



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 02:07 PM UTC

PDB ID : 8OPC / pdb_00008opc
EMDB ID : EMD-17048
Title : Virus-like Particle based on PVY coat protein with helical architecture encapsidating ssRNA
Authors : Kavcic, L.; Kezar, A.; Podobnik, M.
Deposited on : 2023-04-07
Resolution : 2.99 Å(reported)
Based on initial model : 6HXZ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

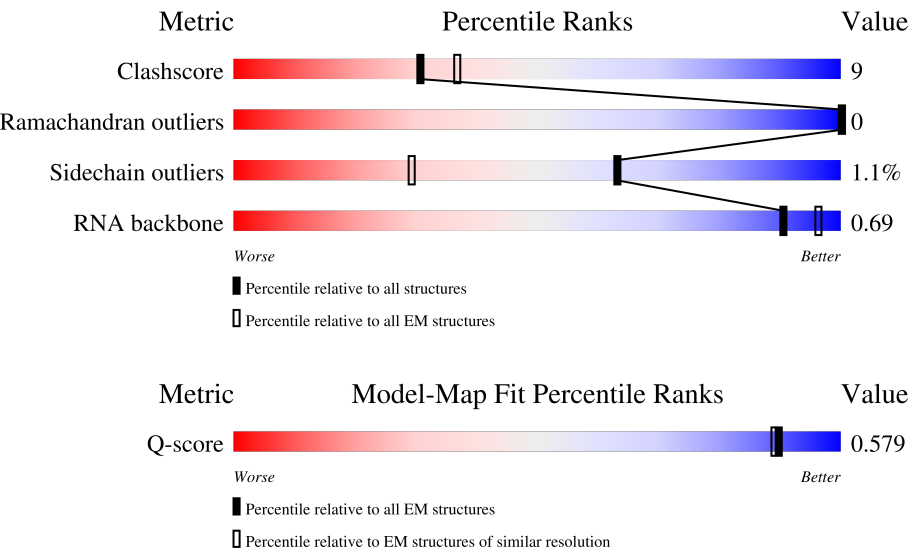
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.99 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.



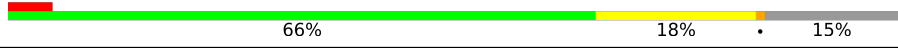
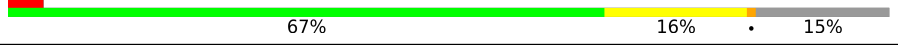
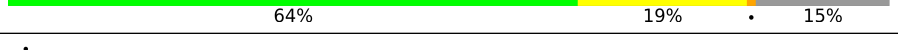
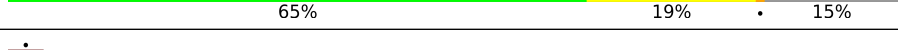
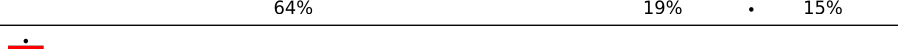
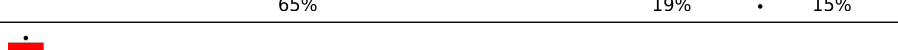
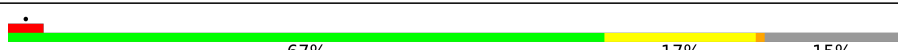
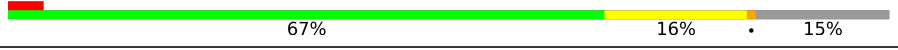
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13287 (2.49 - 3.49)

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	267	65%19%15%
1	Ac	267	62%21%15%
1	Ae	267	65%19%15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Ag	267	
1	Ai	267	
1	Ak	267	
1	Am	267	
1	Ao	267	
1	Aq	267	
1	As	267	
1	Au	267	
1	Aw	267	
1	Ay	267	
1	Ba	267	
1	Bc	267	
1	Be	267	
1	Bg	267	
1	Bi	267	
1	Bk	267	
1	Bm	267	
1	Bo	267	
1	Bq	267	
1	Bs	267	
1	Bu	267	
1	Bw	267	
1	By	267	
1	Ca	267	
1	Cc	267	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
2	Bj	5	
2	Bl	5	
2	Bn	5	
2	Bp	5	
2	Br	5	
2	Bt	5	
2	Bv	5	
2	Bx	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	Bz	5	 60% 40%
2	Cb	5	 60% 40%
2	Cd	5	 60% 40%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 53088 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 (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ac	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ae	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ag	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ai	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ak	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Am	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ao	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Aq	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	As	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Au	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Aw	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ay	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ba	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bc	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Be	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bg	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Bi	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bk	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bm	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bo	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bq	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bs	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bu	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Bw	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	By	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Ca	226	Total	C	N	O	S	0	0
			1796	1125	315	342	14		
1	Cc	226	Total	C	N	O	S	0	0
			1796	1125	315	342	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	C	N	O	P	0	0
			100	45	10	40	5		
2	Ad	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Af	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Ah	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Aj	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Al	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	An	5	Total	C	N	O	P	0	0
			100	45	10	40	5		
2	Ap	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

Continued on next page...

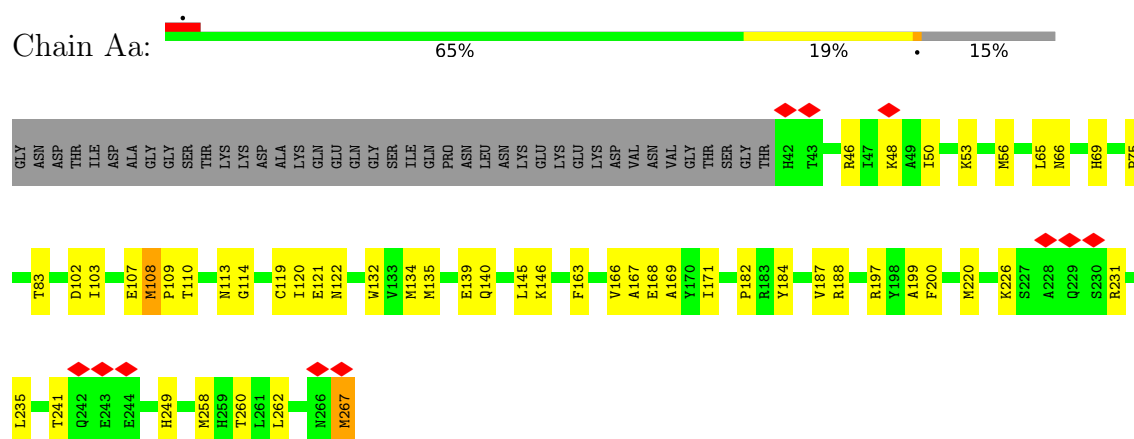
Continued from previous page...

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

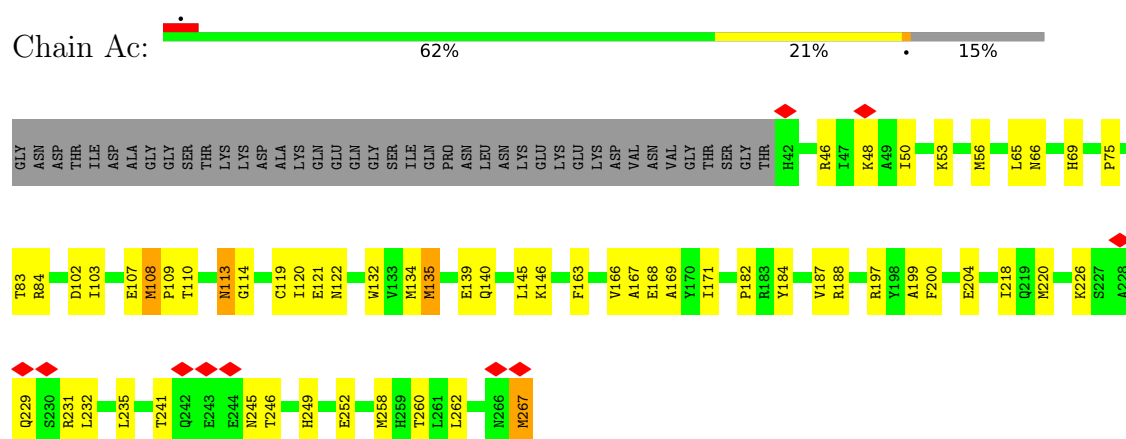
3 Residue-property plots

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.

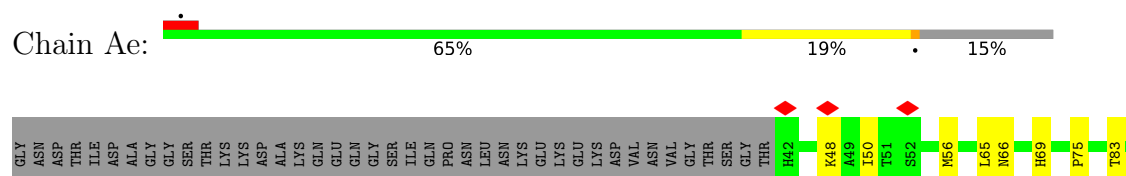
- Molecule 1: Genome polyprotein (Fragment)



- Molecule 1: Genome polyprotein (Fragment)

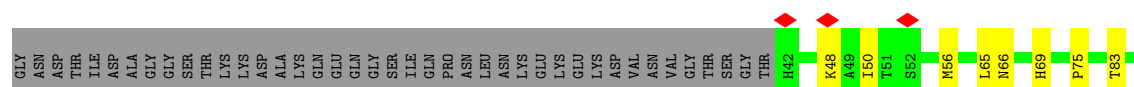


- Molecule 1: Genome polyprotein (Fragment)

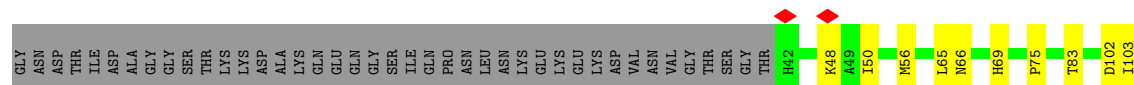




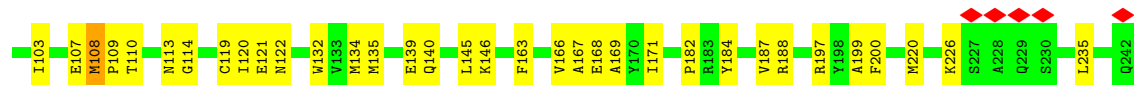
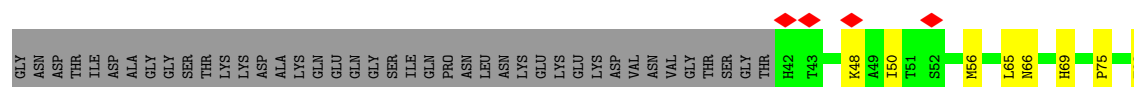
• Molecule 1: Genome polyprotein (Fragment)

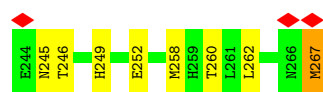


• Molecule 1: Genome polyprotein (Fragment)



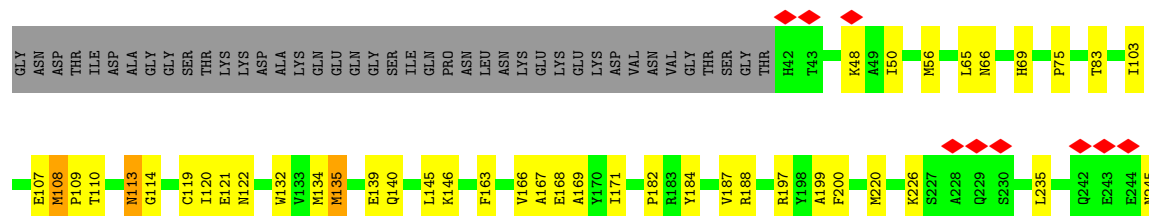
• Molecule 1: Genome polyprotein (Fragment)





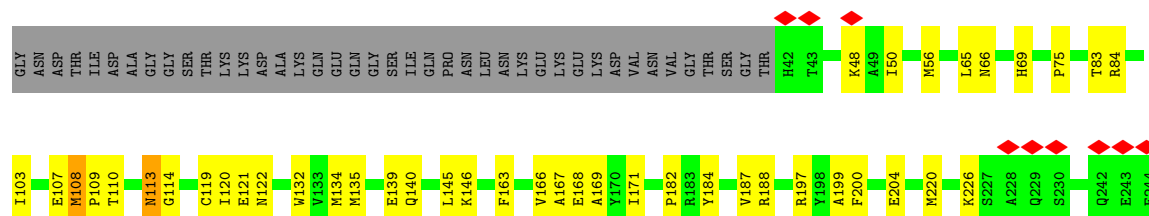
• Molecule 1: Genome polyprotein (Fragment)

Chain Am: 67% 16% 15%



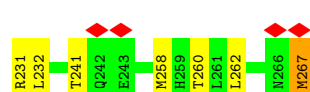
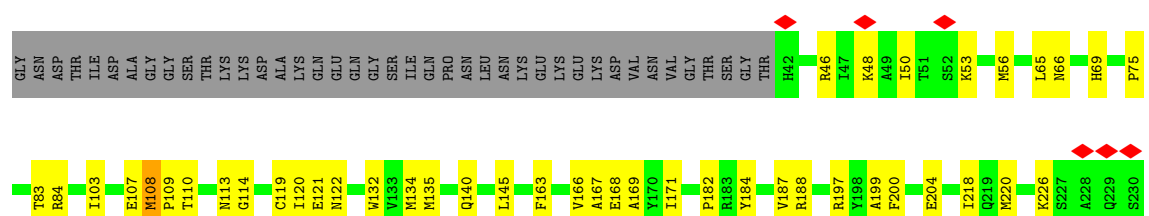
• Molecule 1: Genome polyprotein (Fragment)

Chain Ao: 66% 17% 15%



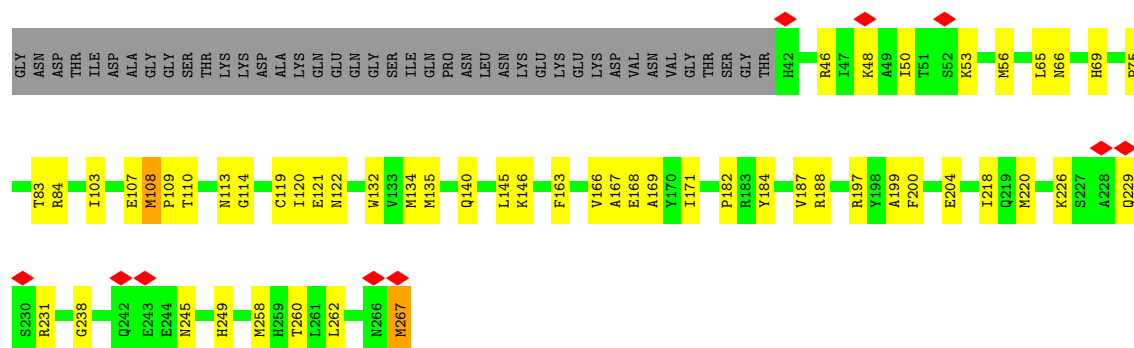
• Molecule 1: Genome polyprotein (Fragment)

Chain Aq: 66% 18% 15%



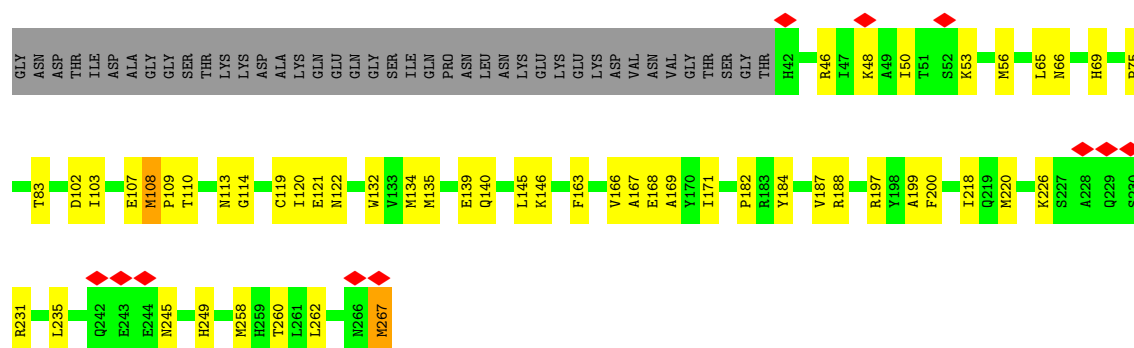
• Molecule 1: Genome polyprotein (Fragment)

Chain As: 



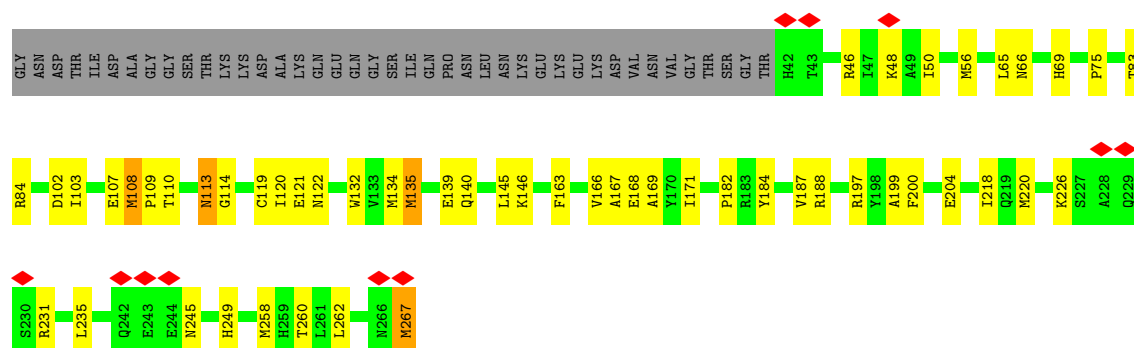
• Molecule 1: Genome polypeptide (Fragment)

Chain Au: 



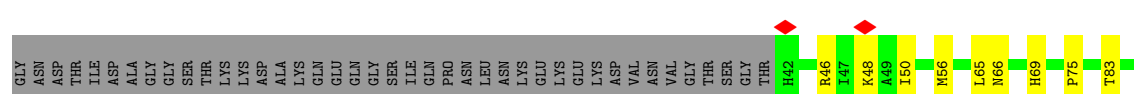
• Molecule 1: Genome polypeptide (Fragment)

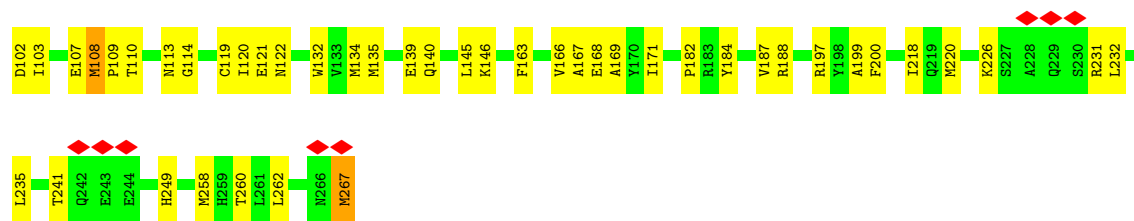
Chain Aw: 



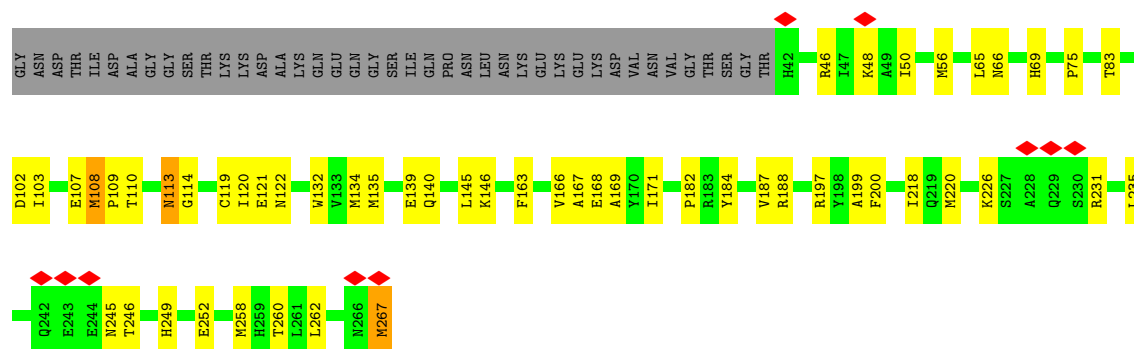
• Molecule 1: Genome polypeptide (Fragment)

Chain Ay: 

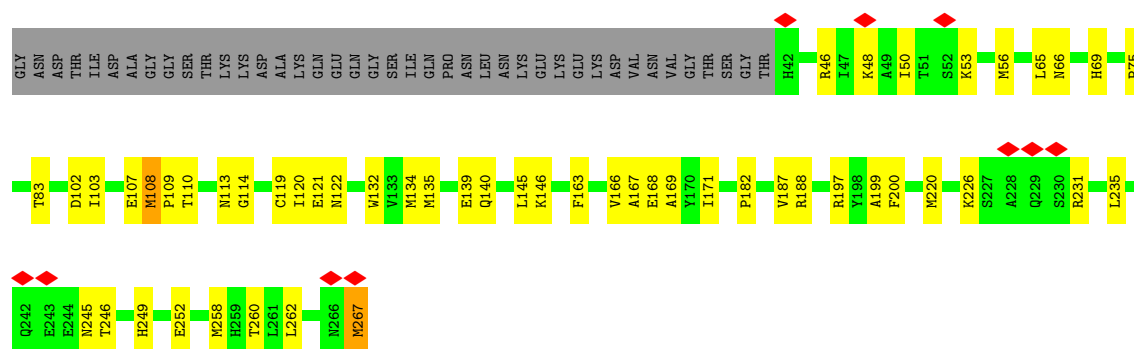




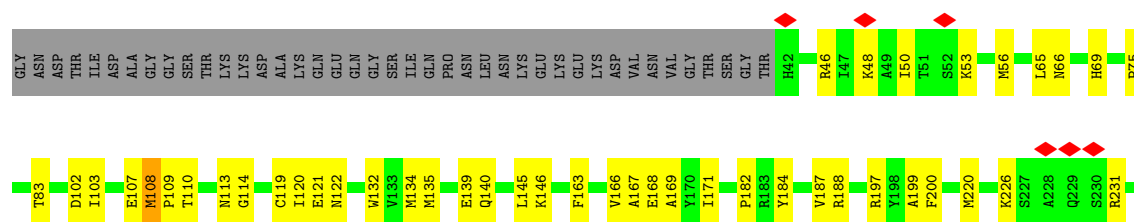
• Molecule 1: Genome polyprotein (Fragment)



• Molecule 1: Genome polyprotein (Fragment)

