:HA	1.95	0.47
1:Ck:206:ALA:CB	1:Cm:91:MET:HE2	2.44	0.47
1:Cs:93:LEU:HD23	1:Cs:102:LEU:HB2	1.95	0.47
1:Ao:210:MET:HE2	1:Aq:108:ILE:HA	1.95	0.47
1:Bc:210:MET:HE2	1:Be:108:ILE:HA	1.96	0.47
1:Bi:284:GLU:OE2	1:Bi:296:HIS:NE2	2.44	0.47
1:Ck:93:LEU:HD23	1:Ck:102:LEU:HB2	1.95	0.47
1:Aa:154:VAL:HG11	1:Ac:110:TYR:HE2	1.77	0.47
1:Ag:93:LEU:HD23	1:Ag:102:LEU:HB2	1.95	0.47
1:Ag:283:THR:HG23	1:Bo:256:GLN:HE22	1.79	0.47
1:Ag:284:GLU:HG3	1:Ag:285:ARG:H	1.80	0.47
1:Am:154:VAL:HG11	1:Ao:110:TYR:HE2	1.77	0.47
1:Aq:195:GLN:HE21	2:Ar:2:U:H5'	1.80	0.47
1:Aq:210:MET:HE2	1:As:108:ILE:HA	1.96	0.47
1:Au:284:GLU:HG3	1:Au:285:ARG:H	1.80	0.47
1:Bi:93:LEU:HD23	1:Bi:102:LEU:HB2	1.95	0.47
1:Bq:93:LEU:HD23	1:Bq:102:LEU:HB2	1.95	0.47
1:Bq:284:GLU:HG3	1:Bq:285:ARG:H	1.80	0.47
1:Cc:291:VAL:HG23	1:Cc:292:SER:N	2.30	0.47
1:Cc:284:GLU:HG3	1:Cc:285:ARG:H	1.80	0.47
1:Cg:223:LEU:HD21	1:Ci:243:ASN:C	2.39	0.47
1:Cg:284:GLU:HG3	1:Cg:285:ARG:H	1.80	0.47
1:Co:154:VAL:HG11	1:Cq:110:TYR:HE2	1.77	0.47
1:Cq:284:GLU:OE2	1:Cq:296:HIS:NE2	2.44	0.47
1:Ae:284:GLU:HG3	1:Ae:285:ARG:H	1.80	0.47
1:Ak:272:LEU:N	1:Bc:252:GLU:OE1	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ak:291:VAL:HG23	1:Ak:292:SER:N	2.30	0.47
1:Ay:206:ALA:CB	1:Ba:91:MET:HE2	2.45	0.47
1:Ba:93:LEU:HD23	1:Ba:102:LEU:HB2	1.95	0.47
1:Be:284:GLU:HG3	1:Be:285:ARG:H	1.80	0.47
1:Bg:284:GLU:HG3	1:Bg:285:ARG:H	1.80	0.47
1:Bs:284:GLU:HG3	1:Bs:285:ARG:H	1.80	0.47
1:Cc:284:GLU:HG3	1:Cc:285:ARG:H	1.80	0.47
1:Cc:284:GLU:OE2	1:Cc:296:HIS:NE2	2.44	0.47
1:Aa:284:GLU:OE2	1:Aa:296:HIS:NE2	2.44	0.47
1:Ak:283:THR:OG1	1:Bc:269:MET:HE3	2.15	0.47
1:Au:291:VAL:HG23	1:Au:292:SER:N	2.30	0.47
1:Aw:93:LEU:HD21	1:Aw:104:LEU:HG	1.97	0.47
1:Bm:291:VAL:HG23	1:Bm:292:SER:N	2.30	0.47
1:Bu:283:THR:OG1	1:Cm:269:MET:HE3	2.15	0.47
1:Ce:284:GLU:OE2	1:Ce:296:HIS:NE2	2.43	0.47
1:Aa:218:MET:HE1	1:Aa:230:LYS:HA	1.97	0.47
1:Aa:284:GLU:HG3	1:Aa:285:ARG:H	1.80	0.47
1:Aa:291:VAL:HG23	1:Aa:292:SER:N	2.30	0.47
1:Ac:284:GLU:HG3	1:Ac:285:ARG:H	1.80	0.47
1:Ae:93:LEU:HD21	1:Ae:104:LEU:HG	1.97	0.47
1:Ae:284:GLU:OE2	1:Ae:296:HIS:NE2	2.44	0.47
1:Ai:284:GLU:HG3	1:Ai:285:ARG:H	1.80	0.47
1:Ak:284:GLU:CD	1:Ak:296:HIS:HE2	2.23	0.47
1:Am:284:GLU:HG3	1:Am:285:ARG:H	1.80	0.47
1:Ay:139:ASP:OD2	1:Bs:89:PRO:HG3	2.15	0.47
1:Ay:284:GLU:HG3	1:Ay:285:ARG:H	1.80	0.47
1:Ba:284:GLU:HG3	1:Ba:285:ARG:H	1.80	0.47
1:Ba:291:VAL:HG23	1:Ba:292:SER:N	2.30	0.47
1:Bi:291:VAL:HG23	1:Bi:292:SER:N	2.30	0.47
1:Bo:284:GLU:HG3	1:Bo:285:ARG:H	1.80	0.47
1:Bs:211:ARG:HH11	1:Bu:111:LYS:HB3	1.80	0.47
1:Bs:269:MET:O	1:Ci:228:ASN:HB2	2.14	0.47
1:Bw:291:VAL:HG23	1:Bw:292:SER:N	2.30	0.47
1:Ca:284:GLU:HG3	1:Ca:285:ARG:H	1.80	0.47
1:Cg:93:LEU:HD21	1:Cg:104:LEU:HG	1.97	0.47
1:Ck:291:VAL:HG23	1:Ck:292:SER:N	2.30	0.47
1:Cm:154:VAL:HG11	1:Co:110:TYR:HE2	1.76	0.47
1:Aa:284:GLU:CD	1:Aa:296:HIS:HE2	2.23	0.46
1:Ac:291:VAL:HG23	1:Ac:292:SER:N	2.30	0.46
1:Ag:93:LEU:HD21	1:Ag:104:LEU:HG	1.97	0.46
1:Ai:291:VAL:HG23	1:Ai:292:SER:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:291:VAL:HG23	1:Bc:292:SER:N	2.30	0.46
1:Be:283:THR:HG23	1:Cm:256:GLN:HE22	1.79	0.46
1:Bg:165:ILE:HG22	2:Bh:5:U:H1'	1.97	0.46
1:Bm:93:LEU:HD21	1:Bm:104:LEU:HG	1.97	0.46
1:Bm:173:ASP:HB2	1:Cg:81:ILE:HG13	1.96	0.46
1:Bo:291:VAL:HG23	1:Bo:292:SER:N	2.30	0.46
1:Bq:93:LEU:HD21	1:Bq:104:LEU:HG	1.97	0.46
1:By:284:GLU:OE2	1:By:296:HIS:NE2	2.44	0.46
1:Ce:206:ALA:HB2	1:Cg:91:MET:HE2	1.96	0.46
1:Cg:291:VAL:HG23	1:Cg:292:SER:N	2.30	0.46
1:Ck:284:GLU:HG3	1:Ck:285:ARG:H	1.80	0.46
1:Co:284:GLU:HG3	1:Co:285:ARG:H	1.80	0.46
1:Bi:284:GLU:HG3	1:Bi:285:ARG:H	1.80	0.46
1:Bo:93:LEU:HD21	1:Bo:104:LEU:HG	1.97	0.46
1:By:218:MET:HE1	1:By:230:LYS:HA	1.97	0.46
1:Ce:291:VAL:HG23	1:Ce:292:SER:N	2.30	0.46
1:Cq:218:MET:HE1	1:Cq:230:LYS:HA	1.98	0.46
1:Cs:218:MET:HE1	1:Cs:230:LYS:HA	1.97	0.46
1:Ag:291:VAL:HG23	1:Ag:292:SER:N	2.30	0.46
1:Ai:93:LEU:HD21	1:Ai:104:LEU:HG	1.97	0.46
1:Ao:93:LEU:HD21	1:Ao:104:LEU:HG	1.97	0.46
1:Ao:284:GLU:HG3	1:Ao:285:ARG:H	1.80	0.46
1:As:218:MET:HE1	1:As:230:LYS:HA	1.97	0.46
1:As:291:VAL:HG23	1:As:292:SER:N	2.30	0.46
1:Aw:291:VAL:HG23	1:Aw:292:SER:N	2.30	0.46
1:Ay:93:LEU:HD21	1:Ay:104:LEU:HG	1.97	0.46
1:Bi:284:GLU:CD	1:Bi:296:HIS:HE2	2.23	0.46
1:Bk:284:GLU:CD	1:Bk:296:HIS:HE2	2.23	0.46
1:Ce:93:LEU:HD21	1:Ce:104:LEU:HG	1.97	0.46
1:Ci:284:GLU:HG3	1:Ci:285:ARG:H	1.80	0.46
1:Ci:291:VAL:HG23	1:Ci:292:SER:N	2.31	0.46
1:Co:93:LEU:HD21	1:Co:104:LEU:HG	1.97	0.46
1:Cq:93:LEU:HD21	1:Cq:104:LEU:HG	1.97	0.46
1:Ac:93:LEU:HD21	1:Ac:104:LEU:HG	1.97	0.46
1:Ac:284:GLU:CD	1:Ac:296:HIS:HE2	2.23	0.46
1:Ay:284:GLU:CD	1:Ay:296:HIS:HE2	2.23	0.46
1:Bc:220:ARG:NH2	2:Bd:5:U:O3'	2.48	0.46
1:Bo:284:GLU:OE2	1:Bo:296:HIS:NE2	2.44	0.46
1:Bu:284:GLU:HG3	1:Bu:285:ARG:H	1.80	0.46
1:Bu:284:GLU:CD	1:Bu:296:HIS:HE2	2.23	0.46
1:Bw:165:ILE:HG22	2:Bx:5:U:C2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:By:284:GLU:HG3	1:By:285:ARG:H	1.80	0.46
1:Ce:200:PHE:CE1	1:Cg:94:PRO:HG3	2.50	0.46
1:Ci:93:LEU:HD21	1:Ci:104:LEU:HG	1.97	0.46
1:Ci:284:GLU:CD	1:Ci:296:HIS:HE2	2.23	0.46
1:Ae:200:PHE:HE1	1:Ag:102:LEU:HD21	1.81	0.46
1:Ag:210:MET:HE2	1:Ai:108:ILE:HA	1.98	0.46
1:Am:93:LEU:HD21	1:Am:104:LEU:HG	1.97	0.46
1:Au:93:LEU:HD21	1:Au:104:LEU:HG	1.97	0.46
1:Be:291:VAL:HG23	1:Be:292:SER:N	2.30	0.46
1:Bi:93:LEU:HD21	1:Bi:104:LEU:HG	1.97	0.46
1:Bk:284:GLU:HG3	1:Bk:285:ARG:H	1.80	0.46
1:Bs:154:VAL:HG11	1:Bu:110:TYR:HE2	1.76	0.46
1:Ck:154:VAL:HG11	1:Cm:110:TYR:HE2	1.79	0.46
1:Cm:210:MET:HE2	1:Co:108:ILE:HA	1.96	0.46
1:Am:291:VAL:HG23	1:Am:292:SER:N	2.30	0.46
1:Ao:284:GLU:OE2	1:Ao:296:HIS:NE2	2.44	0.46
1:Aq:220:ARG:NH2	2:Ar:5:U:O3'	2.48	0.46
1:Aw:283:THR:HG23	1:Ce:256:GLN:HE22	1.79	0.46
1:Ba:93:LEU:HD21	1:Ba:104:LEU:HG	1.97	0.46
1:Be:218:MET:HE1	1:Be:230:LYS:HA	1.97	0.46
1:Bg:93:LEU:HD21	1:Bg:104:LEU:HG	1.97	0.46
1:Bk:291:VAL:HG23	1:Bk:292:SER:N	2.30	0.46
1:Bm:284:GLU:CD	1:Bm:296:HIS:HE2	2.23	0.46
1:Bq:291:VAL:HG23	1:Bq:292:SER:N	2.30	0.46
1:Bw:218:MET:HE1	1:Bw:230:LYS:HA	1.97	0.46
1:Cc:93:LEU:HD21	1:Cc:104:LEU:HG	1.97	0.46
1:As:283:THR:OG1	1:Bk:269:MET:HE3	2.16	0.46
1:Bg:284:GLU:CD	1:Bg:296:HIS:HE2	2.23	0.46
1:Bu:291:VAL:HG23	1:Bu:292:SER:N	2.30	0.46
1:Bw:93:LEU:HD21	1:Bw:104:LEU:HG	1.97	0.46
1:Ca:284:GLU:CD	1:Ca:296:HIS:HE2	2.23	0.46
1:Ce:154:VAL:HA	1:Ce:157:ILE:HD12	1.98	0.46
1:Ce:159:ASN:CG	1:Cg:119:ASN:HB2	2.41	0.46
1:Ck:93:LEU:HD21	1:Ck:104:LEU:HG	1.97	0.46
1:Ae:291:VAL:HG23	1:Ae:292:SER:N	2.30	0.46
1:Ai:200:PHE:HE1	1:Ak:102:LEU:HD21	1.80	0.46
1:Ai:284:GLU:CD	1:Ai:296:HIS:HE2	2.23	0.46
1:As:284:GLU:HG3	1:As:285:ARG:H	1.80	0.46
1:Au:218:MET:HE1	1:Au:230:LYS:HA	1.97	0.46
1:Bm:154:VAL:HA	1:Bm:157:ILE:HD12	1.98	0.46
1:Bm:218:MET:HE1	1:Bm:230:LYS:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:93:LEU:HD21	1:Bu:104:LEU:HG	1.97	0.46
1:Cq:291:VAL:HG23	1:Cq:292:SER:N	2.30	0.46
1:Cs:284:GLU:CD	1:Cs:296:HIS:HE2	2.23	0.46
1:Cs:291:VAL:HG23	1:Cs:292:SER:N	2.30	0.46
1:Aq:218:MET:HE1	1:Aq:230:LYS:HA	1.97	0.46
1:Aw:284:GLU:OE2	1:Aw:296:HIS:NE2	2.44	0.46
1:Be:284:GLU:CD	1:Be:296:HIS:HE2	2.23	0.46
1:Bg:218:MET:HE1	1:Bg:230:LYS:HA	1.98	0.46
1:Bk:218:MET:HE1	1:Bk:230:LYS:HA	1.97	0.46
1:Bo:154:VAL:HA	1:Bo:157:ILE:HD12	1.98	0.46
1:By:284:GLU:CD	1:By:296:HIS:HE2	2.23	0.46
1:By:291:VAL:HG23	1:By:292:SER:N	2.30	0.46
1:Ca:218:MET:HE1	1:Ca:230:LYS:HA	1.97	0.46
1:Cc:284:GLU:CD	1:Cc:296:HIS:HE2	2.23	0.46
1:Cg:154:VAL:HA	1:Cg:157:ILE:HD12	1.98	0.46
1:Ci:195:GLN:HE21	2:Cj:2:U:H5'	1.79	0.46
1:Co:291:VAL:HG23	1:Co:292:SER:N	2.30	0.46
1:Cq:284:GLU:CD	1:Cq:296:HIS:HE2	2.23	0.46
1:Ac:283:THR:HG23	1:Bk:256:GLN:HE22	1.80	0.46
1:Ae:159:ASN:CG	1:Ag:119:ASN:HB2	2.41	0.46
1:Ae:206:ALA:HB2	1:Ag:91:MET:HE2	1.97	0.46
1:Ae:284:GLU:CD	1:Ae:296:HIS:HE2	2.23	0.46
1:Am:218:MET:HE1	1:Am:230:LYS:HA	1.97	0.46
1:Aq:224:LEU:HD11	2:At:1:U:OP2	2.15	0.46
1:Aq:283:THR:HG23	1:By:256:GLN:HE22	1.80	0.46
1:As:272:LEU:N	1:Bk:252:GLU:OE1	2.44	0.46
1:Au:154:VAL:HA	1:Au:157:ILE:HD12	1.98	0.46
1:Ay:159:ASN:CG	1:Ba:119:ASN:HB2	2.41	0.46
1:Bs:93:LEU:HD21	1:Bs:104:LEU:HG	1.97	0.46
1:Bs:284:GLU:CD	1:Bs:296:HIS:HE2	2.23	0.46
1:Bs:291:VAL:HG23	1:Bs:292:SER:N	2.30	0.46
1:Co:218:MET:HE1	1:Co:230:LYS:HA	1.97	0.46
1:Cq:284:GLU:HG3	1:Cq:285:ARG:H	1.80	0.46
1:Aa:93:LEU:HD21	1:Aa:104:LEU:HG	1.97	0.45
1:Ac:218:MET:HE1	1:Ac:230:LYS:HA	1.97	0.45
1:Aq:291:VAL:HG23	1:Aq:292:SER:N	2.30	0.45
1:As:93:LEU:HD21	1:As:104:LEU:HG	1.97	0.45
1:Aw:154:VAL:HA	1:Aw:157:ILE:HD12	1.98	0.45
1:Bk:93:LEU:HD21	1:Bk:104:LEU:HG	1.97	0.45
1:Bk:286:HIS:HD2	1:Cc:270:PHE:O	1.99	0.45
1:Bw:284:GLU:HG3	1:Bw:285:ARG:H	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cc:154:VAL:HA	1:Cc:157:ILE:HD12	1.98	0.45
1:Ce:218:MET:HE1	1:Ce:230:LYS:HA	1.97	0.45
1:Ae:154:VAL:HA	1:Ae:157:ILE:HD12	1.98	0.45
1:Ag:154:VAL:HA	1:Ag:157:ILE:HD12	1.98	0.45
1:Aq:93:LEU:HD21	1:Aq:104:LEU:HG	1.97	0.45
1:Ay:291:VAL:HG23	1:Ay:292:SER:N	2.30	0.45
1:Bk:154:VAL:HA	1:Bk:157:ILE:HD12	1.98	0.45
1:Bq:154:VAL:HA	1:Bq:157:ILE:HD12	1.98	0.45
1:Ca:291:VAL:HG23	1:Ca:292:SER:N	2.30	0.45
1:Ce:284:GLU:CD	1:Ce:296:HIS:HE2	2.23	0.45
1:Co:154:VAL:HA	1:Co:157:ILE:HD12	1.98	0.45
1:Ac:154:VAL:HA	1:Ac:157:ILE:HD12	1.98	0.45
1:Ao:154:VAL:HA	1:Ao:157:ILE:HD12	1.98	0.45
1:Be:154:VAL:HA	1:Be:157:ILE:HD12	1.98	0.45
1:Bg:284:GLU:OE2	1:Bg:296:HIS:NE2	2.44	0.45
1:Bg:291:VAL:HG23	1:Bg:292:SER:N	2.30	0.45
1:Bk:224:LEU:HD23	1:Bk:224:LEU:HA	1.81	0.45
1:Ci:154:VAL:HA	1:Ci:157:ILE:HD12	1.98	0.45
1:Cm:93:LEU:HD21	1:Cm:104:LEU:HG	1.97	0.45
1:Cm:291:VAL:HG23	1:Cm:292:SER:N	2.30	0.45
1:Co:284:GLU:CD	1:Co:296:HIS:HE2	2.23	0.45
1:Cs:284:GLU:HG3	1:Cs:285:ARG:H	1.80	0.45
1:Ag:284:GLU:OE2	1:Ag:296:HIS:NE2	2.44	0.45
1:Ai:104:LEU:HD23	1:Ai:104:LEU:HA	1.80	0.45
1:Ak:93:LEU:HD21	1:Ak:104:LEU:HG	1.97	0.45
1:As:284:GLU:CD	1:As:296:HIS:HE2	2.23	0.45
1:Ay:154:VAL:HA	1:Ay:157:ILE:HD12	1.98	0.45
1:Bc:93:LEU:HD21	1:Bc:104:LEU:HG	1.97	0.45
