



Full wwPDB EM Validation Report ⓘ

May 18, 2026 – 01:38 PM JST

PDB ID : 9V2W / pdb_00009v2w
EMDB ID : EMD-64742
Title : Cryo-EM structure of the histone deacetylase complex Rpd3L in complex with di-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 : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

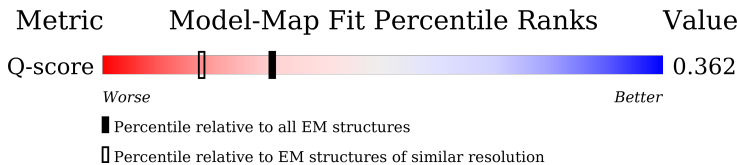
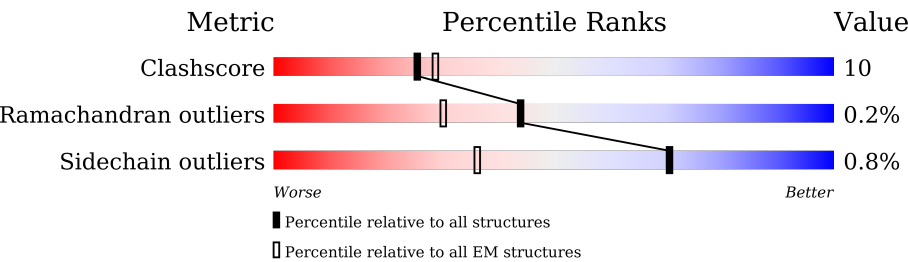
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1096	<div><div>6%</div><div>50%</div><div>13%</div><div>37%</div></div>
2	B	107	<div><div>79%</div><div>21%</div></div>
2	M	107	<div><div>76%</div><div>24%</div></div>
2	O	107	<div><div>73%</div><div>27%</div></div>

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Mol	Chain	Length	Quality of chain
2	S	107	
3	C	378	
4	D	93	
4	N	93	
4	P	93	
4	T	93	
5	E	119	
6	F	311	
7	G	119	
8	H	98	
8	Q	98	
8	U	98	
8	W	98	
9	I	105	
10	J	206	
11	K	249	
12	L	79	
12	R	79	
12	V	79	
12	Z	79	
13	X	329	
14	Y	329	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 39938 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	694	Total	C	N	O	S	0	0
			5799	3728	979	1076	16		

- Molecule 2 is a protein called Histone H2A.

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

- Molecule 3 is a protein called Histone deacetylase RPD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	378	Total	C	N	O	S	0	0
			2999	1908	506	560	25		

- Molecule 4 is a protein called Histone H2B.

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

- Molecule 5 is a protein called Transcriptional regulatory protein DEP1.

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

- Molecule 6 is a protein called Transcriptional regulatory protein SDS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1328	831	238	258	1		

- Molecule 7 is a protein called Transcriptional regulatory protein SAP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	119	Total	C	N	O	S	0	0
			1002	630	185	185	2		

- Molecule 8 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	97	Total	C	N	O	S	0	0
			800	506	153	138	3		
8	Q	98	Total	C	N	O	S	0	0
			811	512	157	139	3		
8	U	97	Total	C	N	O	S	0	0
			800	506	153	138	3		
8	W	98	Total	C	N	O	S	0	0
			811	512	157	139	3		

- Molecule 9 is a protein called Transcriptional regulatory protein PHO23.

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

- Molecule 10 is a protein called Transcriptional regulatory protein RXT2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1167	741	210	214	2		

- Molecule 11 is a protein called Histone deacetylase complex subunit CTI6.

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

- Molecule 12 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	77	Total	C	N	O	S	0	0
			618	391	119	107	1		
12	R	79	Total	C	N	O	S	0	0
			637	403	124	109	1		
12	V	79	Total	C	N	O	S	0	0
			637	403	124	109	1		
12	Z	78	Total	C	N	O	S	0	0
			629	397	123	108	1		

- Molecule 13 is a DNA chain called DNA (329-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	X	329	Total	C	N	O	P	0	0
			6786	3211	1286	1961	328		

- Molecule 14 is a DNA chain called DNA (329-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Y	329	Total	C	N	O	P	0	0
			6697	3185	1201	1983	328		

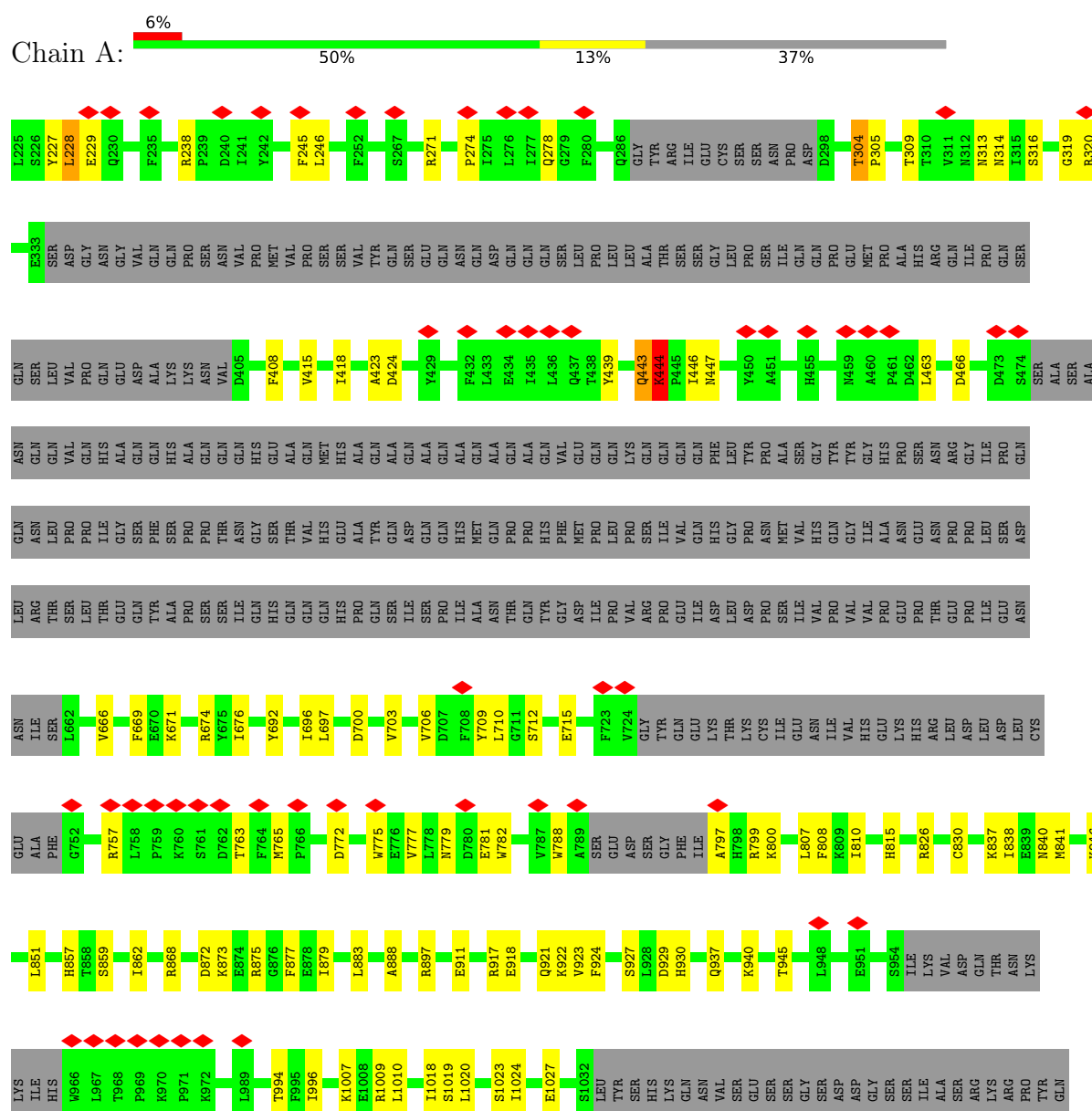
- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

3 Residue-property plots

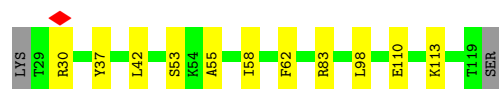
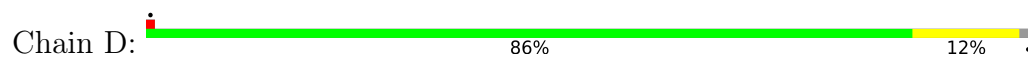
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Transcriptional regulatory protein SIN3

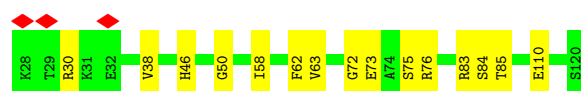
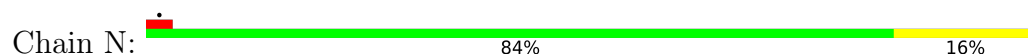




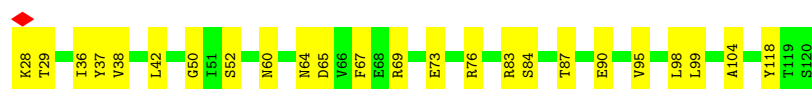
- Molecule 4: Histone H2B



- Molecule 4: Histone H2B



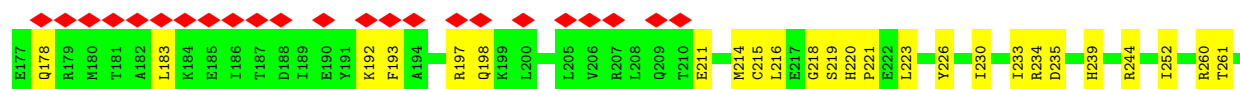
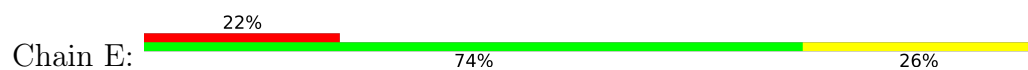
- Molecule 4: Histone H2B



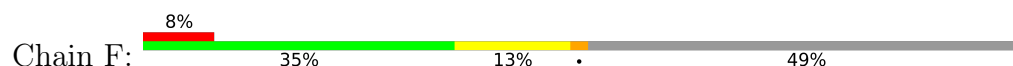
- Molecule 4: Histone H2B

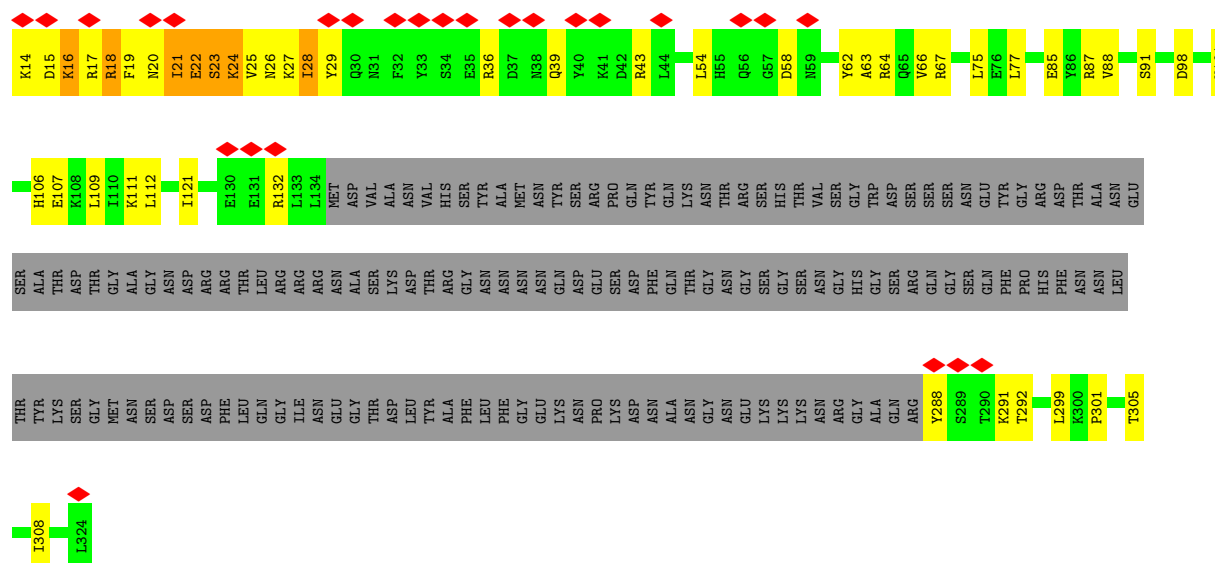


- Molecule 5: Transcriptional regulatory protein DEP1

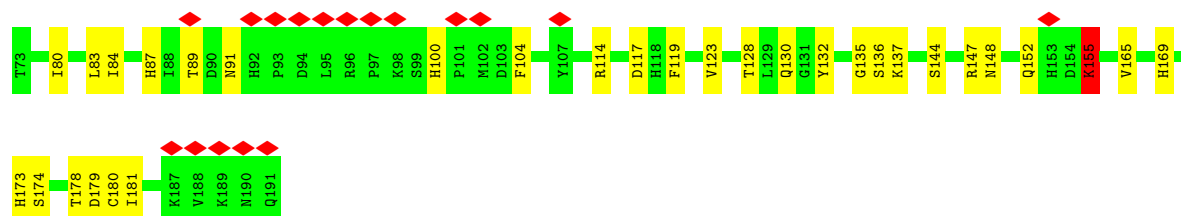
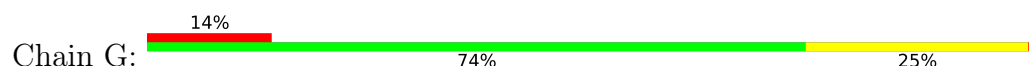


- Molecule 6: Transcriptional regulatory protein SDS3

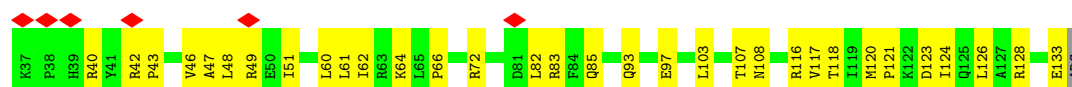




• Molecule 7: Transcriptional regulatory protein SAP30



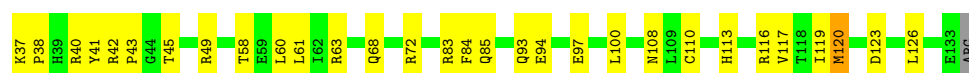
• Molecule 8: Histone H3



• Molecule 8: Histone H3



• Molecule 8: Histone H3

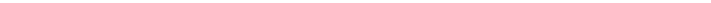


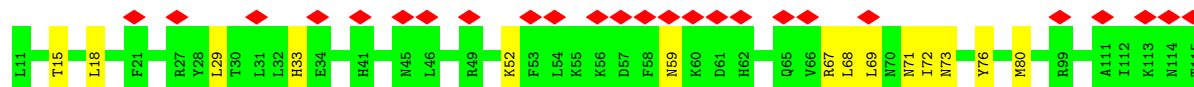
- Molecule 8: Histone H3

Chain W: 76% 24%



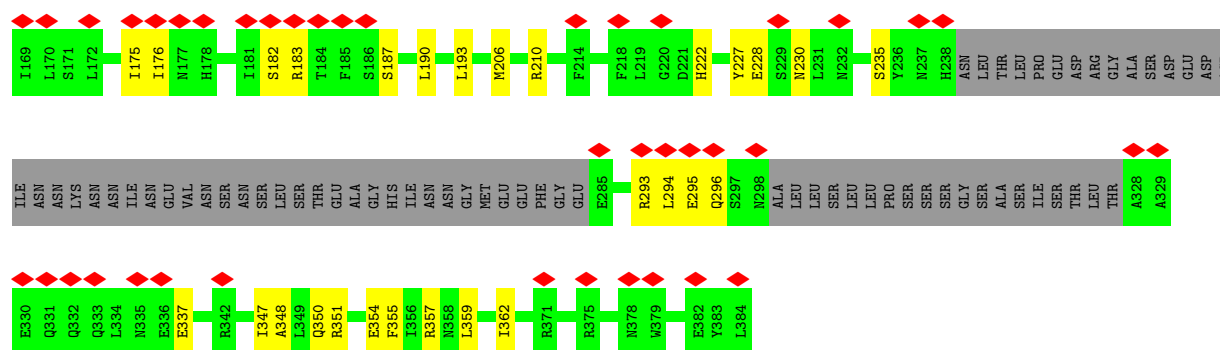
- Molecule 9: Transcriptional regulatory protein PHO23