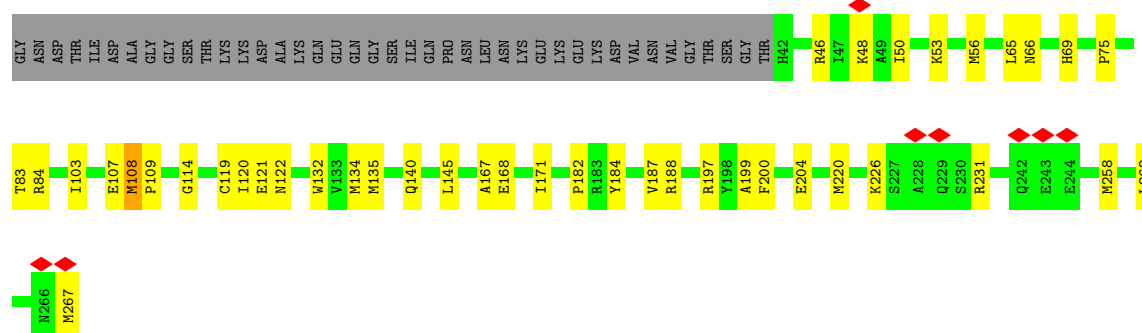


• Molecule 1: Genome polyprotein (Fragment)

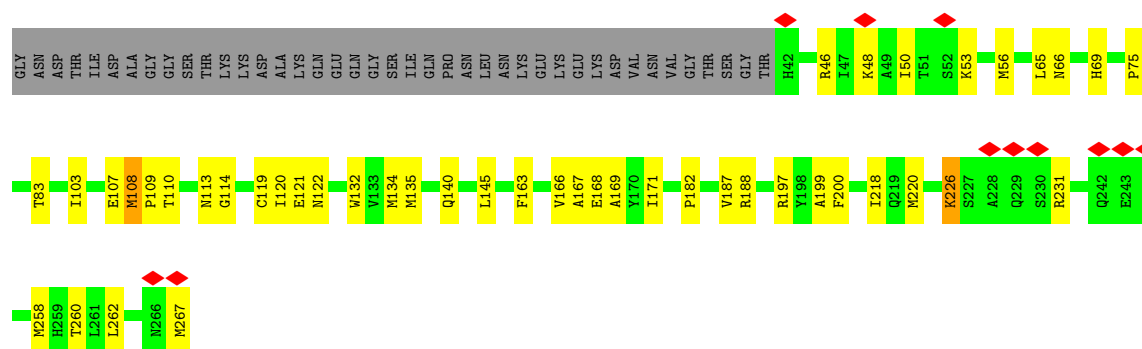




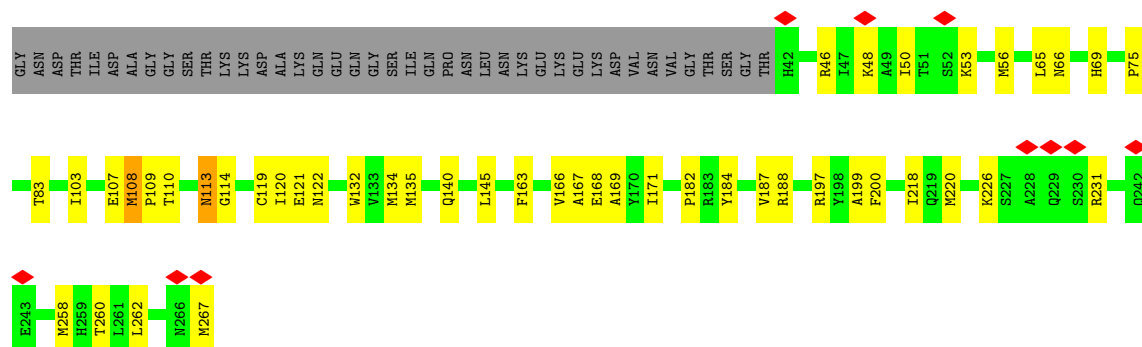
- Molecule 1: Genome polyprotein (Fragment)



- Molecule 1: Genome polyprotein (Fragment)

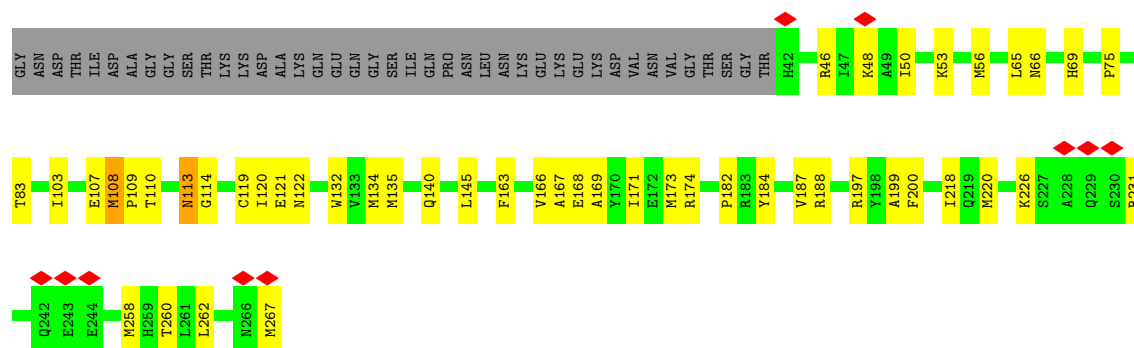


- Molecule 1: Genome polyprotein (Fragment)



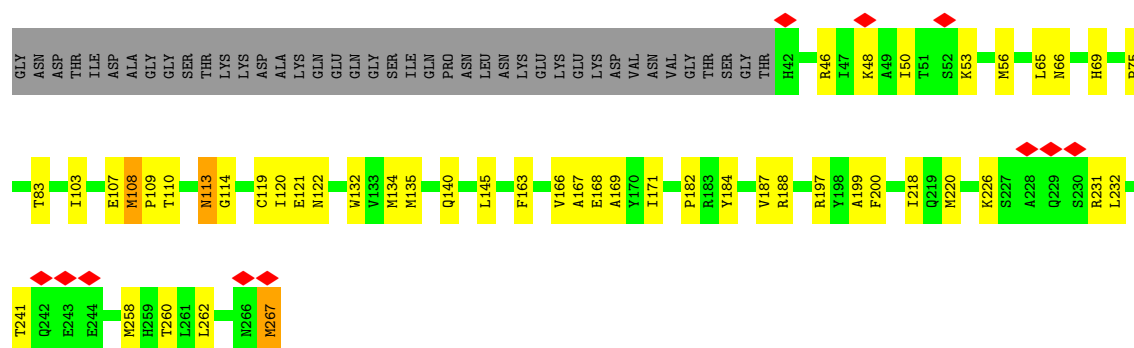
- Molecule 1: Genome polyprotein (Fragment)

Chain Bm: 



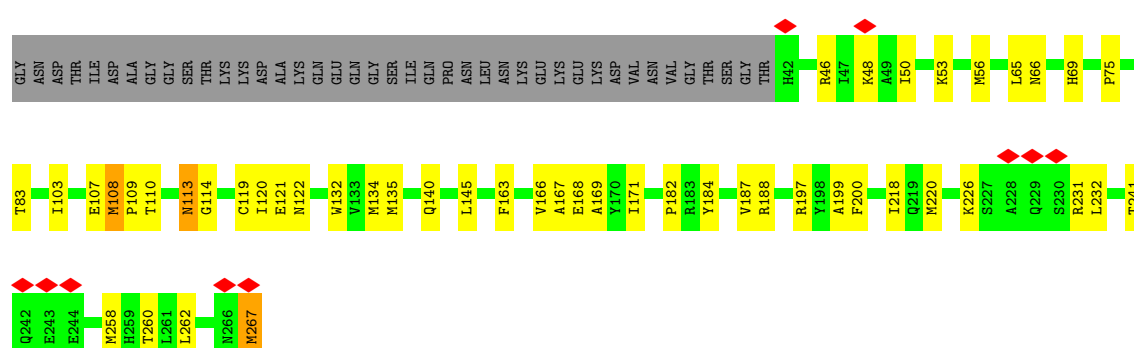
• Molecule 1: Genome polyprotein (Fragment)

Chain Bo: 



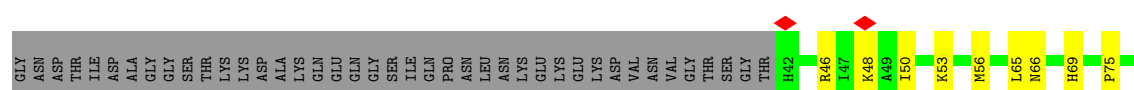
• Molecule 1: Genome polyprotein (Fragment)

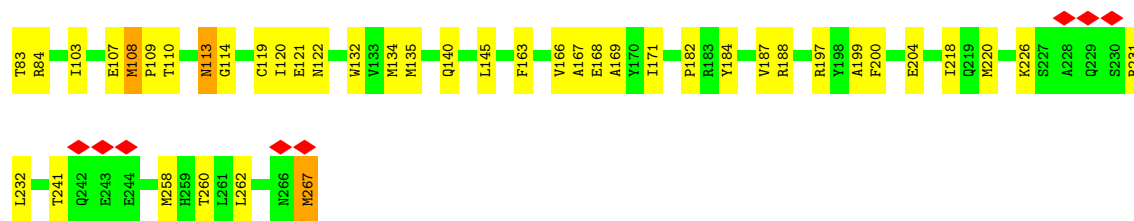
Chain Bq: 



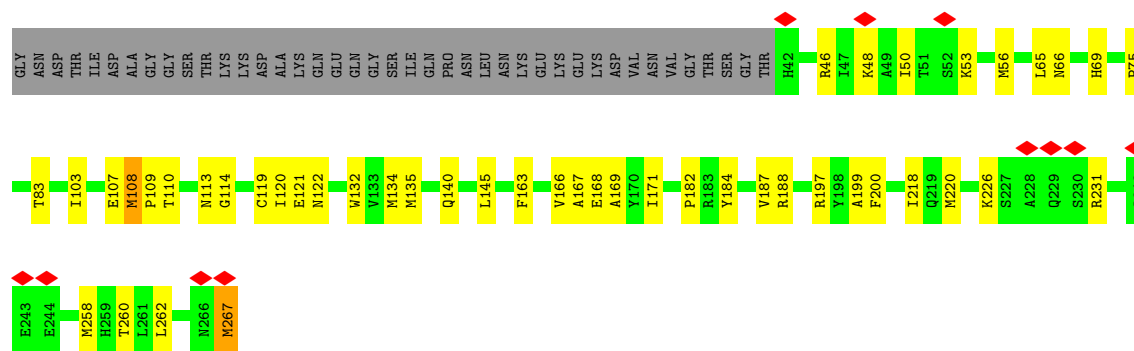
• Molecule 1: Genome polyprotein (Fragment)

Chain Bs: 

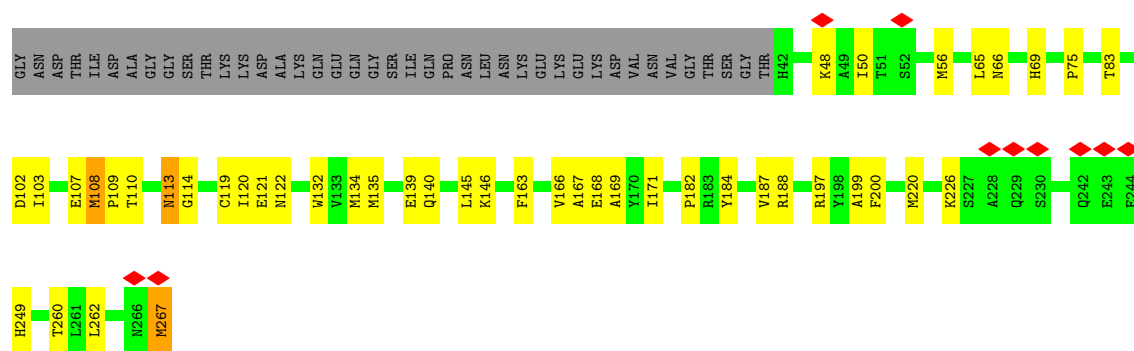




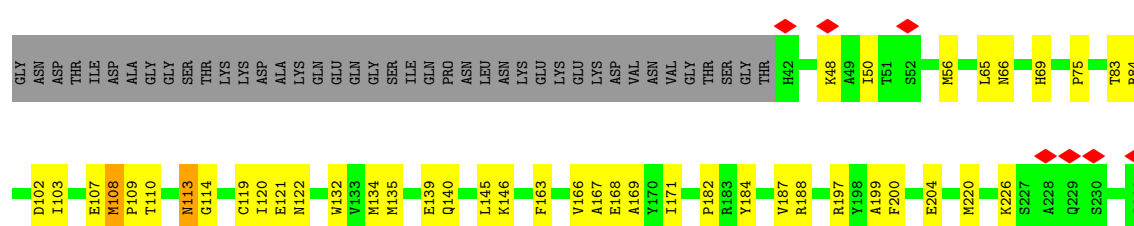
• Molecule 1: Genome polyprotein (Fragment)

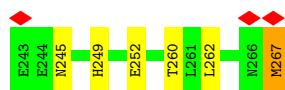


• Molecule 1: Genome polyprotein (Fragment)



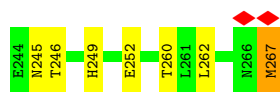
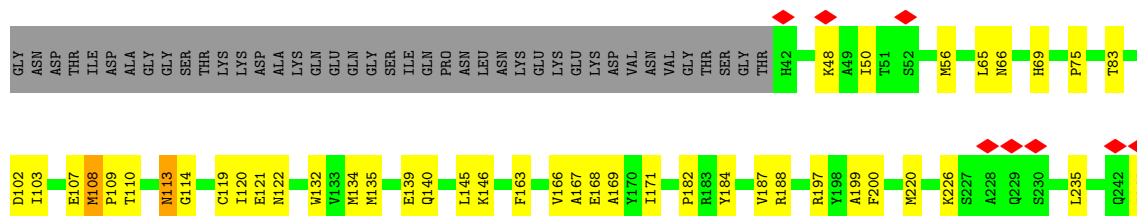
• Molecule 1: Genome polyprotein (Fragment)





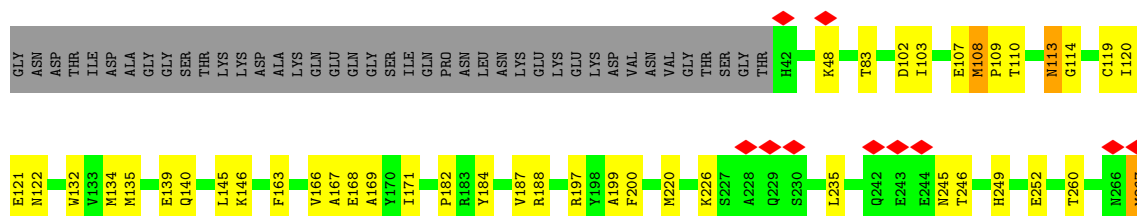
- Molecule 1: Genome polyprotein (Fragment)

Chain Ca: 66% 18% 15%



- Molecule 1: Genome polyprotein (Fragment)

Chain Cc: 69% 15% 15%



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

Chain Ab: 60% 40%



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

Chain Ad: 60% 40%



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

Chain Af: 80% 20%



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

Chain Ah:  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:  60% 40%



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

Chain An:  60% 40%



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

Chain Ap:  60% 40%



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

Chain Ar:  60% 40%



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

Chain At:  60% 40%



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

Chain Av:  60% 40%



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

Chain Ax:  60% 40%



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

Chain Az:  60% 40%



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

Chain Bb:  60% 40%



- 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:  60% 40%

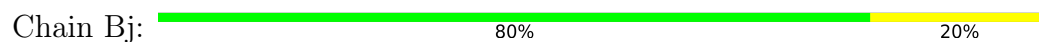


- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain Bh:  60% 40%



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



- 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')



- 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 Bx:  60% 40%



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

Chain Bz:  60% 40%



- 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:  60% 40%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-40.960°, rise=3.966 Å, axial sym=C1	Depositor
Number of segments used	10266	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; patchCTF correction	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.379	Depositor
Minimum map value	-2.558	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.275	Depositor
Recommended contour level	0.665	Depositor
Map size (Å)	285.0, 285.0, 285.0	wwPDB
Map dimensions	300, 300, 300	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	0.32	0/1833	0.49	2/2482 (0.1%)
1	Ac	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Ae	0.32	0/1833	0.49	2/2482 (0.1%)
1	Ag	0.32	0/1833	0.49	2/2482 (0.1%)
1	Ai	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Ak	0.32	0/1833	0.49	2/2482 (0.1%)
1	Am	0.33	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Ao	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Aq	0.32	0/1833	0.49	2/2482 (0.1%)
1	As	0.32	0/1833	0.49	2/2482 (0.1%)
1	Au	0.32	0/1833	0.49	2/2482 (0.1%)
1	Aw	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Ay	0.32	0/1833	0.49	2/2482 (0.1%)
1	Ba	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Bc	0.32	0/1833	0.49	2/2482 (0.1%)
1	Be	0.32	0/1833	0.49	2/2482 (0.1%)
1	Bg	0.32	0/1833	0.49	2/2482 (0.1%)
1	Bi	0.32	0/1833	0.49	2/2482 (0.1%)
1	Bk	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Bm	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Bo	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Bq	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Bs	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Bu	0.32	0/1833	0.49	2/2482 (0.1%)
1	Bw	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	By	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Ca	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
1	Cc	0.32	1/1833 (0.1%)	0.49	2/2482 (0.1%)
2	Ab	0.16	0/109	0.26	0/166
2	Ad	0.16	0/109	0.26	0/166
2	Af	0.16	0/109	0.26	0/166
2	Ah	0.16	0/109	0.26	0/166
2	Aj	0.16	0/109	0.26	0/166
2	Al	0.16	0/109	0.26	0/166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	An	0.16	0/109	0.26	0/166
2	Ap	0.16	0/109	0.26	0/166
2	Ar	0.16	0/109	0.26	0/166
2	At	0.16	0/109	0.26	0/166
2	Av	0.16	0/109	0.26	0/166
2	Ax	0.16	0/109	0.26	0/166
2	Az	0.16	0/109	0.26	0/166
2	Bb	0.16	0/109	0.26	0/166
2	Bd	0.16	0/109	0.26	0/166
2	Bf	0.16	0/109	0.26	0/166
2	Bh	0.16	0/109	0.26	0/166
2	Bj	0.16	0/109	0.26	0/166
2	Bl	0.16	0/109	0.26	0/166
2	Bn	0.16	0/109	0.26	0/166
2	Bp	0.16	0/109	0.26	0/166
2	Br	0.16	0/109	0.26	0/166
2	Bt	0.16	0/109	0.26	0/166
2	Bv	0.16	0/109	0.26	0/166
2	Bx	0.16	0/109	0.26	0/166
2	Bz	0.17	0/109	0.26	0/166
2	Cb	0.16	0/109	0.26	0/166
2	Cd	0.16	0/109	0.26	0/166
All	All	0.32	15/54376 (0.0%)	0.48	56/74144 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Ai	113	ASN	C-N	-5.04	1.27	1.33
1	Ba	113	ASN	C-N	-5.03	1.27	1.33
1	Bs	113	ASN	C-N	-5.03	1.27	1.33
1	Cc	113	ASN	C-N	-5.03	1.27	1.33
1	Bm	113	ASN	C-N	-5.02	1.27	1.33
1	Ac	113	ASN	C-N	-5.02	1.27	1.33
1	Ao	113	ASN	C-N	-5.02	1.27	1.33
1	Aw	113	ASN	C-N	-5.02	1.27	1.33
1	By	113	ASN	C-N	-5.02	1.27	1.33
1	Ca	113	ASN	C-N	-5.02	1.27	1.33
1	Am	113	ASN	C-N	-5.02	1.27	1.33
1	Bw	113	ASN	C-N	-5.01	1.27	1.33
1	Bk	113	ASN	C-N	-5.01	1.27	1.33
1	Bq	113	ASN	C-N	-5.01	1.27	1.33
1	Bo	113	ASN	C-N	-5.00	1.27	1.33

