



Full wwPDB EM Validation Report ⓘ

Aug 17, 2026 – 01:37 PM JST

PDB ID : 23WQ / pdb_000023wq
EMDB ID : EMD-69324
Title : Cryo-EM structure of EcBPAN-guide RNA-target DNA complex
Authors : Liu, M.; Yu, Q.; Shi, D.J.; Xing, Q.; Ma, L.X.
Deposited on : 2026-02-23
Resolution : 3.27 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.dev133
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) : 2.50

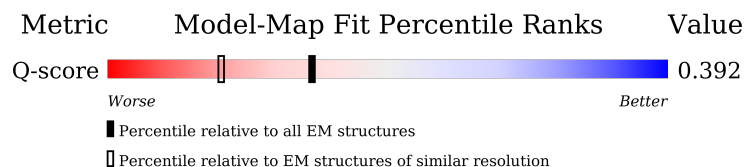
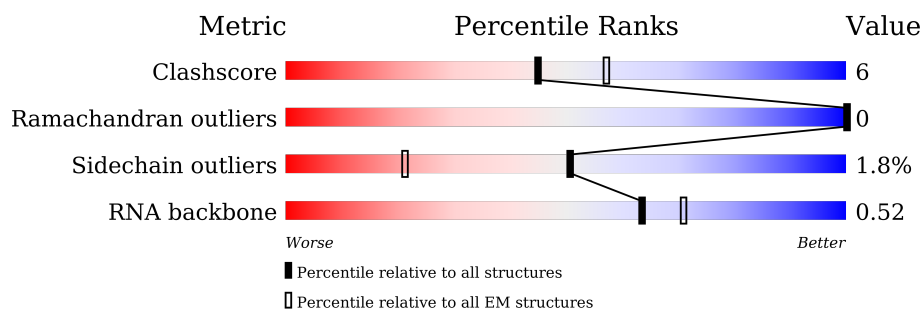
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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.



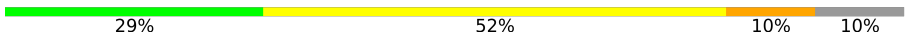
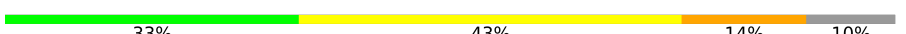
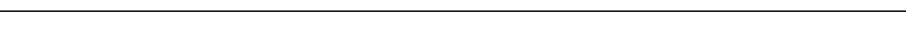
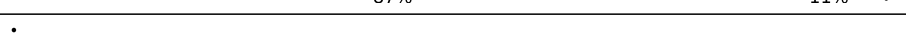
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14508 (2.77 - 3.77)

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	A	21	
1	C	21	
1	E	21	

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Mol	Chain	Length	Quality of chain
1	H	21	
1	I	21	
1	K	21	
1	N	21	
1	O	21	
2	B	21	
2	D	21	
2	F	21	
2	G	21	
2	J	21	
2	L	21	
2	M	21	
2	P	21	
3	1	390	
3	2	390	
3	3	390	
3	4	390	
3	5	390	
3	6	390	
3	7	390	
3	8	390	
4	a	731	
4	b	731	
4	c	731	
4	d	731	

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Mol	Chain	Length	Quality of chain
4	e	731	
4	f	731	
4	g	731	
4	h	731	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 77641 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 RNA chain called RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*CP*CP*CP*UP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	19	Total 400	C 180	N 70	O 131	P 19	0	0
1	C	19	Total 400	C 180	N 70	O 131	P 19	0	0
1	E	19	Total 400	C 180	N 70	O 131	P 19	0	0
1	H	19	Total 400	C 180	N 70	O 131	P 19	0	0
1	K	19	Total 400	C 180	N 70	O 131	P 19	0	0
1	N	19	Total 400	C 180	N 70	O 131	P 19	0	0
1	O	19	Total 400	C 180	N 70	O 131	P 19	0	0
1	I	19	Total 400	C 180	N 70	O 131	P 19	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	20	Total 412	C 197	N 73	O 122	P 20	0	0
2	D	20	Total 412	C 197	N 73	O 122	P 20	0	0
2	F	20	Total 412	C 197	N 73	O 122	P 20	0	0
2	G	20	Total 412	C 197	N 73	O 122	P 20	0	0
2	L	20	Total 412	C 197	N 73	O 122	P 20	0	0
2	M	20	Total 412	C 197	N 73	O 122	P 20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	20	Total	C	N	O	P	0	0
			412	197	73	122	20		
2	J	20	Total	C	N	O	P	0	0
			412	197	73	122	20		

- Molecule 3 is a protein called EcbAgaN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	380	Total	C	N	O	S	0	0
			3047	1960	505	569	13		
3	2	383	Total	C	N	O	S	0	0
			3074	1978	511	572	13		
3	4	384	Total	C	N	O	S	0	0
			3083	1983	512	575	13		
3	3	386	Total	C	N	O	S	0	0
			3100	1995	515	577	13		
3	8	383	Total	C	N	O	S	0	0
			3074	1978	511	572	13		
3	7	384	Total	C	N	O	S	0	0
			3083	1984	513	573	13		
3	5	389	Total	C	N	O	S	0	0
			3122	2010	518	580	14		
3	6	389	Total	C	N	O	S	0	0
			3122	2010	518	580	14		

- Molecule 4 is a protein called EcAgo.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	730	Total	C	N	O	S	0	0
			5797	3683	1013	1078	23		
4	e	731	Total	C	N	O	S	0	0
			5805	3688	1014	1079	24		
4	g	731	Total	C	N	O	S	0	0
			5805	3688	1014	1079	24		
4	h	731	Total	C	N	O	S	0	0
			5805	3688	1014	1079	24		
4	a	731	Total	C	N	O	S	0	0
			5805	3688	1014	1079	24		
4	b	731	Total	C	N	O	S	0	0
			5805	3688	1014	1079	24		
4	c	731	Total	C	N	O	S	0	0
			5805	3688	1014	1079	24		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	731	Total	C	N	O	S	0	0
			5805	3688	1014	1079	24		

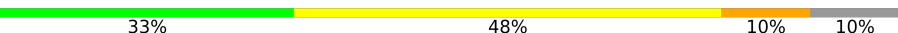
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	C	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	H	1	Total	Mg	0
			1	1	
5	K	1	Total	Mg	0
			1	1	
5	N	1	Total	Mg	0
			1	1	
5	O	1	Total	Mg	0
			1	1	
5	I	1	Total	Mg	0
			1	1	

3 Residue-property plots [i](#)

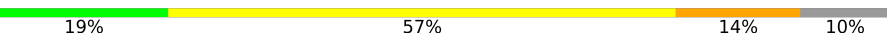
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*C P*CP*CP*UP*GP*G)-3')

Chain A: 

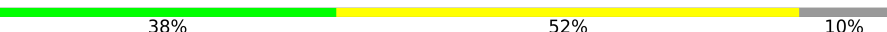


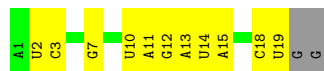
- Molecule 1: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*C P*CP*CP*UP*GP*G)-3')

Chain C: 

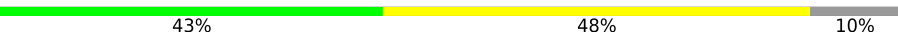


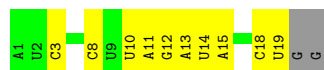
- Molecule 1: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*C P*CP*CP*UP*GP*G)-3')

Chain E: 

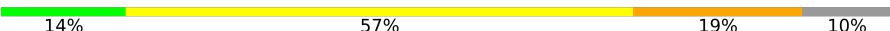


- Molecule 1: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*C P*CP*CP*UP*GP*G)-3')

Chain H: 



- Molecule 1: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*C P*CP*CP*UP*GP*G)-3')

Chain K: 



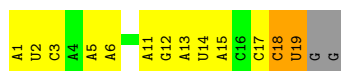
- Molecule 1: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*CP*CP*CP*UP*GP*G)-3')



- Molecule 1: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*CP*CP*CP*UP*GP*G)-3')



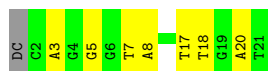
- Molecule 1: RNA (5'-R(P*AP*UP*CP*AP*AP*AP*GP*CP*UP*UP*AP*GP*AP*UP*AP*CP*CP*CP*UP*GP*G)-3')



- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')



- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')



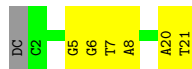
- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')





- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')

Chain G: 67% 29% 5%



- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')

Chain L: 67% 29% 5%



- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')

Chain M: 76% 19% 5%



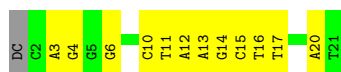
- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')

Chain P: 48% 48% 5%



- Molecule 2: DNA (5'-D(*CP*CP*AP*GP*GP*GP*TP*AP*TP*CP*TP*AP*AP*GP*CP*TP*TP*TP*GP*AP*T)-3')

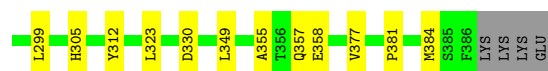
Chain J: 38% 57% 5%



- Molecule 3: EcbAgaN

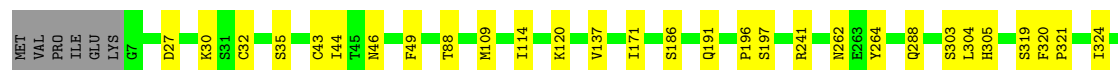
Chain 1: 87% 10% 3%





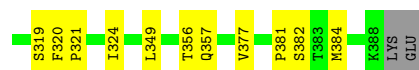
• Molecule 3: EcbAgaN

Chain 2: 87% 11% .



• Molecule 3: EcbAgaN

Chain 4: 88% 11% .



• Molecule 3: EcbAgaN

Chain 3: 91% 8% ..



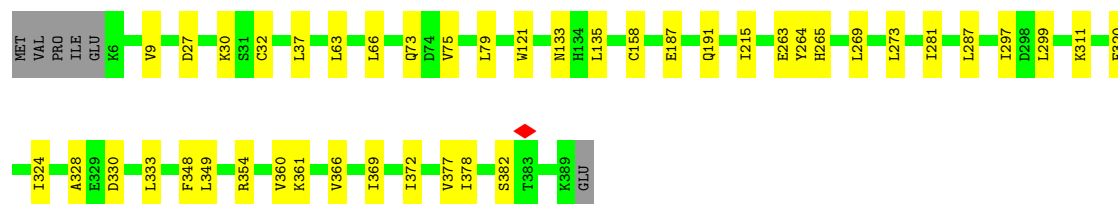
• Molecule 3: EcbAgaN

Chain 8: 88% 10% .

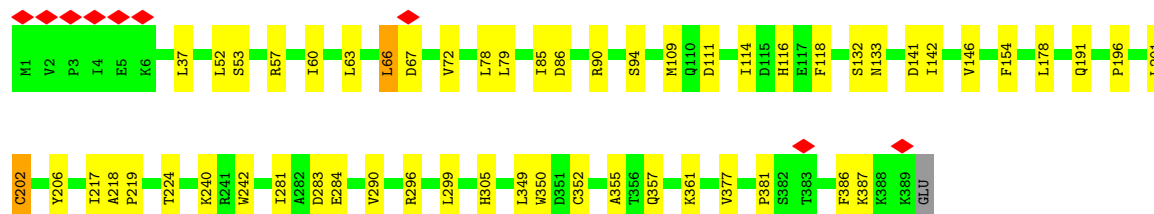
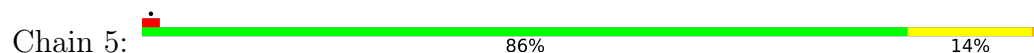


• Molecule 3: EcbAgaN

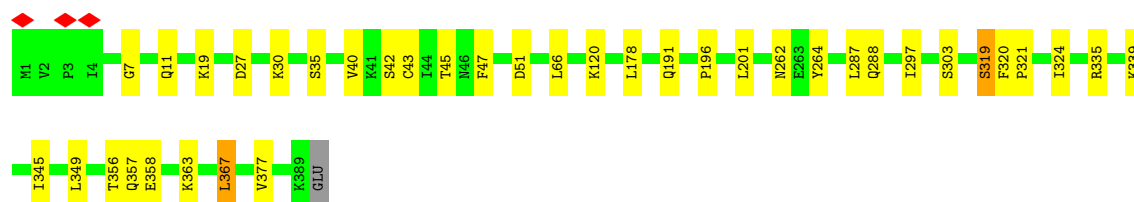
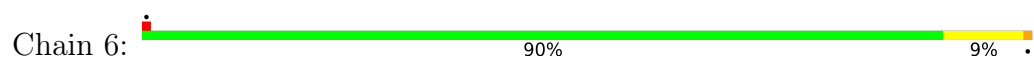
Chain 7: 87% 11% .



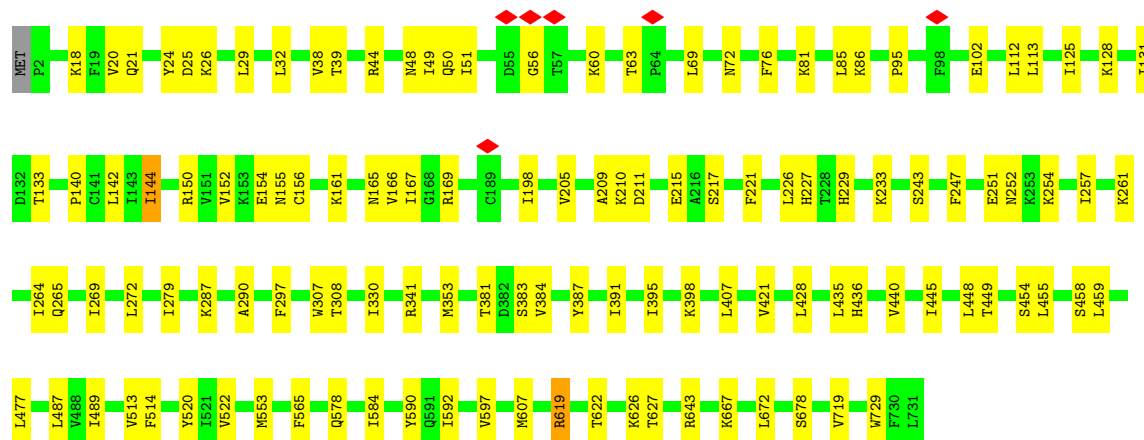
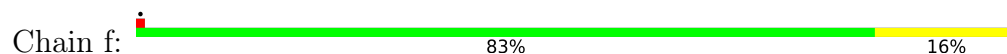
• Molecule 3: EcbAgaN



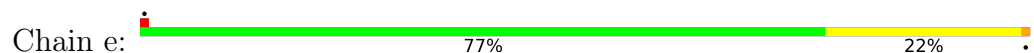
• Molecule 3: EcbAgaN

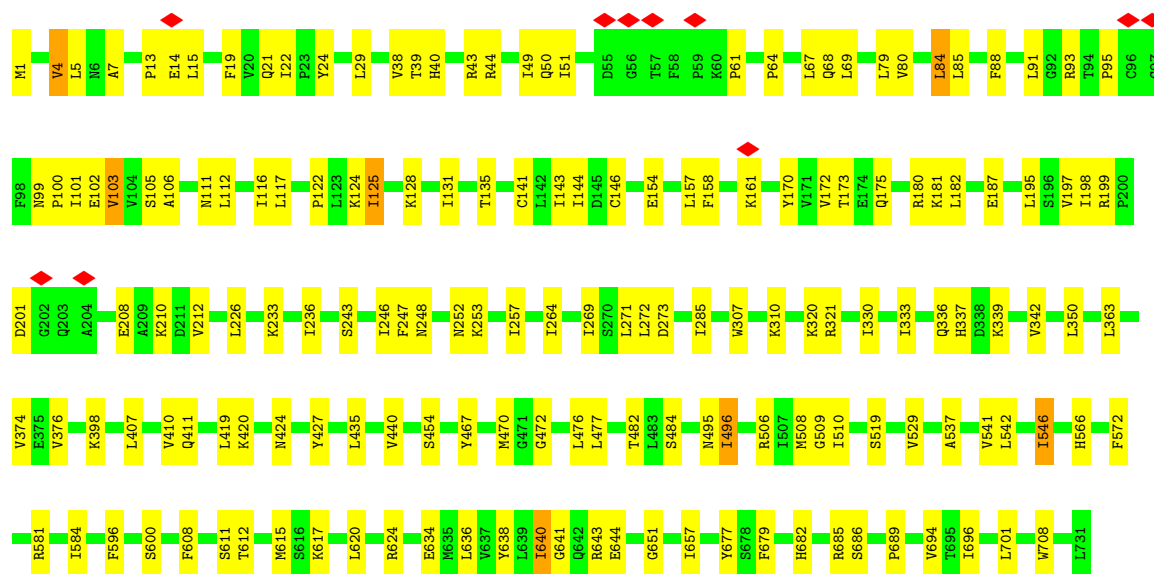


• Molecule 4: EcAgo



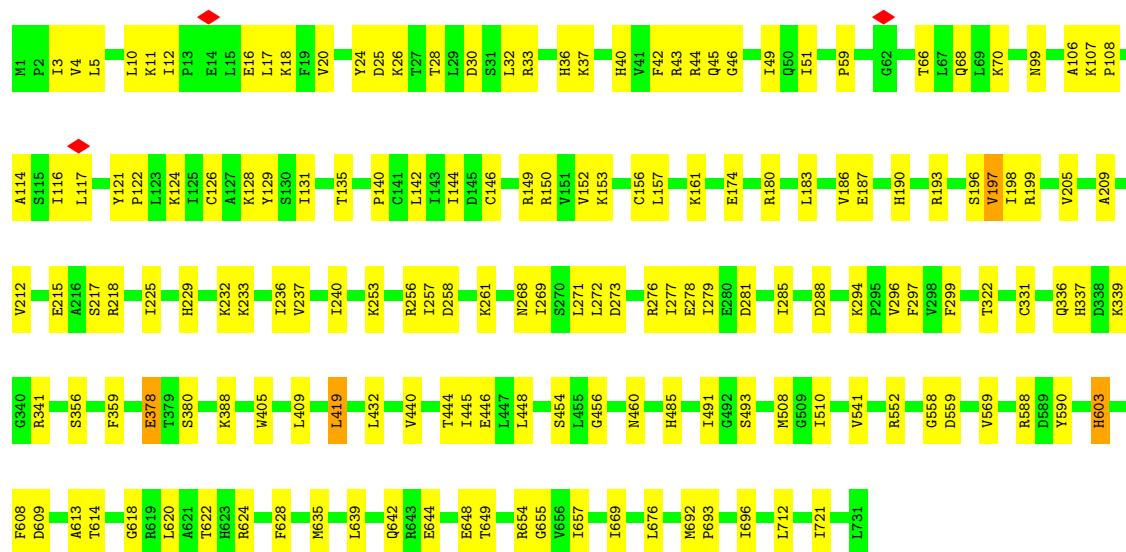
• Molecule 4: EcAgo





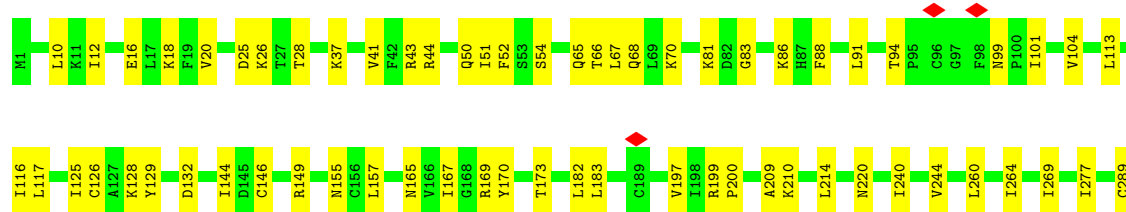
• Molecule 4: EcAgo

Chain g: 78% 22% .



