



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:41 PM UTC

PDB ID : 9VJA / pdb_00009vja
EMDB ID : EMD-65108
Title : Type I-A CRISPR integrase prespacer catching complex, State II
Authors : Li, Z.X.; Li, Y.T.; Lu, M.L.; Xiao, Y.B.
Deposited on : 2025-06-19
Resolution : 3.01 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

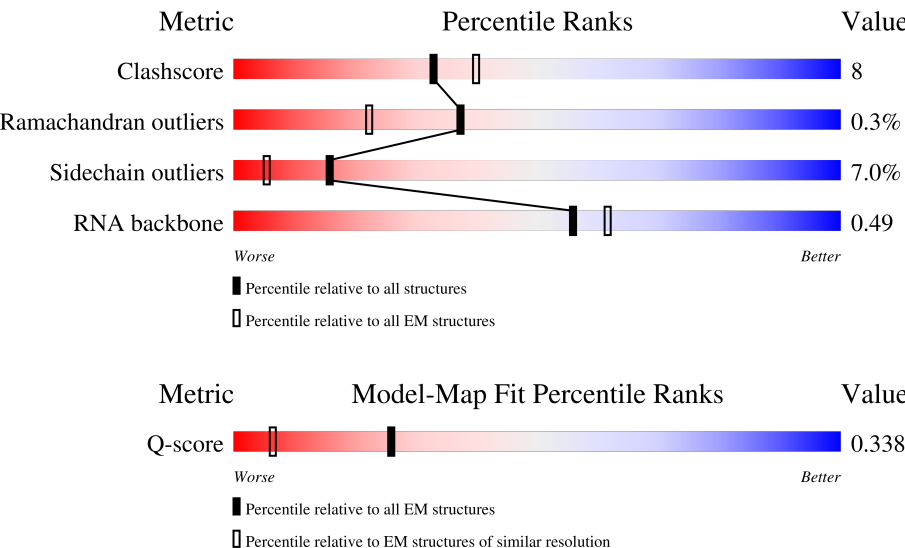
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.01 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	13882 (2.51 - 3.51)

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	K	288	<div> <div>6%</div> <div>56%</div> <div>38%</div> <div>6%</div> </div>
1	L	288	<div> <div>23%</div> <div>55%</div> <div>38%</div> <div>6%</div> </div>
2	N	51	<div> <div>18%</div> <div>73%</div> <div>16%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
3	T	51	
4	g	55	
5	t	83	
6	A	219	
6	B	219	
6	C	219	
6	D	219	
7	S	1337	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26425 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 CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	286	Total	C	N	O	S	0	0
			2347	1508	407	423	9		
1	L	285	Total	C	N	O	S	0	0
			2333	1497	405	422	9		

- Molecule 2 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	45	Total	C	N	O	P	0	0
			928	442	179	262	45		

- Molecule 3 is a DNA chain called DNA (51-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	45	Total	C	N	O	P	0	0
			917	441	153	278	45		

- Molecule 4 is a RNA chain called RNA (55-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	28	Total	C	N	O	P	0	0
			586	262	90	206	28		

- Molecule 5 is a RNA chain called RNA (83-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	t	62	Total	C	N	O	P	0	0
			1322	592	237	431	62		

- Molecule 6 is a protein called Type II-A CRISPR-associated protein Csn2.

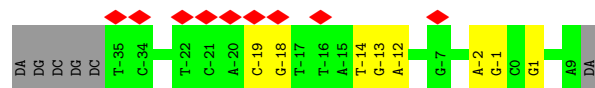
Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
6	B	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
6	C	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		
6	D	219	Total	C	N	O	S	0	0
			1790	1158	276	351	5		

- Molecule 7 is a protein called CRISPR-associated endonuclease Cas9.

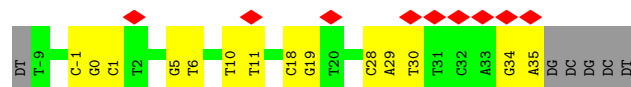
Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	1323	Total	C	N	O	S	0	0
			10832	6942	1849	2015	26		



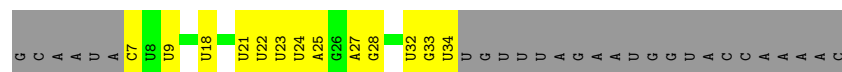
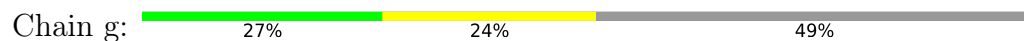
- Molecule 2: DNA (51-MER)



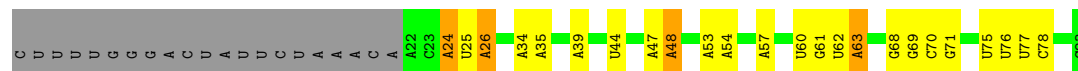
- Molecule 3: DNA (51-MER)



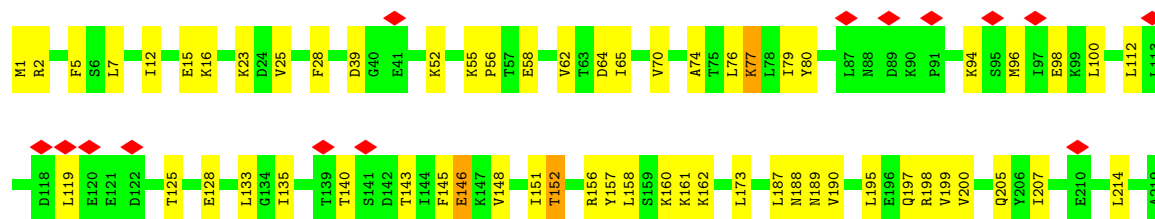
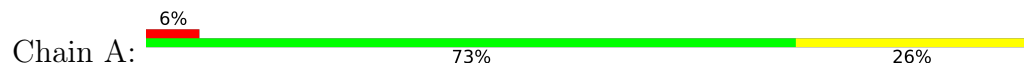
- Molecule 4: RNA (55-MER)



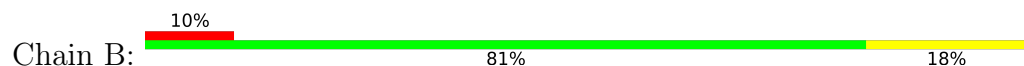
- Molecule 5: RNA (83-MER)

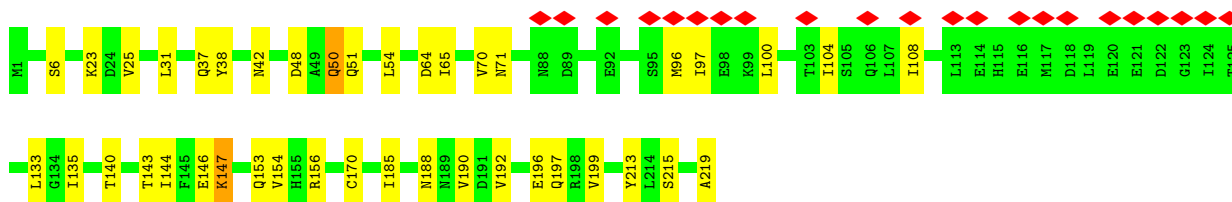


- Molecule 6: Type II-A CRISPR-associated protein Csn2

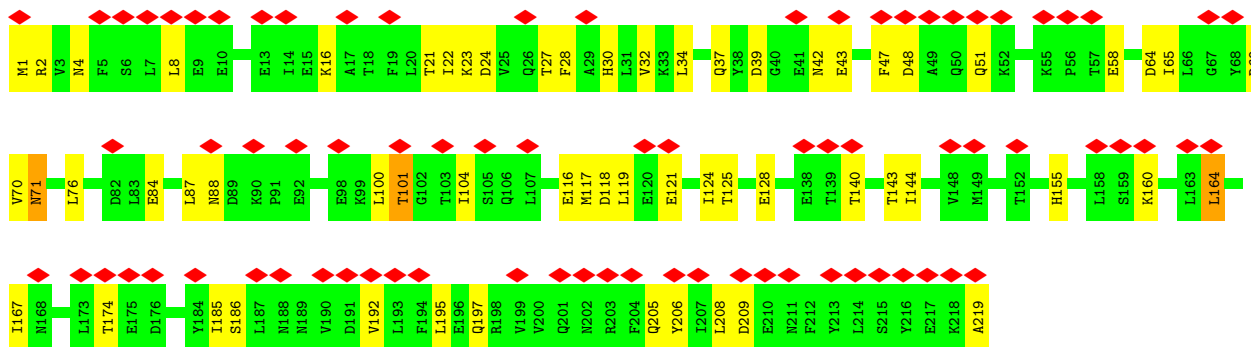
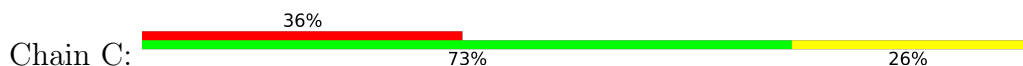


- Molecule 6: Type II-A CRISPR-associated protein Csn2

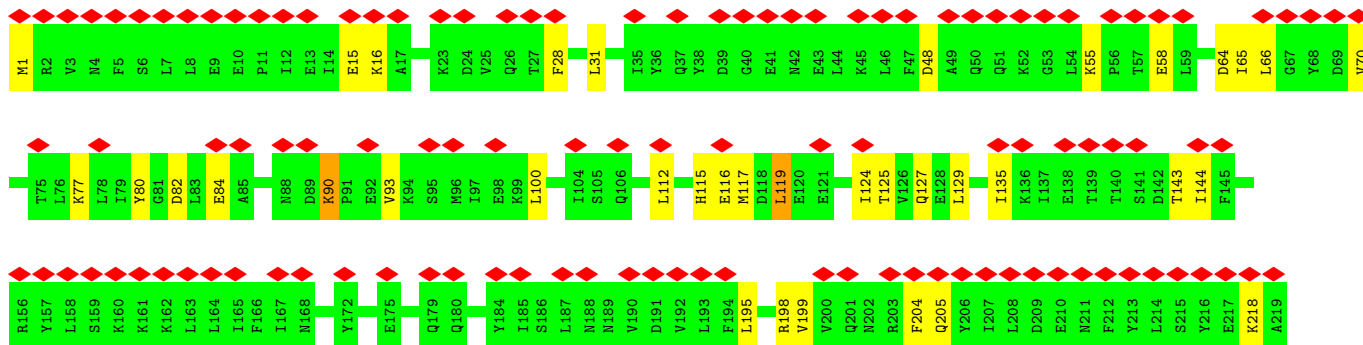
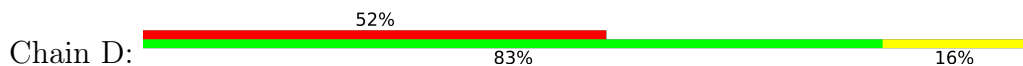




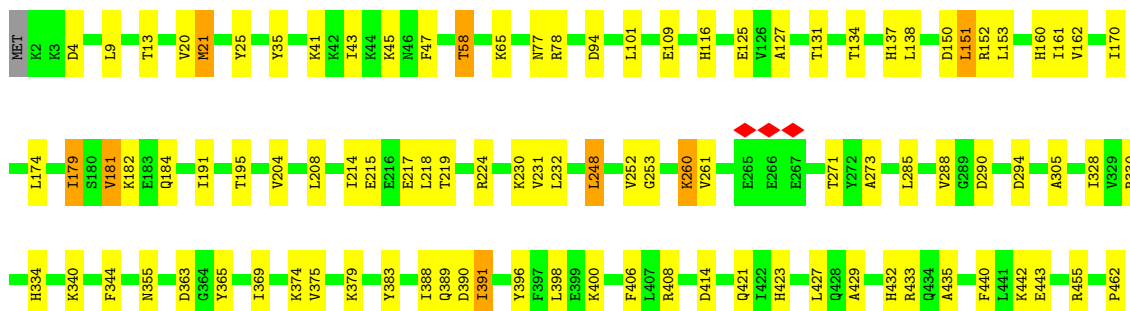
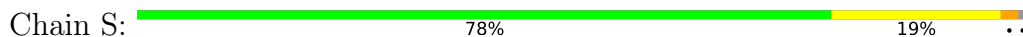
• Molecule 6: Type II-A CRISPR-associated protein Csn2