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ao	122	ASN	N-CA-C	6.41	119.77	112.97
1	Ag	122	ASN	N-CA-C	6.41	119.76	112.97
1	Ay	122	ASN	N-CA-C	6.41	119.76	112.97
1	Ae	122	ASN	N-CA-C	6.40	119.76	112.97
1	Bu	122	ASN	N-CA-C	6.40	119.76	112.97
1	Au	122	ASN	N-CA-C	6.40	119.75	112.97
1	Bi	122	ASN	N-CA-C	6.39	119.75	112.97
1	As	122	ASN	N-CA-C	6.39	119.75	112.97
1	Aw	122	ASN	N-CA-C	6.39	119.75	112.97
1	Bq	122	ASN	N-CA-C	6.39	119.74	112.97
1	Bo	122	ASN	N-CA-C	6.39	119.74	112.97
1	Ai	122	ASN	N-CA-C	6.38	119.74	112.97
1	Ca	122	ASN	N-CA-C	6.38	119.74	112.97
1	Ak	122	ASN	N-CA-C	6.38	119.74	112.97
1	Ac	122	ASN	N-CA-C	6.38	119.73	112.97
1	Bg	122	ASN	N-CA-C	6.38	119.73	112.97
1	Bs	122	ASN	N-CA-C	6.38	119.73	112.97
1	Be	122	ASN	N-CA-C	6.37	119.72	112.97
1	Bk	122	ASN	N-CA-C	6.37	119.72	112.97
1	By	122	ASN	N-CA-C	6.37	119.72	112.97
1	Am	122	ASN	N-CA-C	6.37	119.72	112.97
1	Bc	122	ASN	N-CA-C	6.36	119.72	112.97
1	Ba	122	ASN	N-CA-C	6.36	119.71	112.97
1	Cc	122	ASN	N-CA-C	6.36	119.71	112.97
1	Aa	122	ASN	N-CA-C	6.35	119.70	112.97
1	Aq	122	ASN	N-CA-C	6.35	119.70	112.97
1	Bm	122	ASN	N-CA-C	6.33	119.69	112.97
1	Bw	122	ASN	N-CA-C	6.33	119.68	112.97
1	By	226	LYS	CB-CA-C	-5.40	109.88	117.23
1	Bg	226	LYS	CB-CA-C	-5.37	109.93	117.23
1	As	226	LYS	CB-CA-C	-5.37	109.93	117.23
1	Ba	226	LYS	CB-CA-C	-5.36	109.94	117.23
1	Ay	226	LYS	CB-CA-C	-5.36	109.94	117.23
1	Bw	226	LYS	CB-CA-C	-5.36	109.94	117.23
1	Cc	226	LYS	CB-CA-C	-5.36	109.94	117.23
1	Bo	226	LYS	CB-CA-C	-5.36	109.94	117.23
1	Ca	226	LYS	CB-CA-C	-5.36	109.94	117.23
1	Bm	226	LYS	CB-CA-C	-5.36	109.95	117.23
1	Aa	226	LYS	CB-CA-C	-5.35	109.95	117.23
1	Ac	226	LYS	CB-CA-C	-5.35	109.95	117.23
1	Ae	226	LYS	CB-CA-C	-5.35	109.95	117.23
1	Ag	226	LYS	CB-CA-C	-5.35	109.95	117.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Ao	226	LYS	CB-CA-C	-5.35	109.95	117.23
1	Bc	226	LYS	CB-CA-C	-5.35	109.95	117.23
1	Aq	226	LYS	CB-CA-C	-5.35	109.96	117.23
1	Bi	226	LYS	CB-CA-C	-5.35	109.96	117.23
1	Aw	226	LYS	CB-CA-C	-5.34	109.96	117.23
1	Ai	226	LYS	CB-CA-C	-5.34	109.96	117.23
1	Bk	226	LYS	CB-CA-C	-5.34	109.97	117.23
1	Bq	226	LYS	CB-CA-C	-5.34	109.97	117.23
1	Bu	226	LYS	CB-CA-C	-5.34	109.97	117.23
1	Ak	226	LYS	CB-CA-C	-5.34	109.97	117.23
1	Au	226	LYS	CB-CA-C	-5.34	109.97	117.23
1	Bs	226	LYS	CB-CA-C	-5.34	109.97	117.23
1	Am	226	LYS	CB-CA-C	-5.34	109.97	117.23
1	Be	226	LYS	CB-CA-C	-5.33	109.99	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1796	0	1775	50	0
1	Ac	1796	0	1775	59	0
1	Ae	1796	0	1775	53	0
1	Ag	1796	0	1775	45	0
1	Ai	1796	0	1775	45	0
1	Ak	1796	0	1775	48	0
1	Am	1796	0	1775	45	0
1	Ao	1796	0	1775	43	0
1	Aq	1796	0	1775	49	0
1	As	1796	0	1775	51	0
1	Au	1796	0	1775	52	0
1	Aw	1796	0	1775	51	0
1	Ay	1796	0	1775	53	0
1	Ba	1796	0	1775	55	0
1	Bc	1796	0	1775	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Be	1796	0	1775	52	0
1	Bg	1796	0	1775	35	0
1	Bi	1796	0	1775	43	0
1	Bk	1796	0	1775	44	0
1	Bm	1796	0	1775	43	0
1	Bo	1796	0	1775	49	0
1	Bq	1796	0	1775	48	0
1	Bs	1796	0	1775	49	0
1	Bu	1796	0	1775	44	0
1	Bw	1796	0	1775	42	0
1	By	1796	0	1775	45	0
1	Ca	1796	0	1775	47	0
1	Cc	1796	0	1775	38	0
2	Ab	100	0	51	2	0
2	Ad	100	0	51	2	0
2	Af	100	0	51	1	0
2	Ah	100	0	51	2	0
2	Aj	100	0	51	1	0
2	Al	100	0	51	2	0
2	An	100	0	51	2	0
2	Ap	100	0	51	2	0
2	Ar	100	0	51	2	0
2	At	100	0	51	2	0
2	Av	100	0	51	2	0
2	Ax	100	0	51	2	0
2	Az	100	0	51	2	0
2	Bb	100	0	51	2	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	2	0
2	Bp	100	0	51	2	0
2	Br	100	0	51	2	0
2	Bt	100	0	51	2	0
2	Bv	100	0	51	2	0
2	Bx	100	0	51	2	0
2	Bz	100	0	51	2	0
2	Cb	100	0	51	2	0
2	Cd	100	0	51	2	0
All	All	53088	0	51128	925	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (925) 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:Bo:103:ILE:HG23	1:Bo:107:GLU:HG3	1.71	0.73
1:Bq:103:ILE:HG23	1:Bq:107:GLU:HG3	1.71	0.73
1:Bc:103:ILE:HG23	1:Bc:107:GLU:HG3	1.71	0.73
1:Bm:103:ILE:HG23	1:Bm:107:GLU:HG3	1.71	0.73
1:Bs:103:ILE:HG23	1:Bs:107:GLU:HG3	1.71	0.73
1:Bi:103:ILE:HG23	1:Bi:107:GLU:HG3	1.71	0.73
1:Ba:103:ILE:HG23	1:Ba:107:GLU:HG3	1.71	0.73
1:Bk:103:ILE:HG23	1:Bk:107:GLU:HG3	1.71	0.73
1:Ak:103:ILE:HG23	1:Ak:107:GLU:HG3	1.71	0.73
1:Am:103:ILE:HG23	1:Am:107:GLU:HG3	1.71	0.73
1:Ao:103:ILE:HG23	1:Ao:107:GLU:HG3	1.71	0.73
1:Aw:103:ILE:HG23	1:Aw:107:GLU:HG3	1.71	0.72
1:Ay:103:ILE:HG23	1:Ay:107:GLU:HG3	1.71	0.72
1:Bi:103:ILE:HG23	1:Bi:107:GLU:HG3	1.71	0.72
1:Au:103:ILE:HG23	1:Au:107:GLU:HG3	1.71	0.72
1:Be:103:ILE:HG23	1:Be:107:GLU:HG3	1.71	0.72
1:Ag:103:ILE:HG23	1:Ag:107:GLU:HG3	1.71	0.72
1:As:103:ILE:HG23	1:As:107:GLU:HG3	1.71	0.72
1:Bu:103:ILE:HG23	1:Bu:107:GLU:HG3	1.71	0.72
1:Bw:103:ILE:HG23	1:Bw:107:GLU:HG3	1.71	0.72
1:Ae:103:ILE:HG23	1:Ae:107:GLU:HG3	1.71	0.72
1:By:103:ILE:HG23	1:By:107:GLU:HG3	1.71	0.72
1:Ac:103:ILE:HG23	1:Ac:107:GLU:HG3	1.71	0.72
1:Ca:103:ILE:HG23	1:Ca:107:GLU:HG3	1.71	0.72
1:Aa:103:ILE:HG23	1:Aa:107:GLU:HG3	1.71	0.72
1:Bg:103:ILE:HG23	1:Bg:107:GLU:HG3	1.71	0.72
1:Aq:103:ILE:HG23	1:Aq:107:GLU:HG3	1.71	0.71
1:Cc:103:ILE:HG23	1:Cc:107:GLU:HG3	1.71	0.71
1:Ae:258:MET:HG3	1:Am:267:MET:HE3	1.82	0.62
1:Am:249:HIS:HB2	1:Ba:231:ARG:HH22	1.66	0.61
1:Ao:258:MET:HG3	1:Cc:267:MET:HE3	1.83	0.61
1:Am:258:MET:HG3	1:Ca:267:MET:HE3	1.84	0.60
1:Bc:249:HIS:HB2	1:Bq:231:ARG:HH22	1.67	0.60
1:Ag:56:MET:HG2	1:Bi:166:VAL:HG22	1.84	0.60
1:Ag:258:MET:HG3	1:Ao:267:MET:HE3	1.83	0.60
1:Aq:267:MET:HE3	1:Bo:258:MET:HG3	1.84	0.60
1:Ak:249:HIS:HB2	1:Ay:231:ARG:HH22	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ao:249:HIS:HB2	1:Bc:231:ARG:HH22	1.67	0.60
1:Aq:258:MET:HG3	1:Ay:267:MET:HE3	1.84	0.60
1:Ac:231:ARG:HH22	1:Ca:249:HIS:HB2	1.66	0.59
1:Bg:258:MET:HG3	1:Bo:267:MET:HE3	1.84	0.59
1:Ac:258:MET:HG3	1:Ak:267:MET:HE3	1.85	0.59
1:Au:249:HIS:HB2	1:Bi:231:ARG:HH22	1.67	0.59
1:Be:231:ARG:HH22	1:Bw:249:HIS:HB2	1.66	0.59
1:Bm:258:MET:HG3	1:Bu:267:MET:HE3	1.84	0.59
1:Ag:249:HIS:HB2	1:Au:231:ARG:HH22	1.67	0.59
1:Ai:249:HIS:HB2	1:Aw:231:ARG:HH22	1.66	0.59
1:Au:56:MET:HG2	1:Aw:166:VAL:HG22	1.85	0.59
1:Ba:249:HIS:HB2	1:Bo:231:ARG:HH22	1.67	0.59
1:Be:249:HIS:HB2	1:Bs:231:ARG:HH22	1.67	0.59
1:Bk:56:MET:HG2	1:Bm:166:VAL:HG22	1.85	0.59
1:Ca:56:MET:HG2	1:Cc:166:VAL:HG22	1.85	0.59
1:Aw:258:MET:HG3	1:Be:267:MET:HE3	1.84	0.59
1:Bg:56:MET:HG2	1:Bi:166:VAL:HG22	1.85	0.59
1:Ai:56:MET:HG2	1:Ak:166:VAL:HG22	1.85	0.59
1:Ae:56:MET:HG2	1:Ag:166:VAL:HG22	1.85	0.59
1:Ai:258:MET:HG3	1:Bw:267:MET:HE3	1.85	0.59
1:Ay:56:MET:HG2	1:Ba:166:VAL:HG22	1.85	0.59
1:Ae:267:MET:HE3	1:Bc:258:MET:HG3	1.85	0.58
1:Aq:56:MET:HG2	1:As:166:VAL:HG22	1.85	0.58
1:As:56:MET:HG2	1:Au:166:VAL:HG22	1.85	0.58
1:Ay:249:HIS:HB2	1:Bm:231:ARG:HH22	1.67	0.58
1:Aa:231:ARG:HH22	1:By:249:HIS:HB2	1.67	0.58
1:Ag:267:MET:HE3	1:Be:258:MET:HG3	1.85	0.58
1:Bi:56:MET:HG2	1:Bk:166:VAL:HG22	1.85	0.58
1:Bo:56:MET:HG2	1:Bq:166:VAL:HG22	1.85	0.58
1:Ac:249:HIS:HB2	1:Aq:231:ARG:HH22	1.67	0.58
1:Ak:258:MET:HG3	1:By:267:MET:HE3	1.85	0.58
1:Aw:56:MET:HG2	1:Ay:166:VAL:HG22	1.86	0.58
1:Aa:166:VAL:HG22	1:Be:56:MET:HG2	1.84	0.58
1:Ae:249:HIS:HB2	1:As:231:ARG:HH22	1.66	0.58
1:Bk:258:MET:HG3	1:Bs:267:MET:HE3	1.85	0.58
1:As:249:HIS:HB2	1:Bg:231:ARG:HH22	1.67	0.58
1:Au:258:MET:HG3	1:Bc:267:MET:HE3	1.86	0.58
1:Aw:249:HIS:HB2	1:Bk:231:ARG:HH22	1.67	0.58
1:Bw:56:MET:HG2	1:By:166:VAL:HG22	1.85	0.58
1:Ak:56:MET:HG2	1:Am:166:VAL:HG22	1.85	0.58
1:Am:56:MET:HG2	1:Ao:166:VAL:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:56:MET:HG2	1:Bo:166:VAL:HG22	1.86	0.58
1:By:56:MET:HG2	1:Ca:166:VAL:HG22	1.85	0.58
1:Aw:267:MET:HE3	1:Bu:258:MET:HG3	1.86	0.58
1:Bc:56:MET:HG2	1:Be:166:VAL:HG22	1.85	0.58
1:Bs:56:MET:HG2	1:Bu:166:VAL:HG22	1.85	0.58
1:Ac:56:MET:HG2	1:Ae:166:VAL:HG22	1.86	0.57
1:Aa:249:HIS:HB2	1:Bu:231:ARG:HH22	1.67	0.57
1:Ac:267:MET:HE3	1:Ba:258:MET:HG3	1.87	0.57
1:Ba:56:MET:HG2	1:Bc:166:VAL:HG22	1.85	0.57
1:Bi:258:MET:HG3	1:Bq:267:MET:HE3	1.86	0.57
1:Ae:231:ARG:HH22	1:Cc:249:HIS:HB2	1.67	0.57
1:As:258:MET:HG3	1:Ba:267:MET:HE3	1.86	0.57
1:Aa:56:MET:HG2	1:Ac:166:VAL:HG22	1.86	0.57
1:Ao:56:MET:HG2	1:Bw:166:VAL:HG22	1.85	0.57
1:As:267:MET:HE3	1:Bq:258:MET:HG3	1.87	0.57
1:Aa:258:MET:HG3	1:Ai:267:MET:HE3	1.87	0.57
1:Bq:56:MET:HG2	1:Bs:166:VAL:HG22	1.85	0.57
1:Ac:184:TYR:OH	2:Ad:4:U:O2	2.20	0.56
1:Aq:166:VAL:HG22	1:Bu:56:MET:HG2	1.87	0.56
1:Au:267:MET:HE3	1:Bs:258:MET:HG3	1.87	0.56
1:Aa:267:MET:HE3	1:Ay:258:MET:HG3	1.89	0.55
1:Bu:184:TYR:OH	2:Bv:4:U:O2	2.20	0.55
1:By:184:TYR:OH	2:Bz:4:U:O2	2.20	0.55
1:Ai:66:ASN:HB3	1:Ak:113:ASN:HD21	1.72	0.55
1:Ao:135:MET:HE1	1:Ao:140:GLN:HG3	1.89	0.55
1:Bk:66:ASN:HB3	1:Bm:113:ASN:HD21	1.72	0.55
1:Bs:135:MET:HE1	1:Bs:140:GLN:HG3	1.89	0.55
1:Be:135:MET:HE1	1:Be:140:GLN:HG3	1.89	0.54
1:Bu:135:MET:HE1	1:Bu:140:GLN:HG3	1.89	0.54
1:Bw:135:MET:HE1	1:Bw:140:GLN:HG3	1.89	0.54
1:Au:66:ASN:HB3	1:Aw:113:ASN:HD21	1.73	0.54
1:Bc:135:MET:HE1	1:Bc:140:GLN:HG3	1.89	0.54
1:Aa:135:MET:HE1	1:Aa:140:GLN:HG3	1.89	0.54
1:Ae:66:ASN:HB3	1:Ag:113:ASN:HD21	1.72	0.54
1:By:135:MET:HE1	1:By:140:GLN:HG3	1.89	0.54
1:Ay:66:ASN:HB3	1:Ba:113:ASN:HD21	1.72	0.54
1:Bq:135:MET:HE1	1:Bq:140:GLN:HG3	1.89	0.54
1:Am:135:MET:HE1	1:Am:140:GLN:HG3	1.89	0.54
1:Ba:135:MET:HE1	1:Ba:140:GLN:HG3	1.89	0.54
1:Ag:56:MET:HG2	1:Ai:166:VAL:CG2	2.38	0.54
1:Ao:50:ILE:HG12	1:Bw:169:ALA:HB1	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bo:135:MET:HE1	1:Bo:140:GLN:HG3	1.89	0.54
1:Ca:135:MET:HE1	1:Ca:140:GLN:HG3	1.89	0.54
1:Ac:135:MET:HE1	1:Ac:140:GLN:HG3	1.89	0.54
1:Ag:66:ASN:HB3	1:Ai:113:ASN:HD21	1.72	0.54
1:Aq:135:MET:HE1	1:Aq:140:GLN:HG3	1.89	0.54
1:As:66:ASN:HB3	1:Au:113:ASN:HD21	1.73	0.54
1:Ay:56:MET:HG2	1:Ba:166:VAL:CG2	2.38	0.54
1:Bg:66:ASN:HB3	1:Bi:113:ASN:HD21	1.72	0.54
1:Bw:66:ASN:HB3	1:By:113:ASN:HD21	1.72	0.54
1:Ak:66:ASN:HB3	1:Am:113:ASN:HD21	1.73	0.53
1:Bc:66:ASN:HB3	1:Be:113:ASN:HD21	1.72	0.53
1:Bs:66:ASN:HB3	1:Bu:113:ASN:HD21	1.72	0.53
1:Ae:56:MET:HG2	1:Ag:166:VAL:CG2	2.39	0.53
1:By:66:ASN:HB3	1:Ca:113:ASN:HD21	1.73	0.53
1:Aa:113:ASN:HD21	1:Be:66:ASN:HB3	1.72	0.53
1:Aa:166:VAL:CG2	1:Be:56:MET:HG2	2.38	0.53
1:Ay:135:MET:HE1	1:Ay:140:GLN:HG3	1.89	0.53
1:Bi:135:MET:HE1	1:Bi:140:GLN:HG3	1.89	0.53
1:Bk:56:MET:HG2	1:Bm:166:VAL:CG2	2.38	0.53
1:By:56:MET:HG2	1:Ca:166:VAL:CG2	2.39	0.53
1:Ca:66:ASN:HB3	1:Cc:113:ASN:HD21	1.73	0.53
1:Ac:66:ASN:HB3	1:Ae:113:ASN:HD21	1.74	0.53
1:Ba:66:ASN:HB3	1:Bc:113:ASN:HD21	1.73	0.53
1:Bg:135:MET:HE1	1:Bg:140:GLN:HG3	1.89	0.53
1:Ai:135:MET:HE1	1:Ai:140:GLN:HG3	1.89	0.53
1:Ak:56:MET:HG2	1:Am:166:VAL:CG2	2.39	0.53
1:Ak:135:MET:HE1	1:Ak:140:GLN:HG3	1.89	0.53
1:As:135:MET:HE1	1:As:140:GLN:HG3	1.89	0.53
1:Bm:135:MET:HE1	1:Bm:140:GLN:HG3	1.89	0.53
1:Ae:135:MET:HE1	1:Ae:140:GLN:HG3	1.89	0.53
1:Aq:56:MET:HG2	1:As:166:VAL:CG2	2.38	0.53
1:Bi:56:MET:HG2	1:Bk:166:VAL:CG2	2.39	0.53
1:Bi:66:ASN:HB3	1:Bk:113:ASN:HD21	1.73	0.53
1:Ac:50:ILE:HG12	1:Ae:169:ALA:HB1	1.91	0.53
1:Aw:66:ASN:HB3	1:Ay:113:ASN:HD21	1.74	0.53
1:Cc:135:MET:HE1	1:Cc:140:GLN:HG3	1.89	0.53
1:Aw:135:MET:HE1	1:Aw:140:GLN:HG3	1.89	0.53
1:Bg:56:MET:HG2	1:Bi:166:VAL:CG2	2.38	0.53
1:Bo:66:ASN:HB3	1:Bq:113:ASN:HD21	1.72	0.53
1:Bm:66:ASN:HB3	1:Bo:113:ASN:HD21	1.73	0.53
1:Bw:50:ILE:HG12	1:By:169:ALA:HB1	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Am:66:ASN:HB3	1:Ao:113:ASN:HD21	1.72	0.53
1:Au:56:MET:HG2	1:Aw:166:VAL:CG2	2.38	0.53
1:Au:135:MET:HE1	1:Au:140:GLN:HG3	1.89	0.53
1:Bm:56:MET:HG2	1:Bo:166:VAL:CG2	2.39	0.53
1:Bq:66:ASN:HB3	1:Bs:113:ASN:HD21	1.73	0.53
1:Am:56:MET:HG2	1:Ao:166:VAL:CG2	2.38	0.52
1:Aq:66:ASN:HB3	1:As:113:ASN:HD21	1.73	0.52
1:Bs:50:ILE:HG12	1:Bu:169:ALA:HB1	1.91	0.52
1:Bs:56:MET:HG2	1:Bu:166:VAL:CG2	2.39	0.52
1:Ai:56:MET:HG2	1:Ak:166:VAL:CG2	2.38	0.52
1:Aq:50:ILE:HG12	1:As:169:ALA:HB1	1.91	0.52
1:Bk:135:MET:HE1	1:Bk:140:GLN:HG3	1.89	0.52
1:Ag:135:MET:HE1	1:Ag:140:GLN:HG3	1.89	0.52
1:Ao:56:MET:HG2	1:Bw:166:VAL:CG2	2.39	0.52
1:As:56:MET:HG2	1:Au:166:VAL:CG2	2.39	0.52
1:Bq:56:MET:HG2	1:Bs:166:VAL:CG2	2.39	0.52
1:Bw:184:TYR:OH	2:Bx:4:U:O2	2.20	0.52
1:Bc:50:ILE:HG12	1:Be:169:ALA:HB1	1.91	0.52
1:Aa:56:MET:HG2	1:Ac:166:VAL:CG2	2.40	0.52
1:Aa:66:ASN:HB3	1:Ac:113:ASN:HD21	1.74	0.52
1:Ae:50:ILE:HG12	1:Ag:169:ALA:HB1	1.91	0.52
1:Aw:56:MET:HG2	1:Ay:166:VAL:CG2	2.39	0.52
1:Ba:50:ILE:HG12	1:Bc:169:ALA:HB1	1.91	0.52
1:Bo:56:MET:HG2	1:Bq:166:VAL:CG2	2.38	0.52
1:Bw:56:MET:HG2	1:By:166:VAL:CG2	2.38	0.52
1:Aa:262:LEU:HD23	1:Ac:260:THR:HG22	1.92	0.52
1:Ao:66:ASN:HB3	1:Bw:113:ASN:HD21	1.73	0.52
1:Au:197:ARG:O	1:Au:200:PHE:HE1	1.93	0.52
1:Bg:50:ILE:HG12	1:Bi:169:ALA:HB1	1.91	0.52
1:Bi:197:ARG:O	1:Bi:200:PHE:HE1	1.93	0.52
1:Bm:197:ARG:O	1:Bm:200:PHE:HE1	1.93	0.52
1:Ca:56:MET:HG2	1:Cc:166:VAL:CG2	2.39	0.52
1:Ag:50:ILE:HG12	1:Ai:169:ALA:HB1	1.90	0.52
1:Bk:262:LEU:HD23	1:Bm:260:THR:HG22	1.92	0.52
1:Am:50:ILE:HG12	1:Ao:169:ALA:HB1	1.91	0.52
1:Au:262:LEU:HD23	1:Aw:260:THR:HG22	1.92	0.52
1:Ay:197:ARG:O	1:Ay:200:PHE:HE1	1.93	0.52
1:Bc:262:LEU:HD23	1:Be:260:THR:HG22	1.92	0.52
1:Bs:262:LEU:HD23	1:Bu:260:THR:HG22	1.92	0.52
1:By:50:ILE:HG12	1:Ca:169:ALA:HB1	1.91	0.52
1:Ac:197:ARG:O	1:Ac:200:PHE:HE1	1.93	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ae:262:LEU:HD23	1:Ag:260:THR:HG22	1.92	0.52
1:Ag:197:ARG:O	1:Ag:200:PHE:HE1	1.93	0.52
1:Ag:262:LEU:HD23	1:Ai:260:THR:HG22	1.92	0.52
1:Am:197:ARG:O	1:Am:200:PHE:HE1	1.93	0.52
1:Am:262:LEU:HD23	1:Ao:260:THR:HG22	1.92	0.52
1:Aq:166:VAL:CG2	1:Bu:56:MET:HG2	2.40	0.52
1:As:184:TYR:OH	2:At:4:U:O2	2.20	0.52
1:Bi:50:ILE:HG12	1:Bk:169:ALA:HB1	1.91	0.52
1:Ac:56:MET:HG2	1:Ae:166:VAL:CG2	2.40	0.51
1:Ba:56:MET:HG2	1:Bc:166:VAL:CG2	2.39	0.51
1:Bc:56:MET:HG2	1:Be:166:VAL:CG2	2.38	0.51
1:Bq:262:LEU:HD23	1:Bs:260:THR:HG22	1.92	0.51
1:Ca:197:ARG:O	1:Ca:200:PHE:HE1	1.93	0.51
1:Ak:197:ARG:O	1:Ak:200:PHE:HE1	1.93	0.51
1:Aq:262:LEU:HD23	1:As:260:THR:HG22	1.92	0.51
1:Ba:197:ARG:O	1:Ba:200:PHE:HE1	1.93	0.51
1:Bq:50:ILE:HG12	1:Bs:169:ALA:HB1	1.91	0.51
1:Cc:197:ARG:O	1:Cc:200:PHE:HE1	1.93	0.51
1:Aq:197:ARG:O	1:Aq:200:PHE:HE1	1.93	0.51
1:Bg:262:LEU:HD23	1:Bi:260:THR:HG22	1.92	0.51
1:Ai:197:ARG:O	1:Ai:200:PHE:HE1	1.93	0.51
1:Ak:262:LEU:HD23	1:Am:260:THR:HG22	1.92	0.51
1:Aq:113:ASN:HD21	1:Bu:66:ASN:HB3	1.75	0.51
1:Ay:50:ILE:HG12	1:Ba:169:ALA:HB1	1.91	0.51
1:Ba:262:LEU:HD23	1:Bc:260:THR:HG22	1.92	0.51
1:By:262:LEU:HD23	1:Ca:260:THR:HG22	1.92	0.51
1:Au:184:TYR:OH	2:Av:4:U:O2	2.20	0.51
1:Bs:184:TYR:OH	2:Bt:4:U:O2	2.20	0.51
1:Bw:262:LEU:HD23	1:By:260:THR:HG22	1.92	0.51
1:Ca:50:ILE:HG12	1:Cc:169:ALA:HB1	1.91	0.51
1:Aa:169:ALA:HB1	1:Be:50:ILE:HG12	1.92	0.51
1:Ai:50:ILE:HG12	1:Ak:169:ALA:HB1	1.91	0.51
1:Bi:262:LEU:HD23	1:Bk:260:THR:HG22	1.92	0.51
1:Bk:50:ILE:HG12	1:Bm:169:ALA:HB1	1.91	0.51
1:Aq:169:ALA:HB1	1:Bu:50:ILE:HG12	1.93	0.51
1:Bo:50:ILE:HG12	1:Bq:169:ALA:HB1	1.91	0.51
1:Bq:197:ARG:O	1:Bq:200:PHE:HE1	1.93	0.51
1:Bu:48:LYS:HD3	1:Bu:48:LYS:N	2.26	0.51
1:As:50:ILE:HG12	1:Au:169:ALA:HB1	1.91	0.51
1:Ba:114:GLY:HA3	1:Ba:134:MET:SD	2.51	0.51
1:Bs:48:LYS:HD3	1:Bs:48:LYS:N	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ca:114:GLY:HA3	1:Ca:134:MET:SD	2.51	0.51
1:Ca:262:LEU:HD23	1:Cc:260:THR:HG22	1.92	0.51
1:Ac:114:GLY:HA3	1:Ac:134:MET:SD	2.51	0.51
1:Ae:197:ARG:O	1:Ae:200:PHE:HE1	1.93	0.51
1:Aw:197:ARG:O	1:Aw:200:PHE:HE1	1.93	0.51
1:Bg:197:ARG:O	1:Bg:200:PHE:HE1	1.93	0.51
1:Bu:197:ARG:O	1:Bu:200:PHE:HE1	1.93	0.51
1:Bw:114:GLY:HA3	1:Bw:134:MET:SD	2.51	0.51
1:Aa:48:LYS:HD3	1:Aa:48:LYS:N	2.26	0.51
1:Aa:50:ILE:HG12	1:Ac:169:ALA:HB1	1.93	0.51
1:Aq:114:GLY:HA3	1:Aq:134:MET:SD	2.51	0.51
1:As:114:GLY:HA3	1:As:134:MET:SD	2.51	0.51
1:Ay:114:GLY:HA3	1:Ay:134:MET:SD	2.51	0.51
1:Be:114:GLY:HA3	1:Be:134:MET:SD	2.51	0.51
1:Be:197:ARG:O	1:Be:200:PHE:HE1	1.93	0.51
1:Bm:114:GLY:HA3	1:Bm:134:MET:SD	2.51	0.51
1:Bo:197:ARG:O	1:Bo:200:PHE:HE1	1.93	0.51
1:Bs:114:GLY:HA3	1:Bs:134:MET:SD	2.51	0.51
1:Bs:197:ARG:O	1:Bs:200:PHE:HE1	1.93	0.51
1:Bw:197:ARG:O	1:Bw:200:PHE:HE1	1.93	0.51
1:Aa:197:ARG:O	1:Aa:200:PHE:HE1	1.93	0.50
1:Ae:114:GLY:HA3	1:Ae:134:MET:SD	2.51	0.50
1:Bc:48:LYS:HD3	1:Bc:48:LYS:N	2.26	0.50
1:Be:48:LYS:HD3	1:Be:48:LYS:N	2.26	0.50
1:Bg:114:GLY:HA3	1:Bg:134:MET:SD	2.51	0.50
1:Bk:197:ARG:O	1:Bk:200:PHE:HE1	1.93	0.50
1:Ak:50:ILE:HG12	1:Am:169:ALA:HB1	1.91	0.50
1:Au:48:LYS:HD3	1:Au:48:LYS:N	2.26	0.50
1:Aw:50:ILE:HG12	1:Ay:169:ALA:HB1	1.92	0.50
1:Bc:114:GLY:HA3	1:Bc:134:MET:SD	2.51	0.50
1:Bm:50:ILE:HG12	1:Bo:169:ALA:HB1	1.92	0.50
1:Bq:48:LYS:HD3	1:Bq:48:LYS:N	2.26	0.50
1:Ac:48:LYS:HD3	1:Ac:48:LYS:N	2.26	0.50