Chain I:  24% 87% 13%



- Molecule 10: Transcriptional regulatory protein RXT2

Chain J: 

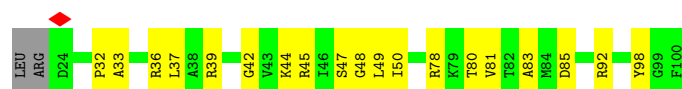


- Molecule 11: Histone deacetylase complex subunit CTI6

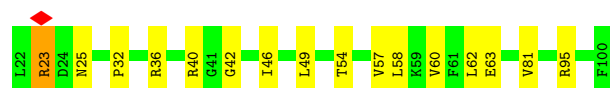
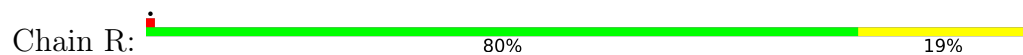
Chain K:  9% 14% 84%



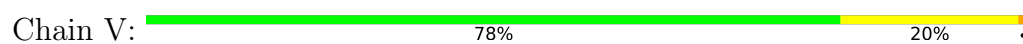
- Molecule 12: Histone H4



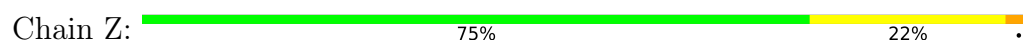
- Molecule 12: Histone H4



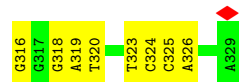
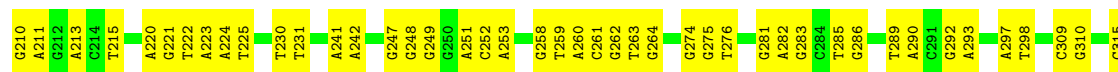
- Molecule 12: Histone H4



- Molecule 12: Histone H4

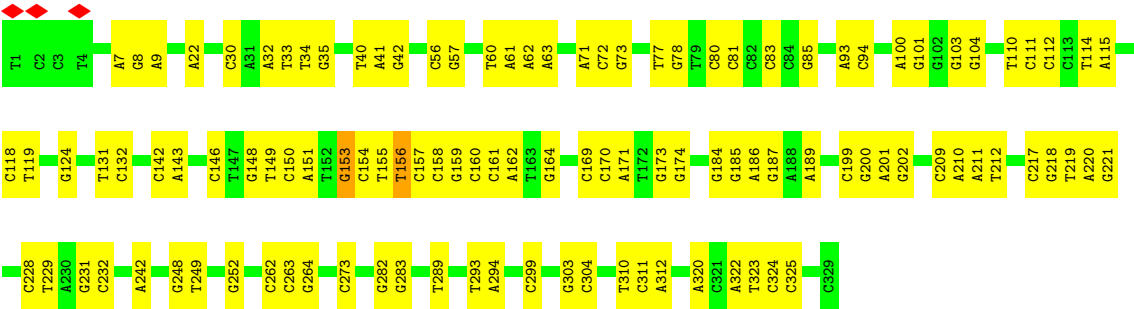


- Molecule 13: DNA (329-MER)



- Molecule 14: DNA (329-MER)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	205066	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	0.519	Depositor
Minimum map value	-0.012	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	0.33	0/5928	0.63	2/7994 (0.0%)
2	B	0.60	0/835	0.63	0/1127
2	M	0.60	0/835	0.63	0/1127
2	O	0.60	0/835	0.66	1/1127 (0.1%)
2	S	0.60	0/835	0.64	0/1127
3	C	0.46	0/3076	0.64	0/4161
4	D	0.41	0/726	0.58	0/978
4	N	0.40	0/741	0.55	0/997
4	P	0.75	0/741	0.64	0/997
4	T	0.82	0/726	0.68	0/978
5	E	0.33	0/1039	0.56	0/1397
6	F	0.42	0/1346	0.70	0/1803
7	G	0.38	0/1026	0.70	1/1383 (0.1%)
8	H	0.39	0/812	0.67	0/1090
8	Q	0.89	0/823	0.83	0/1104
8	U	0.88	0/812	0.78	0/1090
8	W	0.43	0/823	0.64	0/1104
9	I	0.23	0/876	0.59	0/1182
10	J	0.28	0/1185	0.60	0/1594
11	K	0.18	0/344	0.45	0/459
12	L	0.44	0/625	0.66	0/838
12	R	0.88	0/644	0.82	0/863
12	V	0.90	0/644	0.83	0/863
12	Z	0.46	0/636	0.61	0/852
13	X	0.19	0/7626	0.44	2/11779 (0.0%)
14	Y	0.19	0/7500	0.41	2/11564 (0.0%)
All	All	0.43	0/42039	0.58	8/59578 (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
5	E	0	1
7	G	0	1
12	R	0	1
12	Z	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	X	173	DG	P-O3'-C3'	-9.45	106.03	120.20
14	Y	153	DG	P-O3'-C3'	-7.13	109.51	120.20
14	Y	156	DT	P-O3'-C3'	-6.79	110.01	120.20
13	X	172	DG	P-O3'-C3'	-6.72	110.13	120.20
1	A	676	ILE	N-CA-C	-5.86	108.15	113.71
2	O	37	GLY	N-CA-C	-5.62	106.30	115.46
7	G	155	LYS	N-CA-C	-5.41	104.14	111.55
1	A	229	GLU	N-CA-C	-5.36	106.58	113.01

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	219	SER	Peptide
7	G	104	PHE	Peptide
12	R	23	ARG	Sidechain
12	Z	23	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	5799	0	5746	113	0
2	B	825	0	882	16	0
2	M	825	0	882	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	825	0	882	26	0
2	S	825	0	882	37	0
3	C	2999	0	2882	47	0
4	D	715	0	737	16	0
4	N	730	0	755	13	0
4	P	730	0	755	23	0
4	T	715	0	737	25	0
5	E	1022	0	1026	22	0
6	F	1328	0	1340	60	0
7	G	1002	0	977	23	0
8	H	800	0	840	42	0
8	Q	811	0	853	42	0
8	U	800	0	840	33	0
8	W	811	0	853	35	0
9	I	864	0	875	10	0
10	J	1167	0	1189	18	0
11	K	340	0	312	3	0
12	L	618	0	657	27	0
12	R	637	0	681	15	0
12	V	637	0	681	24	0
12	Z	629	0	670	18	0
13	X	6786	0	3688	175	0
14	Y	6697	0	3699	167	0
15	C	1	0	0	0	0
All	All	39938	0	34321	725	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 10.