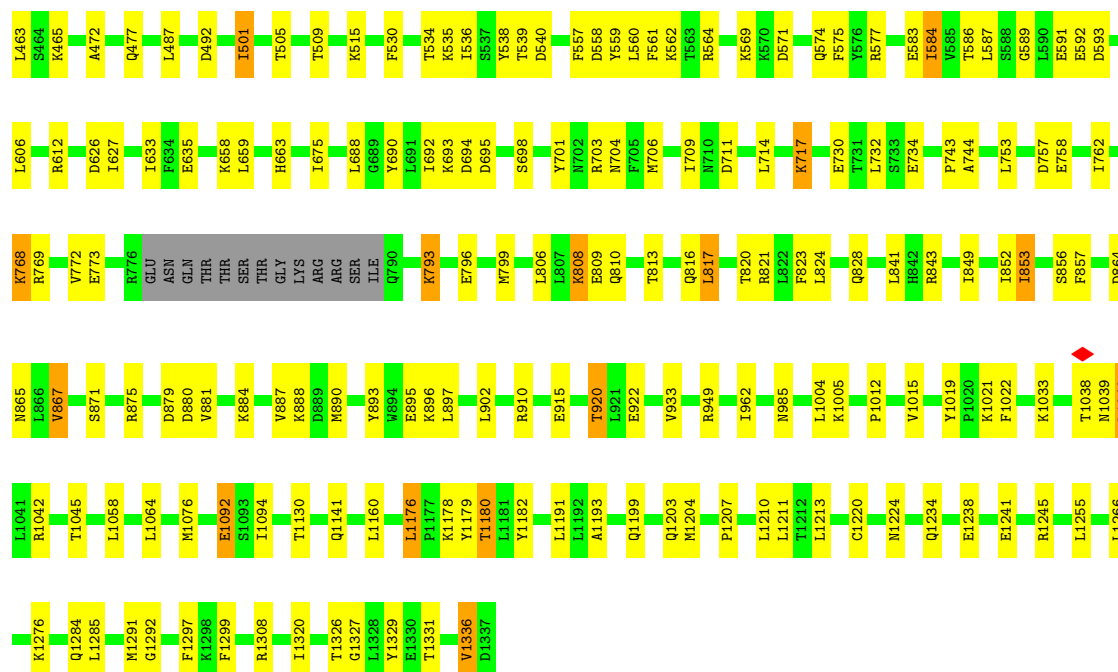


• Molecule 6: Type II-A CRISPR-associated protein Csn2



• Molecule 7: CRISPR-associated endonuclease Cas9





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80591	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.951	Depositor
Minimum map value	-0.393	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.06	Depositor
Map size (\AA)	357.888, 357.888, 357.888	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.932, 0.932, 0.932	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	K	0.21	0/2395	0.46	0/3232
1	L	0.21	0/2379	0.47	0/3209
2	N	0.22	0/1044	0.42	0/1609
3	T	0.19	0/1024	0.45	0/1578
4	g	0.21	0/651	0.30	0/1010
5	t	0.19	0/1479	0.25	0/2302
6	A	0.18	0/1817	0.35	0/2456
6	B	0.20	0/1817	0.32	0/2456
6	C	0.15	0/1817	0.35	0/2456
6	D	0.13	0/1817	0.33	0/2456
7	S	0.20	0/11049	0.34	0/14863
All	All	0.19	0/27289	0.37	0/37627

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	K	2347	0	2371	85	0
1	L	2333	0	2361	72	0
2	N	928	0	506	5	0
3	T	917	0	514	9	0
4	g	586	0	295	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	t	1322	0	666	14	0
6	A	1790	0	1811	36	0
6	B	1790	0	1811	25	0
6	C	1790	0	1811	36	0
6	D	1790	0	1811	20	0
7	S	10832	0	10924	150	0
All	All	26425	0	24881	429	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 8.