1:Ai:262:LEU:HD23	1:Ak:260:THR:HG22	1.92	0.50
1:Aq:48:LYS:HD3	1:Aq:48:LYS:N	2.26	0.50
1:Au:50:ILE:HG12	1:Aw:169:ALA:HB1	1.91	0.50
1:Bk:114:GLY:HA3	1:Bk:134:MET:SD	2.51	0.50
1:By:48:LYS:HD3	1:By:48:LYS:N	2.26	0.50
1:By:197:ARG:O	1:By:200:PHE:HE1	1.93	0.50
1:Ca:184:TYR:OH	2:Cb:4:U:O2	2.20	0.50
1:Cc:48:LYS:HD3	1:Cc:48:LYS:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Cc:114:GLY:HA3	1:Cc:134:MET:SD	2.51	0.50
1:Ao:114:GLY:HA3	1:Ao:134:MET:SD	2.51	0.50
1:Ao:197:ARG:O	1:Ao:200:PHE:HE1	1.93	0.50
1:As:197:ARG:O	1:As:200:PHE:HE1	1.93	0.50
1:As:262:LEU:HD23	1:Au:260:THR:HG22	1.92	0.50
1:Ba:184:TYR:OH	2:Bb:4:U:O2	2.20	0.50
1:Bo:114:GLY:HA3	1:Bo:134:MET:SD	2.51	0.50
1:Ak:48:LYS:HD3	1:Ak:48:LYS:N	2.26	0.50
1:Aw:114:GLY:HA3	1:Aw:134:MET:SD	2.51	0.50
1:Bc:197:ARG:O	1:Bc:200:PHE:HE1	1.93	0.50
1:Bg:48:LYS:HD3	1:Bg:48:LYS:N	2.26	0.50
1:Bw:48:LYS:HD3	1:Bw:48:LYS:N	2.26	0.50
1:Ai:48:LYS:HD3	1:Ai:48:LYS:N	2.26	0.50
1:Am:48:LYS:HD3	1:Am:48:LYS:N	2.26	0.50
1:Am:114:GLY:HA3	1:Am:134:MET:SD	2.51	0.50
1:Ao:262:LEU:HD23	1:Bw:260:THR:HG22	1.93	0.50
1:Ay:262:LEU:HD23	1:Ba:260:THR:HG22	1.92	0.50
1:Bi:48:LYS:HD3	1:Bi:48:LYS:N	2.26	0.50
1:Ag:114:GLY:HA3	1:Ag:134:MET:SD	2.51	0.50
1:Ai:114:GLY:HA3	1:Ai:134:MET:SD	2.51	0.50
1:Bo:48:LYS:HD3	1:Bo:48:LYS:N	2.26	0.50
1:Bo:262:LEU:HD23	1:Bq:260:THR:HG22	1.92	0.50
1:Ca:48:LYS:HD3	1:Ca:48:LYS:N	2.26	0.50
1:Aw:48:LYS:HD3	1:Aw:48:LYS:N	2.26	0.50
1:Aw:262:LEU:HD23	1:Ay:260:THR:HG22	1.93	0.50
1:Bi:114:GLY:HA3	1:Bi:134:MET:SD	2.51	0.50
1:Bm:262:LEU:HD23	1:Bo:260:THR:HG22	1.93	0.50
1:Ag:48:LYS:HD3	1:Ag:48:LYS:N	2.26	0.49
1:As:48:LYS:HD3	1:As:48:LYS:N	2.26	0.49
1:Ba:48:LYS:HD3	1:Ba:48:LYS:N	2.26	0.49
1:Bu:114:GLY:HA3	1:Bu:134:MET:SD	2.51	0.49
1:By:114:GLY:HA3	1:By:134:MET:SD	2.51	0.49
1:Ae:48:LYS:HD3	1:Ae:48:LYS:N	2.26	0.49
1:Ao:48:LYS:HD3	1:Ao:48:LYS:N	2.26	0.49
1:Au:114:GLY:HA3	1:Au:134:MET:SD	2.51	0.49
1:Ay:48:LYS:HD3	1:Ay:48:LYS:N	2.26	0.49
1:Bm:48:LYS:HD3	1:Bm:48:LYS:N	2.26	0.49
1:Aa:114:GLY:HA3	1:Aa:134:MET:SD	2.51	0.49
1:Ak:114:GLY:HA3	1:Ak:134:MET:SD	2.51	0.49
1:Bq:114:GLY:HA3	1:Bq:134:MET:SD	2.51	0.49
1:Cc:184:TYR:OH	2:Cd:4:U:O2	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:48:LYS:HD3	1:Bk:48:LYS:N	2.26	0.49
1:Aq:260:THR:HG22	1:Bu:262:LEU:HD23	1.94	0.49
1:Ac:262:LEU:HD23	1:Ae:260:THR:HG22	1.94	0.49
1:Au:48:LYS:HD3	1:Au:48:LYS:H	1.79	0.48
1:Ag:48:LYS:HD3	1:Ag:48:LYS:H	1.79	0.48
1:As:48:LYS:HD3	1:As:48:LYS:H	1.79	0.48
1:Bm:48:LYS:HD3	1:Bm:48:LYS:H	1.79	0.48
1:Ac:48:LYS:HD3	1:Ac:48:LYS:H	1.78	0.48
1:Bk:48:LYS:HD3	1:Bk:48:LYS:H	1.79	0.48
1:Aw:48:LYS:HD3	1:Aw:48:LYS:H	1.79	0.48
1:Aa:260:THR:HG22	1:Be:262:LEU:HD23	1.95	0.48
1:Ay:48:LYS:HD3	1:Ay:48:LYS:H	1.78	0.48
1:Bo:48:LYS:HD3	1:Bo:48:LYS:H	1.79	0.48
1:Am:48:LYS:HD3	1:Am:48:LYS:H	1.79	0.48
1:Ae:48:LYS:HD3	1:Ae:48:LYS:H	1.79	0.48
1:Ai:48:LYS:HD3	1:Ai:48:LYS:H	1.79	0.48
1:Ak:48:LYS:HD3	1:Ak:48:LYS:H	1.79	0.48
1:Aa:48:LYS:HD3	1:Aa:48:LYS:H	1.79	0.48
1:Ag:66:ASN:HB3	1:Ai:113:ASN:ND2	2.29	0.48
1:Ca:48:LYS:HD3	1:Ca:48:LYS:H	1.79	0.48
1:Ac:197:ARG:NH2	1:Ca:146:LYS:HD3	2.29	0.47
1:Bq:184:TYR:OH	2:Br:4:U:O2	2.20	0.47
1:Ai:66:ASN:HB3	1:Ak:113:ASN:ND2	2.30	0.47
1:Ao:48:LYS:HD3	1:Ao:48:LYS:H	1.79	0.47
1:Bc:121:GLU:OE2	1:Bc:182:PRO:HA	2.15	0.47
1:Ca:66:ASN:HB3	1:Cc:113:ASN:ND2	2.30	0.47
1:Ay:184:TYR:OH	2:Az:4:U:O2	2.20	0.47
1:Be:146:LYS:HD3	1:Bs:197:ARG:NH2	2.29	0.47
1:Bg:48:LYS:HD3	1:Bg:48:LYS:H	1.79	0.47
1:Bk:66:ASN:HB3	1:Bm:113:ASN:ND2	2.30	0.47
1:Bk:121:GLU:OE2	1:Bk:182:PRO:HA	2.15	0.47
1:As:121:GLU:OE2	1:As:182:PRO:HA	2.15	0.47
1:Ba:48:LYS:HD3	1:Ba:48:LYS:H	1.79	0.47
1:Be:48:LYS:HD3	1:Be:48:LYS:H	1.78	0.47
1:Bi:121:GLU:OE2	1:Bi:182:PRO:HA	2.15	0.47
1:Bo:121:GLU:OE2	1:Bo:182:PRO:HA	2.15	0.47
1:Bs:66:ASN:HB3	1:Bu:113:ASN:ND2	2.30	0.47
1:Cc:121:GLU:OE2	1:Cc:182:PRO:HA	2.15	0.47
1:Ak:121:GLU:OE2	1:Ak:182:PRO:HA	2.15	0.47
1:Ao:65:LEU:HD21	1:Bw:163:PHE:HE2	1.80	0.47
1:Aq:121:GLU:OE2	1:Aq:182:PRO:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Au:66:ASN:HB3	1:Aw:113:ASN:ND2	2.30	0.47
1:Aw:121:GLU:OE2	1:Aw:182:PRO:HA	2.15	0.47
1:Ay:66:ASN:HB3	1:Ba:113:ASN:ND2	2.30	0.47
1:Ba:121:GLU:OE2	1:Ba:182:PRO:HA	2.15	0.47
1:Bg:66:ASN:HB3	1:Bi:113:ASN:ND2	2.30	0.47
1:Bq:48:LYS:HD3	1:Bq:48:LYS:H	1.79	0.47
1:Bw:48:LYS:HD3	1:Bw:48:LYS:H	1.79	0.47
1:Ae:146:LYS:HD3	1:As:197:ARG:NH2	2.29	0.47
1:Ai:121:GLU:OE2	1:Ai:182:PRO:HA	2.15	0.47
1:Ai:146:LYS:HD3	1:Aw:197:ARG:NH2	2.30	0.47
1:Am:66:ASN:HB3	1:Ao:113:ASN:ND2	2.30	0.47
1:Am:121:GLU:OE2	1:Am:182:PRO:HA	2.15	0.47
1:Au:121:GLU:OE2	1:Au:182:PRO:HA	2.15	0.47
1:Be:121:GLU:OE2	1:Be:182:PRO:HA	2.15	0.47
1:Bi:48:LYS:HD3	1:Bi:48:LYS:H	1.79	0.47
1:Bs:121:GLU:OE2	1:Bs:182:PRO:HA	2.15	0.47
1:Bu:121:GLU:OE2	1:Bu:182:PRO:HA	2.15	0.47
1:By:48:LYS:HD3	1:By:48:LYS:H	1.79	0.47
1:Aa:113:ASN:ND2	1:Be:66:ASN:HB3	2.29	0.47
1:Aq:48:LYS:HD3	1:Aq:48:LYS:H	1.78	0.47
1:Bm:121:GLU:OE2	1:Bm:182:PRO:HA	2.15	0.47
1:Cc:48:LYS:HD3	1:Cc:48:LYS:H	1.79	0.47
1:Ag:146:LYS:HD3	1:Au:197:ARG:NH2	2.30	0.47
1:Ak:146:LYS:HD3	1:Ay:197:ARG:NH2	2.30	0.47
1:As:66:ASN:HB3	1:Au:113:ASN:ND2	2.30	0.47
1:Bi:66:ASN:HB3	1:Bk:113:ASN:ND2	2.30	0.47
1:Bi:168:GLU:HG3	1:Bi:197:ARG:HB2	1.97	0.47
1:Aa:121:GLU:OE2	1:Aa:182:PRO:HA	2.15	0.47
1:Ae:168:GLU:HG3	1:Ae:197:ARG:HB2	1.97	0.47
1:Ag:121:GLU:OE2	1:Ag:182:PRO:HA	2.15	0.47
1:Aw:168:GLU:HG3	1:Aw:197:ARG:HB2	1.97	0.47
1:Ba:66:ASN:HB3	1:Bc:113:ASN:ND2	2.30	0.47
1:Bc:146:LYS:HD3	1:Bq:197:ARG:NH2	2.30	0.47
1:Bg:121:GLU:OE2	1:Bg:182:PRO:HA	2.15	0.47
1:Bo:66:ASN:HB3	1:Bq:113:ASN:ND2	2.30	0.47
1:Ca:121:GLU:OE2	1:Ca:182:PRO:HA	2.15	0.47
1:Ai:168:GLU:HG3	1:Ai:197:ARG:HB2	1.97	0.46
1:Ao:66:ASN:HB3	1:Bw:113:ASN:ND2	2.30	0.46
1:Aq:66:ASN:HB3	1:As:113:ASN:ND2	2.30	0.46
1:Au:168:GLU:HG3	1:Au:197:ARG:HB2	1.97	0.46
1:Bq:121:GLU:OE2	1:Bq:182:PRO:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:168:GLU:HG3	1:Ag:197:ARG:HB2	1.97	0.46
1:Am:146:LYS:HD3	1:Ba:197:ARG:NH2	2.30	0.46
1:Ao:121:GLU:OE2	1:Ao:182:PRO:HA	2.15	0.46
1:As:168:GLU:HG3	1:As:197:ARG:HB2	1.97	0.46
1:Ba:65:LEU:HD21	1:Bc:163:PHE:HE2	1.81	0.46
1:Bm:168:GLU:HG3	1:Bm:197:ARG:HB2	1.97	0.46
1:Bw:66:ASN:HB3	1:By:113:ASN:ND2	2.30	0.46
1:Aa:197:ARG:NH2	1:By:146:LYS:HD3	2.30	0.46
1:Ac:121:GLU:OE2	1:Ac:182:PRO:HA	2.15	0.46
1:Ae:66:ASN:HB3	1:Ag:113:ASN:ND2	2.30	0.46
1:Ae:197:ARG:NH2	1:Cc:146:LYS:HD3	2.31	0.46
1:Bc:66:ASN:HB3	1:Be:113:ASN:ND2	2.30	0.46
1:Bg:168:GLU:HG3	1:Bg:197:ARG:HB2	1.97	0.46
1:Bk:168:GLU:HG3	1:Bk:197:ARG:HB2	1.97	0.46
1:Bq:65:LEU:HD21	1:Bs:163:PHE:HE2	1.81	0.46
1:Bs:48:LYS:HD3	1:Bs:48:LYS:H	1.79	0.46
1:Bu:48:LYS:HD3	1:Bu:48:LYS:H	1.78	0.46
1:Ca:168:GLU:HG3	1:Ca:197:ARG:HB2	1.97	0.46
1:Ak:168:GLU:HG3	1:Ak:197:ARG:HB2	1.97	0.46
1:Ay:121:GLU:OE2	1:Ay:182:PRO:HA	2.15	0.46
1:Bm:66:ASN:HB3	1:Bo:113:ASN:ND2	2.31	0.46
1:By:66:ASN:HB3	1:Ca:113:ASN:ND2	2.30	0.46
1:By:121:GLU:OE2	1:By:182:PRO:HA	2.15	0.46
1:Cc:168:GLU:HG3	1:Cc:197:ARG:HB2	1.97	0.46
1:Aa:66:ASN:HB3	1:Ac:113:ASN:ND2	2.31	0.46
1:Aq:168:GLU:HG3	1:Aq:197:ARG:HB2	1.97	0.46
1:Ac:168:GLU:HG3	1:Ac:197:ARG:HB2	1.97	0.46
1:Ak:65:LEU:HD21	1:Am:163:PHE:HE2	1.81	0.46
1:Ae:121:GLU:OE2	1:Ae:182:PRO:HA	2.15	0.46
1:Ay:168:GLU:HG3	1:Ay:197:ARG:HB2	1.98	0.46
1:Bw:121:GLU:OE2	1:Bw:182:PRO:HA	2.15	0.46
1:By:65:LEU:HD21	1:Ca:163:PHE:HE2	1.81	0.46
1:Ba:168:GLU:HG3	1:Ba:197:ARG:HB2	1.97	0.46
1:Bq:66:ASN:HB3	1:Bs:113:ASN:ND2	2.30	0.46
1:Aa:184:TYR:OH	2:Ab:4:U:O2	2.20	0.46
1:Bi:65:LEU:HD21	1:Bk:163:PHE:HE2	1.81	0.46
1:Bo:168:GLU:HG3	1:Bo:197:ARG:HB2	1.97	0.46
1:Aa:168:GLU:HG3	1:Aa:197:ARG:HB2	1.98	0.46
1:Ag:65:LEU:HD21	1:Ai:163:PHE:HE2	1.81	0.46
1:Ao:184:TYR:OH	2:Ap:4:U:O2	2.20	0.46
1:By:168:GLU:HG3	1:By:197:ARG:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bc:48:LYS:HD3	1:Bc:48:LYS:H	1.78	0.45
1:Ak:66:ASN:HB3	1:Am:113:ASN:ND2	2.30	0.45
1:Am:168:GLU:HG3	1:Am:197:ARG:HB2	1.97	0.45
1:Bk:184:TYR:OH	2:Bl:4:U:O2	2.20	0.45
1:Bs:132:TRP:CD1	1:Bs:145:LEU:HD13	2.52	0.45
1:Ca:65:LEU:HD21	1:Cc:163:PHE:HE2	1.82	0.45
1:Aa:135:MET:CG	1:Be:75:PRO:HB3	2.47	0.45
1:Ae:65:LEU:HD21	1:Ag:163:PHE:HE2	1.82	0.45
1:Ai:132:TRP:CD1	1:Ai:145:LEU:HD13	2.52	0.45
1:Ao:146:LYS:HD3	1:Bc:197:ARG:NH2	2.31	0.45
1:Ao:168:GLU:HG3	1:Ao:197:ARG:HB2	1.97	0.45
1:As:146:LYS:HD3	1:Bg:197:ARG:NH2	2.32	0.45
1:Aw:132:TRP:CD1	1:Aw:145:LEU:HD13	2.52	0.45
1:Bc:245:ASN:HD22	1:Bq:231:ARG:HD3	1.81	0.45
1:Be:132:TRP:CD1	1:Be:145:LEU:HD13	2.52	0.45
1:Be:197:ARG:NH2	1:Bw:146:LYS:HD3	2.31	0.45
1:Bg:65:LEU:HD21	1:Bi:163:PHE:HE2	1.82	0.45
1:Bq:168:GLU:HG3	1:Bq:197:ARG:HB2	1.97	0.45
1:Bu:168:GLU:HG3	1:Bu:197:ARG:HB2	1.97	0.45
1:Ac:66:ASN:HB3	1:Ae:113:ASN:ND2	2.31	0.45
1:Ao:132:TRP:CD1	1:Ao:145:LEU:HD13	2.52	0.45
1:Aq:65:LEU:HD21	1:As:163:PHE:HE2	1.82	0.45
1:Ay:146:LYS:HD3	1:Bm:197:ARG:NH2	2.31	0.45
1:Bk:132:TRP:CD1	1:Bk:145:LEU:HD13	2.52	0.45
1:Bs:168:GLU:HG3	1:Bs:197:ARG:HB2	1.97	0.45
1:Bw:132:TRP:CD1	1:Bw:145:LEU:HD13	2.52	0.45
1:Bw:168:GLU:HG3	1:Bw:197:ARG:HB2	1.97	0.45
1:Ak:132:TRP:CD1	1:Ak:145:LEU:HD13	2.52	0.45
1:As:65:LEU:HD21	1:Au:163:PHE:HE2	1.81	0.45
1:Ba:146:LYS:HD3	1:Bo:197:ARG:NH2	2.31	0.45
1:Bc:132:TRP:CD1	1:Bc:145:LEU:HD13	2.52	0.45
1:Bc:168:GLU:HG3	1:Bc:197:ARG:HB2	1.97	0.45
1:Bo:132:TRP:CD1	1:Bo:145:LEU:HD13	2.52	0.45
1:Bq:132:TRP:CD1	1:Bq:145:LEU:HD13	2.52	0.45
1:Au:65:LEU:HD21	1:Aw:163:PHE:HE2	1.82	0.45
1:Au:146:LYS:HD3	1:Bi:197:ARG:NH2	2.32	0.45
1:Aw:66:ASN:HB3	1:Ay:113:ASN:ND2	2.31	0.45
1:Ay:132:TRP:CD1	1:Ay:145:LEU:HD13	2.52	0.45
1:Ba:139:GLU:HG2	1:Bm:46:ARG:HH21	1.82	0.45
1:Bc:103:ILE:CG2	1:Bc:107:GLU:HG3	2.46	0.45
1:Be:168:GLU:HG3	1:Be:197:ARG:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:132:TRP:CD1	1:Bm:145:LEU:HD13	2.52	0.45
1:Cc:132:TRP:CD1	1:Cc:145:LEU:HD13	2.52	0.45
1:Aa:146:LYS:HD3	1:Bu:197:ARG:NH2	2.31	0.45
1:Ac:65:LEU:HD21	1:Ae:163:PHE:HE2	1.81	0.45
1:Ac:132:TRP:CD1	1:Ac:145:LEU:HD13	2.52	0.45
1:Ac:146:LYS:HD3	1:Aq:197:ARG:NH2	2.31	0.45
1:Ae:132:TRP:CD1	1:Ae:145:LEU:HD13	2.52	0.45
1:Bg:132:TRP:CD1	1:Bg:145:LEU:HD13	2.52	0.45
1:Bo:184:TYR:OH	2:Bp:4:U:O2	2.20	0.45
1:Ca:132:TRP:CD1	1:Ca:145:LEU:HD13	2.52	0.45
1:Ai:65:LEU:HD21	1:Ak:163:PHE:HE2	1.82	0.45
1:Ai:199:ALA:HA	1:Ai:220:MET:HE1	1.99	0.45
1:As:132:TRP:CD1	1:As:145:LEU:HD13	2.52	0.45
1:Bc:65:LEU:HD21	1:Be:163:PHE:HE2	1.82	0.45
1:Bm:65:LEU:HD21	1:Bo:163:PHE:HE2	1.82	0.45
1:Bs:65:LEU:HD21	1:Bu:163:PHE:HE2	1.82	0.45
1:Aa:132:TRP:CD1	1:Aa:145:LEU:HD13	2.52	0.45
1:Ag:199:ALA:HA	1:Ag:220:MET:HE1	1.99	0.45
1:Ak:245:ASN:HD22	1:Ay:231:ARG:HD3	1.82	0.45
1:Aq:132:TRP:CD1	1:Aq:145:LEU:HD13	2.52	0.45
1:Aw:65:LEU:HD21	1:Ay:163:PHE:HE2	1.82	0.45
1:Ay:103:ILE:CG2	1:Ay:107:GLU:HG3	2.46	0.45
1:Bk:167:ALA:O	1:Bk:171:ILE:HG13	2.17	0.45
1:Bu:132:TRP:CD1	1:Bu:145:LEU:HD13	2.52	0.45
1:Ae:167:ALA:O	1:Ae:171:ILE:HG13	2.17	0.44
1:Ak:184:TYR:OH	2:Al:4:U:O2	2.20	0.44
1:Am:132:TRP:CD1	1:Am:145:LEU:HD13	2.52	0.44
1:Aq:113:ASN:ND2	1:Bu:66:ASN:HB3	2.32	0.44
1:Au:167:ALA:O	1:Au:171:ILE:HG13	2.18	0.44
1:Aw:184:TYR:OH	2:Ax:4:U:O2	2.20	0.44
1:Be:245:ASN:HD22	1:Bs:231:ARG:HD3	1.82	0.44
1:Bk:65:LEU:HD21	1:Bm:163:PHE:HE2	1.82	0.44
1:Bo:199:ALA:HA	1:Bo:220:MET:HE1	2.00	0.44
1:Cc:167:ALA:O	1:Cc:171:ILE:HG13	2.17	0.44
1:Aa:163:PHE:HE2	1:Be:65:LEU:HD21	1.82	0.44
1:Ai:103:ILE:CG2	1:Ai:107:GLU:HG3	2.46	0.44
1:Am:245:ASN:HD22	1:Ba:231:ARG:HD3	1.82	0.44
1:Aq:163:PHE:HE2	1:Bu:65:LEU:HD21	1.83	0.44
1:As:167:ALA:O	1:As:171:ILE:HG13	2.17	0.44
1:Ba:103:ILE:CG2	1:Ba:107:GLU:HG3	2.46	0.44
1:Bc:199:ALA:HA	1:Bc:220:MET:HE1	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bm:199:ALA:HA	1:Bm:220:MET:HE1	2.00	0.44
1:Bq:199:ALA:HA	1:Bq:220:MET:HE1	1.99	0.44
1:Ak:199:ALA:HA	1:Ak:220:MET:HE1	1.99	0.44
1:Am:65:LEU:HD21	1:Ao:163:PHE:HE2	1.82	0.44
1:As:199:ALA:HA	1:As:220:MET:HE1	1.99	0.44
1:Au:132:TRP:CD1	1:Au:145:LEU:HD13	2.52	0.44
1:Aw:167:ALA:O	1:Aw:171:ILE:HG13	2.18	0.44
1:Ay:65:LEU:HD21	1:Ba:163:PHE:HE2	1.82	0.44
1:Be:199:ALA:HA	1:Be:220:MET:HE1	1.99	0.44
1:Bi:167:ALA:O	1:Bi:171:ILE:HG13	2.18	0.44
1:Bk:199:ALA:HA	1:Bk:220:MET:HE1	1.99	0.44
1:Ag:132:TRP:CD1	1:Ag:145:LEU:HD13	2.52	0.44
1:Ag:167:ALA:O	1:Ag:171:ILE:HG13	2.18	0.44
1:Au:199:ALA:HA	1:Au:220:MET:HE1	1.99	0.44
1:Ba:132:TRP:CD1	1:Ba:145:LEU:HD13	2.52	0.44
1:Bm:167:ALA:O	1:Bm:171:ILE:HG13	2.17	0.44
1:Bw:65:LEU:HD21	1:By:163:PHE:HE2	1.82	0.44
1:Aa:75:PRO:HB3	1:Ac:135:MET:CG	2.47	0.44
1:Ai:167:ALA:O	1:Ai:171:ILE:HG13	2.17	0.44
1:Aw:139:GLU:HG2	1:Bi:46:ARG:HH21	1.83	0.44
1:Ba:199:ALA:HA	1:Ba:220:MET:HE1	1.99	0.44
1:Bg:167:ALA:O	1:Bg:171:ILE:HG13	2.17	0.44
1:Bo:65:LEU:HD21	1:Bq:163:PHE:HE2	1.82	0.44
1:Bo:103:ILE:CG2	1:Bo:107:GLU:HG3	2.46	0.44
1:Ca:167:ALA:O	1:Ca:171:ILE:HG13	2.17	0.44
1:Ac:167:ALA:O	1:Ac:171:ILE:HG13	2.17	0.44
1:Am:199:ALA:HA	1:Am:220:MET:HE1	1.99	0.44
1:Bc:139:GLU:HG2	1:Bo:46:ARG:HH21	1.83	0.44
1:Be:46:ARG:HH21	1:By:139:GLU:HG2	1.83	0.44
1:Bi:132:TRP:CD1	1:Bi:145:LEU:HD13	2.52	0.44
1:Ca:199:ALA:HA	1:Ca:220:MET:HE1	1.99	0.44
1:Ae:75:PRO:HB3	1:Ag:135:MET:CG	2.48	0.44
1:Ak:167:ALA:O	1:Ak:171:ILE:HG13	2.17	0.44
1:Aq:199:ALA:HA	1:Aq:220:MET:HE1	1.99	0.44
1:Ae:199:ALA:HA	1:Ae:220:MET:HE1	2.00	0.44
1:As:75:PRO:HB3	1:Au:135:MET:CG	2.48	0.44
1:Aw:146:LYS:HD3	1:Bk:197:ARG:NH2	2.32	0.44
1:Ay:139:GLU:HG2	1:Bk:46:ARG:HH21	1.83	0.44
1:Bq:75:PRO:HB3	1:Bs:135:MET:CG	2.48	0.44
1:By:75:PRO:HB3	1:Ca:135:MET:CG	2.48	0.44
1:Aq:167:ALA:O	1:Aq:171:ILE:HG13	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bk:103:ILE:CG2	1:Bk:107:GLU:HG3	2.46	0.44
1:Bo:75:PRO:HB3	1:Bq:135:MET:CG	2.48	0.44
1:Bo:167:ALA:O	1:Bo:171:ILE:HG13	2.17	0.44
1:Bw:199:ALA:HA	1:Bw:220:MET:HE1	1.99	0.44
1:By:199:ALA:HA	1:By:220:MET:HE1	2.00	0.44
1:Ae:231:ARG:HD3	1:Cc:245:ASN:HD22	1.82	0.43
1:Am:75:PRO:HB3	1:Ao:135:MET:CG	2.48	0.43
1:Aq:75:PRO:HB3	1:As:135:MET:CG	2.48	0.43
1:Aw:75:PRO:HB3	1:Ay:135:MET:CG	2.48	0.43
1:Ay:75:PRO:HB3	1:Ba:135:MET:CG	2.48	0.43
1:Ba:245:ASN:HD22	1:Bo:231:ARG:HD3	1.83	0.43
1:Bc:167:ALA:O	1:Bc:171:ILE:HG13	2.17	0.43
1:Bi:75:PRO:HB3	1:Bk:135:MET:CG	2.48	0.43
1:Bk:75:PRO:HB3	1:Bm:135:MET:CG	2.48	0.43
1:Aa:65:LEU:HD21	1:Ac:163:PHE:HE2	1.83	0.43
1:Ae:245:ASN:HD22	1:As:231:ARG:HD3	1.83	0.43
1:Ak:103:ILE:CG2	1:Ak:107:GLU:HG3	2.46	0.43
1:Au:139:GLU:HG2	1:Bg:46:ARG:HH21	1.84	0.43
1:Ay:167:ALA:O	1:Ay:171:ILE:HG13	2.17	0.43
1:Bc:75:PRO:HB3	1:Be:135:MET:CG	2.48	0.43
1:Bi:199:ALA:HA	1:Bi:220:MET:HE1	1.99	0.43
1:Bm:75:PRO:HB3	1:Bo:135:MET:CG	2.48	0.43
1:Aa:199:ALA:HA	1:Aa:220:MET:HE1	2.00	0.43
1:Ac:245:ASN:HD22	1:Aq:231:ARG:HD3	1.83	0.43
1:Ak:75:PRO:HB3	1:Am:135:MET:CG	2.48	0.43
1:Aq:135:MET:CG	1:Bu:75:PRO:HB3	2.47	0.43
1:Aw:199:ALA:HA	1:Aw:220:MET:HE1	2.00	0.43
1:Bs:75:PRO:HB3	1:Bu:135:MET:CG	2.48	0.43
1:Bs:199:ALA:HA	1:Bs:220:MET:HE1	1.99	0.43
1:Bw:167:ALA:O	1:Bw:171:ILE:HG13	2.17	0.43
1:By:132:TRP:CD1	1:By:145:LEU:HD13	2.52	0.43
1:By:167:ALA:O	1:By:171:ILE:HG13	2.17	0.43
1:Cc:199:ALA:HA	1:Cc:220:MET:HE1	1.99	0.43
1:Ag:75:PRO:HB3	1:Ai:135:MET:CG	2.49	0.43
1:Am:103:ILE:CG2	1:Am:107:GLU:HG3	2.46	0.43
1:Ba:235:LEU:HD23	1:Bo:218:ILE:HG22	2.00	0.43
1:Bg:199:ALA:HA	1:Bg:220:MET:HE1	1.99	0.43
1:Ai:75:PRO:HB3	1:Ak:135:MET:CG	2.48	0.43
1:Bu:167:ALA:O	1:Bu:171:ILE:HG13	2.17	0.43
1:Bw:75:PRO:HB3	1:By:135:MET:CG	2.48	0.43
1:Ay:199:ALA:HA	1:Ay:220:MET:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ba:75:PRO:HB3	1:Bc:135:MET:CG	2.48	0.43
1:Bw:120:ILE:HG23	1:Bw:171:ILE:HD11	2.01	0.43
1:Ca:75:PRO:HB3	1:Cc:135:MET:CG	2.48	0.43
1:Aa:167:ALA:O	1:Aa:171:ILE:HG13	2.17	0.43
1:Ao:167:ALA:O	1:Ao:171:ILE:HG13	2.18	0.43
1:Ao:199:ALA:HA	1:Ao:220:MET:HE1	1.99	0.43
1:As:69:HIS:CD2	1:Au:110:THR:HG23	2.54	0.43
1:Bc:119:CYS:C	1:Bc:121:GLU:N	2.77	0.43
1:Bo:120:ILE:HG23	1:Bo:171:ILE:HD11	2.01	0.43
1:Aa:120:ILE:HG23	1:Aa:171:ILE:HD11	2.01	0.43
1:Ac:139:GLU:HG2	1:Bu:46:ARG:HH21	1.84	0.43
1:Ag:184:TYR:OH	2:Ah:4:U:O2	2.20	0.43
1:Ak:139:GLU:HG2	1:Aw:46:ARG:HH21	1.84	0.43
1:Am:83:THR:HG22	2:An:1:U:H5"	2.01	0.43
1:Am:119:CYS:O	1:Am:120:ILE:C	2.62	0.43
1:Ao:120:ILE:HG23	1:Ao:171:ILE:HD11	2.01	0.43
1:Aw:83:THR:HG22	2:Ax:1:U:H5"	2.01	0.43
1:Aw:235:LEU:HD23	1:Bk:218:ILE:HG22	2.01	0.43
1:Be:120:ILE:HG23	1:Be:171:ILE:HD11	2.01	0.43
1:Be:167:ALA:O	1:Be:171:ILE:HG13	2.17	0.43
1:Bk:83:THR:HG22	2:Bl:1:U:H5"	2.01	0.43
1:Bu:199:ALA:HA	1:Bu:220:MET:HE1	1.99	0.43
1:Aa:69:HIS:CD2	1:Ac:110:THR:HG23	2.54	0.43
1:Ac:46:ARG:HH21	1:Cc:139:GLU:HG2	1.84	0.43
1:Ag:83:THR:HG22	2:Ah:1:U:H5"	2.01	0.43
1:Ai:245:ASN:HD22	1:Aw:231:ARG:HD3	1.83	0.43
1:Aq:110:THR:HG23	1:Bu:69:HIS:CD2	2.53	0.43