All (725) 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:A:319:GLY:O	14:Y:161:DC:H5''	1.09	1.27
12:Z:35:ARG:NH1	13:X:262:DG:OP2	1.77	1.18
2:M:11:ARG:NH2	13:X:298:DT:O2	1.79	1.14
12:R:36:ARG:NH2	14:Y:242:DA:OP1	1.83	1.11
2:O:11:ARG:NH2	13:X:119:DT:O2	1.83	1.10
6:F:15:ASP:HB2	6:F:16:LYS:NZ	1.65	1.10
12:V:36:ARG:NH2	13:X:62:DA:OP1	1.83	1.10
4:D:83:ARG:HH12	13:X:220:DA:H3'	1.17	1.05
1:A:319:GLY:O	14:Y:161:DC:C5'	2.06	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:16:THR:HA	14:Y:212:DT:H5''	1.44	0.95
2:S:42:ARG:HA	14:Y:294:DA:OP1	1.69	0.92
8:H:85:GLN:HA	13:X:230:DT:H5''	1.51	0.92
8:H:72:ARG:HH22	13:X:231:DT:P	1.93	0.91
8:W:39:HIS:HD2	13:X:186:DA:O4'	1.53	0.91
4:P:37:TYR:OH	13:X:123:DG:H5''	1.70	0.91
8:W:42:ARG:N	14:Y:146:DC:OP1	2.06	0.87
1:A:227:TYR:CZ	13:X:182:DC:OP1	2.28	0.87
1:A:319:GLY:C	14:Y:161:DC:H5''	2.00	0.86
14:Y:155:DT:H3'	14:Y:156:DT:C4	2.11	0.85
4:T:53:SER:N	13:X:21:DC:OP1	2.09	0.85
8:H:72:ARG:NH2	13:X:231:DT:OP1	2.09	0.85
2:O:77:ARG:HD2	14:Y:201:DA:H4'	1.56	0.84
6:F:15:ASP:HB2	6:F:16:LYS:HZ3	1.39	0.84
8:H:42:ARG:HG2	13:X:324:DC:OP1	1.77	0.84
4:D:83:ARG:NH1	13:X:220:DA:H3'	1.94	0.83
8:H:46:VAL:HB	14:Y:85:DG:OP1	1.79	0.82
8:W:41:TYR:HD2	13:X:264:DG:OP1	1.63	0.81
4:T:37:TYR:HE1	14:Y:303:DG:OP1	1.65	0.79
8:Q:83:ARG:HE	14:Y:232:DC:H5'	1.47	0.79
8:U:41:TYR:HA	13:X:145:DC:H5''	1.64	0.78
6:F:15:ASP:HB2	6:F:16:LYS:HZ1	1.49	0.76
8:W:41:TYR:CD2	13:X:264:DG:OP1	2.40	0.74
8:W:46:VAL:HB	13:X:263:DT:P	2.28	0.74
8:Q:68:GLN:HE21	8:Q:72:ARG:HH21	1.35	0.73
1:A:319:GLY:HA3	14:Y:161:DC:P	2.29	0.73
2:S:42:ARG:CA	14:Y:294:DA:OP1	2.37	0.72
4:T:37:TYR:OH	14:Y:303:DG:H5''	1.90	0.72
8:U:116:ARG:HD3	13:X:72:DA:H3'	1.70	0.72
5:E:214:MET:HE3	6:F:121:ILE:HG12	1.70	0.71
2:M:57:TYR:HB2	4:N:110:GLU:HG2	1.72	0.71
6:F:16:LYS:HE2	6:F:17:ARG:CZ	2.21	0.70
4:D:30:ARG:HH21	13:X:207:DC:H4'	1.57	0.70
8:W:39:HIS:CD2	13:X:186:DA:O4'	2.42	0.70
2:S:43:VAL:N	14:Y:294:DA:OP1	2.25	0.70
4:P:36:ILE:HD11	13:X:123:DG:O5'	1.91	0.70
14:Y:156:DT:H2''	14:Y:157:DC:C5	2.26	0.70
3:C:23:TYR:HB3	3:C:63:ILE:HG12	1.74	0.70
4:T:37:TYR:CE1	14:Y:303:DG:OP1	2.45	0.70
2:S:42:ARG:HG2	14:Y:294:DA:H5'	1.73	0.69
6:F:15:ASP:CB	6:F:16:LYS:HZ3	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:154:DC:H2'	13:X:155:DA:H8	1.57	0.69
8:H:40:ARG:HH12	8:H:43:PRO:HD3	1.58	0.69
8:W:107:THR:HG21	8:W:124:ILE:HD13	1.75	0.68
5:E:252:ILE:HG12	6:F:87:ARG:HE	1.57	0.68
4:T:95:VAL:HG13	4:T:99:LEU:HD12	1.76	0.68
2:S:11:ARG:NH1	13:X:32:DA:C2	2.60	0.68
8:H:60:LEU:HD11	2:M:104:GLN:HE22	1.59	0.67
12:Z:23:ARG:C	12:Z:25:ASN:H	2.03	0.67
1:A:408:PHE:HB2	1:A:444:LYS:HZ1	1.59	0.67
1:A:424:ASP:HA	14:Y:171:DA:N7	2.09	0.67
4:D:53:SER:N	13:X:200:DC:OP1	2.22	0.67
8:W:39:HIS:CE1	14:Y:146:DC:C5'	2.78	0.67
8:H:118:THR:N	13:X:251:DA:OP1	2.27	0.66
2:B:42:ARG:HA	14:Y:115:DA:OP1	1.96	0.66
2:S:17:ARG:HE	13:X:32:DA:P	2.19	0.66
8:Q:79:LYS:HD3	8:Q:82:LEU:HD13	1.78	0.66
12:V:45:ARG:HA	14:Y:263:DC:OP1	1.96	0.66
8:Q:46:VAL:HB	13:X:84:DT:P	2.36	0.66
10:J:222:HIS:CE1	10:J:296:GLN:H	2.15	0.65
4:D:30:ARG:HH21	13:X:207:DC:C4'	2.10	0.65
5:E:216:LEU:HG	5:E:218:GLY:H	1.62	0.65
8:Q:121:PRO:HG2	12:R:49:LEU:HD12	1.79	0.65
2:O:27:VAL:HG13	2:O:48:PRO:HB2	1.79	0.65
4:P:73:GLU:OE1	4:P:76:ARG:NH2	2.30	0.65
6:F:16:LYS:HE2	6:F:17:ARG:NE	2.12	0.65
1:A:917:ARG:NH1	1:A:918:GLU:OE2	2.30	0.64
2:M:42:ARG:HB3	13:X:292:DG:H4'	1.77	0.64
8:U:108:ASN:ND2	12:V:42:GLY:O	2.29	0.64
1:A:1010:LEU:HD21	1:A:1254:HIS:HB2	1.79	0.64
2:S:29:ARG:NH1	4:T:32:GLU:OE2	2.30	0.64
1:A:674:ARG:NH2	14:Y:112:DC:H2'	2.13	0.63
10:J:222:HIS:NE2	10:J:295:GLU:HA	2.14	0.63
8:Q:133:GLU:OE2	12:R:95:ARG:NH2	2.31	0.63
3:C:209:HIS:HE1	3:C:235:ASN:HB3	1.62	0.63
8:H:83:ARG:HH21	14:Y:103:DG:H5'	1.64	0.63
8:H:108:ASN:ND2	12:L:42:GLY:O	2.32	0.62
8:H:120:MET:SD	12:L:47:SER:OG	2.58	0.62
6:F:16:LYS:HD2	6:F:17:ARG:H	1.63	0.62
8:H:46:VAL:HG22	8:H:49:ARG:HH21	1.64	0.62
14:Y:72:DC:H2'	14:Y:73:DG:C8	2.35	0.62
1:A:929:ASP:HB2	1:A:1234:ASN:HD21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:52:SER:HA	14:Y:201:DA:H5''	1.82	0.62
8:U:83:ARG:HG3	12:V:80:THR:HG22	1.82	0.62
1:A:1023:SER:OG	1:A:1273:ARG:NH2	2.32	0.62
4:P:84:SER:H	14:Y:221:DG:P	2.23	0.62
6:F:15:ASP:O	6:F:18:ARG:HB3	1.99	0.62
13:X:172:DG:H2'	14:Y:157:DC:N4	2.15	0.62
1:A:320:ARG:O	14:Y:162:DA:OP1	2.17	0.61
4:D:98:LEU:HD23	12:L:92:ARG:HH21	1.64	0.61
2:S:28:GLY:HA3	13:X:31:DG:H3'	1.82	0.61
9:I:69:LEU:HD12	9:I:72:ILE:HD11	1.82	0.61
2:S:17:ARG:NE	13:X:32:DA:OP2	2.34	0.61
12:V:46:ILE:N	14:Y:263:DC:OP1	2.32	0.61
5:E:193:PHE:HA	5:E:197:ARG:HB2	1.82	0.61
3:C:287:SER:HB3	3:C:357:PRO:HG3	1.82	0.61
4:P:50:GLY:HA3	14:Y:202:DG:OP1	2.00	0.61
4:P:83:ARG:HB3	14:Y:221:DG:OP1	2.00	0.61
8:W:108:ASN:ND2	12:Z:42:GLY:O	2.34	0.61
4:D:37:TYR:OH	14:Y:124:DG:OP1	2.12	0.61
2:O:75:LYS:HB3	13:X:133:DC:OP1	1.99	0.61
2:O:58:LEU:HD11	4:P:99:LEU:HD21	1.82	0.61
8:U:41:TYR:O	14:Y:264:DG:H4'	2.01	0.61
6:F:24:LYS:HA	6:F:27:LYS:HD2	1.83	0.60
8:U:117:VAL:N	13:X:72:DA:OP1	2.30	0.60
10:J:354:GLU:HG2	10:J:357:ARG:HE	1.64	0.60
2:S:32:ARG:HD3	13:X:31:DG:P	2.41	0.60
8:H:117:VAL:H	13:X:251:DA:P	2.24	0.60
1:A:1141:ASN:HD21	1:A:1262:THR:HG22	1.65	0.60
3:C:135:ASN:ND2	3:C:172:GLU:O	2.34	0.60
12:V:79:LYS:N	14:Y:283:DG:OP1	2.31	0.60
8:W:118:THR:OG1	14:Y:73:DG:H5''	2.02	0.60
8:H:128:ARG:HE	8:H:133:GLU:HG3	1.66	0.60
7:G:178:THR:HG23	7:G:180:CYS:H	1.67	0.59
8:H:64:LYS:HG2	14:Y:94:DC:OP1	2.01	0.59
8:H:46:VAL:HB	14:Y:85:DG:P	2.42	0.59
12:V:32:PRO:HG2	13:X:62:DA:H2'	1.83	0.59
1:A:666:VAL:HG22	6:F:18:ARG:HA	1.84	0.59
4:N:58:ILE:O	4:N:62:PHE:N	2.35	0.59
12:Z:65:VAL:HG22	12:Z:93:GLN:HE22	1.67	0.59
13:X:172:DG:H8	13:X:172:DG:H5''	1.66	0.59
13:X:285:DT:H2''	13:X:286:DG:H5''	1.84	0.59
1:A:227:TYR:OH	13:X:182:DC:OP1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:73:GLU:OE1	4:N:76:ARG:NH2	2.36	0.59
4:P:84:SER:N	14:Y:221:DG:OP1	2.36	0.59
8:W:39:HIS:HE1	14:Y:146:DC:C5'	2.15	0.59
8:H:40:ARG:NH2	13:X:248:DG:H5'	2.18	0.58
8:H:66:PRO:HD3	14:Y:93:DA:O5'	2.03	0.58
1:A:274:PRO:HG3	1:A:316:SER:HB3	1.86	0.58
2:O:11:ARG:NH1	13:X:118:DA:H2	2.01	0.58
5:E:244:ARG:NH1	6:F:98:ASP:OD2	2.35	0.58
13:X:173:DG:H5''	13:X:173:DG:N3	2.18	0.58
1:A:921:GLN:NE2	1:A:1186:LEU:O	2.37	0.58
12:L:48:GLY:H	14:Y:83:DC:P	2.26	0.58
13:X:180:DG:N2	14:Y:151:DA:N7	2.52	0.58
6:F:17:ARG:HB3	6:F:21:ILE:HG23	1.86	0.57
2:S:11:ARG:NH1	13:X:32:DA:H2	2.02	0.57
6:F:16:LYS:HD2	6:F:17:ARG:HG3	1.84	0.57
8:U:116:ARG:NH1	8:U:120:MET:HG3	2.19	0.57
12:L:32:PRO:HG2	13:X:241:DA:OP2	2.05	0.57
12:L:78:ARG:NH1	12:L:80:THR:O	2.37	0.57
12:Z:36:ARG:NH2	14:Y:63:DA:OP1	2.38	0.57
8:W:38:PRO:HB2	8:W:40:ARG:HG2	1.87	0.57
8:H:116:ARG:NH2	8:H:123:ASP:OD1	2.36	0.57
8:Q:79:LYS:HB2	8:Q:82:LEU:HD22	1.86	0.57
13:X:325:DC:H2'	13:X:326:DA:C8	2.40	0.57
7:G:148:ASN:HA	7:G:155:LYS:HA	1.86	0.57
13:X:172:DG:H2'	14:Y:157:DC:H41	1.69	0.57
2:B:17:ARG:HG2	2:B:20:ARG:HH21	1.70	0.56
14:Y:157:DC:C4	14:Y:158:DC:N4	2.73	0.56
2:M:17:ARG:HG2	2:M:20:ARG:HH21	1.70	0.56
8:Q:72:ARG:NH2	14:Y:232:DC:OP2	2.36	0.56
13:X:103:DA:H2''	13:X:104:DG:H5''	1.87	0.56
8:H:42:ARG:H	13:X:324:DC:H5'	1.71	0.56
12:R:60:VAL:HA	12:R:63:GLU:HG2	1.87	0.56
12:V:47:SER:HA	14:Y:262:DC:H5''	1.86	0.56
1:A:424:ASP:OD2	13:X:155:DA:OP1	2.24	0.56
3:C:268:VAL:HG12	3:C:306:MET:HB3	1.86	0.56
14:Y:149:DT:H2''	14:Y:150:DC:H5''	1.86	0.56
2:B:88:ARG:NH2	2:B:100:VAL:O	2.39	0.56
1:A:872:ASP:OD2	1:A:875:ARG:NH1	2.33	0.56
2:O:17:ARG:HG2	2:O:20:ARG:HH21	1.70	0.56
2:M:88:ARG:NH2	2:M:100:VAL:O	2.39	0.56
2:O:44:GLY:HA2	13:X:113:DG:H5''	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:32:PRO:HD2	13:X:62:DA:H3'	1.86	0.56
6:F:24:LYS:HB3	7:G:181:ILE:HG12	1.87	0.56
1:A:415:VAL:HA	1:A:418:ILE:HD12	1.88	0.55
2:O:88:ARG:NH2	2:O:100:VAL:O	2.39	0.55
2:S:17:ARG:HG2	2:S:20:ARG:HH21	1.70	0.55
13:X:222:DT:H2'	13:X:223:DA:C8	2.41	0.55
2:S:88:ARG:NH2	2:S:100:VAL:O	2.39	0.55
6:F:67:ARG:HH12	7:G:144:SER:HB3	1.71	0.55
8:U:84:PHE:N	13:X:52:DT:OP1	2.24	0.55
7:G:89:THR:C	7:G:91:ASN:H	2.15	0.55
2:S:76:THR:OG1	14:Y:312:DA:H3'	2.06	0.55
8:W:39:HIS:CE1	14:Y:146:DC:H5''	2.40	0.55
13:X:14:DT:H2''	13:X:15:DA:H5'	1.88	0.55
1:A:1138:LEU:HB3	1:A:1303:ILE:HB	1.88	0.55
8:Q:65:LEU:HD12	13:X:92:DA:H2'	1.87	0.55
13:X:215:DT:H1'	14:Y:118:DC:H42	1.70	0.55
4:N:83:ARG:HB3	14:Y:42:DG:OP1	2.07	0.55
1:A:1076:LYS:HD3	1:A:1267:ALA:HB1	1.89	0.55
8:Q:84:PHE:O	14:Y:231:DG:H3'	2.07	0.55
2:M:77:ARG:HD2	14:Y:22:DA:H4'	1.88	0.55
8:W:79:LYS:HD3	8:W:82:LEU:HD13	1.89	0.55
2:O:79:ILE:HG22	2:O:81:ARG:H	1.72	0.55
13:X:282:DA:H2''	13:X:283:DG:H5''	1.87	0.54
8:H:64:LYS:HB2	14:Y:94:DC:OP2	2.05	0.54
12:L:32:PRO:HB2	13:X:241:DA:P	2.48	0.54
2:S:16:THR:HA	13:X:32:DA:H5''	1.89	0.54
8:U:37:LYS:HD2	8:U:38:PRO:HD2	1.88	0.54
1:A:922:LYS:HD2	6:F:288:TYR:HD1	1.73	0.54
2:M:79:ILE:HG22	2:M:81:ARG:H	1.72	0.54
8:Q:46:VAL:HB	13:X:84:DT:OP1	2.08	0.54
13:X:207:DC:H2''	13:X:208:DT:C5	2.43	0.54
1:A:423:ALA:CB	14:Y:170:DC:H5	2.20	0.54
7:G:173:HIS:ND1	7:G:174:SER:O	2.41	0.54
13:X:140:DA:H2''	13:X:141:DT:C2	2.43	0.54
13:X:172:DG:C4	14:Y:157:DC:H5	2.26	0.54
2:B:79:ILE:HG22	2:B:81:ARG:H	1.72	0.54
13:X:324:DC:H2'	13:X:325:DC:C6	2.43	0.54
1:A:309:THR:OG1	1:A:313:ASN:ND2	2.41	0.53
8:U:45:THR:HG21	13:X:145:DC:OP1	2.08	0.53
1:A:1225:GLU:HG3	1:A:1229:ARG:HH12	1.74	0.53
3:C:135:ASN:HD21	3:C:173:LEU:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:152:GLN:C	7:G:155:LYS:HZ1	2.16	0.53
2:S:57:TYR:HB2	4:T:110:GLU:HG2	1.91	0.53
8:Q:58:THR:HG21	2:S:81:ARG:HB2	1.90	0.53
13:X:172:DG:H1'	14:Y:159:DG:N2	2.22	0.53
1:A:703:VAL:HA	1:A:706:VAL:HG12	1.90	0.53
2:B:104:GLN:NE2	8:W:94:GLU:OE2	2.41	0.53
4:D:37:TYR:CE1	14:Y:124:DG:OP1	2.62	0.53
7:G:83:LEU:O	7:G:87:HIS:N	2.41	0.53
8:H:82:LEU:HD21	12:L:81:VAL:HG23	1.89	0.53
8:U:83:ARG:HD3	14:Y:282:DG:H5''	1.91	0.53
8:W:39:HIS:HD2	13:X:186:DA:C4'	2.22	0.53
14:Y:33:DT:H2'	14:Y:34:DT:H71	1.91	0.53
8:H:117:VAL:N	13:X:251:DA:OP1	2.38	0.53
2:S:79:ILE:HG22	2:S:81:ARG:H	1.72	0.53
12:Z:90:LEU:HA	12:Z:93:GLN:HE21	1.72	0.53
1:A:278:GLN:NE2	1:A:314:ASN:O	2.41	0.53
1:A:1018:ILE:HG22	1:A:1024:ILE:HD11	1.90	0.53
6:F:58:ASP:HB3	6:F:62:TYR:HB3	1.91	0.53
10:J:293:ARG:NH2	10:J:295:GLU:OE1	2.41	0.53
2:M:11:ARG:NH1	14:Y:33:DT:O2	2.32	0.53
5:E:292:GLU:O	6:F:36:ARG:NH2	2.41	0.53
5:E:275:ARG:NH1	6:F:62:TYR:OH	2.41	0.53
7:G:119:PHE:HB3	7:G:169:HIS:HE1	1.74	0.52
9:I:80:MET:HE1	10:J:348:ALA:HB2	1.90	0.52
14:Y:173:DG:H2''	14:Y:174:DG:C8	2.44	0.52
12:L:45:ARG:HH21	14:Y:83:DC:H4'	1.74	0.52
12:V:36:ARG:CZ	13:X:62:DA:OP1	2.56	0.52
3:C:221:LEU:HD11	3:C:372:VAL:HG23	1.92	0.52
3:C:285:ASN:OD1	3:C:358:SER:N	2.42	0.52
4:D:83:ARG:HA	13:X:220:DA:OP1	2.10	0.52
7:G:136:SER:OG	7:G:137:LYS:N	2.42	0.52
3:C:365:THR:HG23	3:C:368:TYR:H	1.74	0.52
2:M:63:LEU:HD11	4:N:38:VAL:HG13	1.92	0.52
13:X:173:DG:N1	14:Y:156:DT:N3	2.58	0.52
13:X:258:DG:H2''	13:X:259:DT:H5'	1.91	0.52
5:E:211:GLU:HB2	5:E:214:MET:O	2.09	0.52
8:H:64:LYS:HD3	8:H:93:GLN:HE22	1.75	0.52
8:Q:39:HIS:CE1	13:X:7:DA:H1'	2.44	0.52
8:U:63:ARG:NH2	14:Y:273:DC:H5'	2.24	0.52
13:X:315:DC:H2''	13:X:316:DG:H5''	1.91	0.52
3:C:181:LEU:HB3	3:C:267:VAL:HG23	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:80:THR:HG22	13:X:282:DA:OP1	2.09	0.52
2:S:32:ARG:HD3	13:X:31:DG:OP2	2.10	0.52
13:X:37:DA:H2''	13:X:38:DG:C8	2.45	0.52
1:A:994:THR:HG21	1:A:1212:ARG:HG3	1.92	0.52
14:Y:153:DG:H2'	14:Y:154:DC:N3	2.25	0.52
6:F:17:ARG:O	6:F:18:ARG:C	2.53	0.52
13:X:223:DA:H2'	13:X:224:DA:C8	2.45	0.52
10:J:351:ARG:O	10:J:355:PHE:N	2.43	0.51
13:X:172:DG:H5''	13:X:172:DG:C8	2.45	0.51
14:Y:153:DG:H2'	14:Y:154:DC:C2	2.46	0.51
1:A:1020:LEU:HG	1:A:1273:ARG:HG2	1.92	0.51
13:X:200:DC:H2''	13:X:201:DA:C8	2.45	0.51
14:Y:32:DA:H3'	14:Y:33:DT:H71	1.93	0.51
1:A:757:ARG:NH1	1:A:781:GLU:OE1	2.42	0.51
3:C:20:ARG:HB3	3:C:140:ASP:H	1.74	0.51
12:Z:23:ARG:C	12:Z:25:ASN:N	2.63	0.51
3:C:220:GLU:H	3:C:223:ASP:HB2	1.76	0.51
10:J:182:SER:O	10:J:187:SER:OG	2.27	0.51
4:N:30:ARG:HD3	14:Y:30:DC:H4'	1.92	0.51
8:W:117:VAL:N	14:Y:73:DG:OP1	2.35	0.51
1:A:779:ASN:HD21	1:A:782:TRP:HB2	1.74	0.51
4:P:60:ASN:O	4:P:64:ASN:ND2	2.43	0.51
1:A:841:MET:HE3	1:A:846:LYS:HG2	1.93	0.51
14:Y:157:DC:H2''	14:Y:158:DC:C6	2.45	0.51
12:L:32:PRO:CB	13:X:241:DA:OP2	2.59	0.51
13:X:21:DC:H2''	13:X:22:DA:C8	2.46	0.51
2:M:68:ASN:OD1	2:M:71:ARG:NH2	2.44	0.51
14:Y:155:DT:H3'	14:Y:156:DT:C5	2.46	0.51
1:A:862:ILE:HD11	3:C:32:TYR:CZ	2.46	0.50
8:U:49:ARG:HD3	14:Y:189:DA:O3'	2.10	0.50
12:Z:60:VAL:O	12:Z:64:ASN:ND2	2.43	0.50
11:K:471:ASP:O	11:K:475:ASN:ND2	2.44	0.50
2:S:68:ASN:OD1	2:S:71:ARG:NH2	2.44	0.50
13:X:274:DG:N1	14:Y:57:DG:O6	2.44	0.50
13:X:85:DG:H2''	13:X:86:DC:H5''	1.92	0.50
1:A:1024:ILE:HB	1:A:1027:GLU:HB2	1.93	0.50
2:B:68:ASN:OD1	2:B:71:ARG:NH2	2.44	0.50
10:J:227:TYR:H	10:J:230:ASN:HB2	1.76	0.50
11:K:247:ARG:HG3	11:K:250:LYS:HE2	1.93	0.50
8:U:42:ARG:HG2	13:X:145:DC:OP1	2.11	0.50
13:X:174:DA:N6	14:Y:154:DC:H5''	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:197:DT:H2''	13:X:198:DG:N7	2.26	0.50
1:A:788:TRP:HE1	3:C:214:PHE:H	1.60	0.50
5:E:198:GLN:HE22	6:F:132:ARG:HB3	1.77	0.50
8:H:72:ARG:CZ	13:X:231:DT:OP1	2.60	0.50
9:I:76:TYR:HB3	9:I:80:MET:HE2	1.94	0.50
2:S:85:LEU:O	2:S:89:ASN:ND2	2.45	0.50
3:C:184:ASP:HB3	3:C:207:SER:HA	1.92	0.50
2:S:30:VAL:HG13	4:T:67:PHE:HE1	1.75	0.50
1:A:875:ARG:HH12	6:F:301:PRO:HB3	1.76	0.50
2:S:54:VAL:HG21	4:T:95:VAL:HG21	1.94	0.50
14:Y:161:DC:H2'	14:Y:162:DA:C8	2.47	0.50
1:A:319:GLY:CA	14:Y:161:DC:P	3.00	0.50
3:C:185:ILE:O	3:C:275:SER:OG	2.22	0.50
2:O:68:ASN:OD1	2:O:71:ARG:NH2	2.44	0.50
2:O:85:LEU:O	2:O:89:ASN:ND2	2.45	0.50
13:X:166:DC:H41	14:Y:164:DG:H21	1.58	0.50
2:O:30:VAL:HG13	4:P:67:PHE:HE1	1.77	0.49
13:X:319:DA:H2''	13:X:320:DT:C2	2.47	0.49
3:C:182:TYR:HB3	3:C:205:THR:HA	1.94	0.49
2:O:63:LEU:HD13	4:P:42:LEU:HB2	1.94	0.49
2:B:85:LEU:O	2:B:89:ASN:ND2	2.45	0.49
8:H:121:PRO:HG3	12:L:50:ILE:HA	1.93	0.49
2:M:85:LEU:O	2:M:89:ASN:ND2	2.45	0.49
4:T:71:ALA:O	4:T:75:SER:OG	2.29	0.49
8:U:68:GLN:HE21	8:U:72:ARG:HH21	1.59	0.49
8:U:119:ILE:HD12	12:V:50:ILE:HD13	1.94	0.49
9:I:68:LEU:HD23	9:I:71:ASN:HD22	1.77	0.49
13:X:28:DC:H2''	13:X:29:DT:C5	2.46	0.49
1:A:304:THR:N	1:A:305:PRO:HD2	2.28	0.49
8:H:85:GLN:HE21	12:L:83:ALA:H	1.60	0.49
13:X:150:DA:H2''	13:X:151:DG:C8	2.47	0.49
9:I:73:ASN:ND2	10:J:337:GLU:OE2	2.45	0.49
4:T:37:TYR:HH	14:Y:303:DG:H5''	1.75	0.49
8:W:43:PRO:HD2	14:Y:71:DA:H5'	1.93	0.49
14:Y:173:DG:C6	14:Y:174:DG:N2	2.80	0.49
4:D:37:TYR:CZ	14:Y:124:DG:OP1	2.65	0.49
1:A:922:LYS:HG3	1:A:923:VAL:HG23	1.95	0.49
5:E:235:ASP:O	5:E:239:HIS:N	2.45	0.49
7:G:128:THR:O	7:G:132:TYR:N	2.46	0.49
10:J:175:ILE:O	10:J:183:ARG:NH2	2.44	0.49
12:L:98:TYR:HB3	4:N:58:ILE:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:23:ARG:O	12:Z:25:ASN:N	2.46	0.49
13:X:175:DA:H2'	13:X:175:DA:N3	2.28	0.49
14:Y:154:DC:H4'	14:Y:155:DT:OP2	2.13	0.49
5:E:234:ARG:HD3	6:F:106:HIS:CG	2.48	0.49
2:M:42:ARG:NH2	13:X:292:DG:O4'	2.43	0.49
2:O:115:LEU:HD11	8:U:108:ASN:HD21	1.78	0.48
2:S:29:ARG:NH2	14:Y:304:DC:OP1	2.45	0.48
2:S:32:ARG:NE	13:X:31:DG:OP1	2.43	0.48
12:V:45:ARG:CA	14:Y:263:DC:OP1	2.61	0.48
8:Q:65:LEU:HG	13:X:93:DG:OP2	2.13	0.48
14:Y:142:DC:H2''	14:Y:143:DA:H5'	1.95	0.48
1:A:423:ALA:CB	14:Y:170:DC:C5	2.96	0.48
14:Y:131:DT:H2''	14:Y:132:DC:C5	2.48	0.48
2:S:27:VAL:HG13	2:S:48:PRO:HB2	1.96	0.48
2:S:42:ARG:NH2	14:Y:293:DT:O4'	2.45	0.48
3:C:316:ARG:HG3	3:C:347:TYR:HA	1.95	0.48
6:F:25:VAL:HA	6:F:28:ILE:HB	1.96	0.48
1:A:671:LYS:NZ	1:A:715:GLU:OE1	2.47	0.48
9:I:68:LEU:HA	9:I:71:ASN:HD22	1.78	0.48
12:V:46:ILE:O	14:Y:262:DC:H3'	2.13	0.48
13:X:136:DC:H2''	13:X:137:DG:H5''	1.96	0.48
13:X:157:DC:N3	13:X:158:DA:N6	2.62	0.48
13:X:172:DG:H1'	14:Y:159:DG:H22	1.79	0.48
6:F:15:ASP:H	6:F:18:ARG:NE	2.12	0.48
13:X:323:DT:O2	14:Y:8:DG:N2	2.45	0.48
14:Y:156:DT:H2''	14:Y:157:DC:C6	2.48	0.48
1:A:830:CYS:SG	1:A:857:HIS:ND1	2.86	0.48
5:E:261:THR:OG1	10:J:228:GLU:OE1	2.31	0.48
6:F:305:THR:HA	6:F:308:ILE:HG12	1.95	0.48
8:Q:84:PHE:HD1	12:R:81:VAL:HB	1.78	0.48
8:W:39:HIS:HE1	14:Y:146:DC:H5'	1.78	0.48
8:W:46:VAL:HB	13:X:263:DT:OP2	2.12	0.48
13:X:224:DA:H2'	13:X:225:DT:C6	2.49	0.48
1:A:423:ALA:HB3	14:Y:170:DC:H5	1.77	0.48
12:Z:57:VAL:HA	12:Z:60:VAL:HG12	1.95	0.48
1:A:837:LYS:NZ	1:A:841:MET:SD	2.87	0.48
8:Q:46:VAL:HG21	13:X:84:DT:H3'	1.96	0.48
1:A:463:LEU:HA	1:A:466:ASP:HB2	1.96	0.47
5:E:215:CYS:HB3	5:E:220:HIS:CG	2.48	0.47
8:H:72:ARG:NH2	13:X:231:DT:P	2.73	0.47
12:V:48:GLY:H	14:Y:262:DC:P	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:62:ILE:O	8:W:93:GLN:NE2	2.46	0.47
14:Y:169:DC:H2''	14:Y:170:DC:O2	2.14	0.47
1:A:996:ILE:HG23	1:A:1007:LYS:HB3	1.97	0.47
8:H:42:ARG:HG2	13:X:324:DC:P	2.54	0.47
2:O:43:VAL:N	13:X:114:DA:OP1	2.42	0.47
4:P:36:ILE:CD1	13:X:123:DG:O5'	2.62	0.47
13:X:110:DT:H2''	13:X:111:DA:N7	2.28	0.47
3:C:20:ARG:H	3:C:140:ASP:HB2	1.79	0.47
14:Y:159:DG:OP2	14:Y:160:DC:N4	2.48	0.47
1:A:443:GLN:O	1:A:444:LYS:C	2.58	0.47
1:A:911:GLU:OE2	6:F:101:LYS:NZ	2.39	0.47
2:B:43:VAL:O	14:Y:114:DT:H5''	2.15	0.47
8:H:103:LEU:HD21	8:H:124:ILE:HG23	1.96	0.47
8:H:121:PRO:HG2	12:L:49:LEU:HG	1.97	0.47
8:Q:42:ARG:NH2	14:Y:325:DC:OP2	2.48	0.47
8:Q:46:VAL:N	13:X:84:DT:OP1	2.47	0.47
1:A:1210:LEU:O	1:A:1214:LEU:N	2.47	0.47
4:P:69:ARG:HB3	4:P:98:LEU:HD22	1.97	0.47
8:U:100:LEU:HD11	12:V:58:LEU:HD13	1.95	0.47
13:X:221:DG:N2	14:Y:110:DT:O2	2.48	0.47
1:A:319:GLY:HA2	14:Y:161:DC:OP1	2.14	0.47
1:A:439:TYR:HB3	1:A:444:LYS:HG2	1.95	0.47
3:C:110:CYS:O	3:C:162:TYR:OH	2.32	0.47
3:C:141:VAL:HG11	3:C:329:LEU:HD13	1.96	0.47
2:S:47:ALA:N	2:S:48:PRO:HD2	2.30	0.47
13:X:117:DA:H2''	13:X:118:DA:H5'	1.96	0.47
13:X:171:DC:H5	13:X:172:DG:C2	2.33	0.47
13:X:175:DA:H2''	13:X:176:DG:C8	2.50	0.47
14:Y:8:DG:H2''	14:Y:9:DA:C8	2.49	0.47
8:H:48:LEU:HD23	8:H:51:ILE:HD12	1.97	0.47
10:J:190:LEU:HD23	10:J:193:LEU:HD12	1.96	0.47
12:R:54:THR:HA	12:R:57:VAL:HG22	1.96	0.47
1:A:423:ALA:HB1	14:Y:170:DC:C5	2.50	0.47
3:C:82:TYR:OH	3:C:162:TYR:O	2.21	0.47
8:Q:81:ASP:OD1	8:Q:81:ASP:N	2.48	0.47
8:W:41:TYR:HA	14:Y:146:DC:OP1	2.14	0.47
1:A:1269:PHE:O	1:A:1273:ARG:N	2.48	0.46
8:Q:83:ARG:HA	14:Y:232:DC:OP1	2.15	0.46
4:D:58:ILE:O	4:D:62:PHE:N	2.47	0.46
8:U:38:PRO:HB2	8:U:40:ARG:HG2	1.97	0.46
13:X:130:DC:H2''	13:X:131:DG:N7	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:VAL:HB	3:C:376:ILE:HD11	1.97	0.46
6:F:98:ASP:HA	6:F:101:LYS:HG2	1.97	0.46
12:R:46:ILE:N	13:X:83:DG:OP1	2.42	0.46
13:X:10:DT:H2''	13:X:11:DA:C8	2.50	0.46
14:Y:219:DT:H2''	14:Y:220:DA:N7	2.31	0.46
8:H:116:ARG:HB3	13:X:251:DA:OP1	2.16	0.46
2:O:81:ARG:HB2	8:U:58:THR:HG21	1.97	0.46
13:X:260:DA:H1'	13:X:261:DC:C4	2.51	0.46
1:A:1162:LYS:HA	1:A:1165:ASN:HB2	1.98	0.46
12:L:33:ALA:HA	12:L:36:ARG:HE	1.81	0.46
2:M:77:ARG:NH1	14:Y:22:DA:H4'	2.31	0.46
4:P:99:LEU:O	4:P:104:ALA:HB2	2.15	0.46
8:Q:108:ASN:HD21	2:S:115:LEU:HD11	1.80	0.46
12:V:45:ARG:HG2	14:Y:263:DC:H5''	1.97	0.46
6:F:85:GLU:HA	6:F:88:VAL:HG22	1.97	0.46
13:X:210:DG:H2''	13:X:211:DA:C8	2.50	0.46
13:X:318:DG:H2''	13:X:319:DA:C8	2.51	0.46
14:Y:209:DC:H2''	14:Y:210:DA:C8	2.51	0.46
13:X:174:DA:C6	14:Y:154:DC:H2'	2.50	0.46
13:X:252:DC:H2'	13:X:253:DA:C8	2.51	0.46
1:A:1197:ASP:OD1	1:A:1197:ASP:N	2.48	0.46
2:B:11:ARG:HA	13:X:213:DA:H5''	1.97	0.46
2:O:11:ARG:NH1	14:Y:212:DT:O2	2.35	0.46
2:S:63:LEU:HD13	4:T:42:LEU:HB2	1.98	0.46
8:W:73:GLU:HG3	12:Z:23:ARG:HA	1.97	0.46
1:A:709:TYR:HB2	7:G:100:HIS:HE1	1.80	0.46
10:J:175:ILE:HG13	10:J:176:ILE:HG23	1.97	0.46
8:W:39:HIS:HE1	14:Y:146:DC:H5''	1.80	0.46
1:A:700:ASP:HA	1:A:703:VAL:HG22	1.98	0.46
1:A:826:ARG:NH2	3:C:28:ASP:OD2	2.45	0.46
8:H:47:ALA:N	14:Y:85:DG:OP1	2.49	0.46
10:J:359:LEU:HA	10:J:362:ILE:HG12	1.97	0.46
12:L:32:PRO:HD3	13:X:242:DA:OP2	2.16	0.45
4:T:73:GLU:OE2	12:V:72:TYR:OH	2.29	0.45
8:W:39:HIS:CE1	14:Y:146:DC:H5'	2.50	0.45
14:Y:80:DC:H2''	14:Y:81:DC:C5	2.51	0.45
1:A:945:THR:HG22	1:A:1146:ILE:HG21	1.97	0.45
3:C:164:ASN:ND2	3:C:192:GLY:O	2.49	0.45
6:F:67:ARG:NH2	7:G:147:ARG:HB2	2.31	0.45
2:M:32:ARG:NE	14:Y:32:DA:OP2	2.46	0.45
14:Y:110:DT:H2''	14:Y:111:DC:C5	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Y:199:DC:H2''	14:Y:200:DG:C8	2.51	0.45
1:A:1019:SER:HA	1:A:1024:ILE:HG13	1.99	0.45
2:B:109:PRO:HA	8:W:55:GLN:HB3	1.97	0.45
3:C:45:ILE:HD13	3:C:146:ALA:HA	1.97	0.45
12:L:32:PRO:HD2	13:X:241:DA:H3'	1.98	0.45
4:T:84:SER:N	13:X:41:DA:OP1	2.44	0.45
1:A:666:VAL:HG13	6:F:15:ASP:OD2	2.16	0.45
3:C:41:LYS:O	3:C:44:ARG:NH1	2.50	0.45
12:L:47:SER:HB3	12:L:49:LEU:HD23	1.98	0.45
2:M:11:ARG:HG2	13:X:298:DT:H4'	1.97	0.45
8:Q:61:LEU:HD13	12:R:36:ARG:HB3	1.99	0.45
8:W:64:LYS:O	8:W:68:GLN:N	2.42	0.45
13:X:112:DC:H2''	13:X:113:DG:C8	2.52	0.45
1:A:924:PHE:O	1:A:927:SER:OG	2.26	0.45
6:F:17:ARG:HA	6:F:20:ASN:HB3	1.97	0.45
12:L:78:ARG:NH2	12:L:85:ASP:OD2	2.44	0.45
3:C:150:HIS:HD2	3:C:190:GLY:HA2	1.81	0.45
3:C:174:LEU:O	3:C:202:ARG:NH2	2.49	0.45
2:O:16:THR:O	2:O:19:SER:OG	2.34	0.45
8:U:68:GLN:O	8:U:72:ARG:HG2	2.17	0.45
1:A:1145:TYR:HE1	1:A:1314:ILE:HD13	1.82	0.45
8:H:83:ARG:HH21	14:Y:103:DG:C5'	2.30	0.45
14:Y:184:DG:H2''	14:Y:185:DG:C8	2.52	0.45
3:C:62:GLU:HA	5:E:265:GLN:HE22	1.81	0.44
12:L:78:ARG:HD2	14:Y:104:DG:H5''	2.00	0.44
12:V:45:ARG:HG2	14:Y:263:DC:C5'	2.47	0.44
12:Z:79:LYS:HG2	13:X:281:DG:OP1	2.17	0.44
13:X:78:DC:H2''	13:X:79:DG:C8	2.53	0.44
1:A:868:ARG:NH2	1:A:873:LYS:O	2.50	0.44
3:C:74:MET:HE2	3:C:83:ILE:HD11	1.99	0.44
5:E:260:ARG:NH1	10:J:235:SER:O	2.48	0.44
4:P:28:LYS:HB3	4:P:29:THR:H	1.66	0.44
1:A:1179:THR:HA	1:A:1182:LYS:HG2	1.98	0.44
6:F:24:LYS:HG2	7:G:179:ASP:OD2	2.17	0.44
6:F:24:LYS:HG3	7:G:181:ILE:HD11	1.99	0.44
10:J:222:HIS:CD2	10:J:294:LEU:HG	2.53	0.44
11:K:245:MET:SD	11:K:245:MET:N	2.91	0.44
12:L:32:PRO:HG2	13:X:241:DA:P	2.57	0.44
2:M:42:ARG:HB2	4:N:85:THR:HG22	1.99	0.44
8:Q:48:LEU:HD23	8:Q:51:ILE:HD12	1.99	0.44
13:X:223:DA:H2'	13:X:224:DA:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:15:ASP:H	6:F:18:ARG:HB3	1.81	0.44
13:X:195:DT:H1'	13:X:196:DC:H5'	1.99	0.44
1:A:879:ILE:O	1:A:883:LEU:N	2.49	0.44
2:B:32:ARG:HD3	13:X:210:DG:P	2.58	0.44
2:B:102:ILE:HG23	4:D:58:ILE:HD13	1.99	0.44
8:W:41:TYR:HD2	13:X:264:DG:P	2.39	0.44
13:X:222:DT:H2'	13:X:223:DA:H8	1.83	0.44
14:Y:186:DA:H2''	14:Y:187:DG:C8	2.53	0.44
1:A:227:TYR:HE1	1:A:246:LEU:HD13	1.83	0.44
1:A:799:ARG:HH22	3:C:360:MET:HG2	1.83	0.44
5:E:223:LEU:HA	5:E:226:TYR:HB3	2.00	0.44
14:Y:56:DC:H2''	14:Y:57:DG:C8	2.53	0.44
1:A:807:LEU:HD23	1:A:810:ILE:HD12	1.98	0.44
2:M:41:GLU:HB2	4:N:84:SER:HB3	2.00	0.44
8:Q:84:PHE:N	14:Y:232:DC:OP1	2.46	0.44
4:T:89:ARG:HG2	12:V:75:HIS:CE1	2.53	0.44
8:U:120:MET:HE1	13:X:72:DA:H4'	2.00	0.44
13:X:230:DT:H1'	13:X:231:DT:H5'	2.00	0.44
6:F:39:GLN:O	6:F:43:ARG:NE	2.50	0.44
2:M:55:LEU:HD22	4:N:63:VAL:HG13	2.00	0.44
4:T:90:GLU:HG2	12:V:75:HIS:CE1	2.53	0.44
1:A:797:ALA:HB3	1:A:800:LYS:HA	2.00	0.43
1:A:1313:SER:OG	1:A:1315:GLN:NE2	2.51	0.43
8:U:119:ILE:HG13	8:U:119:ILE:O	2.18	0.43
1:A:696:ILE:HG23	7:G:114:ARG:HB3	1.98	0.43
1:A:826:ARG:NH2	1:A:859:SER:OG	2.51	0.43
1:A:1155:TYR:O	1:A:1159:LEU:N	2.51	0.43
12:L:45:ARG:HH21	14:Y:83:DC:C4'	2.30	0.43
8:Q:62:ILE:HB	8:Q:93:GLN:HE21	1.82	0.43
3:C:17:ASP:N	3:C:17:ASP:OD1	2.51	0.43
6:F:24:LYS:HA	6:F:24:LYS:HD3	1.54	0.43
8:H:107:THR:HG21	8:H:124:ILE:HG12	1.99	0.43
2:M:11:ARG:NH1	13:X:297:DA:H2	2.16	0.43
2:M:16:THR:O	2:M:19:SER:OG	2.34	0.43
4:P:87:THR:OG1	4:P:90:GLU:OE1	2.31	0.43
8:Q:54:TYR:HB3	12:R:40:ARG:HG3	2.00	0.43
8:Q:108:ASN:ND2	12:R:42:GLY:O	2.51	0.43
14:Y:248:DG:H2''	14:Y:249:DT:C5	2.53	0.43
1:A:765:MET:HE2	1:A:775:TRP:HB2	2.00	0.43
6:F:16:LYS:H	6:F:16:LYS:HG3	1.52	0.43
12:L:39:ARG:NH1	12:L:44:LYS:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:123:ASP:OD1	8:U:113:HIS:NE2	2.41	0.43
4:T:83:ARG:NH1	13:X:41:DA:H2'	2.34	0.43
8:U:61:LEU:N	8:U:97:GLU:OE2	2.51	0.43
13:X:11:DA:O4'	14:Y:320:DA:N6	2.51	0.43
1:A:227:TYR:HB3	1:A:245:PHE:HE2	1.83	0.43
1:A:879:ILE:HD11	6:F:308:ILE:HG22	2.00	0.43
9:I:15:THR:HA	9:I:18:LEU:HD12	1.99	0.43
2:S:42:ARG:NH2	14:Y:293:DT:C4'	2.82	0.43
8:W:118:THR:HG1	14:Y:73:DG:H5''	1.80	0.43
14:Y:119:DT:H6	14:Y:119:DT:H2'	1.63	0.43
1:A:1133:ARG:HG2	1:A:1278:THR:HA	2.01	0.43
6:F:63:ALA:HA	6:F:66:VAL:HG12	2.00	0.43
10:J:206:MET:O	10:J:210:ARG:NH2	2.52	0.43
13:X:174:DA:H2	14:Y:153:DG:H21	1.66	0.43
1:A:228:LEU:HD12	1:A:228:LEU:HA	1.70	0.43
1:A:706:VAL:HG22	1:A:710:LEU:HD23	2.00	0.43
1:A:930:HIS:ND1	3:C:358:SER:OG	2.48	0.43
8:H:61:LEU:HD12	12:L:37:LEU:HD23	2.01	0.43
2:O:47:ALA:N	2:O:48:PRO:HD2	2.33	0.43
13:X:309:DC:H2''	13:X:310:DG:N7	2.33	0.43
1:A:692:TYR:HD1	1:A:697:LEU:HB2	1.84	0.43
3:C:269:LEU:HD21	3:C:295:VAL:HG22	2.00	0.43
8:Q:72:ARG:HH22	14:Y:232:DC:P	2.41	0.43
4:T:83:ARG:HA	13:X:41:DA:OP1	2.18	0.43
8:W:108:ASN:HB2	12:Z:43:VAL:HG22	2.00	0.43
13:X:248:DG:H2''	13:X:249:DG:C8	2.54	0.43
14:Y:217:DC:H2''	14:Y:218:DG:C8	2.54	0.43
14:Y:228:DC:H4'	14:Y:229:DT:H5'	2.01	0.43
1:A:826:ARG:HD2	1:A:862:ILE:HG21	2.01	0.43
8:Q:64:LYS:HB2	13:X:93:DG:OP1	2.18	0.43
4:T:83:ARG:NH2	13:X:42:DG:OP2	2.52	0.43
8:H:62:ILE:N	8:H:97:GLU:OE2	2.51	0.43
8:Q:118:THR:HB	14:Y:252:DG:H5''	2.00	0.43
1:A:937:GLN:OE1	1:A:940:LYS:NZ	2.48	0.42
12:L:32:PRO:CG	13:X:241:DA:OP2	2.66	0.42
8:Q:69:ARG:NH2	13:X:92:DA:OP1	2.51	0.42
8:Q:84:PHE:CD1	12:R:81:VAL:HB	2.54	0.42
2:O:63:LEU:HD11	4:P:38:VAL:HG13	2.00	0.42
12:Z:78:ARG:NH1	12:Z:80:THR:O	2.52	0.42
14:Y:157:DC:C5	14:Y:158:DC:N4	2.87	0.42
13:X:89:DT:H2''	13:X:90:DT:H72	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:X:176:DG:H2'	13:X:177:DC:C6	2.54	0.42
13:X:292:DG:H2''	13:X:293:DA:C8	2.54	0.42
1:A:1201:GLU:OE2	1:A:1209:ARG:NH2	2.52	0.42
6:F:26:ASN:HA	6:F:29:TYR:HD2	1.85	0.42
8:H:120:MET:N	8:H:123:ASP:OD2	2.52	0.42
14:Y:77:DT:H2''	14:Y:78:DG:C8	2.55	0.42
1:A:669:PHE:HB3	6:F:17:ARG:CZ	2.49	0.42
3:C:356:ARG:HA	3:C:357:PRO:HD3	1.92	0.42
6:F:17:ARG:O	6:F:21:ILE:N	2.52	0.42
4:P:83:ARG:HA	14:Y:221:DG:OP2	2.20	0.42
8:W:46:VAL:HG22	8:W:49:ARG:HH21	1.83	0.42
13:X:137:DG:H2''	13:X:138:DG:H5'	2.02	0.42
1:A:319:GLY:HA3	14:Y:161:DC:O5'	2.18	0.42
1:A:710:LEU:HD12	1:A:712:SER:H	1.84	0.42
5:E:178:GLN:HE21	5:E:183:LEU:HD12	1.83	0.42
5:E:264:HIS:O	5:E:268:HIS:N	2.48	0.42
2:O:21:ALA:HB2	4:P:118:TYR:HB2	2.01	0.42
2:B:16:THR:O	2:B:19:SER:OG	2.34	0.42
5:E:271:VAL:HG22	6:F:66:VAL:HG23	2.02	0.42
6:F:22:GLU:O	6:F:23:SER:C	2.62	0.42
1:A:446:ILE:HG23	1:A:447:ASN:OD1	2.19	0.42
1:A:1009:ARG:HH12	1:A:1070:HIS:CD2	2.38	0.42
1:A:1138:LEU:N	1:A:1303:ILE:O	2.49	0.42
3:C:114:ASP:N	3:C:114:ASP:OD1	2.53	0.42
8:Q:75:ALA:HB1	8:Q:82:LEU:HD23	2.01	0.42
14:Y:60:DT:H2''	14:Y:61:DA:C8	2.54	0.42
8:H:126:LEU:HD22	8:W:113:HIS:CG	2.54	0.42
12:V:84:MET:SD	12:V:84:MET:N	2.93	0.42
8:W:120:MET:SD	12:Z:47:SER:OG	2.70	0.42
13:X:36:DT:H2''	13:X:37:DA:C8	2.55	0.42
13:X:174:DA:H2''	13:X:175:DA:C5	2.55	0.42
14:Y:322:DA:H2'	14:Y:323:DT:H71	2.02	0.42
3:C:369:LEU:HA	3:C:372:VAL:HG12	2.02	0.42
7:G:123:VAL:HG11	7:G:165:VAL:HG11	2.02	0.42
4:T:76:ARG:HB3	4:T:80:TYR:CZ	2.55	0.42
13:X:167:DA:N1	14:Y:162:DA:N6	2.68	0.42
13:X:197:DT:H2''	13:X:198:DG:C8	2.54	0.42
14:Y:34:DT:N3	14:Y:35:DG:O6	2.53	0.42
14:Y:160:DC:H2''	14:Y:161:DC:C2	2.55	0.42
1:A:1291:ARG:HH21	1:A:1296:ASN:HA	1.83	0.41
12:R:32:PRO:HB2	14:Y:242:DA:OP2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:41:TYR:O	13:X:263:DT:H4'	2.20	0.41
13:X:99:DC:H2''	13:X:100:DT:C6	2.55	0.41
14:Y:310:DT:H2''	14:Y:311:DC:C6	2.54	0.41
8:Q:113:HIS:CG	8:U:126:LEU:HD22	2.55	0.41
2:S:58:LEU:HD11	4:T:99:LEU:HD11	2.01	0.41
2:S:102:ILE:HG23	4:T:58:ILE:HD13	2.02	0.41
13:X:180:DG:H2''	13:X:181:DA:H5'	2.02	0.41
14:Y:100:DA:H2''	14:Y:101:DG:N7	2.35	0.41
2:B:63:LEU:HD13	4:D:42:LEU:HB2	2.02	0.41
6:F:64:ARG:HH22	7:G:117:ASP:HB3	1.86	0.41
2:S:26:PRO:HD3	4:T:37:TYR:CD1	2.55	0.41
12:Z:30:THR:HG21	14:Y:63:DA:H5''	2.00	0.41
1:A:319:GLY:C	14:Y:161:DC:C5'	2.81	0.41
1:A:851:LEU:HA	1:A:851:LEU:HD23	1.90	0.41
6:F:109:LEU:HD23	6:F:112:LEU:HD12	2.02	0.41
9:I:29:LEU:O	9:I:33:HIS:N	2.52	0.41
12:L:44:LYS:HG3	2:M:115:LEU:HB3	2.02	0.41
4:N:72:GLY:O	4:N:75:SER:OG	2.36	0.41
8:Q:113:HIS:NE2	8:U:123:ASP:OD1	2.44	0.41
13:X:107:DG:H2'	13:X:108:DT:H71	2.02	0.41
8:Q:47:ALA:N	13:X:84:DT:OP1	2.48	0.41
2:S:26:PRO:HD3	4:T:37:TYR:CG	2.56	0.41
14:Y:148:DG:H1'	14:Y:149:DT:C2	2.55	0.41
1:A:868:ARG:HH12	1:A:877:PHE:HB2	1.86	0.41
6:F:107:GLU:OE2	6:F:111:LYS:NZ	2.52	0.41
8:Q:126:LEU:HD22	8:U:113:HIS:CG	2.55	0.41
8:U:43:PRO:HA	14:Y:264:DG:H5'	2.02	0.41
13:X:275:DG:H2'	13:X:276:DT:H71	2.01	0.41
1:A:808:PHE:CE2	3:C:280:ARG:HG2	2.56	0.41
1:A:840:ASN:ND2	7:G:135:GLY:O	2.54	0.41
1:A:1216:ASN:ND2	1:A:1218:ASP:OD2	2.54	0.41
3:C:31:ASN:ND2	3:C:46:ARG:HH22	2.18	0.41
6:F:75:LEU:HD12	6:F:75:LEU:HA	1.84	0.41
8:Q:100:LEU:HD11	12:R:58:LEU:HD13	2.03	0.41
13:X:42:DG:N2	14:Y:289:DT:O2	2.53	0.41
1:A:788:TRP:NE1	3:C:214:PHE:H	2.18	0.41
2:B:43:VAL:N	14:Y:115:DA:OP1	2.50	0.41
6:F:77:LEU:HD23	6:F:77:LEU:HA	1.89	0.41
13:X:247:DG:H2''	13:X:248:DG:C8	2.56	0.41
13:X:289:DT:H2''	13:X:290:DA:N7	2.35	0.41
14:Y:40:DT:H2''	14:Y:41:DA:N7	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:VAL:HG21	3:C:174:LEU:HD21	2.02	0.41
1:A:815:HIS:CE1	3:C:41:LYS:HD3	2.56	0.41
3:C:151:HIS:O	3:C:158:SER:OG	2.32	0.41
5:E:230:ILE:HA	5:E:233:ILE:HG22	2.03	0.41
6:F:16:LYS:HA	6:F:19:PHE:CZ	2.56	0.41
7:G:80:ILE:HD13	7:G:83:LEU:HD21	2.03	0.41
9:I:67:ARG:O	9:I:71:ASN:ND2	2.53	0.41
10:J:347:ILE:HA	10:J:350:GLN:HG2	2.03	0.41
2:M:76:THR:O	4:N:50:GLY:N	2.46	0.41
2:O:100:VAL:HG22	12:V:96:THR:HG23	2.02	0.41
4:P:36:ILE:HD13	13:X:123:DG:H2'	2.02	0.41
4:P:95:VAL:O	4:P:99:LEU:HB2	2.21	0.41
8:Q:73:GLU:OE1	12:R:25:ASN:ND2	2.54	0.41
14:Y:61:DA:H2''	14:Y:62:DA:C8	2.56	0.41
1:A:309:THR:O	1:A:313:ASN:ND2	2.54	0.41
1:A:1073:ARG:HH21	1:A:1260:ALA:HB1	1.85	0.41
3:C:279:ASP:OD1	3:C:280:ARG:N	2.46	0.41
4:T:77:LEU:O	4:T:81:ASN:ND2	2.54	0.41
8:W:118:THR:HG23	14:Y:72:DC:O3'	2.21	0.41
12:Z:35:ARG:O	12:Z:39:ARG:N	2.47	0.41
14:Y:7:DA:H2''	14:Y:8:DG:C8	2.56	0.41
1:A:238:ARG:NH2	1:A:271:ARG:H	2.18	0.40
1:A:772:ASP:HA	1:A:775:TRP:CZ3	2.57	0.40
1:A:838:ILE:HD12	1:A:888:ALA:HA	2.02	0.40
1:A:1194:MET:HE1	1:A:1223:TRP:CE2	2.56	0.40
2:B:80:PRO:HD3	4:D:55:ALA:HB2	2.03	0.40
5:E:275:ARG:NH2	6:F:54:LEU:O	2.54	0.40
8:H:62:ILE:O	8:H:93:GLN:NE2	2.55	0.40
8:H:85:GLN:NE2	12:L:83:ALA:H	2.18	0.40
2:M:16:THR:HA	14:Y:33:DT:H5''	2.03	0.40
2:M:64:GLU:HA	4:N:46:HIS:HE1	1.85	0.40
2:O:32:ARG:HD3	14:Y:211:DA:OP2	2.20	0.40
8:Q:65:LEU:HD12	13:X:92:DA:C2'	2.51	0.40
2:S:42:ARG:HH21	14:Y:293:DT:C1'	2.33	0.40
8:U:85:GLN:NE2	12:V:83:ALA:H	2.19	0.40
1:A:897:ARG:HB3	6:F:299:LEU:HD11	2.03	0.40
1:A:1291:ARG:NH2	1:A:1318:ALA:O	2.53	0.40
8:Q:45:THR:HG21	14:Y:324:DC:H4'	2.02	0.40
12:R:62:LEU:HD23	12:R:62:LEU:HA	1.90	0.40
4:D:110:GLU:HA	4:D:113:LYS:HB2	2.04	0.40
6:F:22:GLU:O	6:F:25:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:LEU:HD22	7:G:130:GLN:HA	2.03	0.40
4:P:65:ASP:OD2	12:V:98:TYR:OH	2.39	0.40
2:S:11:ARG:NH2	14:Y:299:DC:O2	2.54	0.40
8:U:60:LEU:HD22	8:U:93:GLN:HG2	2.03	0.40
4:D:83:ARG:CA	13:X:220:DA:OP1	2.69	0.40
6:F:17:ARG:HG2	7:G:179:ASP:HA	2.03	0.40
2:O:104:GLN:NE2	8:U:94:GLU:OE2	2.55	0.40
13:X:171:DC:H5	13:X:172:DG:N3	2.20	0.40
1:A:1133:ARG:HB2	1:A:1136:PHE:HE1	1.86	0.40
3:C:166:ILE:O	3:C:170:ILE:N	2.54	0.40
3:C:358:SER:OG	3:C:359:ASN:N	2.54	0.40
5:E:192:LYS:O	5:E:197:ARG:N	2.38	0.40
6:F:17:ARG:HA	6:F:20:ASN:CB	2.52	0.40
6:F:87:ARG:O	6:F:91:SER:N	2.51	0.40
7:G:83:LEU:HD12	7:G:84:ILE:HG13	2.03	0.40
9:I:52:LYS:O	9:I:59:ASN:ND2	2.55	0.40
8:U:110:CYS:SG	8:U:126:LEU:HD23	2.61	0.40
13:X:51:DT:H2''	13:X:52:DT:H71	2.03	0.40
13:X:185:DG:H2''	13:X:186:DA:H5'	2.03	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	676/1096 (62%)	626 (93%)	49 (7%)	1 (0%)	48	78
2	B	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	M	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	O	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	S	105/107 (98%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	376/378 (100%)	350 (93%)	26 (7%)	0	100	100
4	D	89/93 (96%)	88 (99%)	1 (1%)	0	100	100
4	N	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
4	P	91/93 (98%)	91 (100%)	0	0	100	100
4	T	89/93 (96%)	88 (99%)	1 (1%)	0	100	100
5	E	117/119 (98%)	106 (91%)	10 (8%)	1 (1%)	14	42
6	F	154/311 (50%)	139 (90%)	13 (8%)	2 (1%)	9	33
7	G	117/119 (98%)	102 (87%)	15 (13%)	0	100	100
8	H	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
8	Q	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
8	U	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
8	W	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
9	I	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
10	J	135/206 (66%)	133 (98%)	2 (2%)	0	100	100
11	K	36/249 (14%)	36 (100%)	0	0	100	100
12	L	75/79 (95%)	71 (95%)	4 (5%)	0	100	100
12	R	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
12	V	77/79 (98%)	77 (100%)	0	0	100	100
12	Z	76/79 (96%)	71 (93%)	4 (5%)	1 (1%)	9	33
All	All	3181/4091 (78%)	3023 (95%)	153 (5%)	5 (0%)	44	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	Z	24	ASP
6	F	22	GLU
6	F	292	THR
1	A	444	LYS
5	E	221	PRO