1:Bm:284:GLU:HG3	1:Bm:285:ARG:H	1.80	0.45
1:By:154:VAL:HA	1:By:157:ILE:HD12	1.98	0.45
1:Cg:284:GLU:OE2	1:Cg:296:HIS:NE2	2.44	0.45
1:Ae:206:ALA:CB	1:Ag:91:MET:HE2	2.46	0.45
1:Aq:284:GLU:CD	1:Aq:296:HIS:HE2	2.23	0.45
1:As:154:VAL:HA	1:As:157:ILE:HD12	1.98	0.45
1:Bs:223:LEU:HD21	1:Bu:243:ASN:C	2.41	0.45
1:Ca:93:LEU:HD21	1:Ca:104:LEU:HG	1.97	0.45
1:Cg:214:ASP:OD2	1:Ci:111:LYS:HE2	2.17	0.45
1:Ck:218:MET:HE1	1:Ck:230:LYS:HA	1.97	0.45
1:Co:284:GLU:OE2	1:Co:296:HIS:NE2	2.44	0.45
1:Ag:218:MET:HE1	1:Ag:230:LYS:HA	1.98	0.45
1:Aq:284:GLU:HG3	1:Aq:285:ARG:H	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:93:LEU:HD21	1:Be:104:LEU:HG	1.97	0.45
1:Bo:284:GLU:CD	1:Bo:296:HIS:HE2	2.23	0.45
1:Bw:284:GLU:CD	1:Bw:296:HIS:HE2	2.23	0.45
1:Bw:284:GLU:OE2	1:Bw:296:HIS:NE2	2.44	0.45
1:By:93:LEU:HD21	1:By:104:LEU:HG	1.97	0.45
1:Ci:218:MET:HE1	1:Ci:230:LYS:HA	1.98	0.45
1:Cs:93:LEU:HD21	1:Cs:104:LEU:HG	1.97	0.45
1:Cs:154:VAL:HA	1:Cs:157:ILE:HD12	1.98	0.45
1:Ai:218:MET:HE1	1:Ai:230:LYS:HA	1.98	0.45
1:Ay:200:PHE:CE1	1:Ba:94:PRO:HG3	2.51	0.45
1:Bs:218:MET:HE1	1:Bs:230:LYS:HA	1.97	0.45
1:Co:224:LEU:HD23	1:Co:224:LEU:HA	1.81	0.45
1:Aa:154:VAL:HA	1:Aa:157:ILE:HD12	1.98	0.45
1:Ag:284:GLU:CD	1:Ag:296:HIS:HE2	2.23	0.45
1:Ai:154:VAL:HA	1:Ai:157:ILE:HD12	1.98	0.45
1:Ao:218:MET:HE1	1:Ao:230:LYS:HA	1.97	0.45
1:Ao:291:VAL:HG23	1:Ao:292:SER:N	2.30	0.45
1:Au:284:GLU:CD	1:Au:296:HIS:HE2	2.23	0.45
1:Ay:218:MET:HE1	1:Ay:230:LYS:HA	1.97	0.45
1:Bs:154:VAL:HA	1:Bs:157:ILE:HD12	1.98	0.45
1:Cg:284:GLU:CD	1:Cg:296:HIS:HE2	2.23	0.45
1:Ak:154:VAL:HA	1:Ak:157:ILE:HD12	1.98	0.45
1:Ao:284:GLU:CD	1:Ao:296:HIS:HE2	2.23	0.45
1:As:168:TYR:CZ	1:Bk:213:LEU:HD21	2.52	0.45
1:Bc:284:GLU:CD	1:Bc:296:HIS:HE2	2.23	0.45
1:Be:224:LEU:HD11	2:Bh:1:U:OP2	2.17	0.45
1:Bi:218:MET:HE1	1:Bi:230:LYS:HA	1.97	0.45
1:Ca:154:VAL:HA	1:Ca:157:ILE:HD12	1.98	0.45
1:Cc:218:MET:HE1	1:Cc:230:LYS:HA	1.97	0.45
1:Ck:206:ALA:CB	1:Cm:91:MET:CE	2.95	0.45
1:Cm:284:GLU:CD	1:Cm:296:HIS:HE2	2.23	0.45
1:Aw:218:MET:HE1	1:Aw:230:LYS:HA	1.97	0.45
1:Ba:154:VAL:HA	1:Ba:157:ILE:HD12	1.98	0.45
1:Bm:154:VAL:HG11	1:Bo:110:TYR:HE2	1.76	0.45
1:Bu:154:VAL:HA	1:Bu:157:ILE:HD12	1.98	0.45
1:Bu:218:MET:HE1	1:Bu:230:LYS:HA	1.97	0.45
1:Ce:200:PHE:CD1	1:Cg:94:PRO:HG3	2.51	0.45
1:Cg:195:GLN:HE21	2:Ch:2:U:H5'	1.82	0.45
1:Ak:218:MET:HE1	1:Ak:230:LYS:HA	1.97	0.44
1:Bq:284:GLU:OE2	1:Bq:296:HIS:NE2	2.44	0.44
1:Cg:218:MET:HE1	1:Cg:230:LYS:HA	1.97	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ck:154:VAL:HA	1:Ck:157:ILE:HD12	1.98	0.44
1:Ck:214:ASP:OD2	1:Cm:111:LYS:HE2	2.17	0.44
1:Aw:284:GLU:CD	1:Aw:296:HIS:HE2	2.23	0.44
2:Ax:5:U:O3'	2:Az:1:U:H5'	2.17	0.44
1:Bi:154:VAL:HA	1:Bi:157:ILE:HD12	1.98	0.44
1:Cm:154:VAL:HA	1:Cm:157:ILE:HD12	1.98	0.44
1:Ae:218:MET:HE1	1:Ae:230:LYS:HA	1.97	0.44
1:Am:154:VAL:HA	1:Am:157:ILE:HD12	1.98	0.44
1:Am:284:GLU:OE2	1:Am:296:HIS:NE2	2.44	0.44
1:Bc:218:MET:HE1	1:Bc:230:LYS:HA	1.97	0.44
1:Bs:214:ASP:OD2	1:Bu:111:LYS:HE2	2.17	0.44
1:Bw:154:VAL:HA	1:Bw:157:ILE:HD12	1.98	0.44
1:Ck:284:GLU:CD	1:Ck:296:HIS:HE2	2.23	0.44
1:Cq:104:LEU:HD23	1:Cq:104:LEU:HA	1.80	0.44
1:Ak:214:ASP:OD2	1:Am:111:LYS:HE2	2.18	0.44
1:Bc:104:LEU:HD23	1:Bc:104:LEU:HA	1.80	0.44
1:Bc:154:VAL:HA	1:Bc:157:ILE:HD12	1.98	0.44
1:Bq:218:MET:HE1	1:Bq:230:LYS:HA	1.97	0.44
1:Bw:205:GLU:CD	1:Bw:234:ARG:HH21	2.26	0.44
1:Ak:205:GLU:CD	1:Ak:234:ARG:HH21	2.26	0.44
1:Ak:206:ALA:HB2	1:Am:91:MET:HE2	1.99	0.44
1:Ao:205:GLU:CD	1:Ao:234:ARG:HH21	2.26	0.44
1:Aq:292:SER:HB2	1:Aq:295:VAL:HG22	2.00	0.44
1:Ba:218:MET:HE1	1:Ba:230:LYS:HA	1.97	0.44
1:Ba:284:GLU:CD	1:Ba:296:HIS:HE2	2.23	0.44
1:Bi:195:GLN:HE21	2:Bj:2:U:H5'	1.82	0.44
1:Bo:218:MET:HE1	1:Bo:230:LYS:HA	1.98	0.44
1:Bs:183:LYS:HD2	1:Ck:234:ARG:HH22	1.82	0.44
1:Bw:104:LEU:HD23	1:Bw:104:LEU:HA	1.80	0.44
1:By:292:SER:HB2	1:By:295:VAL:HG22	2.00	0.44
1:Ca:154:VAL:HG11	1:Cc:110:TYR:HE2	1.79	0.44
1:Ca:292:SER:HB2	1:Ca:295:VAL:HG22	2.00	0.44
1:Cm:205:GLU:CD	1:Cm:234:ARG:HH21	2.26	0.44
1:Cm:218:MET:HE1	1:Cm:230:LYS:HA	1.97	0.44
1:Cq:154:VAL:HA	1:Cq:157:ILE:HD12	1.98	0.44
1:Cs:292:SER:HB2	1:Cs:295:VAL:HG22	2.00	0.44
1:Aa:291:VAL:O	1:Ac:296:HIS:CD2	2.71	0.44
1:Aa:292:SER:HB2	1:Aa:295:VAL:HG22	2.00	0.44
1:Ak:292:SER:HB2	1:Ak:295:VAL:HG22	2.00	0.44
1:Ba:292:SER:HB2	1:Ba:295:VAL:HG22	2.00	0.44
1:Be:205:GLU:CD	1:Be:234:ARG:HH21	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bg:205:GLU:CD	1:Bg:234:ARG:HH21	2.26	0.44
1:Bg:292:SER:HB2	1:Bg:295:VAL:HG22	2.00	0.44
1:Bk:168:TYR:CZ	1:Cc:213:LEU:HD21	2.52	0.44
1:Bq:292:SER:HB2	1:Bq:295:VAL:HG22	2.00	0.44
1:Cc:206:ALA:HB2	1:Ce:91:MET:HE2	1.99	0.44
1:Cg:211:ARG:HH11	1:Ci:111:LYS:HB3	1.82	0.44
1:Ci:200:PHE:HE1	1:Ck:102:LEU:HD21	1.82	0.44
1:Ck:292:SER:HB2	1:Ck:295:VAL:HG22	2.00	0.44
1:Co:205:GLU:CD	1:Co:234:ARG:HH21	2.26	0.44
1:Ag:220:ARG:NH2	2:Ah:5:U:O3'	2.51	0.44
1:Ag:292:SER:HB2	1:Ag:295:VAL:HG22	2.00	0.44
1:Ai:292:SER:HB2	1:Ai:295:VAL:HG22	2.00	0.44
1:As:292:SER:HB2	1:As:295:VAL:HG22	2.00	0.44
1:Ba:205:GLU:CD	1:Ba:234:ARG:HH21	2.26	0.44
1:Bg:154:VAL:HA	1:Bg:157:ILE:HD12	1.98	0.44
1:Bg:291:VAL:O	1:Bi:296:HIS:CD2	2.71	0.44
1:Bi:292:SER:HB2	1:Bi:295:VAL:HG22	2.00	0.44
1:Bk:292:SER:HB2	1:Bk:295:VAL:HG22	2.00	0.44
1:Bq:284:GLU:CD	1:Bq:296:HIS:HE2	2.23	0.44
1:Bs:205:GLU:CD	1:Bs:234:ARG:HH21	2.26	0.44
1:Bu:292:SER:HB2	1:Bu:295:VAL:HG22	2.00	0.44
1:Ca:205:GLU:CD	1:Ca:234:ARG:HH21	2.26	0.44
1:Ci:284:GLU:OE2	1:Ci:296:HIS:NE2	2.43	0.44
1:Co:292:SER:HB2	1:Co:295:VAL:HG22	2.00	0.44
1:Cq:205:GLU:CD	1:Cq:234:ARG:HH21	2.26	0.44
1:Ac:210:MET:HE2	1:Ae:108:ILE:HA	1.99	0.44
1:Ac:292:SER:HB2	1:Ac:295:VAL:HG22	2.00	0.44
1:Am:284:GLU:CD	1:Am:296:HIS:HE2	2.23	0.44
1:Am:292:SER:HB2	1:Am:295:VAL:HG22	2.00	0.44
1:Aq:154:VAL:HA	1:Aq:157:ILE:HD12	1.98	0.44
1:Aw:292:SER:HB2	1:Aw:295:VAL:HG22	2.00	0.44
1:Be:292:SER:HB2	1:Be:295:VAL:HG22	2.00	0.44
1:Bg:200:PHE:HE1	1:Bi:102:LEU:HD21	1.83	0.44
1:Bg:224:LEU:HD23	1:Bg:224:LEU:HA	1.81	0.44
1:Bk:205:GLU:CD	1:Bk:234:ARG:HH21	2.26	0.44
1:Bo:292:SER:HB2	1:Bo:295:VAL:HG22	2.00	0.44
1:By:291:VAL:O	1:Ca:296:HIS:CD2	2.71	0.44
1:Ci:292:SER:HB2	1:Ci:295:VAL:HG22	2.00	0.44
1:Ae:205:GLU:CD	1:Ae:234:ARG:HH21	2.26	0.44
1:Ai:284:GLU:OE2	1:Ai:296:HIS:NE2	2.44	0.44
1:As:291:VAL:O	1:Au:296:HIS:CD2	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:292:SER:HB2	1:Au:295:VAL:HG22	2.00	0.44
1:Ay:284:GLU:OE2	1:Ay:296:HIS:NE2	2.44	0.44
1:Ay:292:SER:HB2	1:Ay:295:VAL:HG22	2.00	0.44
1:Bc:205:GLU:CD	1:Bc:234:ARG:HH21	2.26	0.44
1:Bc:292:SER:HB2	1:Bc:295:VAL:HG22	2.00	0.44
1:Bo:200:PHE:HE1	1:Bq:102:LEU:HD21	1.83	0.44
1:Bq:195:GLN:NE2	2:Br:2:U:H5'	2.31	0.44
1:Bs:292:SER:HB2	1:Bs:295:VAL:HG22	2.00	0.44
1:Ce:292:SER:HB2	1:Ce:295:VAL:HG22	2.00	0.44
1:Ck:200:PHE:HE1	1:Cm:102:LEU:HD21	1.83	0.44
1:Cm:292:SER:HB2	1:Cm:295:VAL:HG22	2.00	0.44
1:Co:195:GLN:HE21	2:Cp:2:U:H5'	1.82	0.44
1:Cq:200:PHE:HE1	1:Cs:102:LEU:HD21	1.83	0.44
1:Cs:205:GLU:CD	1:Cs:234:ARG:HH21	2.26	0.44
1:Ak:224:LEU:HD23	1:Ak:224:LEU:HA	1.81	0.43
1:Am:200:PHE:HE1	1:Ao:102:LEU:HD21	1.83	0.43
1:Ao:292:SER:HB2	1:Ao:295:VAL:HG22	2.00	0.43
1:Au:205:GLU:CD	1:Au:234:ARG:HH21	2.26	0.43
1:Bo:205:GLU:CD	1:Bo:234:ARG:HH21	2.26	0.43
1:Bu:224:LEU:HD11	2:Bx:1:U:OP2	2.18	0.43
1:Bw:200:PHE:HE1	1:By:102:LEU:HD21	1.83	0.43
1:Ce:205:GLU:CD	1:Ce:234:ARG:HH21	2.26	0.43
1:Ce:219:PRO:O	1:Ce:222:GLY:N	2.51	0.43
1:Cg:292:SER:HB2	1:Cg:295:VAL:HG22	2.00	0.43
1:Ci:205:GLU:CD	1:Ci:234:ARG:HH21	2.26	0.43
1:Cq:292:SER:HB2	1:Cq:295:VAL:HG22	2.00	0.43
1:Cs:261:ALA:CB	2:Ct:4:U:H1'	2.47	0.43
1:Aa:200:PHE:HE1	1:Ac:102:LEU:HD21	1.83	0.43
1:Ai:206:ALA:HB2	1:Ak:91:MET:HE2	2.00	0.43
1:Aq:205:GLU:CD	1:Aq:234:ARG:HH21	2.26	0.43
1:Au:200:PHE:HE1	1:Aw:102:LEU:HD21	1.83	0.43
1:Au:291:VAL:O	1:Aw:296:HIS:CD2	2.71	0.43
1:Bi:154:VAL:HG11	1:Bk:110:TYR:HE2	1.81	0.43
1:Bm:200:PHE:HE1	1:Bo:102:LEU:HD21	1.83	0.43
1:Bm:291:VAL:O	1:Bo:296:HIS:CD2	2.71	0.43
1:Bm:292:SER:HB2	1:Bm:295:VAL:HG22	2.00	0.43
1:Bq:159:ASN:ND2	1:Bs:119:ASN:HB2	2.33	0.43
1:Cc:200:PHE:HE1	1:Ce:102:LEU:HD21	1.83	0.43
1:Cc:292:SER:HB2	1:Cc:295:VAL:HG22	2.00	0.43
1:Ce:206:ALA:CB	1:Cg:91:MET:CE	2.96	0.43
1:Cm:284:GLU:OE2	1:Cm:296:HIS:NE2	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cm:291:VAL:O	1:Co:296:HIS:CD2	2.71	0.43
1:Cq:291:VAL:O	1:Cs:296:HIS:CD2	2.71	0.43
1:Ae:292:SER:HB2	1:Ae:295:VAL:HG22	2.00	0.43
1:Ao:291:VAL:O	1:Aq:296:HIS:CD2	2.71	0.43
1:Ay:206:ALA:HB2	1:Ba:91:MET:HE2	2.00	0.43
1:Ay:224:LEU:HD23	1:Ay:224:LEU:HA	1.81	0.43
1:Ba:219:PRO:O	1:Ba:222:GLY:N	2.51	0.43
1:Bq:205:GLU:CD	1:Bq:234:ARG:HH21	2.26	0.43
1:Bs:284:GLU:OE2	1:Bs:296:HIS:NE2	2.44	0.43
1:Bu:284:GLU:OE2	1:Bu:296:HIS:NE2	2.44	0.43
1:Bw:292:SER:HB2	1:Bw:295:VAL:HG22	2.00	0.43
1:Cc:195:GLN:HE21	2:Cd:2:U:H5'	1.84	0.43
1:Ai:283:THR:O	1:Bq:256:GLN:CD	2.61	0.43
1:As:200:PHE:HE1	1:Au:102:LEU:HD21	1.83	0.43
1:Ay:205:GLU:CD	1:Ay:234:ARG:HH21	2.26	0.43
1:Ay:219:PRO:O	1:Ay:222:GLY:N	2.51	0.43
1:Be:284:GLU:OE2	1:Be:296:HIS:NE2	2.44	0.43
1:Bo:219:PRO:O	1:Bo:222:GLY:N	2.51	0.43
1:Bs:123:THR:N	1:Bs:126:GLN:OE1	2.52	0.43
1:By:205:GLU:CD	1:By:234:ARG:HH21	2.26	0.43
1:Bi:123:THR:N	1:Bi:126:GLN:OE1	2.52	0.43
1:Ae:123:THR:N	1:Ae:126:GLN:OE1	2.52	0.43
1:Ag:283:THR:O	1:Bo:256:GLN:CD	2.61	0.43
1:Ak:284:GLU:OE2	1:Ak:296:HIS:NE2	2.43	0.43
1:Am:272:LEU:N	1:Be:252:GLU:OE1	2.46	0.43
1:As:205:GLU:CD	1:As:234:ARG:HH21	2.26	0.43
1:Bc:123:THR:N	1:Bc:126:GLN:OE1	2.52	0.43
1:Be:291:VAL:O	1:Be:296:HIS:CD2	2.71	0.43
2:Bn:5:U:O3'	2:Bp:1:U:C5'	2.65	0.43
1:Cc:205:GLU:CD	1:Cc:234:ARG:HH21	2.26	0.43
1:Aa:283:THR:O	1:Bi:256:GLN:CD	2.62	0.43
1:Ak:219:PRO:O	1:Ak:222:GLY:N	2.51	0.43
1:Am:205:GLU:CD	1:Am:234:ARG:HH21	2.26	0.43
1:Ay:173:ASP:HB2	1:Bs:81:ILE:CG1	2.49	0.43
1:Bi:205:GLU:CD	1:Bi:234:ARG:HH21	2.26	0.43
1:Bs:168:TYR:CZ	1:Ck:213:LEU:HD21	2.53	0.43
1:Bu:205:GLU:CD	1:Bu:234:ARG:HH21	2.26	0.43
