



Full wwPDB EM Validation Report ⓘ

Apr 27, 2026 – 10:55 AM JST

PDB ID : 9V2V / pdb_00009v2v
EMDB ID : EMD-64741
Title : Cryo-EM structure of the histone deacetylase complex Rpd3L in complex with mono-nucleosome
Authors : Zhao, H.; Li, H.; Wang, C.; Yang, X.; Li, H.; Zou, B.; Dong, S.; Zhang, N.; Zhou, Y.; Yi, L.; Zhang, Y.; Xie, Y.; Qin, D.; Chao, W.; Pei, D.; He, J.
Deposited on : 2025-05-21
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

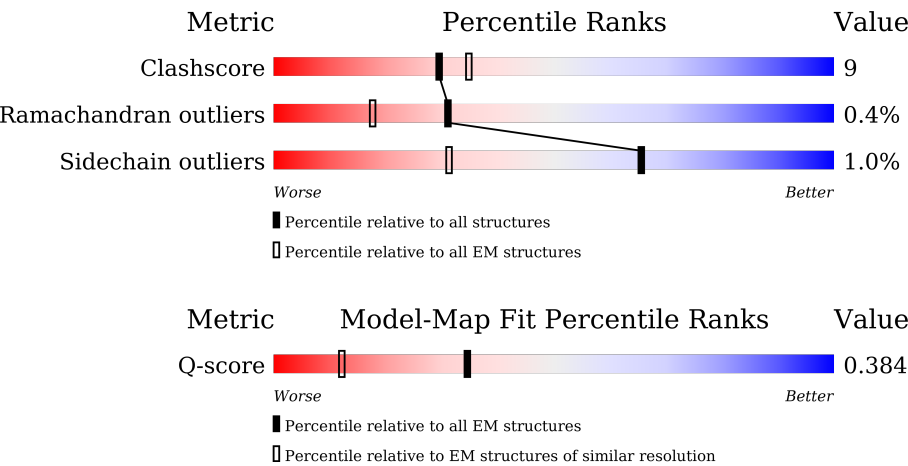
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	683	<div><div>10%</div><div><div></div><div>65%</div><div>17%</div><div>18%</div></div></div>
1	B	683	<div><div>27%</div><div><div></div><div>52%</div><div>13%</div><div>•</div><div>33%</div></div></div>
2	C	385	<div><div>•</div><div><div></div><div>76%</div><div>23%</div><div>•</div></div></div>
2	D	385	<div><div>10%</div><div><div></div><div>70%</div><div>25%</div><div>• •</div></div></div>

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Mol	Chain	Length	Quality of chain
3	E	119	
4	F	311	
5	G	121	
6	H	211	
7	I	105	
8	J	218	
9	K	249	
10	O	107	
10	S	107	
11	P	93	
11	T	93	
12	Q	98	
12	U	98	
13	R	79	
13	V	79	
14	X	155	
15	Y	155	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 34241 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 Transcriptional regulatory protein SIN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	562	Total	C	N	O	S	0	0
			4734	3044	801	874	15		
1	B	456	Total	C	N	O	S	0	0
			3824	2443	661	704	16		

- Molecule 2 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	385	Total	C	N	O	S	0	0
			3054	1942	517	570	25		
2	D	369	Total	C	N	O	S	0	0
			2929	1861	496	547	25		

- Molecule 3 is a protein called Transcriptional regulatory protein DEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	119	Total	C	N	O	S	0	0
			1022	642	188	188	4		

- Molecule 4 is a protein called Transcriptional regulatory protein SDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	166	Total	C	N	O	S	0	0
			1392	869	252	269	2		

- Molecule 5 is a protein called Transcriptional regulatory protein SAP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	121	Total	C	N	O	S	0	0
			1021	642	190	187	2		

- Molecule 6 is a protein called Transcriptional regulatory protein RXT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	180	Total	C	N	O	S	0	0
			1438	923	244	269	2		

- Molecule 7 is a protein called Transcriptional regulatory protein PHO23.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	105	Total	C	N	O	S	0	0
			864	545	147	167	5		

- Molecule 8 is a protein called Transcriptional regulatory protein RXT2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	157	Total	C	N	O	S	0	0
			1293	823	229	239	2		

- Molecule 9 is a protein called Histone deacetylase complex subunit CTI6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	40	Total	C	N	O	S	0	0
			340	211	55	71	3		

- Molecule 10 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	107	Total	C	N	O		0	0
			825	519	163	143			
10	S	107	Total	C	N	O		0	0
			825	519	163	143			

- Molecule 11 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	93	Total	C	N	O	S	0	0
			730	460	131	137	2		
11	T	91	Total	C	N	O	S	0	0
			715	451	128	134	2		

- Molecule 12 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	98	Total	C	N	O	S	0	0
			811	512	157	139	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	U	97	Total	C	N	O	S	0	0
			800	506	153	138	3		

- Molecule 13 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	79	Total	C	N	O	S	0	0
			637	403	124	109	1		
13	V	79	Total	C	N	O	S	0	0
			637	403	124	109	1		

- Molecule 14 is a DNA chain called DNA (155-MER).

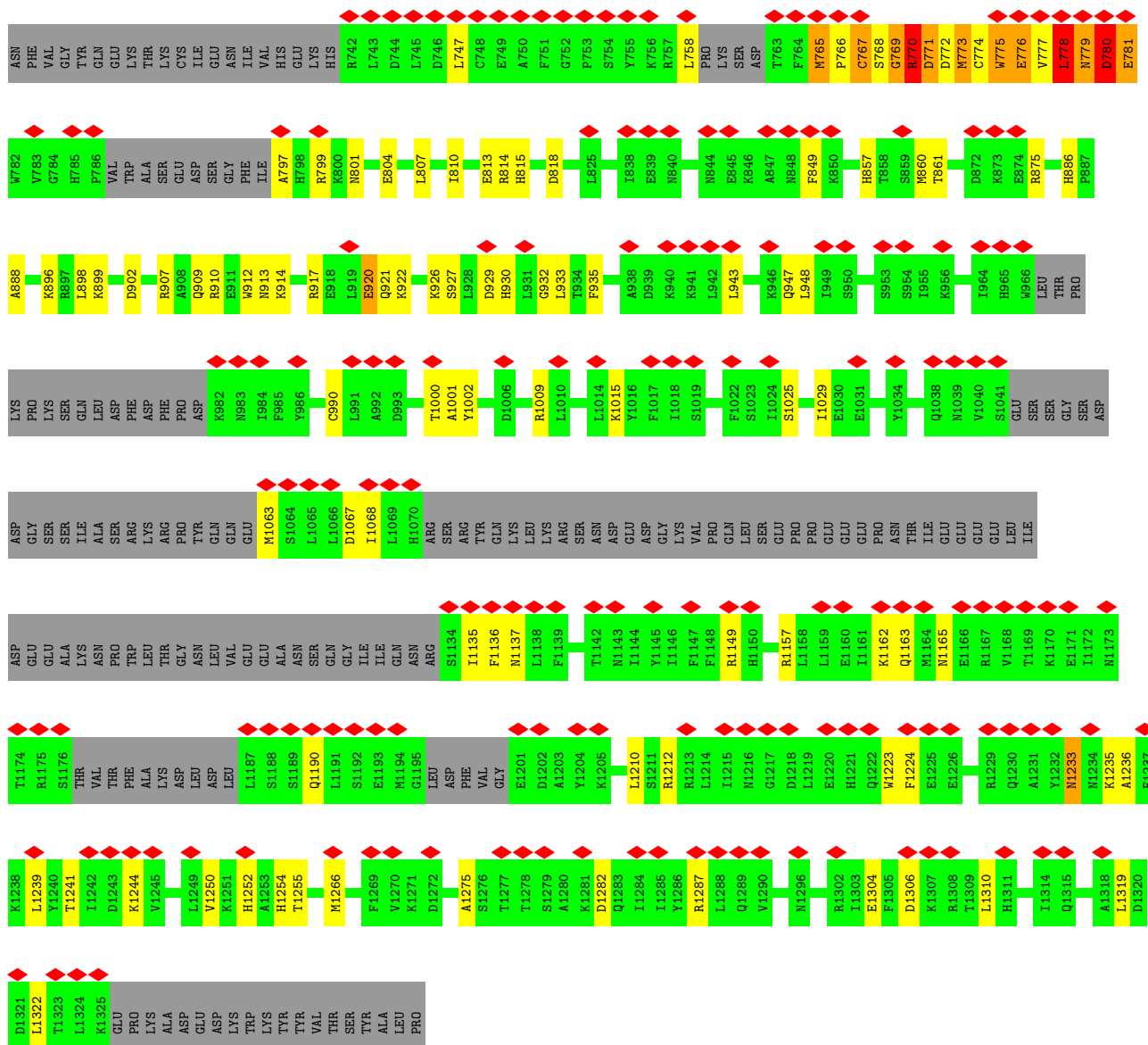
Mol	Chain	Residues	Atoms					AltConf	Trace
14	X	155	Total	C	N	O	P	0	0
			3195	1513	602	926	154		

- Molecule 15 is a DNA chain called DNA (155-MER).

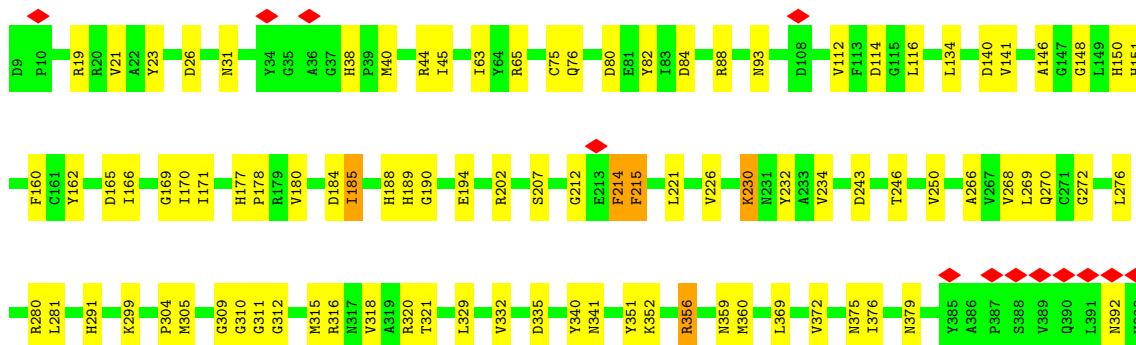
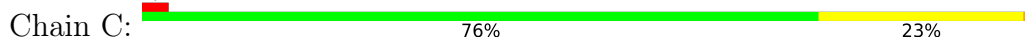
Mol	Chain	Residues	Atoms					AltConf	Trace
15	Y	155	Total	C	N	O	P	0	0
			3154	1500	570	930	154		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

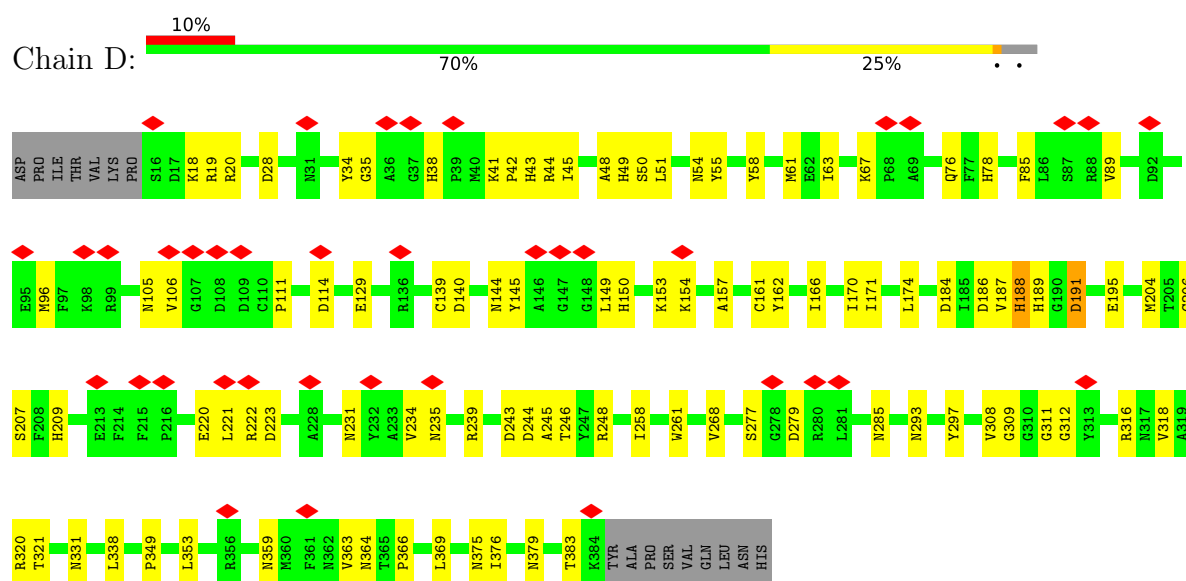
Mol	Chain	Residues	Atoms		AltConf
16	C	1	Total	Zn	0
			1	1	