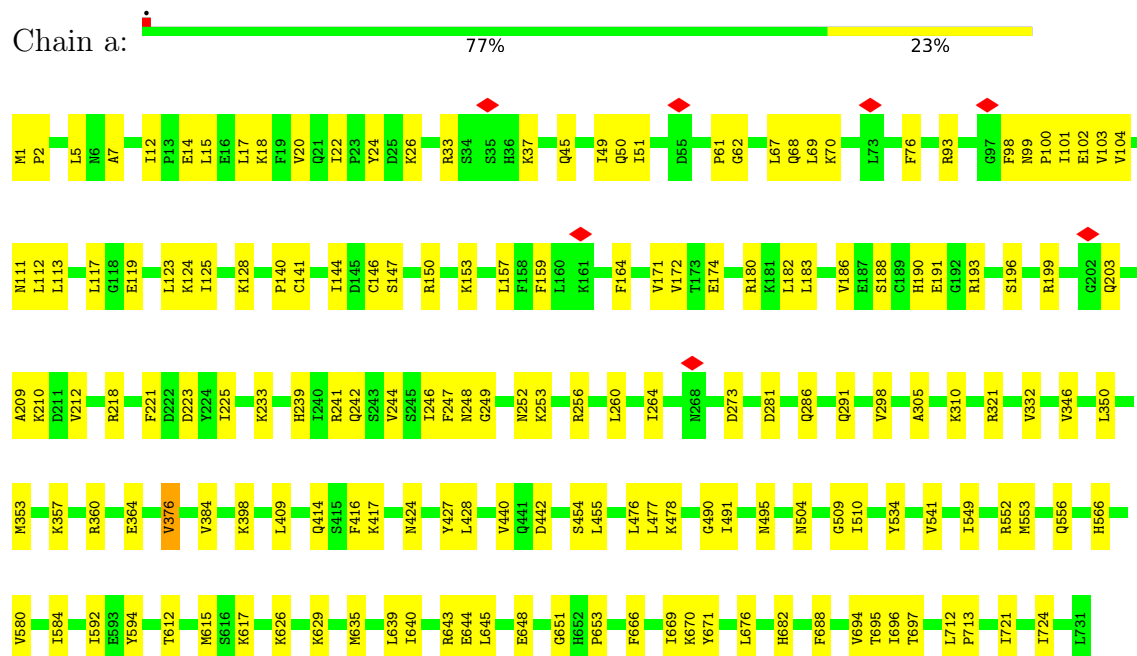
• Molecule 4: EcAgo

Chain h: 85% 15%

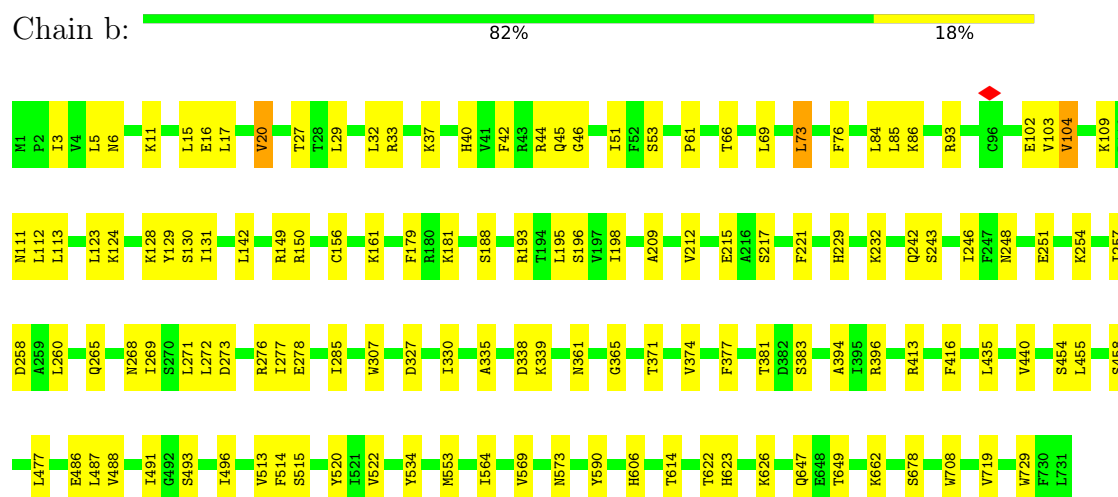




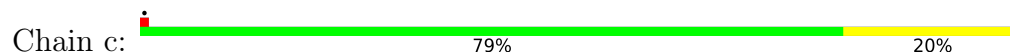
• Molecule 4: EcAgo

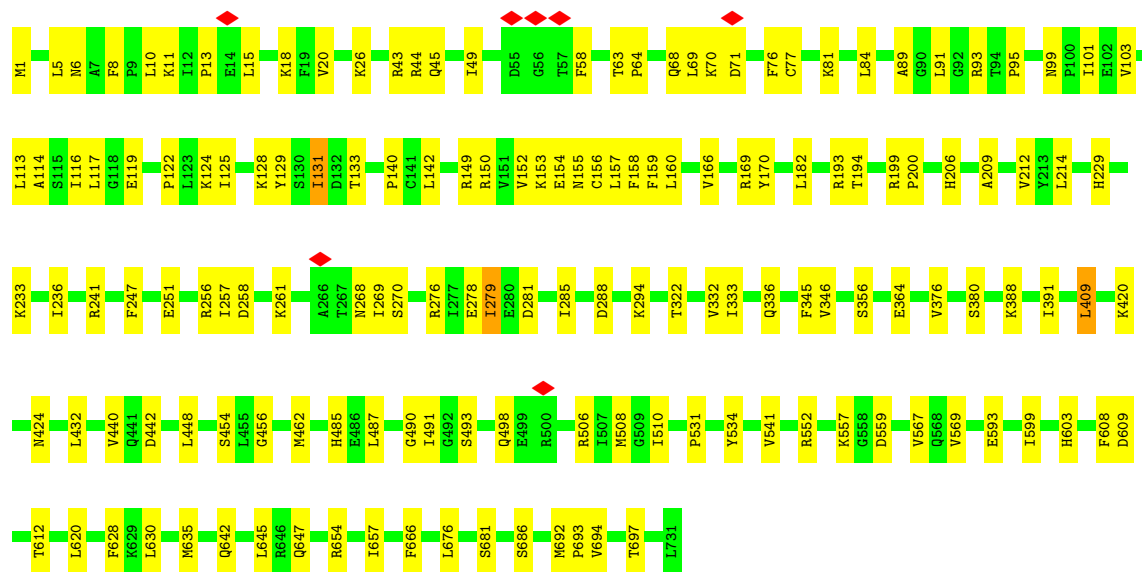


• Molecule 4: EcAgo

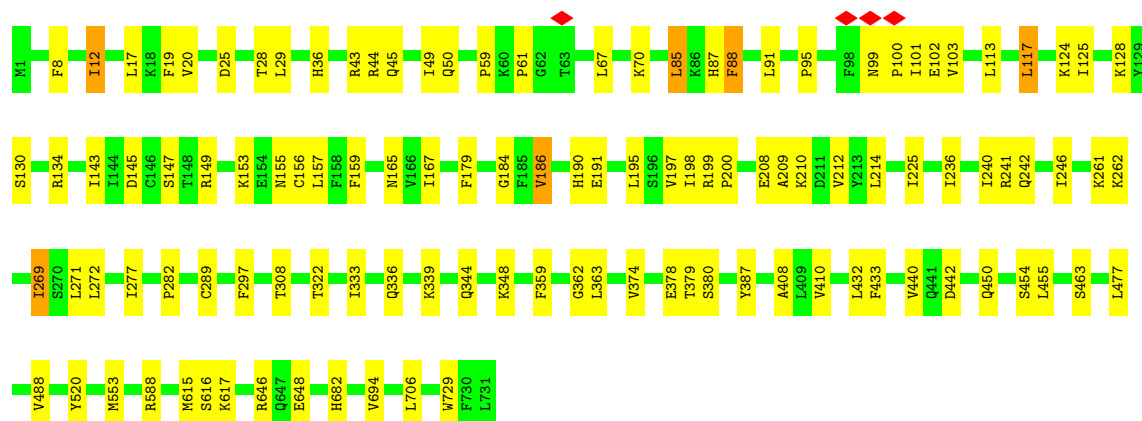
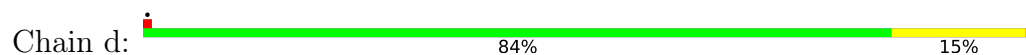


• Molecule 4: EcAgo





• Molecule 4: EcAgo



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	309746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02158	Depositor
Map size ($\text{\AA}$)	362.87997, 362.87997, 362.87997	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.567, 0.567, 0.567	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	A	0.16	0/446	0.31	0/691
1	C	0.15	0/446	0.31	0/691
1	E	0.15	0/446	0.29	0/691
1	H	0.21	0/446	0.34	0/691
1	I	0.13	0/446	0.30	0/691
1	K	0.13	0/446	0.30	0/691
1	N	0.22	0/446	0.35	0/691
1	O	0.20	0/446	0.36	0/691
2	B	0.19	0/461	0.32	0/710
2	D	0.16	0/461	0.32	0/710
2	F	0.19	0/461	0.33	0/710
2	G	0.19	0/461	0.32	0/710
2	J	0.16	0/461	0.31	0/710
2	L	0.16	0/461	0.32	0/710
2	M	0.19	0/461	0.33	0/710
2	P	0.16	0/461	0.32	0/710
3	1	0.25	0/3122	0.28	0/4236
3	2	0.33	0/3149	0.30	0/4269
3	3	0.21	0/3175	0.28	0/4303
3	4	0.27	0/3158	0.28	0/4281
3	5	0.26	0/3198	0.29	0/4335
3	6	0.33	0/3198	0.30	0/4335
3	7	0.21	0/3158	0.27	0/4280
3	8	0.27	0/3149	0.28	0/4269
4	a	0.13	0/5929	0.24	0/8009
4	b	0.15	0/5929	0.24	0/8009
4	c	0.15	0/5929	0.26	0/8009
4	d	0.17	0/5929	0.24	0/8009
4	e	0.13	0/5929	0.26	0/8009
4	f	0.15	0/5921	0.23	0/7998
4	g	0.16	0/5929	0.27	0/8009
4	h	0.17	0/5929	0.25	0/8009