All (429) 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:L:273:VAL:HA	1:L:277:ASN:HB2	1.62	0.80
1:K:273:VAL:O	1:K:277:ASN:ND2	2.22	0.70
7:S:875:ARG:NH2	7:S:880:ASP:O	2.25	0.68
4:g:32:U:H3	5:t:24:A:H61	1.41	0.68
6:C:23:LYS:HD2	6:C:209:ASP:HA	1.76	0.68
1:K:16:TYR:OH	1:K:56:ARG:NH1	2.26	0.68
6:A:200:VAL:O	6:A:205:GLN:NE2	2.28	0.67
1:K:213:LEU:O	1:K:217:LEU:HB2	1.93	0.67
7:S:21:MET:HE2	7:S:25:TYR:HA	1.76	0.67
1:K:7:VAL:HG12	1:K:41:LEU:HB3	1.77	0.66
6:A:39:ASP:HA	6:A:56:PRO:HG3	1.78	0.66
1:K:64:VAL:H	1:K:76:LYS:HZ3	1.42	0.66
1:K:228:ILE:O	1:K:232:ASN:ND2	2.28	0.66
7:S:693:LYS:NZ	7:S:695:ASP:OD2	2.29	0.65
7:S:1203:GLN:NE2	7:S:1291:MET:SD	2.69	0.65
3:T:1:DC:H5'	7:S:1092:GLU:HG3	1.79	0.65
1:L:112:LYS:HD2	1:L:219:GLU:HB2	1.79	0.65
7:S:116:HIS:HB3	7:S:125:GLU:HG3	1.77	0.64
1:K:83:ARG:NH2	1:L:206:ASN:O	2.31	0.64
1:L:16:TYR:OH	1:L:56:ARG:NH1	2.30	0.64
7:S:864:ASP:O	7:S:910:ARG:NH1	2.31	0.64
1:K:165:THR:HG23	1:K:167:GLU:H	1.63	0.63
7:S:985:ASN:ND2	7:S:1204:MET:O	2.31	0.63
1:L:272:VAL:HG13	1:L:276:LEU:HB3	1.79	0.63
7:S:161:ILE:HG23	7:S:423:HIS:HB3	1.81	0.63
1:L:204:HIS:O	1:L:207:GLN:NE2	2.32	0.62
7:S:1199:GLN:HB3	7:S:1292:GLY:HA2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1:MET:SD	6:A:2:ARG:NH1	2.73	0.62
7:S:58:THR:HA	7:S:743:PRO:HG2	1.81	0.62
1:L:140:ARG:HD3	1:L:144:PRO:HD2	1.82	0.62
1:K:39:VAL:HG13	1:K:63:LEU:HB3	1.81	0.61
1:K:3:TRP:N	1:K:38:ASP:OD2	2.33	0.61
1:L:205:ALA:HB3	1:L:207:GLN:HE22	1.64	0.61
1:L:206:ASN:OD1	1:L:206:ASN:N	2.32	0.61
7:S:893:TYR:HD1	7:S:896:LYS:HE3	1.64	0.61
6:D:65:ILE:HG21	6:D:144:ILE:HG23	1.81	0.61
7:S:569:LYS:HG3	7:S:587:LEU:HD21	1.82	0.61
7:S:703:ARG:HH22	7:S:714:LEU:HD21	1.66	0.61
7:S:260:LYS:HE2	7:S:261:VAL:HG22	1.82	0.61
1:L:191:LEU:HD11	1:L:213:LEU:HD13	1.82	0.61
7:S:137:HIS:HA	7:S:328:ILE:HD11	1.82	0.61
6:B:143:THR:OG1	6:B:146:GLU:OE1	2.20	0.60
1:L:111:GLN:HG3	1:L:220:PRO:HB3	1.84	0.60
5:t:35:A:O2'	7:S:101:LEU:O	2.20	0.59
6:B:37:GLN:O	6:B:42:ASN:ND2	2.32	0.59
1:L:44:THR:OG1	1:L:45:THR:N	2.33	0.59
1:K:198:THR:O	1:K:198:THR:OG1	2.20	0.58
1:L:111:GLN:O	1:L:115:ASN:ND2	2.32	0.58
6:B:42:ASN:O	7:S:577:ARG:NH2	2.36	0.58
7:S:13:THR:HG23	7:S:744:ALA:HB1	1.85	0.58
6:C:197:GLN:HB3	6:D:198:ARG:HH12	1.66	0.58
1:L:9:ASN:ND2	1:L:43:GLU:O	2.36	0.58
6:C:185:ILE:HD13	6:C:192:VAL:HG21	1.85	0.58
1:K:125:TYR:HB3	1:K:128:LYS:HB2	1.85	0.58
6:B:199:VAL:HG11	6:B:219:ALA:HB3	1.85	0.58
6:C:2:ARG:NH1	6:C:48:ASP:O	2.37	0.58
7:S:231:VAL:HB	7:S:248:LEU:HD11	1.86	0.58
6:C:4:ASN:HA	6:C:8:LEU:HD21	1.86	0.58
7:S:150:ASP:OD1	7:S:150:ASP:N	2.32	0.58
7:S:808:LYS:HG2	7:S:810:GLN:H	1.68	0.58
7:S:35:TYR:HB2	7:S:1331:THR:HG22	1.85	0.57
3:T:-1:DC:H2''	3:T:0:DG:C8	2.39	0.57
1:K:190:GLU:HB3	1:K:269:THR:HG21	1.86	0.57
6:A:79:ILE:HG12	6:C:117:MET:HE1	1.87	0.57
6:C:32:VAL:HG22	6:C:167:ILE:HG21	1.87	0.57
7:S:260:LYS:HD3	7:S:260:LYS:H	1.69	0.57
1:L:67:CYS:HA	1:L:73:PRO:HA	1.87	0.57
6:B:48:ASP:OD2	6:B:50:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:171:ASP:OD1	1:K:233:ARG:NH2	2.38	0.57
6:A:94:LYS:NZ	6:A:98:GLU:OE2	2.38	0.57
1:L:92:ARG:NH1	1:L:276:LEU:O	2.37	0.57
1:L:111:GLN:OE1	1:L:268:TYR:OH	2.22	0.57
1:K:237:PHE:HA	1:K:240:MET:HE3	1.87	0.56
6:C:84:GLU:O	6:C:88:ASN:ND2	2.35	0.56
7:S:562:LYS:O	7:S:612:ARG:NH2	2.38	0.56
7:S:363:ASP:OD2	7:S:379:LYS:NZ	2.38	0.56
6:A:74:ALA:O	6:A:77:LYS:NZ	2.33	0.56
1:L:259:MET:HE2	1:L:263:ASN:HB3	1.88	0.56
7:S:78:ARG:NH1	7:S:162:VAL:O	2.39	0.56
6:A:156:ARG:HD3	6:A:188:ASN:HB3	1.88	0.56
6:A:158:LEU:HD13	6:A:160:LYS:HZ3	1.70	0.56
7:S:558:ASP:HA	7:S:562:LYS:HD3	1.87	0.56
1:L:172:ILE:HD11	1:L:233:ARG:HD2	1.86	0.55
7:S:530:PHE:O	7:S:534:THR:OG1	2.20	0.55
1:L:184:LEU:HD11	1:L:211:PHE:HB2	1.89	0.55
7:S:388:ILE:HG22	7:S:389:GLN:H	1.70	0.55
3:T:5:DG:H2''	3:T:6:DT:H5''	1.88	0.55
5:t:34:A:H2'	5:t:35:A:H8	1.72	0.55
6:B:23:LYS:O	6:B:197:GLN:NE2	2.40	0.55
6:C:39:ASP:OD1	6:C:39:ASP:N	2.39	0.55
7:S:45:LYS:NZ	7:S:1327:GLY:O	2.35	0.55
1:K:222:ARG:HG3	1:K:223:PRO:HD3	1.89	0.55
7:S:675:ILE:HG22	7:S:688:LEU:HB2	1.88	0.55
7:S:1193:ALA:HB2	7:S:1199:GLN:HG3	1.87	0.55
5:t:53:A:O2'	7:S:58:THR:O	2.24	0.55
6:C:16:LYS:HD2	6:C:186:SER:HA	1.88	0.55
7:S:1176:LEU:HG	7:S:1180:THR:HG21	1.88	0.55
1:K:139:LEU:H	1:K:140:ARG:HH21	1.54	0.54
5:t:47:A:H4'	7:S:465:LYS:HD2	1.89	0.54
7:S:224:ARG:NH1	7:S:252:VAL:O	2.39	0.54
7:S:501:ILE:HD13	7:S:633:ILE:HD12	1.89	0.54
1:K:53:LEU:O	1:K:57:LEU:HB2	2.08	0.54
1:L:136:ARG:HH12	1:L:139:LEU:HD23	1.73	0.54
1:L:112:LYS:NZ	1:L:116:GLN:OE1	2.29	0.54
6:D:80:TYR:HE1	6:D:135:ILE:HB	1.73	0.54
7:S:435:ALA:HB1	7:S:442:LYS:HB2	1.89	0.54
1:K:225:VAL:HG12	1:K:247:LEU:HD11	1.89	0.54
3:T:10:DT:H2''	3:T:11:DT:C5	2.43	0.54
4:g:21:U:O2'	7:S:1094:ILE:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:249:MET:N	1:K:249:MET:SD	2.81	0.53
6:A:143:THR:N	6:A:146:GLU:OE2	2.41	0.53
7:S:184:GLN:HE21	7:S:305:ALA:HB2	1.71	0.53
6:B:51:GLN:O	7:S:574:GLN:NE2	2.41	0.53
6:C:22:ILE:HG23	6:C:208:LEU:HD22	1.90	0.53
1:K:65:LEU:HD13	1:K:192:VAL:HG23	1.90	0.53
1:K:5:THR:HG23	1:K:39:VAL:HB	1.91	0.53
7:S:43:ILE:HD11	7:S:45:LYS:HE3	1.91	0.53
6:C:167:ILE:HG12	6:C:195:LEU:HD21	1.91	0.53
1:K:132:LEU:HD13	1:K:135:MET:HG2	1.90	0.53
6:A:28:PHE:HE1	6:A:195:LEU:HG	1.73	0.53
6:C:1:MET:HE2	6:C:2:ARG:HH11	1.73	0.53
7:S:564:ARG:NH1	7:S:571:ASP:OD2	2.41	0.53
7:S:806:LEU:HB3	7:S:809:GLU:HB2	1.91	0.53
1:K:123:ARG:H	1:K:123:ARG:HD2	1.74	0.53
2:N:-2:DA:H2'	2:N:-1:DG:H5'	1.91	0.53
7:S:260:LYS:HG2	7:S:261:VAL:HG13	1.90	0.52
7:S:1039:ASN:H	7:S:1042:ARG:HD3	1.74	0.52
1:K:163:ASP:O	1:K:168:GLN:NE2	2.42	0.52
7:S:271:THR:HG22	7:S:273:ALA:H	1.73	0.52
7:S:920:THR:OG1	7:S:922:GLU:OE1	2.26	0.52
1:L:69:ASP:OD1	1:L:69:ASP:N	2.43	0.52
1:K:96:TRP:HE1	1:K:277:ASN:CG	2.18	0.52
1:K:219:GLU:OE1	1:K:222:ARG:NH1	2.43	0.52
1:K:219:GLU:HA	1:K:222:ARG:HH11	1.74	0.52
1:K:185:SER:OG	1:K:189:ARG:NH2	2.36	0.51
7:S:477:GLN:HE21	7:S:492:ASP:HA	1.75	0.51
6:A:25:VAL:HG22	6:A:197:GLN:HE21	1.75	0.51
6:B:170:CYS:HB2	6:B:196:GLU:HG2	1.93	0.51
6:D:1:MET:HG2	6:D:48:ASP:HA	1.91	0.51
7:S:717:LYS:HE3	7:S:717:LYS:H	1.75	0.51
1:K:96:TRP:HB3	1:K:101:LYS:HE3	1.92	0.51
1:L:24:LYS:HZ1	6:B:6:SER:HB2	1.74	0.51
1:L:83:ARG:HD3	1:L:193:GLN:HG3	1.92	0.51
1:K:40:LEU:N	1:K:63:LEU:O	2.34	0.51
1:K:96:TRP:HE3	1:K:101:LYS:HE2	1.76	0.51
1:L:271:HIS:O	1:L:275:VAL:N	2.43	0.51
5:t:34:A:H2'	5:t:35:A:C8	2.45	0.51
6:A:15:GLU:HG3	6:A:16:LYS:HG2	1.92	0.51
1:K:41:LEU:HD21	1:K:189:ARG:HD2	1.92	0.51
5:t:48:A:O2'	7:S:77:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:1191:LEU:HD11	7:S:1291:MET:HE2	1.92	0.50
1:K:57:LEU:O	1:K:62:ILE:HG12	2.10	0.50
6:A:16:LYS:HE3	6:A:189:ASN:HA	1.92	0.50
6:C:30:HIS:NE2	6:C:43:GLU:OE2	2.38	0.50
7:S:856:SER:O	7:S:1039:ASN:N	2.44	0.50
1:K:217:LEU:HD21	1:K:272:VAL:HG11	1.93	0.50
1:K:105:TRP:HD1	1:K:108:ILE:HD11	1.77	0.50
7:S:1284:GLN:HB3	7:S:1297:PHE:HB2	1.92	0.50
3:T:18:DC:H2''	3:T:19:DG:N7	2.26	0.50
1:K:165:THR:HG22	1:K:168:GLN:HG3	1.92	0.50
7:S:1038:THR:HG23	7:S:1042:ARG:HE	1.77	0.50
1:L:233:ARG:HG3	1:L:234:LYS:HD3	1.94	0.49
5:t:70:C:H2'	5:t:71:G:H8	1.77	0.49
7:S:217:GLU:HA	7:S:230:LYS:HZ2	1.77	0.49
7:S:334:HIS:NE2	7:S:365:TYR:OH	2.35	0.49
7:S:440:PHE:HA	7:S:443:GLU:HG2	1.94	0.49
7:S:884:LYS:HE3	7:S:888:LYS:HE3	1.93	0.49
1:L:98:GLU:HA	1:L:101:LYS:HG2	1.95	0.49
1:L:250:ASN:HD22	1:L:251:THR:H	1.60	0.49
7:S:887:VAL:HG11	7:S:915:GLU:HA	1.94	0.49
7:S:897:LEU:HD22	7:S:902:LEU:HD12	1.94	0.49
6:D:66:LEU:H	6:D:66:LEU:HD23	1.77	0.49
6:A:100:LEU:HB2	6:C:104:ILE:HD11	1.94	0.49
1:K:21:LEU:HB3	1:K:32:ILE:HG12	1.95	0.49
1:K:9:ASN:HD22	1:K:10:LYS:HG3	1.77	0.49
3:T:29:DA:H1'	3:T:30:DT:H5'	1.93	0.49
1:K:89:GLN:O	1:K:89:GLN:NE2	2.45	0.49
7:S:539:THR:OG1	7:S:586:THR:O	2.29	0.49
6:C:117:MET:HE3	6:C:119:LEU:HD21	1.95	0.48
1:L:275:VAL:HA	1:L:280:GLU:HB3	1.94	0.48
6:C:64:ASP:HB2	6:D:64:ASP:HB2	1.95	0.48
1:K:191:LEU:O	1:K:194:THR:OG1	2.31	0.48
7:S:583:GLU:N	7:S:583:GLU:OE1	2.47	0.48
7:S:769:ARG:HD3	7:S:1004:LEU:HD12	1.95	0.48
1:K:23:PHE:HB3	1:K:30:GLU:HB2	1.94	0.48
1:K:212:ASN:OD1	1:K:212:ASN:N	2.45	0.48
1:L:119:HIS:CD2	1:L:227:GLN:HG2	2.48	0.48
1:K:87:SER:OG	1:L:210:ASP:OD1	2.32	0.48
1:L:86:SER:O	1:L:89:GLN:N	2.45	0.48
1:L:140:ARG:HD2	1:L:147:ARG:HG3	1.95	0.48
7:S:462:PRO:HG2	7:S:472:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:163:ASP:OD1	1:L:163:ASP:N	2.45	0.48
6:A:12:ILE:HD11	6:A:214:LEU:HD21	1.94	0.48
6:D:199:VAL:HG13	6:D:205:GLN:HE22	1.79	0.48
1:K:191:LEU:HD22	1:K:198:THR:HB	1.96	0.48
3:T:28:DC:H2''	3:T:29:DA:C8	2.49	0.48
6:B:133:LEU:HG	6:D:124:ILE:HD11	1.96	0.48
6:C:65:ILE:HG21	6:C:144:ILE:HG23	1.95	0.48
1:K:263:ASN:O	1:K:266:THR:OG1	2.27	0.48
7:S:703:ARG:NH1	7:S:711:ASP:OD2	2.47	0.47
7:S:1220:CYS:O	7:S:1276:LYS:NZ	2.46	0.47
6:D:15:GLU:HG3	6:D:16:LYS:HG2	1.96	0.47
7:S:429:ALA:O	7:S:433:ARG:HG2	2.13	0.47
6:A:156:ARG:HD3	6:A:188:ASN:HD22	1.80	0.47
7:S:540:ASP:HA	7:S:584:ILE:HA	1.95	0.47
1:K:109:ILE:O	1:K:113:ILE:HG12	2.14	0.47
7:S:94:ASP:OD2	7:S:152:ARG:NH1	2.47	0.47
1:K:105:TRP:CZ3	1:K:203:LYS:HB2	2.50	0.47
4:g:24:U:H2'	4:g:25:A:H8	1.79	0.47
1:K:13:LYS:HG3	6:B:213:TYR:CE1	2.49	0.47
1:L:68:ASP:HB3	1:L:74:ILE:HD13	1.96	0.47
4:g:18:U:O2'	7:S:414:ASP:O	2.32	0.47
6:B:213:TYR:CE2	6:B:215:SER:HB3	2.50	0.47
6:C:143:THR:OG1	6:C:144:ILE:N	2.48	0.47
7:S:821:ARG:HG2	7:S:849:ILE:HD11	1.97	0.47
1:L:166:ARG:H	1:L:173:ASN:ND2	2.13	0.47
6:B:50:GLN:H	6:B:50:GLN:HG3	1.58	0.47
6:C:34:LEU:HA	6:C:37:GLN:HG2	1.96	0.47
7:S:294:ASP:OD1	7:S:294:ASP:N	2.47	0.47
7:S:717:LYS:HE3	7:S:717:LYS:N	2.30	0.47
7:S:215:GLU:O	7:S:219:THR:OG1	2.33	0.46
7:S:828:GLN:O	7:S:893:TYR:OH	2.30	0.46