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	646/1006 (64%)	641 (99%)	5 (1%)	73	77
2	B	84/84 (100%)	83 (99%)	1 (1%)	63	72
2	M	84/84 (100%)	82 (98%)	2 (2%)	43	62
2	O	84/84 (100%)	83 (99%)	1 (1%)	63	72
2	S	84/84 (100%)	83 (99%)	1 (1%)	63	72
3	C	320/320 (100%)	319 (100%)	1 (0%)	86	84
4	D	78/80 (98%)	78 (100%)	0	100	100
4	N	80/80 (100%)	80 (100%)	0	100	100
4	P	80/80 (100%)	80 (100%)	0	100	100
4	T	78/80 (98%)	78 (100%)	0	100	100
5	E	111/111 (100%)	111 (100%)	0	100	100
6	F	148/275 (54%)	140 (95%)	8 (5%)	20	47
7	G	110/110 (100%)	109 (99%)	1 (1%)	70	76
8	H	85/86 (99%)	85 (100%)	0	100	100
8	Q	86/86 (100%)	86 (100%)	0	100	100
8	U	85/86 (99%)	84 (99%)	1 (1%)	63	72
8	W	86/86 (100%)	86 (100%)	0	100	100
9	I	101/101 (100%)	101 (100%)	0	100	100
10	J	131/187 (70%)	131 (100%)	0	100	100
11	K	38/232 (16%)	38 (100%)	0	100	100
12	L	64/66 (97%)	64 (100%)	0	100	100
12	R	66/66 (100%)	65 (98%)	1 (2%)	57	69
12	V	66/66 (100%)	65 (98%)	1 (2%)	57	69
12	Z	65/66 (98%)	64 (98%)	1 (2%)	57	69
All	All	2860/3606 (79%)	2836 (99%)	24 (1%)	70	77