1:Au:75:PRO:HB3	1:Aw:135:MET:CG	2.48	0.43
1:Ay:83:THR:HG22	2:Az:1:U:H5"	2.01	0.43
1:Ba:83:THR:HG22	2:Bb:1:U:H5"	2.01	0.43
1:Ba:167:ALA:O	1:Ba:171:ILE:HG13	2.17	0.43
1:Be:139:GLU:HG2	1:Bq:46:ARG:HH21	1.83	0.43
1:Bs:83:THR:HG22	2:Bt:1:U:H5"	2.01	0.43
1:Bu:120:ILE:HG23	1:Bu:171:ILE:HD11	2.01	0.43
1:Aa:46:ARG:HH21	1:Ca:139:GLU:HG2	1.84	0.43
1:Ac:235:LEU:HD23	1:Aq:218:ILE:HG22	2.01	0.43
1:Ak:69:HIS:CD2	1:Am:110:THR:HG23	2.54	0.43
1:Ak:83:THR:HG22	2:Al:1:U:H5"	2.01	0.43
1:Ao:83:THR:HG22	2:Ap:1:U:H5"	2.01	0.43
1:Aq:120:ILE:HG23	1:Aq:171:ILE:HD11	2.01	0.43
1:Aw:69:HIS:CD2	1:Ay:110:THR:HG23	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ay:120:ILE:HG23	1:Ay:171:ILE:HD11	2.01	0.43
1:Bg:75:PRO:HB3	1:Bi:135:MET:CG	2.48	0.43
1:Bm:69:HIS:CD2	1:Bo:110:THR:HG23	2.54	0.43
1:Bm:83:THR:HG22	2:Bn:1:U:H5''	2.01	0.43
1:Bq:167:ALA:O	1:Bq:171:ILE:HG13	2.17	0.43
1:By:69:HIS:CD2	1:Ca:110:THR:HG23	2.54	0.43
1:Ae:146:LYS:HD3	1:As:197:ARG:HH22	1.84	0.42
1:Ai:83:THR:HG22	2:Aj:1:U:H5''	2.01	0.42
1:Am:184:TYR:OH	2:An:4:U:O2	2.20	0.42
1:Bc:83:THR:HG22	2:Bd:1:U:H5''	2.01	0.42
1:Bc:119:CYS:O	1:Bc:120:ILE:C	2.62	0.42
1:Be:83:THR:HG22	2:Bf:1:U:H5''	2.01	0.42
1:Bi:83:THR:HG22	2:Bj:1:U:H5''	2.01	0.42
1:Bs:167:ALA:O	1:Bs:171:ILE:HG13	2.17	0.42
1:Cc:83:THR:HG22	2:Cd:1:U:H5''	2.01	0.42
1:Aa:231:ARG:HD3	1:By:245:ASN:HD22	1.83	0.42
1:Ae:83:THR:HG22	2:Af:1:U:H5''	2.01	0.42
1:Ae:139:GLU:HG2	1:Aq:46:ARG:HH21	1.85	0.42
1:Ae:218:ILE:HG22	1:Cc:235:LEU:HD23	2.01	0.42
1:Au:69:HIS:CD2	1:Aw:110:THR:HG23	2.55	0.42
1:Ay:119:CYS:O	1:Ay:120:ILE:C	2.62	0.42
1:Bo:83:THR:HG22	2:Bp:1:U:H5''	2.01	0.42
1:Bq:83:THR:HG22	2:Br:1:U:H5''	2.01	0.42
1:Bq:120:ILE:HG23	1:Bq:171:ILE:HD11	2.01	0.42
1:Ac:199:ALA:HA	1:Ac:220:MET:HE1	2.00	0.42
1:Ai:69:HIS:CD2	1:Ak:110:THR:HG23	2.55	0.42
1:Ai:119:CYS:O	1:Ai:120:ILE:C	2.62	0.42
1:Ak:120:ILE:HG23	1:Ak:171:ILE:HD11	2.01	0.42
1:Aq:69:HIS:CD2	1:As:110:THR:HG23	2.55	0.42
1:As:187:VAL:HG12	1:As:188:ARG:NH2	2.35	0.42
1:Ay:69:HIS:CD2	1:Ba:110:THR:HG23	2.55	0.42
1:Ba:119:CYS:C	1:Ba:121:GLU:N	2.77	0.42
1:Ba:120:ILE:HG23	1:Ba:171:ILE:HD11	2.01	0.42
1:Bc:187:VAL:HG12	1:Bc:188:ARG:NH2	2.35	0.42
1:Bg:69:HIS:CD2	1:Bi:110:THR:HG23	2.55	0.42
1:Bi:69:HIS:CD2	1:Bk:110:THR:HG23	2.54	0.42
1:Bo:119:CYS:C	1:Bo:121:GLU:N	2.77	0.42
1:Bq:69:HIS:CD2	1:Bs:110:THR:HG23	2.54	0.42
1:Bw:119:CYS:C	1:Bw:121:GLU:N	2.77	0.42
1:Aa:83:THR:HG22	2:Ab:1:U:H5''	2.01	0.42
1:Aa:139:GLU:HG2	1:Bs:46:ARG:HH21	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:120:ILE:HG23	1:Ai:171:ILE:HD11	2.01	0.42
1:Ak:187:VAL:HG12	1:Ak:188:ARG:NH2	2.35	0.42
1:Am:187:VAL:HG12	1:Am:188:ARG:NH2	2.35	0.42
1:As:83:THR:HG22	2:At:1:U:H5''	2.01	0.42
1:As:238:GLY:O	1:Bi:226:LYS:NZ	2.50	0.42
1:Au:83:THR:HG22	2:Av:1:U:H5''	2.01	0.42
1:Ba:187:VAL:HG12	1:Ba:188:ARG:NH2	2.35	0.42
1:Bg:83:THR:HG22	2:Bh:1:U:H5''	2.01	0.42
1:Bm:103:ILE:CG2	1:Bm:107:GLU:HG3	2.46	0.42
1:By:120:ILE:HG23	1:By:171:ILE:HD11	2.01	0.42
1:Ca:187:VAL:HG12	1:Ca:188:ARG:NH2	2.35	0.42
1:Ac:69:HIS:CD2	1:Ae:110:THR:HG23	2.54	0.42
1:Ac:197:ARG:HH22	1:Ca:146:LYS:HD3	1.84	0.42
1:Ac:231:ARG:HD3	1:Ca:245:ASN:HD22	1.82	0.42
1:Am:167:ALA:O	1:Am:171:ILE:HG13	2.17	0.42
1:Ao:119:CYS:C	1:Ao:121:GLU:N	2.76	0.42
1:Aq:83:THR:HG22	2:Ar:1:U:H5''	2.01	0.42
1:Aq:184:TYR:OH	2:Ar:4:U:O2	2.20	0.42
1:Au:187:VAL:HG12	1:Au:188:ARG:NH2	2.35	0.42
1:Ay:187:VAL:HG12	1:Ay:188:ARG:NH2	2.35	0.42
1:Bc:46:ARG:HH21	1:Bw:139:GLU:HG2	1.84	0.42
1:Bm:120:ILE:HG23	1:Bm:171:ILE:HD11	2.01	0.42
1:Bo:119:CYS:O	1:Bo:120:ILE:C	2.62	0.42
1:Bq:187:VAL:HG12	1:Bq:188:ARG:NH2	2.35	0.42
1:Bu:83:THR:HG22	2:Bv:1:U:H5''	2.01	0.42
1:By:83:THR:HG22	2:Bz:1:U:H5''	2.01	0.42
1:Ak:235:LEU:HD23	1:Ay:218:ILE:HG22	2.02	0.42
1:Am:69:HIS:CD2	1:Ao:110:THR:HG23	2.55	0.42
1:Ao:187:VAL:HG12	1:Ao:188:ARG:NH2	2.35	0.42
1:Bc:69:HIS:CD2	1:Be:110:THR:HG23	2.55	0.42
1:Bc:246:THR:HG22	1:Bq:232:LEU:HD22	2.02	0.42
1:Bg:120:ILE:HG23	1:Bg:171:ILE:HD11	2.01	0.42
1:Bo:69:HIS:CD2	1:Bq:110:THR:HG23	2.55	0.42
1:Bs:119:CYS:O	1:Bs:120:ILE:C	2.62	0.42
1:Bs:187:VAL:HG12	1:Bs:188:ARG:NH2	2.35	0.42
1:Bw:83:THR:HG22	2:Bx:1:U:H5''	2.01	0.42
1:By:187:VAL:HG12	1:By:188:ARG:NH2	2.35	0.42
1:Ca:120:ILE:HG23	1:Ca:171:ILE:HD11	2.01	0.42
1:Ae:69:HIS:CD2	1:Ag:110:THR:HG23	2.55	0.42
1:Ae:120:ILE:HG23	1:Ae:171:ILE:HD11	2.01	0.42
1:Ag:69:HIS:CD2	1:Ai:110:THR:HG23	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ai:139:GLU:HG2	1:Au:46:ARG:HH21	1.84	0.42
1:Ai:187:VAL:HG12	1:Ai:188:ARG:NH2	2.35	0.42
1:Am:120:ILE:HG23	1:Am:171:ILE:HD11	2.01	0.42
1:Ao:69:HIS:CD2	1:Bw:110:THR:HG23	2.54	0.42
1:Ao:75:PRO:HB3	1:Bw:135:MET:CG	2.49	0.42
1:Aq:187:VAL:HG12	1:Aq:188:ARG:NH2	2.35	0.42
1:Ay:235:LEU:HD23	1:Bm:218:ILE:HG22	2.02	0.42
1:Ba:69:HIS:CD2	1:Bc:110:THR:HG23	2.54	0.42
1:Ba:102:ASP:OD1	1:Bm:53:LYS:HE3	2.20	0.42
1:Bg:187:VAL:HG12	1:Bg:188:ARG:NH2	2.35	0.42
1:Bo:187:VAL:HG12	1:Bo:188:ARG:NH2	2.35	0.42
1:Ca:69:HIS:CD2	1:Cc:110:THR:HG23	2.55	0.42
1:Ca:83:THR:HG22	2:Cb:1:U:H5"	2.01	0.42
1:Cc:187:VAL:HG12	1:Cc:188:ARG:NH2	2.35	0.42
1:Aa:187:VAL:HG12	1:Aa:188:ARG:NH2	2.35	0.42
1:Ac:83:THR:HG22	2:Ad:1:U:H5"	2.01	0.42
1:Ao:245:ASN:HD22	1:Bc:231:ARG:HD3	1.84	0.42
1:Au:120:ILE:HG23	1:Au:171:ILE:HD11	2.01	0.42
1:Bc:120:ILE:HG23	1:Bc:171:ILE:HD11	2.01	0.42
1:Be:187:VAL:HG12	1:Be:188:ARG:NH2	2.35	0.42
1:Bm:184:TYR:OH	2:Bn:4:U:O2	2.20	0.42
1:Bw:69:HIS:CD2	1:By:110:THR:HG23	2.55	0.42
1:By:119:CYS:C	1:By:121:GLU:N	2.76	0.42
1:Cc:120:ILE:HG23	1:Cc:171:ILE:HD11	2.01	0.42
1:Ac:120:ILE:HG23	1:Ac:171:ILE:HD11	2.01	0.42
1:Ai:108:MET:N	1:Ai:109:PRO:CD	2.83	0.42
1:Bk:69:HIS:CD2	1:Bm:110:THR:HG23	2.55	0.42
1:Bk:120:ILE:HG23	1:Bk:171:ILE:HD11	2.01	0.42
1:Bs:69:HIS:CD2	1:Bu:110:THR:HG23	2.55	0.42
1:Bs:120:ILE:HG23	1:Bs:171:ILE:HD11	2.01	0.42
1:Aa:108:MET:N	1:Aa:109:PRO:CD	2.83	0.42
1:Aa:119:CYS:C	1:Aa:121:GLU:N	2.77	0.42
1:Ae:119:CYS:O	1:Ae:120:ILE:C	2.62	0.42
1:Aq:119:CYS:O	1:Aq:120:ILE:C	2.62	0.42
1:As:119:CYS:O	1:As:120:ILE:C	2.62	0.42
1:Aw:187:VAL:HG12	1:Aw:188:ARG:NH2	2.35	0.42
1:Ay:102:ASP:OD1	1:Bk:53:LYS:HE3	2.20	0.42
1:Bc:146:LYS:HD3	1:Bq:197:ARG:HH22	1.84	0.42
1:Bk:108:MET:N	1:Bk:109:PRO:CD	2.83	0.42
1:Bm:119:CYS:C	1:Bm:121:GLU:N	2.76	0.42
1:Ac:75:PRO:HB3	1:Ae:135:MET:CG	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:218:ILE:HG22	1:Ca:235:LEU:HD23	2.01	0.41
1:Ae:241:THR:HG21	1:Cc:252:GLU:HG2	2.02	0.41
1:Ag:187:VAL:HG12	1:Ag:188:ARG:NH2	2.35	0.41
1:Aq:108:MET:N	1:Aq:109:PRO:CD	2.83	0.41
1:As:108:MET:N	1:As:109:PRO:CD	2.83	0.41
1:Ay:108:MET:N	1:Ay:109:PRO:CD	2.83	0.41
1:Bc:108:MET:N	1:Bc:109:PRO:CD	2.83	0.41
1:Bi:120:ILE:HG23	1:Bi:171:ILE:HD11	2.01	0.41
1:Bm:187:VAL:HG12	1:Bm:188:ARG:NH2	2.35	0.41
1:Bu:197:ARG:H	1:Bu:197:ARG:HG2	1.71	0.41
1:Bw:108:MET:N	1:Bw:109:PRO:CD	2.83	0.41
1:Bw:187:VAL:HG12	1:Bw:188:ARG:NH2	2.35	0.41
1:Ac:108:MET:N	1:Ac:109:PRO:CD	2.83	0.41
1:Ac:187:VAL:HG12	1:Ac:188:ARG:NH2	2.35	0.41
1:Ae:108:MET:N	1:Ae:109:PRO:CD	2.83	0.41
1:Ag:119:CYS:O	1:Ag:120:ILE:C	2.62	0.41
1:Ak:119:CYS:C	1:Ak:121:GLU:N	2.77	0.41
1:Ao:119:CYS:O	1:Ao:120:ILE:C	2.62	0.41
1:Bc:235:LEU:HD23	1:Bq:218:ILE:HG22	2.01	0.41
1:Bc:245:ASN:HD22	1:Bq:231:ARG:CD	2.33	0.41
1:Bi:108:MET:N	1:Bi:109:PRO:CD	2.83	0.41
1:Bi:187:VAL:HG12	1:Bi:188:ARG:NH2	2.35	0.41
1:Bq:103:ILE:CG2	1:Bq:107:GLU:HG3	2.46	0.41
1:Bs:108:MET:N	1:Bs:109:PRO:CD	2.83	0.41
1:Bu:187:VAL:HG12	1:Bu:188:ARG:NH2	2.35	0.41
1:By:119:CYS:O	1:By:120:ILE:C	2.62	0.41
1:Ca:119:CYS:O	1:Ca:120:ILE:C	2.62	0.41
1:Cc:108:MET:N	1:Cc:109:PRO:CD	2.83	0.41
1:Aa:110:THR:HG23	1:Be:69:HIS:CD2	2.54	0.41
1:Ac:119:CYS:O	1:Ac:120:ILE:C	2.62	0.41
1:Ak:119:CYS:O	1:Ak:120:ILE:C	2.62	0.41
1:Aw:245:ASN:HD22	1:Bk:231:ARG:HD3	1.84	0.41
1:Ba:108:MET:N	1:Ba:109:PRO:CD	2.83	0.41
1:Bc:252:GLU:HG2	1:Bq:241:THR:HG21	2.02	0.41
1:Bg:108:MET:N	1:Bg:109:PRO:CD	2.83	0.41
1:Bi:119:CYS:O	1:Bi:120:ILE:C	2.62	0.41
1:Bo:108:MET:N	1:Bo:109:PRO:CD	2.83	0.41
1:Aa:197:ARG:HH22	1:By:146:LYS:HD3	1.86	0.41
1:Ae:232:LEU:HD22	1:Cc:246:THR:HG22	2.03	0.41
1:Ag:108:MET:N	1:Ag:109:PRO:CD	2.83	0.41
1:Ag:120:ILE:HG23	1:Ag:171:ILE:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:139:GLU:HG2	1:As:46:ARG:HH21	1.85	0.41
1:Ag:146:LYS:HD3	1:Au:197:ARG:HH22	1.85	0.41
1:Ag:245:ASN:HD22	1:Au:231:ARG:HD3	1.84	0.41
1:Am:108:MET:N	1:Am:109:PRO:CD	2.83	0.41
1:Am:139:GLU:HG2	1:Ay:46:ARG:HH21	1.85	0.41
1:Au:108:MET:N	1:Au:109:PRO:CD	2.83	0.41
1:Aw:120:ILE:HG23	1:Aw:171:ILE:HD11	2.01	0.41
1:Ba:246:THR:HG22	1:Bo:232:LEU:HD22	2.02	0.41
1:Be:108:MET:N	1:Be:109:PRO:CD	2.83	0.41
1:Bg:119:CYS:O	1:Bg:120:ILE:C	2.62	0.41
1:Bu:119:CYS:C	1:Bu:121:GLU:N	2.76	0.41
1:Ac:146:LYS:HD3	1:Aq:197:ARG:HH22	1.86	0.41
1:Ae:187:VAL:HG12	1:Ae:188:ARG:NH2	2.35	0.41
1:Ae:235:LEU:HD23	1:As:218:ILE:HG22	2.02	0.41
1:Am:146:LYS:HD3	1:Ba:197:ARG:HH22	1.85	0.41
1:As:119:CYS:C	1:As:121:GLU:N	2.76	0.41
1:Au:119:CYS:O	1:Au:120:ILE:C	2.62	0.41
1:Au:235:LEU:HD23	1:Bi:218:ILE:HG22	2.02	0.41
1:Ay:119:CYS:C	1:Ay:121:GLU:N	2.77	0.41
1:Be:146:LYS:HD3	1:Bs:197:ARG:HH22	1.84	0.41
1:Be:252:GLU:HG2	1:Bs:241:THR:HG21	2.03	0.41
1:Bg:84:ARG:NE	1:Bg:204:GLU:OE2	2.53	0.41
1:Bq:108:MET:N	1:Bq:109:PRO:CD	2.83	0.41
1:Bs:119:CYS:C	1:Bs:121:GLU:N	2.77	0.41
1:Ca:108:MET:N	1:Ca:109:PRO:CD	2.83	0.41
1:As:120:ILE:HG23	1:As:171:ILE:HD11	2.01	0.41
1:Au:245:ASN:HD22	1:Bi:231:ARG:HD3	1.84	0.41
1:Be:184:TYR:OH	2:Bf:4:U:O2	2.20	0.41
1:Ca:119:CYS:C	1:Ca:121:GLU:N	2.77	0.41
1:Ac:246:THR:HG22	1:Aq:232:LEU:HD22	2.02	0.41
1:Am:119:CYS:C	1:Am:121:GLU:N	2.77	0.41
1:Aw:102:ASP:OD1	1:Bi:53:LYS:HE3	2.21	0.41
1:Aw:108:MET:N	1:Aw:109:PRO:CD	2.83	0.41
1:Ai:235:LEU:HD23	1:Aw:218:ILE:HG22	2.02	0.41
1:Ak:146:LYS:HD3	1:Ay:197:ARG:HH22	1.85	0.41
1:Ao:139:GLU:HG2	1:Ba:46:ARG:HH21	1.85	0.41
1:Aq:84:ARG:NE	1:Aq:204:GLU:OE2	2.53	0.41
1:Be:102:ASP:OD1	1:Bq:53:LYS:HE3	2.21	0.41
1:Bg:184:TYR:OH	2:Bh:4:U:O2	2.20	0.41
1:Bu:119:CYS:O	1:Bu:120:ILE:C	2.62	0.41
1:Ac:84:ARG:NE	1:Ac:204:GLU:OE2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ac:252:GLU:HG2	1:Aq:241:THR:HG21	2.03	0.41
1:Ae:102:ASP:OD1	1:Aq:53:LYS:HE3	2.21	0.41
1:Ae:197:ARG:HH22	1:Cc:146:LYS:HD3	1.86	0.41
1:Ae:243:GLU:O	1:As:229:GLN:NE2	2.52	0.41
1:Ag:235:LEU:HD23	1:Au:218:ILE:HG22	2.03	0.41
1:Am:235:LEU:HD23	1:Ba:218:ILE:HG22	2.03	0.41
1:Ao:84:ARG:NE	1:Ao:204:GLU:OE2	2.53	0.41
1:Ao:108:MET:N	1:Ao:109:PRO:CD	2.83	0.41
1:Ba:245:ASN:HD22	1:Bo:231:ARG:CD	2.34	0.41
1:Be:245:ASN:HD22	1:Bs:231:ARG:CD	2.34	0.41
1:Bk:119:CYS:O	1:Bk:120:ILE:C	2.62	0.41
1:Bm:108:MET:N	1:Bm:109:PRO:CD	2.83	0.41
1:Bs:84:ARG:NE	1:Bs:204:GLU:OE2	2.53	0.41
1:By:84:ARG:NE	1:By:204:GLU:OE2	2.53	0.41
1:By:108:MET:N	1:By:109:PRO:CD	2.83	0.41
1:Aa:53:LYS:HE3	1:Ca:102:ASP:OD1	2.21	0.41
1:Aa:119:CYS:O	1:Aa:120:ILE:C	2.62	0.41
1:Be:53:LYS:HE3	1:By:102:ASP:OD1	2.21	0.41
1:Be:235:LEU:HD23	1:Bs:218:ILE:HG22	2.02	0.41
1:Bk:187:VAL:HG12	1:Bk:188:ARG:NH2	2.35	0.41
1:Bw:197:ARG:H	1:Bw:197:ARG:HG2	1.71	0.41
1:Aa:102:ASP:OD1	1:Bs:53:LYS:HE3	2.20	0.40
1:Ac:245:ASN:HD22	1:Aq:231:ARG:CD	2.34	0.40
1:Ai:119:CYS:C	1:Ai:121:GLU:N	2.77	0.40
1:Ak:246:THR:HG22	1:Ay:232:LEU:HD22	2.03	0.40
1:Aq:119:CYS:C	1:Aq:121:GLU:N	2.77	0.40
1:Aw:84:ARG:NE	1:Aw:204:GLU:OE2	2.53	0.40
1:Be:246:THR:HG22	1:Bs:232:LEU:HD22	2.03	0.40
1:Bg:197:ARG:H	1:Bg:197:ARG:HG2	1.71	0.40
1:Bk:119:CYS:C	1:Bk:121:GLU:N	2.76	0.40
1:Ac:102:ASP:OD1	1:Bu:53:LYS:HE3	2.21	0.40
1:Ac:119:CYS:C	1:Ac:121:GLU:N	2.77	0.40
1:Ac:241:THR:HG21	1:Ca:252:GLU:HG2	2.04	0.40
1:As:84:ARG:NE	1:As:204:GLU:OE2	2.53	0.40
1:Aw:103:ILE:CG2	1:Aw:107:GLU:HG3	2.46	0.40
1:Ba:119:CYS:O	1:Ba:120:ILE:C	2.62	0.40
1:Ba:252:GLU:HG2	1:Bo:241:THR:HG21	2.03	0.40
1:Be:119:CYS:O	1:Be:120:ILE:C	2.62	0.40
1:Cc:119:CYS:O	1:Cc:120:ILE:C	2.62	0.40
1:Ac:53:LYS:HE3	1:Cc:102:ASP:OD1	2.21	0.40
1:Ag:102:ASP:OD1	1:As:53:LYS:HE3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Ag:119:CYS:C	1:Ag:121:GLU:N	2.76	0.40
1:Ak:252:GLU:HG2	1:Ay:241:THR:HG21	2.03	0.40
1:As:245:ASN:HD22	1:Bg:231:ARG:HD3	1.85	0.40
1:Au:102:ASP:OD1	1:Bg:53:LYS:HE3	2.21	0.40
1:Ba:146:LYS:HD3	1:Bo:197:ARG:HH22	1.86	0.40
1:Bg:119:CYS:C	1:Bg:121:GLU:N	2.77	0.40
1:Bu:108:MET:N	1:Bu:109:PRO:CD	2.83	0.40
1:Aa:241:THR:HG21	1:By:252:GLU:HG2	2.04	0.40
1:Ac:229:GLN:NE2	1:Ca:243:GLU:O	2.53	0.40
1:Ac:232:LEU:HD22	1:Ca:246:THR:HG22	2.03	0.40
1:Ai:146:LYS:HD3	1:Aw:197:ARG:HH22	1.85	0.40
1:Ak:245:ASN:HD22	1:Ay:231:ARG:CD	2.34	0.40
1:Au:119:CYS:C	1:Au:121:GLU:N	2.76	0.40
1:Aw:119:CYS:O	1:Aw:120:ILE:C	2.62	0.40
1:Bc:53:LYS:HE3	1:Bw:102:ASP:OD1	2.21	0.40
1:Bc:102:ASP:OD1	1:Bo:53:LYS:HE3	2.21	0.40
1:Bw:119:CYS:O	1:Bw:120:ILE:C	2.62	0.40
1:Aa:235:LEU:HD23	1:Bu:218:ILE:HG22	2.02	0.40
1:Ae:119:CYS:C	1:Ae:121:GLU:N	2.77	0.40
1:Ae:231:ARG:CD	1:Cc:245:ASN:HD22	2.34	0.40
1:Ai:102:ASP:OD1	1:Au:53:LYS:HE3	2.21	0.40
1:Ak:108:MET:N	1:Ak:109:PRO:CD	2.83	0.40
1:Au:146:LYS:HD3	1:Bi:197:ARG:HH22	1.87	0.40
1:Be:197:ARG:H	1:Be:197:ARG:HG2	1.71	0.40
1:Bm:173:MET:HE2	1:Bm:174:ARG:HG2	2.04	0.40
1:Bq:119:CYS:C	1:Bq:121:GLU:N	2.77	0.40
1:Cc:119:CYS:C	1:Cc:121:GLU:N	2.77	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	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ac	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ae	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ag	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ai	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ak	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Am	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ao	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Aq	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	As	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Au	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Aw	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ay	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ba	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bc	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Be	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bg	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bi	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bk	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bm	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bo	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bq	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bs	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bu	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Bw	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	By	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Ca	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
1	Cc	224/267 (84%)	212 (95%)	12 (5%)	0	100	100
All	All	6272/7476 (84%)	5936 (95%)	336 (5%)	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	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Ac	196/229 (86%)	193 (98%)	3 (2%)	57	80
1	Ae	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Ag	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Ai	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Ak	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Am	196/229 (86%)	193 (98%)	3 (2%)	57	80
1	Ao	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Aq	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	As	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Au	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Aw	196/229 (86%)	193 (98%)	3 (2%)	57	80
1	Ay	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Ba	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bc	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Be	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bg	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bi	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bk	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bm	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bo	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bq	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bs	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bu	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Bw	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	By	196/229 (86%)	194 (99%)	2 (1%)	68	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ca	196/229 (86%)	194 (99%)	2 (1%)	68	84
1	Cc	196/229 (86%)	194 (99%)	2 (1%)	68	84
All	All	5488/6412 (86%)	5429 (99%)	59 (1%)	63	83