1:K:271:HIS:HA	1:K:274:LYS:HE2	1.96	0.46
7:S:9:LEU:HD12	7:S:772:VAL:HG12	1.95	0.46
1:L:272:VAL:O	1:L:277:ASN:N	2.43	0.46
6:C:1:MET:N	6:C:47:PHE:O	2.36	0.46
7:S:151:LEU:HD23	7:S:151:LEU:HA	1.80	0.46
1:K:122:GLN:HB3	1:K:123:ARG:CZ	2.46	0.46
6:C:118:ASP:OD1	6:C:118:ASP:N	2.48	0.46
6:D:115:HIS:CG	6:D:116:GLU:H	2.34	0.46
7:S:224:ARG:HH11	7:S:253:GLY:HA3	1.80	0.46
7:S:1213:LEU:HD22	7:S:1238:GLU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:105:TRP:O	1:K:108:ILE:HG13	2.15	0.46
1:L:86:SER:O	1:L:88:LEU:N	2.49	0.46
1:L:260:PHE:O	1:L:264:ILE:HG12	2.15	0.46
6:D:112:LEU:HD22	6:D:119:LEU:HD23	1.98	0.46
7:S:1130:THR:HG22	7:S:1141:GLN:HG2	1.99	0.45
1:L:9:ASN:HD21	1:L:71:ARG:HE	1.64	0.45
2:N:-14:DT:H2''	2:N:-13:DG:H5'	1.97	0.45
5:t:61:G:C6	5:t:63:A:H8	2.35	0.45
6:B:38:TYR:OH	6:B:54:LEU:O	2.29	0.45
6:B:70:VAL:HG13	6:B:154:VAL:HG21	1.99	0.45
6:D:90:LYS:HD3	6:D:93:VAL:HG11	1.98	0.45
7:S:627:ILE:HG21	7:S:659:LEU:HD13	1.99	0.45
1:K:119:HIS:ND1	1:K:155:TYR:OH	2.41	0.45
1:K:218:MET:HE2	1:K:218:MET:HB3	1.86	0.45
1:L:186:ILE:HD12	1:L:248:PHE:HE1	1.82	0.45
6:C:69:ASP:O	6:C:71:ASN:N	2.49	0.45
7:S:793:LYS:H	7:S:793:LYS:HD2	1.81	0.45
1:K:59:ASP:OD1	1:K:59:ASP:N	2.42	0.45
1:K:186:ILE:HD11	1:K:262:THR:HA	1.97	0.45
1:L:117:SER:HB3	1:L:136:ARG:HD3	1.98	0.45
1:L:123:ARG:O	1:L:123:ARG:NE	2.43	0.45
7:S:635:GLU:HG2	7:S:663:HIS:CE1	2.51	0.45
7:S:559:TYR:HD2	7:S:575:PHE:HE1	1.63	0.45
1:K:40:LEU:HD23	1:K:64:VAL:HG23	1.99	0.45
1:L:22:VAL:HG12	1:L:31:LEU:HG	1.97	0.45
7:S:1005:LYS:HB3	7:S:1058:LEU:HD22	1.99	0.45
1:L:120:LEU:HD21	1:L:159:LEU:HD22	1.99	0.45
6:C:205:GLN:HE21	6:C:219:ALA:HB3	1.81	0.45
7:S:591:GLU:HG2	7:S:592:GLU:HG2	1.99	0.45
1:K:214:ALA:O	1:K:218:MET:N	2.49	0.45
1:K:239:ILE:HD11	1:K:243:LYS:HE3	1.98	0.45
7:S:569:LYS:HD3	7:S:593:ASP:HA	1.98	0.45
7:S:1182:TYR:HB3	7:S:1320:ILE:HD13	1.98	0.45
7:S:817:LEU:HD12	7:S:823:PHE:HD1	1.82	0.44
5:t:53:A:H2'	5:t:54:A:C8	2.52	0.44
7:S:692:ILE:HG22	7:S:693:LYS:HG3	1.99	0.44
7:S:890:MET:HE1	7:S:893:TYR:HB3	1.99	0.44
3:T:18:DC:H2''	3:T:19:DG:C8	2.52	0.44
6:B:185:ILE:HG23	6:B:190:VAL:HG23	1.99	0.44
7:S:174:LEU:HD22	7:S:421:GLN:HB2	1.99	0.44
1:L:272:VAL:HG12	1:L:277:ASN:ND2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:1039:ASN:OD1	7:S:1040:LEU:N	2.50	0.44
1:K:156:PHE:HA	1:K:160:PHE:CD2	2.52	0.44
1:K:191:LEU:HD11	1:K:213:LEU:HD22	2.00	0.44
6:D:80:TYR:CE1	6:D:135:ILE:HB	2.53	0.44
6:D:84:GLU:OE1	6:D:127:GLN:NE2	2.48	0.44
6:A:156:ARG:HA	6:A:190:VAL:HG11	1.99	0.44
5:t:53:A:H2'	5:t:54:A:H8	1.82	0.44
6:B:156:ARG:NH1	6:B:188:ASN:O	2.50	0.44
7:S:557:PHE:HA	7:S:561:PHE:HD1	1.83	0.44
1:K:159:LEU:HD13	1:K:159:LEU:HA	1.88	0.44
7:S:4:ASP:HB3	7:S:768:LYS:HD2	2.00	0.44
1:K:218:MET:HE3	1:K:222:ARG:HH22	1.83	0.44
1:L:63:LEU:HB2	1:L:189:ARG:HD3	2.00	0.44
3:T:34:DG:H2''	3:T:35:DA:H5'	2.00	0.43
6:B:65:ILE:HG21	6:B:144:ILE:HG23	2.00	0.43
6:C:125:THR:HG23	6:C:128:GLU:H	1.84	0.43
7:S:730:GLU:HB3	7:S:734:GLU:HG3	2.00	0.43
7:S:853:ILE:HG23	7:S:865:ASN:HD21	1.83	0.43
1:K:120:LEU:HD23	1:K:120:LEU:HA	1.87	0.43
1:L:205:ALA:HB3	1:L:207:GLN:NE2	2.33	0.43
6:C:58:GLU:HB3	6:C:160:LYS:O	2.18	0.43
7:S:285:LEU:HD12	7:S:290:ASP:HA	1.99	0.43
7:S:340:LYS:NZ	7:S:396:TYR:OH	2.41	0.43
7:S:757:ASP:OD2	7:S:949:ARG:NH2	2.51	0.43
6:D:204:PHE:HA	6:D:218:LYS:HA	2.01	0.43
7:S:758:GLU:OE2	7:S:1326:THR:OG1	2.33	0.43
1:L:100:ARG:O	1:L:103:GLN:HG2	2.18	0.43
5:t:34:A:H5''	7:S:160:HIS:CD2	2.54	0.43
7:S:355:ASN:OD1	7:S:383:TYR:OH	2.37	0.43
7:S:390:ASP:O	7:S:391:ILE:HG12	2.19	0.43
7:S:1038:THR:HG23	7:S:1042:ARG:HB3	2.00	0.43
1:K:262:THR:O	1:K:266:THR:HG23	2.18	0.43
1:L:25:ALA:HB3	1:L:28:HIS:HB3	2.01	0.43
7:S:762:ILE:HG12	7:S:1329:TYR:CZ	2.53	0.43
7:S:1004:LEU:HD23	7:S:1004:LEU:HA	1.89	0.43
1:L:203:LYS:HE2	1:L:204:HIS:CE1	2.53	0.43
6:D:28:PHE:HE1	6:D:195:LEU:HG	1.82	0.43
7:S:344:PHE:CZ	7:S:391:ILE:HG21	2.53	0.43
1:L:120:LEU:HD12	1:L:132:LEU:HD11	1.99	0.43
6:D:55:LYS:HG3	6:D:58:GLU:HG2	2.01	0.43
7:S:400:LYS:HB3	7:S:406:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:-19:DC:H2"	2:N:-18:DG:N7	2.34	0.43
6:C:21:THR:OG1	6:C:206:TYR:O	2.35	0.43
1:K:191:LEU:HD21	1:K:213:LEU:HD13	2.01	0.42
1:K:42:LEU:HD12	1:K:66:PHE:CD1	2.54	0.42
7:S:138:LEU:HD11	7:S:153:LEU:HB3	2.00	0.42
7:S:1207:PRO:HD2	7:S:1210:LEU:HD12	2.01	0.42
1:L:98:GLU:HA	1:L:101:LYS:HE2	2.00	0.42
6:B:153:GLN:O	6:D:117:MET:HE1	2.19	0.42
7:S:709:ILE:C	7:S:717:LYS:HE2	2.43	0.42
7:S:962:ILE:HG12	7:S:1015:VAL:HG22	2.00	0.42
1:L:42:LEU:HD22	1:L:47:ILE:HD12	2.00	0.42
1:L:60:GLU:HB3	1:L:62:ILE:HG12	2.00	0.42
7:S:1241:GLU:O	7:S:1245:ARG:HG2	2.19	0.42
1:L:89:GLN:HG2	1:L:194:THR:O	2.19	0.42
2:N:1:DG:N7	7:S:1308:ARG:NH1	2.62	0.42
6:C:76:LEU:HD23	6:C:76:LEU:HA	1.92	0.42
7:S:134:THR:OG1	7:S:137:HIS:ND1	2.43	0.42
7:S:161:ILE:HG21	7:S:427:LEU:HB2	2.02	0.42
7:S:330:ARG:HD3	7:S:408:ARG:HG3	2.00	0.42
1:K:219:GLU:HA	1:K:222:ARG:NH1	2.34	0.42
7:S:20:VAL:HB	7:S:47:PHE:HB3	2.01	0.42
7:S:824:LEU:HD12	7:S:824:LEU:HA	1.84	0.42
1:K:69:ASP:C	1:K:71:ARG:H	2.27	0.42
1:L:64:VAL:HG13	1:L:77:ILE:HB	2.02	0.42
6:A:23:LYS:HE2	6:A:207:ILE:HG23	2.02	0.42
6:A:62:VAL:HG12	6:A:65:ILE:HD13	2.01	0.42
6:A:145:PHE:HA	6:A:173:LEU:HD21	2.00	0.42
6:C:28:PHE:O	6:C:32:VAL:HG23	2.19	0.42
1:K:75:GLY:HA2	1:L:80:PHE:H	1.84	0.42
6:A:96:MET:HE3	6:A:100:LEU:HD11	2.02	0.42
6:A:148:VAL:O	6:A:152:THR:OG1	2.38	0.42
6:B:108:ILE:HD13	6:B:108:ILE:HA	1.86	0.42
7:S:768:LYS:HE2	7:S:768:LYS:HB2	1.89	0.42
6:A:100:LEU:HD22	6:C:100:LEU:HD22	2.01	0.42
7:S:191:ILE:O	7:S:195:THR:OG1	2.31	0.42
1:K:93:GLN:HE22	1:K:197:PHE:H	1.68	0.41
1:K:115:ASN:HB3	1:K:223:PRO:HG2	2.02	0.41
1:K:89:GLN:HE21	1:K:93:GLN:HB3	1.84	0.41
1:L:56:ARG:HH22	7:S:698:SER:HB3	1.85	0.41
1:L:89:GLN:NE2	1:L:196:CYS:SG	2.93	0.41
6:A:12:ILE:HD13	6:A:12:ILE:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:104:ILE:HG21	6:D:129:LEU:HD11	2.01	0.41
7:S:536:ILE:HD13	7:S:589:GLY:HA3	2.02	0.41
7:S:1042:ARG:O	7:S:1045:THR:OG1	2.36	0.41
6:A:112:LEU:HG	6:A:119:LEU:HD12	2.02	0.41
6:C:155:HIS:ND1	6:C:164:LEU:HB2	2.35	0.41
7:S:793:LYS:HE3	7:S:793:LYS:HB3	1.94	0.41
6:A:133:LEU:HD22	6:C:121:GLU:HB2	2.01	0.41
1:K:100:ARG:HD2	1:K:103:GLN:NE2	2.36	0.41
1:K:107:ALA:O	1:K:111:GLN:HG2	2.20	0.41
1:K:112:LYS:HE2	1:K:219:GLU:HB3	2.01	0.41
1:K:275:VAL:HG12	1:K:280:GLU:HB2	2.03	0.41
5:t:25:U:H2'	5:t:26:A:C8	2.55	0.41
6:A:52:LYS:HE3	6:A:52:LYS:HB2	1.92	0.41
6:D:115:HIS:CG	6:D:116:GLU:N	2.89	0.41
7:S:248:LEU:HD23	7:S:248:LEU:HA	1.94	0.41
7:S:658:LYS:HE3	7:S:658:LYS:HB3	1.90	0.41
7:S:808:LYS:H	7:S:808:LYS:HD3	1.85	0.41
7:S:1012:PRO:HB3	7:S:1019:TYR:CG	2.56	0.41
7:S:538:TYR:HA	7:S:587:LEU:HA	2.01	0.41
7:S:793:LYS:HA	7:S:796:GLU:HG2	2.03	0.41
7:S:820:THR:HG22	7:S:1224:ASN:HD22	1.85	0.41
7:S:852:ILE:HD11	7:S:867:VAL:HG13	2.01	0.41
1:K:8:VAL:O	1:K:43:GLU:HB2	2.19	0.41
1:L:104:VAL:HG21	1:L:276:LEU:HG	2.03	0.41
2:N:-13:DG:H2''	2:N:-12:DA:C8	2.55	0.41
6:A:62:VAL:HG11	6:A:151:ILE:HD13	2.03	0.41
6:A:156:ARG:NH2	6:C:116:GLU:OE2	2.53	0.41
6:B:147:LYS:HA	6:B:147:LYS:HD3	1.93	0.41
6:C:101:THR:HG23	6:C:124:ILE:HB	2.02	0.41
7:S:505:THR:HB	7:S:515:LYS:HD2	2.03	0.41
5:t:60:U:H2'	5:t:61:G:O4'	2.20	0.41
6:C:2:ARG:NH2	6:C:51:GLN:HG2	2.36	0.41
1:K:10:LYS:NZ	1:K:27:ASP:H	2.19	0.41
1:K:132:LEU:O	1:K:135:MET:HG3	2.20	0.41
1:L:179:GLY:N	1:L:244:LEU:HD21	2.36	0.41
6:A:80:TYR:CE1	6:A:135:ILE:HB	2.56	0.41
6:A:80:TYR:HE1	6:A:135:ILE:HB	1.85	0.41
6:A:146:GLU:H	6:A:146:GLU:HG3	1.58	0.41
6:C:24:ASP:O	6:C:27:THR:N	2.49	0.41
7:S:232:LEU:HG	7:S:248:LEU:HD12	2.01	0.41
7:S:535:LYS:HG3	7:S:704:ASN:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:238:PRO:HA	1:L:241:LYS:HE2	2.02	0.41
4:g:21:U:H2'	4:g:22:U:C6	2.56	0.41
7:S:41:LYS:HD3	7:S:41:LYS:HA	1.90	0.41
7:S:182:LYS:HB3	7:S:182:LYS:HE3	1.88	0.41
1:K:162:ASN:OD1	1:K:162:ASN:N	2.55	0.40
1:K:267:ASP:HA	1:K:270:LYS:HG2	2.03	0.40
1:L:87:SER:OG	1:L:88:LEU:N	2.51	0.40
1:L:219:GLU:H	1:L:219:GLU:CD	2.29	0.40
4:g:24:U:H2'	4:g:25:A:C8	2.56	0.40
6:A:64:ASP:OD1	6:B:64:ASP:N	2.54	0.40
7:S:374:LYS:HG3	7:S:375:VAL:HG23	2.03	0.40
7:S:816:GLN:OE1	7:S:816:GLN:N	2.49	0.40
1:K:172:ILE:HG12	1:K:233:ARG:NH2	2.36	0.40
1:L:18:ASN:O	1:L:20:HIS:ND1	2.43	0.40
1:L:91:THR:O	1:L:95:ALA:N	2.54	0.40
7:S:181:VAL:HG22	7:S:182:LYS:HB2	2.04	0.40
7:S:1178:LYS:HE3	7:S:1179:TYR:CZ	2.56	0.40
1:K:132:LEU:HD12	1:K:135:MET:HE2	2.02	0.40
4:g:7:C:H1'	7:S:706:MET:HE2	2.04	0.40
6:A:64:ASP:OD1	6:A:64:ASP:N	2.53	0.40
6:B:96:MET:O	6:B:100:LEU:HG	2.22	0.40
7:S:732:LEU:HD11	7:S:753:LEU:HD13	2.02	0.40
1:L:118:LEU:HA	1:L:121:ALA:HB3	2.03	0.40
1:L:219:GLU:N	1:L:220:PRO:HD2	2.37	0.40
7:S:170:ILE:HG21	7:S:179:ILE:HG13	2.04	0.40
7:S:1021:LYS:HG3	7:S:1022:PHE:H	1.85	0.40
1:K:105:TRP:CD1	1:K:108:ILE:HD11	2.56	0.40
1:L:24:LYS:NZ	6:B:6:SER:HB2	2.35	0.40
1:L:232:ASN:HD22	1:L:235:GLU:HG3	1.85	0.40
4:g:23:U:H2'	4:g:24:U:C6	2.56	0.40
6:A:55:LYS:H	6:A:55:LYS:HG2	1.65	0.40
6:A:160:LYS:HE2	6:A:161:LYS:HG3	2.03	0.40
7:S:127:ALA:O	7:S:131:THR:HG22	2.22	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	K	284/288 (99%)	255 (90%)	29 (10%)	0	100	100
1	L	283/288 (98%)	260 (92%)	21 (7%)	2 (1%)	18	51
6	A	217/219 (99%)	206 (95%)	10 (5%)	1 (0%)	24	59
6	B	217/219 (99%)	205 (94%)	12 (6%)	0	100	100
6	C	217/219 (99%)	199 (92%)	17 (8%)	1 (0%)	24	59
6	D	217/219 (99%)	203 (94%)	14 (6%)	0	100	100
7	S	1319/1337 (99%)	1222 (93%)	94 (7%)	3 (0%)	43	75
All	All	2754/2789 (99%)	2550 (93%)	197 (7%)	7 (0%)	37	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	87	SER
7	S	1336	VAL
6	A	140	THR
6	C	70	VAL
7	S	58	THR
1	L	209	ASN
7	S	204	VAL