1:Cg:205:GLU:CD	1:Cg:234:ARG:HH21	2.26	0.43
1:Co:200:PHE:HE1	1:Cq:102:LEU:HD21	1.83	0.43
1:Cs:219:PRO:O	1:Cs:222:GLY:N	2.51	0.43
1:Aa:224:LEU:HD23	1:Aa:224:LEU:HA	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:205:GLU:CD	1:Ac:234:ARG:HH21	2.26	0.43
1:Ai:219:PRO:O	1:Ai:222:GLY:N	2.51	0.43
1:Ai:220:ARG:NH2	2:Aj:5:U:O3'	2.52	0.43
1:Am:123:THR:N	1:Am:126:GLN:OE1	2.52	0.43
1:Ao:200:PHE:HE1	1:Aq:102:LEU:HD21	1.83	0.43
1:Ay:154:VAL:HG11	1:Ba:110:TYR:HE2	1.83	0.43
1:Be:200:PHE:HE1	1:Bg:102:LEU:HD21	1.83	0.43
1:Bg:283:THR:O	1:Co:256:GLN:CD	2.62	0.43
1:Bm:205:GLU:CD	1:Bm:234:ARG:HH21	2.26	0.43
1:Bw:195:GLN:NE2	2:Bx:2:U:H5'	2.33	0.43
1:Cc:219:PRO:O	1:Cc:222:GLY:N	2.51	0.43
1:Cg:123:THR:N	1:Cg:126:GLN:OE1	2.52	0.43
1:Ag:183:LYS:HD2	1:Ay:234:ARG:HH22	1.83	0.43
1:Ag:205:GLU:CD	1:Ag:234:ARG:HH21	2.26	0.43
1:Ai:205:GLU:CD	1:Ai:234:ARG:HH21	2.26	0.43
1:Ao:104:LEU:HD23	1:Ao:104:LEU:HA	1.80	0.43
1:Aq:200:PHE:HE1	1:As:102:LEU:HD21	1.84	0.43
1:As:104:LEU:O	1:As:108:ILE:HG13	2.19	0.43
1:Au:123:THR:N	1:Au:126:GLN:OE1	2.52	0.43
1:Au:224:LEU:HD23	1:Au:224:LEU:HA	1.81	0.43
1:Bi:104:LEU:O	1:Bi:108:ILE:HG13	2.19	0.43
1:Bi:283:THR:O	1:Cq:256:GLN:CD	2.62	0.43
1:Bk:208:ILE:HD13	1:Bk:219:PRO:HG3	2.01	0.43
1:Bm:219:PRO:O	1:Bm:222:GLY:N	2.51	0.43
1:Bq:123:THR:N	1:Bq:126:GLN:OE1	2.52	0.43
1:Bw:291:VAL:O	1:By:296:HIS:CD2	2.72	0.43
1:Cc:104:LEU:O	1:Cc:108:ILE:HG13	2.19	0.43
1:Co:291:VAL:O	1:Cq:296:HIS:CD2	2.72	0.43
1:Cs:104:LEU:O	1:Cs:108:ILE:HG13	2.19	0.43
1:Ag:170:THR:CG2	1:Ag:177:GLN:HE21	2.32	0.43
1:Ai:170:THR:CG2	1:Ai:177:GLN:HE21	2.32	0.43
1:Aq:208:ILE:HD13	1:Aq:219:PRO:HG3	2.01	0.43
1:As:208:ILE:HD13	1:As:219:PRO:HG3	2.01	0.43
1:Ay:200:PHE:CD1	1:Ba:94:PRO:HG3	2.54	0.43
1:Ba:123:THR:N	1:Ba:126:GLN:OE1	2.52	0.43
1:Bc:200:PHE:HE1	1:Be:102:LEU:HD21	1.84	0.43
1:Bm:104:LEU:O	1:Bm:108:ILE:HG13	2.19	0.43
1:Bq:158:GLU:OE1	1:Bs:114:GLN:HG3	2.19	0.43
1:Bu:170:THR:CG2	1:Bu:177:GLN:HE21	2.32	0.43
1:Cc:208:ILE:HD13	1:Cc:219:PRO:HG3	2.01	0.43
1:Cg:170:THR:CG2	1:Cg:177:GLN:HE21	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ck:205:GLU:CD	1:Ck:234:ARG:HH21	2.26	0.43
1:Ck:224:LEU:HD23	1:Ck:224:LEU:HA	1.81	0.43
1:Ck:284:GLU:OE2	1:Ck:296:HIS:NE2	2.43	0.43
1:Cm:200:PHE:HE1	1:Co:102:LEU:HD21	1.84	0.43
1:Aa:205:GLU:CD	1:Aa:234:ARG:HH21	2.26	0.43
1:Aa:208:ILE:HD13	1:Aa:219:PRO:HG3	2.01	0.43
1:Ac:104:LEU:O	1:Ac:108:ILE:HG13	2.19	0.43
1:Ac:200:PHE:HE1	1:Ae:102:LEU:HD21	1.84	0.43
1:Au:208:ILE:HD13	1:Au:219:PRO:HG3	2.01	0.43
1:Aw:205:GLU:CD	1:Aw:234:ARG:HH21	2.26	0.43
1:Bi:146:ARG:NH1	1:Bk:100:ALA:O	2.52	0.43
1:Bi:208:ILE:HD13	1:Bi:219:PRO:HG3	2.01	0.43
1:Bo:291:VAL:O	1:Bq:296:HIS:CD2	2.72	0.43
1:By:104:LEU:O	1:By:108:ILE:HG13	2.19	0.43
1:By:200:PHE:HE1	1:Ca:102:LEU:HD21	1.83	0.43
1:Ca:210:MET:HE2	1:Cc:108:ILE:HA	2.00	0.43
1:Cc:123:THR:N	1:Cc:126:GLN:OE1	2.52	0.43
1:Ci:170:THR:CG2	1:Ci:177:GLN:HE21	2.32	0.43
1:Aa:220:ARG:NH2	2:Ab:5:U:O3'	2.52	0.42
1:Ae:206:ALA:CB	1:Ag:91:MET:CE	2.97	0.42
1:Ag:224:LEU:HD23	1:Ag:224:LEU:HA	1.81	0.42
1:Ak:123:THR:N	1:Ak:126:GLN:OE1	2.52	0.42
1:As:165:ILE:HG22	2:At:5:U:C2	2.53	0.42
1:As:183:LYS:HD2	1:Bk:234:ARG:HH22	1.84	0.42
1:Aw:104:LEU:O	1:Aw:108:ILE:HG13	2.19	0.42
1:Aw:219:PRO:O	1:Aw:222:GLY:N	2.51	0.42
1:Aw:224:LEU:HA	1:Aw:224:LEU:HD23	1.81	0.42
1:Ba:104:LEU:O	1:Ba:108:ILE:HG13	2.19	0.42
1:Be:283:THR:O	1:Cm:256:GLN:CD	2.61	0.42
1:Bg:170:THR:CG2	1:Bg:177:GLN:HE21	2.32	0.42
1:Bg:272:LEU:N	1:By:252:GLU:OE1	2.46	0.42
1:Bi:104:LEU:HD23	1:Bi:104:LEU:HA	1.80	0.42
1:Bu:214:ASP:OD2	1:Bw:111:LYS:HE2	2.19	0.42
1:Co:123:THR:N	1:Co:126:GLN:OE1	2.52	0.42
1:Cs:208:ILE:HD13	1:Cs:219:PRO:HG3	2.01	0.42
1:Aq:291:VAL:O	1:As:296:HIS:CD2	2.72	0.42
1:Aw:170:THR:CG2	1:Aw:177:GLN:HE21	2.32	0.42
1:Ba:269:MET:O	1:Bq:228:ASN:HB2	2.19	0.42
1:Bc:284:GLU:OE2	1:Bc:296:HIS:NE2	2.44	0.42
1:Bm:208:ILE:HD13	1:Bm:219:PRO:HG3	2.01	0.42
1:Bq:206:ALA:CB	1:Bs:91:MET:HE2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bs:104:LEU:O	1:Bs:108:ILE:HG13	2.19	0.42
1:Bu:200:PHE:HE1	1:Bw:102:LEU:HD21	1.84	0.42
1:Ce:208:ILE:HD13	1:Ce:219:PRO:HG3	2.01	0.42
1:Cg:206:ALA:HB2	1:Ci:91:MET:HE2	2.00	0.42
1:Cq:208:ILE:HD13	1:Cq:219:PRO:HG3	2.01	0.42
1:Ac:168:TYR:CZ	1:Au:213:LEU:HD21	2.54	0.42
1:Ae:208:ILE:HD13	1:Ae:219:PRO:HG3	2.01	0.42
1:Ag:219:PRO:O	1:Ag:222:GLY:N	2.51	0.42
1:Ag:286:HIS:HD2	1:Ay:270:PHE:O	2.02	0.42
1:Ao:104:LEU:O	1:Ao:108:ILE:HG13	2.19	0.42
2:Ap:5:U:O3'	2:Ar:1:U:H5'	2.20	0.42
1:Aw:283:THR:O	1:Ce:256:GLN:CD	2.61	0.42
1:Bc:104:LEU:O	1:Bc:108:ILE:HG13	2.19	0.42
1:Be:104:LEU:O	1:Be:108:ILE:HG13	2.19	0.42
1:Bk:123:THR:N	1:Bk:126:GLN:OE1	2.52	0.42
1:Bs:200:PHE:CE1	1:Bu:94:PRO:HG3	2.53	0.42
1:Cq:170:THR:CG2	1:Cq:177:GLN:HE21	2.32	0.42
1:Ae:170:THR:CG2	1:Ae:177:GLN:HE21	2.32	0.42
1:Ag:104:LEU:O	1:Ag:108:ILE:HG13	2.19	0.42
1:Ak:170:THR:CG2	1:Ak:177:GLN:HE21	2.32	0.42
1:Bg:168:TYR:CZ	1:By:213:LEU:HD21	2.55	0.42
1:Bo:214:ASP:OD2	1:Bq:111:LYS:HE2	2.19	0.42
1:Bw:170:THR:CG2	1:Bw:177:GLN:HE21	2.32	0.42
1:By:123:THR:N	1:By:126:GLN:OE1	2.52	0.42
1:By:208:ILE:HD13	1:By:219:PRO:HG3	2.01	0.42
1:Ce:170:THR:CG2	1:Ce:177:GLN:HE21	2.32	0.42
1:Cg:104:LEU:O	1:Cg:108:ILE:HG13	2.19	0.42
1:Cs:123:THR:N	1:Cs:126:GLN:OE1	2.52	0.42
1:Aa:123:THR:N	1:Aa:126:GLN:OE1	2.52	0.42
1:Ac:123:THR:N	1:Ac:126:GLN:OE1	2.52	0.42
1:Ac:208:ILE:HD13	1:Ac:219:PRO:HG3	2.01	0.42
1:Ai:168:TYR:CZ	1:Ba:213:LEU:HD21	2.55	0.42
1:Ai:286:HIS:HD2	1:Ba:270:PHE:O	2.01	0.42
1:Ak:200:PHE:HE1	1:Am:102:LEU:HD21	1.84	0.42
1:Am:291:VAL:O	1:Ao:296:HIS:CD2	2.72	0.42
1:Aq:123:THR:N	1:Aq:126:GLN:OE1	2.52	0.42
1:As:115:ARG:NH1	1:As:245:ARG:HH12	2.18	0.42
1:As:170:THR:CG2	1:As:177:GLN:HE21	2.32	0.42
1:Au:170:THR:CG2	1:Au:177:GLN:HE21	2.32	0.42
1:Ay:104:LEU:O	1:Ay:108:ILE:HG13	2.19	0.42
1:Bc:227:LEU:HD12	1:Bc:228:ASN:H	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Be:291:VAL:O	1:Bg:296:HIS:CD2	2.72	0.42
1:Bu:220:ARG:NH2	2:Bv:5:U:O3'	2.53	0.42
1:Bw:227:LEU:HD12	1:Bw:228:ASN:H	1.85	0.42
1:Ca:208:ILE:HD13	1:Ca:219:PRO:HG3	2.01	0.42
1:Ca:219:PRO:O	1:Ca:222:GLY:N	2.51	0.42
1:Cg:208:ILE:HD13	1:Cg:219:PRO:HG3	2.01	0.42
1:Ck:170:THR:CG2	1:Ck:177:GLN:HE21	2.32	0.42
1:Ck:227:LEU:HD12	1:Ck:228:ASN:H	1.85	0.42
1:Co:208:ILE:HD13	1:Co:219:PRO:HG3	2.01	0.42
1:Ac:224:LEU:HA	1:Ac:224:LEU:HD23	1.81	0.42
1:Ao:224:LEU:HD23	1:Ao:224:LEU:HA	1.81	0.42
1:Aq:170:THR:CG2	1:Aq:177:GLN:HE21	2.32	0.42
1:Bm:104:LEU:HD23	1:Bm:104:LEU:HA	1.80	0.42
1:Bm:234:ARG:HG3	1:Bm:235:TYR:CD2	2.55	0.42
1:Bu:104:LEU:O	1:Bu:108:ILE:HG13	2.19	0.42
1:Bw:208:ILE:HD13	1:Bw:219:PRO:HG3	2.01	0.42
1:Co:104:LEU:O	1:Co:108:ILE:HG13	2.19	0.42
1:Cq:219:PRO:O	1:Cq:222:GLY:N	2.51	0.42
1:Cs:115:ARG:NH1	1:Cs:245:ARG:HH12	2.18	0.42
1:Cs:170:THR:CG2	1:Cs:177:GLN:HE21	2.32	0.42
1:Ac:115:ARG:NH1	1:Ac:245:ARG:HH12	2.18	0.42
1:Ae:234:ARG:HG3	1:Ae:235:TYR:CD2	2.55	0.42
1:Ag:183:LYS:HD2	1:Ay:234:ARG:NH2	2.35	0.42
1:Ag:227:LEU:HD12	1:Ag:228:ASN:H	1.85	0.42
1:Ai:227:LEU:HD12	1:Ai:228:ASN:H	1.85	0.42
1:Ao:208:ILE:HD13	1:Ao:219:PRO:HG3	2.01	0.42
1:Aw:208:ILE:HD13	1:Aw:219:PRO:HG3	2.01	0.42
1:Ay:170:THR:CG2	1:Ay:177:GLN:HE21	2.32	0.42
1:Ay:234:ARG:HG3	1:Ay:235:TYR:CD2	2.55	0.42
1:Ba:284:GLU:OE2	1:Ba:296:HIS:NE2	2.43	0.42
1:Be:208:ILE:HD13	1:Be:219:PRO:HG3	2.01	0.42
1:Bg:104:LEU:O	1:Bg:108:ILE:HG13	2.19	0.42
1:Bg:123:THR:N	1:Bg:126:GLN:OE1	2.52	0.42
1:Bg:208:ILE:HD13	1:Bg:219:PRO:HG3	2.01	0.42
1:Bi:170:THR:CG2	1:Bi:177:GLN:HE21	2.32	0.42
1:Bk:219:PRO:O	1:Bk:222:GLY:N	2.51	0.42
1:Bq:104:LEU:O	1:Bq:108:ILE:HG13	2.19	0.42
1:Bs:234:ARG:HG3	1:Bs:235:TYR:CD2	2.55	0.42
1:Bu:168:TYR:CZ	1:Cm:213:LEU:HD21	2.55	0.42
1:Ca:224:LEU:HD11	2:Cd:1:U:OP2	2.19	0.42
1:Cc:115:ARG:NH1	1:Cc:245:ARG:HH12	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cc:206:ALA:CB	1:Ce:91:MET:HE2	2.49	0.42
1:Cg:104:LEU:HD23	1:Cg:104:LEU:HA	1.80	0.42
1:Ci:227:LEU:HD12	1:Ci:228:ASN:H	1.85	0.42
1:Cm:104:LEU:O	1:Cm:108:ILE:HG13	2.19	0.42
1:Ag:208:ILE:HD13	1:Ag:219:PRO:HG3	2.01	0.42
1:Ak:206:ALA:CB	1:Am:91:MET:HE2	2.49	0.42
1:Am:283:THR:O	1:Bu:256:GLN:CD	2.62	0.42
1:Ao:224:LEU:HD11	2:Ar:1:U:OP2	2.20	0.42
1:As:234:ARG:HG3	1:As:235:TYR:CD2	2.55	0.42
1:Au:214:ASP:OD2	1:Aw:111:LYS:HE2	2.20	0.42
1:Ba:183:LYS:HD2	1:Bs:234:ARG:NH2	2.35	0.42
1:Be:168:TYR:CZ	1:Bw:213:LEU:HD21	2.55	0.42
1:Bi:115:ARG:NH1	1:Bi:245:ARG:HH12	2.18	0.42
1:Bi:123:THR:N	1:Bi:126:GLN:OE1	2.52	0.42
1:Bm:115:ARG:NH1	1:Bm:245:ARG:HH12	2.18	0.42
1:Bm:214:ASP:OD2	1:Bo:111:LYS:HE2	2.20	0.42
1:Bo:123:THR:N	1:Bo:126:GLN:OE1	2.52	0.42
1:Bw:104:LEU:O	1:Bw:108:ILE:HG13	2.19	0.42
1:Cg:234:ARG:HG3	1:Cg:235:TYR:CD2	2.55	0.42
1:Ck:104:LEU:O	1:Ck:108:ILE:HG13	2.19	0.42
1:Co:214:ASP:OD2	1:Cq:111:LYS:HE2	2.19	0.42
1:Cq:214:ASP:OD2	1:Cs:111:LYS:HE2	2.20	0.42
1:Cs:234:ARG:HG3	1:Cs:235:TYR:CD2	2.55	0.42
1:Ae:200:PHE:CE1	1:Ag:94:PRO:HG3	2.54	0.42
1:Ag:234:ARG:HG3	1:Ag:235:TYR:CD2	2.55	0.42
1:Ak:234:ARG:HG3	1:Ak:235:TYR:CD2	2.55	0.42
1:As:183:LYS:HD2	1:Bk:234:ARG:NH2	2.35	0.42
1:Au:219:PRO:O	1:Au:222:GLY:N	2.51	0.42
1:Ba:227:LEU:HD12	1:Ba:228:ASN:H	1.85	0.42
1:Be:206:ALA:HB2	1:Bg:91:MET:HE2	2.02	0.42
1:Be:227:LEU:HD12	1:Be:228:ASN:H	1.85	0.42
1:Bk:234:ARG:HG3	1:Bk:235:TYR:CD2	2.55	0.42
1:Bo:208:ILE:HD13	1:Bo:219:PRO:HG3	2.01	0.42
1:Bq:234:ARG:HG3	1:Bq:235:TYR:CD2	2.55	0.42
1:Bs:115:ARG:NH1	1:Bs:245:ARG:HH12	2.18	0.42
1:Bw:123:THR:N	1:Bw:126:GLN:OE1	2.52	0.42
1:By:115:ARG:NH1	1:By:245:ARG:HH12	2.18	0.42
1:Cc:170:THR:CG2	1:Cc:177:GLN:HE21	2.32	0.42
1:Ce:123:THR:N	1:Ce:126:GLN:OE1	2.52	0.42
1:Cm:227:LEU:HD12	1:Cm:228:ASN:H	1.85	0.42
1:Ac:183:LYS:HD2	1:Au:234:ARG:HH22	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:272:LEU:N	1:Aw:252:GLU:OE1	2.40	0.42
1:Ai:234:ARG:HG3	1:Ai:235:TYR:CD2	2.55	0.42
1:Ak:183:LYS:HD2	1:Bc:234:ARG:HH22	1.85	0.42
1:Am:227:LEU:HD12	1:Am:228:ASN:H	1.85	0.42
1:Ay:123:THR:N	1:Ay:126:GLN:OE1	2.52	0.42
1:Ay:208:ILE:HD13	1:Ay:219:PRO:HG3	2.01	0.42