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.20	0/79987	0.27	0/109577

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	A	400	0	205	6	0
1	C	400	0	205	17	0
1	E	400	0	205	6	0
1	H	400	0	205	5	0
1	I	400	0	205	9	0
1	K	400	0	205	13	0
1	N	400	0	205	5	0
1	O	400	0	205	13	0
2	B	412	0	228	4	0
2	D	412	0	228	8	0
2	F	412	0	228	4	0
2	G	412	0	228	8	0
2	J	412	0	228	8	0
2	L	412	0	228	7	0
2	M	412	0	228	3	0
2	P	412	0	228	9	0
3	1	3047	0	3007	28	0
3	2	3074	0	3046	21	0
3	3	3100	0	3076	20	0
3	4	3083	0	3052	24	0
3	5	3122	0	3104	29	0
3	6	3122	0	3104	20	0
3	7	3083	0	3059	25	0
3	8	3074	0	3046	26	0
4	a	5805	0	5813	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	b	5805	0	5813	81	0
4	c	5805	0	5813	106	0
4	d	5805	0	5813	75	0
4	e	5805	0	5813	103	0
4	f	5797	0	5802	72	0
4	g	5805	0	5813	106	0
4	h	5805	0	5813	69	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	K	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
All	All	77641	0	74451	950	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (950) 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)
4:c:128:LYS:HE3	4:c:149:ARG:HB2	1.55	0.88
4:d:199:ARG:HD3	4:d:200:PRO:HD2	1.61	0.81
4:d:615:MET:HE3	4:d:616:SER:H	1.47	0.79
4:g:692:MET:HE3	4:g:693:PRO:HD2	1.64	0.78
4:e:93:ARG:HE	4:e:105:SER:HA	1.51	0.76
4:h:183:LEU:HD12	4:h:197:VAL:HG11	1.69	0.74
2:P:20:DA:H62	4:a:454:SER:HB2	1.54	0.73
1:E:7:G:H5"	4:b:248:ASN:HD22	1.54	0.72
4:c:485:HIS:HE1	4:c:559:ASP:HB3	1.55	0.72
3:2:319:SER:HB2	3:2:321:PRO:HD2	1.71	0.71
4:b:15:LEU:HD23	4:b:273:ASP:HB2	1.71	0.71
4:g:4:VAL:HB	4:g:608:PHE:HB2	1.72	0.71
4:b:33:ARG:HG3	4:b:37:LYS:HE3	1.73	0.71
4:b:131:ILE:HD11	4:b:142:LEU:HD12	1.73	0.70
4:h:155:ASN:HD22	4:h:210:LYS:HA	1.56	0.70
4:b:381:THR:HG23	4:b:383:SER:H	1.57	0.70
1:C:1:A:H5"	4:c:442:ASP:HB2	1.72	0.70
2:G:7:DT:H3	1:H:15:A:H61	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:319:SER:HB2	3:6:321:PRO:HD2	1.72	0.70
4:e:482:THR:HG22	4:e:484:SER:H	1.55	0.69
4:e:112:LEU:HD21	4:e:247:PHE:HE2	1.58	0.69
4:g:341:ARG:HB3	4:g:448:LEU:HD21	1.73	0.69
4:g:635:MET:HE3	4:g:669:ILE:HG12	1.75	0.68
4:b:487:LEU:HD12	4:b:514:PHE:HB3	1.76	0.68
4:f:165:ASN:HD21	4:f:167:ILE:HB	1.59	0.68
4:h:607:MET:HE2	4:h:622:THR:HG21	1.76	0.68
4:b:271:LEU:HD13	4:b:277:ILE:HD11	1.77	0.67
4:f:85:LEU:HD23	4:f:95:PRO:HG2	1.75	0.67
4:f:381:THR:HG23	4:f:383:SER:H	1.59	0.67
1:A:1:A:H5'	4:d:442:ASP:HB2	1.76	0.66
3:4:349:LEU:HD23	3:4:377:VAL:HG13	1.78	0.66
4:c:608:PHE:HB3	4:c:620:LEU:HD22	1.78	0.66
3:3:100:MET:HE1	3:3:142:ILE:HD12	1.78	0.66
4:e:454:SER:HB2	2:J:20:DA:H62	1.59	0.66
1:O:14:U:H2'	1:O:15:A:H8	1.61	0.66
4:e:172:VAL:HG21	4:e:180:ARG:HB3	1.78	0.65
4:d:271:LEU:HG	4:d:272:LEU:H	1.62	0.65
4:f:113:LEU:HD22	4:f:125:ILE:HD12	1.76	0.65
3:5:60:ILE:HA	3:5:63:LEU:HD13	1.78	0.65
3:8:349:LEU:HD23	3:8:377:VAL:HG13	1.79	0.65
4:c:170:TYR:HB3	4:c:182:LEU:HD11	1.77	0.65
4:h:16:GLU:HB3	4:h:66:THR:HB	1.77	0.65
4:b:6:ASN:HD22	4:b:606:HIS:HB2	1.61	0.65
4:a:12:ILE:HD11	4:a:69:LEU:HB3	1.78	0.64
4:e:427:TYR:HH	4:e:708:TRP:CD1	2.15	0.64
1:K:18:C:H42	2:L:4:DG:H1	1.43	0.64
2:L:8:DA:H2''	4:g:99:ASN:HD21	1.60	0.64
4:b:179:PHE:HB2	4:b:181:LYS:HZ1	1.62	0.64
4:g:339:LYS:HE2	4:g:378:GLU:HB3	1.78	0.64
4:a:193:ARG:HH22	4:a:209:ALA:HB3	1.61	0.64
3:5:349:LEU:HD23	3:5:377:VAL:HG13	1.80	0.64
4:h:264:ILE:HG23	4:h:269:ILE:HG13	1.80	0.63
4:d:101:ILE:HG23	4:d:102:GLU:HG3	1.79	0.63
4:e:38:VAL:HG12	4:e:39:THR:HG23	1.80	0.63
4:f:155:ASN:HD22	4:f:210:LYS:HA	1.63	0.63
4:a:18:LYS:HZ1	4:a:62:GLY:H	1.46	0.63
3:1:349:LEU:HD23	3:1:377:VAL:HG13	1.80	0.63
4:e:14:GLU:HG3	4:e:68:GLN:HE22	1.64	0.63
4:b:11:LYS:HE3	4:b:278:GLU:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:27:ASP:HB3	3:3:30:LYS:HB2	1.81	0.62
1:I:14:U:H2'	1:I:15:A:H8	1.64	0.62
4:a:332:VAL:HG12	4:a:409:LEU:HB2	1.81	0.62
4:d:25:ASP:HB3	4:d:28:THR:HG22	1.80	0.62
4:a:645:LEU:HD11	4:a:653:PRO:HD3	1.80	0.62
4:e:93:ARG:HH21	4:e:106:ALA:H	1.45	0.62
3:2:262:ASN:HD22	3:2:264:TYR:HD2	1.48	0.62
4:d:157:LEU:HD12	4:d:209:ALA:HB3	1.81	0.62
4:a:112:LEU:HD12	4:a:239:HIS:CE1	2.35	0.62
3:6:262:ASN:HD22	3:6:264:TYR:HD2	1.48	0.62
3:1:281:ILE:HD11	3:1:299:LEU:HD22	1.81	0.62
4:f:156:CYS:HB2	4:f:209:ALA:HB1	1.81	0.61
3:8:319:SER:HB2	3:8:321:PRO:HD2	1.82	0.61
4:a:209:ALA:HA	4:a:212:VAL:HG22	1.83	0.61
3:7:27:ASP:HB3	3:7:30:LYS:HB2	1.80	0.61
1:I:18:C:H42	2:J:4:DG:H1	1.47	0.61
4:c:154:GLU:HB2	4:c:158:PHE:HD2	1.66	0.61
4:d:102:GLU:HG2	4:d:130:SER:HB3	1.81	0.61
4:b:44:ARG:HH21	4:b:46:GLY:HA2	1.65	0.61
4:h:68:GLN:HG3	4:h:70:LYS:HG2	1.83	0.60
3:4:36:LEU:HD13	3:4:63:LEU:HB3	1.83	0.60
3:4:319:SER:HB2	3:4:321:PRO:HD2	1.83	0.60
4:a:249:GLY:HA2	4:a:651:GLY:HA2	1.84	0.60
1:K:10:U:H2'	1:K:11:A:C8	2.37	0.60
4:a:124:LYS:HB2	4:a:153:LYS:HZ2	1.65	0.60
4:g:131:ILE:HD11	4:g:142:LEU:HD12	1.83	0.60
3:5:79:LEU:HD11	3:5:118:PHE:HA	1.83	0.60
4:a:357:LYS:HA	4:a:360:ARG:HH12	1.67	0.59
1:O:7:G:H4'	4:a:244:VAL:HB	1.84	0.59
4:h:116:ILE:HG23	4:h:117:LEU:HD23	1.82	0.59
4:c:676:LEU:HG	4:c:693:PRO:HG3	1.83	0.59
4:b:330:ILE:HB	4:b:374:VAL:HG23	1.82	0.59
4:f:477:LEU:HD21	4:f:678:SER:HB3	1.85	0.59
4:b:17:LEU:HD13	4:b:272:LEU:HD23	1.85	0.59
4:c:332:VAL:HG12	4:c:409:LEU:HB2	1.84	0.59
4:g:271:LEU:HB2	4:g:277:ILE:HD11	1.85	0.59
4:f:330:ILE:HD13	4:f:407:LEU:HB3	1.85	0.59
3:6:349:LEU:HD23	3:6:377:VAL:HG13	1.83	0.59
4:d:165:ASN:HD21	4:d:167:ILE:HB	1.67	0.59
3:2:349:LEU:HD23	3:2:377:VAL:HG13	1.84	0.58
2:F:6:DG:H2''	4:b:44:ARG:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:99:ASN:HD21	4:d:101:ILE:HG22	1.67	0.58
3:5:281:ILE:HD11	3:5:299:LEU:HD22	1.84	0.58
4:h:615:MET:HE3	4:h:616:SER:N	2.18	0.58
4:a:424:ASN:HB3	4:a:427:TYR:HB2	1.86	0.58
4:b:40:HIS:CE1	4:b:53:SER:HB2	2.39	0.58
3:6:27:ASP:HB3	3:6:30:LYS:HB2	1.85	0.58
4:g:485:HIS:HE1	4:g:559:ASP:HB3	1.67	0.58
4:g:588:ARG:HA	4:g:588:ARG:NE	2.19	0.58
4:h:25:ASP:HB3	4:h:28:THR:HG22	1.84	0.58
4:a:639:LEU:HD11	4:a:676:LEU:HD21	1.86	0.58
4:g:261:LYS:HG3	4:g:279:ILE:HD11	1.84	0.58
4:e:43:ARG:HB3	4:e:50:GLN:HB2	1.86	0.58
3:7:328:ALA:HB2	3:7:369:ILE:HD13	1.86	0.58
4:c:18:LYS:HE2	4:c:64:PRO:HB3	1.84	0.58
4:g:3:ILE:HD11	4:g:285:ILE:H	1.69	0.58
4:g:25:ASP:HB2	4:g:28:THR:HG22	1.84	0.58
4:b:73:LEU:HA	4:b:76:PHE:HB3	1.86	0.58
4:b:156:CYS:HB2	4:b:209:ALA:HB1	1.86	0.58
4:h:334:CYS:HB3	4:h:339:LYS:HZ1	1.69	0.58
4:a:617:LYS:HG3	4:a:648:GLU:HA	1.86	0.58
3:1:72:VAL:HG22	3:1:109:MET:HE2	1.86	0.57
4:b:276:ARG:HH22	4:b:278:GLU:HG3	1.68	0.57
4:d:156:CYS:HA	4:d:159:PHE:HD2	1.69	0.57
4:e:321:ARG:HE	3:5:94:SER:HB3	1.69	0.57
1:C:1:A:H61	4:c:424:ASN:HD21	1.52	0.57
4:g:603:HIS:HE1	4:g:654:ARG:HB3	1.70	0.57
4:c:81:LYS:HD2	4:c:133:THR:HG21	1.86	0.57
4:d:333:ILE:HD12	4:d:410:VAL:HG22	1.84	0.57
4:d:336:GLN:HE22	4:d:380:SER:HA	1.69	0.57
4:e:1:MET:HE1	4:e:611:SER:HB3	1.87	0.57
4:g:11:LYS:NZ	4:g:277:ILE:HA	2.20	0.57
4:g:721:ILE:HD11	4:h:396:ARG:HH21	1.69	0.57
1:I:19:U:H3	2:J:3:DA:H61	1.53	0.57
4:a:353:MET:HE1	4:a:455:LEU:HD23	1.87	0.57
4:a:617:LYS:HE2	4:a:643:ARG:HH12	1.70	0.57
4:c:268:ASN:HA	4:c:276:ARG:HE	1.69	0.57
3:1:79:LEU:HD11	3:1:118:PHE:HA	1.87	0.57
4:a:584:ILE:HD12	4:a:592:ILE:HD12	1.87	0.57
3:2:35:SER:HB2	3:2:43:CYS:HB3	1.86	0.57
4:c:166:VAL:HA	4:c:169:ARG:HD2	1.86	0.57
4:f:264:ILE:HG23	4:f:269:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1:A:H61	4:a:424:ASN:HD21	1.52	0.56
1:O:10:U:H2'	1:O:11:A:C8	2.40	0.56
4:a:721:ILE:HD11	4:b:396:ARG:HE	1.70	0.56
4:f:20:VAL:HB	4:f:63:THR:HG21	1.86	0.56
1:C:10:U:H2'	1:C:11:A:C8	2.40	0.56
4:h:334:CYS:HB3	4:h:339:LYS:NZ	2.21	0.56
4:a:17:LEU:HB2	4:a:67:LEU:HB3	1.87	0.56
4:b:69:LEU:HD22	4:b:76:PHE:HB2	1.86	0.56
4:e:88:PHE:HB2	4:e:95:PRO:HG3	1.87	0.56
4:g:268:ASN:HA	4:g:276:ARG:HD2	1.86	0.56
4:a:112:LEU:HD12	4:a:239:HIS:HE1	1.71	0.56
4:d:113:LEU:HG	4:d:117:LEU:HD11	1.86	0.56
4:b:5:LEU:HB2	4:b:285:ILE:HD13	1.88	0.56
4:c:43:ARG:HH21	4:c:45:GLN:HB2	1.71	0.56
3:3:324:ILE:HG22	3:3:369:ILE:HD11	1.87	0.56
4:h:379:THR:HG21	4:h:387:TYR:HE1	1.70	0.56
3:7:324:ILE:HG22	3:7:369:ILE:HD11	1.87	0.56
1:O:18:C:H42	2:P:4:DG:H1	1.52	0.56
3:1:150:GLU:H	3:1:150:GLU:CD	2.14	0.56
4:c:89:ALA:HB2	4:c:95:PRO:HG3	1.88	0.55
4:d:124:LYS:HE2	4:d:153:LYS:HD3	1.88	0.55
4:e:102:GLU:HB3	4:e:128:LYS:HD2	1.87	0.55
1:C:8:C:H4'	4:c:150:ARG:HE	1.70	0.55
1:C:14:U:H2'	1:C:15:A:C8	2.41	0.55
4:g:17:LEU:HD11	4:g:273:ASP:HB3	1.88	0.55
3:5:217:ILE:HG12	3:5:219:PRO:HG3	1.88	0.55
4:b:335:ALA:HB3	4:b:338:ASP:HB2	1.88	0.55
4:c:420:LYS:HE2	4:c:498:GLN:HB3	1.89	0.55
3:2:288:GLN:HE22	3:6:339:LYS:HE3	1.72	0.55
1:C:19:U:H3	2:D:3:DA:H61	1.54	0.55
1:K:14:U:H2'	1:K:15:A:C8	2.42	0.55
4:d:339:LYS:HZ1	4:d:378:GLU:HB3	1.71	0.55
4:a:68:GLN:HG3	4:a:70:LYS:H	1.71	0.55
4:b:242:GLN:O	4:b:246:ILE:HG13	2.07	0.55
3:5:37:LEU:HD21	3:5:206:TYR:HB2	1.89	0.55
2:B:19:DG:H21	4:d:646:ARG:HH12	1.55	0.55
4:a:24:TYR:HB2	4:a:49:ILE:HG13	1.88	0.55
4:a:612:THR:HA	4:a:615:MET:HE1	1.89	0.55
4:c:20:VAL:HG21	4:c:58:PHE:HZ	1.72	0.55
4:c:257:ILE:HG13	4:c:258:ASP:N	2.21	0.55
3:1:293:LYS:HD3	3:1:296:ARG:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:600:SER:HB2	4:e:657:ILE:HB	1.88	0.55
4:h:427:TYR:HH	4:h:708:TRP:CD1	2.24	0.55
4:a:93:ARG:HB2	4:a:103:VAL:HG13	1.89	0.55
4:b:29:LEU:HD12	4:b:32:LEU:HD11	1.89	0.55
4:b:254:LYS:HZ3	4:b:257:ILE:HD11	1.72	0.55
4:e:424:ASN:HD21	1:I:1:A:H61	1.55	0.54
1:O:14:U:H2'	1:O:15:A:C8	2.40	0.54
4:h:616:SER:HA	4:h:619:ARG:HG2	1.87	0.54
4:d:269:ILE:HD11	4:d:277:ILE:HB	1.89	0.54
4:e:122:PRO:HG2	4:e:158:PHE:CE2	2.43	0.54
4:g:10:LEU:HD11	4:g:277:ILE:HG22	1.90	0.54
4:h:338:ASP:HA	4:h:341:ARG:HD3	1.89	0.54
3:2:27:ASP:HB3	3:2:30:LYS:HB2	1.88	0.54
4:g:493:SER:HB2	4:g:508:MET:HG2	1.88	0.54
3:4:62:GLY:HA2	3:4:105:LEU:HB2	1.90	0.54
3:4:381:PRO:HG2	3:4:384:MET:HG3	1.89	0.54
4:g:225:ILE:HG13	4:g:233:LYS:HB2	1.89	0.54
4:a:5:LEU:HG	4:a:7:ALA:H	1.73	0.54
4:c:485:HIS:CE1	4:c:559:ASP:HB3	2.40	0.54
3:1:96:MET:HE1	3:1:135:LEU:HD13	1.89	0.54
4:e:246:ILE:HG22	4:e:252:ASN:HB2	1.88	0.54
4:c:508:MET:HE1	4:c:534:TYR:CE2	2.43	0.54
4:d:588:ARG:HH11	4:d:588:ARG:HG3	1.72	0.54
4:g:285:ILE:HG22	4:g:288:ASP:HB2	1.89	0.54
4:c:261:LYS:HG3	4:c:279:ILE:HD11	1.89	0.54
4:e:5:LEU:HD12	4:e:285:ILE:HD13	1.89	0.54
4:e:85:LEU:HA	4:e:88:PHE:CE2	2.43	0.54
4:e:651:GLY:H	1:I:6:A:H4'	1.72	0.54
4:g:122:PRO:HB2	4:g:152:VAL:HG13	1.89	0.54
4:a:332:VAL:HG11	4:a:346:VAL:HG11	1.89	0.54
4:g:157:LEU:H	4:g:157:LEU:HD12	1.71	0.54
3:1:141:ASP:HB3	3:1:154:PHE:HD1	1.73	0.53
4:e:634:GLU:HG3	4:e:657:ILE:HG23	1.90	0.53
4:c:149:ARG:HE	4:c:150:ARG:H	1.54	0.53
3:4:89:PRO:HG3	4:g:322:THR:HG21	1.90	0.53
4:e:407:LEU:HB2	4:e:470:MET:HE2	1.90	0.53
3:1:293:LYS:HZ2	3:1:296:ARG:HG3	1.71	0.53
4:e:19:PHE:HE2	4:e:21:GLN:HE22	1.55	0.53
2:G:5:DG:H2'	2:G:6:DG:H8	1.72	0.53
1:N:10:U:H2'	1:N:11:A:C8	2.44	0.53
2:P:12:DA:H4'	4:a:495:ASN:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:20:VAL:HG21	4:b:61:PRO:HA	1.90	0.53
3:5:191:GLN:HB3	3:5:196:PRO:HG3	1.90	0.53
3:5:350:TRP:CD1	3:5:352:CYS:HG	2.26	0.53
3:2:339:LYS:HE2	3:6:288:GLN:HE22	1.72	0.53
3:7:32:CYS:SG	3:7:63:LEU:HD12	2.48	0.53
1:H:10:U:H2'	1:H:11:A:C8	2.44	0.53
1:K:10:U:H2'	1:K:11:A:H8	1.73	0.53
2:L:20:DA:H62	4:g:454:SER:HB2	1.73	0.53
4:b:513:VAL:HG22	4:b:522:VAL:HA	1.90	0.53
4:b:623:HIS:HB2	4:b:626:LYS:HE2	1.89	0.53
4:c:131:ILE:HD11	4:c:142:LEU:HD12	1.91	0.53
4:c:155:ASN:OD1	4:c:157:LEU:HD12	2.08	0.53
3:5:111:ASP:HB3	3:5:114:ILE:HB	1.91	0.53
3:3:269:LEU:O	3:3:273:LEU:HD12	2.08	0.53
4:h:129:TYR:HD2	4:h:260:LEU:HD22	1.73	0.53
4:a:247:PHE:HA	4:a:252:ASN:HB3	1.88	0.53
4:f:25:ASP:H	4:f:29:LEU:HD13	1.73	0.53
4:h:43:ARG:HB3	4:h:50:GLN:HB3	1.90	0.53
1:A:10:U:H2'	1:A:11:A:C8	2.43	0.53
4:g:16:GLU:HB3	4:g:66:THR:HB	1.91	0.53
3:7:330:ASP:HA	3:7:333:LEU:HD12	1.91	0.53
4:e:7:ALA:HB1	4:e:141:CYS:HB2	1.90	0.53
1:C:10:U:H2'	1:C:11:A:H8	1.74	0.53
2:L:6:DG:H1'	4:g:44:ARG:HH11	1.74	0.53
4:f:215:GLU:OE1	4:f:217:SER:HB3	2.09	0.53
1:O:1:A:H2	4:a:416:PHE:HB2	1.74	0.53
4:c:129:TYR:HE2	4:c:256:ARG:HB3	1.74	0.53
4:e:339:LYS:HA	4:e:342:VAL:HG12	1.91	0.53
4:g:146:CYS:HB3	4:g:253:LYS:HG3	1.91	0.53
3:1:94:SER:HB3	4:a:321:ARG:HE	1.74	0.52
3:7:354:ARG:HD3	3:7:382:SER:HB2	1.91	0.52
4:e:496:ILE:HD11	4:e:708:TRP:CG	2.44	0.52
4:g:20:VAL:HG23	4:g:51:ILE:HB	1.91	0.52
1:O:19:U:H3	2:P:3:DA:H61	1.54	0.52
4:h:341:ARG:HD2	4:h:341:ARG:N	2.23	0.52
4:e:330:ILE:HB	4:e:374:VAL:HG23	1.89	0.52
1:H:10:U:H2'	1:H:11:A:H8	1.74	0.52
4:g:129:TYR:HE1	4:g:256:ARG:HB3	1.73	0.52
4:h:173:THR:HG22	4:h:183:LEU:HD22	1.91	0.52
4:c:336:GLN:HE22	4:c:380:SER:HA	1.73	0.52
3:8:222:GLY:HA2	3:7:215:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:622:THR:HG22	4:f:626:LYS:HG3	1.91	0.52
2:P:5:DG:H4'	4:a:26:LYS:HE3	1.91	0.52
4:c:93:ARG:HE	4:c:103:VAL:HG21	1.74	0.52
4:a:640:ILE:HD12	4:a:644:GLU:HG2	1.91	0.52
4:c:11:LYS:HE3	4:c:278:GLU:H	1.74	0.52
4:d:29:LEU:HD13	4:d:49:ILE:HD13	1.90	0.52
4:e:93:ARG:HB2	4:e:103:VAL:HB	1.92	0.52
4:g:493:SER:HB3	4:g:569:VAL:HG21	1.92	0.52
4:b:477:LEU:HD21	4:b:678:SER:HB3	1.91	0.52
4:f:131:ILE:HD13	4:f:144:ILE:HG23	1.90	0.52
2:P:8:DA:H2'	4:a:98:PHE:HE2	1.73	0.52
4:d:208:GLU:HG2	4:d:210:LYS:H	1.75	0.52
3:3:366:VAL:HG12	3:3:372:ILE:HG21	1.91	0.52
1:K:19:U:H3	2:L:3:DA:H61	1.58	0.52
4:d:588:ARG:HG3	4:d:588:ARG:NH1	2.25	0.52
3:1:240:LYS:HA	3:4:357:GLN:HG3	1.91	0.52
4:g:618:GLY:HA3	4:g:642:GLN:HG2	1.92	0.52
3:1:271:TYR:CG	3:2:241:ARG:HD3	2.45	0.51
4:e:111:ASN:HA	4:e:125:ILE:HG22	1.92	0.51
4:e:542:LEU:O	4:e:546:ILE:HG22	2.09	0.51
4:g:271:LEU:HG	4:g:272:LEU:H	1.75	0.51
4:a:14:GLU:HA	4:a:68:GLN:HE22	1.75	0.51
4:a:510:ILE:HG21	4:a:541:VAL:HG11	1.90	0.51
4:b:112:LEU:HD13	4:b:243:SER:HB2	1.92	0.51
4:c:114:ALA:HB1	4:c:119:GLU:HA	1.92	0.51
3:8:357:GLN:HG3	3:5:240:LYS:HA	1.93	0.51
4:e:61:PRO:HB2	4:e:64:PRO:HG3	1.91	0.51
4:g:107:LYS:HG3	4:g:108:PRO:HD2	1.92	0.51
4:c:270:SER:HA	4:c:276:ARG:HA	1.92	0.51
3:7:281:ILE:HD11	3:7:299:LEU:HD22	1.92	0.51
4:f:81:LYS:HE2	4:f:133:THR:HG22	1.92	0.51
4:f:445:ILE:HD12	4:f:448:LEU:HD13	1.92	0.51
1:E:10:U:H2'	1:E:11:A:C8	2.46	0.51
1:N:14:U:H2'	1:N:15:A:C8	2.46	0.51
4:c:113:LEU:HD23	4:c:125:ILE:HD11	1.92	0.51
3:2:88:THR:HG22	4:h:473:VAL:HG21	1.92	0.51
4:f:341:ARG:HH22	4:f:449:THR:HG22	1.75	0.51
4:e:79:LEU:HG	4:e:272:LEU:HD12	1.92	0.51
4:e:170:TYR:HD2	4:e:182:LEU:HD22	1.74	0.51
4:b:209:ALA:HA	4:b:212:VAL:HG22	1.93	0.51
4:c:91:LEU:HD11	4:c:269:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:122:PRO:HB3	4:c:154:GLU:HB3	1.91	0.51
3:1:287:LEU:HD21	3:1:293:LYS:HB3	1.91	0.51
3:2:46:ASN:HD21	3:2:49:PHE:HD1	1.59	0.51
4:f:261:LYS:HG2	4:f:279:ILE:HD11	1.92	0.51
4:d:186:VAL:HG11	4:d:195:LEU:HD13	1.93	0.51
3:6:335:ARG:HH21	3:6:345:ILE:HG13	1.75	0.51
4:a:18:LYS:HZ1	4:a:61:PRO:HA	1.74	0.51