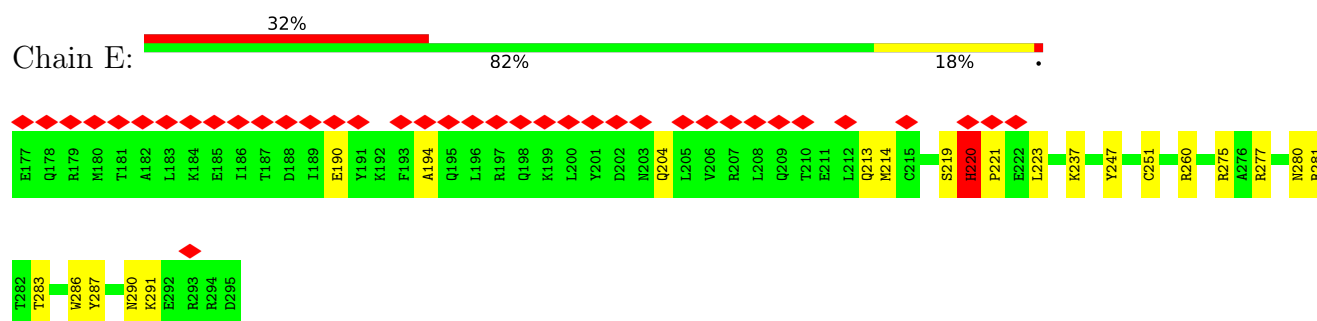
• Molecule 2: Histone deacetylase RPD3



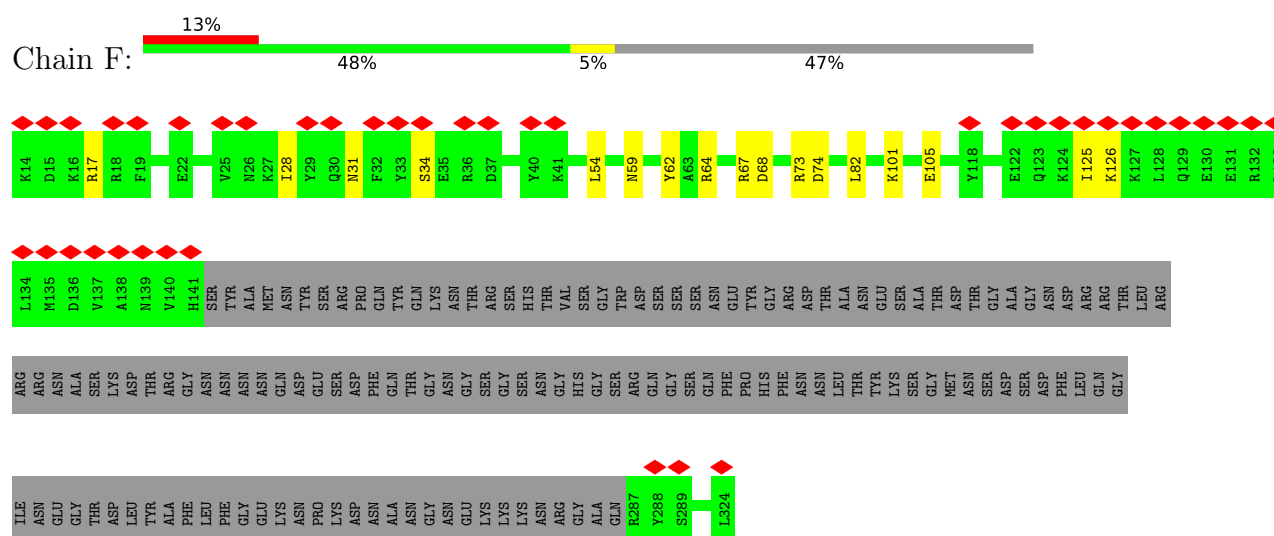
• Molecule 2: Histone deacetylase RPD3



• Molecule 3: Transcriptional regulatory protein DEP1

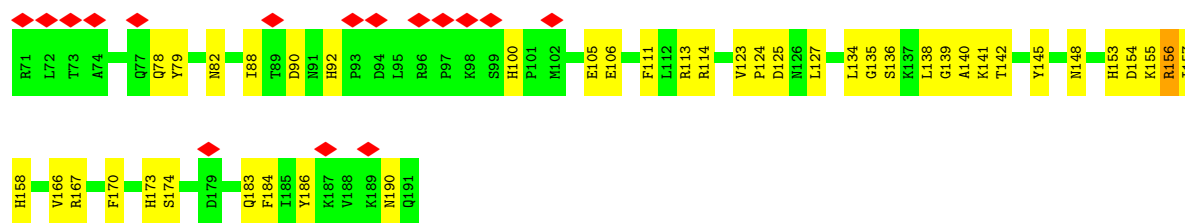


• Molecule 4: Transcriptional regulatory protein SDS3

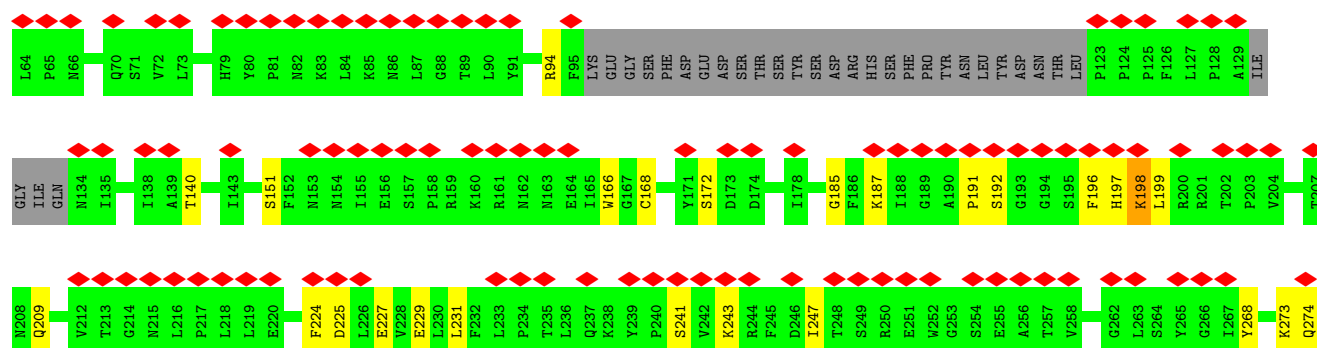
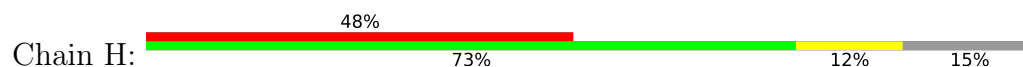


• Molecule 5: Transcriptional regulatory protein SAP30

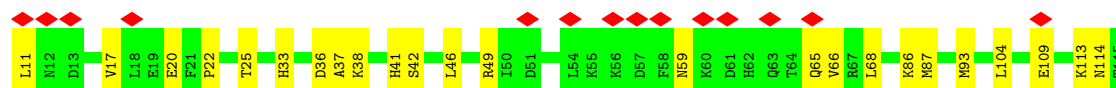
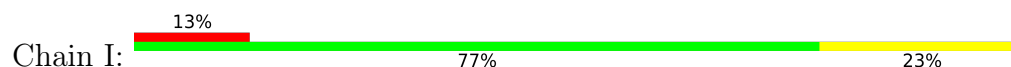




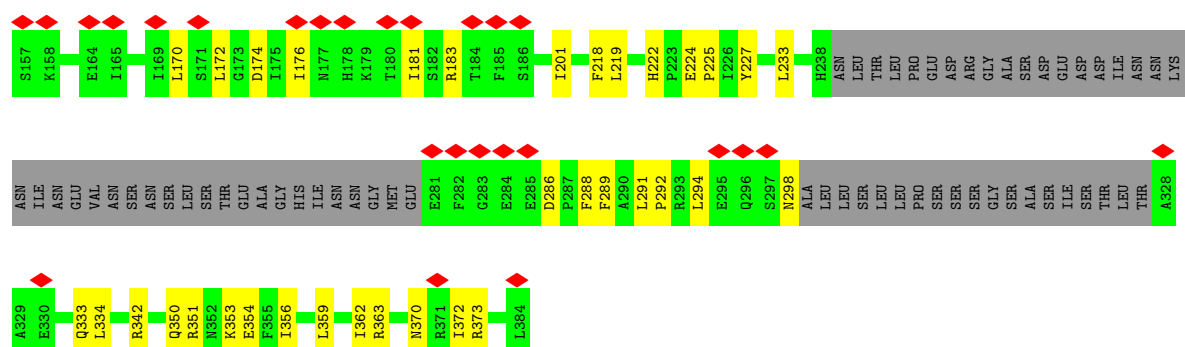
• Molecule 6: Transcriptional regulatory protein RXT3



• Molecule 7: Transcriptional regulatory protein PHO23

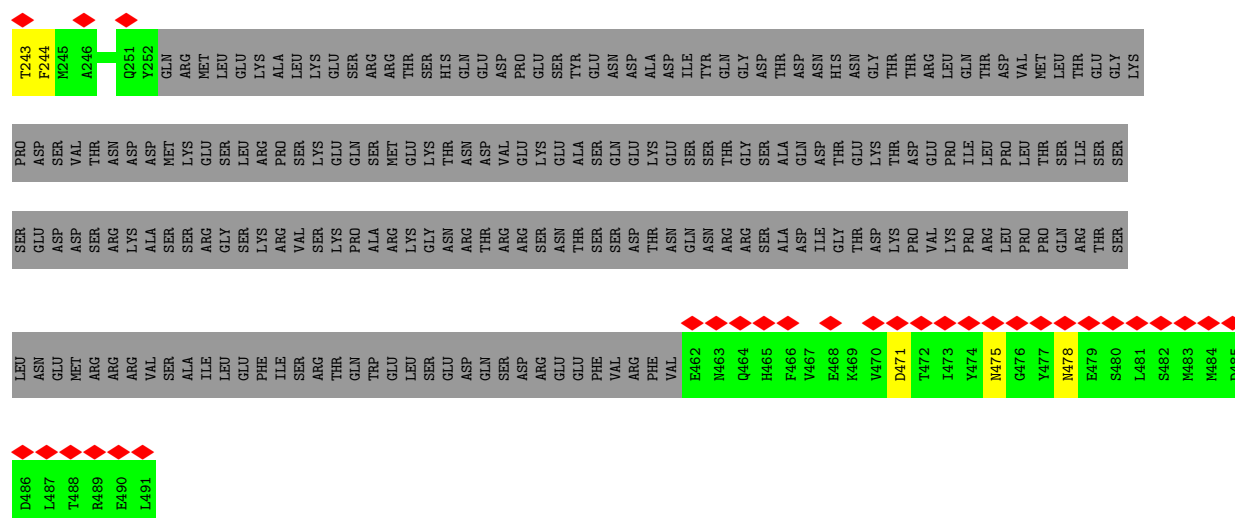


• Molecule 8: Transcriptional regulatory protein RXT2



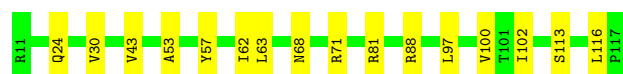
• Molecule 9: Histone deacetylase complex subunit CTI6





- Molecule 10: Histone H2A

Chain O: 85% 15%



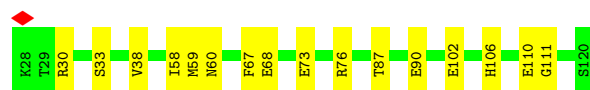
- Molecule 10: Histone H2A

Chain S: 85% 13% ..



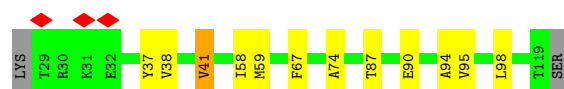
- Molecule 11: Histone H2B

Chain P: 83% 17%



- Molecule 11: Histone H2B

Chain T: 85% 12% ..

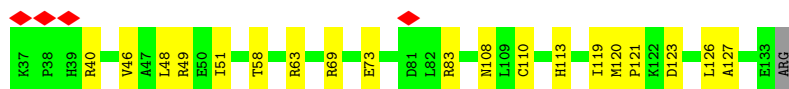
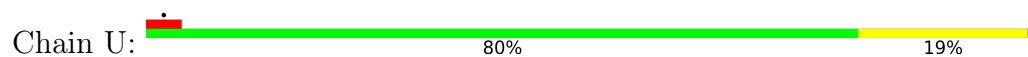


- Molecule 12: Histone H3

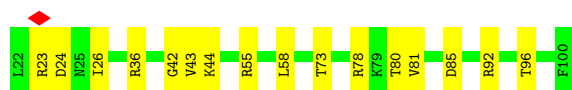
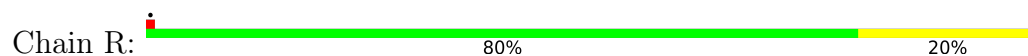
Chain Q: 83% 17%



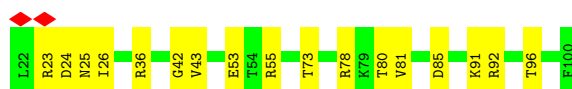
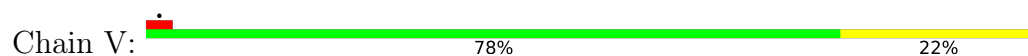
• Molecule 12: Histone H3



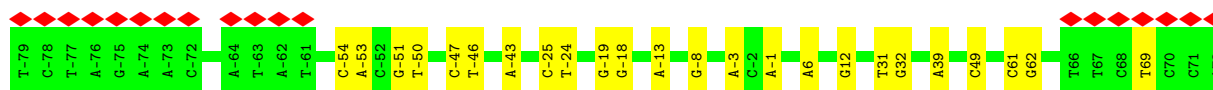
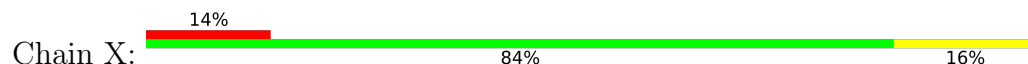
• Molecule 13: Histone H4



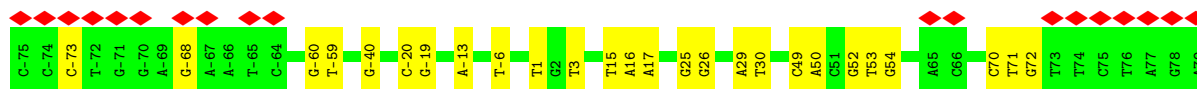
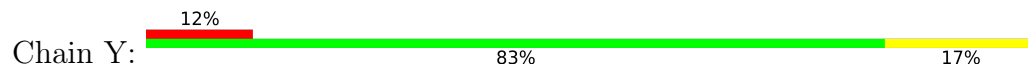
• Molecule 13: Histone H4



• Molecule 14: DNA (155-MER)



• Molecule 15: DNA (155-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	451544	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.535	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	426.0, 426.0, 426.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71, 0.71, 0.71	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.73	0/4838	0.77	4/6517 (0.1%)
1	B	0.34	0/3898	0.70	5/5240 (0.1%)
2	C	1.07	0/3133	0.83	1/4240 (0.0%)
2	D	0.42	0/3003	0.69	0/4059
3	E	0.64	0/1039	0.77	0/1397
4	F	0.62	0/1411	0.68	0/1891
5	G	0.63	0/1045	0.83	2/1408 (0.1%)
6	H	0.26	0/1474	0.60	0/2004
7	I	0.38	0/876	0.67	0/1182
8	J	0.49	0/1313	0.70	0/1767
9	K	0.19	0/344	0.49	0/459
10	O	1.01	0/835	0.87	1/1127 (0.1%)
10	S	0.95	0/835	0.80	0/1127
11	P	1.01	0/741	0.80	0/997
11	T	0.96	0/726	0.86	1/978 (0.1%)
12	Q	1.12	0/823	0.87	0/1104
12	U	1.06	0/812	0.81	0/1090
13	R	1.23	0/644	0.83	0/863
13	V	1.23	0/644	0.83	0/863
14	X	0.79	0/3589	0.64	0/5543
15	Y	0.82	0/3533	0.64	0/5446
All	All	0.76	0/35556	0.73	14/49302 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
5	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1275	ALA	N-CA-C	-8.43	104.13	114.75
11	T	41	VAL	N-CA-C	-7.72	104.39	113.42
1	A	1143	ASN	N-CA-C	-7.60	105.17	114.75
5	G	153	HIS	N-CA-C	-6.96	104.06	114.64
1	A	857	HIS	N-CA-C	-6.57	106.22	114.56
1	B	1244	LYS	N-CA-C	-6.55	106.50	114.75
10	O	24	GLN	N-CA-C	-6.38	106.04	113.88
1	B	1287	ARG	N-CA-C	-6.13	104.41	113.61
5	G	184	PHE	N-CA-C	-5.63	107.06	114.04
2	C	148	GLY	N-CA-C	-5.50	107.42	115.72
1	B	780	ASP	N-CA-C	-5.24	106.88	113.28
1	A	676	ILE	N-CA-C	-5.21	106.81	113.22
1	A	923	VAL	N-CA-C	-5.12	108.84	113.71
1	B	1163	GLN	N-CA-C	-5.09	108.09	114.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	770	ARG	Sidechain
5	G	156	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4734	0	4696	85	0
1	B	3824	0	3822	70	0
2	C	3054	0	2935	69	0
2	D	2929	0	2810	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1022	0	1026	20	0
4	F	1392	0	1402	29	0
5	G	1021	0	1001	42	0
6	H	1438	0	1424	16	0
7	I	864	0	875	19	0
8	J	1293	0	1321	27	0
9	K	340	0	312	3	0
10	O	825	0	882	14	0
10	S	825	0	882	15	0
11	P	730	0	755	12	0
11	T	715	0	737	9	0
12	Q	811	0	853	13	0
12	U	800	0	840	16	0
13	R	637	0	681	12	0
13	V	637	0	681	13	0
14	X	3195	0	1740	25	0
15	Y	3154	0	1742	23	0
16	C	1	0	0	0	0
All	All	34241	0	31417	480	0