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	K	254/255 (100%)	221 (87%)	33 (13%)	4	18
1	L	253/255 (99%)	214 (85%)	39 (15%)	2	13
6	A	202/202 (100%)	187 (93%)	15 (7%)	13	40
6	B	202/202 (100%)	193 (96%)	9 (4%)	24	57
6	C	202/202 (100%)	195 (96%)	7 (4%)	32	64
6	D	202/202 (100%)	193 (96%)	9 (4%)	24	57
7	S	1174/1192 (98%)	1112 (95%)	62 (5%)	20	52
All	All	2489/2510 (99%)	2315 (93%)	174 (7%)	16	42

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	6	VAL
1	K	9	ASN
1	K	22	VAL
1	K	31	LEU
1	K	32	ILE
1	K	34	LEU
1	K	44	THR
1	K	49	LEU
1	K	62	ILE
1	K	78	LEU
1	K	88	LEU
1	K	93	GLN
1	K	123	ARG
1	K	139	LEU
1	K	142	PHE
1	K	148	GLU
1	K	159	LEU
1	K	160	PHE
1	K	172	ILE
1	K	176	LEU
1	K	190	GLU
1	K	191	LEU
1	K	198	THR
1	K	211	PHE
1	K	212	ASN
1	K	213	LEU
1	K	217	LEU
1	K	229	ILE
1	K	233	ARG

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Mol	Chain	Res	Type
1	K	253	MET
1	K	257	LYS
1	K	267	ASP
1	K	276	LEU
1	L	6	VAL
1	L	7	VAL
1	L	15	SER
1	L	32	ILE
1	L	39	VAL
1	L	40	LEU
1	L	41	LEU
1	L	44	THR
1	L	47	ILE
1	L	49	LEU
1	L	64	VAL
1	L	72	LEU
1	L	76	LYS
1	L	77	ILE
1	L	80	PHE
1	L	90	LEU
1	L	109	ILE
1	L	123	ARG
1	L	125	TYR
1	L	159	LEU
1	L	166	ARG
1	L	182	LEU
1	L	191	LEU
1	L	202	LEU
1	L	206	ASN
1	L	210	ASP
1	L	211	PHE
1	L	213	LEU
1	L	225	VAL
1	L	230	TYR
1	L	239	ILE
1	L	242	ARG
1	L	244	LEU
1	L	250	ASN
1	L	256	LYS
1	L	258	GLN
1	L	261	LEU
1	L	276	LEU

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Mol	Chain	Res	Type
1	L	283	VAL
6	A	5	PHE
6	A	7	LEU
6	A	58	GLU
6	A	70	VAL
6	A	76	LEU
6	A	77	LYS
6	A	125	THR
6	A	128	GLU
6	A	146	GLU
6	A	152	THR
6	A	157	TYR
6	A	162	LYS
6	A	187	LEU
6	A	198	ARG
6	A	199	VAL
6	B	25	VAL
6	B	31	LEU
6	B	50	GLN
6	B	71	ASN
6	B	97	ILE
6	B	135	ILE
6	B	140	THR
6	B	147	LYS
6	B	192	VAL
6	C	42	ASN
6	C	71	ASN
6	C	87	LEU
6	C	101	THR
6	C	140	THR
6	C	164	LEU
6	C	174	THR
6	D	31	LEU
6	D	70	VAL
6	D	77	LYS
6	D	82	ASP
6	D	90	LYS
6	D	100	LEU
6	D	119	LEU
6	D	125	THR
6	D	143	THR
7	S	21	MET

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Mol	Chain	Res	Type
7	S	65	LYS
7	S	109	GLU
7	S	151	LEU
7	S	179	ILE
7	S	181	VAL
7	S	208	LEU
7	S	214	ILE
7	S	218	LEU
7	S	248	LEU
7	S	260	LYS
7	S	288	VAL
7	S	369	ILE
7	S	391	ILE
7	S	398	LEU
7	S	432	HIS
7	S	455	ARG
7	S	463	LEU
7	S	487	LEU
7	S	501	ILE
7	S	509	THR
7	S	560	LEU
7	S	584	ILE
7	S	606	LEU
7	S	626	ASP
7	S	690	TYR
7	S	694	ASP
7	S	701	TYR
7	S	717	LYS
7	S	768	LYS
7	S	773	GLU
7	S	793	LYS
7	S	799	MET
7	S	808	LYS
7	S	813	THR
7	S	817	LEU
7	S	841	LEU
7	S	843	ARG
7	S	853	ILE
7	S	857	PHE
7	S	867	VAL
7	S	871	SER
7	S	879	ASP

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Mol	Chain	Res	Type
7	S	881	VAL
7	S	895	GLU
7	S	920	THR
7	S	933	VAL
7	S	1033	LYS
7	S	1040	LEU
7	S	1064	LEU
7	S	1076	MET
7	S	1092	GLU
7	S	1160	LEU
7	S	1176	LEU
7	S	1180	THR
7	S	1211	LEU
7	S	1234	GLN
7	S	1255	LEU
7	S	1266	LEU
7	S	1285	LEU
7	S	1299	PHE
7	S	1336	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	9	ASN
1	K	89	GLN
1	K	93	GLN
1	K	103	GLN
1	K	115	ASN
1	K	116	GLN
1	K	271	HIS
1	L	89	GLN
1	L	168	GLN
1	L	207	GLN
1	L	232	ASN
1	L	250	ASN
1	L	258	GLN
1	L	277	ASN
1	L	278	GLN
6	A	127	GLN
6	A	155	HIS
6	A	202	ASN
6	B	86	GLN

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Mol	Chain	Res	Type
6	C	86	GLN
6	C	153	GLN
6	C	168	ASN
6	C	197	GLN
6	C	202	ASN
6	D	106	GLN
7	S	37	ASN
7	S	77	ASN
7	S	116	HIS
7	S	178	ASN
7	S	184	GLN
7	S	186	GLN
7	S	187	GLN
7	S	194	GLN
7	S	198	ASN
7	S	377	GLN
7	S	403	GLN
7	S	477	GLN
7	S	596	ASN
7	S	638	GLN
7	S	721	GLN
7	S	851	HIS
7	S	905	GLN
7	S	926	HIS
7	S	929	GLN
7	S	960	GLN
7	S	1202	ASN
7	S	1262	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	g	27/55 (49%)	5 (18%)	0
5	t	61/83 (73%)	14 (22%)	0
All	All	88/138 (63%)	19 (21%)	0

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	g	9	U
4	g	27	A

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Mol	Chain	Res	Type
4	g	28	G
4	g	33	G
4	g	34	U
5	t	24	A
5	t	26	A
5	t	39	A
5	t	44	U
5	t	48	A
5	t	57	A
5	t	62	U
5	t	63	A
5	t	68	G
5	t	69	G
5	t	75	U
5	t	76	U
5	t	77	U
5	t	78	C

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.

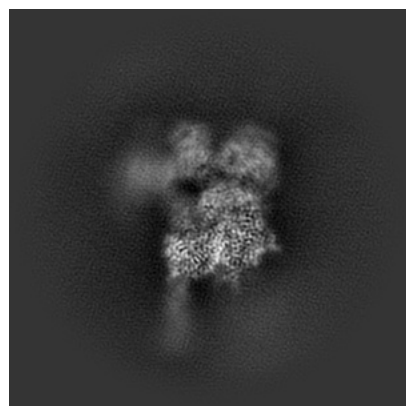
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65108. These allow visual inspection of the internal detail of the map and identification of artifacts.

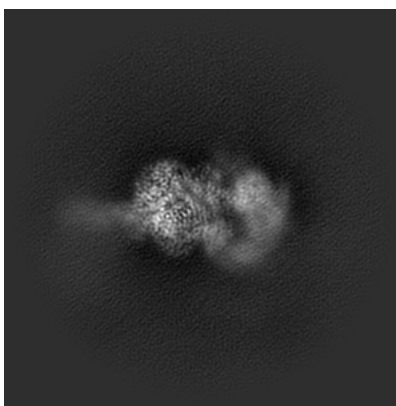
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

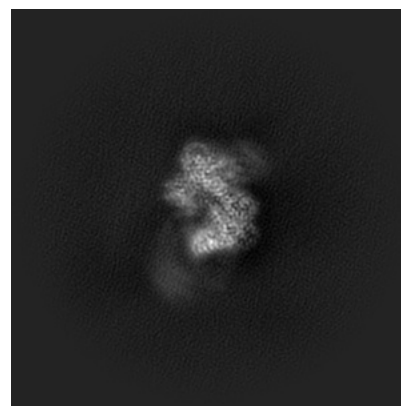
6.1.1 Primary map



X

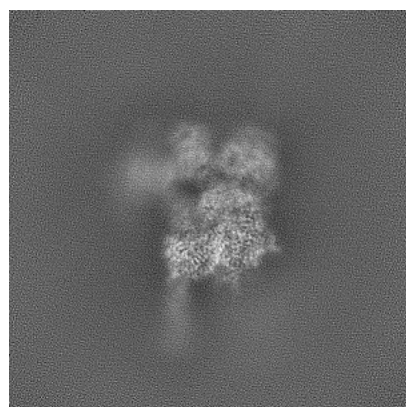


Y

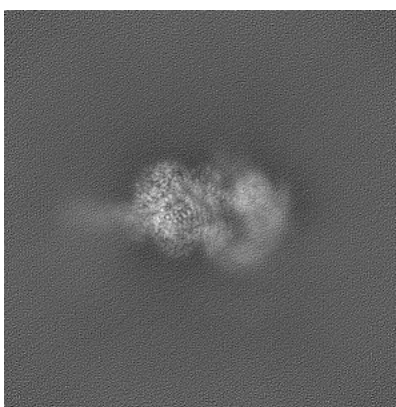


Z

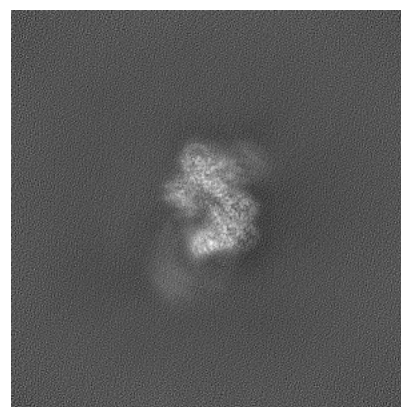
6.1.2 Raw map



X



Y

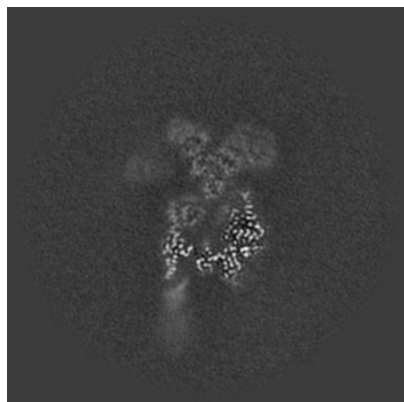


Z

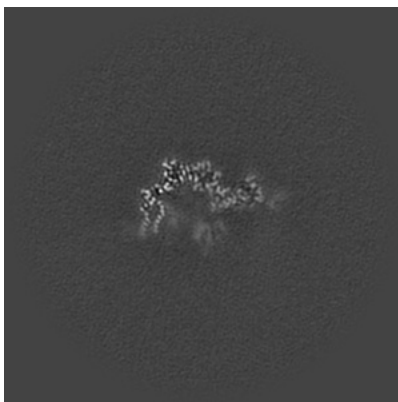
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