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Aa	108	MET
1	Aa	267	MET
1	Ac	108	MET
1	Ac	135	MET
1	Ac	267	MET
1	Ae	108	MET
1	Ae	267	MET
1	Ag	108	MET
1	Ag	267	MET
1	Ai	108	MET
1	Ai	267	MET
1	Ak	108	MET
1	Ak	267	MET
1	Am	108	MET
1	Am	135	MET
1	Am	267	MET
1	Ao	108	MET
1	Ao	267	MET
1	Aq	108	MET
1	Aq	267	MET
1	As	108	MET
1	As	267	MET
1	Au	108	MET
1	Au	267	MET
1	Aw	108	MET
1	Aw	135	MET
1	Aw	267	MET
1	Ay	108	MET
1	Ay	267	MET
1	Ba	108	MET
1	Ba	267	MET
1	Bc	108	MET
1	Bc	267	MET
1	Be	108	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Be	267	MET
1	Bg	108	MET
1	Bg	267	MET
1	Bi	108	MET
1	Bi	267	MET
1	Bk	108	MET
1	Bk	267	MET
1	Bm	108	MET
1	Bm	267	MET
1	Bo	108	MET
1	Bo	267	MET
1	Bq	108	MET
1	Bq	267	MET
1	Bs	108	MET
1	Bs	267	MET
1	Bu	108	MET
1	Bu	267	MET
1	Bw	108	MET
1	Bw	267	MET
1	By	108	MET
1	By	267	MET
1	Ca	108	MET
1	Ca	267	MET
1	Cc	108	MET
1	Cc	267	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	Aa	69	HIS
1	Aa	98	GLN
1	Aa	158	GLN
1	Aa	217	HIS
1	Aa	245	ASN
1	Ac	69	HIS
1	Ac	98	GLN
1	Ac	158	GLN
1	Ac	217	HIS
1	Ac	245	ASN
1	Ae	69	HIS
1	Ae	98	GLN
1	Ae	158	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Ae	217	HIS
1	Ae	245	ASN
1	Ag	69	HIS
1	Ag	98	GLN
1	Ag	158	GLN
1	Ag	217	HIS
1	Ag	245	ASN
1	Ai	69	HIS
1	Ai	98	GLN
1	Ai	158	GLN
1	Ai	217	HIS
1	Ai	245	ASN
1	Ak	69	HIS
1	Ak	98	GLN
1	Ak	158	GLN
1	Ak	217	HIS
1	Ak	245	ASN
1	Am	69	HIS
1	Am	98	GLN
1	Am	158	GLN
1	Am	217	HIS
1	Am	245	ASN
1	Ao	69	HIS
1	Ao	98	GLN
1	Ao	158	GLN
1	Ao	217	HIS
1	Ao	245	ASN
1	Aq	69	HIS
1	Aq	98	GLN
1	Aq	158	GLN
1	Aq	217	HIS
1	As	69	HIS
1	As	98	GLN
1	As	158	GLN
1	As	217	HIS
1	As	245	ASN
1	Au	69	HIS
1	Au	98	GLN
1	Au	158	GLN
1	Au	217	HIS
1	Au	245	ASN
1	Aw	69	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Aw	98	GLN
1	Aw	158	GLN
1	Aw	217	HIS
1	Aw	245	ASN
1	Ay	69	HIS
1	Ay	98	GLN
1	Ay	158	GLN
1	Ay	217	HIS
1	Ay	245	ASN
1	Ba	69	HIS
1	Ba	98	GLN
1	Ba	158	GLN
1	Ba	217	HIS
1	Ba	245	ASN
1	Bc	69	HIS
1	Bc	98	GLN
1	Bc	158	GLN
1	Bc	217	HIS
1	Bc	245	ASN
1	Be	69	HIS
1	Be	98	GLN
1	Be	158	GLN
1	Be	217	HIS
1	Be	245	ASN
1	Bg	69	HIS
1	Bg	98	GLN
1	Bg	158	GLN
1	Bg	217	HIS
1	Bi	69	HIS
1	Bi	98	GLN
1	Bi	158	GLN
1	Bi	217	HIS
1	Bk	69	HIS
1	Bk	98	GLN
1	Bk	158	GLN
1	Bk	217	HIS
1	Bm	69	HIS
1	Bm	98	GLN
1	Bm	158	GLN
1	Bm	217	HIS
1	Bo	69	HIS
1	Bo	98	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Bo	158	GLN
1	Bo	217	HIS
1	Bq	69	HIS
1	Bq	98	GLN
1	Bq	158	GLN
1	Bq	217	HIS
1	Bs	69	HIS
1	Bs	98	GLN
1	Bs	158	GLN
1	Bs	217	HIS
1	Bu	69	HIS
1	Bu	98	GLN
1	Bu	158	GLN
1	Bu	217	HIS
1	Bw	69	HIS
1	Bw	98	GLN
1	Bw	158	GLN
1	Bw	217	HIS
1	Bw	245	ASN
1	By	69	HIS
1	By	98	GLN
1	By	158	GLN
1	By	217	HIS
1	By	245	ASN
1	Ca	69	HIS
1	Ca	98	GLN
1	Ca	158	GLN
1	Ca	217	HIS
1	Ca	245	ASN
1	Cc	69	HIS
1	Cc	98	GLN
1	Cc	158	GLN
1	Cc	217	HIS
1	Cc	245	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Ab	4/5 (80%)	0	0
2	Ad	4/5 (80%)	0	0
2	Af	4/5 (80%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
All	All	112/140 (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.