3:1:357:GLN:HG3	3:4:240:LYS:HA	1.91	0.51
4:f:44:ARG:HD2	2:G:6:DG:H4'	1.91	0.51
4:g:114:ALA:HA	4:g:121:TYR:HD2	1.75	0.51
4:g:510:ILE:HG21	4:g:541:VAL:HG11	1.92	0.51
4:a:428:LEU:HD12	4:a:712:LEU:HD21	1.93	0.51
4:b:93:ARG:HH21	4:b:104:VAL:HG13	1.76	0.51
1:A:14:U:H2'	1:A:15:A:C8	2.46	0.51
4:a:157:LEU:HD22	4:a:210:LYS:HG3	1.92	0.51
4:a:260:LEU:O	4:a:264:ILE:HG13	2.11	0.51
4:a:694:VAL:HA	4:a:697:THR:HG22	1.91	0.51
4:b:40:HIS:NE2	4:b:51:ILE:HG23	2.26	0.51
4:b:45:GLN:O	4:b:45:GLN:HG3	2.11	0.51
3:5:72:VAL:HG22	3:5:109:MET:HE2	1.92	0.51
2:D:5:DG:H1'	4:c:26:LYS:HE3	1.93	0.51
3:6:7:GLY:HA2	3:6:11:GLN:HB2	1.92	0.51
3:8:89:PRO:HG3	4:c:322:THR:HG21	1.92	0.50
4:f:353:MET:HE1	4:f:455:LEU:HB3	1.92	0.50
1:E:10:U:H2'	1:E:11:A:H8	1.76	0.50
1:K:8:C:H4'	4:g:150:ARG:HE	1.75	0.50
4:d:43:ARG:HG2	4:d:45:GLN:HE22	1.76	0.50
2:G:5:DG:H2'	2:G:6:DG:C8	2.46	0.50
4:g:209:ALA:HA	4:g:212:VAL:HG22	1.93	0.50
4:a:305:ALA:HB1	4:a:310:LYS:HE2	1.93	0.50
4:b:488:VAL:HG12	4:b:564:ILE:HB	1.92	0.50
4:d:102:GLU:H	4:d:130:SER:HA	1.75	0.50
4:e:477:LEU:HD11	4:e:682:HIS:HB2	1.93	0.50
4:a:666:PHE:HZ	4:a:671:TYR:HD2	1.58	0.50
4:c:630:LEU:H	4:c:635:MET:HA	1.76	0.50
4:d:615:MET:HE3	4:d:616:SER:N	2.22	0.50
4:g:183:LEU:HD11	4:g:205:VAL:HG21	1.93	0.50
4:b:493:SER:HB3	4:b:569:VAL:HG21	1.93	0.50
3:8:240:LYS:HA	3:5:357:GLN:HG3	1.92	0.50
4:f:38:VAL:HG13	4:f:39:THR:HG23	1.93	0.50
4:g:116:ILE:HB	4:g:121:TYR:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:170:TYR:HD2	4:h:182:LEU:HD11	1.75	0.50
4:b:113:LEU:HD21	4:b:123:LEU:HB2	1.93	0.50
4:c:603:HIS:HB3	4:c:657:ILE:HD11	1.92	0.50
3:6:357:GLN:HG2	3:6:358:GLU:HG2	1.93	0.50
3:1:85:ILE:HG12	4:a:552:ARG:HD3	1.94	0.50
3:4:85:ILE:HG23	4:g:552:ARG:HD2	1.94	0.50
4:f:86:LYS:HE3	4:f:272:LEU:HD13	1.94	0.50
2:D:20:DA:H62	4:c:454:SER:HB2	1.77	0.50
4:h:169:ARG:HH21	4:h:220:ASN:HA	1.77	0.50
4:b:377:PHE:HE2	4:b:394:ALA:HA	1.76	0.50
3:6:287:LEU:HD11	3:6:297:ILE:HD11	1.94	0.50
4:f:24:TYR:HB3	4:f:49:ILE:HG13	1.93	0.50
4:a:147:SER:HA	4:a:248:ASN:HD21	1.75	0.50
4:f:112:LEU:HG	4:f:243:SER:HB3	1.94	0.50
4:f:384:VAL:HG13	4:f:428:LEU:HD22	1.93	0.50
4:d:85:LEU:HD22	4:d:100:PRO:HB3	1.92	0.50
3:7:366:VAL:HG12	3:7:372:ILE:HG21	1.93	0.50
2:D:8:DA:H2'	4:c:99:ASN:HD21	1.77	0.50
4:d:128:LYS:HD2	4:d:149:ARG:HB2	1.94	0.50
3:2:357:GLN:HG2	3:2:358:GLU:HG2	1.94	0.49
1:C:14:U:H2'	1:C:15:A:H8	1.76	0.49
4:d:36:HIS:NE2	4:d:59:PRO:HG3	2.27	0.49
3:8:85:ILE:HG23	4:c:552:ARG:HD2	1.94	0.49
3:8:382:SER:HB3	3:5:355:ALA:HA	1.93	0.49
4:g:388:LYS:HG3	4:g:432:LEU:HD11	1.93	0.49
4:a:150:ARG:HH22	4:a:218:ARG:N	2.10	0.49
4:d:155:ASN:HD22	4:d:210:LYS:HA	1.76	0.49
3:1:355:ALA:HA	3:4:382:SER:HB3	1.93	0.49
2:M:19:DG:H21	4:h:646:ARG:HH12	1.60	0.49
4:f:597:VAL:HG21	4:f:672:LEU:HD12	1.93	0.49
4:b:477:LEU:HD23	4:b:520:TYR:HD2	1.76	0.49
1:K:14:U:H2'	1:K:15:A:H8	1.77	0.49
4:g:215:GLU:HG3	4:g:217:SER:H	1.77	0.49
4:g:356:SER:HB3	4:g:456:GLY:HA3	1.95	0.49
4:h:128:LYS:HD2	4:h:149:ARG:HB2	1.93	0.49
4:b:188:SER:HB3	4:b:196:SER:HB3	1.95	0.49
4:c:388:LYS:HG3	4:c:432:LEU:HD11	1.94	0.49
3:4:36:LEU:HD21	3:4:166:ARG:NH2	2.28	0.49
4:c:336:GLN:NE2	4:c:380:SER:HA	2.27	0.49
4:d:113:LEU:HB2	4:d:125:ILE:HG12	1.93	0.49
4:e:116:ILE:HG22	4:e:117:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:712:LEU:HD12	4:a:713:PRO:HD2	1.95	0.49
4:b:84:LEU:HD23	4:b:269:ILE:HG21	1.95	0.49
3:8:27:ASP:HB3	3:8:30:LYS:HB2	1.95	0.49
4:f:112:LEU:H	4:f:112:LEU:HD22	1.78	0.49
4:a:68:GLN:HE21	4:a:70:LYS:HG2	1.78	0.49
3:5:53:SER:O	3:5:57:ARG:HG3	2.13	0.49
4:e:612:THR:HA	4:e:615:MET:HE1	1.94	0.49
2:F:19:DG:H5'	4:b:647:GLN:OE1	2.12	0.49
2:F:20:DA:H62	4:b:454:SER:HB2	1.77	0.49
1:K:1:A:H1'	4:g:444:THR:HG23	1.94	0.49
4:h:41:VAL:HB	4:h:52:PHE:HB2	1.94	0.49
4:e:175:GLN:HE21	4:e:181:LYS:HB2	1.77	0.49
4:g:721:ILE:HD11	4:h:396:ARG:HE	1.78	0.49
4:h:729:TRP:H	4:h:729:TRP:CD1	2.30	0.49
4:a:509:GLY:C	4:a:510:ILE:HD12	2.38	0.49
3:1:293:LYS:HZ1	3:1:330:ASP:CG	2.20	0.48
4:f:307:TRP:HE1	2:G:21:DT:H2''	1.77	0.48
4:e:99:ASN:HB2	4:e:100:PRO:HD3	1.93	0.48
1:E:14:U:H2'	1:E:15:A:H8	1.78	0.48
4:g:187:GLU:OE1	4:g:198:ILE:HG13	2.14	0.48
1:O:7:G:H1'	4:a:241:ARG:HH12	1.78	0.48
4:a:188:SER:HB3	4:a:196:SER:HB3	1.95	0.48
4:a:298:VAL:HG23	4:a:478:LYS:HG2	1.96	0.48
4:c:68:GLN:HE21	4:c:70:LYS:H	1.61	0.48
4:c:508:MET:HE1	4:c:534:TYR:CD2	2.49	0.48
4:g:128:LYS:HD2	4:g:149:ARG:HB2	1.95	0.48
4:a:566:HIS:HB3	4:a:696:ILE:HD11	1.95	0.48
3:4:27:ASP:HB3	3:4:30:LYS:HB2	1.96	0.48
4:g:135:THR:HA	4:g:140:PRO:HA	1.94	0.48
4:c:229:HIS:HE1	4:c:236:ILE:HG21	1.79	0.48
4:g:12:ILE:HD12	4:g:70:LYS:HD2	1.96	0.48
4:g:648:GLU:HG2	4:g:649:THR:HG23	1.96	0.48
4:e:350:LEU:HD23	4:e:363:LEU:HD23	1.96	0.48
1:C:15:A:H61	2:D:7:DT:H3	1.60	0.48
2:J:14:DG:H2'	2:J:15:DC:C6	2.48	0.48
4:a:174:GLU:HG3	4:a:180:ARG:HE	1.79	0.48
4:a:629:LYS:HA	4:a:635:MET:HB2	1.96	0.48
3:1:293:LYS:NZ	3:1:296:ARG:HG3	2.28	0.48
4:g:44:ARG:HG3	4:g:46:GLY:H	1.78	0.48
1:O:1:A:H61	4:a:424:ASN:ND2	2.12	0.48
4:a:477:LEU:HD22	4:a:682:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:101:ILE:HB	4:c:131:ILE:HG23	1.95	0.48
3:3:75:VAL:HG12	3:3:79:LEU:HD11	1.96	0.48
3:7:269:LEU:O	3:7:273:LEU:HD12	2.13	0.48
4:f:290:ALA:HB3	4:f:627:THR:HG23	1.96	0.48
4:e:398:LYS:HA	4:e:398:LYS:HD3	1.70	0.48
4:e:572:PHE:HD2	4:e:596:PHE:HB3	1.79	0.48
1:E:14:U:H2'	1:E:15:A:C8	2.48	0.48
1:E:15:A:H5''	4:b:573:ASN:HB3	1.96	0.48
4:h:83:GLY:HA2	4:h:86:LYS:HE2	1.95	0.48
4:a:171:VAL:HG21	4:a:186:VAL:HG23	1.96	0.48
4:a:490:GLY:HA3	4:a:695:THR:HB	1.96	0.48
4:d:87:HIS:CE1	4:d:269:ILE:HA	2.48	0.48
4:f:477:LEU:HD23	4:f:520:TYR:HD2	1.79	0.47
4:b:17:LEU:HD21	4:b:273:ASP:HB3	1.96	0.47
4:b:37:LYS:HZ3	4:b:42:PHE:H	1.62	0.47
4:f:210:LYS:HZ3	4:f:211:ASP:HB3	1.80	0.47
4:h:339:LYS:HE3	4:h:339:LYS:HA	1.95	0.47
4:b:102:GLU:HA	4:b:130:SER:HA	1.95	0.47
4:e:88:PHE:HA	4:e:91:LEU:HB2	1.95	0.47
4:e:208:GLU:HG3	4:e:210:LYS:HG2	1.96	0.47
4:e:495:ASN:HA	4:e:506:ARG:HA	1.96	0.47
1:N:10:U:H2'	1:N:11:A:H8	1.78	0.47
4:h:81:LYS:NZ	4:h:132:ASP:HA	2.30	0.47
4:h:157:LEU:HB2	4:h:209:ALA:HB1	1.96	0.47
1:I:14:U:H2'	1:I:15:A:C8	2.46	0.47
4:c:493:SER:HB3	4:c:569:VAL:HG11	1.97	0.47
3:8:361:LYS:HA	3:8:361:LYS:HD3	1.77	0.47
4:e:419:LEU:HD12	4:e:419:LEU:H	1.78	0.47
4:g:336:GLN:HE22	4:g:380:SER:HA	1.78	0.47
4:a:398:LYS:HA	4:a:398:LYS:HD3	1.69	0.47
4:d:12:ILE:HD11	4:d:70:LYS:HA	1.96	0.47
4:d:408:ALA:HB3	4:d:440:VAL:HG12	1.95	0.47
3:4:32:CYS:SG	3:4:44:ILE:HG23	2.54	0.47
4:f:435:LEU:HD12	4:f:719:VAL:HG11	1.95	0.47
4:e:333:ILE:HB	4:e:410:VAL:HG12	1.96	0.47
4:e:427:TYR:HH	4:e:708:TRP:CG	2.31	0.47
4:g:117:LEU:HB2	4:g:121:TYR:CZ	2.50	0.47
4:h:379:THR:HG21	4:h:387:TYR:CE1	2.48	0.47
4:c:44:ARG:HG3	4:c:49:ILE:HG12	1.94	0.47
4:a:99:ASN:HB3	4:a:100:PRO:HD3	1.97	0.47
4:f:20:VAL:HG12	4:f:51:ILE:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:454:SER:HB2	2:G:20:DA:H62	1.79	0.47
4:e:122:PRO:HB3	4:e:154:GLU:HB2	1.97	0.47
4:c:63:THR:HG23	4:c:63:THR:O	2.15	0.47
4:d:186:VAL:HG22	4:d:197:VAL:HG22	1.97	0.47
4:d:339:LYS:NZ	4:d:378:GLU:HB3	2.29	0.47
4:d:682:HIS:O	4:d:694:VAL:HG11	2.14	0.47
3:4:320:PHE:O	3:4:324:ILE:HG13	2.15	0.47
4:g:229:HIS:HB3	4:g:232:LYS:HG3	1.96	0.47
4:g:331:CYS:HG	4:g:405:TRP:CG	2.33	0.47
4:a:721:ILE:HD11	4:b:396:ARG:HH21	1.79	0.47
3:1:96:MET:HE2	3:1:96:MET:HB2	1.82	0.47
4:e:509:GLY:C	4:e:510:ILE:HD12	2.40	0.47
4:c:157:LEU:HG	4:c:209:ALA:HB3	1.97	0.47
3:5:66:LEU:HD12	3:5:67:ASP:H	1.80	0.47
4:a:1:MET:HB2	4:a:2:PRO:HD3	1.97	0.47
4:a:495:ASN:HB3	4:a:504:ASN:HD21	1.79	0.47
4:b:85:LEU:HB3	4:b:86:LYS:HZ2	1.80	0.47
4:c:81:LYS:HA	4:c:84:LEU:HD12	1.97	0.47
4:e:624:ARG:HH21	4:e:689:PRO:HB3	1.80	0.46
4:f:287:LYS:HE3	4:f:287:LYS:HB3	1.72	0.46
4:e:15:LEU:HD21	4:e:273:ASP:HB2	1.96	0.46
1:C:11:A:H2'	1:C:12:G:H8	1.80	0.46
4:g:174:GLU:HA	4:g:180:ARG:HA	1.97	0.46
4:a:111:ASN:HD22	4:a:119:GLU:HG3	1.80	0.46
4:b:215:GLU:OE1	4:b:217:SER:HB3	2.16	0.46
4:d:379:THR:HG21	4:d:387:TYR:CE1	2.51	0.46
4:e:264:ILE:HG23	4:e:269:ILE:HD11	1.96	0.46
4:e:339:LYS:HZ1	4:e:376:VAL:HB	1.79	0.46
4:e:420:LYS:HA	4:e:420:LYS:HD3	1.72	0.46
4:a:33:ARG:HG3	4:a:37:LYS:HD3	1.98	0.46
4:b:413:ARG:H	4:b:416:PHE:HD2	1.62	0.46
4:c:241:ARG:NH2	4:c:647:GLN:HE22	2.14	0.46
4:d:134:ARG:HB3	4:d:143:ILE:HD11	1.98	0.46
4:d:363:LEU:HD13	4:d:463:SER:HB2	1.96	0.46
4:g:190:HIS:HE1	4:g:196:SER:HB2	1.80	0.46
2:P:13:DA:H2''	2:P:14:DG:H8	1.80	0.46
4:h:408:ALA:HB3	4:h:440:VAL:HG12	1.96	0.46
4:a:172:VAL:HA	4:a:183:LEU:HB2	1.97	0.46
4:f:152:VAL:HG12	4:f:154:GLU:H	1.81	0.46
4:g:336:GLN:NE2	4:g:380:SER:HA	2.31	0.46
4:h:334:CYS:SG	4:h:338:ASP:HB2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:U:H2'	1:A:11:A:H8	1.79	0.46
4:e:199:ARG:HG3	4:e:201:ASP:H	1.80	0.46
4:a:22:ILE:HG12	4:a:51:ILE:HD11	1.98	0.46
4:b:265:GLN:HA	4:b:278:GLU:HG2	1.96	0.46
3:6:40:VAL:HG12	3:6:42:SER:H	1.81	0.46
3:3:40:VAL:HG22	3:3:42:SER:H	1.81	0.46
3:3:75:VAL:O	3:3:79:LEU:HD12	2.16	0.46
4:f:251:GLU:HB2	4:f:619:ARG:HD2	1.97	0.46
4:c:124:LYS:HB2	4:c:153:LYS:HE3	1.97	0.46
4:d:297:PHE:CE2	4:d:308:THR:HG22	2.51	0.46
3:8:320:PHE:O	3:8:324:ILE:HG13	2.15	0.46
4:f:81:LYS:HD3	4:f:81:LYS:HA	1.77	0.46
4:f:297:PHE:CE2	4:f:308:THR:HG22	2.51	0.46
4:a:635:MET:CE	4:a:669:ILE:HG13	2.46	0.46
4:b:16:GLU:HG3	4:b:66:THR:HB	1.96	0.46
1:A:12:G:H2'	1:A:13:A:C8	2.51	0.46
2:G:7:DT:H2'	2:G:8:DA:H8	1.80	0.46
2:L:5:DG:H1'	4:g:26:LYS:HE2	1.98	0.46
4:h:10:LEU:HD11	4:h:277:ILE:HD12	1.98	0.46
4:c:193:ARG:HH22	4:c:209:ALA:HB3	1.81	0.46
3:3:79:LEU:HD12	3:3:79:LEU:H	1.81	0.46
3:8:100:MET:HE2	3:8:100:MET:HB3	1.78	0.46
4:f:102:GLU:HB2	4:f:128:LYS:HB2	1.98	0.46
4:e:175:GLN:NE2	4:e:181:LYS:HB2	2.31	0.46
4:e:243:SER:HB3	4:e:247:PHE:CE2	2.50	0.46
4:c:68:GLN:HB3	4:c:71:ASP:HB2	1.98	0.46
4:d:184:GLY:HA3	4:d:198:ILE:O	2.15	0.46
3:6:45:THR:HG23	3:6:47:PHE:CE2	2.52	0.46
4:a:256:ARG:HA	4:a:256:ARG:HD3	1.67	0.45
4:c:10:LEU:HD13	4:c:142:LEU:HD23	1.98	0.45
4:c:15:LEU:HD23	4:c:15:LEU:HA	1.75	0.45
4:d:450:GLN:HE21	4:d:454:SER:HB2	1.80	0.45
4:d:617:LYS:HB3	4:d:648:GLU:HA	1.98	0.45
4:e:80:VAL:O	4:e:84:LEU:HG	2.16	0.45
3:8:213:GLN:HG3	3:8:214:GLU:HG3	1.98	0.45
4:e:40:HIS:CE1	4:e:51:ILE:HA	2.51	0.45
4:e:102:GLU:HB3	4:e:128:LYS:HB2	1.96	0.45
4:e:641:GLY:H	4:e:644:GLU:HB2	1.81	0.45
4:g:258:ASP:HA	4:g:261:LYS:HE2	1.97	0.45
2:M:6:DG:H1'	4:h:44:ARG:NH1	2.31	0.45
2:J:12:DA:H2''	2:J:13:DA:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:35:SER:HB2	3:6:43:CYS:HB2	1.99	0.45
4:g:131:ILE:HD13	4:g:144:ILE:HB	1.99	0.45
4:b:3:ILE:HB	4:b:285:ILE:HG13	1.98	0.45
4:c:20:VAL:HG21	4:c:58:PHE:CZ	2.50	0.45
4:c:609:ASP:O	4:c:620:LEU:HD23	2.16	0.45
4:d:130:SER:OG	4:d:145:ASP:HB3	2.16	0.45
4:e:307:TRP:HB3	4:e:310:LYS:HG2	1.98	0.45
4:b:435:LEU:HD12	4:b:719:VAL:HG11	1.97	0.45
4:c:156:CYS:O	4:c:160:LEU:HD12	2.17	0.45
3:8:218:ALA:HB1	3:7:9:VAL:HB	1.98	0.45
4:h:297:PHE:CE2	4:h:308:THR:HG22	2.52	0.45
2:J:10:DC:H2'	2:J:11:DT:H71	1.97	0.45
4:c:599:ILE:HG21	4:c:692:MET:SD	2.57	0.45
3:2:32:CYS:SG	3:2:44:ILE:HG23	2.56	0.45
4:e:93:ARG:NH2	4:e:106:ALA:H	2.12	0.45
1:H:14:U:H2'	1:H:15:A:C8	2.52	0.45
2:M:2:DC:H2''	2:M:3:DA:N7	2.32	0.45
1:N:12:G:H2'	1:N:13:A:C8	2.52	0.45
4:c:8:PHE:HZ	4:c:257:ILE:HD12	1.82	0.45
4:c:15:LEU:H	4:c:68:GLN:HE22	1.63	0.45
4:d:729:TRP:H	4:d:729:TRP:CD1	2.34	0.45
3:5:90:ARG:HA	3:5:90:ARG:HD2	1.83	0.45
3:5:283:ASP:C	3:5:284:GLU:HG3	2.41	0.45
3:5:387:LYS:HD2	3:5:387:LYS:N	2.32	0.45
4:h:37:LYS:HD2	4:h:37:LYS:HA	1.69	0.45
4:h:155:ASN:ND2	4:h:157:LEU:HB3	2.32	0.45
4:h:359:PHE:CE2	4:h:362:GLY:HA2	2.51	0.45
4:b:486:GLU:HB2	4:b:515:SER:HB2	1.99	0.45
3:2:335:ARG:HH21	3:2:345:ILE:HG13	1.82	0.45
3:8:19:LYS:HA	3:8:19:LYS:HD3	1.84	0.45
4:e:510:ILE:HG21	4:e:541:VAL:HG11	1.98	0.45
4:e:566:HIS:HB3	4:e:696:ILE:HD11	1.99	0.45
4:h:26:LYS:HD3	4:h:26:LYS:HA	1.58	0.45
4:b:111:ASN:ND2	4:b:124:LYS:HG3	2.32	0.45
4:f:161:LYS:HA	4:f:161:LYS:HD3	1.83	0.45
4:e:157:LEU:O	4:e:161:LYS:HG2	2.16	0.45
4:g:32:LEU:HA	4:g:36:HIS:ND1	2.32	0.45
4:c:160:LEU:HD12	4:c:160:LEU:H	1.81	0.45
3:6:191:GLN:HE21	3:6:196:PRO:HB3	1.83	0.45
3:1:191:GLN:HG3	3:1:196:PRO:HG3	1.99	0.44
3:7:263:GLU:HG3	3:7:297:ILE:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:88:PHE:HD1	4:h:91:LEU:HD12	1.82	0.44
4:a:123:LEU:HB3	4:a:221:PHE:HE1	1.82	0.44
4:a:242:GLN:HE21	4:a:246:ILE:HD12	1.82	0.44
4:b:37:LYS:NZ	4:b:42:PHE:H	2.14	0.44
4:b:729:TRP:CD1	4:b:729:TRP:H	2.35	0.44
4:d:553:MET:HE3	4:d:553:MET:HB3	1.69	0.44
3:3:287:LEU:HG	3:3:294:ASN:HB2	1.99	0.44
4:f:254:LYS:HA	4:f:257:ILE:HB	1.99	0.44
4:f:729:TRP:CD1	4:f:729:TRP:H	2.35	0.44
4:g:294:LYS:HE2	4:g:624:ARG:HH12	1.82	0.44
4:g:603:HIS:CE1	4:g:655:GLY:H	2.35	0.44
4:a:2:PRO:HA	4:a:286:GLN:HB2	1.98	0.44
4:a:100:PRO:HB2	4:a:102:GLU:OE1	2.17	0.44
4:d:242:GLN:O	4:d:246:ILE:HD12	2.18	0.44
1:K:5:A:H2'	1:K:6:A:C8	2.52	0.44
4:a:549:ILE:HG23	4:a:553:MET:HE2	1.98	0.44
4:b:622:THR:OG1	4:b:626:LYS:HG3	2.18	0.44
3:6:320:PHE:O	3:6:324:ILE:HG13	2.17	0.44
3:1:90:ARG:HA	3:1:90:ARG:HD2	1.84	0.44
4:h:20:VAL:HB	4:h:51:ILE:HB	2.00	0.44
4:a:45:GLN:HG2	4:a:50:GLN:HB2	1.98	0.44
4:a:159:PHE:HB3	4:a:164:PHE:HB3	1.99	0.44
4:d:8:PHE:HD1	4:d:282:PRO:HD3	1.82	0.44
4:d:261:LYS:HE3	4:d:262:LYS:HD3	1.99	0.44
3:8:122:ILE:HB	3:8:126:LEU:HD12	1.99	0.44
3:8:381:PRO:HG2	3:8:384:MET:HG3	1.99	0.44
4:g:193:ARG:H	4:g:193:ARG:HG2	1.68	0.44
4:g:692:MET:HE3	4:g:693:PRO:CD	2.43	0.44
4:h:214:LEU:HD23	4:h:214:LEU:HA	1.81	0.44
4:a:146:CYS:HB3	4:a:253:LYS:HG3	1.99	0.44
4:c:247:PHE:CD1	4:c:247:PHE:C	2.95	0.44
4:d:209:ALA:HA	4:d:212:VAL:HG12	2.00	0.44
3:1:263:GLU:HG2	3:1:312:TYR:HB3	2.00	0.44
3:2:320:PHE:O	3:2:324:ILE:HG13	2.17	0.44
3:3:79:LEU:HA	3:3:121:TRP:CD1	2.53	0.44
3:7:311:LYS:HB2	3:7:349:LEU:HD12	2.00	0.44
4:e:248:ASN:O	4:e:253:LYS:HD2	2.18	0.44
4:e:508:MET:HE3	4:e:508:MET:HB3	1.89	0.44
4:a:104:VAL:HA	4:a:128:LYS:HB3	1.98	0.44
4:b:181:LYS:HA	4:b:181:LYS:HD3	1.78	0.44
4:c:332:VAL:HG11	4:c:346:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:45:GLN:HG2	4:d:50:GLN:HG3	1.99	0.44
3:5:361:LYS:HD2	3:5:361:LYS:HA	1.80	0.44
3:1:44:ILE:HD11	3:1:65:ILE:HG12	2.00	0.44
3:1:357:GLN:HG2	3:1:358:GLU:HG2	2.00	0.44
3:7:361:LYS:HD3	3:7:361:LYS:O	2.17	0.44
4:f:26:LYS:HD2	4:f:26:LYS:HA	1.66	0.44
4:f:226:LEU:HB3	4:f:233:LYS:HD3	2.00	0.44
4:e:88:PHE:CD2	4:e:101:ILE:HG21	2.53	0.44
2:F:21:DT:H2''	4:b:307:TRP:HE1	1.83	0.44
4:a:102:GLU:HB3	4:a:128:LYS:HD2	2.00	0.44
4:c:13:PRO:HG2	4:c:69:LEU:HD12	2.00	0.44
3:5:141:ASP:HB3	3:5:154:PHE:HD1	1.82	0.44
4:g:218:ARG:HA	4:g:218:ARG:NE	2.32	0.44
4:b:327:ASP:HA	4:b:371:THR:O	2.17	0.44
4:c:156:CYS:SG	4:c:212:VAL:HG23	2.58	0.44
3:5:381:PRO:HG2	3:5:386:PHE:CD2	2.52	0.44
2:B:18:DT:H5'	4:d:241:ARG:HH12	1.83	0.44
3:8:135:LEU:HB3	3:8:139:GLU:HB2	1.99	0.44