1:Ba:234:ARG:HG3	1:Ba:235:TYR:CD2	2.55	0.42
1:Bc:115:ARG:NH1	1:Bc:245:ARG:HH12	2.18	0.42
1:Be:224:LEU:HD23	1:Be:224:LEU:HA	1.81	0.42
1:Bk:206:ALA:HB2	1:Bm:91:MET:HE2	2.01	0.42
1:Bu:206:ALA:HB2	1:Bw:91:MET:HE2	2.01	0.42
1:Bu:227:LEU:HD12	1:Bu:228:ASN:H	1.85	0.42
1:Ca:195:GLN:HE21	2:Cb:2:U:H5'	1.85	0.42
1:Ca:234:ARG:HG3	1:Ca:235:TYR:CD2	2.55	0.42
1:Cc:234:ARG:HG3	1:Cc:235:TYR:CD2	2.55	0.42
1:Ci:104:LEU:O	1:Ci:108:ILE:HG13	2.19	0.42
1:Ci:234:ARG:HG3	1:Ci:235:TYR:CD2	2.55	0.42
1:Cm:123:THR:N	1:Cm:126:GLN:OE1	2.52	0.42
1:Cm:234:ARG:HG3	1:Cm:235:TYR:CD2	2.55	0.42
1:Ai:104:LEU:O	1:Ai:108:ILE:HG13	2.19	0.41
1:Am:170:THR:CG2	1:Am:177:GLN:HE21	2.32	0.41
1:Am:214:ASP:OD2	1:Ao:111:LYS:HE2	2.19	0.41
1:Am:234:ARG:HG3	1:Am:235:TYR:CD2	2.55	0.41
1:Ao:115:ARG:NH1	1:Ao:245:ARG:HH12	2.18	0.41
1:Aq:234:ARG:HG3	1:Aq:235:TYR:CD2	2.55	0.41
1:As:224:LEU:HA	1:As:224:LEU:HD23	1.81	0.41
1:Ba:224:LEU:HD23	1:Ba:224:LEU:HA	1.81	0.41
1:Bc:168:TYR:CZ	1:Bu:213:LEU:HD21	2.55	0.41
1:Be:234:ARG:HG3	1:Be:235:TYR:CD2	2.55	0.41
1:Bi:210:MET:HE2	1:Bk:108:ILE:HA	2.01	0.41
1:Bk:170:THR:CG2	1:Bk:177:GLN:HE21	2.32	0.41
1:Bq:227:LEU:HD12	1:Bq:228:ASN:H	1.85	0.41
1:Bu:224:LEU:HD23	1:Bu:224:LEU:HA	1.81	0.41
1:By:234:ARG:HG3	1:By:235:TYR:CD2	2.55	0.41
1:Cc:104:LEU:HD23	1:Cc:104:LEU:HA	1.80	0.41
1:Cc:224:LEU:HA	1:Cc:224:LEU:HD23	1.81	0.41
1:Ce:234:ARG:HG3	1:Ce:235:TYR:CD2	2.55	0.41
1:Ck:115:ARG:NH1	1:Ck:245:ARG:HH12	2.18	0.41
1:Aa:104:LEU:O	1:Aa:108:ILE:HG13	2.19	0.41
1:Aa:214:ASP:OD2	1:Ac:111:LYS:HE2	2.19	0.41
1:Ac:170:THR:CG2	1:Ac:177:GLN:HE21	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:234:ARG:HG3	1:Ac:235:TYR:CD2	2.55	0.41
1:Ag:200:PHE:HE1	1:Ai:102:LEU:HD21	1.84	0.41
1:Ai:87:VAL:HG13	1:Ai:91:MET:HE1	2.02	0.41
1:Ai:123:THR:N	1:Ai:126:GLN:OE1	2.52	0.41
1:Ak:104:LEU:O	1:Ak:108:ILE:HG13	2.19	0.41
1:Ak:115:ARG:NH1	1:Ak:245:ARG:HH12	2.18	0.41
1:Am:208:ILE:HD13	1:Am:219:PRO:HG3	2.01	0.41
1:Am:224:LEU:HD11	2:Ap:1:U:OP2	2.20	0.41
1:Ao:214:ASP:OD2	1:Aq:111:LYS:HE2	2.20	0.41
1:Ba:115:ARG:NH1	1:Ba:245:ARG:HH12	2.18	0.41
1:Bi:168:TYR:CZ	1:Ca:213:LEU:HD21	2.54	0.41
1:Bm:224:LEU:HA	1:Bm:224:LEU:HD23	1.81	0.41
1:Bo:224:LEU:HD11	2:Br:1:U:OP2	2.19	0.41
1:Bo:227:LEU:HD12	1:Bo:228:ASN:H	1.85	0.41
1:Bq:87:VAL:HG13	1:Bq:91:MET:HE1	2.02	0.41
1:Bq:208:ILE:HD13	1:Bq:219:PRO:HG3	2.01	0.41
1:Bw:206:ALA:HB2	1:By:91:MET:HE2	2.02	0.41
1:By:227:LEU:HD12	1:By:228:ASN:H	1.85	0.41
1:Ca:104:LEU:O	1:Ca:108:ILE:HG13	2.19	0.41
1:Ca:123:THR:N	1:Ca:126:GLN:OE1	2.52	0.41
1:Ca:200:PHE:HE1	1:Cc:102:LEU:HD21	1.85	0.41
1:Co:219:PRO:O	1:Co:222:GLY:N	2.51	0.41
1:Aa:168:TYR:CZ	1:As:213:LEU:HD21	2.55	0.41
1:Ae:219:PRO:O	1:Ae:222:GLY:N	2.51	0.41
1:Ak:208:ILE:HD13	1:Ak:219:PRO:HG3	2.01	0.41
1:Ak:227:LEU:HD12	1:Ak:228:ASN:H	1.85	0.41
1:Am:104:LEU:O	1:Am:108:ILE:HG13	2.19	0.41
1:Ao:227:LEU:HD12	1:Ao:228:ASN:H	1.85	0.41
1:Aq:104:LEU:O	1:Aq:108:ILE:HG13	2.19	0.41
1:As:283:THR:O	1:Ca:256:GLN:CD	2.62	0.41
1:Aw:234:ARG:HG3	1:Aw:235:TYR:CD2	2.55	0.41
1:Ay:115:ARG:NH1	1:Ay:245:ARG:HH12	2.18	0.41
1:Bc:87:VAL:HG13	1:Bc:91:MET:HE1	2.02	0.41
1:Bc:208:ILE:HD13	1:Bc:219:PRO:HG3	2.01	0.41
1:Be:214:ASP:OD2	1:Bg:111:LYS:HE2	2.19	0.41
1:Bg:234:ARG:HG3	1:Bg:235:TYR:CD2	2.55	0.41
1:Bk:104:LEU:O	1:Bk:108:ILE:HG13	2.19	0.41
1:Bu:234:ARG:HG3	1:Bu:235:TYR:CD2	2.55	0.41
1:By:214:ASP:OD2	1:Ca:111:LYS:HE2	2.20	0.41
1:By:219:PRO:O	1:By:222:GLY:N	2.51	0.41
1:Ca:115:ARG:NH1	1:Ca:245:ARG:HH12	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ck:87:VAL:HG13	1:Ck:91:MET:HE1	2.02	0.41
1:Co:234:ARG:HG3	1:Co:235:TYR:CD2	2.55	0.41
1:Aa:234:ARG:HG3	1:Aa:235:TYR:CD2	2.55	0.41
1:Ag:115:ARG:NH1	1:Ag:245:ARG:HH12	2.18	0.41
1:Ao:283:THR:O	1:Bw:256:GLN:CD	2.62	0.41
1:Aq:115:ARG:NH1	1:Aq:245:ARG:HH12	2.18	0.41
1:As:123:THR:N	1:As:126:GLN:OE1	2.52	0.41
1:As:214:ASP:OD2	1:Au:111:LYS:HE2	2.19	0.41
1:Au:104:LEU:O	1:Au:108:ILE:HG13	2.19	0.41
1:Au:234:ARG:HG3	1:Au:235:TYR:CD2	2.55	0.41
1:Aw:115:ARG:NH1	1:Aw:245:ARG:HH12	2.18	0.41
1:Ay:87:VAL:HG13	1:Ay:91:MET:HE1	2.02	0.41
1:Ay:220:ARG:NH2	2:Az:5:U:O3'	2.53	0.41
1:Ba:87:VAL:HG13	1:Ba:91:MET:HE1	2.02	0.41
1:Ba:170:THR:CG2	1:Ba:177:GLN:HE21	2.32	0.41
1:Bo:104:LEU:O	1:Bo:108:ILE:HG13	2.19	0.41
1:Bo:234:ARG:HG3	1:Bo:235:TYR:CD2	2.55	0.41
1:Bq:168:TYR:CZ	1:Ci:213:LEU:HD21	2.56	0.41
1:Bu:87:VAL:HG13	1:Bu:91:MET:HE1	2.02	0.41
1:Bw:214:ASP:OD2	1:By:111:LYS:HE2	2.19	0.41
1:By:170:THR:CG2	1:By:177:GLN:HE21	2.32	0.41
1:Ca:170:THR:CG2	1:Ca:177:GLN:HE21	2.32	0.41
1:Ce:104:LEU:O	1:Ce:108:ILE:HG13	2.19	0.41
1:Ci:208:ILE:HD13	1:Ci:219:PRO:HG3	2.01	0.41
1:Cq:104:LEU:O	1:Cq:108:ILE:HG13	2.19	0.41
1:Ae:104:LEU:O	1:Ae:108:ILE:HG13	2.19	0.41
1:Ae:104:LEU:HD23	1:Ae:104:LEU:HA	1.80	0.41
1:Ae:200:PHE:CD1	1:Ag:94:PRO:HG3	2.55	0.41
1:Ai:115:ARG:NH1	1:Ai:245:ARG:HH12	2.18	0.41
1:Am:115:ARG:NH1	1:Am:245:ARG:HH12	2.18	0.41
1:Ao:168:TYR:CZ	1:Bg:213:LEU:HD21	2.56	0.41
1:Aq:227:LEU:HD12	1:Aq:228:ASN:H	1.85	0.41
1:As:227:LEU:HD12	1:As:228:ASN:H	1.85	0.41
1:Ay:146:ARG:NH1	1:Ba:100:ALA:O	2.52	0.41
1:Ba:208:ILE:HD13	1:Ba:219:PRO:HG3	2.01	0.41
1:Bg:183:LYS:HD2	1:By:234:ARG:HH22	1.86	0.41
1:Bk:183:LYS:HD2	1:Cc:234:ARG:HH22	1.84	0.41
1:Bm:173:ASP:HB2	1:Cg:81:ILE:CG1	2.50	0.41
1:Bs:87:VAL:HG13	1:Bs:91:MET:HE1	2.02	0.41
1:Bs:208:ILE:HD13	1:Bs:219:PRO:HG3	2.01	0.41
1:Bu:183:LYS:HD2	1:Cm:234:ARG:HH22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cg:87:VAL:HG13	1:Cg:91:MET:HE1	2.02	0.41
1:Ci:115:ARG:NH1	1:Ci:245:ARG:HH12	2.18	0.41
1:Cm:208:ILE:HD13	1:Cm:219:PRO:HG3	2.01	0.41
1:Co:115:ARG:NH1	1:Co:245:ARG:HH12	2.18	0.41
1:Cs:224:LEU:HD23	1:Cs:224:LEU:HA	1.81	0.41
1:Ag:87:VAL:HG13	1:Ag:91:MET:HE1	2.02	0.41
1:Ak:168:TYR:CZ	1:Bc:213:LEU:HD21	2.55	0.41
1:Au:115:ARG:NH1	1:Au:245:ARG:HH12	2.18	0.41
1:Bi:183:LYS:HD2	1:Ca:234:ARG:HH22	1.85	0.41
1:Bs:159:ASN:CG	1:Bu:119:ASN:HB2	2.45	0.41
1:Bu:206:ALA:CB	1:Bw:91:MET:HE2	2.51	0.41
1:Bu:272:LEU:N	1:Cm:252:GLU:OE1	2.44	0.41
1:Ci:87:VAL:HG13	1:Ci:91:MET:HE1	2.02	0.41
1:Ck:208:ILE:HD13	1:Ck:219:PRO:HG3	2.01	0.41
1:Ck:234:ARG:HG3	1:Ck:235:TYR:CD2	2.55	0.41
1:Cm:170:THR:CG2	1:Cm:177:GLN:HE21	2.32	0.41
1:Co:227:LEU:HD12	1:Co:228:ASN:H	1.85	0.41
1:Cs:227:LEU:HD12	1:Cs:228:ASN:H	1.85	0.41
1:Aa:170:THR:CG2	1:Aa:177:GLN:HE21	2.32	0.41
1:Ac:115:ARG:HH12	1:Ac:245:ARG:NH1	2.19	0.41
1:Ac:214:ASP:OD2	1:Ae:111:LYS:HE2	2.20	0.41
1:Ai:206:ALA:CB	1:Ak:91:MET:HE2	2.51	0.41
1:Ai:224:LEU:HD23	1:Ai:224:LEU:HA	1.81	0.41
1:Ak:87:VAL:HG13	1:Ak:91:MET:HE1	2.02	0.41
1:Am:87:VAL:HG13	1:Am:91:MET:HE1	2.02	0.41
1:As:115:ARG:HH12	1:As:245:ARG:NH1	2.19	0.41
1:Bo:84:LEU:H	1:Bo:84:LEU:HG	1.77	0.41
1:Bo:115:ARG:NH1	1:Bo:245:ARG:HH12	2.18	0.41
1:Bs:227:LEU:HD12	1:Bs:228:ASN:H	1.85	0.41
1:Bu:208:ILE:HD13	1:Bu:219:PRO:HG3	2.01	0.41
1:Bw:234:ARG:HG3	1:Bw:235:TYR:CD2	2.55	0.41
1:By:218:MET:HE2	1:By:218:MET:HB2	1.96	0.41
1:Cc:227:LEU:HD12	1:Cc:228:ASN:H	1.85	0.41
1:Cm:87:VAL:HG13	1:Cm:91:MET:HE1	2.02	0.41
1:Cm:115:ARG:NH1	1:Cm:245:ARG:HH12	2.18	0.41
1:Cm:224:LEU:HD23	1:Cm:224:LEU:HA	1.81	0.41
1:Cq:115:ARG:NH1	1:Cq:245:ARG:HH12	2.18	0.41
1:Am:206:ALA:CB	1:Ao:91:MET:HE2	2.51	0.41
1:Ao:123:THR:N	1:Ao:126:GLN:OE1	2.52	0.41
1:Aq:283:THR:O	1:By:256:GLN:CD	2.63	0.41
1:Ba:84:LEU:H	1:Ba:84:LEU:HG	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:214:ASP:OD2	1:Be:111:LYS:HE2	2.21	0.41
1:Bi:272:LEU:N	1:Ca:252:GLU:OE1	2.45	0.41
1:Bk:115:ARG:NH1	1:Bk:245:ARG:HH12	2.18	0.41
1:Bm:170:THR:CG2	1:Bm:177:GLN:HE21	2.32	0.41
1:Bo:206:ALA:HB2	1:Bq:91:MET:HE2	2.03	0.41
1:Bw:218:MET:HE2	1:Bw:218:MET:HB2	1.96	0.41
1:Bw:272:LEU:N	1:Co:252:GLU:OE1	2.46	0.41
1:Cc:115:ARG:HH12	1:Cc:245:ARG:NH1	2.19	0.41
1:Cg:227:LEU:HD12	1:Cg:228:ASN:H	1.85	0.41
1:Co:84:LEU:H	1:Co:84:LEU:HG	1.77	0.41
1:Co:206:ALA:CB	1:Cq:91:MET:HE2	2.51	0.41
1:Cq:227:LEU:HD12	1:Cq:228:ASN:H	1.85	0.41
1:Aa:104:LEU:HD23	1:Aa:104:LEU:HA	1.80	0.41
1:Ac:227:LEU:HD12	1:Ac:228:ASN:H	1.85	0.41
1:Ae:87:VAL:HG13	1:Ae:91:MET:HE1	2.02	0.41
1:Ae:227:LEU:HD12	1:Ae:228:ASN:H	1.85	0.41
1:Ai:183:LYS:HD2	1:Ba:234:ARG:HH22	1.86	0.41
1:Ai:208:ILE:HD13	1:Ai:219:PRO:HG3	2.01	0.41
1:Ai:214:ASP:OD2	1:Ak:111:LYS:HE2	2.21	0.41
1:Am:168:TYR:CZ	1:Be:213:LEU:HD21	2.55	0.41
1:Ao:218:MET:HE2	1:Ao:218:MET:HB2	1.96	0.41
1:Ao:272:LEU:N	1:Bg:252:GLU:OE1	2.46	0.41
1:Aq:168:TYR:CZ	1:Bi:213:LEU:HD21	2.55	0.41
1:As:92:ARG:HE	1:As:92:ARG:HB2	1.72	0.41
1:As:219:PRO:O	1:As:222:GLY:N	2.51	0.41
1:Au:168:TYR:CZ	1:Bm:213:LEU:HD21	2.55	0.41
1:Au:183:LYS:HD2	1:Bm:234:ARG:HH22	1.86	0.41
1:Au:227:LEU:HD12	1:Au:228:ASN:H	1.85	0.41
1:Aw:87:VAL:HG13	1:Aw:91:MET:HE1	2.02	0.41
1:Bc:234:ARG:HG3	1:Bc:235:TYR:CD2	2.55	0.41
1:Be:115:ARG:NH1	1:Be:245:ARG:HH12	2.18	0.41
1:Be:183:LYS:HD2	1:Bw:234:ARG:HH22	1.86	0.41
1:Be:206:ALA:CB	1:Bg:91:MET:HE2	2.51	0.41
1:Bg:218:MET:HE2	1:Bg:218:MET:HB2	1.96	0.41
1:Bi:115:ARG:HH12	1:Bi:245:ARG:NH1	2.19	0.41
1:Bi:219:PRO:O	1:Bi:222:GLY:N	2.51	0.41
1:Bi:234:ARG:HG3	1:Bi:235:TYR:CD2	2.55	0.41
1:Bm:115:ARG:HH12	1:Bm:245:ARG:NH1	2.19	0.41
1:Bm:227:LEU:HD12	1:Bm:228:ASN:H	1.85	0.41
1:Bo:87:VAL:HG13	1:Bo:91:MET:HE1	2.02	0.41
1:Bq:115:ARG:NH1	1:Bq:245:ARG:HH12	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bu:115:ARG:NH1	1:Bu:245:ARG:HH12	2.18	0.41
1:Bw:87:VAL:HG13	1:Bw:91:MET:HE1	2.02	0.41
1:Bw:115:ARG:NH1	1:Bw:245:ARG:HH12	2.18	0.41
1:Bw:206:ALA:CB	1:By:91:MET:HE2	2.51	0.41
1:Bw:219:PRO:O	1:Bw:222:GLY:N	2.51	0.41
1:By:115:ARG:HH12	1:By:245:ARG:NH1	2.19	0.41
1:By:224:LEU:HD23	1:By:224:LEU:HA	1.81	0.41
1:Ce:227:LEU:HD12	1:Ce:228:ASN:H	1.85	0.41
1:Ci:210:MET:HE2	1:Ck:108:ILE:HA	2.03	0.41
1:Cm:219:PRO:O	1:Cm:222:GLY:N	2.51	0.41
1:Cs:115:ARG:HH12	1:Cs:245:ARG:NH1	2.19	0.41
1:Aa:115:ARG:NH1	1:Aa:245:ARG:HH12	2.18	0.41
1:Aa:284:GLU:HG3	1:Aa:285:ARG:N	2.37	0.41
1:Ag:291:VAL:O	1:Ai:296:HIS:CD2	2.74	0.41
1:Am:206:ALA:HB2	1:Ao:91:MET:HE2	2.02	0.41