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

All (480) 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:F:67:ARG:HB3	5:G:156:ARG:NH2	1.05	1.37
4:F:67:ARG:CB	5:G:156:ARG:NH2	1.91	1.33
4:F:67:ARG:HB3	5:G:156:ARG:HH21	1.26	1.00
4:F:67:ARG:HH11	5:G:156:ARG:HE	1.04	0.98
4:F:67:ARG:CB	5:G:156:ARG:HH22	1.70	0.91
1:B:921:GLN:HG2	2:D:349:PRO:HB3	1.62	0.82
14:X:6:DA:N6	15:Y:-6:DT:O4	2.14	0.80
4:F:67:ARG:HH11	5:G:156:ARG:NE	1.80	0.79
3:E:214:MET:HG3	3:E:221:PRO:HG3	1.64	0.79
4:F:67:ARG:CB	5:G:156:ARG:HH21	1.78	0.79
14:X:-1:DA:N6	15:Y:1:DT:O4	2.15	0.78
14:X:-3:DA:N6	15:Y:3:DT:O4	2.16	0.77
4:F:67:ARG:HD2	5:G:156:ARG:NE	1.98	0.77
1:B:1233:ASN:HD21	1:B:1235:LYS:HE3	1.50	0.75
14:X:-50:DT:O4	15:Y:50:DA:N6	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:67:ARG:CG	5:G:156:ARG:NH2	2.53	0.71
4:F:67:ARG:HD2	5:G:156:ARG:CZ	2.21	0.70
5:G:125:ASP:HB2	5:G:156:ARG:HG2	1.73	0.69
10:O:113:SER:HA	10:O:116:LEU:HD12	1.75	0.68
1:A:974:GLN:NE2	1:A:1315:GLN:OE1	2.26	0.68
4:F:67:ARG:NH1	5:G:156:ARG:HE	1.84	0.68
1:A:769:GLY:N	2:C:75:CYS:SG	2.66	0.68
1:A:826:ARG:NH2	1:A:830:CYS:SG	2.68	0.67
1:A:770:ARG:HD2	2:C:76:GLN:HA	1.77	0.67
1:A:939:ASP:OD1	1:A:1157:ARG:NH2	2.28	0.66
3:E:275:ARG:HE	8:J:219:LEU:HD23	1.62	0.65
3:E:220:HIS:H	3:E:221:PRO:HD2	1.62	0.65
2:D:191:ASP:HB3	2:D:195:GLU:HG3	1.79	0.64
1:A:770:ARG:NH1	1:A:774:CYS:O	2.30	0.64
1:A:669:PHE:HB2	4:F:17:ARG:HH12	1.63	0.63
1:B:765:MET:O	1:B:779:ASN:HA	1.97	0.63
2:D:170:ILE:HG22	2:D:268:VAL:HG21	1.80	0.63
5:G:124:PRO:HD2	5:G:157:ILE:HD13	1.81	0.63
2:C:150:HIS:HD2	2:C:190:GLY:HA2	1.63	0.63
2:D:239:ARG:HB3	2:D:363:VAL:HG23	1.81	0.63
10:S:14:ALA:O	10:S:15:LYS:C	2.41	0.62
10:O:102:ILE:HG23	11:P:58:ILE:HD13	1.81	0.62
6:H:197:HIS:O	6:H:198:LYS:C	2.43	0.62
3:E:283:THR:HB	8:J:350:GLN:HG3	1.81	0.62
10:O:81:ARG:HD3	12:U:58:THR:HG22	1.82	0.62
4:F:67:ARG:HD2	5:G:156:ARG:NH2	2.15	0.62
1:A:1135:ILE:HG22	1:A:1306:ASP:HB3	1.83	0.61
2:D:89:VAL:HA	2:D:96:MET:HE1	1.82	0.61
6:H:187:LYS:HE3	6:H:197:HIS:CD2	2.35	0.61
1:A:906:ARG:NH1	1:A:909:GLN:OE1	2.33	0.61
1:B:807:LEU:HD22	1:B:920:GLU:HG2	1.83	0.61
10:O:68:ASN:OD1	10:O:71:ARG:NH1	2.34	0.60
13:V:78:ARG:NH2	13:V:85:ASP:OD2	2.35	0.60
1:A:924:PHE:HE1	2:C:316:ARG:HH11	1.49	0.60
1:A:1201:GLU:OE1	1:A:1206:GLN:NE2	2.34	0.60
2:C:189:HIS:NE2	2:C:194:GLU:OE1	2.28	0.60
11:P:68:GLU:OE2	13:V:91:LYS:NZ	2.34	0.60
1:A:1140:ALA:HB1	1:A:1144:ILE:HB	1.83	0.60
8:J:218:PHE:O	8:J:342:ARG:NH2	2.35	0.60
2:C:272:GLY:O	2:C:291:HIS:NE2	2.35	0.59
2:C:21:VAL:HG22	2:C:141:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:114:ASN:HD22	8:J:170:LEU:HD23	1.67	0.59
6:H:225:ASP:HB2	6:H:273:LYS:HB2	1.85	0.59
11:P:30:ARG:HG3	14:X:49:DC:H4'	1.83	0.59
2:D:44:ARG:NH1	2:D:311:GLY:O	2.34	0.59
1:B:770:ARG:HA	1:B:770:ARG:NH2	2.17	0.59
2:C:23:TYR:HB3	2:C:63:ILE:HG12	1.85	0.59
6:H:224:PHE:HB2	6:H:274:GLN:HA	1.84	0.59
13:R:78:ARG:NH2	13:R:85:ASP:OD2	2.35	0.59
14:X:-53:DA:N6	15:Y:52:DG:O6	2.36	0.59
1:B:810:ILE:HG13	1:B:814:ARG:HH21	1.67	0.58
1:B:917:ARG:HA	1:B:921:GLN:HG3	1.84	0.58
1:A:1138:LEU:HB3	1:A:1303:ILE:HB	1.85	0.58
1:B:922:LYS:O	1:B:926:LYS:NZ	2.37	0.58
5:G:136:SER:OG	5:G:139:GLY:N	2.30	0.58
2:C:44:ARG:HD2	2:C:318:VAL:HG21	1.85	0.58
1:B:1266:MET:SD	1:B:1266:MET:N	2.73	0.58
3:E:286:TRP:O	3:E:290:ASN:ND2	2.37	0.58
1:B:767:CYS:HB2	1:B:770:ARG:HG2	1.86	0.58
4:F:67:ARG:HB3	5:G:156:ARG:HH22	0.75	0.58
2:C:188:HIS:HD2	2:C:215:PHE:HB3	1.69	0.57
2:D:184:ASP:OD1	2:D:186:ASP:N	2.34	0.57
2:D:206:CYS:SG	2:D:207:SER:N	2.76	0.57
2:C:270:GLN:NE2	2:C:309:GLY:O	2.37	0.57
2:D:187:VAL:O	2:D:188:HIS:HB3	2.04	0.57
2:C:40:MET:HG2	2:C:311:GLY:H	1.70	0.57
1:B:1162:LYS:HA	1:B:1165:ASN:HB2	1.86	0.57
2:C:315:MET:HA	2:C:318:VAL:HG22	1.87	0.57
10:S:15:LYS:HD3	10:S:20:ARG:HD2	1.85	0.57
8:J:176:ILE:HA	8:J:183:ARG:HG3	1.87	0.57
2:C:234:VAL:HG13	2:C:376:ILE:HD12	1.87	0.57
1:A:924:PHE:HE2	2:C:356:ARG:HD3	1.70	0.56
3:E:219:SER:HA	3:E:223:LEU:HB2	1.87	0.56
7:I:59:ASN:HD22	8:J:298:ASN:HD22	1.53	0.56
10:O:88:ARG:NH2	10:O:100:VAL:O	2.38	0.56
13:R:73:THR:HG21	13:R:81:VAL:HA	1.87	0.56
1:A:1303:ILE:HG12	1:A:1314:ILE:HG12	1.88	0.56
2:C:221:LEU:HD11	2:C:372:VAL:HG22	1.86	0.56
10:O:57:TYR:HB2	11:P:110:GLU:HG2	1.87	0.56
2:D:366:PRO:HA	2:D:369:LEU:HB2	1.87	0.56
2:D:18:LYS:HD2	2:D:331:ASN:HD22	1.71	0.56
12:Q:63:ARG:HH21	13:R:36:ARG:HH12	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:LEU:HD22	1:A:967:LEU:HD12	1.88	0.56
1:B:943:LEU:H	1:B:947:GLN:HB2	1.71	0.56
5:G:186:TYR:O	5:G:190:ASN:ND2	2.38	0.56
2:C:84:ASP:OD1	2:C:88:ARG:NH1	2.39	0.56
13:V:73:THR:HG21	13:V:81:VAL:HA	1.87	0.56
5:G:148:ASN:HA	5:G:155:LYS:HA	1.88	0.56
1:A:891:ALA:HB3	1:A:892:PRO:HD3	1.89	0.55
2:D:221:LEU:HG	2:D:375:ASN:HD22	1.71	0.55
7:I:104:LEU:HD11	8:J:372:ILE:HG21	1.87	0.55
1:A:768:SER:N	2:C:75:CYS:SG	2.79	0.55
1:A:779:ASN:HD21	1:A:782:TRP:HB2	1.71	0.55
2:D:245:ALA:O	2:D:248:ARG:HG2	2.07	0.55
4:F:67:ARG:CD	5:G:156:ARG:NH2	2.69	0.55
11:P:73:GLU:OE1	11:P:76:ARG:NH2	2.39	0.55
2:C:26:ASP:HA	2:C:65:ARG:HG3	1.87	0.55
2:D:50:SER:O	2:D:54:ASN:ND2	2.40	0.55
1:B:775:TRP:HE3	1:B:776:GLU:H	1.53	0.55
1:A:691:LEU:HD22	1:A:696:ILE:HD12	1.88	0.55
7:I:49:ARG:HD2	7:I:68:LEU:HD11	1.89	0.55
1:A:1161:ILE:HA	1:A:1164:MET:HG2	1.90	0.54
2:D:149:LEU:HD22	2:D:161:CYS:HB2	1.87	0.54
14:X:31:DT:H2"	14:X:32:DG:H5"	1.90	0.54
1:A:935:PHE:HZ	1:A:1157:ARG:HH21	1.54	0.54
1:A:1302:ARG:HH11	1:A:1315:GLN:HG3	1.71	0.54
2:D:19:ARG:HH21	2:D:140:ASP:HB3	1.73	0.54
2:D:209:HIS:HE1	2:D:235:ASN:HB2	1.73	0.54
3:E:275:ARG:NH2	4:F:54:LEU:O	2.41	0.54
5:G:134:LEU:HD11	5:G:142:THR:HG21	1.89	0.54
7:I:22:PRO:HA	7:I:25:THR:HG22	1.90	0.54
2:D:105:ASN:HB3	2:D:157:ALA:HB3	1.90	0.54
7:I:33:HIS:O	7:I:37:ALA:N	2.41	0.54
12:Q:108:ASN:ND2	13:R:42:GLY:O	2.41	0.54
2:C:341:ASN:OD1	2:C:341:ASN:N	2.35	0.53
2:D:222:ARG:NH1	2:D:223:ASP:OD1	2.41	0.53
3:E:220:HIS:N	3:E:221:PRO:HD2	2.23	0.53
4:F:59:ASN:HB3	4:F:62:TYR:HB3	1.90	0.53
6:H:196:PHE:HD2	6:H:209:GLN:HE21	1.56	0.53
14:X:-25:DC:H42	15:Y:25:DG:H1	1.55	0.53
1:A:901:LYS:NZ	1:A:904:GLU:OE2	2.33	0.53
7:I:59:ASN:HD21	7:I:65:GLN:HE21	1.55	0.53
1:A:1029:ILE:HG13	1:A:1032:SER:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:GLY:O	1:B:770:ARG:C	2.51	0.53
2:D:166:ILE:HG12	2:D:308:VAL:HG11	1.91	0.53
12:U:121:PRO:HB3	13:V:53:GLU:HG3	1.90	0.53
2:D:231:ASN:OD1	2:D:383:THR:OG1	2.27	0.53
4:F:68:ASP:OD1	5:G:156:ARG:NH1	2.36	0.53
2:D:244:ASP:O	2:D:246:THR:N	2.41	0.53
8:J:172:LEU:HG	8:J:174:ASP:H	1.74	0.53
1:B:770:ARG:HA	1:B:770:ARG:CZ	2.39	0.52
2:D:85:PHE:HE2	2:D:106:VAL:HG21	1.74	0.52
12:U:83:ARG:HB2	13:V:80:THR:HG22	1.92	0.52
14:X:39:DA:N6	15:Y:-40:DG:O6	2.43	0.52
12:U:110:CYS:SG	12:U:127:ALA:HB2	2.49	0.52
1:A:681:LEU:HD22	1:A:709:TYR:HE1	1.74	0.52
13:R:36:ARG:NH2	15:Y:-13:DA:OP1	2.42	0.52
10:S:30:VAL:HG13	11:T:67:PHE:HE1	1.75	0.52
11:T:94:ALA:O	11:T:98:LEU:HD12	2.10	0.52
1:A:1011:LYS:HG2	1:A:1015:LYS:HE2	1.91	0.52
2:C:19:ARG:HH11	2:C:140:ASP:HB3	1.75	0.52
1:A:662:LEU:N	1:A:664:GLU:OE1	2.43	0.52
1:B:810:ILE:HA	1:B:813:GLU:HB3	1.92	0.52
1:A:904:GLU:HA	1:A:907:ARG:HG2	1.92	0.52
2:C:170:ILE:HG23	2:C:180:VAL:HG21	1.92	0.52
12:Q:42:ARG:NH1	15:Y:70:DC:OP2	2.43	0.51
1:B:1157:ARG:NH1	1:B:1241:THR:OG1	2.43	0.51
2:C:320:ARG:NH2	2:C:352:LYS:O	2.43	0.51
1:A:879:ILE:O	1:A:883:LEU:N	2.42	0.51
3:E:204:GLN:NE2	9:K:471:ASP:OD2	2.43	0.51
5:G:166:VAL:O	5:G:170:PHE:N	2.43	0.51
11:T:87:THR:OG1	11:T:90:GLU:OE1	2.28	0.51
1:B:929:ASP:HA	2:D:359:ASN:HB3	1.93	0.51
2:D:78:HIS:NE2	2:D:153:LYS:O	2.38	0.51
11:P:87:THR:OG1	11:P:90:GLU:OE1	2.28	0.51
2:D:207:SER:N	2:D:234:VAL:O	2.44	0.51
8:J:222:HIS:HB3	8:J:224:GLU:HG2	1.92	0.51
1:A:1141:ASN:HD21	1:A:1262:THR:HG22	1.76	0.51
4:F:28:ILE:HD11	5:G:183:GLN:HE21	1.76	0.51
1:B:909:GLN:O	1:B:913:ASN:N	2.44	0.51
3:E:237:LYS:NZ	4:F:105:GLU:OE1	2.44	0.50
5:G:154:ASP:OD1	5:G:154:ASP:N	2.44	0.50
10:S:54:VAL:HG21	11:T:95:VAL:HG21	1.92	0.50
1:B:861:THR:HG23	2:D:114:ASP:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:SER:O	1:B:769:GLY:C	2.55	0.50
1:B:773:MET:HB2	1:B:775:TRP:CD1	2.47	0.50
2:C:250:VAL:HG21	2:C:369:LEU:HD22	1.93	0.50
3:E:277:ARG:O	3:E:281:ARG:N	2.44	0.50
7:I:36:ASP:OD1	7:I:86:LYS:NZ	2.44	0.50
2:C:312:GLY:HA3	2:C:318:VAL:HG11	1.92	0.50
2:D:261:TRP:HE1	2:D:383:THR:HB	1.75	0.50
7:I:93:MET:HE3	8:J:362:ILE:HG21	1.92	0.50
12:Q:83:ARG:HB2	13:R:80:THR:HG22	1.94	0.50
1:A:811:GLU:OE2	2:C:315:MET:N	2.39	0.50
3:E:214:MET:HE2	3:E:221:PRO:HD3	1.94	0.50
6:H:168:CYS:SG	6:H:172:SER:OG	2.64	0.50
1:A:1172:ILE:HG21	1:A:1198:PHE:HB2	1.94	0.49
1:B:765:MET:HB2	1:B:781:GLU:H	1.77	0.49
1:B:815:HIS:HE1	2:D:43:HIS:CD2	2.30	0.49
5:G:173:HIS:ND1	5:G:174:SER:O	2.45	0.49
10:S:29:ARG:NH2	15:Y:49:DC:OP1	2.44	0.49
1:A:950:SER:O	1:A:972:LYS:NZ	2.45	0.49
2:C:141:VAL:HG11	2:C:329:LEU:HD13	1.93	0.49
1:A:1172:ILE:HD13	1:A:1198:PHE:HB2	1.94	0.49
1:A:1262:THR:O	1:A:1266:MET:N	2.42	0.49
4:F:64:ARG:NH1	5:G:113:ARG:HB2	2.27	0.49
1:A:1145:TYR:O	1:A:1149:ARG:N	2.39	0.49
2:C:82:TYR:OH	2:C:162:TYR:O	2.26	0.49
7:I:109:GLU:OE2	7:I:113:LYS:NZ	2.45	0.49
1:A:978:ASP:OD1	1:A:1311:HIS:ND1	2.35	0.49
10:O:88:ARG:NH1	10:O:97:LEU:O	2.45	0.49
1:B:770:ARG:HH21	1:B:771:ASP:H	1.60	0.49
4:F:64:ARG:HD3	5:G:113:ARG:HD3	1.94	0.49
2:D:204:MET:HE2	2:D:258:ILE:HG12	1.95	0.49
10:O:68:ASN:HA	10:O:71:ARG:HE	1.78	0.49
1:A:779:ASN:ND2	1:A:782:TRP:O	2.46	0.48
12:Q:48:LEU:HD23	12:Q:51:ILE:HD12	1.94	0.48
1:B:778:LEU:O	1:B:779:ASN:C	2.56	0.48
1:B:797:ALA:HB3	1:B:799:ARG:HH22	1.78	0.48
2:D:144:ASN:O	2:D:309:GLY:N	2.38	0.48
15:Y:29:DA:H1'	15:Y:30:DT:H5'	1.94	0.48
2:D:38:HIS:O	2:D:41:LYS:NZ	2.36	0.48
2:D:243:ASP:O	2:D:246:THR:OG1	2.32	0.48
4:F:64:ARG:NH1	5:G:125:ASP:OD1	2.47	0.48
5:G:111:PHE:HE2	5:G:167:ARG:HH22	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:S:14:ALA:O	14:X:-43:DA:H4'	2.14	0.48
2:D:279:ASP:OD1	2:D:279:ASP:N	2.47	0.48
2:D:320:ARG:HD3	2:D:353:LEU:HA	1.96	0.48
6:H:231:LEU:HB3	6:H:268:TYR:HB2	1.96	0.48
8:J:292:PRO:HB2	8:J:294:LEU:HG	1.95	0.48
12:U:120:MET:N	12:U:123:ASP:OD2	2.38	0.47
1:B:1009:ARG:NH1	1:B:1067:ASP:OD1	2.46	0.47
2:D:171:ILE:HG13	2:D:174:LEU:HD12	1.96	0.47
2:D:293:ASN:O	2:D:297:TYR:N	2.47	0.47
4:F:67:ARG:CD	5:G:156:ARG:HH21	2.26	0.47
10:S:13:LYS:C	10:S:15:LYS:N	2.72	0.47
1:A:1234:ASN:HB3	2:C:359:ASN:HD21	1.78	0.47
2:C:40:MET:HE3	2:C:160:PHE:HB3	1.96	0.47
2:D:277:SER:OG	2:D:285:ASN:ND2	2.38	0.47
1:A:851:LEU:HD13	1:A:855:LEU:HD22	1.97	0.47
1:A:870:VAL:HG13	1:A:901:LYS:HG3	1.96	0.47
2:C:112:VAL:HG13	2:C:116:LEU:HD22	1.97	0.47
2:C:180:VAL:HG12	2:C:266:ALA:HB3	1.97	0.47
2:C:188:HIS:CD2	2:C:215:PHE:HB3	2.49	0.47
7:I:42:SER:O	7:I:46:LEU:N	2.44	0.47
15:Y:15:DT:H2''	15:Y:16:DA:C8	2.50	0.47
1:B:990:CYS:SG	1:B:1212:ARG:NH1	2.87	0.47
2:D:51:LEU:O	2:D:55:TYR:N	2.33	0.47
1:A:799:ARG:HH11	2:C:360:MET:HB3	1.80	0.47
1:A:1234:ASN:HB3	2:C:359:ASN:ND2	2.30	0.47
2:D:318:VAL:O	2:D:321:THR:OG1	2.28	0.47
3:E:213:GLN:O	3:E:214:MET:HB2	2.14	0.47
5:G:140:ALA:HA	5:G:145:TYR:CD2	2.49	0.47
13:V:36:ARG:NH2	14:X:-13:DA:OP1	2.47	0.47
14:X:-47:DC:H2''	14:X:-46:DT:C5	2.50	0.47
1:A:710:LEU:HD21	1:A:714:LYS:HA	1.97	0.47
1:A:858:THR:HG23	1:A:860:MET:HE2	1.97	0.47