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	LEU
1	A	304	THR
1	A	443	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	444	LYS
1	A	763	THR
2	B	23	LEU
3	C	143	VAL
6	F	14	LYS
6	F	16	LYS
6	F	18	ARG
6	F	21	ILE
6	F	23	SER
6	F	24	LYS
6	F	28	ILE
6	F	291	LYS
7	G	155	LYS
2	M	23	LEU
2	M	38	ASN
2	O	23	LEU
12	R	23	ARG
2	S	23	LEU
8	U	120	MET
12	V	96	THR
12	Z	24	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
1	A	431	HIS
1	A	663	ASN
1	A	690	ASN
1	A	815	HIS
1	A	836	ASN
1	A	974	GLN
1	A	1004	ASN
1	A	1070	HIS
1	A	1143	ASN
1	A	1163	GLN
1	A	1234	ASN
1	A	1252	HIS
1	A	1274	ASN
1	A	1315	GLN
3	C	31	ASN
3	C	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	135	ASN
3	C	151	HIS
3	C	177	HIS
3	C	189	HIS
3	C	209	HIS
3	C	235	ASN
3	C	263	GLN
3	C	291	HIS
3	C	359	ASN
4	D	60	ASN
4	D	64	ASN
4	D	81	ASN
5	E	178	GLN
5	E	198	GLN
5	E	213	GLN
5	E	265	GLN
5	E	280	ASN
6	F	20	ASN
6	F	26	ASN
6	F	59	ASN
6	F	96	GLN
7	G	100	HIS
7	G	120	GLN
7	G	158	HIS
7	G	169	HIS
7	G	190	ASN
8	H	85	GLN
8	H	93	GLN
8	H	108	ASN
9	I	33	HIS
9	I	59	ASN
9	I	71	ASN
9	I	73	ASN
9	I	88	HIS
10	J	177	ASN
10	J	178	HIS
10	J	222	HIS
10	J	296	GLN
10	J	358	ASN
10	J	360	GLN
10	J	378	ASN
11	K	251	GLN