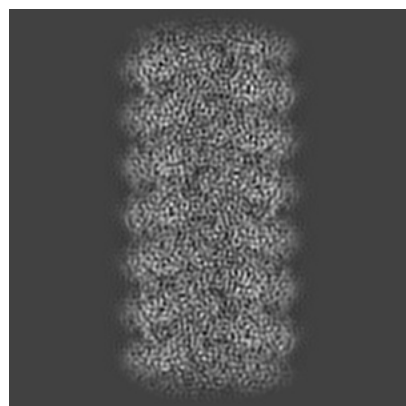
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17048. These allow visual inspection of the internal detail of the map and identification of artifacts.

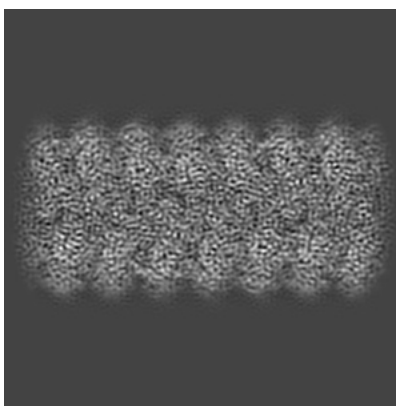
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

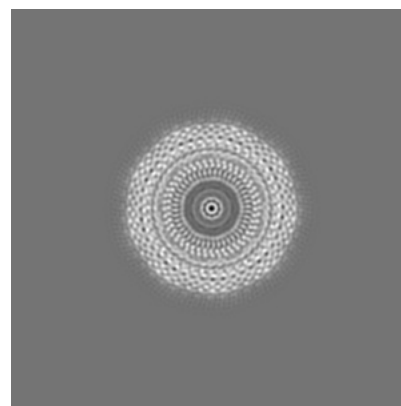
6.1.1 Primary map



X

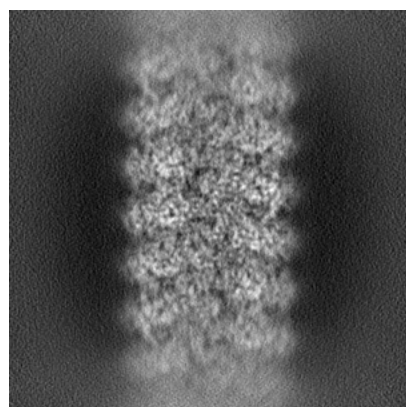


Y

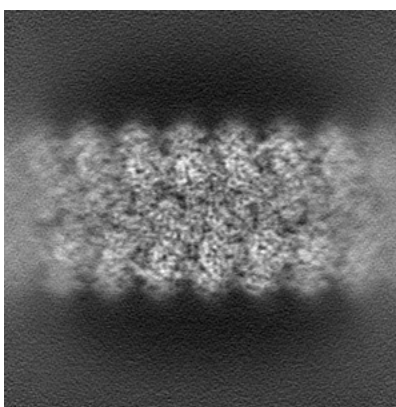


Z

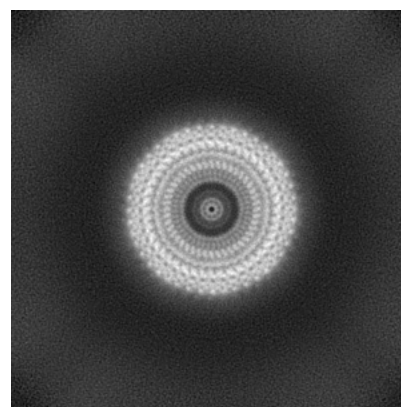
6.1.2 Raw map



X



Y

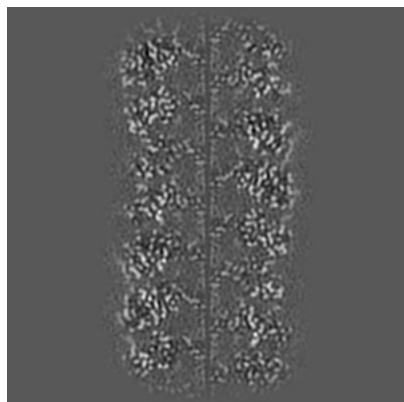


Z

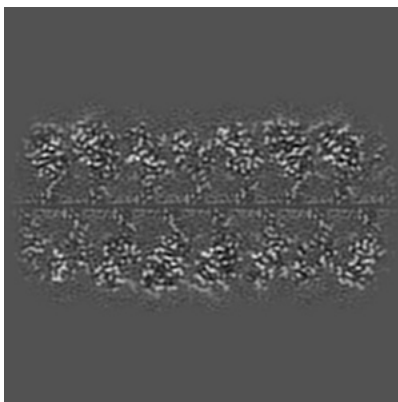
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

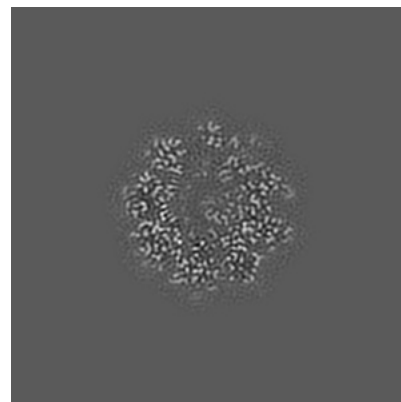
6.2.1 Primary map



X Index: 150

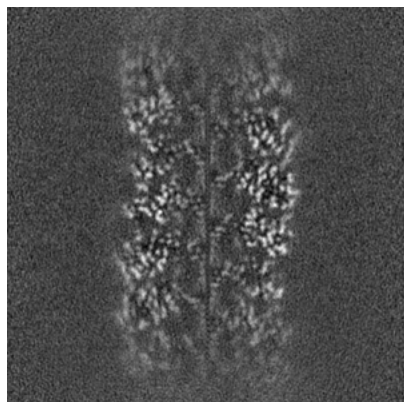


Y Index: 150

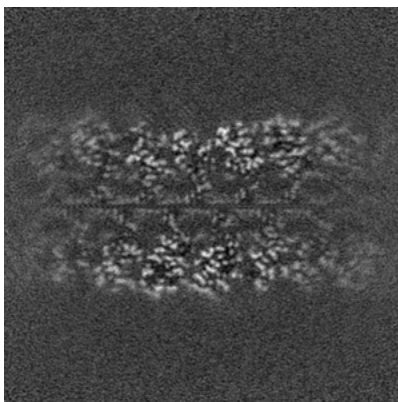


Z Index: 150

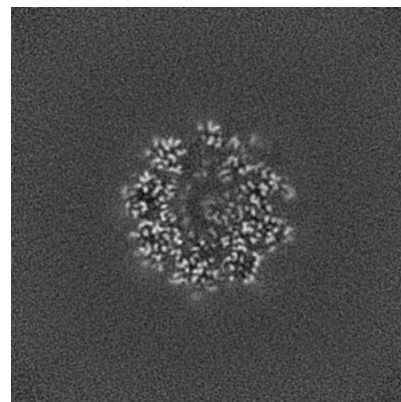
6.2.2 Raw map



X Index: 150



Y Index: 150

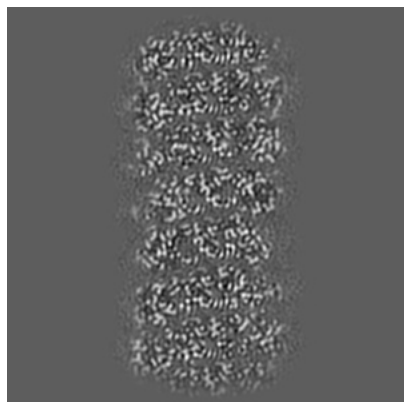


Z Index: 150

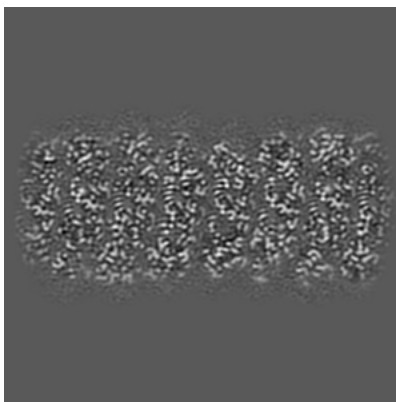
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

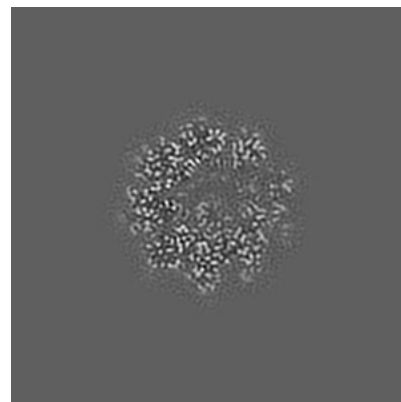
6.3.1 Primary map



X Index: 118

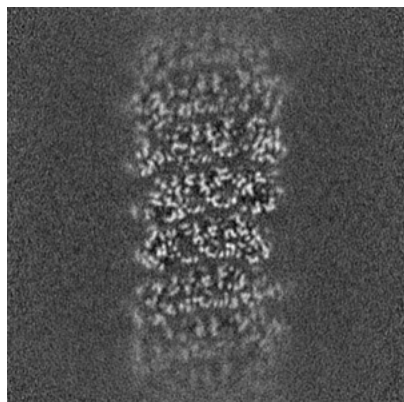


Y Index: 182

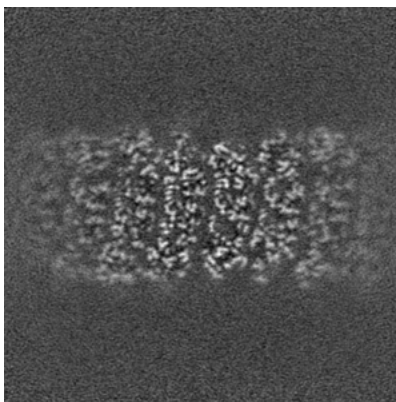


Z Index: 120

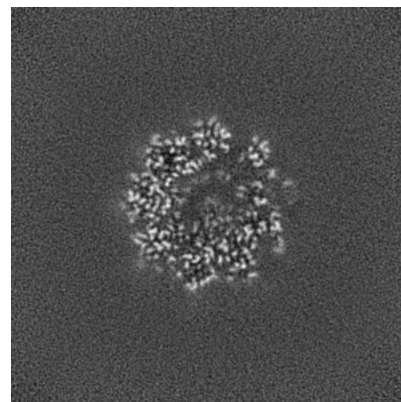
6.3.2 Raw map



X Index: 118



Y Index: 182

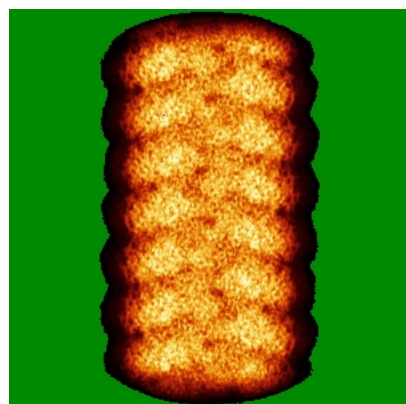


Z Index: 155

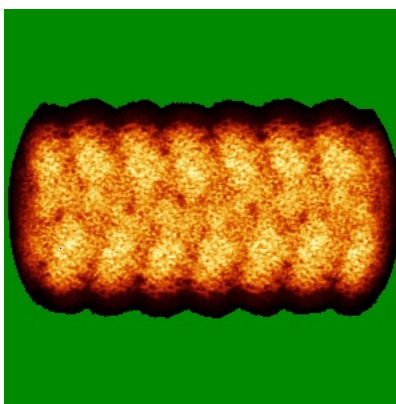
The images above show the largest variance slices of the map in three orthogonal directions.

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

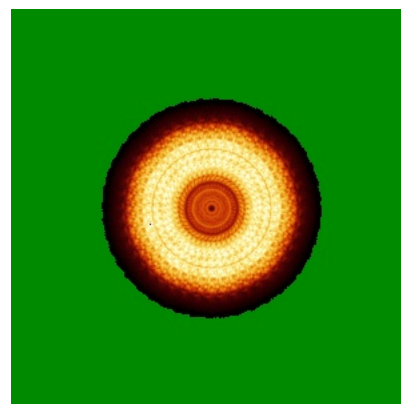
6.4.1 Primary map



X

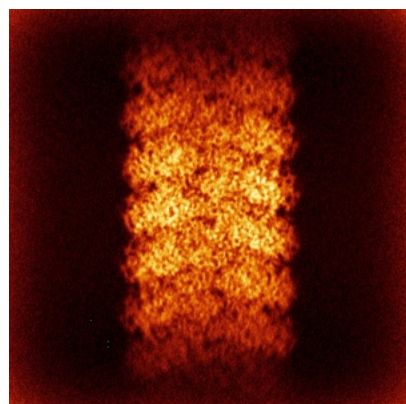


Y

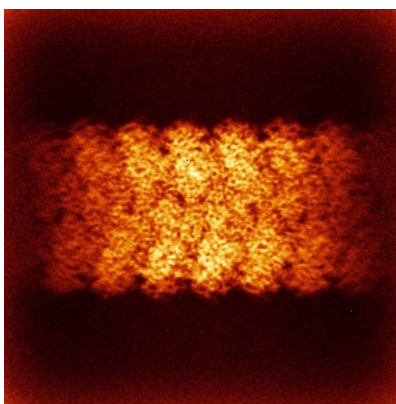


Z

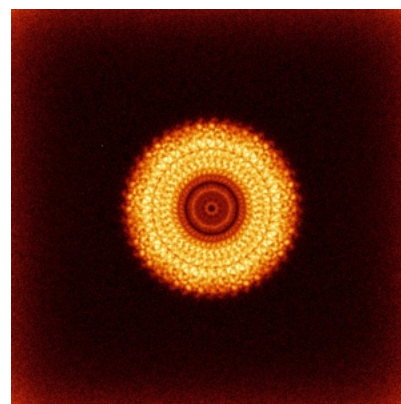
6.4.2 Raw map



X



Y

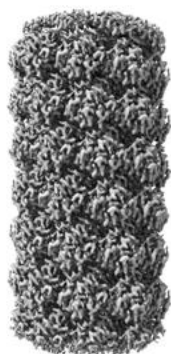


Z

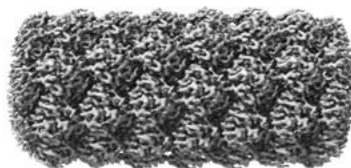
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



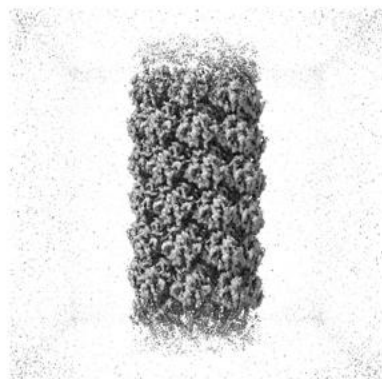
Y



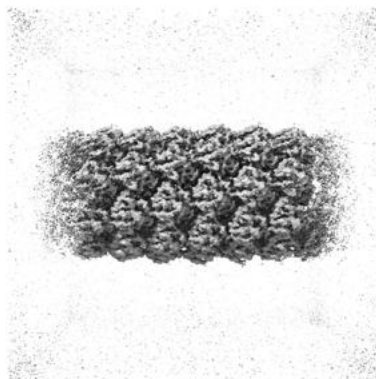
Z

The images above show the 3D surface view of the map at the recommended contour level 0.665. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

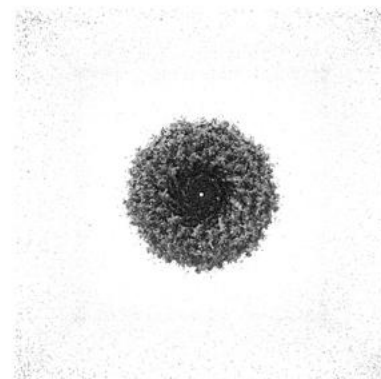
6.5.2 Raw map



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.

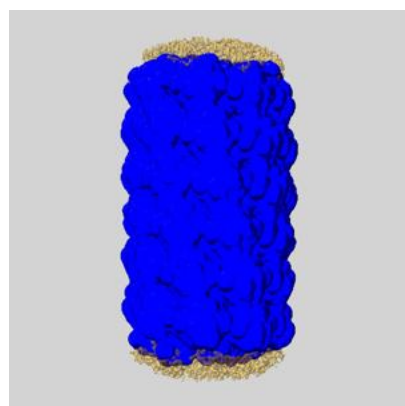
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

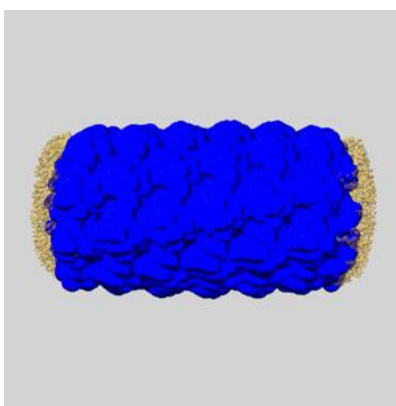
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

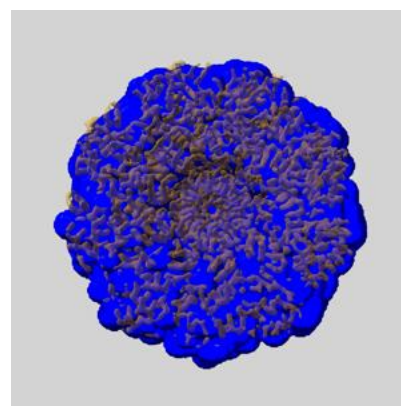
6.6.1 emd_17048_msk_1.map [i](#)