12:Q:103:LEU:HA	12:Q:131:ARG:HH12	1.79	0.47
1:A:704:GLU:HG3	5:G:100:HIS:HE1	1.79	0.47
1:A:911:GLU:OE2	4:F:101:LYS:NZ	2.48	0.46
2:C:243:ASP:OD1	2:C:246:THR:OG1	2.27	0.46
2:C:375:ASN:O	2:C:379:ASN:ND2	2.48	0.46
10:O:30:VAL:HG13	11:P:67:PHE:HE1	1.81	0.46
1:B:773:MET:SD	1:B:773:MET:N	2.88	0.46
2:D:111:PRO:O	2:D:162:TYR:OH	2.32	0.46
12:U:46:VAL:HG22	12:U:49:ARG:HH21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ILE:HG12	1:A:682:TYR:HB2	1.97	0.46
1:B:896:LYS:HA	1:B:899:LYS:HE2	1.97	0.46
1:B:1002:TYR:HB3	1:B:1254:HIS:CD2	2.51	0.46
1:B:1015:LYS:HE2	1:B:1029:ILE:HG22	1.98	0.46
2:D:191:ASP:HB3	2:D:195:GLU:CG	2.44	0.46
5:G:105:GLU:HA	5:G:167:ARG:HH11	1.79	0.46
15:Y:-20:DC:H2''	15:Y:-19:DG:H5''	1.97	0.46
1:A:1178:VAL:HG21	2:C:351:TYR:HB2	1.98	0.46
1:B:1306:ASP:H	1:B:1310:LEU:HA	1.80	0.46
6:H:191:PRO:HA	6:H:196:PHE:CG	2.51	0.46
2:D:376:ILE:HA	2:D:379:ASN:HD22	1.81	0.46
5:G:78:GLN:O	5:G:82:ASN:ND2	2.49	0.46
7:I:17:VAL:HA	7:I:20:GLU:HB3	1.97	0.46
8:J:359:LEU:O	8:J:363:ARG:N	2.41	0.46
11:T:37:TYR:O	11:T:41:VAL:HG13	2.16	0.46
12:U:63:ARG:HH21	13:V:36:ARG:HH12	1.62	0.46
14:X:-25:DC:O2	15:Y:26:DG:N2	2.49	0.46
1:B:948:LEU:HD11	1:B:1149:ARG:HD2	1.97	0.46
3:E:287:TYR:O	3:E:291:LYS:N	2.45	0.45
7:I:11:LEU:HD23	8:J:170:LEU:H	1.81	0.45
14:X:-51:DG:O6	15:Y:50:DA:N6	2.49	0.45
1:A:833:THR:HG22	4:F:82:LEU:HD12	1.97	0.45
2:D:184:ASP:HB3	2:D:207:SER:HA	1.98	0.45
1:B:1135:ILE:HD12	1:B:1282:ASP:HA	1.98	0.45
12:Q:113:HIS:CG	12:U:126:LEU:HD22	2.51	0.45
10:S:14:ALA:HB1	14:X:-43:DA:H4'	1.99	0.45
12:U:48:LEU:HD23	12:U:51:ILE:HD12	1.98	0.45
2:C:335:ASP:N	2:C:335:ASP:OD1	2.47	0.45
2:D:51:LEU:HA	2:D:54:ASN:HB2	1.97	0.45
11:P:59:MET:HB3	11:P:59:MET:HE3	1.72	0.45
2:C:93:ASN:HB3	5:G:88:ILE:HG23	1.98	0.45
11:T:38:VAL:HA	11:T:41:VAL:HG22	1.98	0.45
1:B:930:HIS:HA	1:B:933:LEU:HB3	1.99	0.45
2:C:299:LYS:HB2	2:C:305:MET:HE1	1.99	0.45
1:A:979:PHE:HZ	1:A:1152:THR:HG22	1.81	0.45
2:C:19:ARG:HD2	2:C:141:VAL:HG23	1.98	0.45
2:C:150:HIS:CD2	2:C:190:GLY:HA2	2.48	0.45
8:J:225:PRO:HB2	8:J:227:TYR:CE2	2.52	0.45
1:B:767:CYS:O	1:B:768:SER:C	2.59	0.45
2:D:244:ASP:CG	2:D:245:ALA:H	2.25	0.45
1:A:680:HIS:O	1:A:683:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Q:49:ARG:HH11	12:Q:53:ARG:HH22	1.65	0.44
12:Q:126:LEU:HD22	12:U:113:HIS:CG	2.53	0.44
12:U:69:ARG:NH2	15:Y:17:DA:OP1	2.43	0.44
14:X:61:DC:H2"	14:X:62:DG:H5"	1.98	0.44
1:A:862:ILE:HD13	2:C:31:ASN:HD22	1.81	0.44
2:C:177:HIS:O	2:C:202:ARG:NH2	2.50	0.44
2:D:150:HIS:NE2	2:D:187:VAL:O	2.51	0.44
7:I:87:MET:HE2	8:J:351:ARG:HG2	1.99	0.44
15:Y:71:DT:H2"	15:Y:72:DG:C8	2.52	0.44
10:O:53:ALA:HB3	11:P:111:GLY:HA2	2.00	0.44
2:D:67:LYS:N	2:D:129:GLU:OE1	2.48	0.44
1:A:1196:LEU:HB3	1:A:1227:SER:HB2	1.98	0.44
2:C:114:ASP:OD1	2:C:114:ASP:N	2.49	0.44
1:A:925:PHE:HB3	1:A:1229:ARG:HB3	2.00	0.44
1:B:747:LEU:HG	1:B:758:LEU:HD22	1.99	0.44
5:G:138:LEU:HD23	5:G:141:LYS:HD3	1.99	0.44
8:J:201:ILE:HG23	8:J:356:ILE:HG23	1.98	0.44
14:X:-54:DC:H2"	14:X:-53:DA:C8	2.53	0.44
1:A:665:GLU:HA	1:A:668:PHE:HB2	2.00	0.44
1:A:1153:THR:HB	1:A:1157:ARG:NH1	2.33	0.44
1:B:801:ASN:HD21	1:B:930:HIS:HB3	1.83	0.44
13:R:23:ARG:HD2	13:R:24:ASP:HB2	2.00	0.44
1:B:1319:LEU:HB2	1:B:1322:LEU:HG	2.00	0.44
2:C:134:LEU:HD22	2:C:304:PRO:HB3	2.00	0.44
2:C:272:GLY:HA2	2:C:310:GLY:O	2.17	0.44
7:I:66:VAL:HG11	8:J:333:GLN:HE21	1.83	0.44
9:K:475:ASN:HA	9:K:478:ASN:HB2	1.99	0.44
14:X:69:DT:O2	15:Y:-68:DG:N2	2.51	0.44
1:A:924:PHE:CE2	2:C:356:ARG:HD3	2.51	0.43
1:B:1009:ARG:HB3	1:B:1068:ILE:HD13	2.00	0.43
4:F:125:ILE:HG13	4:F:126:LYS:HD2	2.00	0.43
7:I:11:LEU:HD22	7:I:114:ASN:HD21	1.83	0.43
12:Q:119:ILE:HG12	13:R:43:VAL:HG11	2.00	0.43
12:U:73:GLU:HB2	13:V:25:ASN:HD22	1.83	0.43
13:V:23:ARG:HD2	13:V:24:ASP:HB2	2.00	0.43
1:B:770:ARG:HH22	2:D:76:GLN:HA	1.84	0.43
4:F:73:ARG:NH2	4:F:74:ASP:OD1	2.51	0.43
12:U:40:ARG:HH11	14:X:-8:DG:H21	1.65	0.43
12:U:110:CYS:SG	12:U:126:LEU:HD23	2.58	0.43
2:C:151:HIS:CE1	2:C:215:PHE:HE2	2.36	0.43
6:H:140:THR:HB	6:H:227:GLU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:66:VAL:HG22	8:J:334:LEU:HD13	1.99	0.43
8:J:286:ASP:HB2	8:J:289:PHE:HD2	1.83	0.43
1:B:767:CYS:HA	1:B:780:ASP:OD1	2.18	0.43
2:C:280:ARG:HG3	2:C:281:LEU:HG	2.00	0.43
2:D:150:HIS:NE2	2:D:188:HIS:HB3	2.33	0.43
8:J:233:LEU:HD23	8:J:233:LEU:HA	1.90	0.43
13:R:26:ILE:HG13	13:R:55:ARG:HB3	2.01	0.43
1:A:977:PHE:N	1:A:1312:VAL:O	2.47	0.43
1:B:910:ARG:NH1	7:I:20:GLU:OE1	2.51	0.43
10:S:85:LEU:O	10:S:89:ASN:ND2	2.51	0.43
1:A:1194:MET:HE1	1:A:1223:TRP:CE2	2.54	0.43
1:A:826:ARG:HH12	1:A:863:TYR:HB3	1.83	0.43
2:D:61:MET:HE3	2:D:63:ILE:HB	2.00	0.43
6:H:166:TRP:HZ2	6:H:241:SER:HA	1.84	0.43
1:A:686:LEU:O	1:A:690:ASN:N	2.49	0.43
1:B:777:VAL:HG11	2:D:154:LYS:NZ	2.33	0.43
1:B:886:HIS:CE1	1:B:888:ALA:HB3	2.54	0.43
2:D:244:ASP:C	2:D:246:THR:N	2.77	0.43
6:H:94:ARG:HH21	6:H:151:SER:HA	1.84	0.43
12:U:119:ILE:HG12	13:V:43:VAL:HG11	2.01	0.43
14:X:12:DG:O6	15:Y:-13:DA:N6	2.51	0.43
1:A:799:ARG:NH1	2:C:360:MET:SD	2.91	0.42
1:A:975:LEU:HD13	1:A:975:LEU:HA	1.85	0.42
2:C:45:ILE:HD13	2:C:146:ALA:HA	2.00	0.42
2:C:184:ASP:HB3	2:C:207:SER:HA	2.01	0.42
2:C:185:ILE:HD11	2:C:269:LEU:HD11	2.00	0.42
2:C:276:LEU:HD11	2:C:321:THR:HG21	2.01	0.42
2:D:145:TYR:CD1	2:D:309:GLY:HA3	2.53	0.42
3:E:190:GLU:O	3:E:194:ALA:N	2.52	0.42
6:H:140:THR:HA	6:H:229:GLU:HA	1.99	0.42
1:A:1220:GLU:HB2	1:A:1223:TRP:HD1	1.84	0.42
1:B:914:LYS:HZ3	8:J:181:ILE:HG22	1.84	0.42
10:O:68:ASN:CG	10:O:71:ARG:HH11	2.26	0.42
8:J:291:LEU:HD23	8:J:291:LEU:HA	1.80	0.42
10:S:16:THR:C	10:S:18:SER:N	2.77	0.42
2:D:44:ARG:O	2:D:48:ALA:N	2.46	0.42
2:D:187:VAL:HA	2:D:209:HIS:HB2	2.00	0.42
3:E:280:ASN:HD21	8:J:353:LYS:NZ	2.17	0.42
5:G:127:LEU:HD23	5:G:158:HIS:HD2	1.84	0.42
6:H:185:GLY:HA3	6:H:199:LEU:HD22	2.01	0.42
8:J:225:PRO:HB2	8:J:227:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:33:SER:OG	11:P:60:ASN:ND2	2.51	0.42
1:A:837:LYS:NZ	5:G:135:GLY:HA3	2.35	0.42
1:A:878:GLU:HG3	5:G:79:TYR:OH	2.19	0.42
1:B:1002:TYR:CD1	1:B:1254:HIS:HD2	2.38	0.42
1:B:1210:LEU:HB2	1:B:1224:PHE:CZ	2.54	0.42
2:D:34:TYR:HD2	2:D:42:PRO:HD3	1.84	0.42
2:D:191:ASP:HB3	2:D:195:GLU:CD	2.44	0.42
1:B:770:ARG:HA	1:B:770:ARG:HD3	1.60	0.42
2:D:28:ASP:OD1	2:D:28:ASP:N	2.52	0.42
6:H:227:GLU:OE1	6:H:273:LYS:NZ	2.43	0.42
7:I:38:LYS:HA	7:I:41:HIS:CE1	2.55	0.42
1:A:901:LYS:HA	1:A:901:LYS:HD3	1.79	0.42
1:B:814:ARG:NH1	2:D:316:ARG:HH11	2.18	0.42
1:B:898:LEU:O	1:B:902:ASP:N	2.49	0.42
3:E:260:ARG:HH11	8:J:288:PHE:HA	1.84	0.42
1:B:909:GLN:HA	1:B:912:TRP:HB3	2.01	0.42
2:C:212:GLY:C	2:C:214:PHE:H	2.28	0.42
8:J:370:ASN:OD1	8:J:373:ARG:NH1	2.53	0.42
11:T:74:ALA:HB1	11:T:90:GLU:HB3	2.02	0.42
1:A:1291:ARG:HA	1:A:1294:MET:HG2	2.02	0.42
1:B:932:GLY:HA2	1:B:935:PHE:HB3	2.02	0.42
2:C:221:LEU:HD21	2:C:372:VAL:HG13	2.02	0.42
2:D:20:ARG:HB2	2:D:139:CYS:HA	2.01	0.42
6:H:192:SER:H	6:H:196:PHE:HB2	1.85	0.42
13:R:44:LYS:HB2	10:S:115:LEU:HD21	2.02	0.42
11:T:59:MET:HB3	11:T:59:MET:HE3	1.85	0.42
14:X:-19:DG:H2''	14:X:-18:DG:C8	2.55	0.42
1:A:851:LEU:HD23	1:A:851:LEU:HA	1.89	0.41
1:B:815:HIS:ND1	1:B:818:ASP:OD2	2.52	0.41
1:B:857:HIS:CE1	1:B:860:MET:HG2	2.55	0.41
10:S:78:ILE:HG23	10:S:82:HIS:HB2	2.03	0.41
13:V:26:ILE:HG13	13:V:55:ARG:HB3	2.01	0.41
15:Y:53:DT:H2''	15:Y:54:DG:C8	2.55	0.41
1:B:907:ARG:HA	1:B:910:ARG:HE	1.85	0.41
1:B:917:ARG:HB3	1:B:921:GLN:OE1	2.20	0.41
1:B:1025:SER:HA	1:B:1063:MET:N	2.35	0.41
1:B:1236:ALA:HB1	1:B:1239:LEU:HB2	2.02	0.41
15:Y:-59:DT:H6	15:Y:-59:DT:H2'	1.64	0.41
1:A:1242:ILE:HD12	1:A:1242:ILE:HA	1.91	0.41
2:D:220:GLU:N	2:D:223:ASP:OD2	2.50	0.41
5:G:123:VAL:HB	5:G:157:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:287:TYR:CD2	8:J:354:GLU:HG3	2.54	0.41
14:X:74:DG:N2	15:Y:-73:DC:O2	2.54	0.41
1:A:801:ASN:N	1:A:801:ASN:OD1	2.49	0.41
1:A:948:LEU:HD22	1:A:1149:ARG:HG2	2.03	0.41
1:B:1190:GLN:HE22	1:B:1223:TRP:CG	2.39	0.41
2:C:166:ILE:HG23	2:C:268:VAL:HG11	2.02	0.41
2:D:239:ARG:HB2	2:D:364:ASN:HB2	2.02	0.41
4:F:31:ASN:O	4:F:34:SER:OG	2.37	0.41
10:S:13:LYS:C	10:S:15:LYS:H	2.27	0.41
12:U:108:ASN:ND2	13:V:42:GLY:O	2.53	0.41
1:A:768:SER:N	2:C:80:ASP:OD2	2.53	0.41
1:A:810:ILE:HG23	1:A:916:TRP:CD1	2.56	0.41
1:A:966:TRP:HB3	1:A:967:LEU:H	1.73	0.41
1:B:1002:TYR:HB3	1:B:1254:HIS:NE2	2.35	0.41
1:B:1136:PHE:HD2	1:B:1304:GLU:HA	1.86	0.41
2:C:38:HIS:CD2	2:C:160:PHE:HE1	2.39	0.41
14:X:-24:DT:H6	14:X:-24:DT:H2'	1.65	0.41
1:A:1191:LEU:HD12	1:A:1191:LEU:HA	1.90	0.41
1:B:804:GLU:HG3	1:B:927:SER:HB2	2.02	0.41
1:B:1000:THR:OG1	1:B:1001:ALA:N	2.52	0.41
2:D:35:GLY:O	2:D:38:HIS:ND1	2.46	0.41
1:A:695:ASP:O	5:G:114:ARG:NH1	2.53	0.41
1:A:782:TRP:NE1	2:C:226:VAL:HG11	2.36	0.41
1:A:1225:GLU:O	1:A:1229:ARG:HG3	2.21	0.41
2:C:178:PRO:HA	2:C:202:ARG:HH21	1.85	0.41
5:G:90:ASP:HB2	5:G:92:HIS:CD2	2.56	0.41
9:K:243:THR:OG1	9:K:244:PHE:N	2.53	0.41
10:O:63:LEU:HD11	11:P:38:VAL:HG13	2.02	0.41
11:P:102:GLU:OE2	11:P:106:HIS:NE2	2.54	0.41
12:Q:75:ALA:HB1	12:Q:82:LEU:HD23	2.01	0.41
12:Q:100:LEU:HD11	13:R:58:LEU:HD13	2.02	0.41
10:S:16:THR:O	10:S:17:ARG:C	2.64	0.41
1:A:806:THR:HB	1:A:923:VAL:HG11	2.03	0.41
2:C:340:TYR:CG	3:E:247:TYR:HB3	2.56	0.41
2:D:44:ARG:HH12	2:D:312:GLY:C	2.29	0.41
2:D:58:TYR:HA	2:D:61:MET:HE2	2.02	0.41
2:D:187:VAL:O	2:D:188:HIS:CB	2.68	0.41
10:O:62:ILE:HD13	10:O:62:ILE:HG21	1.85	0.41
1:A:778:LEU:HD21	2:C:171:ILE:HD11	2.03	0.40
1:A:814:ARG:HG2	1:A:916:TRP:CE3	2.56	0.40
1:B:849:PHE:HZ	1:B:888:ALA:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:LYS:C	2:C:232:TYR:H	2.29	0.40
2:C:340:TYR:HD2	3:E:251:CYS:HB2	1.86	0.40
6:H:243:LYS:HA	6:H:247:ILE:HD11	2.02	0.40
12:Q:54:TYR:CE2	13:R:36:ARG:HG2	2.55	0.40
10:O:43:VAL:N	14:X:39:DA:OP1	2.40	0.40
14:X:61:DC:O2	15:Y:-60:DG:N2	2.55	0.40
1:B:765:MET:HB2	1:B:781:GLU:HB2	2.03	0.40
1:B:1252:HIS:O	1:B:1255:THR:OG1	2.33	0.40
2:D:45:ILE:O	2:D:49:HIS:N	2.54	0.40
1:B:1250:VAL:H	1:B:1250:VAL:HG22	1.67	0.40
10:S:63:LEU:HD11	11:T:38:VAL:HG13	2.02	0.40
1:A:799:ARG:HE	2:C:360:MET:HG2	1.86	0.40
2:C:165:ASP:O	2:C:169:GLY:N	2.53	0.40
13:V:55:ARG:HH11	13:V:55:ARG:HD2	1.71	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	
1	A	548/683 (80%)	501 (91%)	46 (8%)	1 (0%)	43	76
1	B	440/683 (64%)	383 (87%)	51 (12%)	6 (1%)	9	36
2	C	383/385 (100%)	352 (92%)	29 (8%)	2 (0%)	24	60
2	D	367/385 (95%)	334 (91%)	31 (8%)	2 (0%)	24	60
3	E	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	14	48
4	F	162/311 (52%)	160 (99%)	2 (1%)	0	100	100
5	G	119/121 (98%)	113 (95%)	6 (5%)	0	100	100
6	H	174/211 (82%)	156 (90%)	17 (10%)	1 (1%)	21	56
7	I	103/105 (98%)	99 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	J	151/218 (69%)	139 (92%)	12 (8%)	0	100	100
9	K	36/249 (14%)	36 (100%)	0	0	100	100
10	O	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
10	S	105/107 (98%)	98 (93%)	5 (5%)	2 (2%)	6	30
11	P	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
11	T	89/93 (96%)	85 (96%)	4 (4%)	0	100	100
12	Q	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
12	U	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
13	R	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
13	V	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
All	All	3335/4224 (79%)	3099 (93%)	221 (7%)	15 (0%)	31	65