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Mol	Chain	Res	Type
12	L	25	ASN
2	M	38	ASN
2	M	104	GLN
4	N	64	ASN
2	O	104	GLN
4	P	46	HIS
4	P	106	HIS
8	Q	39	HIS
8	Q	68	GLN
8	Q	85	GLN
8	Q	93	GLN
8	Q	108	ASN
4	T	46	HIS
4	T	60	ASN
4	T	64	ASN
4	T	81	ASN
8	U	39	HIS
8	U	68	GLN
8	U	108	ASN
12	V	25	ASN
12	V	27	GLN
8	W	39	HIS
12	Z	27	GLN
12	Z	64	ASN
12	Z	93	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

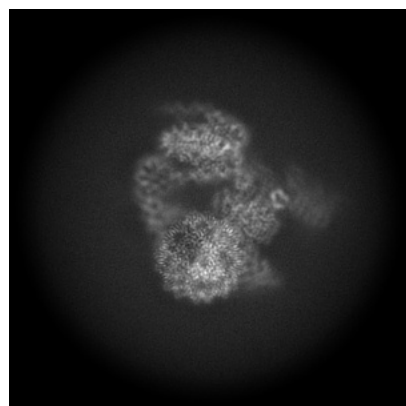
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64742. These allow visual inspection of the internal detail of the map and identification of artifacts.