4:g:609:ASP:O	4:g:620:LEU:HA	2.17	0.44
4:a:112:LEU:HD23	4:a:125:ILE:HG21	2.00	0.44
4:c:258:ASP:HA	4:c:261:LYS:HB3	1.98	0.44
4:c:593:GLU:HB3	4:c:666:PHE:HB2	1.99	0.44
3:8:66:LEU:HD23	3:8:66:LEU:HA	1.75	0.43
3:7:348:PHE:CZ	3:7:378:ILE:HG13	2.53	0.43
2:G:7:DT:H2'	2:G:8:DA:C8	2.53	0.43
4:g:33:ARG:HG3	4:g:37:LYS:HE3	2.00	0.43
4:a:670:LYS:HD3	4:a:670:LYS:HA	1.81	0.43
4:c:251:GLU:HA	4:c:620:LEU:HD12	2.00	0.43
4:c:567:VAL:HG12	4:c:569:VAL:H	1.82	0.43
4:f:69:LEU:HA	4:f:72:ASN:HB2	2.01	0.43
1:C:5:A:H61	2:D:17:DT:H3	1.66	0.43
4:g:106:ALA:HB1	4:g:124:LYS:HE3	2.00	0.43
4:h:363:LEU:HD13	4:h:463:SER:HB2	2.01	0.43
4:a:414:GLN:HE22	4:a:417:LYS:NZ	2.15	0.43
4:d:261:LYS:HB3	4:d:261:LYS:HE2	1.80	0.43
2:B:2:DC:H2''	2:B:3:DA:N7	2.33	0.43
3:4:90:ARG:HA	3:4:90:ARG:HD2	1.84	0.43
4:e:686:SER:HB2	1:I:3:C:H4'	1.99	0.43
2:D:18:DT:H5'	4:c:241:ARG:HH12	1.82	0.43
4:g:16:GLU:CD	4:g:68:GLN:HG2	2.43	0.43
4:g:24:TYR:HA	4:g:49:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:37:LYS:HZ3	4:g:42:PHE:H	1.64	0.43
4:g:183:LEU:HD12	4:g:199:ARG:HD3	2.01	0.43
4:c:345:PHE:HB2	4:c:448:LEU:HD21	2.00	0.43
4:c:506:ARG:O	4:c:531:PRO:HD3	2.18	0.43
4:d:95:PRO:HA	4:d:103:VAL:HG23	2.00	0.43
3:3:339:LYS:HE2	3:3:339:LYS:HB3	1.85	0.43
4:f:18:LYS:HB3	4:f:63:THR:O	2.18	0.43
4:f:56:GLY:H	4:f:60:LYS:NZ	2.16	0.43
4:f:584:ILE:HD12	4:f:592:ILE:HG21	2.01	0.43
1:K:11:A:H2'	1:K:12:G:H8	1.83	0.43
4:g:156:CYS:HB3	4:g:209:ALA:HB1	2.00	0.43
4:b:553:MET:HE3	4:b:553:MET:HB3	1.78	0.43
4:e:101:ILE:HD12	4:e:131:ILE:O	2.19	0.43
4:g:11:LYS:HZ1	4:g:277:ILE:HA	1.83	0.43
4:g:359:PHE:HB2	4:g:460:ASN:HB2	1.98	0.43
4:g:603:HIS:CD2	4:g:657:ILE:HD11	2.53	0.43
4:a:113:LEU:HD11	4:a:117:LEU:HD12	2.01	0.43
4:a:193:ARG:HE	4:a:210:LYS:HE3	1.83	0.43
4:c:294:LYS:HE3	4:c:294:LYS:HB3	1.80	0.43
3:5:37:LEU:HD22	3:5:202:CYS:SG	2.59	0.43
4:e:173:THR:HG22	4:e:212:VAL:HG12	2.00	0.43
4:e:336:GLN:HG2	4:e:337:HIS:N	2.33	0.43
1:O:11:A:H2'	1:O:12:G:O4'	2.18	0.43
4:a:183:LEU:HA	4:a:199:ARG:HH22	1.84	0.43
4:b:161:LYS:HA	4:b:161:LYS:HD3	1.74	0.43
4:d:19:PHE:CE1	4:d:67:LEU:HB3	2.54	0.43
4:d:99:ASN:HB3	4:d:179:PHE:CZ	2.53	0.43
4:e:22:ILE:HD11	4:e:49:ILE:HD12	2.00	0.43
1:C:2:U:H5'	1:C:3:C:OP2	2.19	0.43
4:g:186:VAL:HG22	4:g:197:VAL:HG22	2.01	0.43
4:g:269:ILE:HD12	4:g:278:GLU:HA	2.00	0.43
4:c:5:LEU:HD21	4:c:628:PHE:CD2	2.54	0.43
4:d:455:LEU:HD12	4:d:455:LEU:HA	1.87	0.43
3:6:201:LEU:HD23	3:6:201:LEU:HA	1.81	0.43
3:4:215:ILE:HG23	3:3:189:GLN:HE22	1.83	0.43
4:c:142:LEU:HD13	4:c:142:LEU:HA	1.88	0.43
4:c:199:ARG:NE	4:c:200:PRO:HD2	2.33	0.43
3:5:201:LEU:HD23	3:5:201:LEU:HA	1.88	0.43
3:7:349:LEU:HD23	3:7:377:VAL:HG13	2.01	0.43
4:f:131:ILE:HD11	4:f:142:LEU:HD13	2.01	0.43
4:e:608:PHE:HD2	4:e:620:LEU:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:e:685:ARG:NH1	4:e:701:LEU:HD11	2.34	0.43
4:g:43:ARG:HB3	4:g:45:GLN:HE22	1.83	0.43
4:g:237:VAL:HA	4:g:240:ILE:HD12	2.01	0.43
4:h:18:LYS:H	4:h:18:LYS:HG3	1.60	0.43
4:h:599:ILE:HD11	4:h:692:MET:SD	2.58	0.43
4:a:199:ARG:HB2	4:a:203:GLN:H	1.83	0.43
4:d:379:THR:HG21	4:d:387:TYR:HE1	1.84	0.43
3:6:66:LEU:HD23	3:6:66:LEU:HA	1.83	0.43
3:4:40:VAL:HG12	3:4:43:CYS:H	1.84	0.43
4:f:81:LYS:NZ	4:f:131:ILE:HG13	2.34	0.43
4:e:496:ILE:HD11	4:e:708:TRP:CD1	2.54	0.43
1:C:5:A:H2'	1:C:6:A:C8	2.53	0.43
4:g:5:LEU:HD11	4:g:628:PHE:CE2	2.54	0.43
4:g:157:LEU:HG	4:g:209:ALA:HB3	2.01	0.43
4:h:240:ILE:O	4:h:244:VAL:HG22	2.19	0.43
4:d:17:LEU:HD22	4:d:17:LEU:H	1.84	0.43
3:4:100:MET:HB3	3:4:100:MET:HE2	1.79	0.42
4:e:44:ARG:HD2	2:J:6:DG:H2''	2.00	0.42
4:a:102:GLU:HG2	4:a:128:LYS:HD2	2.01	0.42
4:a:332:VAL:HG23	4:a:376:VAL:HA	2.00	0.42
4:a:476:LEU:HD23	4:a:476:LEU:HA	1.80	0.42
4:c:642:GLN:HA	4:c:645:LEU:HD12	2.00	0.42
3:2:366:VAL:O	3:2:369:ILE:HG12	2.19	0.42
4:h:165:ASN:HD21	4:h:167:ILE:HB	1.84	0.42
4:b:129:TYR:HD2	4:b:260:LEU:HD22	1.83	0.42
4:f:76:PHE:HE2	4:f:140:PRO:HG3	1.84	0.42
4:e:187:GLU:OE1	4:e:198:ILE:HG12	2.19	0.42
4:h:199:ARG:HG3	4:h:200:PRO:HD2	2.00	0.42
4:a:225:ILE:HG22	4:a:233:LYS:HG2	2.01	0.42
4:f:247:PHE:HA	4:f:252:ASN:HD21	1.84	0.42
4:f:387:TYR:O	4:f:391:ILE:HG12	2.19	0.42
4:e:181:LYS:HD2	1:I:11:A:OP1	2.19	0.42
2:L:20:DA:N6	4:g:454:SER:HB2	2.33	0.42
4:h:706:LEU:HD23	4:h:706:LEU:HA	1.87	0.42
4:a:384:VAL:HG13	4:a:428:LEU:HD22	2.00	0.42
4:c:356:SER:HB3	4:c:456:GLY:HA3	2.00	0.42
4:d:344:GLN:O	4:d:348:LYS:HG3	2.19	0.42
3:2:191:GLN:HE21	3:2:196:PRO:HB3	1.85	0.42
3:4:19:LYS:HD3	3:4:19:LYS:HA	1.86	0.42
3:4:201:LEU:HD23	3:4:201:LEU:HA	1.89	0.42
3:8:249:ARG:HD2	3:7:264:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:94:THR:HB	4:h:104:VAL:HB	2.02	0.42
4:a:7:ALA:HB1	4:a:141:CYS:HB2	2.02	0.42
4:c:194:THR:HA	4:c:206:HIS:HB3	2.01	0.42
4:d:432:LEU:O	4:d:432:LEU:HD23	2.20	0.42
3:6:363:LYS:O	3:6:367:LEU:HD12	2.19	0.42
4:f:69:LEU:HD22	4:f:76:PHE:HB2	2.02	0.42
4:e:640:ILE:HD11	1:I:5:A:H5''	2.00	0.42
4:g:639:LEU:HD11	4:g:676:LEU:HD21	2.02	0.42
4:h:336:GLN:O	4:h:339:LYS:HG2	2.19	0.42
4:h:553:MET:HB3	4:h:553:MET:HE3	1.68	0.42
4:c:124:LYS:HD3	4:c:153:LYS:HE2	2.00	0.42
4:d:477:LEU:HB3	4:d:520:TYR:HB2	2.01	0.42
3:4:44:ILE:HD11	3:4:65:ILE:HG12	2.01	0.42
3:8:256:VAL:HG21	3:7:265:HIS:CE1	2.54	0.42
4:e:617:LYS:HE3	4:e:643:ARG:HH22	1.84	0.42
4:g:297:PHE:HB2	4:g:299:PHE:CE1	2.55	0.42
2:P:20:DA:H1'	4:a:688:PHE:HZ	1.84	0.42
4:h:615:MET:HE2	4:h:617:LYS:HB2	2.02	0.42
4:c:156:CYS:HB2	4:c:209:ALA:HB1	2.01	0.42
4:d:155:ASN:ND2	4:d:210:LYS:HA	2.35	0.42
2:B:6:DG:H1'	4:d:44:ARG:HH11	1.83	0.42
3:1:79:LEU:HG	3:1:117:GLU:HB3	2.01	0.42
4:f:21:GLN:HB3	4:f:48:ASN:HD22	1.85	0.42
1:C:11:A:H2'	1:C:12:G:C8	2.55	0.42
1:N:1:A:H8	4:h:412:VAL:HG21	1.85	0.42
4:a:190:HIS:CE1	4:a:191:GLU:HG3	2.54	0.42
4:b:662:LYS:H	4:b:662:LYS:HG2	1.62	0.42
4:c:116:ILE:HB	4:c:117:LEU:HD12	2.02	0.42
4:c:156:CYS:O	4:c:159:PHE:HB2	2.20	0.42
3:2:109:MET:H	3:2:109:MET:HG2	1.64	0.42
3:3:313:ARG:HH22	3:3:316:THR:HA	1.85	0.42
3:3:386:PHE:CZ	3:3:388:LYS:HA	2.55	0.42
4:e:233:LYS:HA	4:e:236:ILE:HD11	2.01	0.42
4:e:476:LEU:HD23	4:e:476:LEU:HA	1.88	0.42
4:g:229:HIS:CD2	4:g:236:ILE:HG13	2.55	0.42
4:b:128:LYS:HD3	4:b:149:ARG:HE	1.84	0.42
4:b:193:ARG:HA	4:b:193:ARG:NE	2.35	0.42
1:A:9:U:OP1	4:d:149:ARG:HD3	2.19	0.42
3:8:285:VAL:O	3:8:296:ARG:HG3	2.19	0.42
3:7:75:VAL:O	3:7:79:LEU:HD12	2.20	0.42
4:f:513:VAL:HG22	4:f:522:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:g:12:ILE:HG21	4:g:70:LYS:HA	2.02	0.42
4:g:446:GLU:H	4:g:446:GLU:HG2	1.69	0.42
4:c:76:PHE:HE2	4:c:140:PRO:HG2	1.84	0.42
4:d:190:HIS:CE1	4:d:191:GLU:HG2	2.55	0.42
3:5:142:ILE:O	3:5:146:VAL:HG22	2.20	0.42
3:6:120:LYS:HB2	3:6:120:LYS:HE2	1.72	0.42
3:8:44:ILE:HD11	3:8:65:ILE:HG23	2.02	0.41
4:e:529:VAL:HG11	4:e:537:ALA:HB2	2.02	0.41
4:h:277:ILE:HD13	4:h:277:ILE:HA	1.88	0.41
4:b:156:CYS:SG	4:b:212:VAL:HG23	2.60	0.41
4:b:496:ILE:HG23	4:b:708:TRP:CE2	2.55	0.41
4:d:88:PHE:HA	4:d:91:LEU:HD12	2.02	0.41
3:1:73:GLN:HE22	4:a:556:GLN:HG3	1.84	0.41
3:2:120:LYS:HB2	3:2:120:LYS:HE2	1.72	0.41
3:2:354:ARG:HG2	3:2:379:SER:HB3	2.03	0.41
4:e:24:TYR:HE1	4:e:29:LEU:HB2	1.85	0.41
4:a:291:GLN:HE21	4:a:626:LYS:HB2	1.85	0.41
4:b:150:ARG:HB3	4:b:221:PHE:CE2	2.54	0.41
4:b:257:ILE:HG13	4:b:258:ASP:N	2.35	0.41
4:b:361:ASN:OD1	4:b:365:GLY:HA3	2.19	0.41
4:c:77:CYS:O	4:c:81:LYS:HG2	2.20	0.41
4:c:103:VAL:O	4:c:128:LYS:HA	2.19	0.41
4:d:20:VAL:HG11	4:d:61:PRO:HA	2.03	0.41
4:f:50:GLN:CD	4:f:50:GLN:H	2.28	0.41
4:f:667:LYS:HB2	4:f:667:LYS:HE2	1.84	0.41
4:g:11:LYS:HZ2	4:g:277:ILE:HA	1.84	0.41
4:g:40:HIS:CD2	4:g:59:PRO:HD3	2.55	0.41
4:g:445:ILE:HD12	4:g:445:ILE:HA	1.89	0.41
4:g:613:ALA:HB2	4:g:620:LEU:HD23	2.02	0.41
4:h:113:LEU:HD22	4:h:125:ILE:HG13	2.01	0.41
4:h:361:ASN:HB3	4:h:365:GLY:HA3	2.03	0.41
3:5:242:TRP:CD1	3:5:386:PHE:HE2	2.38	0.41
3:1:381:PRO:HG2	3:1:384:MET:HE3	2.02	0.41
3:3:113:SER:HA	3:3:116:HIS:CE1	2.56	0.41
3:7:187:GLU:O	3:7:191:GLN:HG2	2.20	0.41
4:g:106:ALA:HB2	4:g:126:CYS:SG	2.60	0.41
4:a:172:VAL:HG12	4:a:182:LEU:HA	2.02	0.41
4:a:350:LEU:HB3	4:a:364:GLU:HG3	2.02	0.41
4:a:353:MET:HE2	4:a:353:MET:HB3	1.96	0.41
4:a:491:ILE:HG21	4:a:534:TYR:OH	2.21	0.41
4:c:490:GLY:O	4:c:491:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:166:VAL:HA	4:f:169:ARG:HD2	2.02	0.41
4:f:395:ILE:HD13	4:f:436:HIS:ND1	2.36	0.41
4:e:320:LYS:HE2	4:e:320:LYS:HB3	1.90	0.41
4:e:467:TYR:CE2	4:e:472:GLY:HA3	2.56	0.41
1:K:15:A:H2'	1:K:16:C:O4'	2.20	0.41
4:g:692:MET:HE2	4:g:696:ILE:HG21	2.03	0.41
4:h:99:ASN:C	4:h:101:ILE:H	2.28	0.41
4:a:76:PHE:CD2	4:a:140:PRO:HG3	2.56	0.41
4:b:109:LYS:H	4:b:109:LYS:HG2	1.60	0.41
4:c:694:VAL:HA	4:c:697:THR:OG1	2.20	0.41
4:d:214:LEU:HD12	4:d:214:LEU:HA	1.81	0.41
3:6:19:LYS:HE2	3:6:19:LYS:HB2	1.84	0.41
3:8:109:MET:H	3:8:109:MET:HG2	1.68	0.41
4:f:150:ARG:HB3	4:f:221:PHE:CE2	2.55	0.41
4:e:13:PRO:HG2	4:e:69:LEU:HD12	2.02	0.41
4:g:624:ARG:HD2	4:g:644:GLU:OE2	2.21	0.41
4:h:640:ILE:HD13	4:h:640:ILE:HA	1.94	0.41
4:a:174:GLU:HG2	4:a:180:ARG:HG2	2.02	0.41
4:b:455:LEU:HD12	4:b:458:SER:OG	2.20	0.41
4:c:214:LEU:HD12	4:c:214:LEU:HA	1.93	0.41
4:c:462:MET:HE3	4:c:462:MET:HB3	1.94	0.41
3:5:52:LEU:HB2	3:5:57:ARG:HG2	2.02	0.41
4:g:558:GLY:HA2	4:g:590:TYR:HB2	2.02	0.41
1:O:1:A:H5''	4:a:442:ASP:HB2	2.03	0.41
2:J:16:DT:H2'	2:J:17:DT:H71	2.03	0.41
4:a:144:ILE:HG21	4:a:260:LEU:HD23	2.03	0.41
4:c:333:ILE:HD13	4:c:391:ILE:HG12	2.03	0.41
4:d:29:LEU:HD13	4:d:49:ILE:HG21	2.03	0.41
4:f:56:GLY:H	4:f:60:LYS:HZ1	1.68	0.41
4:f:487:LEU:HD13	4:f:514:PHE:HB3	2.03	0.41
4:e:4:VAL:HG22	4:e:608:PHE:HB2	2.03	0.41
4:e:143:ILE:C	4:e:144:ILE:HD13	2.46	0.41
4:e:636:LEU:HD21	4:e:638:TYR:HE1	1.86	0.41
4:e:679:PHE:HB3	4:e:694:VAL:HG22	2.01	0.41
1:C:19:U:H3	2:D:3:DA:N6	2.19	0.41
4:g:161:LYS:HA	4:g:161:LYS:HD3	1.90	0.41
2:P:15:DC:H2'	2:P:16:DT:C5	2.56	0.41
4:h:634:GLU:OE2	4:h:634:GLU:N	2.53	0.41
4:a:580:VAL:O	4:a:584:ILE:HG12	2.20	0.41
4:b:339:LYS:C	4:b:339:LYS:HD3	2.46	0.41
3:4:177:ARG:O	3:4:181:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:187:GLU:O	3:3:191:GLN:HG2	2.21	0.41
3:7:79:LEU:HA	3:7:121:TRP:CD1	2.56	0.41
4:f:553:MET:HE3	4:f:553:MET:HB3	1.89	0.41
4:f:643:ARG:H	4:f:643:ARG:HG3	1.64	0.41
4:e:80:VAL:HG23	4:e:271:LEU:HD21	2.02	0.41
4:e:84:LEU:HG	4:e:84:LEU:H	1.77	0.41
4:e:624:ARG:HH12	4:e:677:TYR:HE1	1.69	0.41
1:K:13:A:H2'	1:K:14:U:C6	2.56	0.41
4:h:65:GLN:NE2	4:h:67:LEU:HD23	2.35	0.41
4:a:18:LYS:NZ	4:a:62:GLY:H	2.16	0.41
4:c:6:ASN:ND2	4:c:257:ILE:HD13	2.36	0.41
4:c:241:ARG:HH22	4:c:647:GLN:HE22	1.68	0.41
4:d:359:PHE:CE2	4:d:362:GLY:HA2	2.55	0.41
4:f:150:ARG:HE	1:H:8:C:H4'	1.86	0.41
4:f:261:LYS:HD3	4:f:265:GLN:HE21	1.86	0.41
4:e:581:ARG:HA	4:e:584:ILE:HB	2.02	0.41
4:g:116:ILE:HD12	4:g:229:HIS:NE2	2.35	0.41
4:g:712:LEU:HD23	4:g:712:LEU:HA	1.93	0.41
4:h:477:LEU:HB3	4:h:520:TYR:HB2	2.01	0.41
4:h:692:MET:SD	4:h:693:PRO:HD2	2.61	0.41
4:b:229:HIS:HB3	4:b:232:LYS:HZ1	1.86	0.41
4:b:491:ILE:HD13	4:b:534:TYR:OH	2.21	0.41
4:c:557:LYS:HA	4:c:557:LYS:HD3	1.70	0.41
4:d:128:LYS:HB2	4:d:147:SER:HB3	2.01	0.41
3:3:361:LYS:O	3:3:361:LYS:HD3	2.21	0.40
3:7:66:LEU:HD23	3:7:66:LEU:HA	1.76	0.40
4:f:353:MET:HE3	4:f:459:LEU:HD12	2.04	0.40
4:g:419:LEU:HD13	4:g:419:LEU:HA	1.93	0.40
4:c:603:HIS:HE2	4:c:654:ARG:HB3	1.86	0.40
4:d:706:LEU:HD23	4:d:706:LEU:HA	1.85	0.40
3:5:217:ILE:HG23	3:5:218:ALA:H	1.86	0.40
3:1:86:ASP:HB3	3:1:87:SER:H	1.66	0.40
3:2:381:PRO:HG2	3:2:384:MET:HE3	2.03	0.40
3:4:142:ILE:O	3:4:146:VAL:HG23	2.20	0.40
3:3:170:LYS:HE2	3:3:170:LYS:HB2	1.93	0.40
3:7:320:PHE:O	3:7:324:ILE:HG13	2.22	0.40
4:f:455:LEU:HD12	4:f:458:SER:OG	2.20	0.40
4:f:489:ILE:HD11	4:f:565:PHE:CE2	2.56	0.40
4:e:106:ALA:HB1	4:e:124:LYS:HD2	2.04	0.40
4:e:143:ILE:HD12	4:e:143:ILE:N	2.36	0.40
1:C:2:U:H1'	4:c:462:MET:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:h:144:ILE:HG12	4:h:260:LEU:HD23	2.02	0.40
4:a:113:LEU:HD12	4:a:113:LEU:HA	1.94	0.40
4:c:156:CYS:HB2	4:c:209:ALA:O	2.21	0.40
4:c:261:LYS:HB3	4:c:261:LYS:HE2	1.85	0.40
4:c:510:ILE:HG21	4:c:541:VAL:HG11	2.01	0.40
3:2:363:LYS:HE3	3:2:363:LYS:HB2	1.80	0.40
3:3:297:ILE:N	3:3:297:ILE:HD13	2.37	0.40
3:7:287:LEU:HD23	3:7:287:LEU:HA	1.94	0.40
1:C:3:C:H4'	4:c:686:SER:HB2	2.02	0.40
4:g:261:LYS:HE2	4:g:261:LYS:HB3	1.81	0.40
4:h:128:LYS:NZ	4:h:149:ARG:HD3	2.35	0.40
4:h:341:ARG:HD2	4:h:341:ARG:H	1.86	0.40
4:d:236:ILE:O	4:d:240:ILE:HG12	2.21	0.40
3:8:37:LEU:HD12	3:8:202:CYS:SG	2.61	0.40
4:e:195:LEU:HB3	4:e:197:VAL:HG23	2.04	0.40
4:g:124:LYS:HB2	4:g:153:LYS:HZ2	1.87	0.40
4:b:268:ASN:HA	4:b:276:ARG:HG3	2.03	0.40
4:c:285:ILE:HG22	4:c:288:ASP:HB2	2.03	0.40
3:4:25:HIS:HA	3:4:31:SER:OG	2.22	0.40
3:8:62:GLY:HA2	3:8:105:LEU:HB2	2.03	0.40
3:7:133:ASN:OD1	3:7:133:ASN:O	2.40	0.40
4:f:398:LYS:HD2	4:f:398:LYS:HA	1.92	0.40
4:e:146:CYS:HB3	4:e:253:LYS:HG3	2.04	0.40
4:e:435:LEU:HD23	4:e:435:LEU:HA	1.93	0.40
1:K:12:G:H2'	1:K:13:A:C8	2.57	0.40
1:O:1:A:C2	4:a:416:PHE:HB2	2.53	0.40
4:a:15:LEU:HB2	4:a:273:ASP:HB3	2.02	0.40
4:b:229:HIS:HD2	4:b:232:LYS:HE2	1.86	0.40
4:c:609:ASP:HB3	4:c:612:THR:HG22	2.04	0.40
3:5:132:SER:O	3:5:133:ASN:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1	378/390 (97%)	366 (97%)	12 (3%)	0	100	100
3	2	381/390 (98%)	371 (97%)	10 (3%)	0	100	100
3	3	384/390 (98%)	365 (95%)	19 (5%)	0	100	100
3	4	382/390 (98%)	371 (97%)	11 (3%)	0	100	100
3	5	387/390 (99%)	372 (96%)	15 (4%)	0	100	100
3	6	387/390 (99%)	371 (96%)	16 (4%)	0	100	100
3	7	382/390 (98%)	365 (96%)	17 (4%)	0	100	100
3	8	381/390 (98%)	365 (96%)	16 (4%)	0	100	100
4	a	729/731 (100%)	697 (96%)	32 (4%)	0	100	100
4	b	729/731 (100%)	711 (98%)	18 (2%)	0	100	100
4	c	729/731 (100%)	704 (97%)	25 (3%)	0	100	100
4	d	729/731 (100%)	707 (97%)	22 (3%)	0	100	100
4	e	729/731 (100%)	696 (96%)	33 (4%)	0	100	100
4	f	728/731 (100%)	704 (97%)	24 (3%)	0	100	100
4	g	729/731 (100%)	699 (96%)	30 (4%)	0	100	100
4	h	729/731 (100%)	697 (96%)	32 (4%)	0	100	100
All	All	8893/8968 (99%)	8561 (96%)	332 (4%)	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	
3	1	339/349 (97%)	334 (98%)	5 (2%)	57	73
3	2	342/349 (98%)	333 (97%)	9 (3%)	40	64
3	3	345/349 (99%)	340 (99%)	5 (1%)	59	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	343/349 (98%)	336 (98%)	7 (2%)	48	68
3	5	348/349 (100%)	337 (97%)	11 (3%)	34	60
3	6	348/349 (100%)	342 (98%)	6 (2%)	53	71
3	7	343/349 (98%)	338 (98%)	5 (2%)	57	73
3	8	342/349 (98%)	340 (99%)	2 (1%)	78	82
4	a	639/639 (100%)	631 (99%)	8 (1%)	61	75
4	b	639/639 (100%)	627 (98%)	12 (2%)	50	69
4	c	639/639 (100%)	627 (98%)	12 (2%)	50	69
4	d	639/639 (100%)	627 (98%)	12 (2%)	50	69
4	e	639/639 (100%)	625 (98%)	14 (2%)	45	66
4	f	638/639 (100%)	626 (98%)	12 (2%)	50	69
4	g	639/639 (100%)	624 (98%)	15 (2%)	44	66
4	h	639/639 (100%)	629 (98%)	10 (2%)	55	72
All	All	7861/7904 (100%)	7716 (98%)	145 (2%)	51	70