1:Am:218:MET:HE2	1:Am:218:MET:HB2	1.96	0.41
1:Ao:115:ARG:HH12	1:Ao:245:ARG:NH1	2.19	0.41
1:Ao:284:GLU:HG3	1:Ao:285:ARG:N	2.36	0.41
1:Ay:227:LEU:HD12	1:Ay:228:ASN:H	1.85	0.41
1:Ba:115:ARG:HH12	1:Ba:245:ARG:NH1	2.19	0.41
1:Bc:283:THR:O	1:Ck:256:GLN:CD	2.64	0.41
1:Bg:219:PRO:O	1:Bg:222:GLY:N	2.51	0.41
1:Bi:227:LEU:HD12	1:Bi:228:ASN:H	1.85	0.41
1:Bi:284:GLU:HG3	1:Bi:285:ARG:N	2.37	0.41
1:Bk:206:ALA:CB	1:Bm:91:MET:HE2	2.51	0.41
1:Cc:214:ASP:OD2	1:Ce:111:LYS:HE2	2.20	0.41
1:Cg:115:ARG:NH1	1:Cg:245:ARG:HH12	2.18	0.41
1:Cg:224:LEU:HD23	1:Cg:224:LEU:HA	1.81	0.41
1:Co:218:MET:HE2	1:Co:218:MET:HB2	1.96	0.41
1:Cq:224:LEU:HA	1:Cq:224:LEU:HD23	1.81	0.41
1:Cq:234:ARG:HG3	1:Cq:235:TYR:CD2	2.55	0.41
1:Cs:92:ARG:HE	1:Cs:92:ARG:HB2	1.72	0.41
1:Aa:87:VAL:HG13	1:Aa:91:MET:HE1	2.02	0.40
1:Ac:121:ARG:HH11	1:Ac:121:ARG:HD2	1.77	0.40
1:Ae:115:ARG:NH1	1:Ae:245:ARG:HH12	2.18	0.40
1:Ae:224:LEU:HD23	1:Ae:224:LEU:HA	1.81	0.40
1:Ak:115:ARG:HH12	1:Ak:245:ARG:NH1	2.19	0.40
1:Ao:165:ILE:HG22	2:Ap:5:U:H1'	2.03	0.40
1:Aq:115:ARG:HH12	1:Aq:245:ARG:NH1	2.19	0.40
1:Au:206:ALA:HB2	1:Aw:91:MET:HE2	2.02	0.40
1:Au:269:MET:O	1:Bk:228:ASN:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:284:GLU:HG3	1:Au:285:ARG:N	2.37	0.40
1:Bg:115:ARG:NH1	1:Bg:245:ARG:HH12	2.18	0.40
1:Bg:284:GLU:HG3	1:Bg:285:ARG:N	2.36	0.40
1:Bi:84:LEU:H	1:Bi:84:LEU:HG	1.78	0.40
1:Bm:87:VAL:HG13	1:Bm:91:MET:HE1	2.02	0.40
1:Bm:206:ALA:HB2	1:Bo:91:MET:HE2	2.02	0.40
1:Bo:170:THR:CG2	1:Bo:177:GLN:HE21	2.32	0.40
1:Bu:284:GLU:HG3	1:Bu:285:ARG:N	2.36	0.40
1:Bw:168:TYR:CZ	1:Co:213:LEU:HD21	2.56	0.40
1:Ci:115:ARG:HH12	1:Ci:245:ARG:NH1	2.19	0.40
1:Co:284:GLU:HG3	1:Co:285:ARG:N	2.37	0.40
1:Cq:115:ARG:HH12	1:Cq:245:ARG:NH1	2.19	0.40
1:Ac:219:PRO:O	1:Ac:222:GLY:N	2.51	0.40
1:Am:284:GLU:HG3	1:Am:285:ARG:N	2.37	0.40
1:Ao:234:ARG:HG3	1:Ao:235:TYR:CD2	2.55	0.40
1:Aq:84:LEU:H	1:Aq:84:LEU:HG	1.78	0.40
1:Aq:183:LYS:HD2	1:Bi:234:ARG:HH22	1.86	0.40
1:Aq:284:GLU:HG3	1:Aq:285:ARG:N	2.36	0.40
1:Be:87:VAL:HG13	1:Be:91:MET:HE1	2.02	0.40
1:Bg:214:ASP:OD2	1:Bi:111:LYS:HE2	2.20	0.40
1:Bk:183:LYS:HD2	1:Cc:234:ARG:NH2	2.36	0.40
1:Bo:224:LEU:HA	1:Bo:224:LEU:HD23	1.81	0.40
1:Bq:146:ARG:NH1	1:Bs:100:ALA:O	2.54	0.40
1:Ca:115:ARG:HH12	1:Ca:245:ARG:NH1	2.19	0.40
1:Ca:284:GLU:HG3	1:Ca:285:ARG:N	2.36	0.40
1:Cc:284:GLU:HG3	1:Cc:285:ARG:N	2.37	0.40
1:Ce:115:ARG:NH1	1:Ce:245:ARG:HH12	2.18	0.40
1:Ce:158:GLU:OE1	1:Cg:114:GLN:HG3	2.20	0.40
1:Ci:121:ARG:HH11	1:Ci:121:ARG:HD2	1.77	0.40
1:Co:87:VAL:HG13	1:Co:91:MET:HE1	2.02	0.40
1:Cq:123:THR:N	1:Cq:126:GLN:OE1	2.52	0.40
1:Aa:183:LYS:HD2	1:As:234:ARG:HH22	1.86	0.40
1:Aa:206:ALA:HB2	1:Ac:91:MET:HE2	2.03	0.40
1:Ao:170:THR:CG2	1:Ao:177:GLN:HE21	2.32	0.40
1:Aw:206:ALA:HB2	1:Ay:91:MET:HE2	2.03	0.40
1:Be:123:THR:N	1:Be:126:GLN:OE1	2.52	0.40
1:Bi:87:VAL:HG13	1:Bi:91:MET:HE1	2.03	0.40
1:Bi:218:MET:HE2	1:Bi:218:MET:HB2	1.96	0.40
1:Bo:284:GLU:HG3	1:Bo:285:ARG:N	2.36	0.40
1:Bs:115:ARG:HH12	1:Bs:245:ARG:NH1	2.19	0.40
1:Cc:84:LEU:H	1:Cc:84:LEU:HG	1.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ce:87:VAL:HG13	1:Ce:91:MET:HE1	2.02	0.40
1:Ck:219:PRO:O	1:Ck:222:GLY:N	2.51	0.40
1:Co:115:ARG:HH12	1:Co:245:ARG:NH1	2.19	0.40
1:Cq:284:GLU:HG3	1:Cq:285:ARG:N	2.36	0.40
1:Ac:159:ASN:ND2	1:Ae:119:ASN:HB2	2.36	0.40
1:Ak:121:ARG:HH11	1:Ak:121:ARG:HD2	1.77	0.40
1:Ao:183:LYS:HD2	1:Bg:234:ARG:HH22	1.86	0.40
1:Aq:219:PRO:O	1:Aq:222:GLY:N	2.51	0.40
1:Au:286:HIS:HD2	1:Bm:270:PHE:O	2.04	0.40
1:Ba:284:GLU:HG3	1:Ba:285:ARG:N	2.36	0.40
1:Bg:115:ARG:HH12	1:Bg:245:ARG:NH1	2.19	0.40
1:Bg:227:LEU:HD12	1:Bg:228:ASN:H	1.85	0.40
1:Bk:115:ARG:HH12	1:Bk:245:ARG:NH1	2.19	0.40
1:Bk:227:LEU:HD12	1:Bk:228:ASN:H	1.85	0.40
1:Bo:104:LEU:HD23	1:Bo:104:LEU:HA	1.80	0.40
1:Ca:87:VAL:HG13	1:Ca:91:MET:HE1	2.03	0.40
1:Ca:104:LEU:HA	1:Ca:104:LEU:HD23	1.80	0.40
1:Cc:87:VAL:HG13	1:Cc:91:MET:HE1	2.02	0.40
1:Cc:121:ARG:HH11	1:Cc:121:ARG:HD2	1.77	0.40
1:Cm:115:ARG:HH12	1:Cm:245:ARG:NH1	2.19	0.40
1:Co:206:ALA:HB2	1:Cq:91:MET:HE2	2.02	0.40
1:Aa:115:ARG:HH12	1:Aa:245:ARG:NH1	2.19	0.40
1:Aa:227:LEU:HD12	1:Aa:228:ASN:H	1.85	0.40
1:Ag:284:GLU:HG3	1:Ag:285:ARG:N	2.36	0.40
1:As:284:GLU:HG3	1:As:285:ARG:N	2.37	0.40
1:Aw:123:THR:N	1:Aw:126:GLN:OE1	2.52	0.40
1:Aw:227:LEU:HD12	1:Aw:228:ASN:H	1.85	0.40
1:Ay:183:LYS:HD2	1:Bq:234:ARG:HH22	1.86	0.40
1:Ay:206:ALA:CB	1:Ba:91:MET:CE	3.00	0.40
1:Bc:284:GLU:HG3	1:Bc:285:ARG:N	2.36	0.40
1:Be:115:ARG:HH12	1:Be:245:ARG:NH1	2.19	0.40
1:Bi:159:ASN:ND2	1:Bk:119:ASN:HB2	2.36	0.40
1:Bk:284:GLU:HG3	1:Bk:285:ARG:N	2.36	0.40
2:Bp:5:U:O3'	2:Br:1:U:H5'	2.22	0.40
1:Bw:284:GLU:HG3	1:Bw:285:ARG:N	2.37	0.40
1:Ca:227:LEU:HD12	1:Ca:228:ASN:H	1.85	0.40
1:Cg:224:LEU:HD11	2:Cj:1:U:OP2	2.21	0.40
1:Ci:104:LEU:HD23	1:Ci:104:LEU:HA	1.80	0.40
1:Ci:284:GLU:HG3	1:Ci:285:ARG:N	2.37	0.40
1:Cm:214:ASP:OD2	1:Co:111:LYS:HE2	2.21	0.40
1:Cs:121:ARG:HH11	1:Cs:121:ARG:HD2	1.77	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	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ac	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ae	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ag	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ai	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ak	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Am	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ao	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Aq	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	As	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Au	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Aw	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ay	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ba	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bc	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Be	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bg	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bi	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bk	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bm	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bo	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bq	222/303 (73%)	216 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Bs	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bu	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Bw	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	By	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ca	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Cc	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ce	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Cg	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ci	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Ck	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Cm	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Co	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Cq	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
1	Cs	222/303 (73%)	216 (97%)	6 (3%)	0	100	100
All	All	7992/10908 (73%)	7776 (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	196/253 (78%)	196 (100%)	0	100	100
1	Ac	196/253 (78%)	196 (100%)	0	100	100
1	Ae	196/253 (78%)	196 (100%)	0	100	100
1	Ag	196/253 (78%)	196 (100%)	0	100	100
1	Ai	196/253 (78%)	196 (100%)	0	100	100
1	Ak	196/253 (78%)	196 (100%)	0	100	100
1	Am	196/253 (78%)	196 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ao	196/253 (78%)	196 (100%)	0	100	100
1	Aq	196/253 (78%)	196 (100%)	0	100	100
1	As	196/253 (78%)	196 (100%)	0	100	100
1	Au	196/253 (78%)	196 (100%)	0	100	100
1	Aw	196/253 (78%)	196 (100%)	0	100	100
1	Ay	196/253 (78%)	196 (100%)	0	100	100
1	Ba	196/253 (78%)	196 (100%)	0	100	100
1	Bc	196/253 (78%)	196 (100%)	0	100	100
1	Be	196/253 (78%)	196 (100%)	0	100	100
1	Bg	196/253 (78%)	196 (100%)	0	100	100
1	Bi	196/253 (78%)	196 (100%)	0	100	100
1	Bk	196/253 (78%)	196 (100%)	0	100	100
1	Bm	196/253 (78%)	196 (100%)	0	100	100
1	Bo	196/253 (78%)	196 (100%)	0	100	100
1	Bq	196/253 (78%)	196 (100%)	0	100	100
1	Bs	196/253 (78%)	196 (100%)	0	100	100
1	Bu	196/253 (78%)	196 (100%)	0	100	100
1	Bw	196/253 (78%)	196 (100%)	0	100	100
1	By	196/253 (78%)	196 (100%)	0	100	100
1	Ca	196/253 (78%)	196 (100%)	0	100	100
1	Cc	196/253 (78%)	196 (100%)	0	100	100
1	Ce	196/253 (78%)	196 (100%)	0	100	100
1	Cg	196/253 (78%)	196 (100%)	0	100	100
1	Ci	196/253 (78%)	196 (100%)	0	100	100
1	Ck	196/253 (78%)	196 (100%)	0	100	100
1	Cm	196/253 (78%)	196 (100%)	0	100	100
1	Co	196/253 (78%)	196 (100%)	0	100	100
1	Cq	196/253 (78%)	196 (100%)	0	100	100
1	Cs	196/253 (78%)	196 (100%)	0	100	100
All	All	7056/9108 (78%)	7056 (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 (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	144	GLN
1	Aa	275	ASN
1	Ac	144	GLN
1	Ae	144	GLN
1	Ag	144	GLN
1	Ag	195	GLN
1	Ai	144	GLN
1	Ai	275	ASN
1	Ak	144	GLN
1	Am	144	GLN
1	Am	195	GLN
1	Am	275	ASN
1	Ao	144	GLN
1	Ao	275	ASN
1	Aq	144	GLN
1	Aq	256	GLN
1	Aq	275	ASN
1	As	144	GLN
1	As	195	GLN
1	As	256	GLN
1	Au	144	GLN
1	Au	256	GLN
1	Aw	144	GLN
1	Aw	256	GLN
1	Ay	144	GLN
1	Ay	256	GLN
1	Ba	144	GLN
1	Ba	256	GLN
1	Bc	144	GLN
1	Bc	256	GLN
1	Be	144	GLN
1	Be	256	GLN
1	Be	275	ASN
1	Bg	144	GLN
1	Bg	256	GLN
1	Bi	144	GLN
1	Bi	256	GLN
1	Bk	144	GLN
1	Bk	195	GLN
1	Bk	256	GLN
1	Bk	275	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bm	144	GLN
1	Bm	275	ASN
1	Bo	144	GLN
1	Bo	256	GLN
1	Bq	144	GLN
1	Bq	195	GLN
1	Bq	256	GLN
1	Bs	144	GLN
1	Bs	275	ASN
1	Bu	144	GLN
1	Bw	144	GLN
1	Bw	195	GLN
1	Bw	256	GLN
1	Bw	275	ASN
1	By	144	GLN
1	By	256	GLN
1	By	275	ASN
1	Ca	144	GLN
1	Ca	256	GLN
1	Ca	275	ASN
1	Cc	144	GLN
1	Cc	256	GLN
1	Ce	144	GLN
1	Ce	256	GLN
1	Cg	144	GLN
1	Ci	144	GLN
1	Ck	144	GLN
1	Ck	256	GLN
1	Cm	144	GLN
1	Co	144	GLN
1	Co	256	GLN
1	Cq	144	GLN
1	Cq	256	GLN
1	Cs	144	GLN
1	Cs	177	GLN
1	Cs	195	GLN
1	Cs	256	GLN