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	S	16	THR
1	A	1321	ASP
1	B	766	PRO
1	B	778	LEU
2	D	188	HIS
10	S	15	LYS
1	B	781	GLU
2	C	214	PHE
6	H	198	LYS
1	B	1233	ASN
2	C	215	PHE
1	B	875	ARG
2	D	191	ASP
1	B	769	GLY
3	E	220	HIS

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	A	524/635 (82%)	524 (100%)	0	100	100
1	B	426/635 (67%)	412 (97%)	14 (3%)	33	67
2	C	327/327 (100%)	322 (98%)	5 (2%)	57	80
2	D	312/327 (95%)	310 (99%)	2 (1%)	78	88
3	E	111/111 (100%)	110 (99%)	1 (1%)	70	85
4	F	155/275 (56%)	155 (100%)	0	100	100
5	G	112/112 (100%)	111 (99%)	1 (1%)	70	85
6	H	163/192 (85%)	163 (100%)	0	100	100
7	I	101/101 (100%)	101 (100%)	0	100	100
8	J	146/199 (73%)	146 (100%)	0	100	100
9	K	38/232 (16%)	38 (100%)	0	100	100
10	O	84/84 (100%)	84 (100%)	0	100	100
10	S	84/84 (100%)	83 (99%)	1 (1%)	63	82
11	P	80/80 (100%)	80 (100%)	0	100	100
11	T	78/80 (98%)	77 (99%)	1 (1%)	61	81
12	Q	86/86 (100%)	86 (100%)	0	100	100
12	U	85/86 (99%)	85 (100%)	0	100	100
13	R	66/66 (100%)	64 (97%)	2 (3%)	36	69
13	V	66/66 (100%)	64 (97%)	2 (3%)	36	69
All	All	3044/3778 (81%)	3015 (99%)	29 (1%)	65	84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	765	MET
1	B	767	CYS
1	B	770	ARG
1	B	771	ASP
1	B	772	ASP
1	B	773	MET
1	B	774	CYS
1	B	775	TRP
1	B	776	GLU
1	B	778	LEU
1	B	779	ASN
1	B	780	ASP