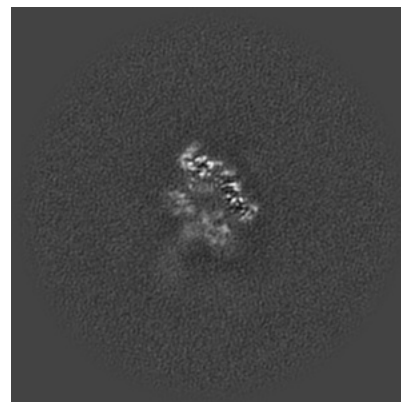
6.2.1 Primary map



X Index: 192

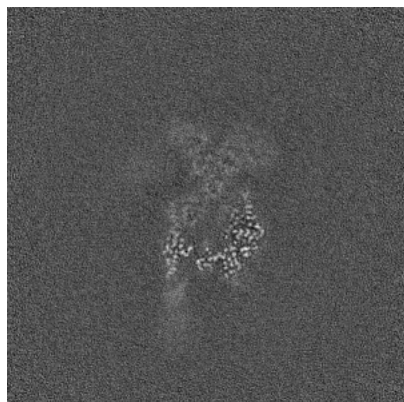


Y Index: 192

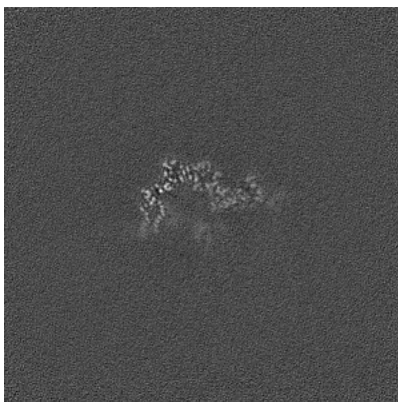


Z Index: 192

6.2.2 Raw map



X Index: 192



Y Index: 192

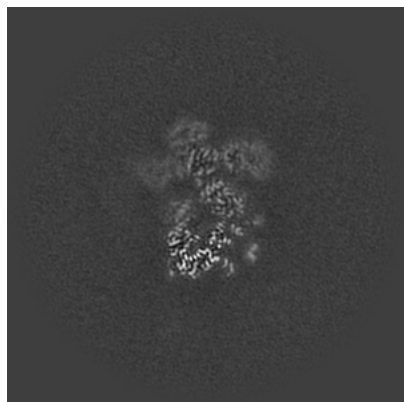


Z Index: 192

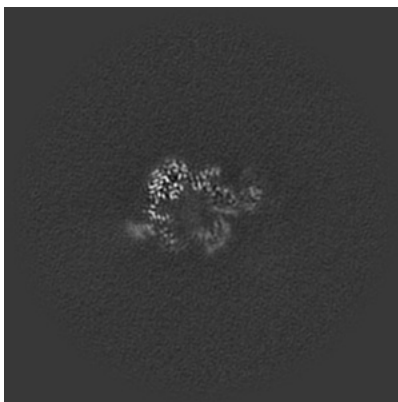
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

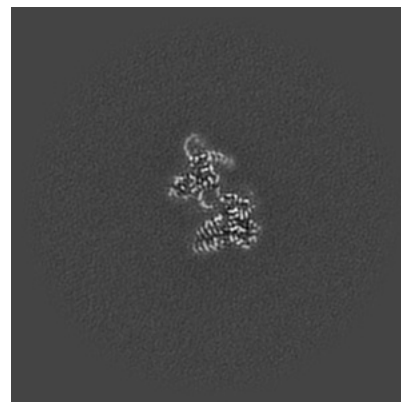
6.3.1 Primary map



X Index: 206

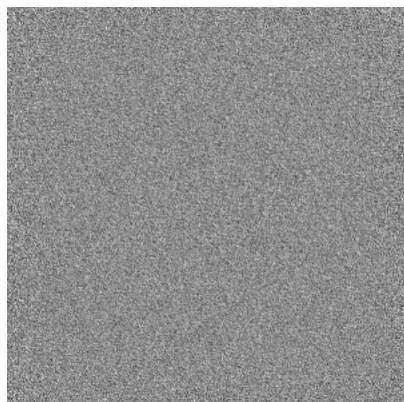


Y Index: 199

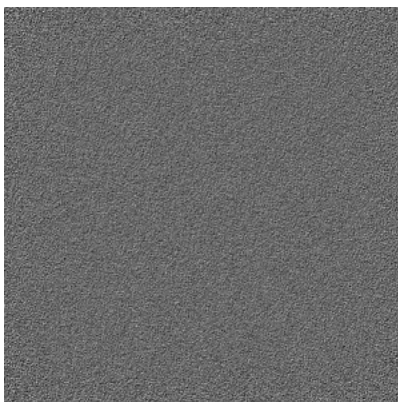


Z Index: 152

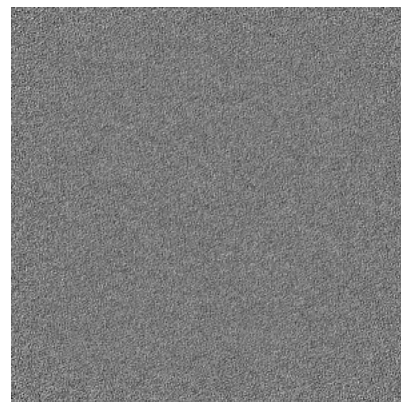
6.3.2 Raw map



X Index: 0



Y Index: 0

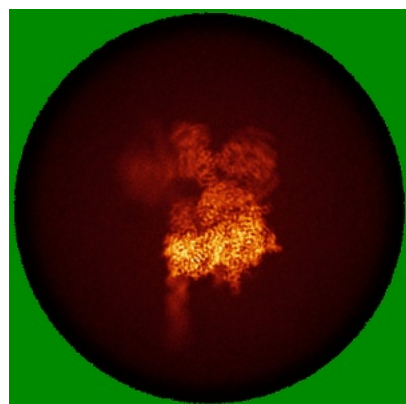


Z Index: 0

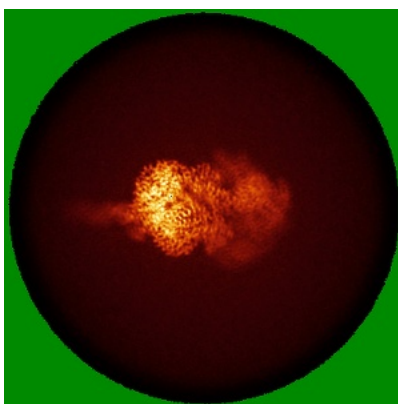
The images above show the largest variance slices of the map in three orthogonal directions.

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

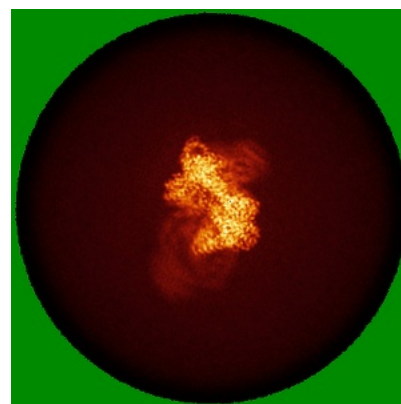
6.4.1 Primary map



X

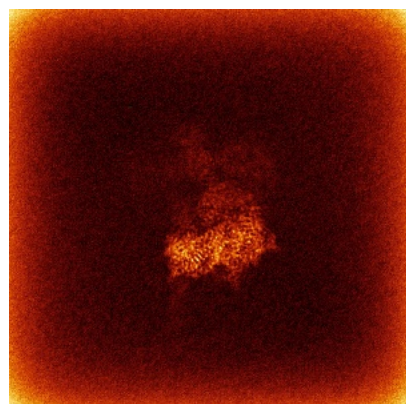


Y

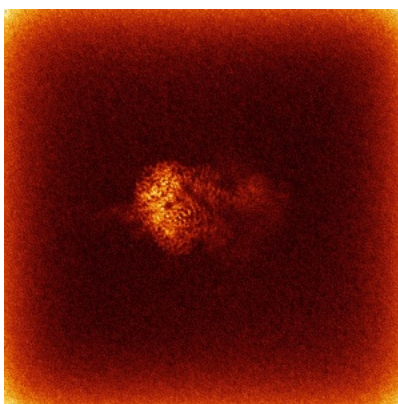


Z

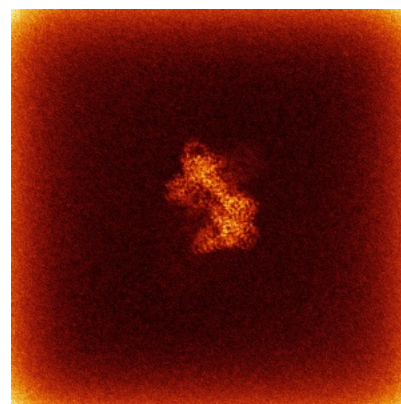
6.4.2 Raw map



X



Y

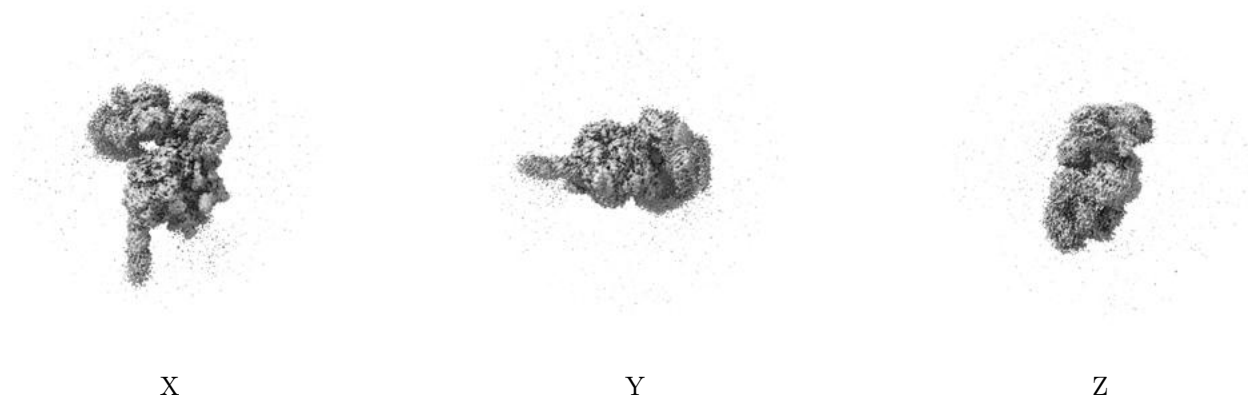


Z

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

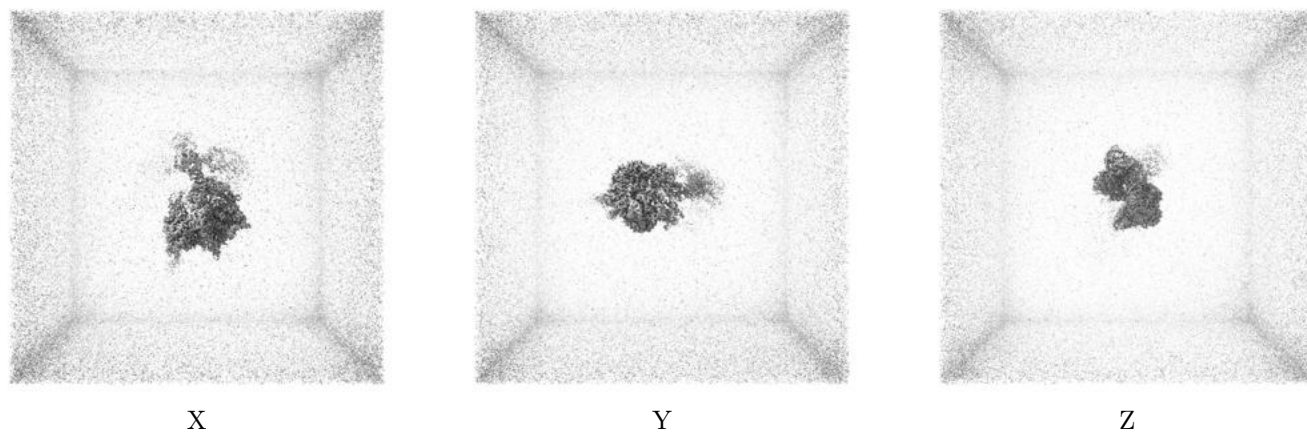
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