5.3.3 RNA ⓘ

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Ab	4/5 (80%)	0	0
2	Ad	4/5 (80%)	0	0
2	Af	4/5 (80%)	0	0
2	Ah	4/5 (80%)	0	0
2	Aj	4/5 (80%)	0	0
2	Al	4/5 (80%)	0	0
2	An	4/5 (80%)	0	0
2	Ap	4/5 (80%)	0	0
2	Ar	4/5 (80%)	0	0
2	At	4/5 (80%)	0	0
2	Av	4/5 (80%)	0	0
2	Ax	4/5 (80%)	0	0
2	Az	4/5 (80%)	0	0
2	Bb	4/5 (80%)	0	0
2	Bd	4/5 (80%)	0	0
2	Bf	4/5 (80%)	0	0
2	Bh	4/5 (80%)	0	0
2	Bj	4/5 (80%)	0	0
2	Bl	4/5 (80%)	0	0
2	Bn	4/5 (80%)	0	0
2	Bp	4/5 (80%)	0	0
2	Br	4/5 (80%)	0	0
2	Bt	4/5 (80%)	0	0
2	Bv	4/5 (80%)	0	0
2	Bx	4/5 (80%)	0	0
2	Bz	4/5 (80%)	0	0
2	Cb	4/5 (80%)	0	0
2	Cd	4/5 (80%)	0	0
2	Cf	4/5 (80%)	0	0
2	Ch	4/5 (80%)	0	0
2	Cj	4/5 (80%)	0	0
2	Cl	4/5 (80%)	0	0
2	Cn	4/5 (80%)	0	0
2	Cp	4/5 (80%)	0	0
2	Cr	4/5 (80%)	0	0
2	Ct	4/5 (80%)	0	0
All	All	144/180 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

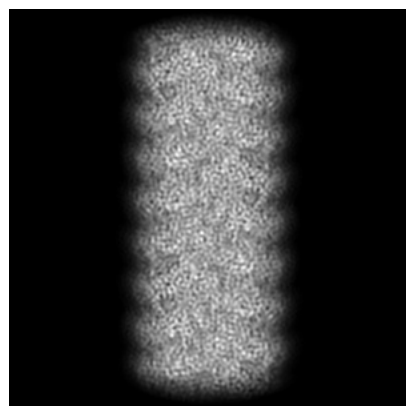
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53865. These allow visual inspection of the internal detail of the map and identification of artifacts.

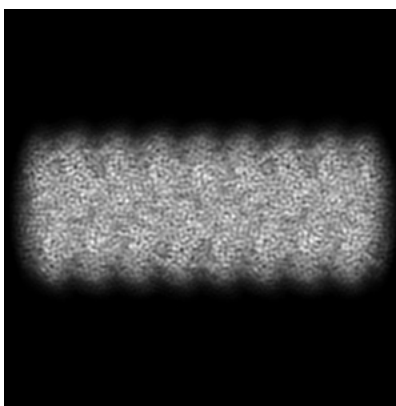
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

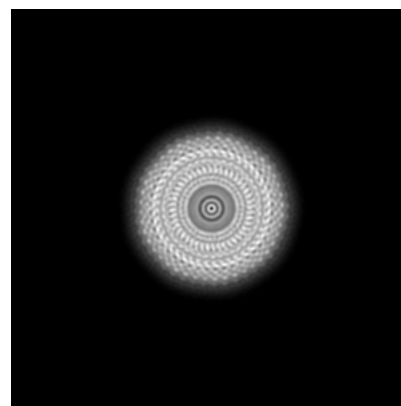
6.1.1 Primary map



X

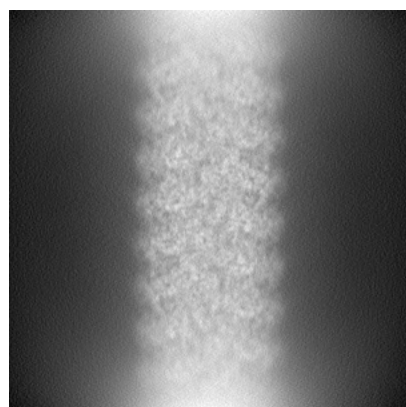


Y

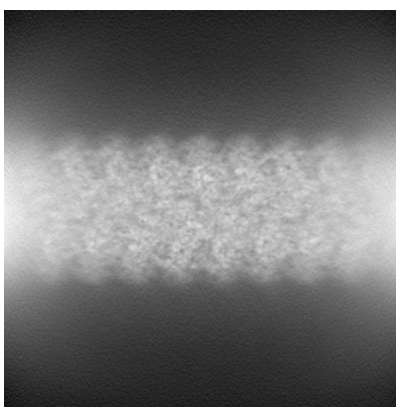


Z

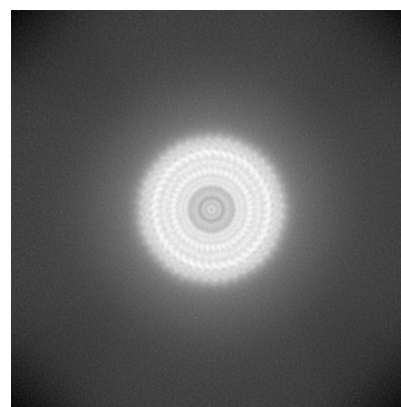
6.1.2 Raw map



X



Y

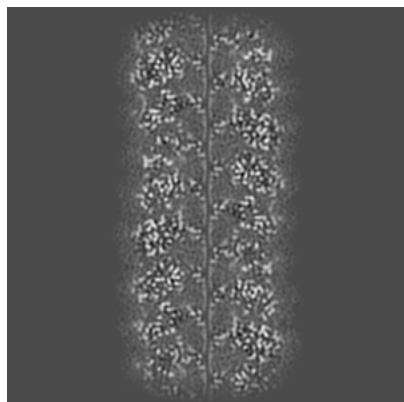


Z

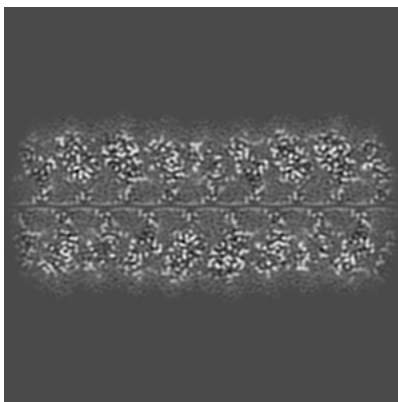
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

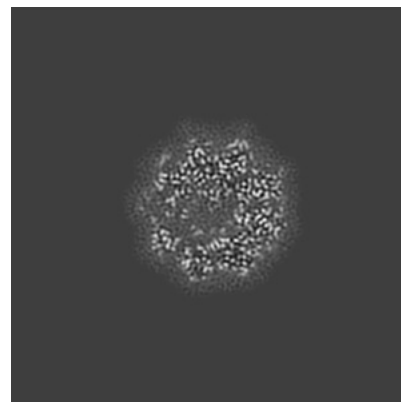
6.2.1 Primary map



X Index: 175

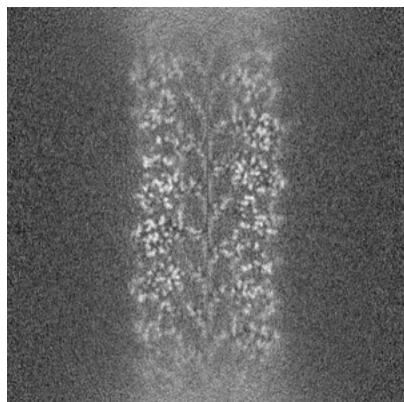


Y Index: 175

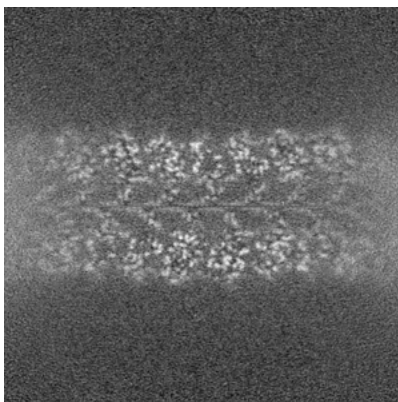


Z Index: 175

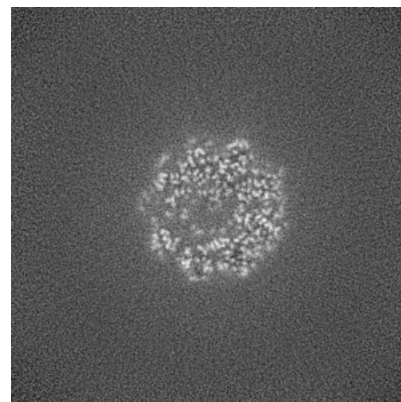
6.2.2 Raw map



X Index: 175



Y Index: 175

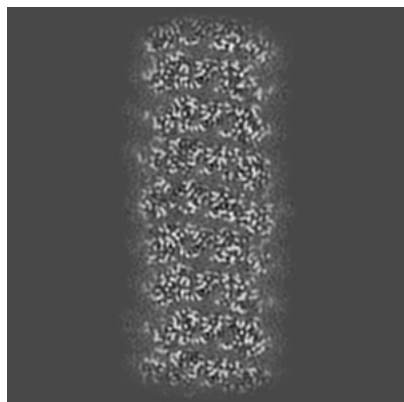


Z Index: 175

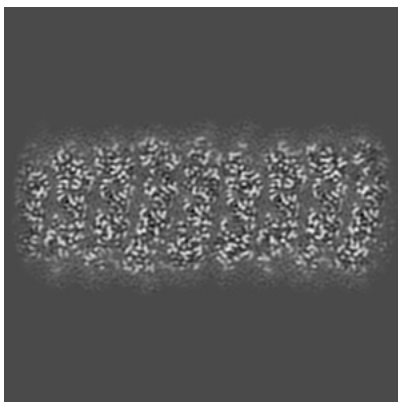
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