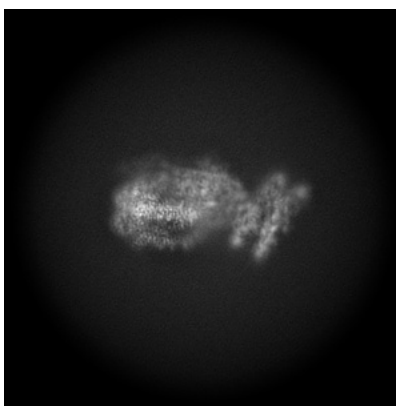
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

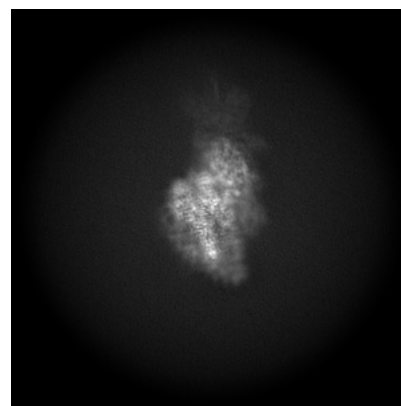
6.1.1 Primary map



X

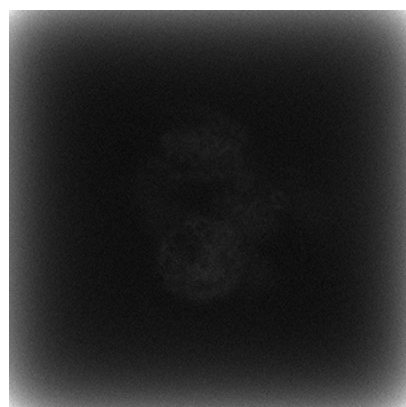


Y



Z

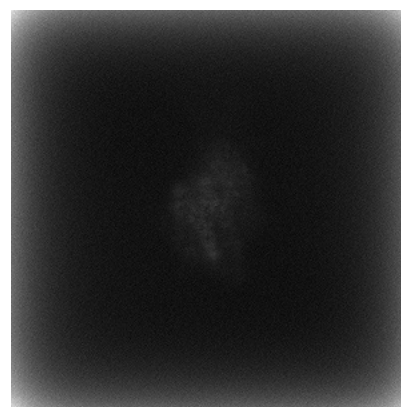
6.1.2 Raw map



X



Y

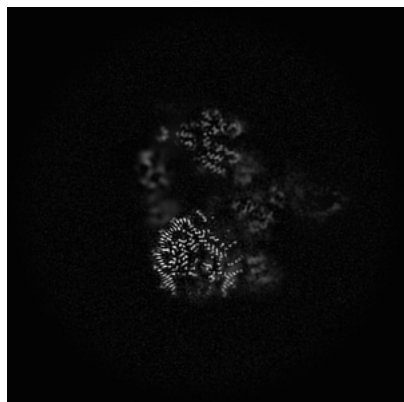


Z

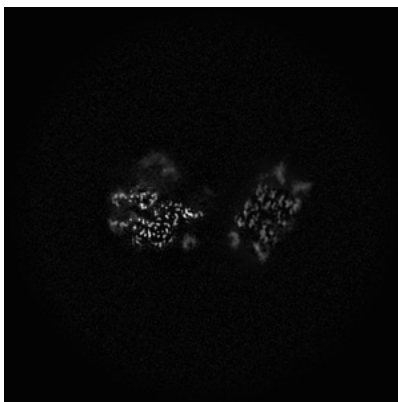
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

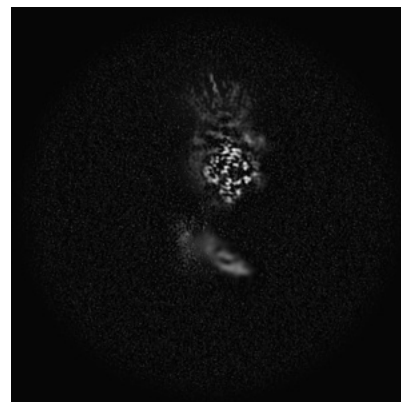
6.2.1 Primary map



X Index: 300

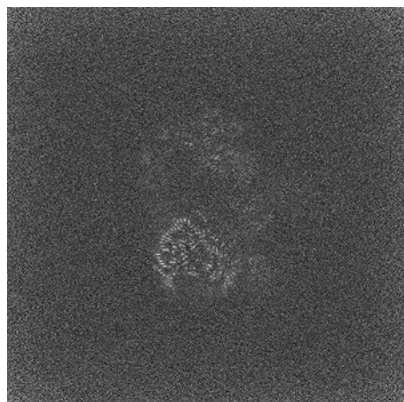


Y Index: 300

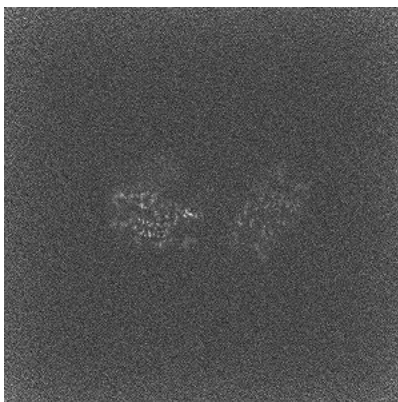


Z Index: 300

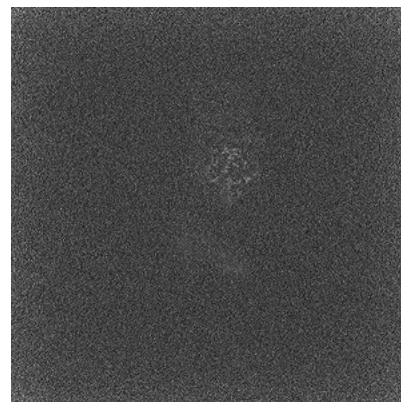
6.2.2 Raw map



X Index: 300



Y Index: 300

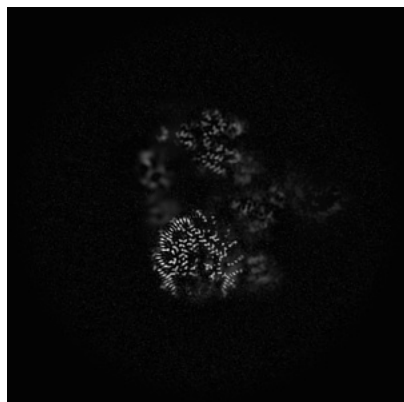


Z Index: 300

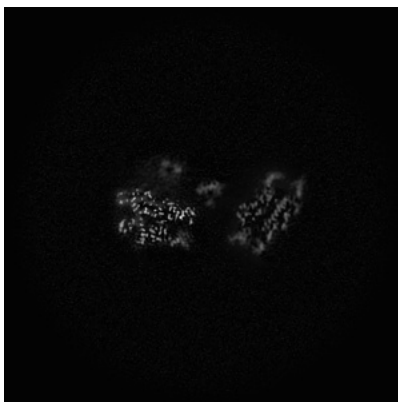
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

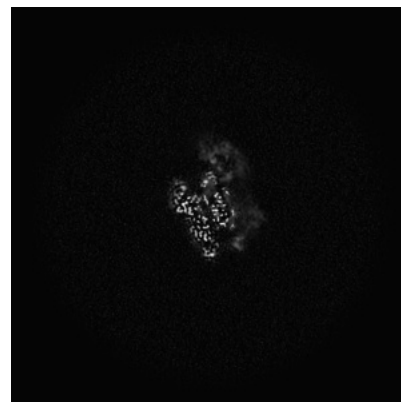
6.3.1 Primary map



X Index: 299

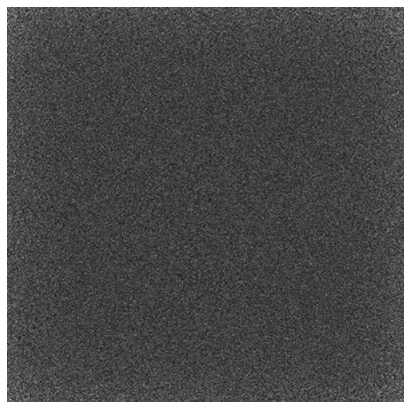


Y Index: 311

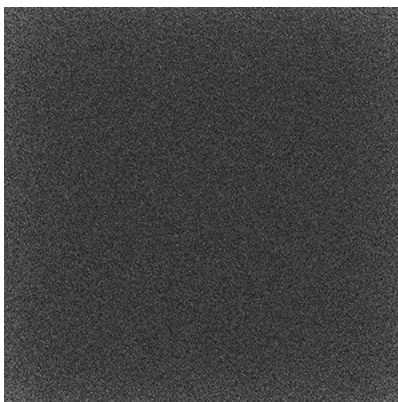


Z Index: 204

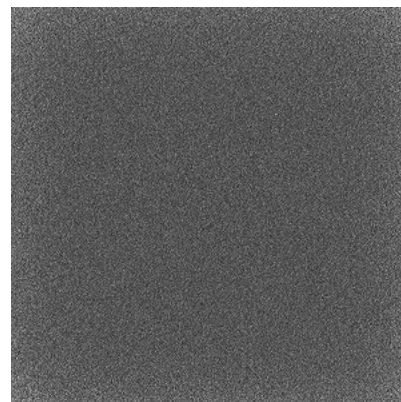
6.3.2 Raw map



X Index: 0



Y Index: 0

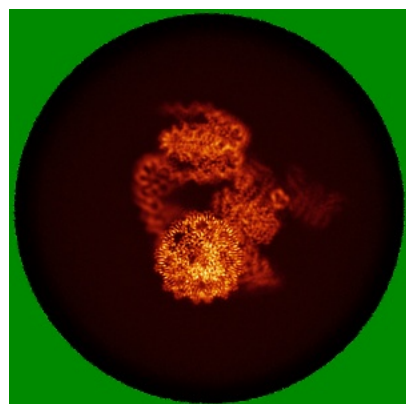


Z Index: 0

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

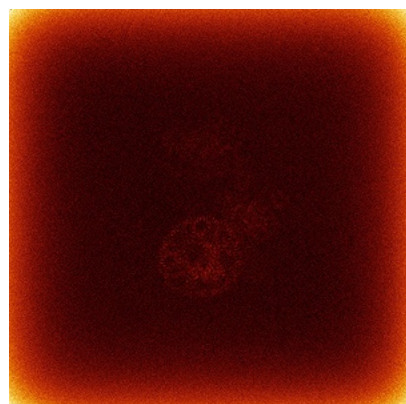


Y



Z

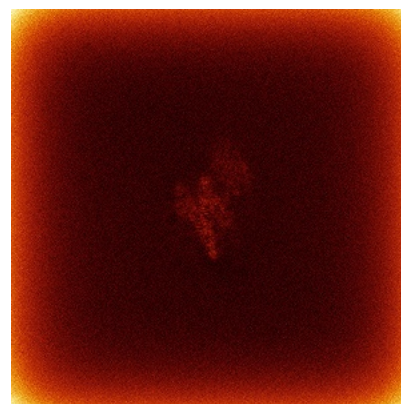
6.4.2 Raw map



X



Y

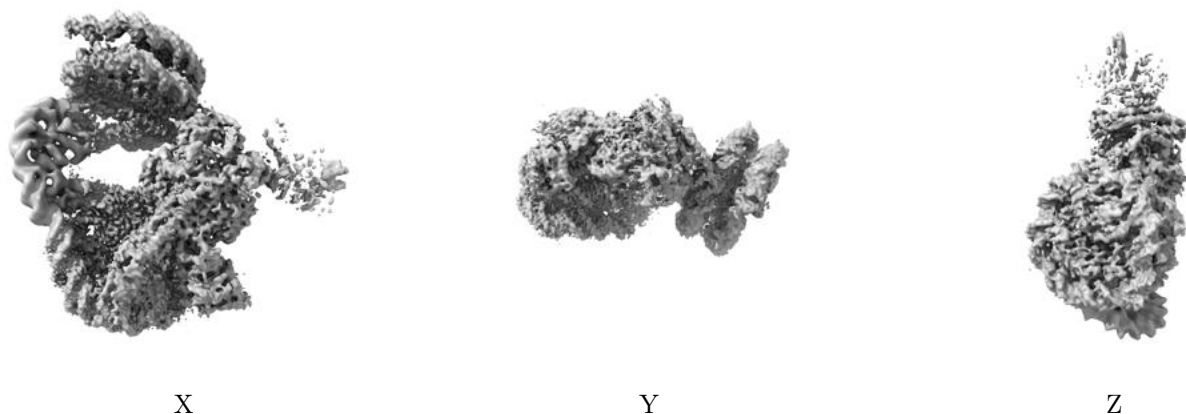


Z

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.

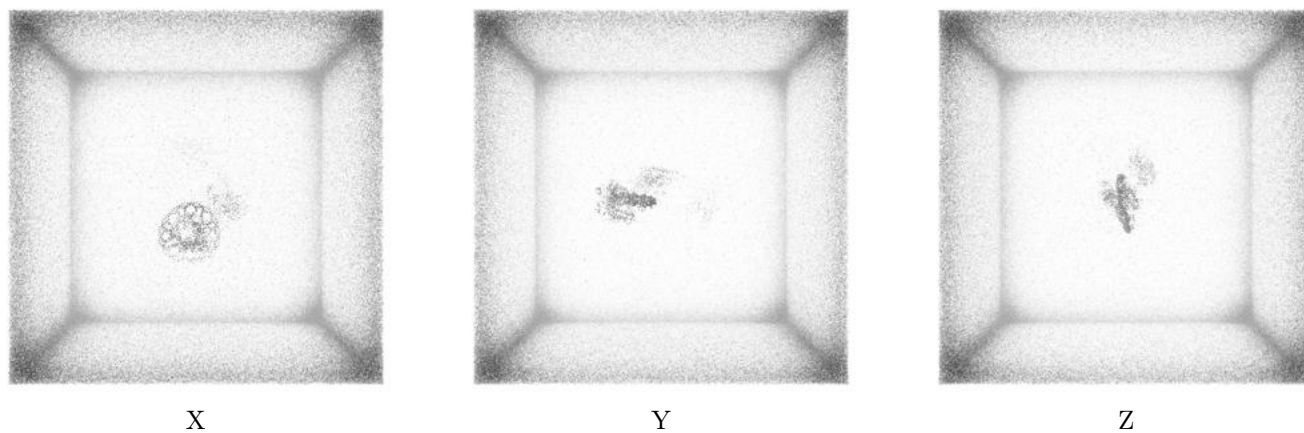
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



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.