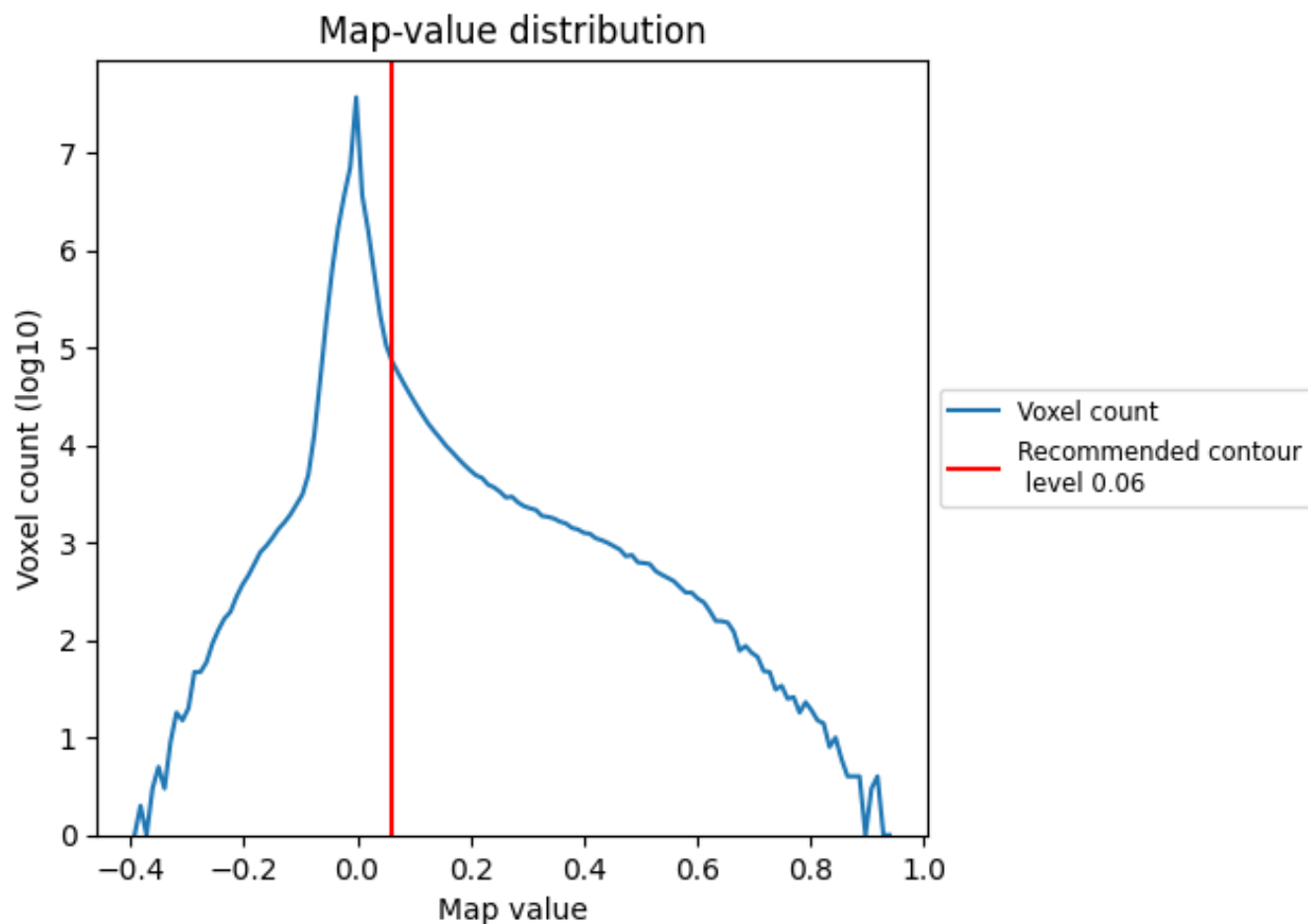
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

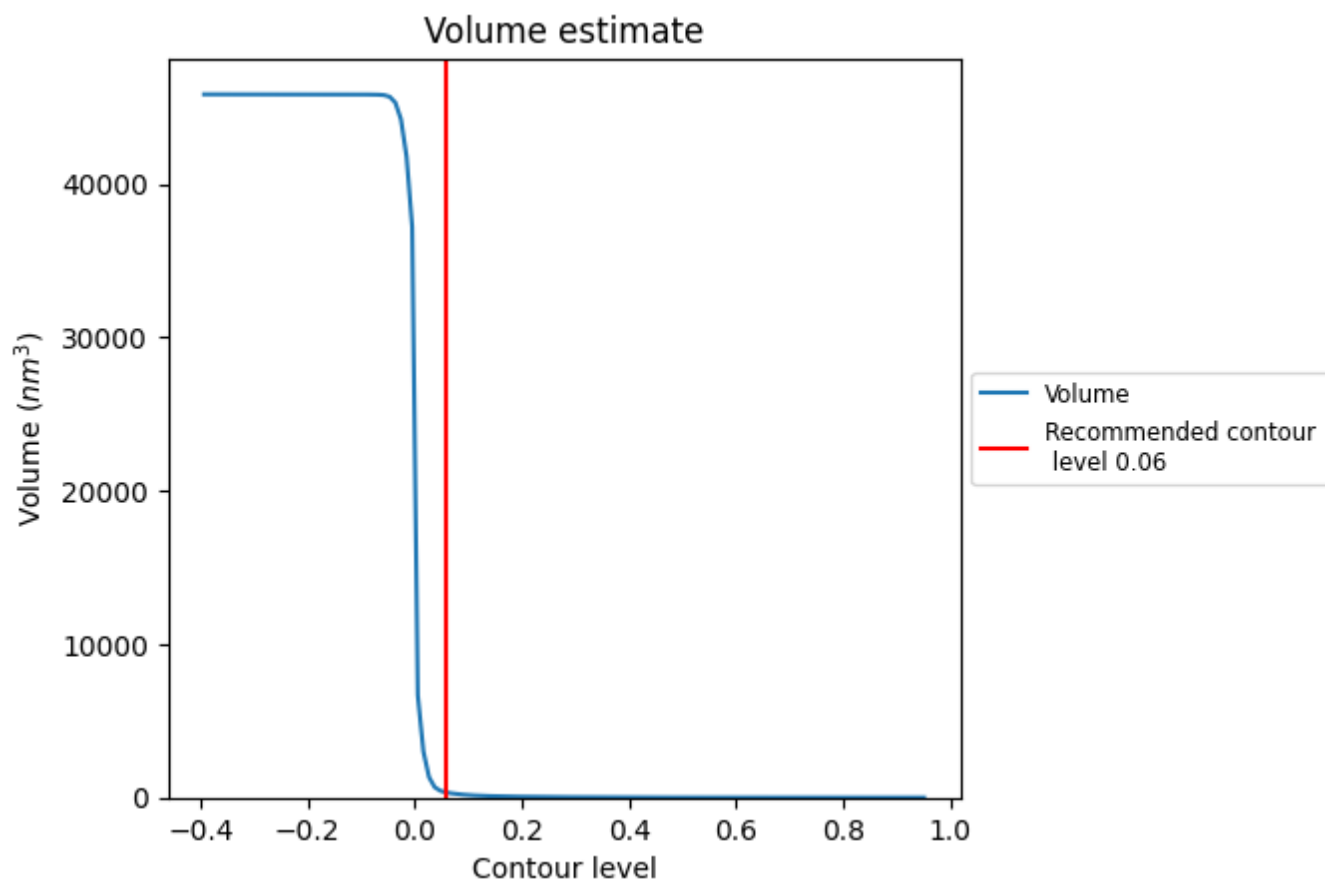
This section contains the results of statistical analysis of the map.

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.

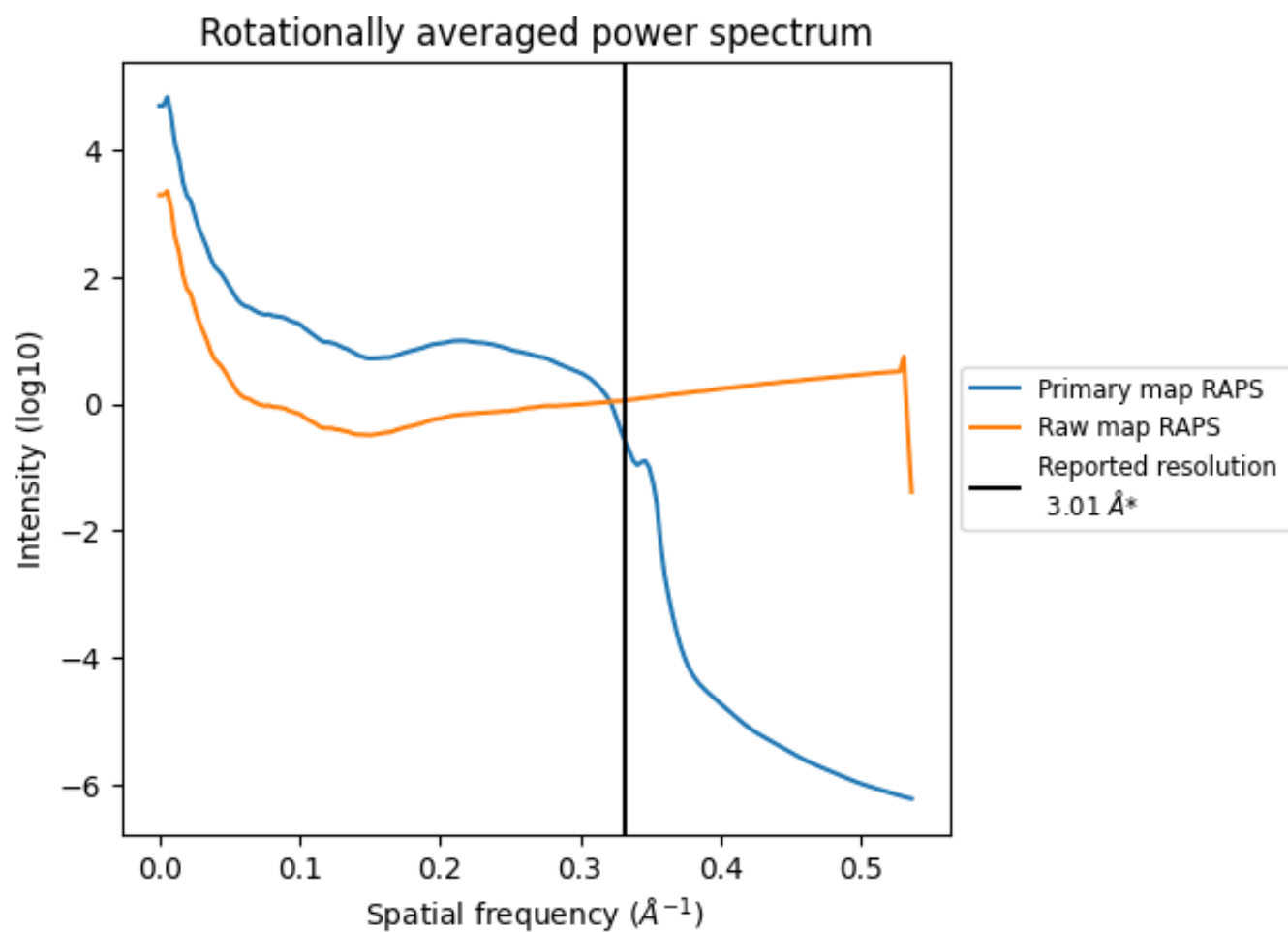
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm^3 ; this corresponds to an approximate mass of 298 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 ⓘ