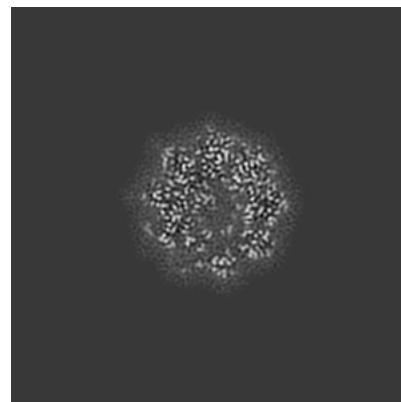
6.3.1 Primary map



X Index: 205

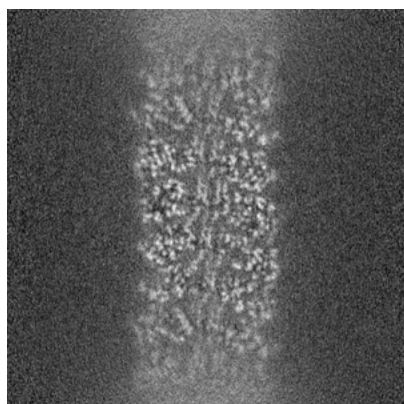


Y Index: 205

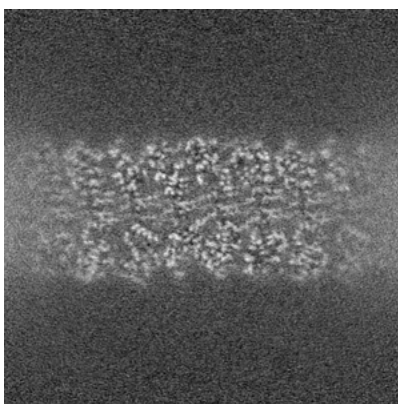


Z Index: 242

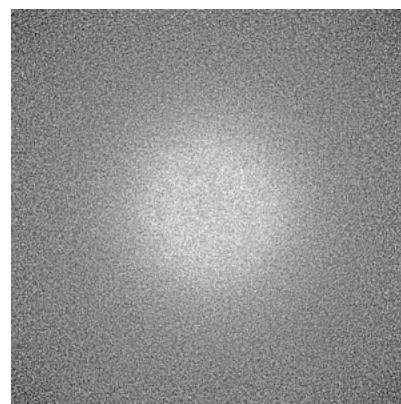
6.3.2 Raw map



X Index: 197



Y Index: 153

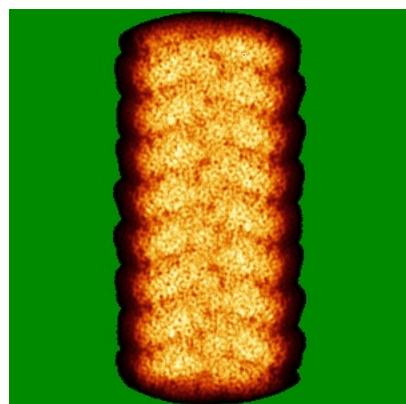


Z Index: 0

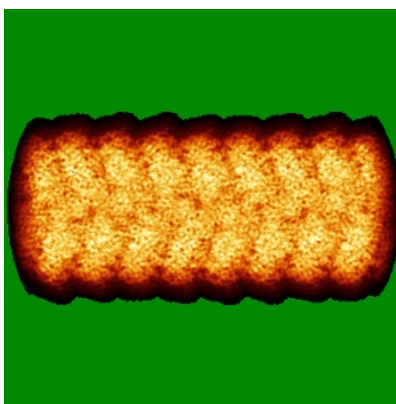
The images above show the largest variance slices of the map in three orthogonal directions.

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

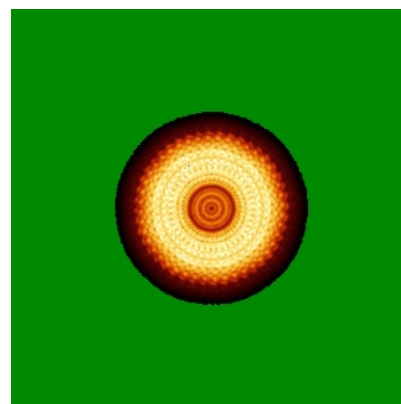
6.4.1 Primary map



X

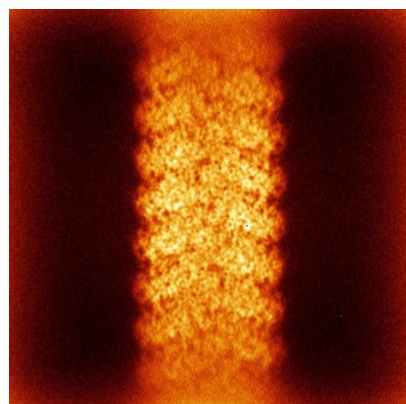


Y

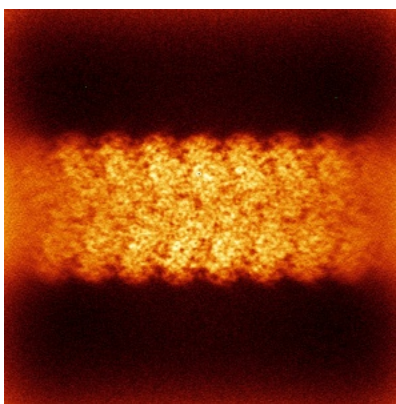


Z

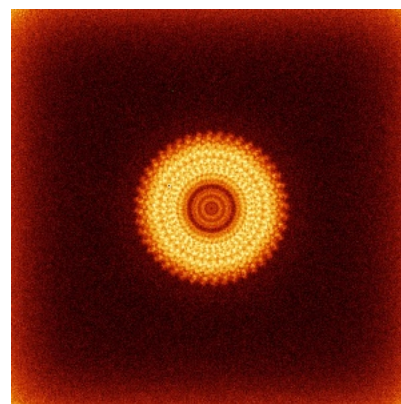
6.4.2 Raw map



X



Y

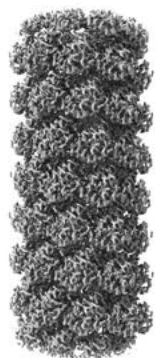


Z

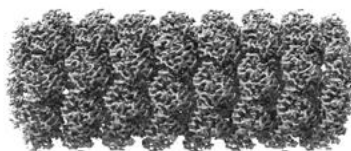
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



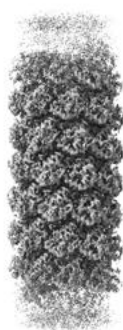
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.34. 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.

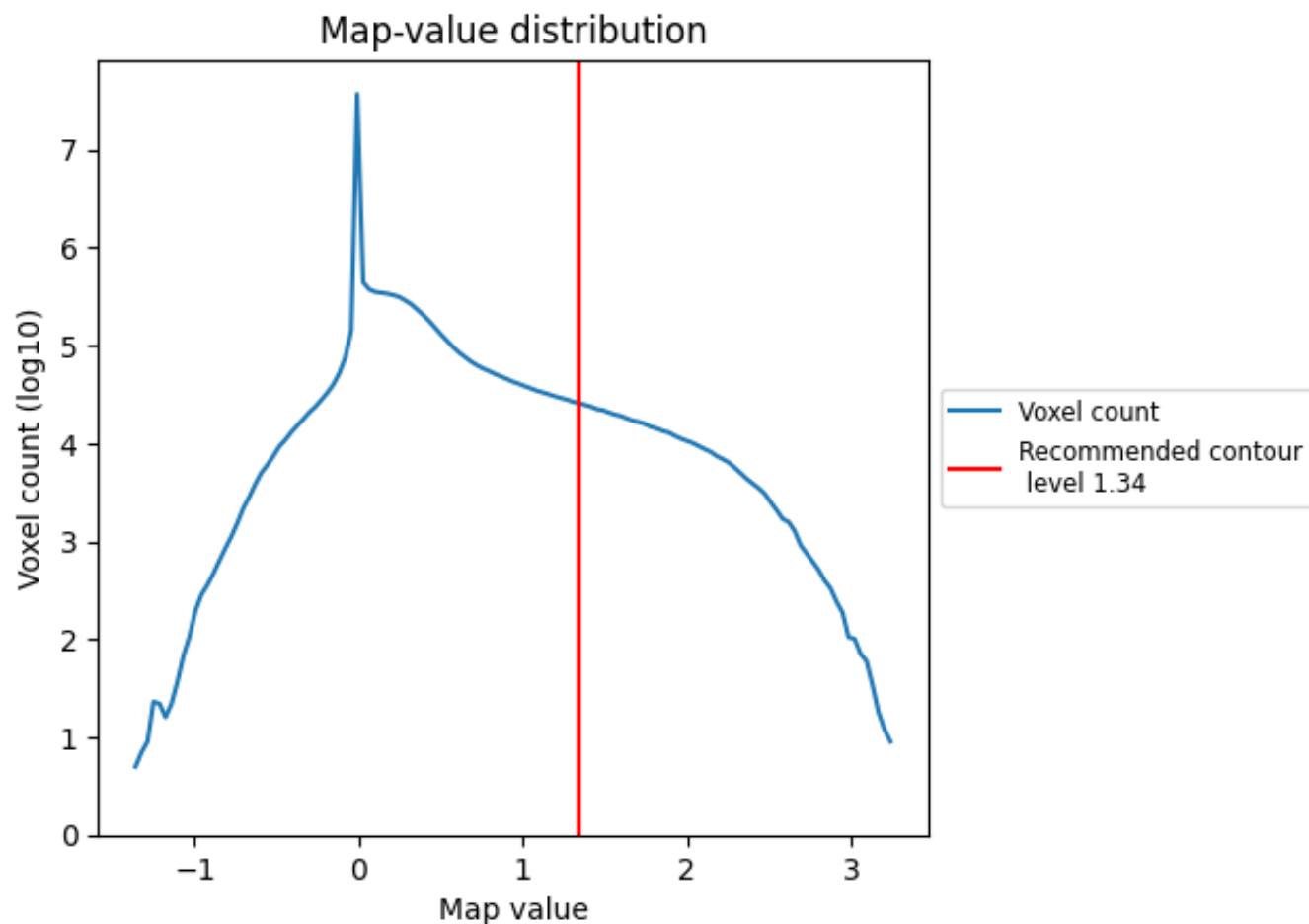
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

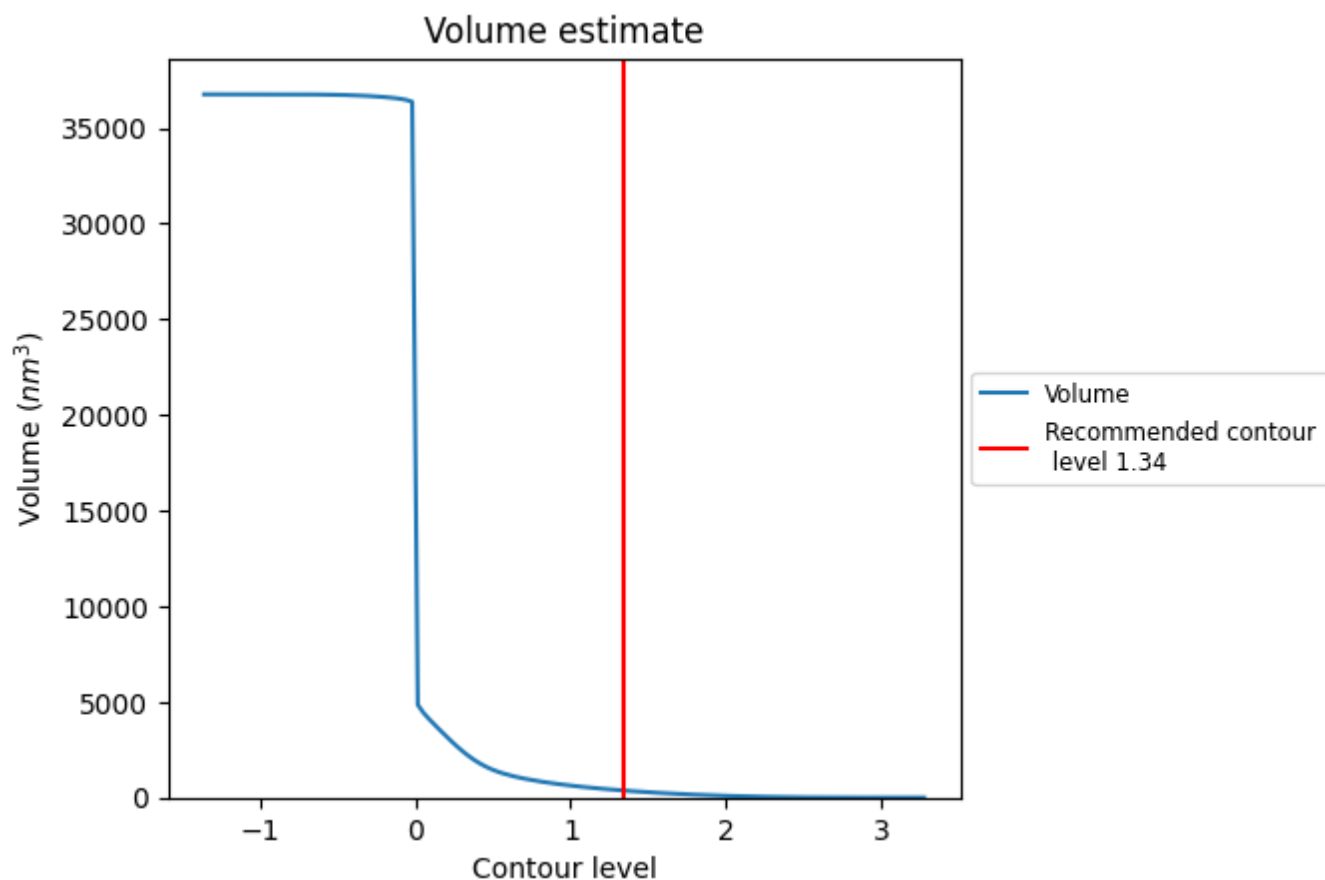
This section contains the results of statistical analysis of the map.

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.