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Mol	Chain	Res	Type
1	B	920	GLU
1	B	1137	ASN
2	C	185	ILE
2	C	230	LYS
2	C	332	VAL
2	C	356	ARG
2	C	392	ASN
2	D	189	HIS
2	D	338	LEU
3	E	220	HIS
5	G	106	GLU
13	R	92	ARG
13	R	96	THR
10	S	16	THR
11	T	58	ILE
13	V	92	ARG
13	V	96	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	678	ASN
1	A	680	HIS
1	A	690	ASN
1	A	836	ASN
1	A	844	ASN
1	A	937	GLN
1	A	983	ASN
1	A	1206	GLN
1	A	1252	HIS
1	A	1274	ASN
1	B	779	ASN
1	B	801	ASN
1	B	815	HIS
1	B	937	GLN
1	B	959	GLN
1	B	1038	GLN
1	B	1137	ASN
1	B	1141	ASN
1	B	1150	HIS
1	B	1233	ASN
1	B	1254	HIS

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Mol	Chain	Res	Type
2	C	38	HIS
2	C	105	ASN
2	C	235	ASN
2	C	317	ASN
2	C	331	ASN
2	C	379	ASN
2	C	392	ASN
2	C	393	HIS
2	D	43	HIS
2	D	105	ASN
2	D	209	HIS
2	D	330	ASN
2	D	359	ASN
2	D	375	ASN
2	D	379	ASN
3	E	204	GLN
3	E	239	HIS
3	E	243	GLN
3	E	253	ASN
3	E	268	HIS
3	E	280	ASN
4	F	61	GLN
4	F	96	GLN
4	F	139	ASN
5	G	82	ASN
5	G	92	HIS
5	G	100	HIS
5	G	126	ASN
5	G	158	HIS
5	G	183	GLN
5	G	190	ASN
6	H	137	ASN
6	H	197	HIS
6	H	205	ASN
6	H	209	GLN
7	I	41	HIS
7	I	59	ASN
7	I	114	ASN
8	J	230	ASN
8	J	232	ASN
8	J	238	HIS
8	J	346	GLN

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Continued from previous page...

Mol	Chain	Res	Type
8	J	378	ASN
9	K	463	ASN
10	O	73	ASN
10	O	104	GLN
11	P	60	ASN
12	Q	113	HIS
13	R	27	GLN
10	S	24	GLN
10	S	73	ASN
10	S	89	ASN
11	T	46	HIS
13	V	25	ASN
13	V	27	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

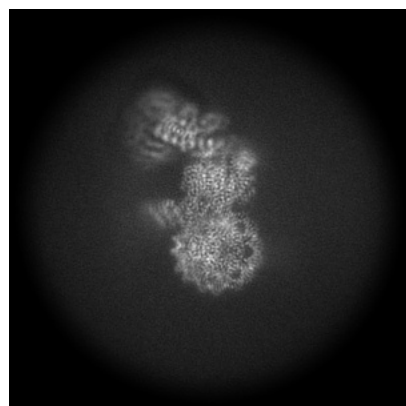
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64741. These allow visual inspection of the internal detail of the map and identification of artifacts.

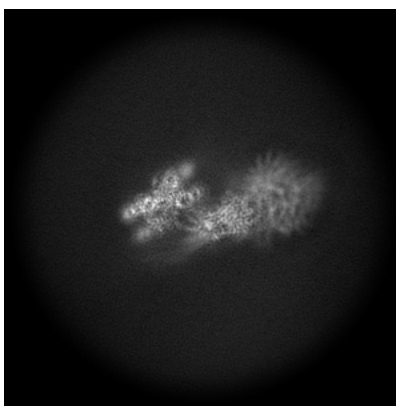
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

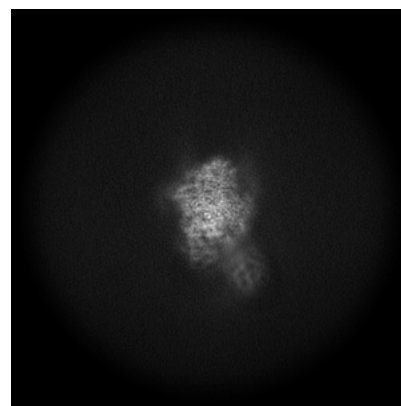
6.1.1 Primary map



X



Y

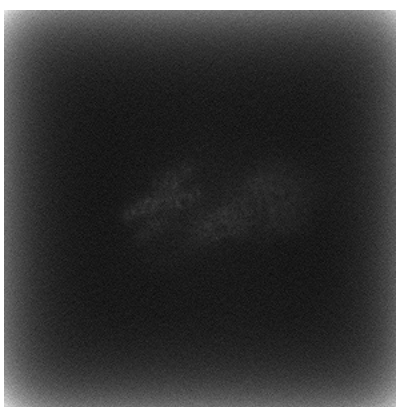


Z

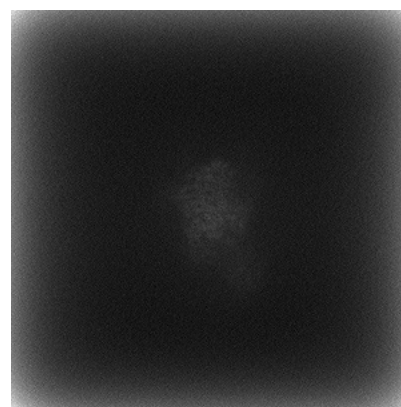
6.1.2 Raw map



X



Y

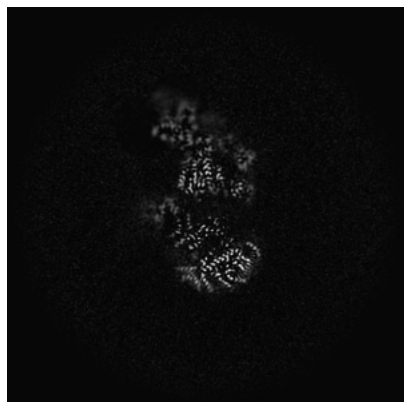


Z

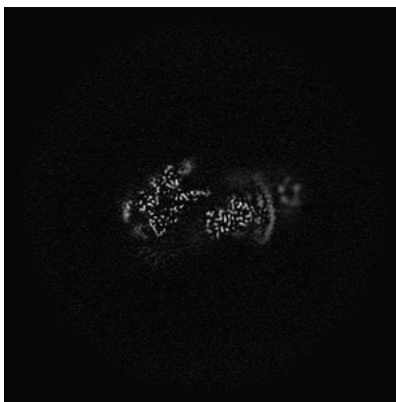
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

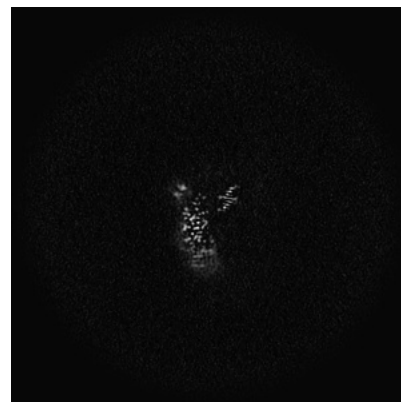
6.2.1 Primary map



X Index: 300

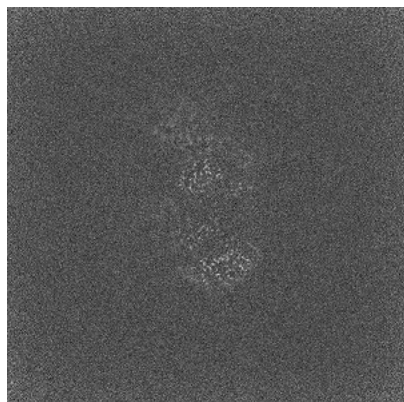


Y Index: 300

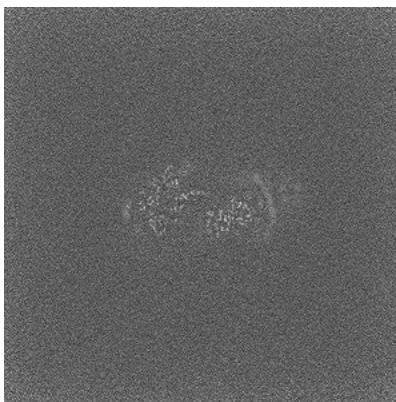


Z Index: 300

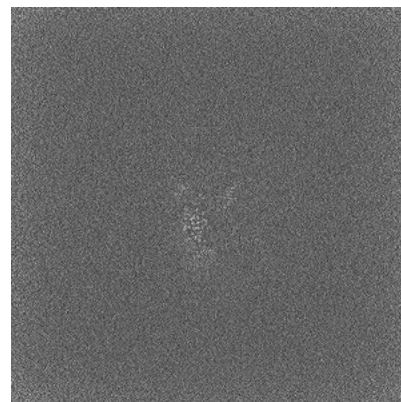
6.2.2 Raw map



X Index: 300



Y Index: 300

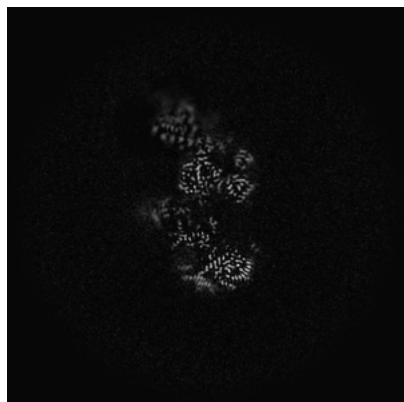


Z Index: 300

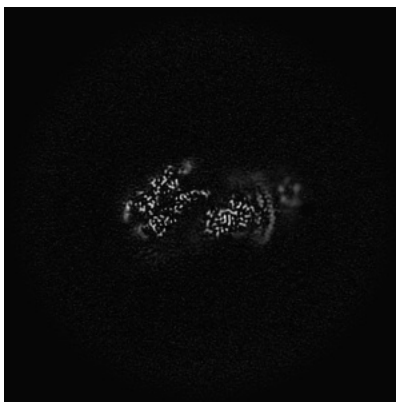
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

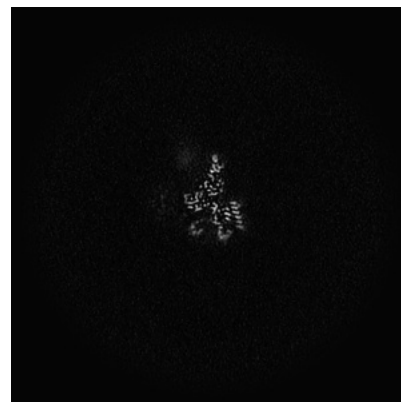
6.3.1 Primary map



X Index: 296

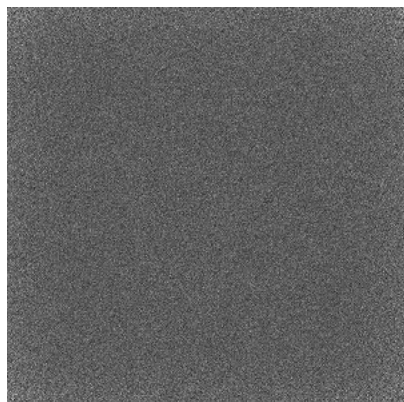


Y Index: 299

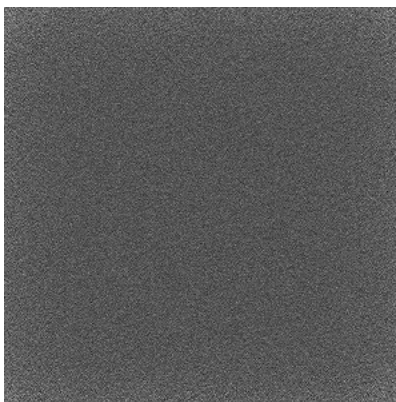


Z Index: 224

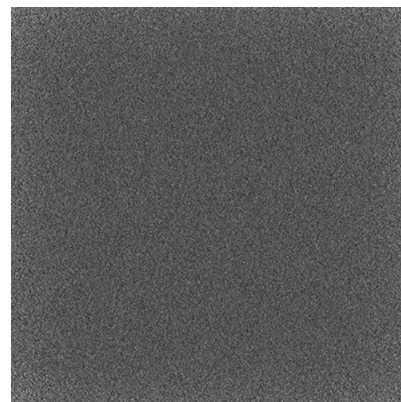
6.3.2 Raw map



X Index: 0



Y Index: 0

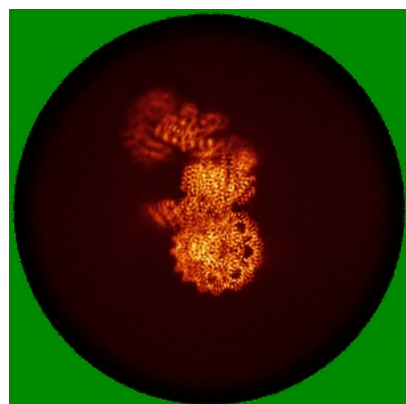


Z Index: 599

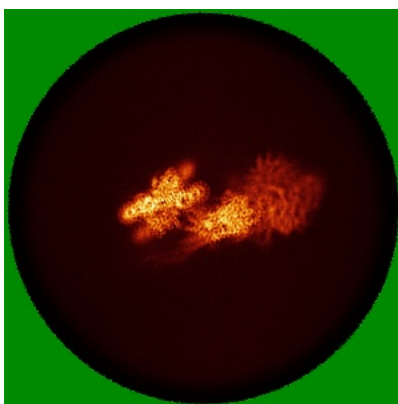
The images above show the largest variance slices of the map in three orthogonal directions.