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1	78	LEU
3	1	150	GLU
3	1	158	CYS
3	1	305	HIS
3	1	323	LEU
3	2	114	ILE
3	2	137	VAL
3	2	171	ILE
3	2	186	SER
3	2	197	SER
3	2	303	SER
3	2	304	LEU
3	2	305	HIS
3	2	356	THR
3	4	88	THR
3	4	137	VAL
3	4	141	ASP
3	4	213	GLN
3	4	215	ILE

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Mol	Chain	Res	Type
3	4	286	ASN
3	4	356	THR
3	3	40	VAL
3	3	158	CYS
3	3	217	ILE
3	3	339	LYS
3	3	360	VAL
3	8	217	ILE
3	8	305	HIS
3	7	37	LEU
3	7	73	GLN
3	7	135	LEU
3	7	158	CYS
3	7	360	VAL
4	f	32	LEU
4	f	144	ILE
4	f	198	ILE
4	f	205	VAL
4	f	227	HIS
4	f	229	HIS
4	f	421	VAL
4	f	440	VAL
4	f	578	GLN
4	f	590	TYR
4	f	607	MET
4	f	619	ARG
4	e	4	VAL
4	e	67	LEU
4	e	84	LEU
4	e	103	VAL
4	e	125	ILE
4	e	135	THR
4	e	226	LEU
4	e	257	ILE
4	e	411	GLN
4	e	440	VAL
4	e	496	ILE
4	e	519	SER
4	e	546	ILE
4	e	640	ILE
4	g	18	LYS
4	g	30	ASP

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Mol	Chain	Res	Type
4	g	197	VAL
4	g	257	ILE
4	g	281	ASP
4	g	296	VAL
4	g	337	HIS
4	g	378	GLU
4	g	409	LEU
4	g	419	LEU
4	g	440	VAL
4	g	491	ILE
4	g	603	HIS
4	g	614	THR
4	g	622	THR
4	h	12	ILE
4	h	54	SER
4	h	126	CYS
4	h	146	CYS
4	h	289	CYS
4	h	322	THR
4	h	332	VAL
4	h	374	VAL
4	h	433	PHE
4	h	445	ILE
4	a	20	VAL
4	a	101	ILE
4	a	223	ASP
4	a	281	ASP
4	a	376	VAL
4	a	440	VAL
4	a	594	TYR
4	a	724	ILE
4	b	20	VAL
4	b	27	THR
4	b	73	LEU
4	b	103	VAL
4	b	104	VAL
4	b	195	LEU
4	b	198	ILE
4	b	251	GLU
4	b	440	VAL
4	b	590	TYR
4	b	614	THR

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Mol	Chain	Res	Type
4	b	649	THR
4	c	1	MET
4	c	131	ILE
4	c	152	VAL
4	c	233	LYS
4	c	279	ILE
4	c	281	ASP
4	c	364	GLU
4	c	376	VAL
4	c	409	LEU
4	c	440	VAL
4	c	487	LEU
4	c	681	SER
4	d	12	ILE
4	d	85	LEU
4	d	88	PHE
4	d	117	LEU
4	d	186	VAL
4	d	225	ILE
4	d	269	ILE
4	d	289	CYS
4	d	322	THR
4	d	374	VAL
4	d	433	PHE
4	d	488	VAL
3	5	66	LEU
3	5	78	LEU
3	5	85	ILE
3	5	86	ASP
3	5	116	HIS
3	5	178	LEU
3	5	202	CYS
3	5	224	THR
3	5	290	VAL
3	5	296	ARG
3	5	305	HIS
3	6	51	ASP
3	6	178	LEU
3	6	303	SER
3	6	319	SER
3	6	356	THR
3	6	367	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (155) such sidechains are listed below:

Mol	Chain	Res	Type
3	1	11	GLN
3	1	129	GLN
3	1	209	ASN
3	1	213	GLN
3	1	286	ASN
3	2	11	GLN
3	2	46	ASN
3	2	175	GLN
3	2	191	GLN
3	2	262	ASN
3	2	268	ASN
3	2	279	ASN
3	2	288	GLN
3	4	8	ASN
3	4	11	GLN
3	4	17	HIS
3	4	25	HIS
3	4	81	GLN
3	4	133	ASN
3	4	279	ASN
3	4	286	ASN
3	4	305	HIS
3	3	11	GLN
3	3	116	HIS
3	3	128	GLN
3	3	189	GLN
3	3	213	GLN
3	3	305	HIS
3	8	8	ASN
3	8	11	GLN
3	8	25	HIS
3	8	73	GLN
3	8	81	GLN
3	8	134	HIS
3	8	148	ASN
3	8	189	GLN
3	8	210	GLN
3	8	268	ASN
3	7	17	HIS
3	7	128	GLN
3	7	292	GLN

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Mol	Chain	Res	Type
3	7	305	HIS
3	7	357	GLN
3	7	359	HIS
4	f	21	GLN
4	f	50	GLN
4	f	155	ASN
4	f	165	ASN
4	f	190	HIS
4	f	203	GLN
4	f	206	HIS
4	f	227	HIS
4	f	248	ASN
4	f	252	ASN
4	f	326	ASN
4	f	424	ASN
4	f	578	GLN
4	f	602	ASN
4	f	647	GLN
4	f	675	GLN
4	f	710	ASN
4	e	21	GLN
4	e	68	GLN
4	e	300	ASN
4	e	315	ASN
4	e	424	ASN
4	e	498	GLN
4	e	503	HIS
4	e	728	GLN
4	g	65	GLN
4	g	99	ASN
4	g	190	HIS
4	g	239	HIS
4	g	248	ASN
4	g	315	ASN
4	g	498	GLN
4	g	505	GLN
4	g	602	ASN
4	g	642	GLN
4	g	675	GLN
4	h	155	ASN
4	h	227	HIS
4	h	229	HIS

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Mol	Chain	Res	Type
4	h	239	HIS
4	h	248	ASN
4	h	337	HIS
4	h	424	ASN
4	h	505	GLN
4	h	647	GLN
4	a	68	GLN
4	a	111	ASN
4	a	220	ASN
4	a	248	ASN
4	a	291	GLN
4	a	300	ASN
4	a	315	ASN
4	a	326	ASN
4	a	336	GLN
4	a	414	GLN
4	a	424	ASN
4	a	441	GLN
4	a	602	ASN
4	a	647	GLN
4	a	728	GLN
4	b	6	ASN
4	b	50	GLN
4	b	65	GLN
4	b	72	ASN
4	b	99	ASN
4	b	248	ASN
4	b	268	ASN
4	b	505	GLN
4	b	550	GLN
4	b	566	HIS
4	b	642	GLN
4	c	36	HIS
4	c	40	HIS
4	c	65	GLN
4	c	68	GLN
4	c	99	ASN
4	c	229	HIS
4	c	248	ASN
4	c	252	ASN
4	c	291	GLN
4	c	424	ASN

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Mol	Chain	Res	Type
4	c	485	HIS
4	c	504	ASN
4	c	545	ASN
4	c	568	GLN
4	c	642	GLN
4	c	647	GLN
4	c	652	HIS
4	d	36	HIS
4	d	40	HIS
4	d	99	ASN
4	d	190	HIS
4	d	268	ASN
4	d	361	ASN
4	d	424	ASN
4	d	450	GLN
4	d	566	HIS
4	d	647	GLN
4	d	661	HIS
3	5	73	GLN
3	5	129	GLN
3	5	175	GLN
3	5	195	ASN
3	6	110	GLN
3	6	116	HIS
3	6	191	GLN
3	6	262	ASN
3	6	267	GLN
3	6	268	ASN
3	6	288	GLN
3	6	305	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	18/21 (85%)	5 (27%)	2 (11%)
1	C	18/21 (85%)	5 (27%)	2 (11%)
1	E	18/21 (85%)	5 (27%)	2 (11%)
1	H	18/21 (85%)	4 (22%)	2 (11%)
1	I	18/21 (85%)	5 (27%)	2 (11%)
1	K	18/21 (85%)	6 (33%)	2 (11%)
1	N	18/21 (85%)	4 (22%)	2 (11%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	O	18/21 (85%)	5 (27%)	2 (11%)
All	All	144/168 (85%)	39 (27%)	16 (11%)

All (39) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	3	C
1	A	13	A
1	A	18	C
1	A	19	U
1	C	2	U
1	C	13	A
1	C	17	C
1	C	18	C
1	C	19	U
1	E	2	U
1	E	3	C
1	E	13	A
1	E	18	C
1	E	19	U
1	H	3	C
1	H	13	A
1	H	18	C
1	H	19	U
1	K	2	U
1	K	3	C
1	K	13	A
1	K	17	C
1	K	18	C
1	K	19	U
1	N	3	C
1	N	13	A
1	N	18	C
1	N	19	U
1	O	2	U
1	O	13	A
1	O	17	C
1	O	18	C
1	O	19	U
1	I	2	U
1	I	13	A

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Mol	Chain	Res	Type
1	I	17	C
1	I	18	C
1	I	19	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	12	G
1	A	18	C
1	C	12	G
1	C	18	C
1	E	12	G
1	E	18	C
1	H	12	G
1	H	18	C
1	K	12	G
1	K	18	C
1	N	12	G
1	N	18	C
1	O	12	G
1	O	18	C
1	I	12	G
1	I	18	C

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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

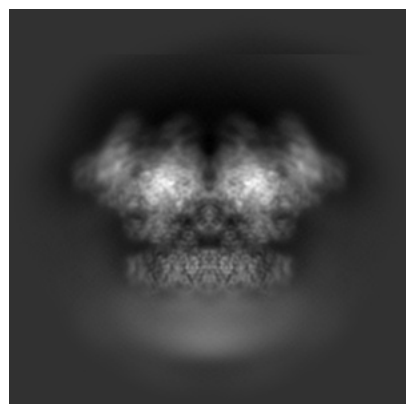
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-69324. These allow visual inspection of the internal detail of the map and identification of artifacts.