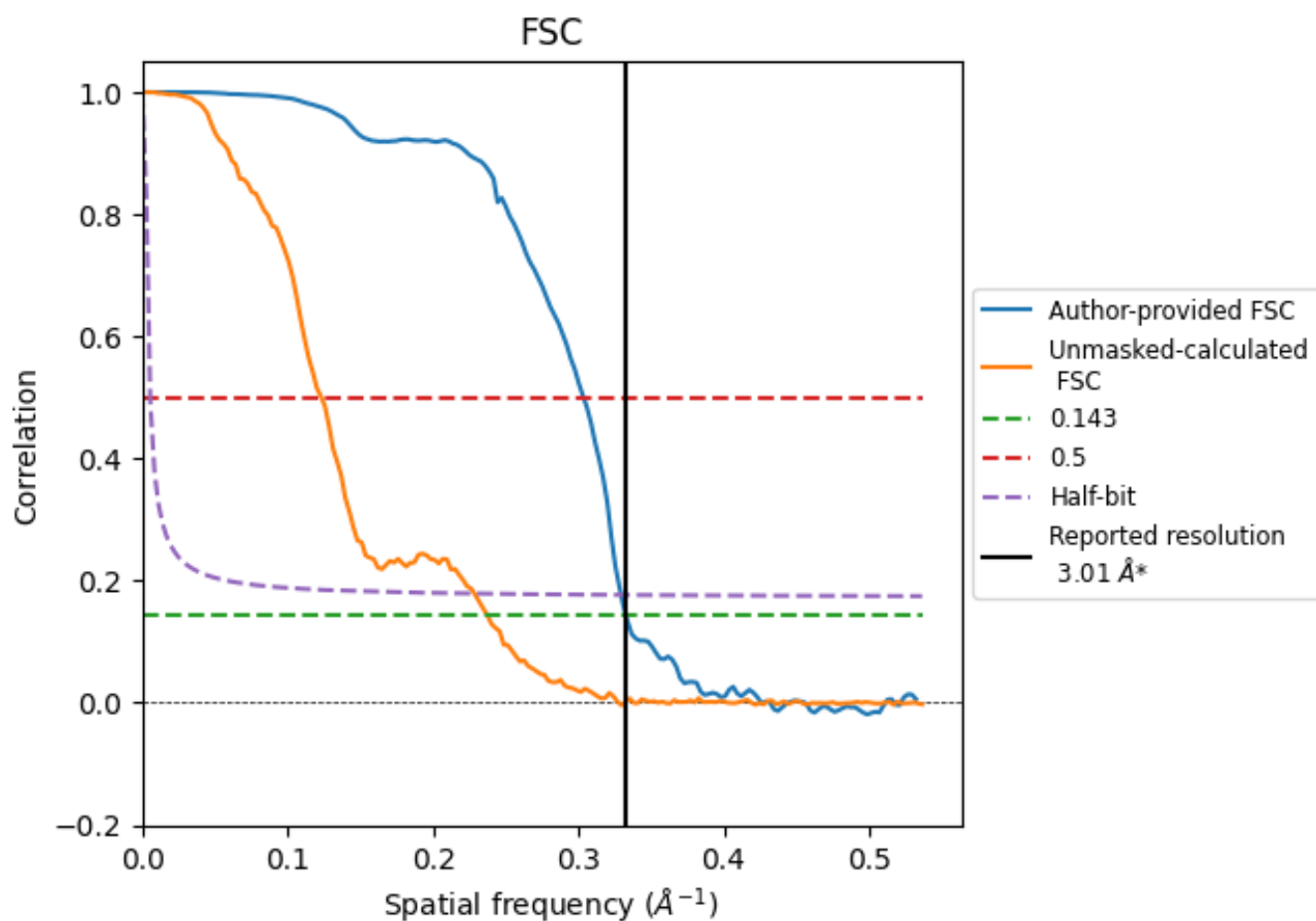


*Reported resolution corresponds to spatial frequency of 0.332 \AA^{-1}

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 0.332 \AA^{-1}

8.2 Resolution estimates [i](#)

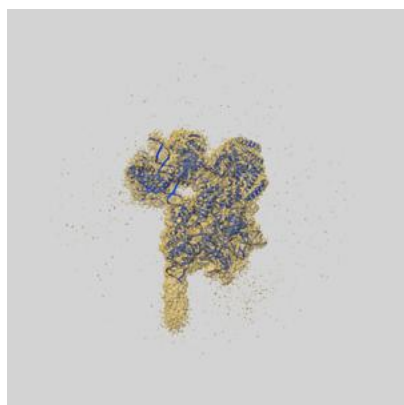
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.01	-	-
Author-provided FSC curve	3.00	3.29	3.04
Unmasked-calculated*	4.21	8.12	4.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.01 by more than 10 %

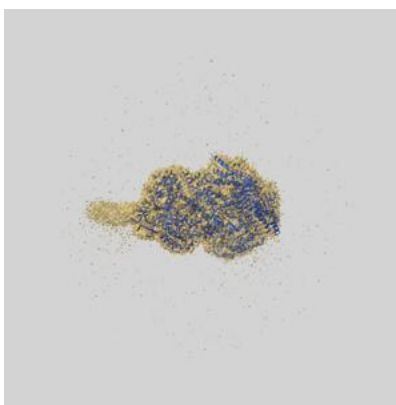
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-65108 and PDB model 9VJA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

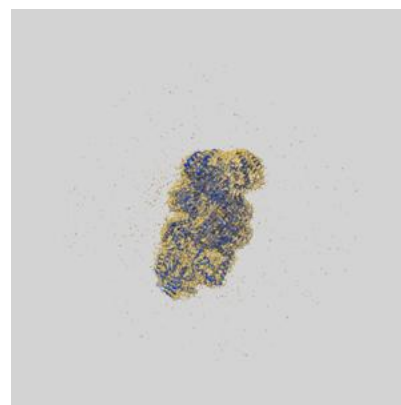
9.1 Map-model overlay [i](#)



X



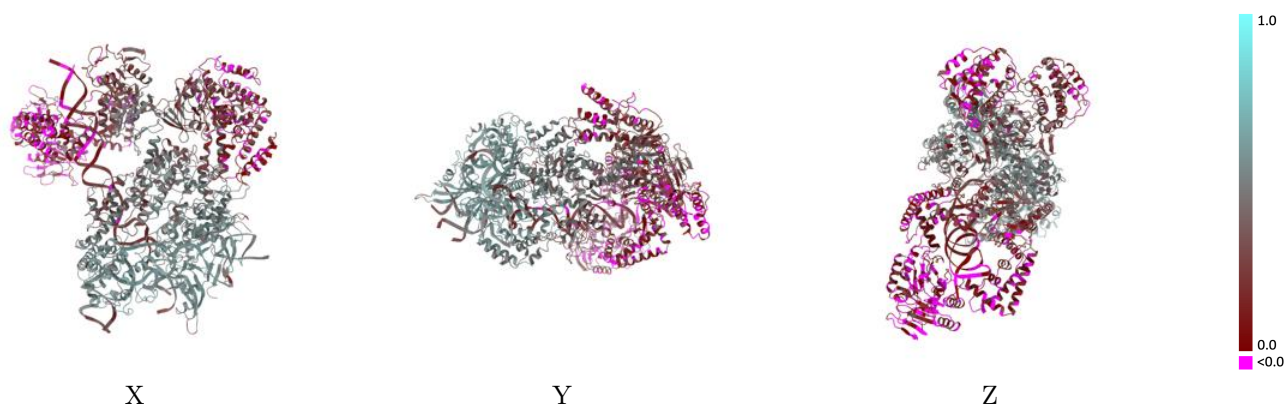
Y



Z

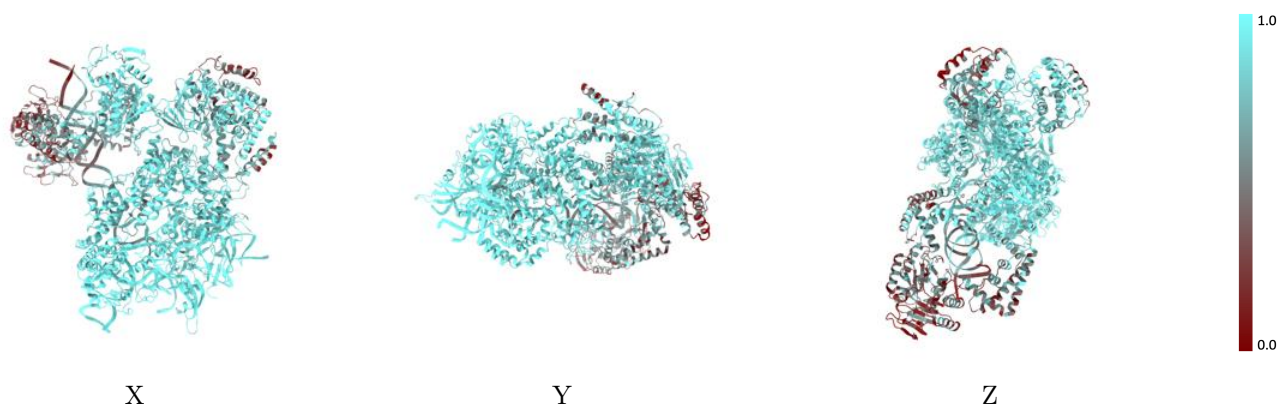
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



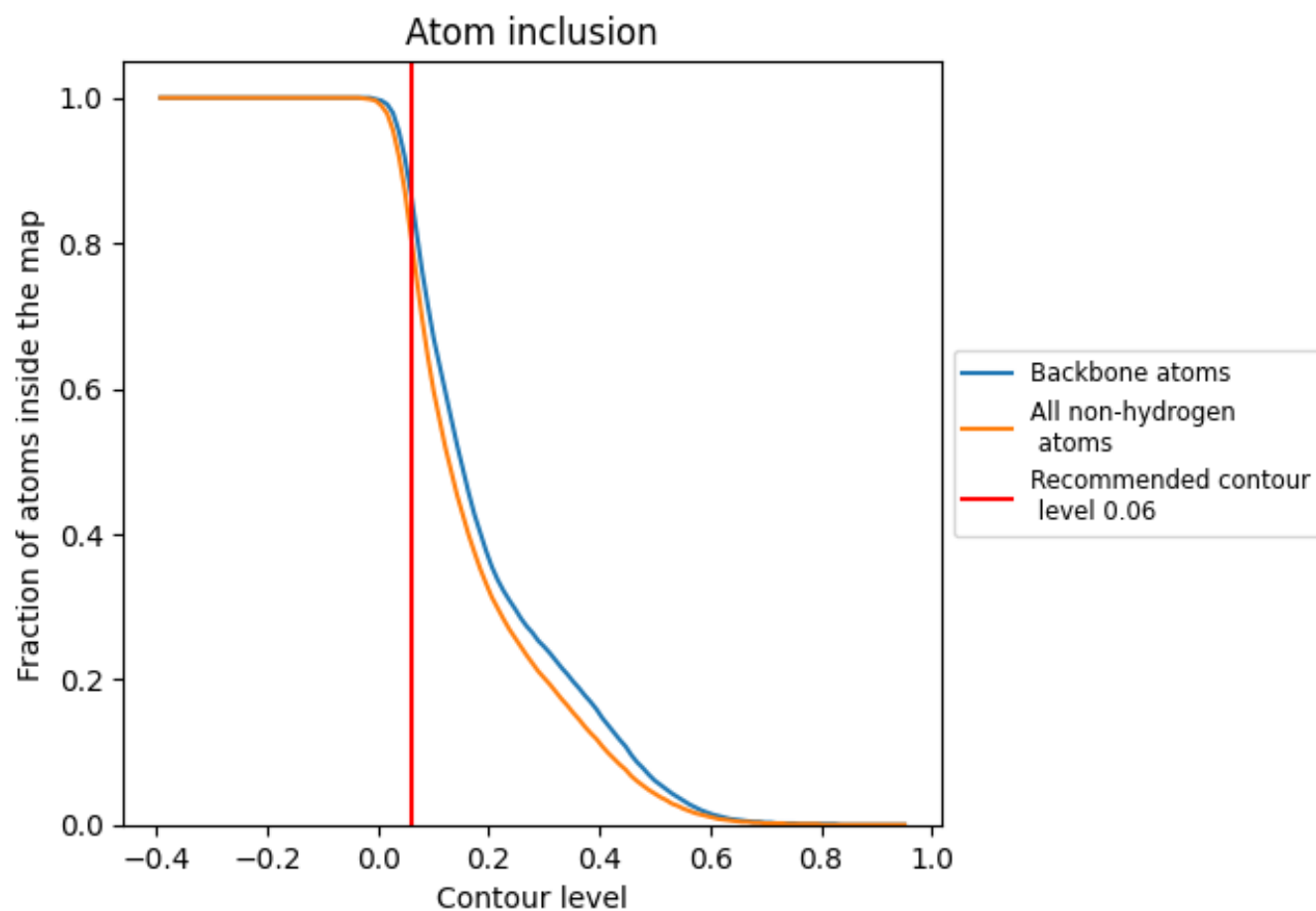
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8050	<div></div> 0.3380
A	<div></div> 0.7940	<div></div> 0.2250
B	<div></div> 0.7800	<div></div> 0.3210
C	<div></div> 0.4880	<div></div> 0.0480
D	<div></div> 0.3870	<div></div> 0.0430
K	<div></div> 0.8020	<div></div> 0.2370
L	<div></div> 0.6620	<div></div> 0.1600
N	<div></div> 0.6830	<div></div> 0.1990
S	<div></div> 0.9520	<div></div> 0.5080
T	<div></div> 0.6880	<div></div> 0.1760
g	<div></div> 0.9900	<div></div> 0.5170
t	<div></div> 0.9920	<div></div> 0.5280

1.0

0.0

<0.0