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

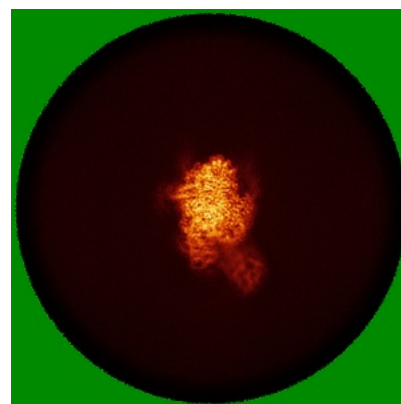
6.4.1 Primary map



X

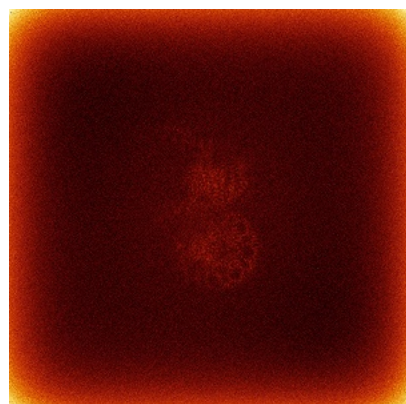


Y

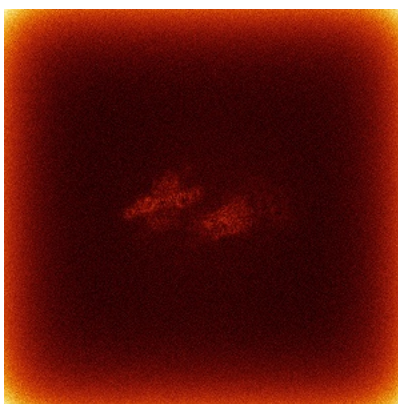


Z

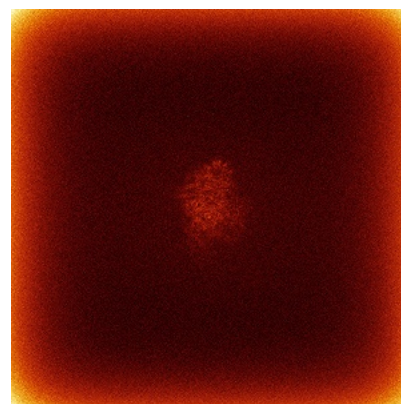
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



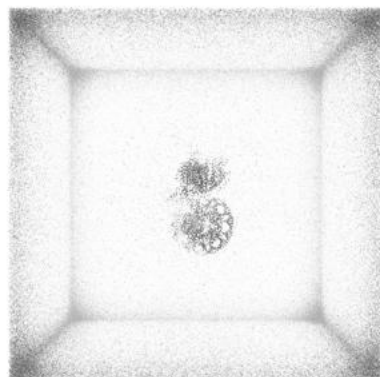
Y



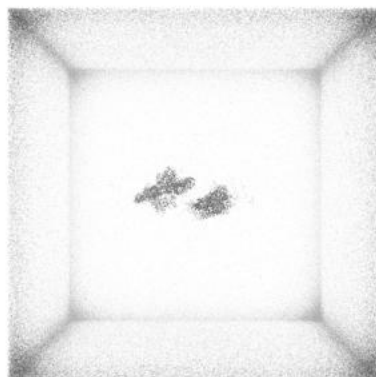
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

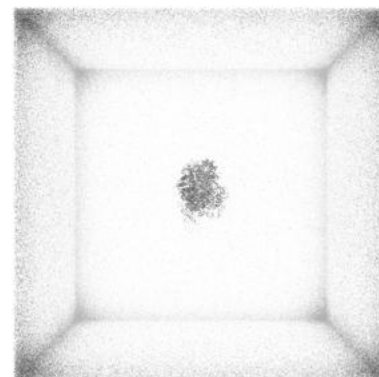
6.5.2 Raw map



X



Y



Z

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

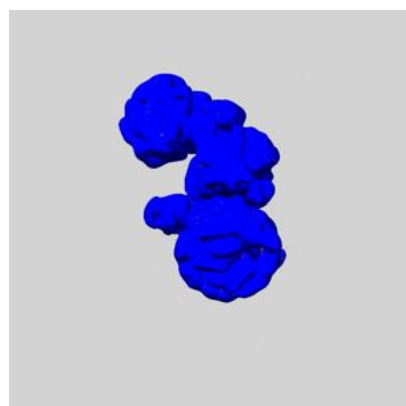
6.6 Mask visualisation [i](#)

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

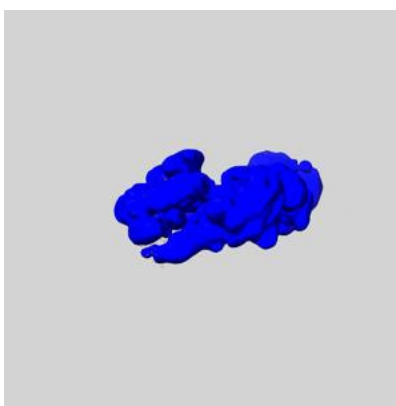
A mask typically either:

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

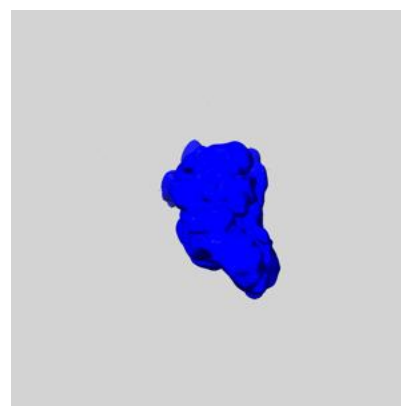
6.6.1 emd_64741_msk_1.map [i](#)



X



Y

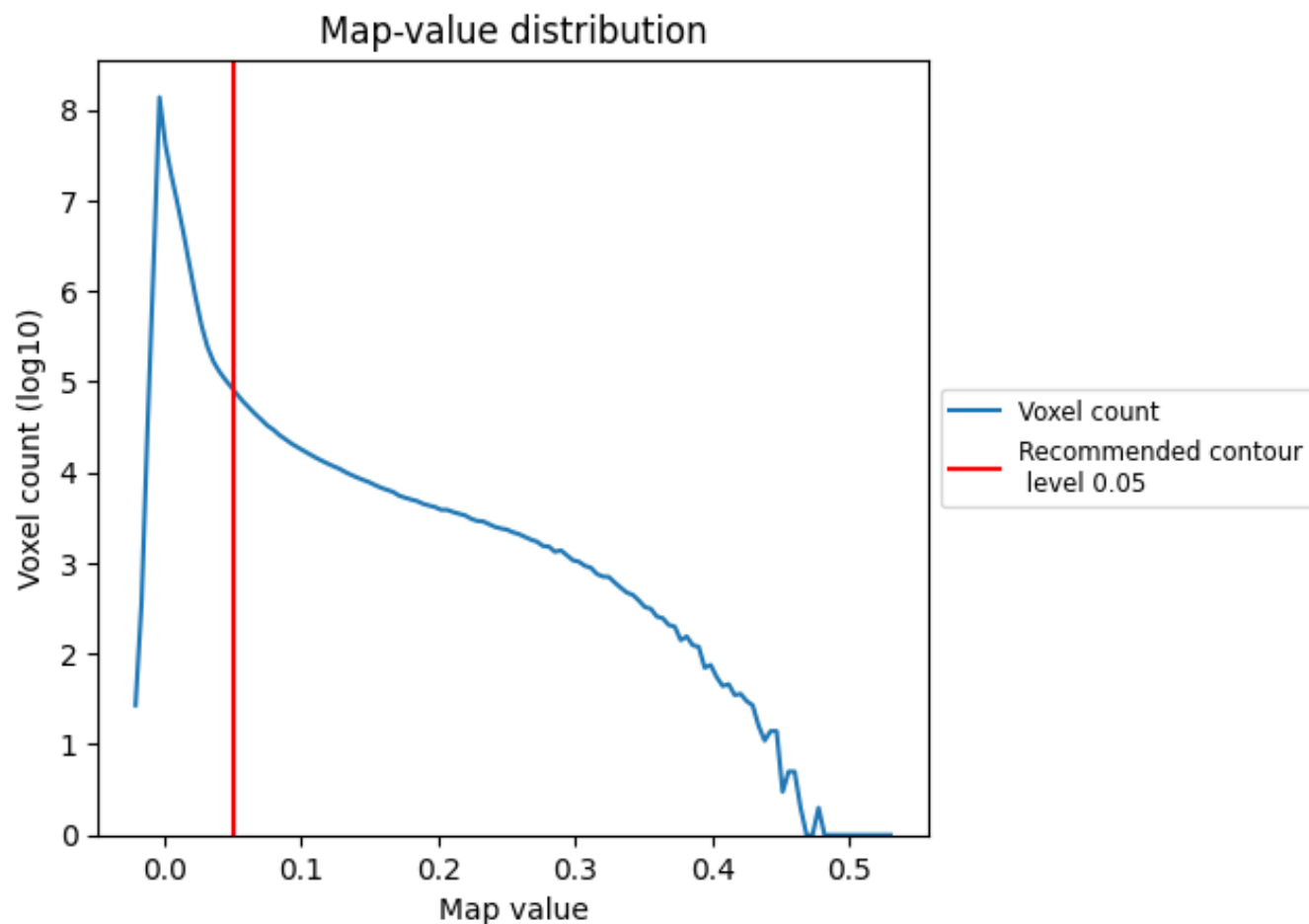


Z

7 Map analysis [i](#)

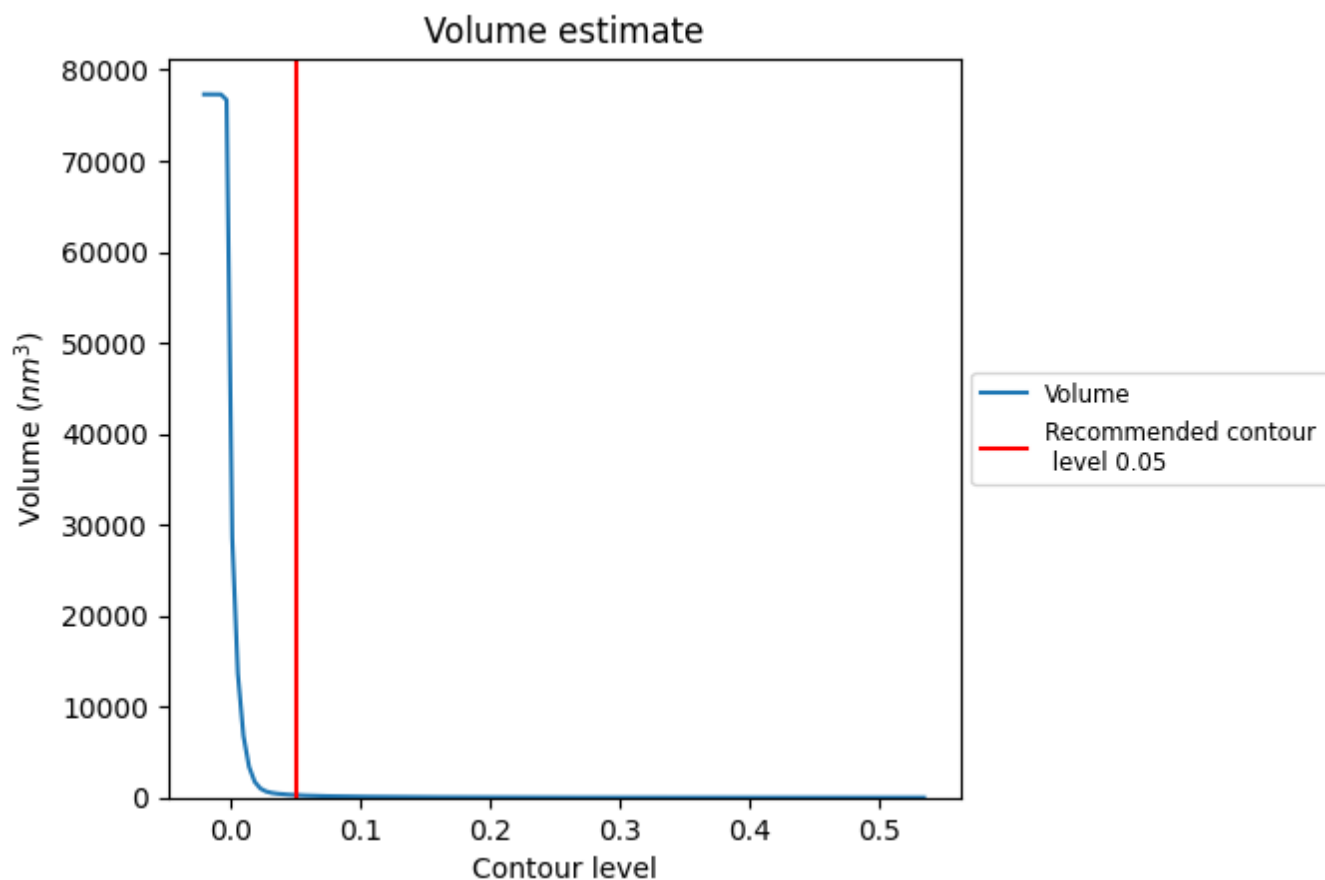
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

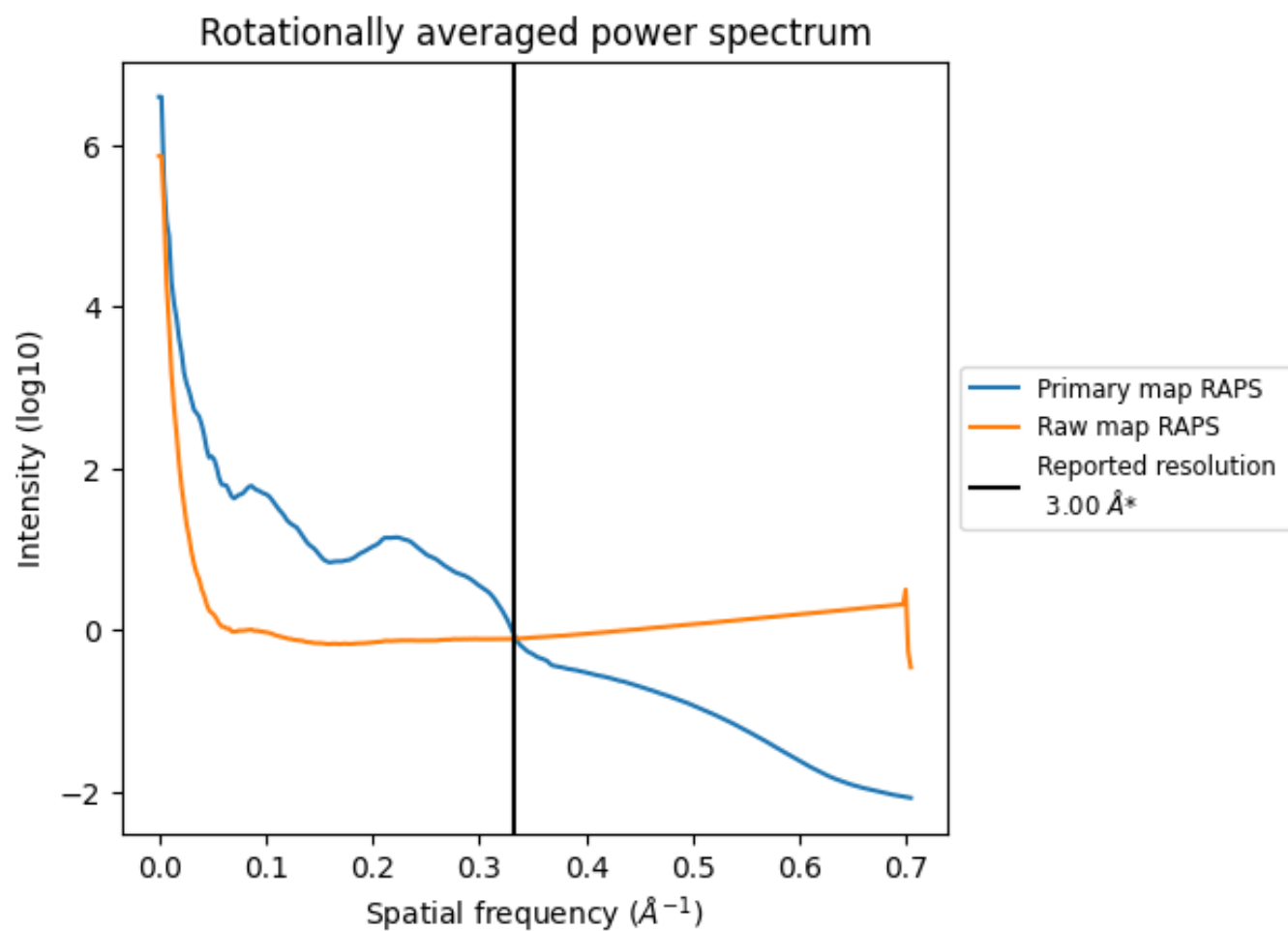
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 268 nm^3 ; this corresponds to an approximate mass of 242 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 ⓘ