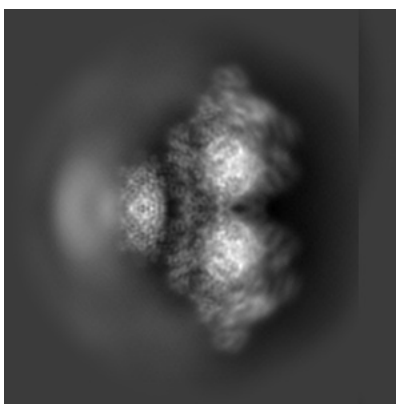
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

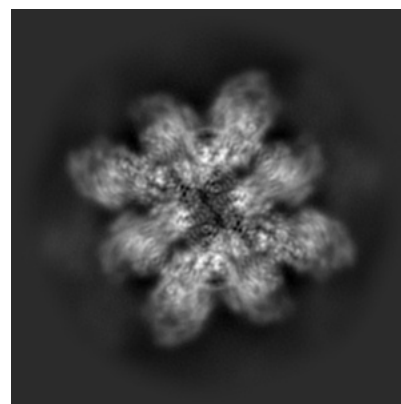
6.1.1 Primary map



X

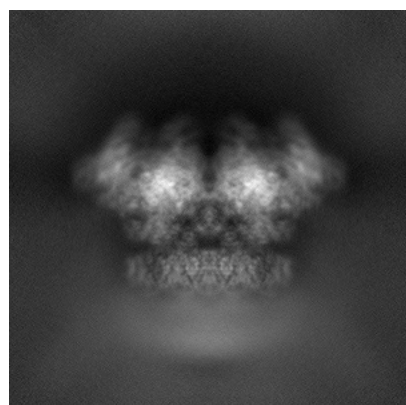


Y

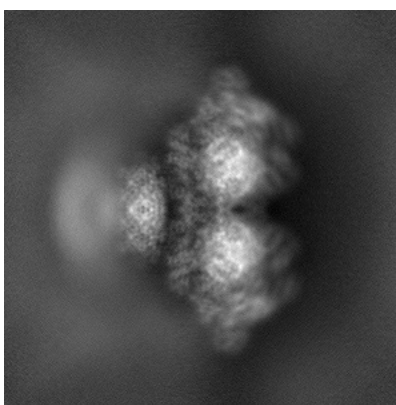


Z

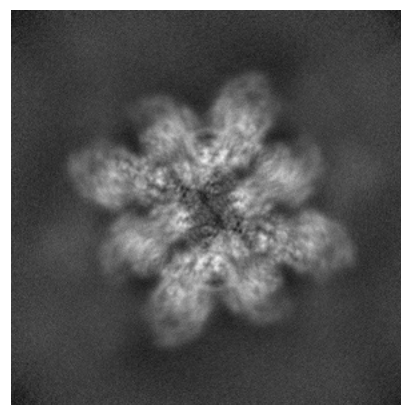
6.1.2 Raw map



X



Y

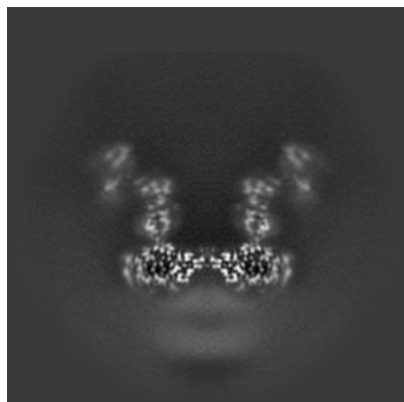


Z

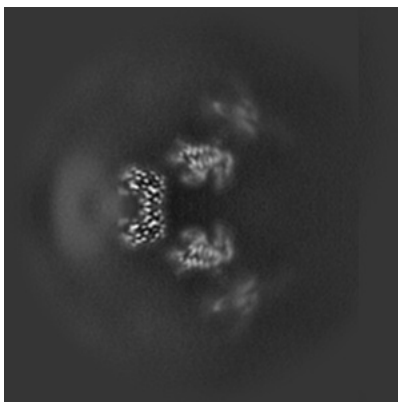
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

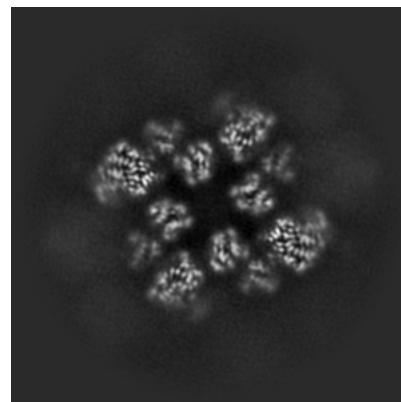
6.2.1 Primary map



X Index: 320

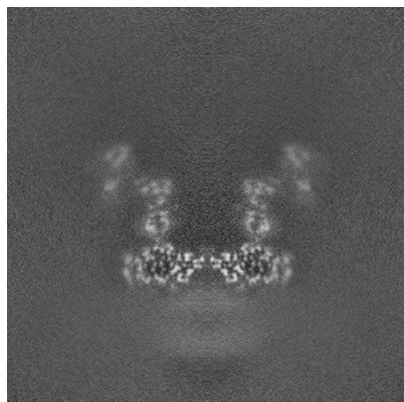


Y Index: 320

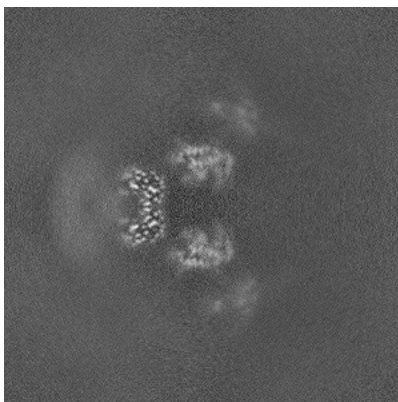


Z Index: 320

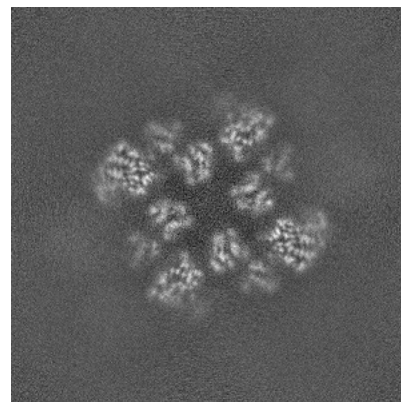
6.2.2 Raw map



X Index: 320



Y Index: 320

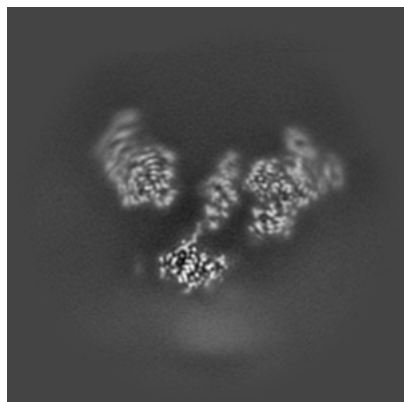


Z Index: 320

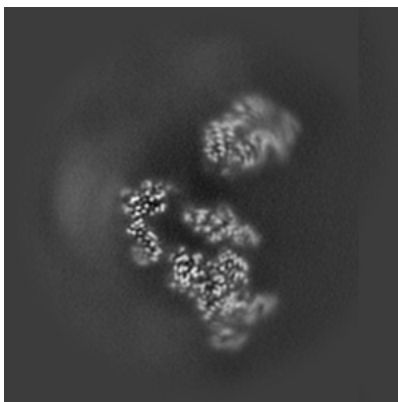
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

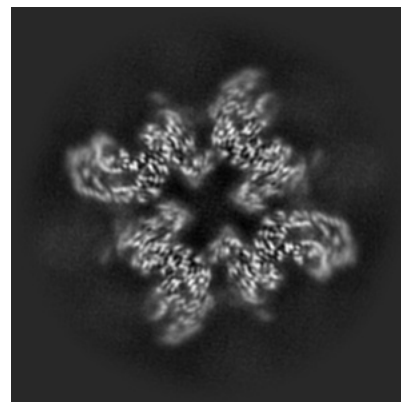
6.3.1 Primary map



X Index: 372

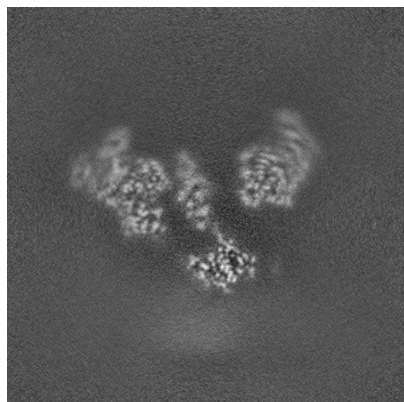


Y Index: 377

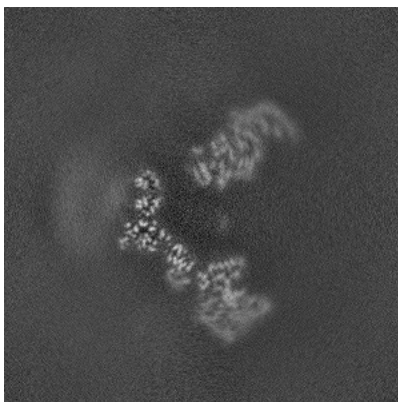


Z Index: 360

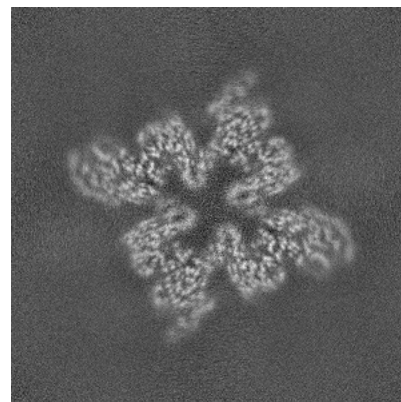
6.3.2 Raw map



X Index: 268



Y Index: 348

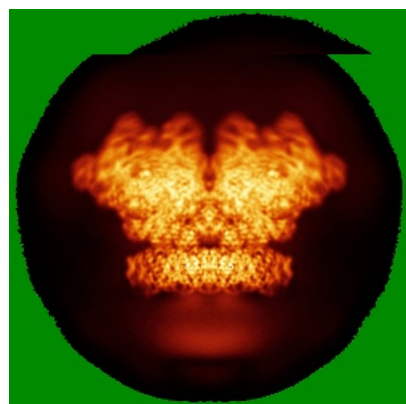


Z Index: 350

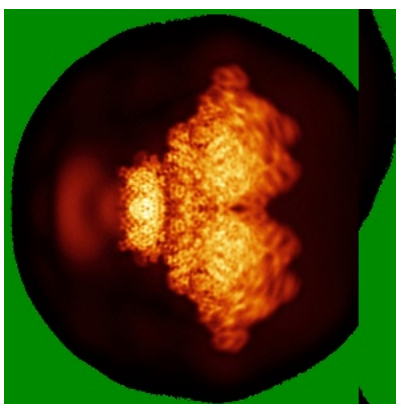
The images above show the largest variance slices of the map in three orthogonal directions.

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

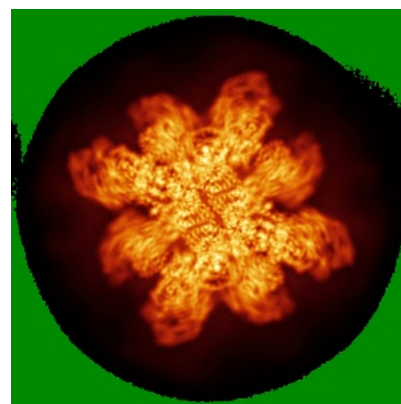
6.4.1 Primary map



X

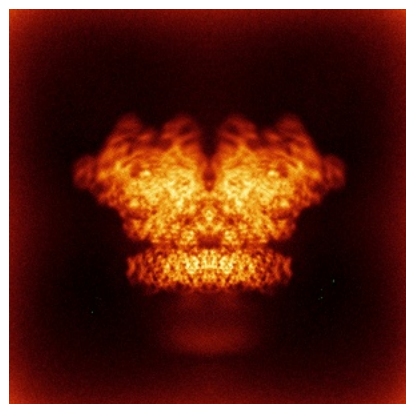


Y

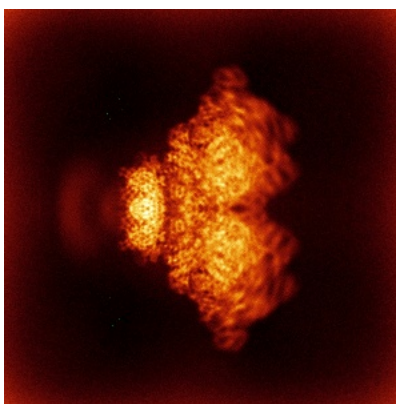


Z

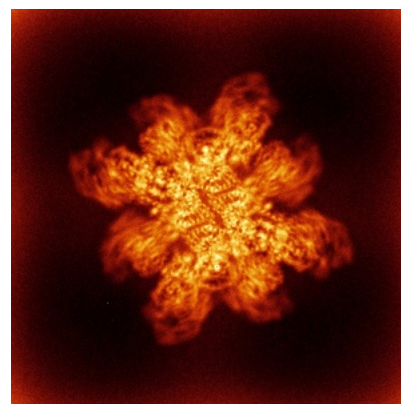
6.4.2 Raw map



X



Y

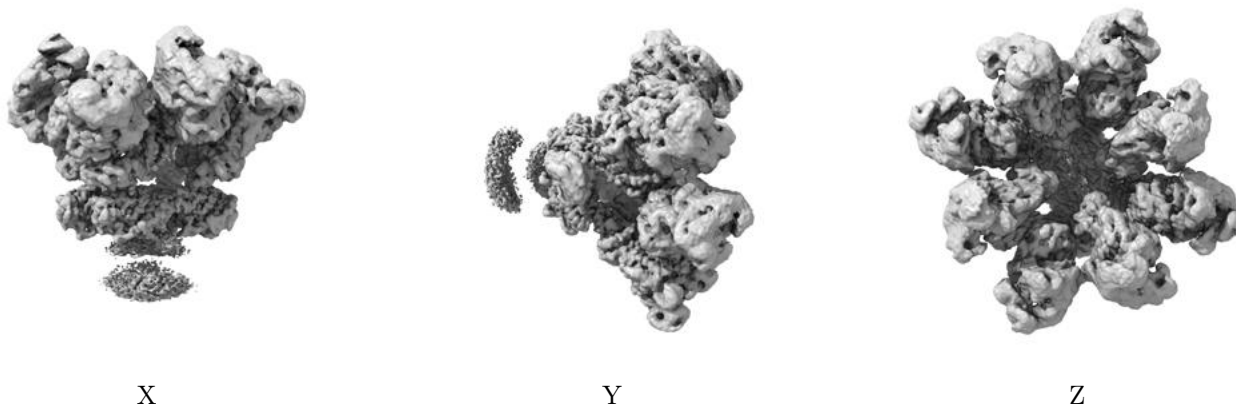


Z

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.

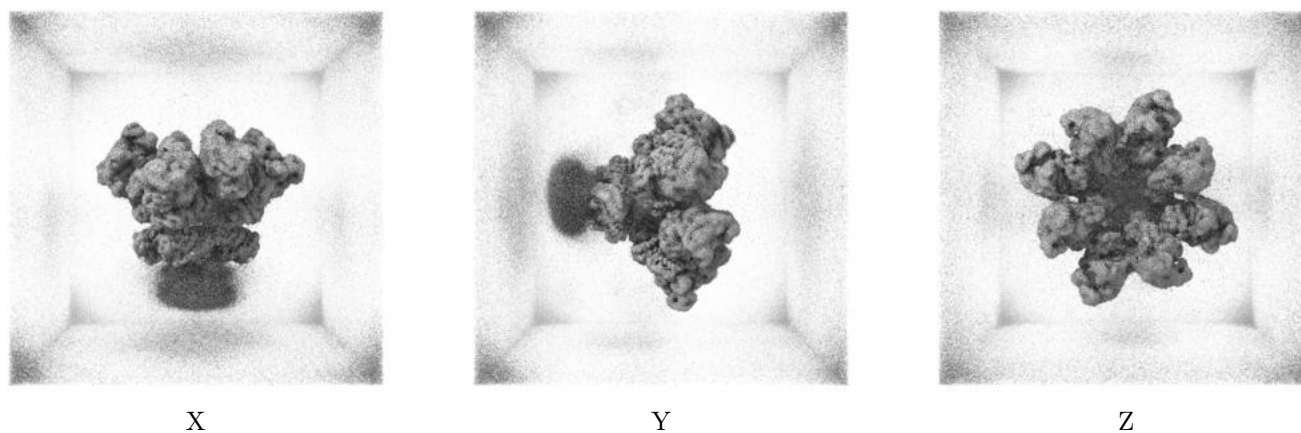
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02158. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

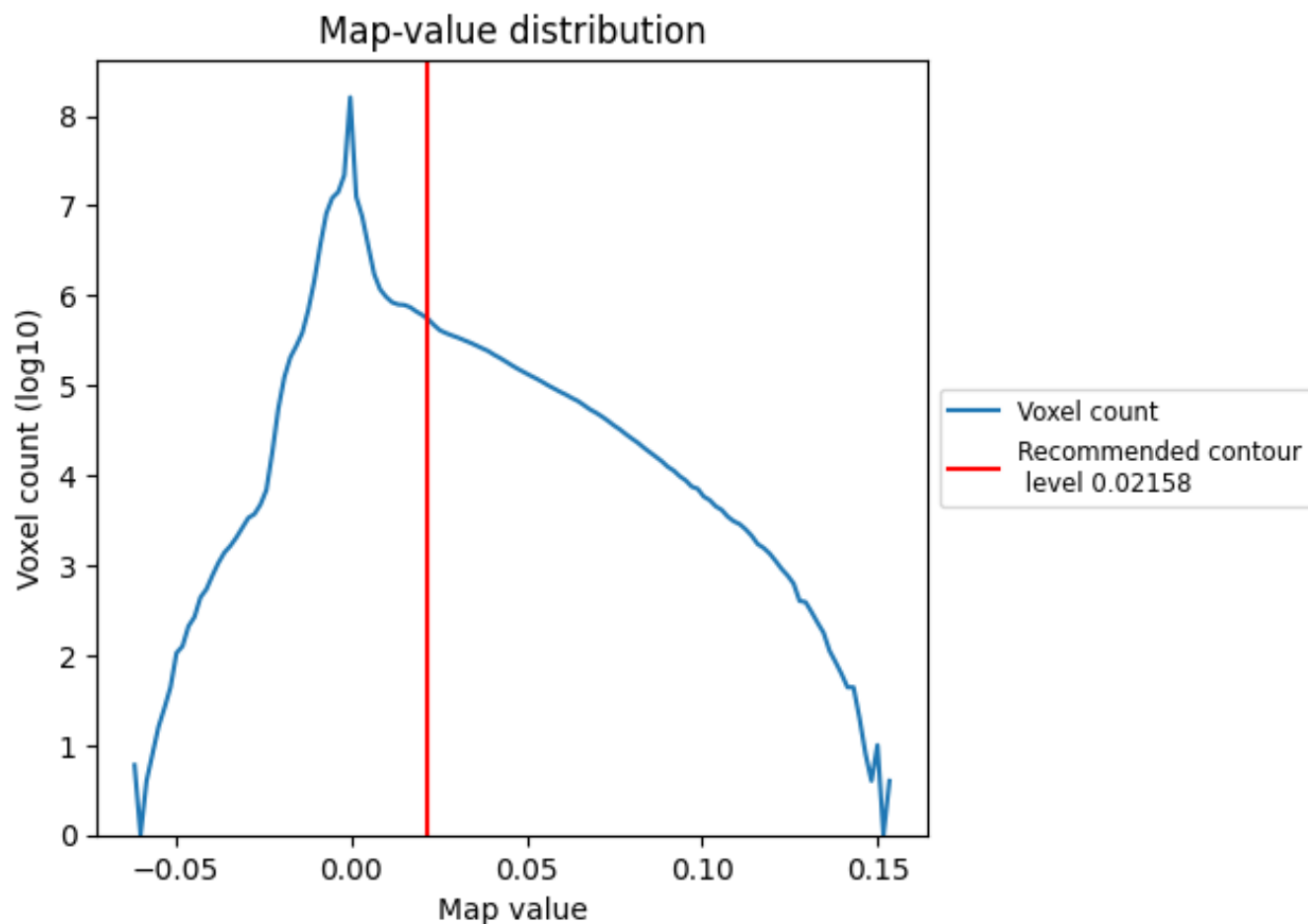
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