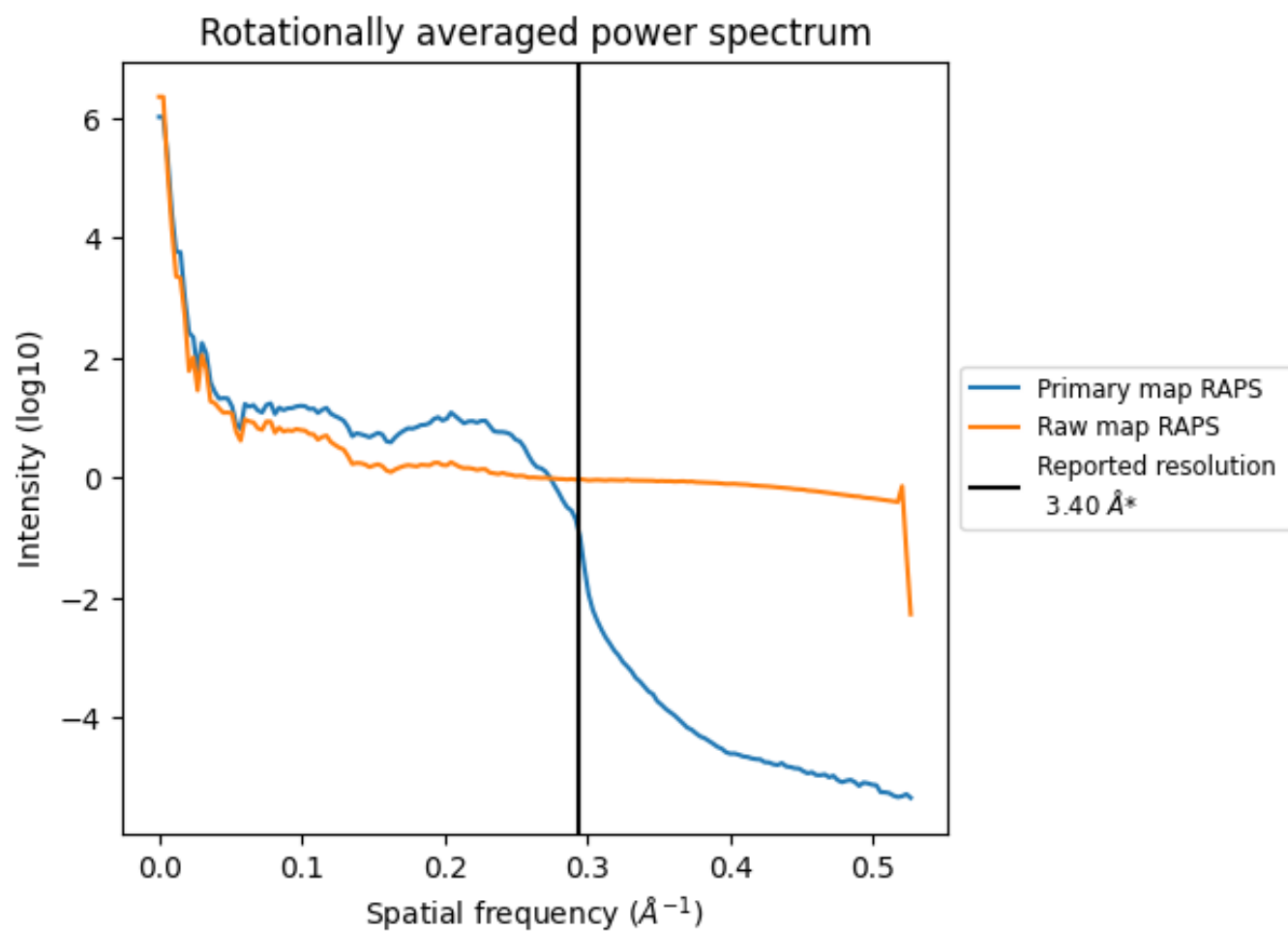
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 369 nm³; this corresponds to an approximate mass of 334 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

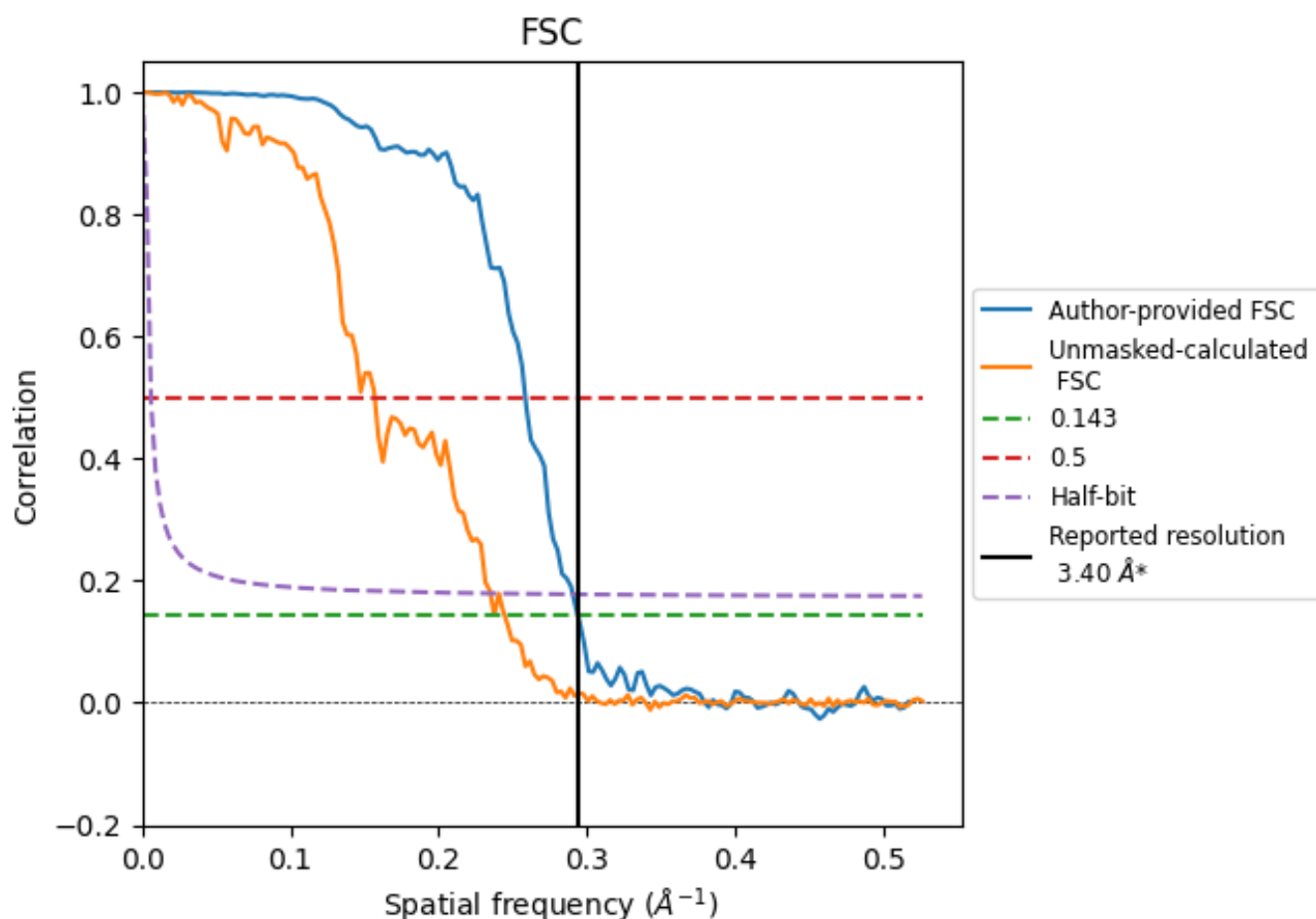


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

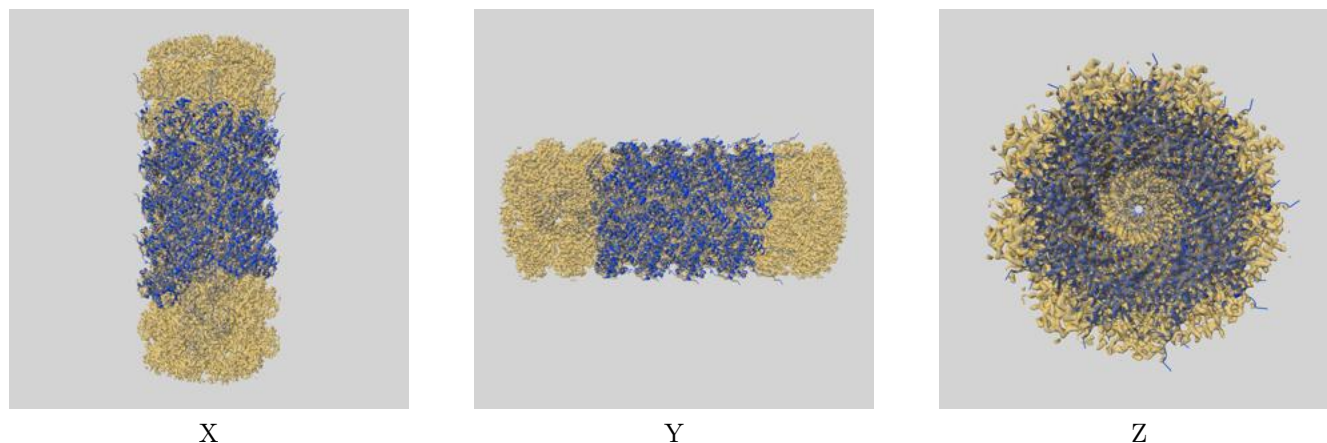
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.40	3.87	3.44
Unmasked-calculated*	4.09	6.37	4.26

*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 4.09 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

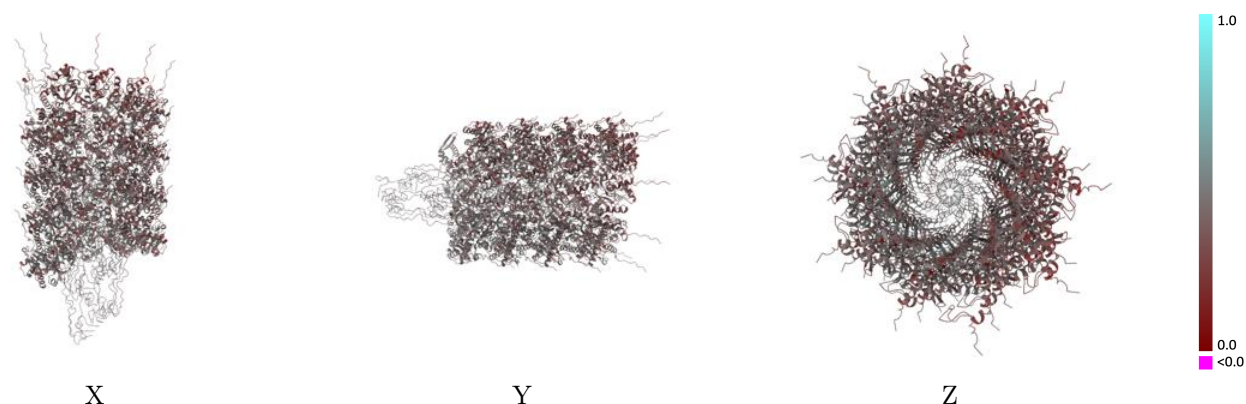
This section contains information regarding the fit between EMDB map EMD-53865 and PDB model 9R9Z. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



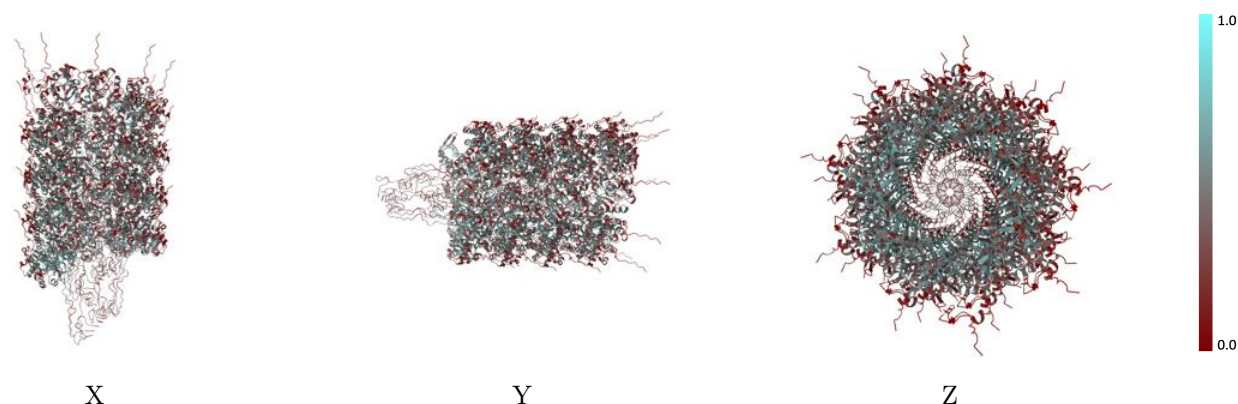
The images above show the 3D surface view of the map at the recommended contour level 1.34 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



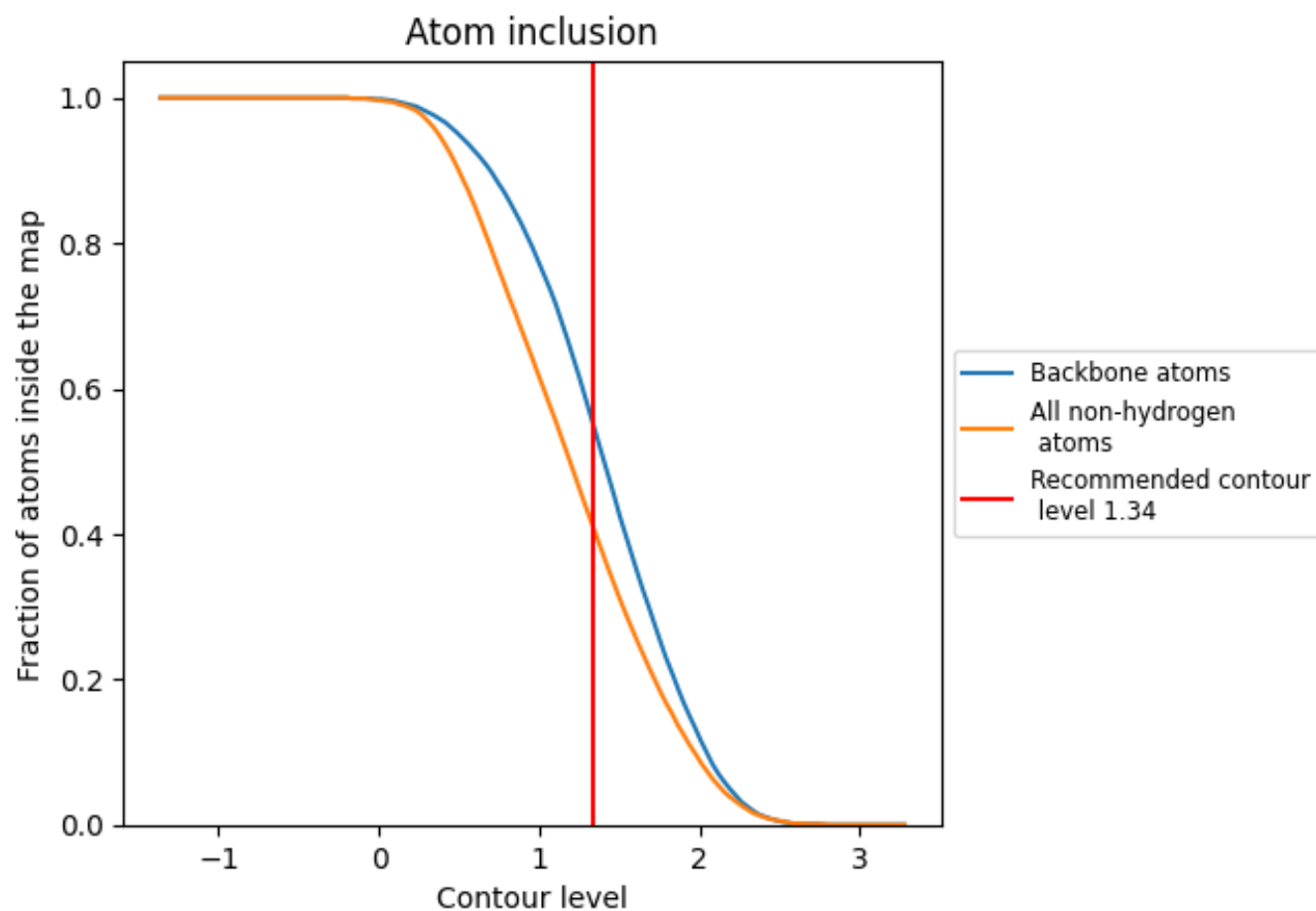
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.34).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 41% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.34) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4070	 0.4010
Aa	 0.3690	 0.3610
Ab	 0.5800	 0.3530
Ac	 0.3530	 0.3490
Ad	 0.6600	 0.4300
Ae	 0.3400	 0.3380
Af	 0.6700	 0.4740
Ag	 0.3590	 0.3580
Ah	 0.6200	 0.4470
Ai	 0.3660	 0.3740
Aj	 0.6600	 0.4470
Ak	 0.3840	 0.3950
Al	 0.6700	 0.4750
Am	 0.4000	 0.4030
An	 0.6100	 0.4420
Ao	 0.3990	 0.3980
Ap	 0.5300	 0.4010
Aq	 0.3910	 0.3920
Ar	 0.5800	 0.3760
As	 0.3790	 0.3800
At	 0.6200	 0.4060
Au	 0.3630	 0.3640
Av	 0.6900	 0.4740
Aw	 0.3580	 0.3660
Ax	 0.6800	 0.4930
Ay	 0.3690	 0.3790
Az	 0.5900	 0.4140
Ba	 0.3970	 0.4050
Bb	 0.6700	 0.4560
Bc	 0.4050	 0.4140
Bd	 0.6500	 0.4560
Be	 0.4180	 0.4210
Bf	 0.6100	 0.4370
Bg	 0.4140	 0.4160
Bh	 0.6100	 0.4210



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bi	 0.4050	 0.4060
Bj	 0.6300	 0.4170
Bk	 0.3790	 0.3860
Bl	 0.6300	 0.4000
Bm	 0.3710	 0.3790
Bn	 0.6900	 0.4930
Bo	 0.3750	 0.3820
Bp	 0.6800	 0.5050
Bq	 0.3960	 0.3950
Br	 0.6000	 0.4180
Bs	 0.4010	 0.4120
Bt	 0.6300	 0.4370
Bu	 0.4220	 0.4310
Bv	 0.6600	 0.4560
Bw	 0.4290	 0.4390
Bx	 0.6700	 0.4580
By	 0.4310	 0.4330
Bz	 0.6500	 0.4430
Ca	 0.4150	 0.4190
Cb	 0.6600	 0.4260
Cc	 0.3860	 0.3980
Cd	 0.6400	 0.4420
Ce	 0.3760	 0.3860
Cf	 0.6900	 0.4970
Cg	 0.3700	 0.3730
Ch	 0.6100	 0.4600
Ci	 0.4090	 0.4080
Cj	 0.6200	 0.4310
Ck	 0.4140	 0.4300
Cl	 0.6600	 0.4600
Cm	 0.4350	 0.4430
Cn	 0.6700	 0.4660
Co	 0.4420	 0.4480
Cp	 0.6100	 0.4540
Cq	 0.4320	 0.4390
Cr	 0.6500	 0.4400
Cs	 0.4220	 0.4220
Ct	 0.5700	 0.3700