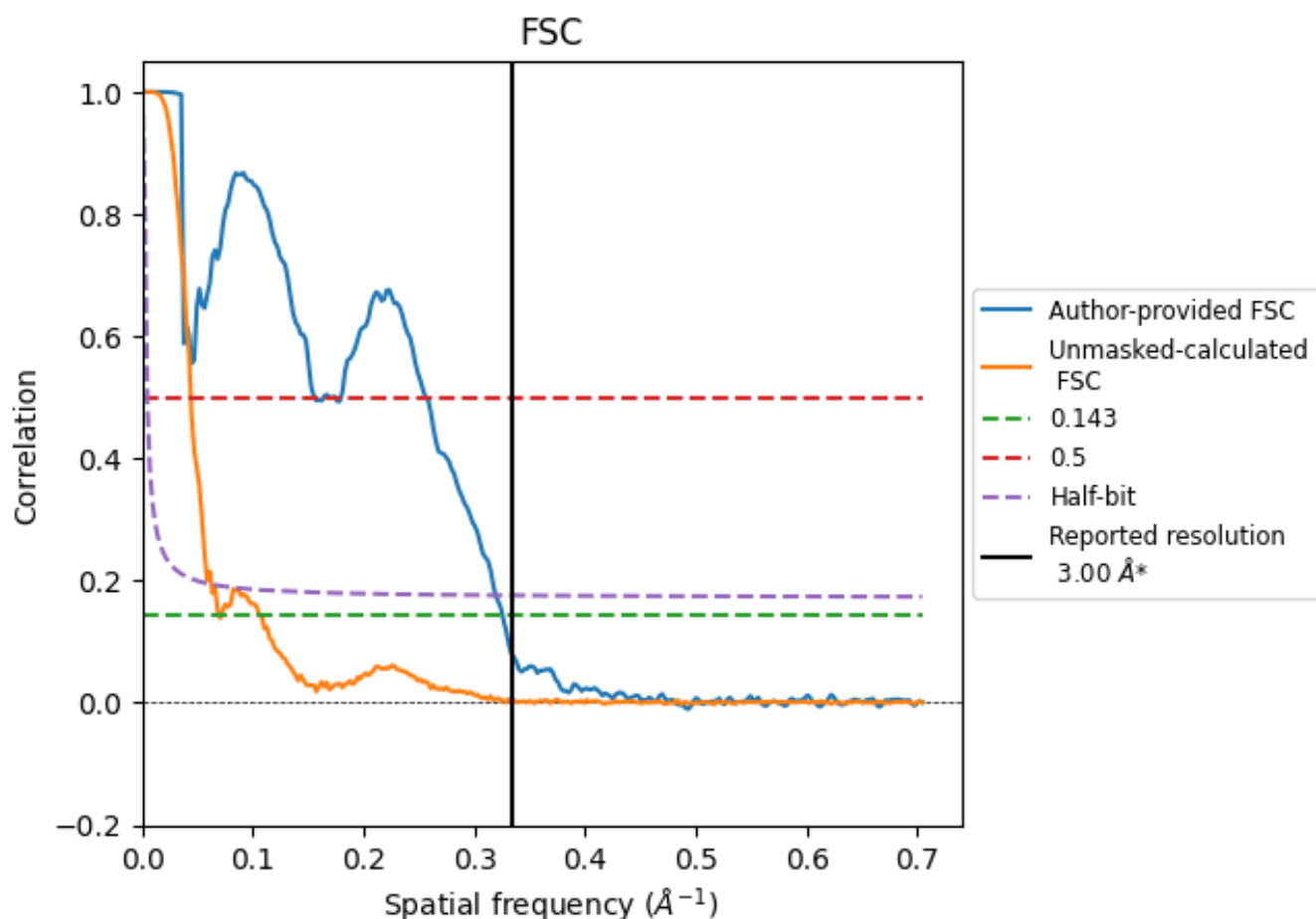


*Reported resolution corresponds to spatial frequency of 0.333 \AA^{-1}

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 0.333 \AA^{-1}

8.2 Resolution estimates [i](#)

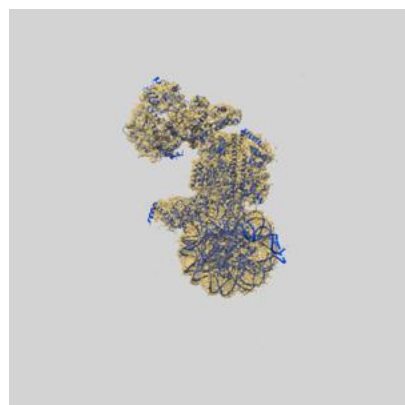
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.07	6.42	3.13
Unmasked-calculated*	14.39	22.78	16.03

*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 14.39 differs from the reported value 3.0 by more than 10 %

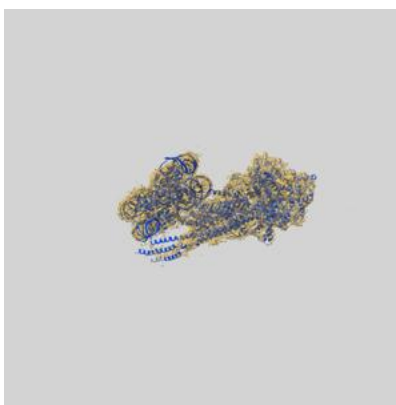
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64741 and PDB model 9V2V. Per-residue inclusion information can be found in section [3](#) on page [7](#).

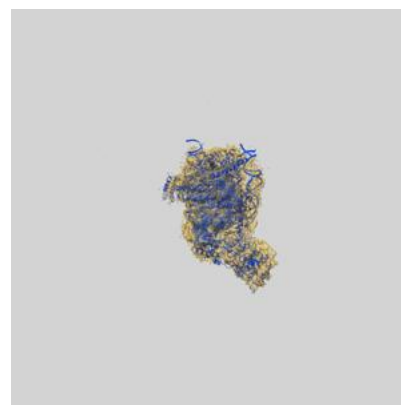
9.1 Map-model overlay [i](#)



X



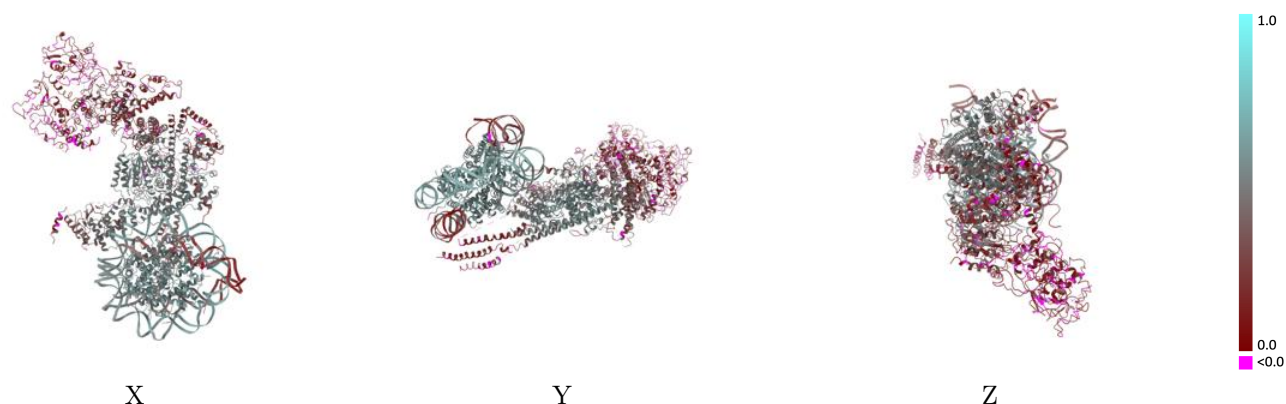
Y



Z

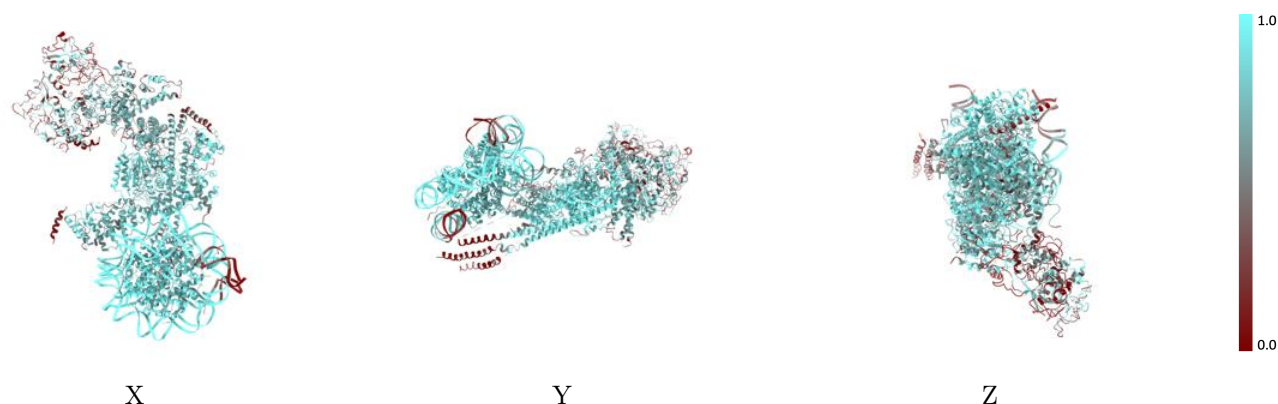
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



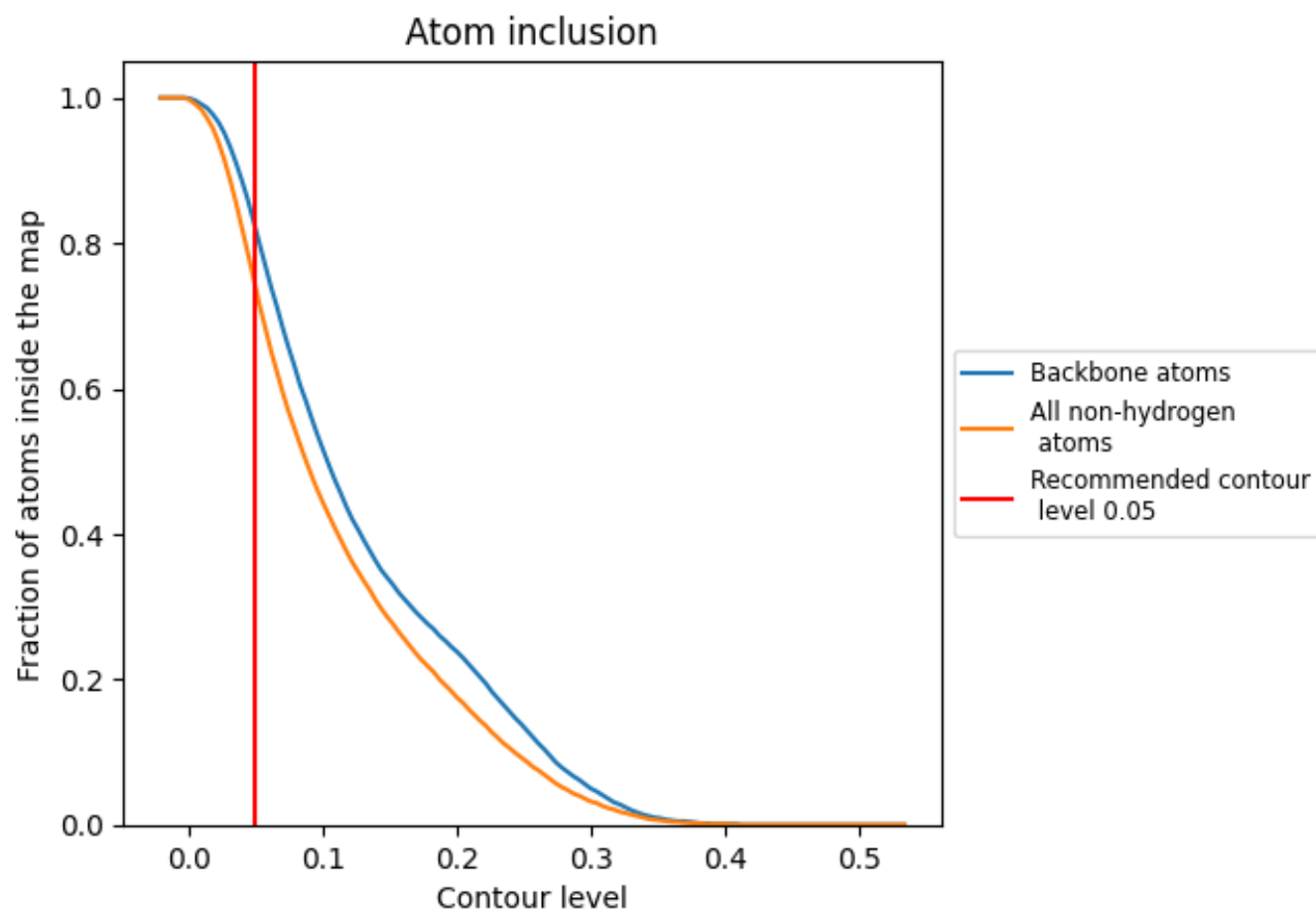
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7380	 0.3840
A	 0.7610	 0.4030
B	 0.4730	 0.1420
C	 0.9050	 0.5200
D	 0.7010	 0.2340
E	 0.6090	 0.3230
F	 0.6340	 0.3580
G	 0.7570	 0.3660
H	 0.3540	 0.1110
I	 0.6390	 0.2760
J	 0.6810	 0.3600
K	 0.2160	 0.1410
O	 0.9320	 0.5560
P	 0.9540	 0.5550
Q	 0.9270	 0.5620
R	 0.9770	 0.5850
S	 0.8430	 0.5530
T	 0.8280	 0.5280
U	 0.8970	 0.5640
V	 0.9050	 0.5790
X	 0.8390	 0.4630
Y	 0.8420	 0.4740