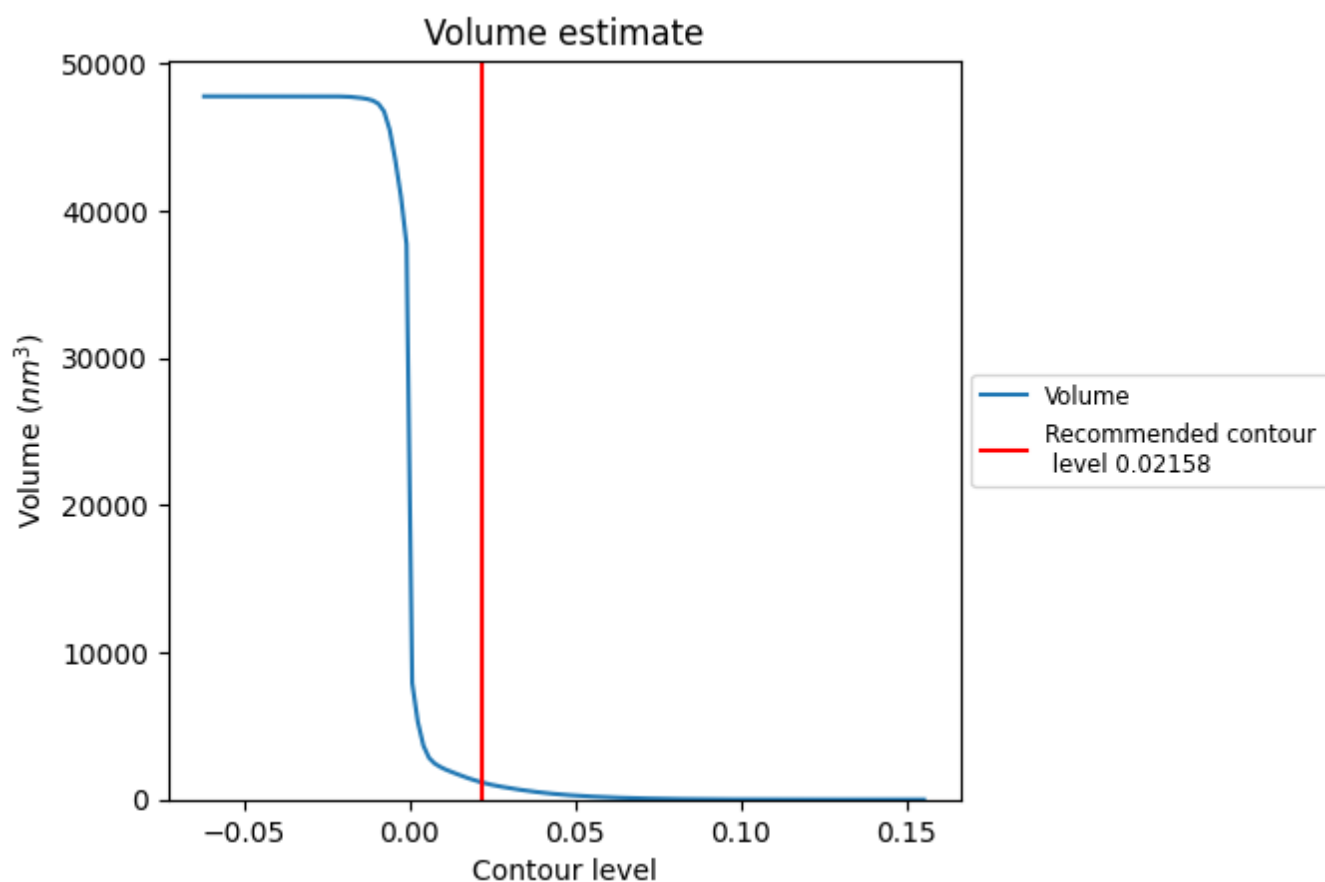
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

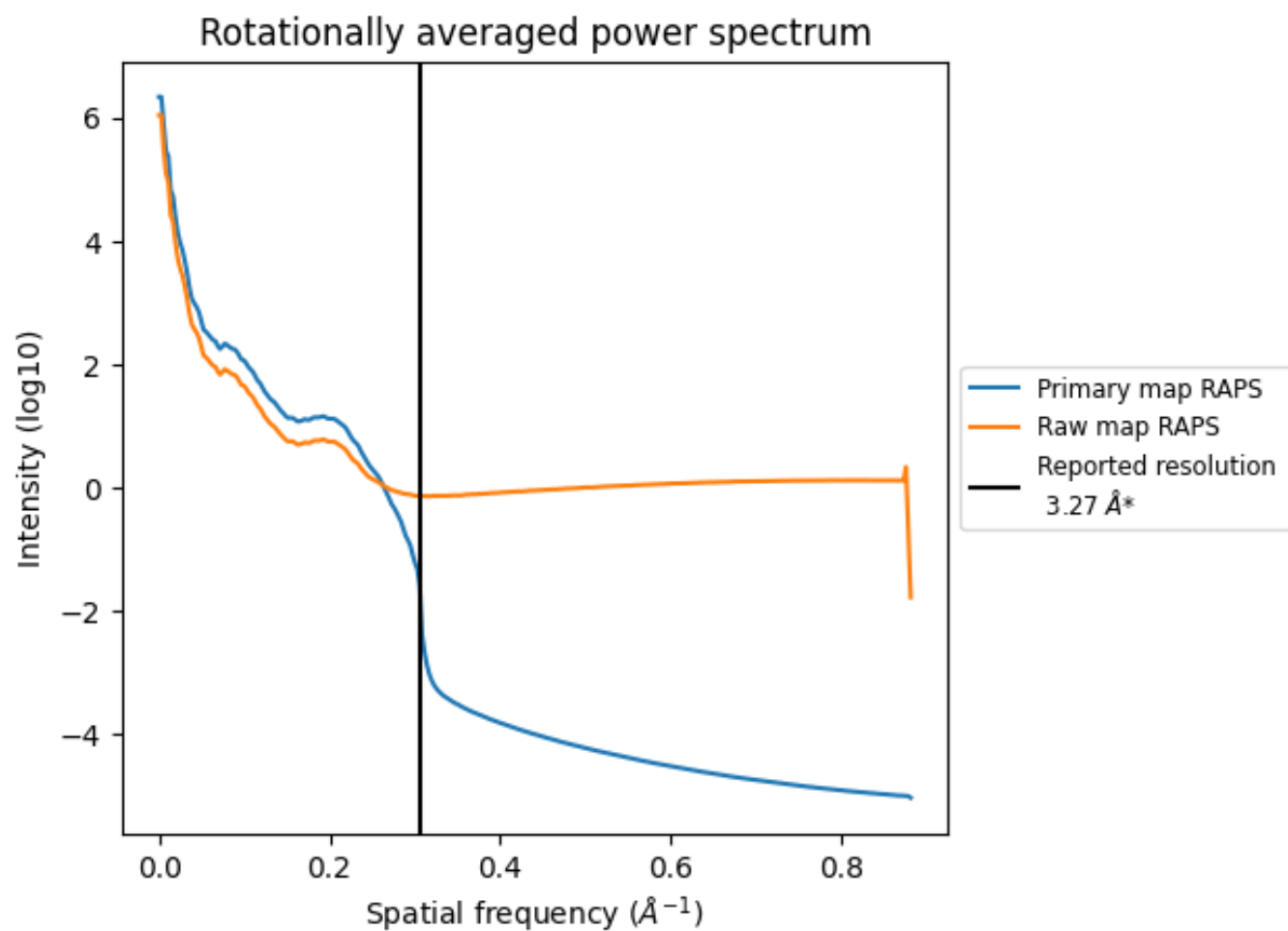
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1182 nm³; this corresponds to an approximate mass of 1068 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 [i](#)

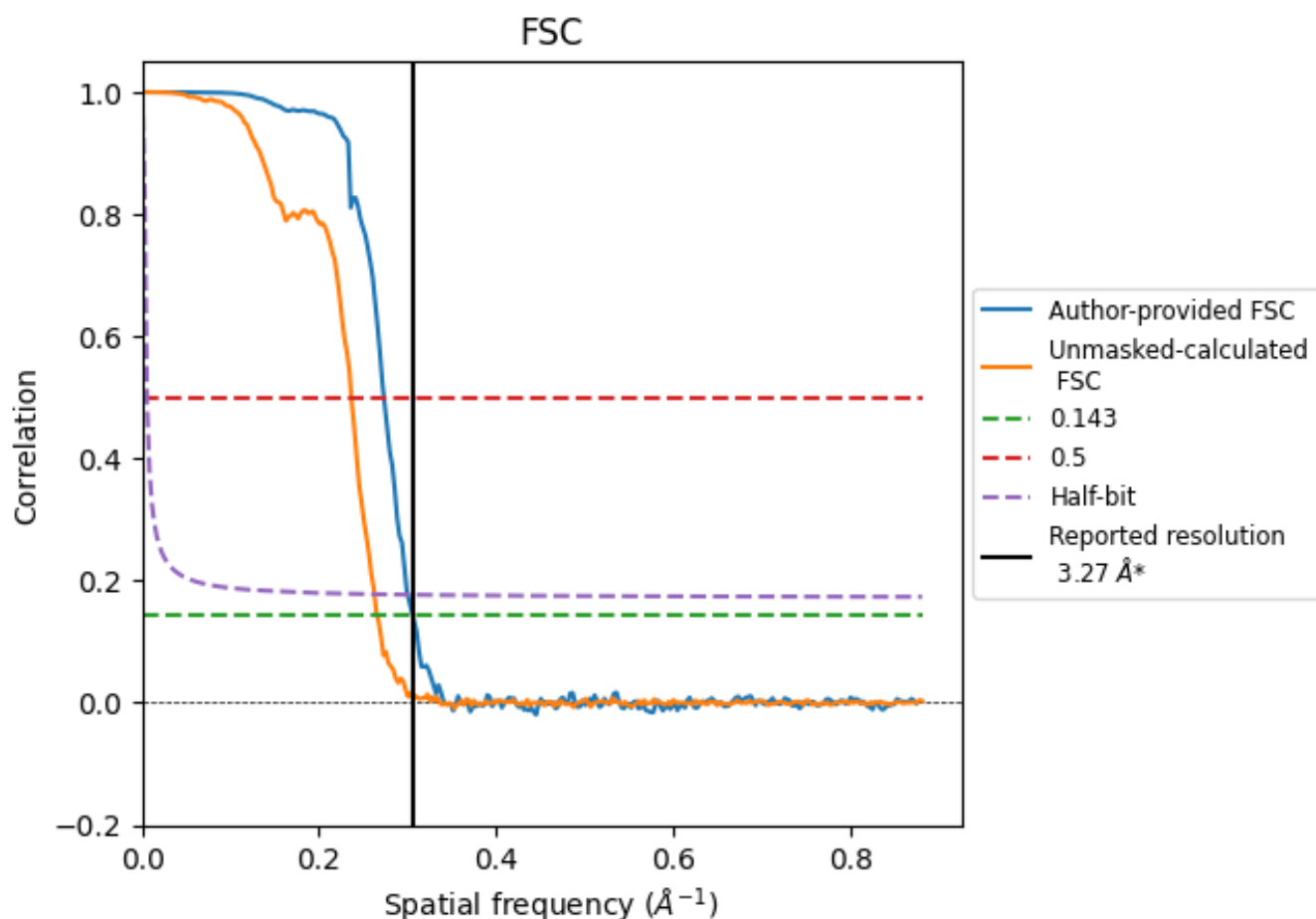


*Reported resolution corresponds to spatial frequency of 0.306 $\text{\AA}^{-1}$

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 $0.306 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

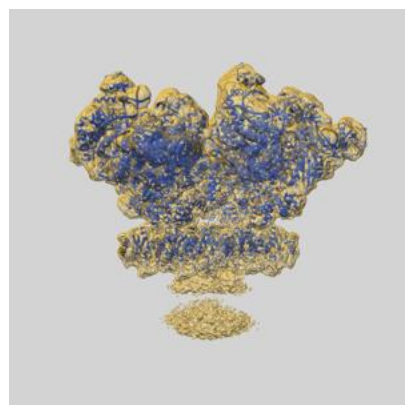
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.27	-	-
Author-provided FSC curve	3.27	3.66	3.33
Unmasked-calculated*	3.77	4.23	3.81

*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 3.77 differs from the reported value 3.27 by more than 10 %

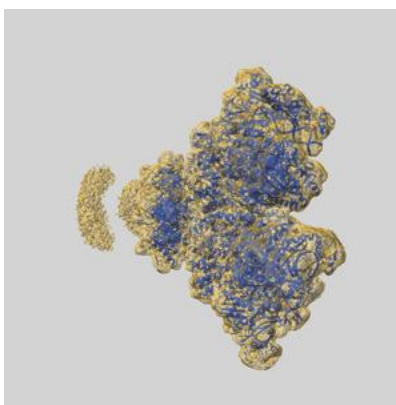
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-69324 and PDB model 23WQ. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

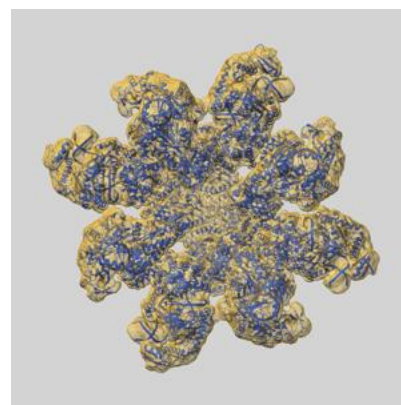
9.1 Map-model overlay [i](#)



X



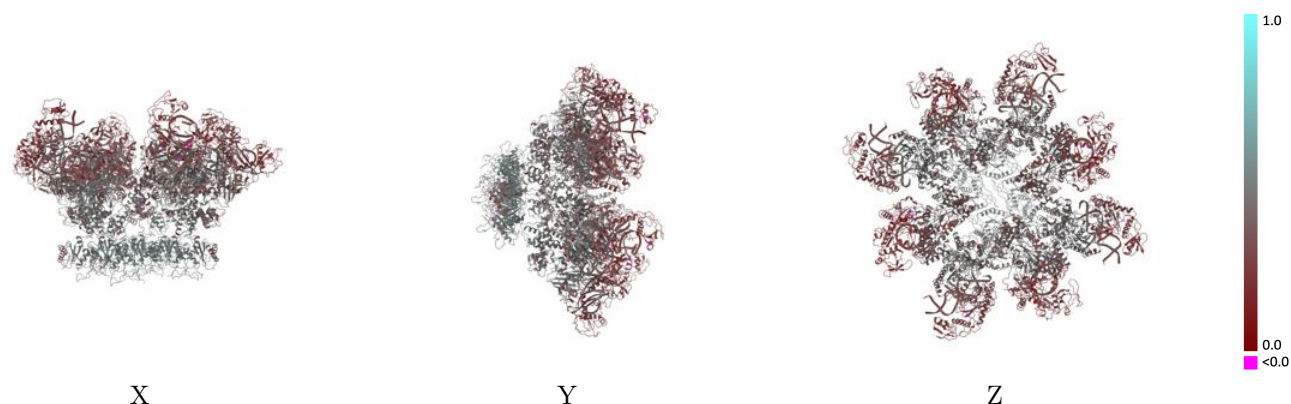
Y



Z

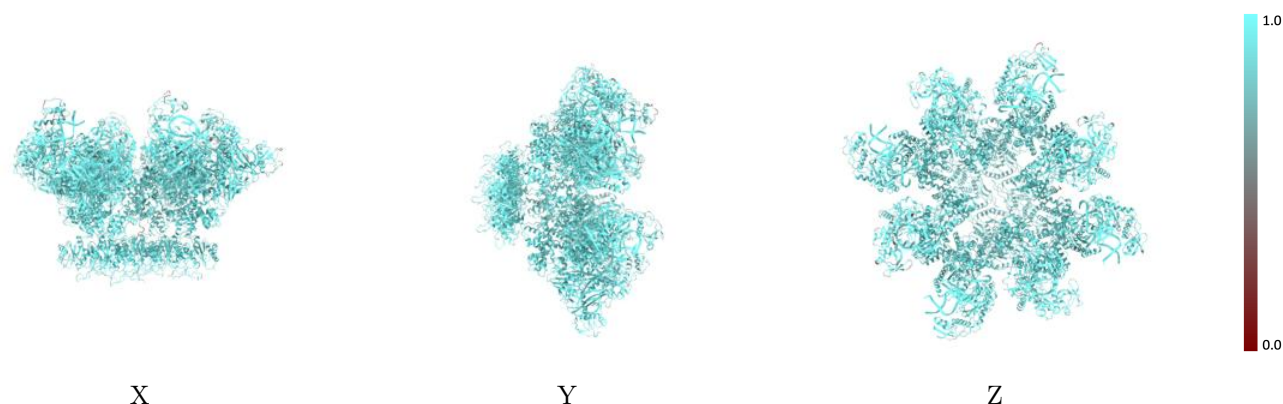
The images above show the 3D surface view of the map at the recommended contour level 0.02158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



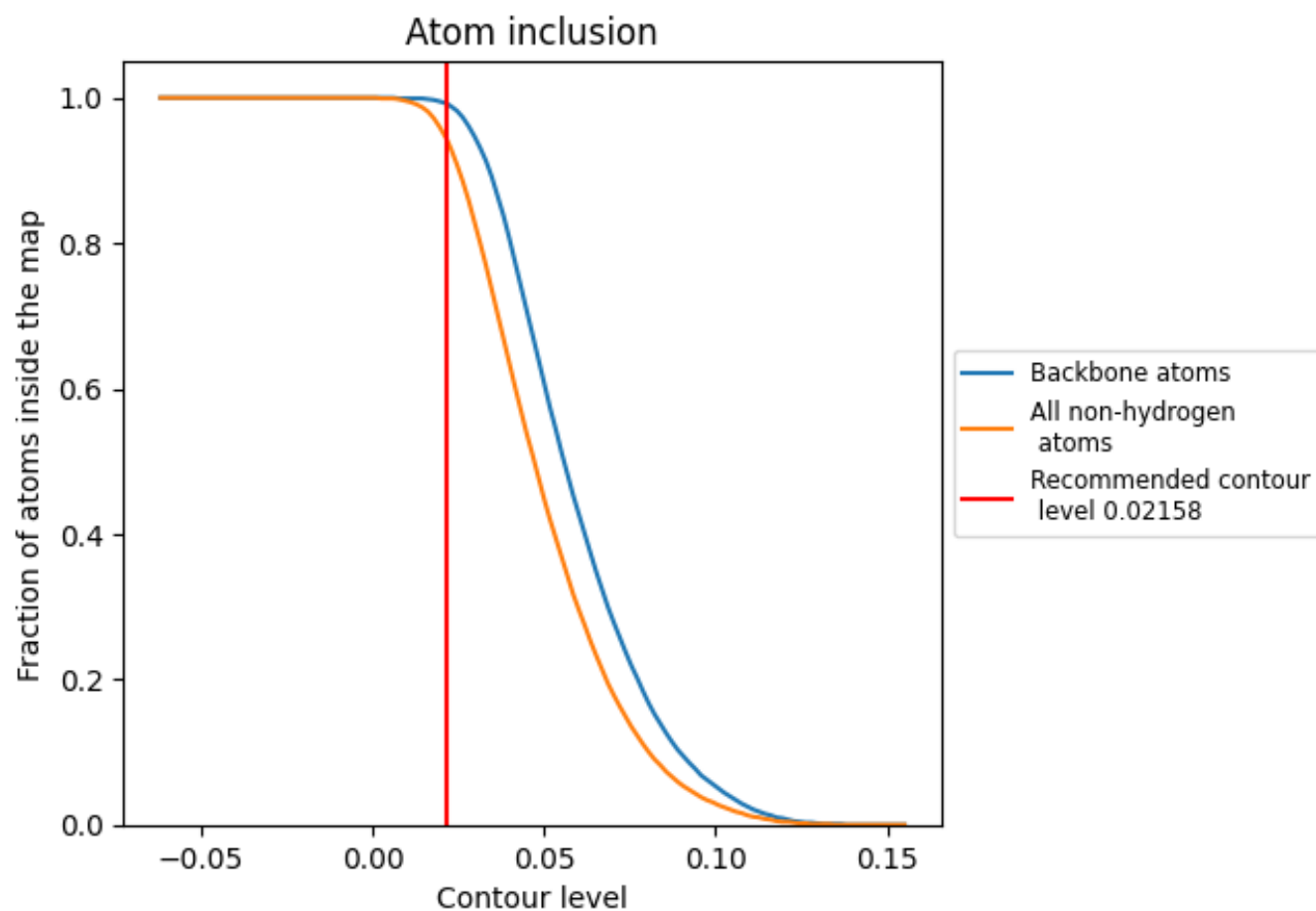
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02158).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (0.02158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.3920
1	 0.9510	 0.4450
2	 0.9610	 0.4970
3	 0.9300	 0.4290
4	 0.9520	 0.4590
5	 0.9240	 0.4350
6	 0.9510	 0.4920
7	 0.9330	 0.4380
8	 0.9520	 0.4600
A	 1.0000	 0.3870
B	 1.0000	 0.3910
C	 1.0000	 0.3420
D	 0.9980	 0.3550
E	 0.9980	 0.3870
F	 1.0000	 0.3900
G	 1.0000	 0.3870
H	 1.0000	 0.3780
I	 0.9980	 0.3320
J	 0.9950	 0.3280
K	 0.9950	 0.3420
L	 0.9980	 0.3480
M	 0.9980	 0.3960
N	 0.9980	 0.3830
O	 0.9980	 0.3320
P	 0.9900	 0.3340
a	 0.9260	 0.3330
b	 0.9430	 0.3770
c	 0.9310	 0.3530
d	 0.9380	 0.3880
e	 0.9270	 0.3320
f	 0.9360	 0.3710
g	 0.9320	 0.3480
h	 0.9440	 0.3910