X



Y

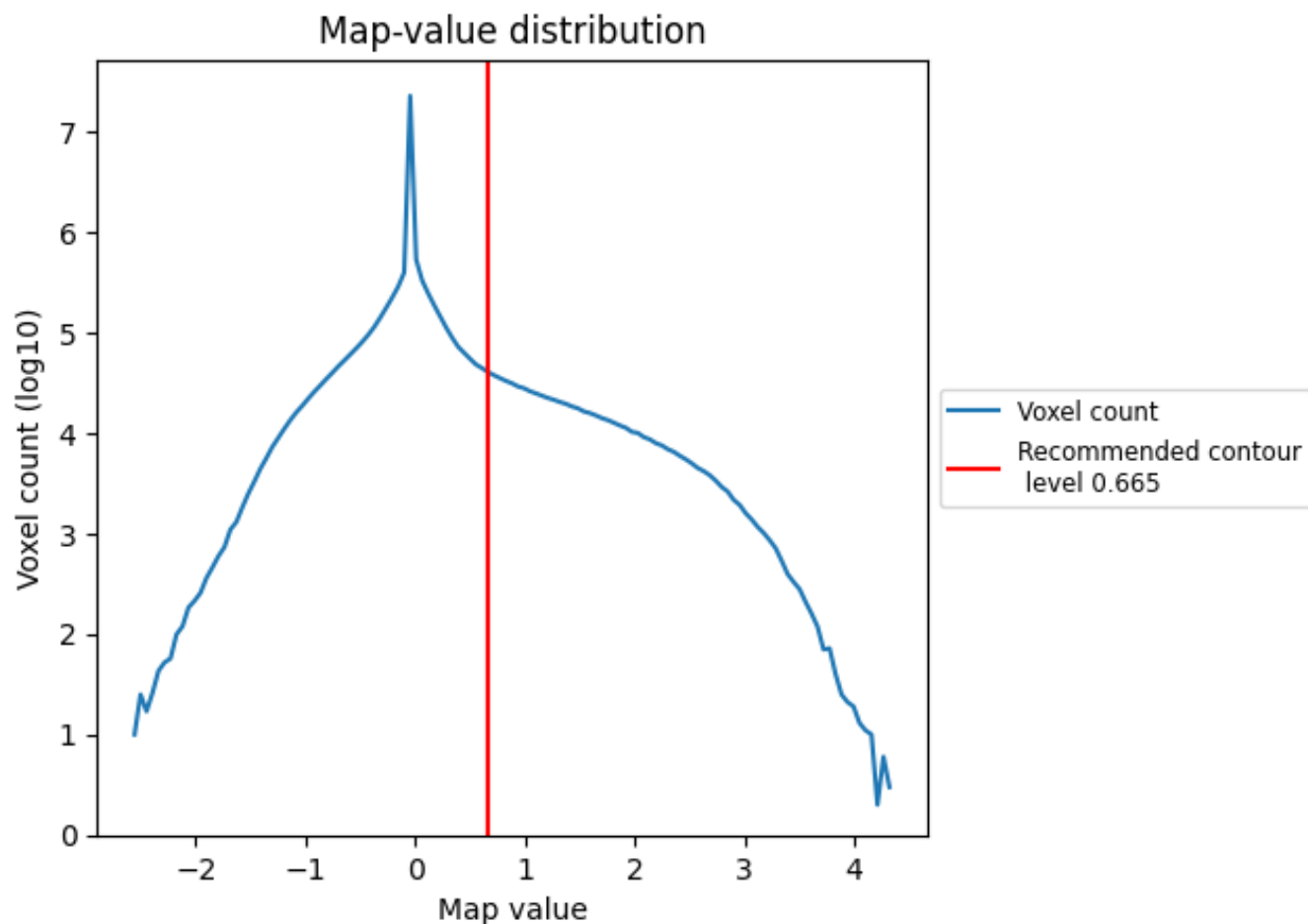


Z

7 Map analysis [i](#)

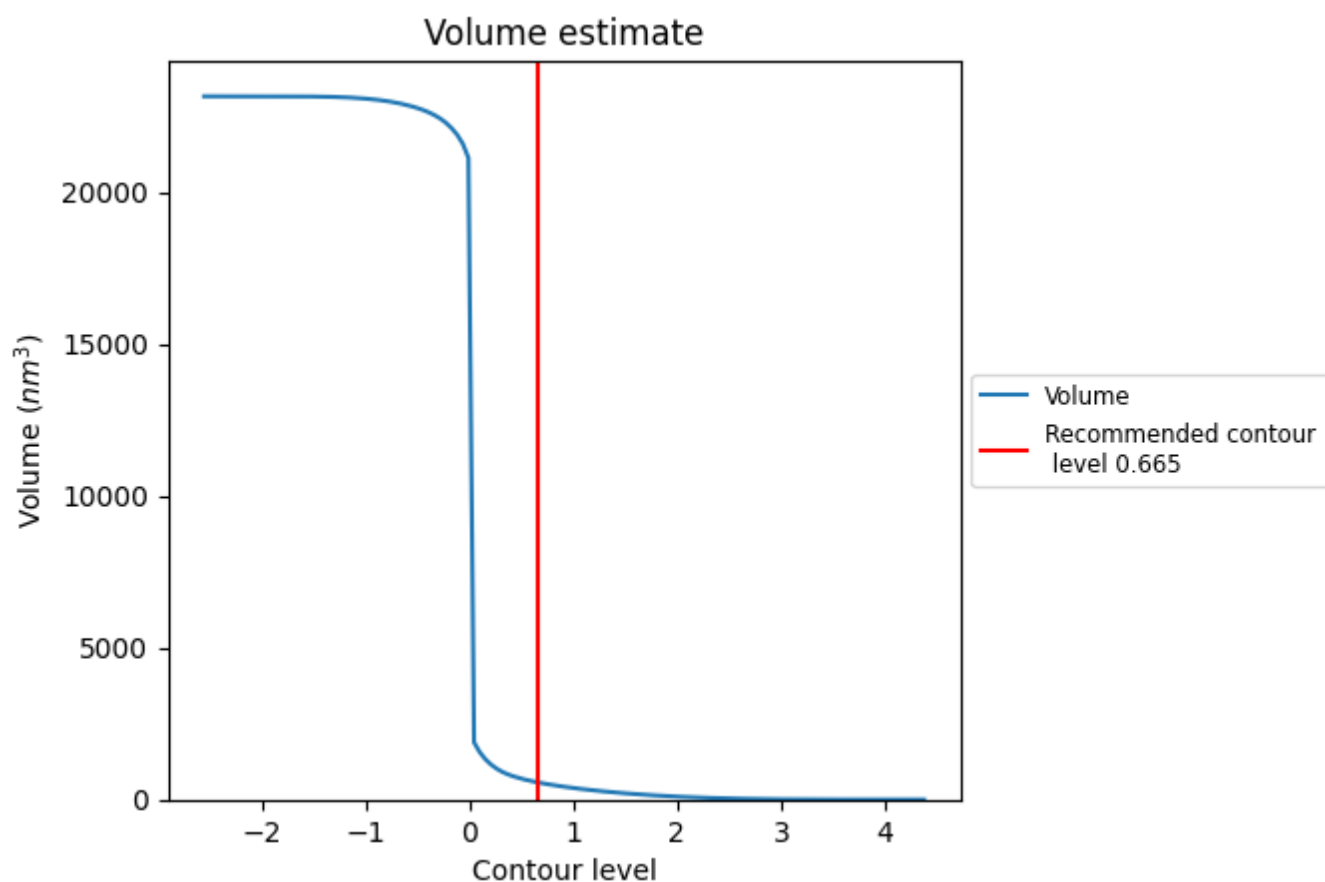
This section contains the results of statistical analysis of the map.

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.

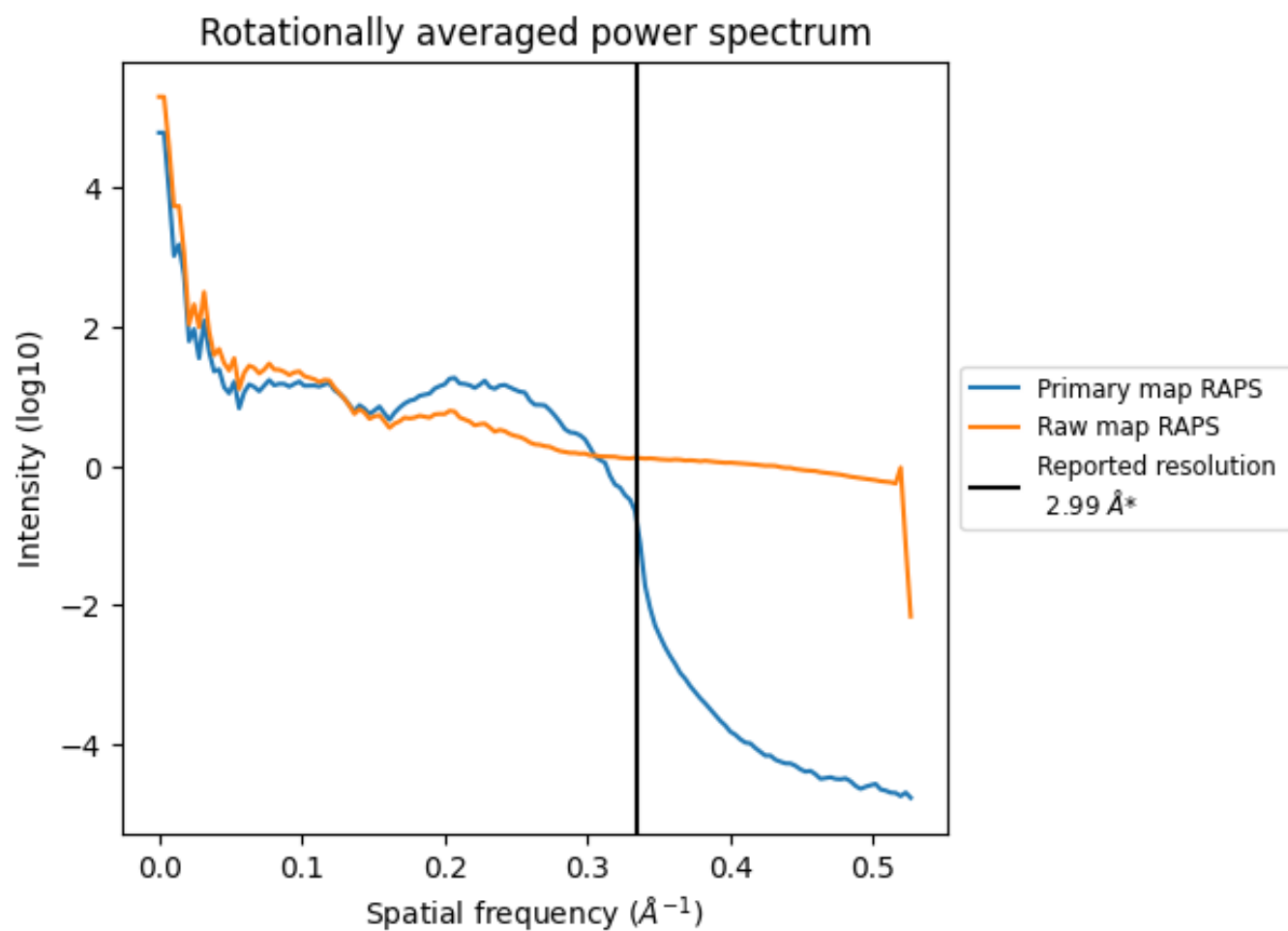
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 560 nm³; this corresponds to an approximate mass of 506 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 ⓘ

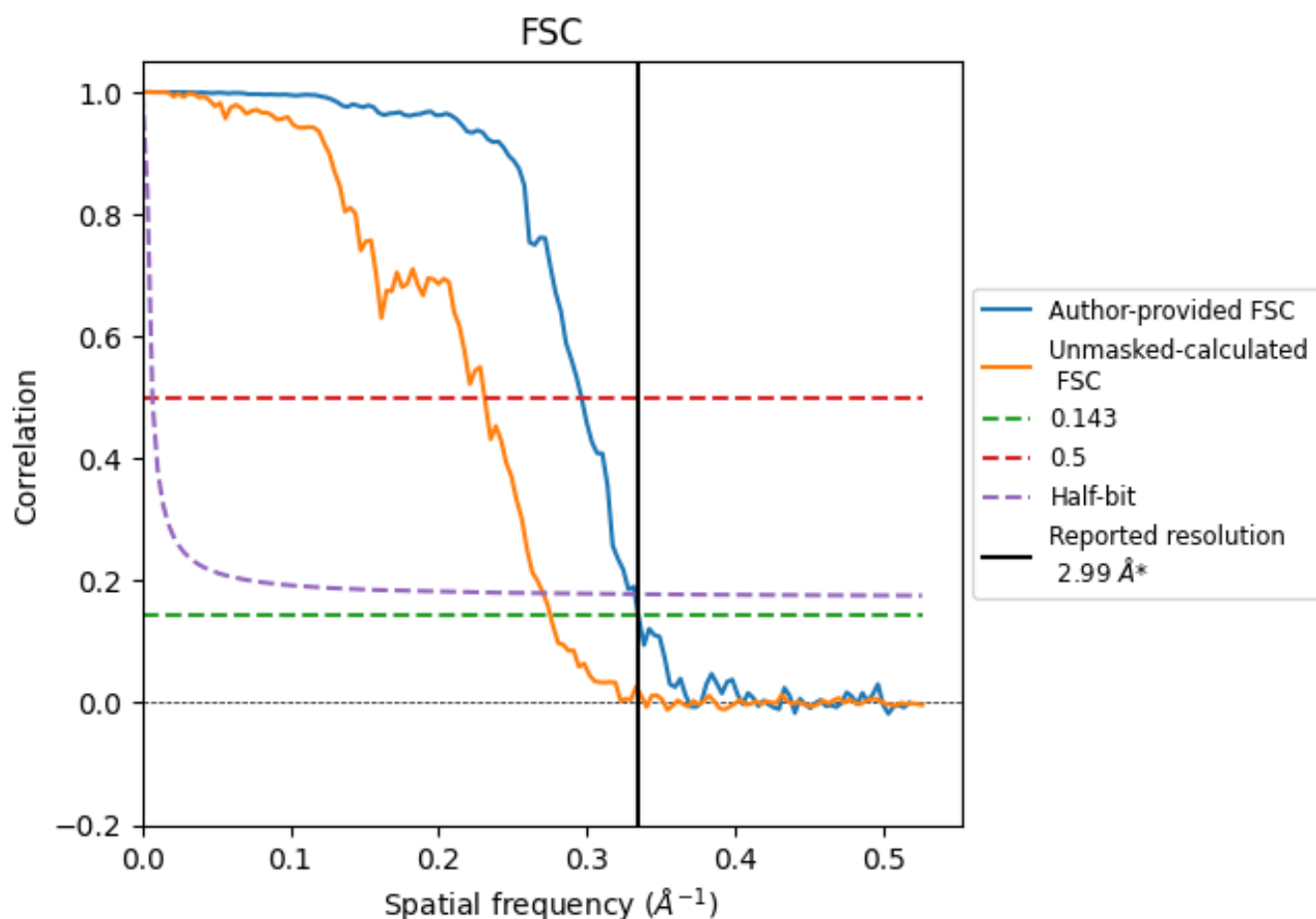


*Reported resolution corresponds to spatial frequency of 0.334 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.334 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

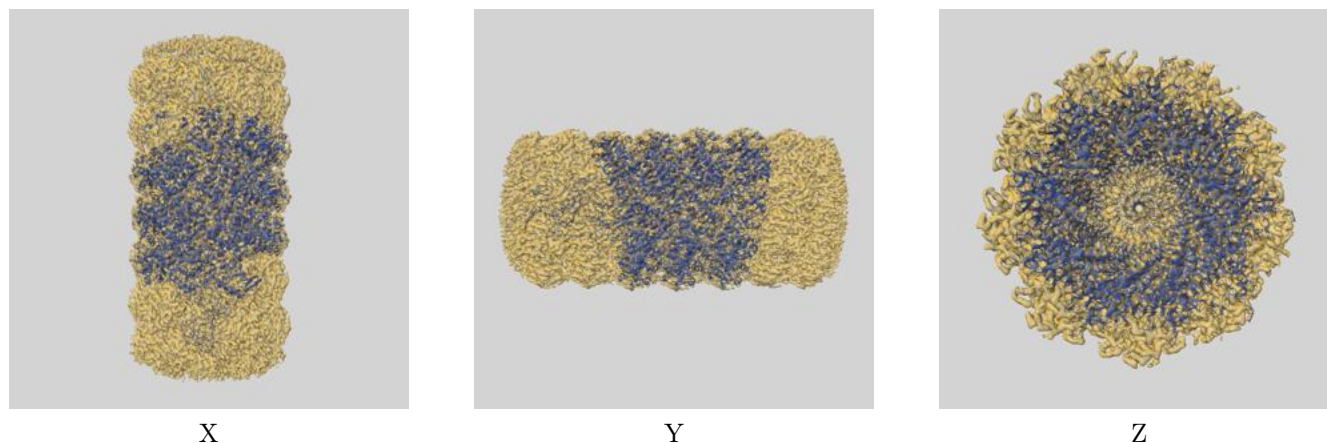
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.99	-	-
Author-provided FSC curve	2.99	3.37	3.01
Unmasked-calculated*	3.63	4.33	3.70

*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 3.63 differs from the reported value 2.99 by more than 10 %

9 Map-model fit [i](#)

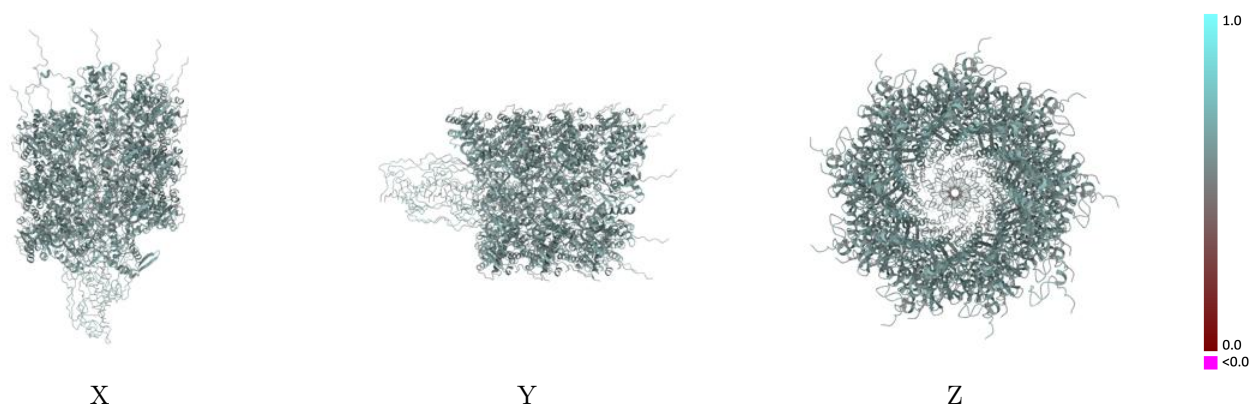
This section contains information regarding the fit between EMDB map EMD-17048 and PDB model 8OPC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



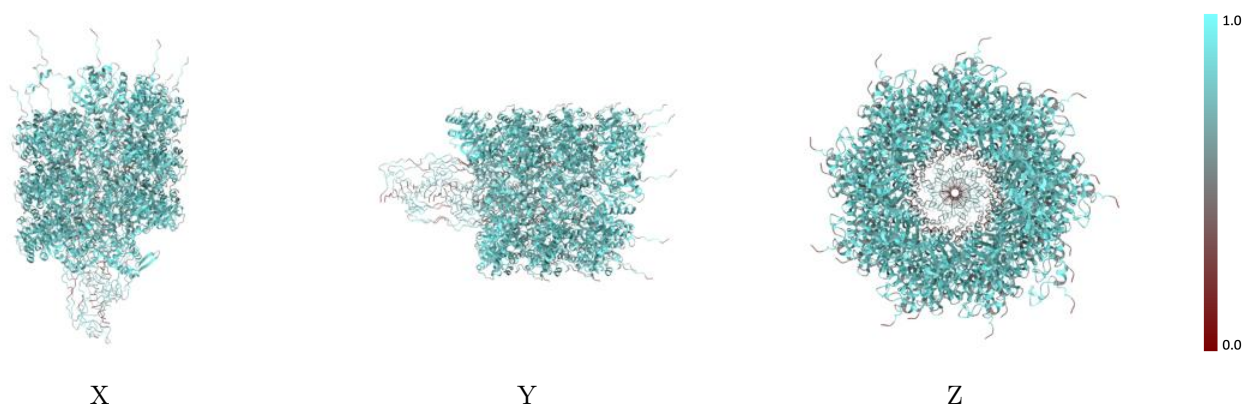
The images above show the 3D surface view of the map at the recommended contour level 0.665 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



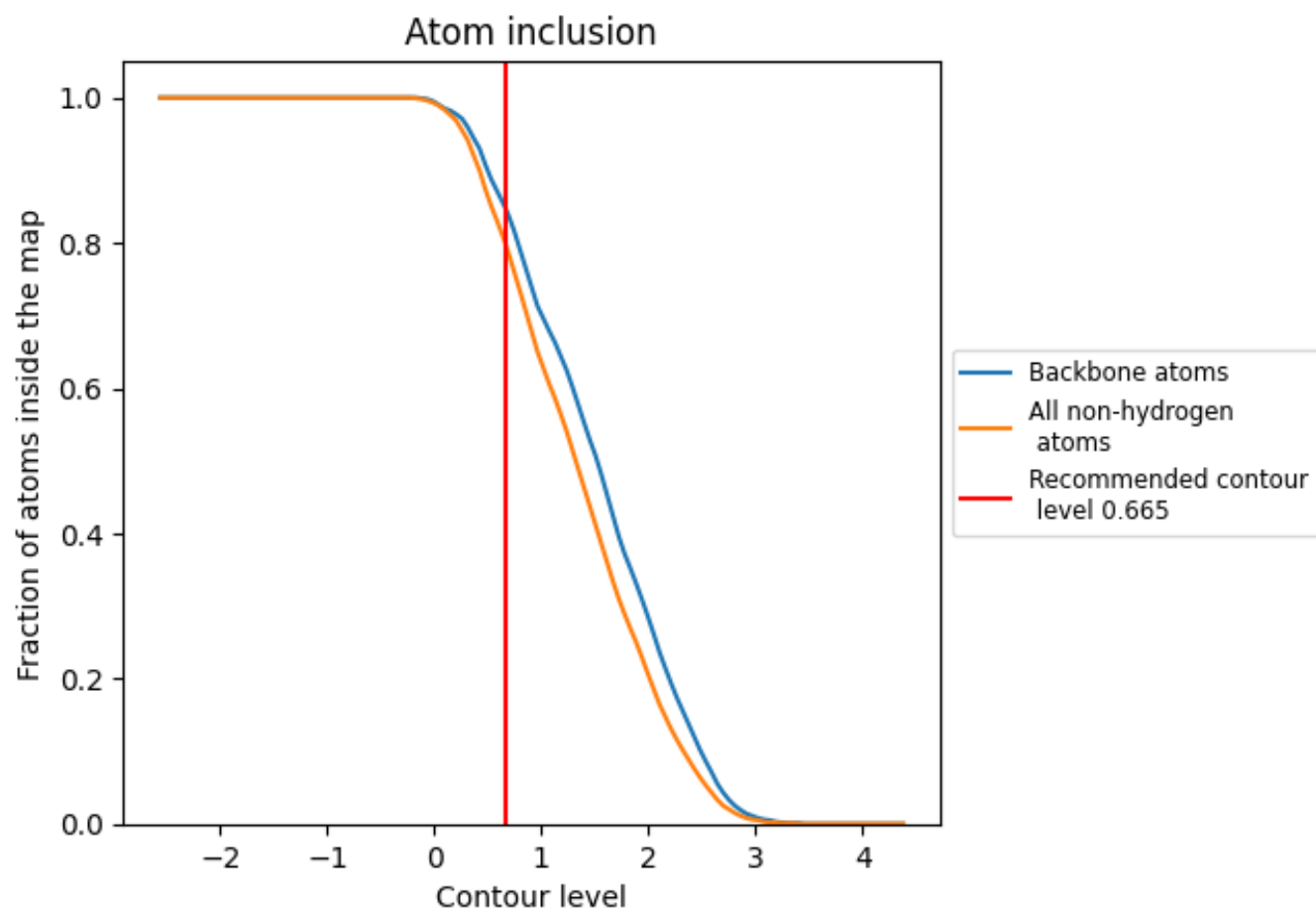
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.665).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 80% 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 (0.665) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.5790
Aa	 0.7890	 0.5760
Ab	 0.9600	 0.5890
Ac	 0.7850	 0.5770
Ad	 0.9500	 0.5960
Ae	 0.7870	 0.5780
Af	 0.9600	 0.5870
Ag	 0.7930	 0.5780
Ah	 0.9600	 0.5980
Ai	 0.7900	 0.5790
Aj	 0.9500	 0.5870
Ak	 0.7880	 0.5790
Al	 0.9500	 0.5960
Am	 0.7890	 0.5780
An	 0.9500	 0.5980
Ao	 0.7900	 0.5780
Ap	 0.9600	 0.5970
Aq	 0.7960	 0.5790
Ar	 0.9400	 0.5970
As	 0.7920	 0.5770
At	 0.9500	 0.5930
Au	 0.7940	 0.5780
Av	 0.9400	 0.5920
Aw	 0.7870	 0.5770
Ax	 0.9500	 0.5900
Ay	 0.7900	 0.5780
Az	 0.9500	 0.5950
Ba	 0.7910	 0.5790
Bb	 0.9600	 0.5920
Bc	 0.7920	 0.5810
Bd	 0.9500	 0.6000
Be	 0.7900	 0.5760
Bf	 0.9500	 0.5970
Bg	 0.7960	 0.5760
Bh	 0.9500	 0.5870



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Bi	 0.7870	 0.5780
Bj	 0.9400	 0.5910
Bk	 0.7910	 0.5790
Bl	 0.9400	 0.5940
Bm	 0.7880	 0.5780
Bn	 0.9500	 0.5960
Bo	 0.7900	 0.5790
Bp	 0.9500	 0.5960
Bq	 0.7890	 0.5780
Br	 0.9500	 0.5960
Bs	 0.7880	 0.5760
Bt	 0.9600	 0.5930
Bu	 0.7890	 0.5750
Bv	 0.9300	 0.5940
Bw	 0.7900	 0.5770
Bx	 0.9600	 0.5960
By	 0.7910	 0.5780
Bz	 0.9400	 0.5930
Ca	 0.7890	 0.5770
Cb	 0.9500	 0.5950
Cc	 0.7890	 0.5780
Cd	 0.9400	 0.5940