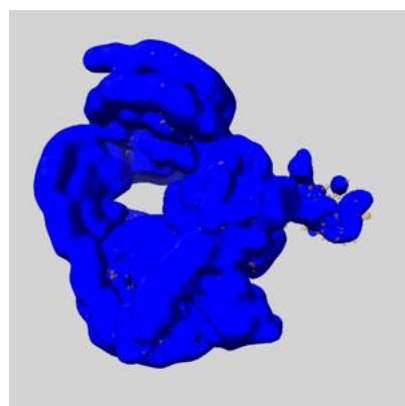
6.6 Mask visualisation [i](#)

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

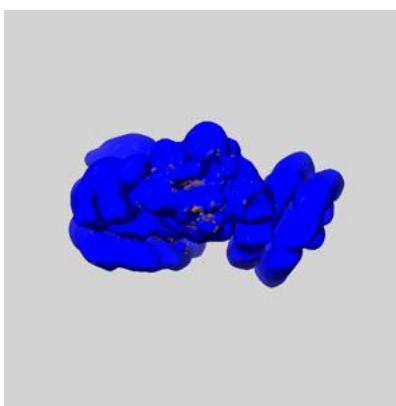
A mask typically either:

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

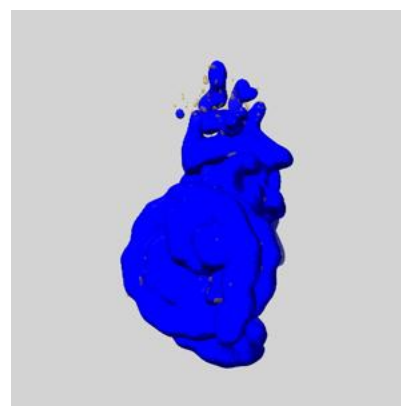
6.6.1 emd_64742_msk_1.map [i](#)



X



Y

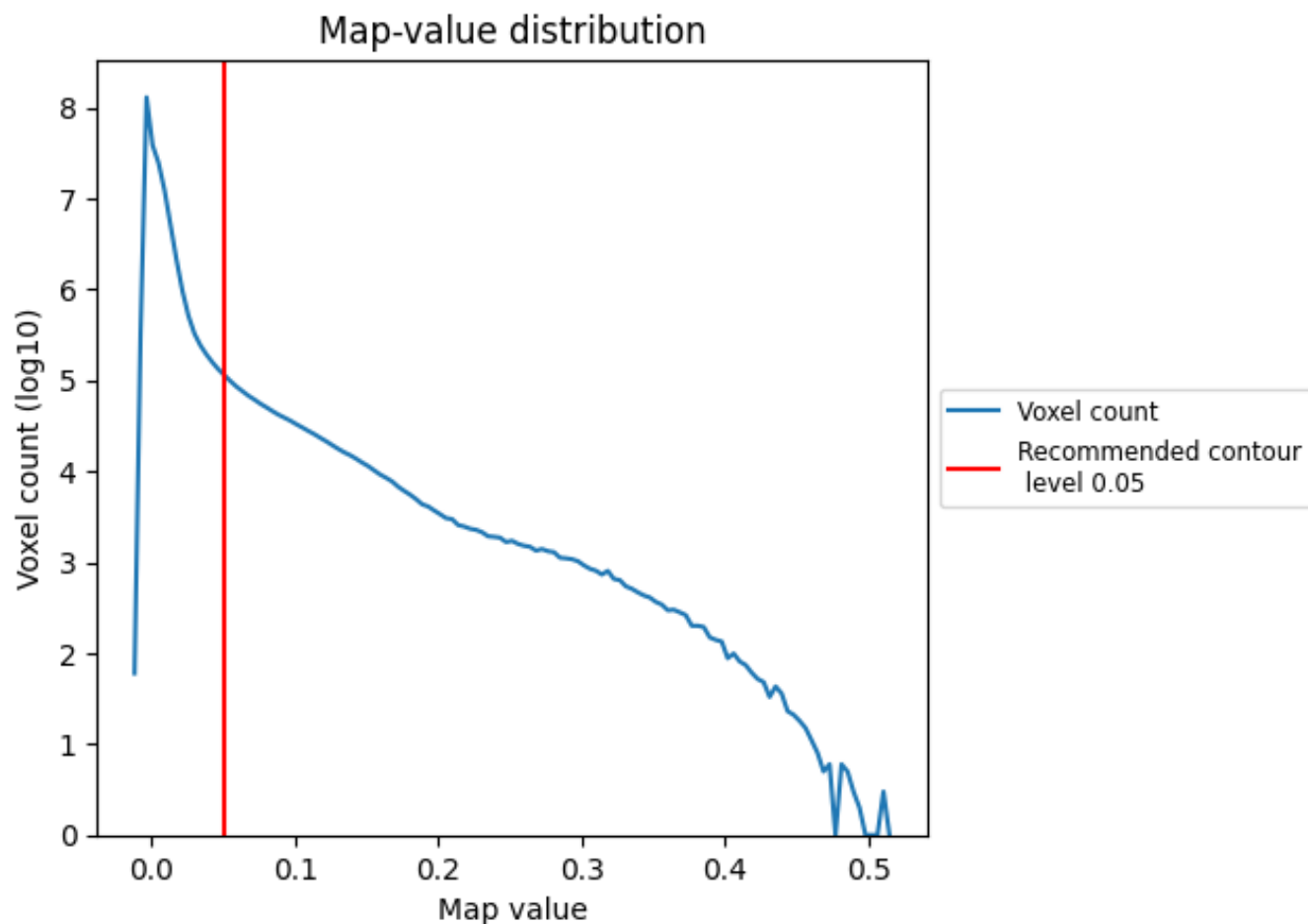


Z

7 Map analysis [i](#)

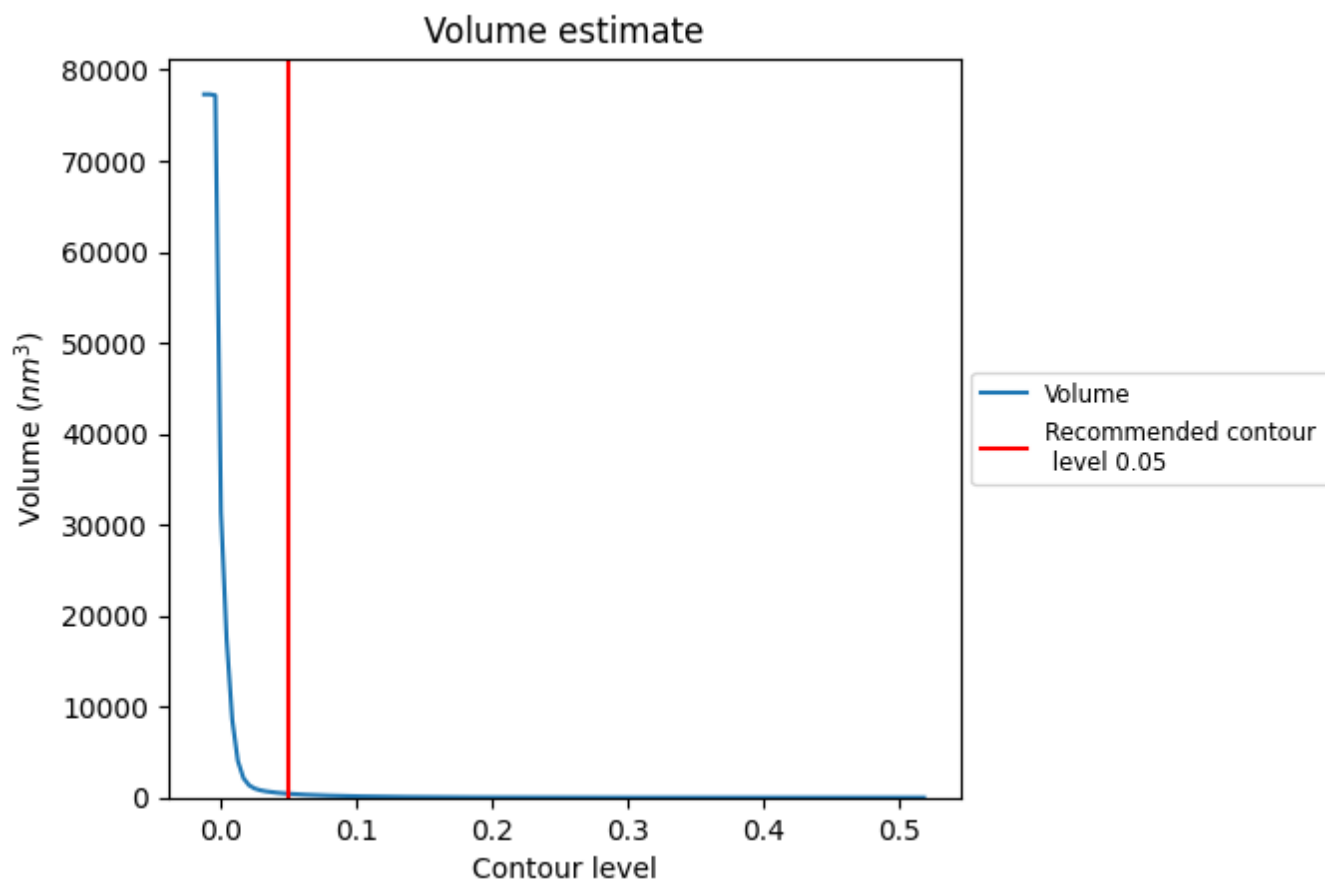
This section contains the results of statistical analysis of the map.

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.

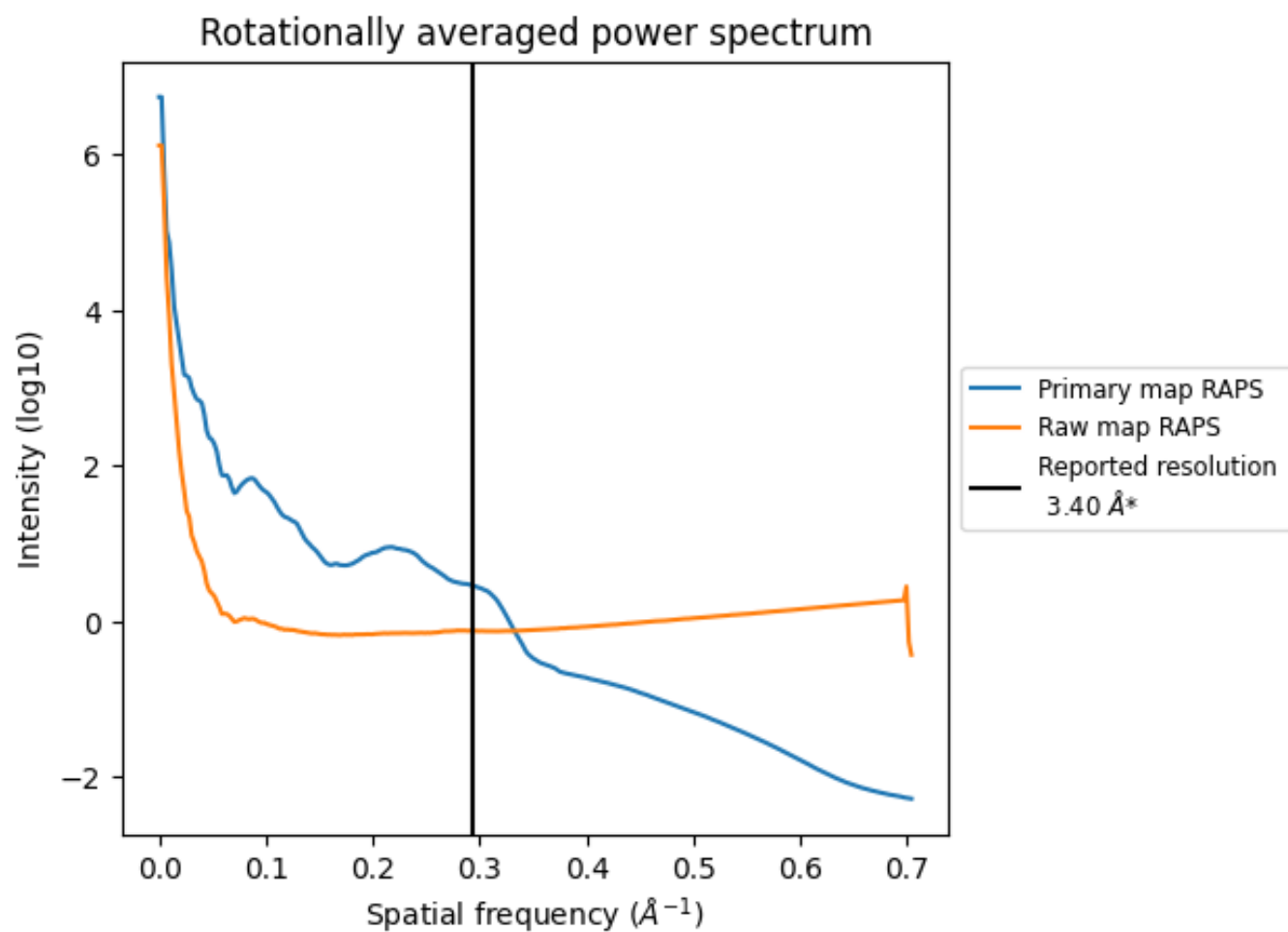
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 425 nm^3 ; this corresponds to an approximate mass of 384 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

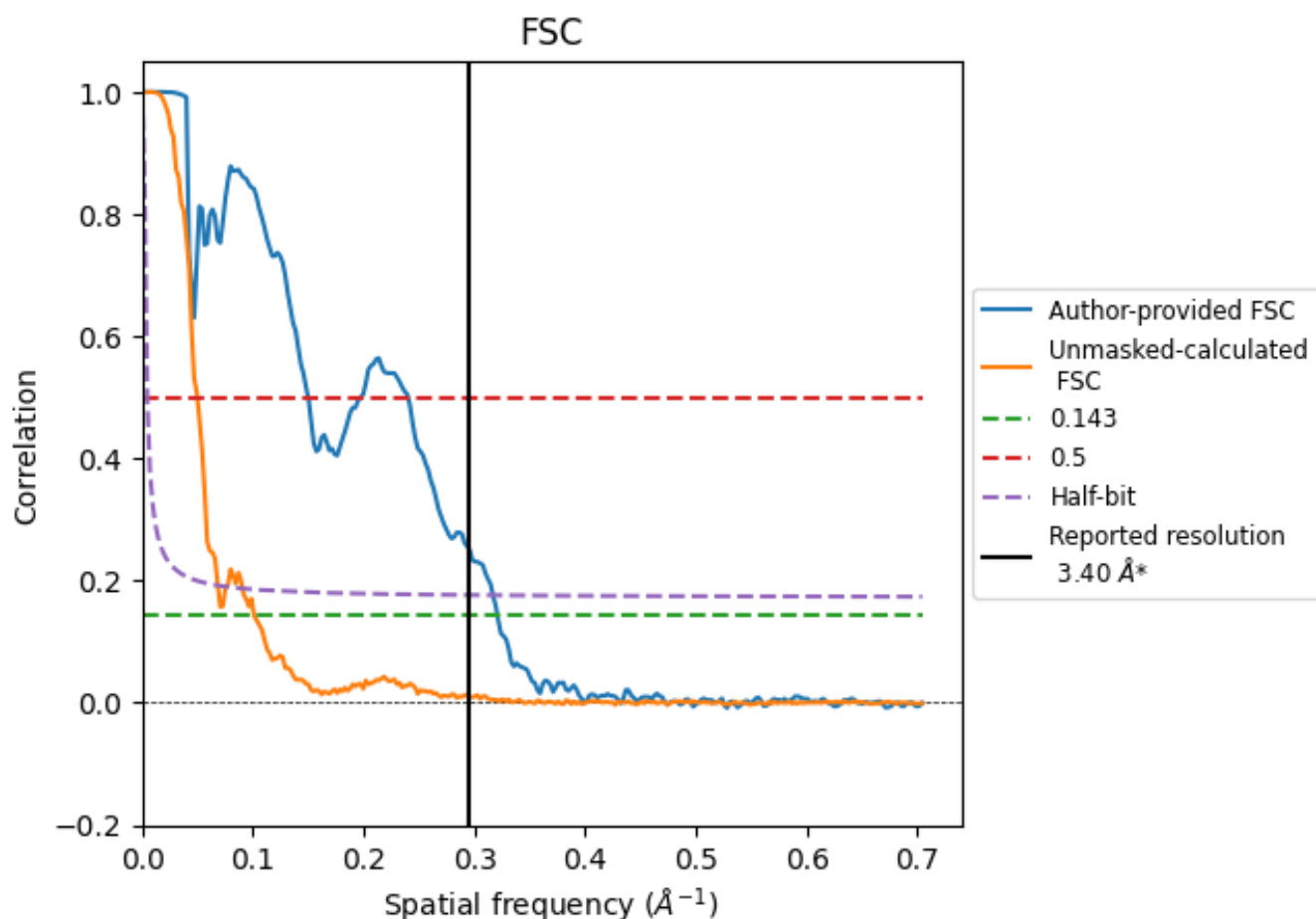


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

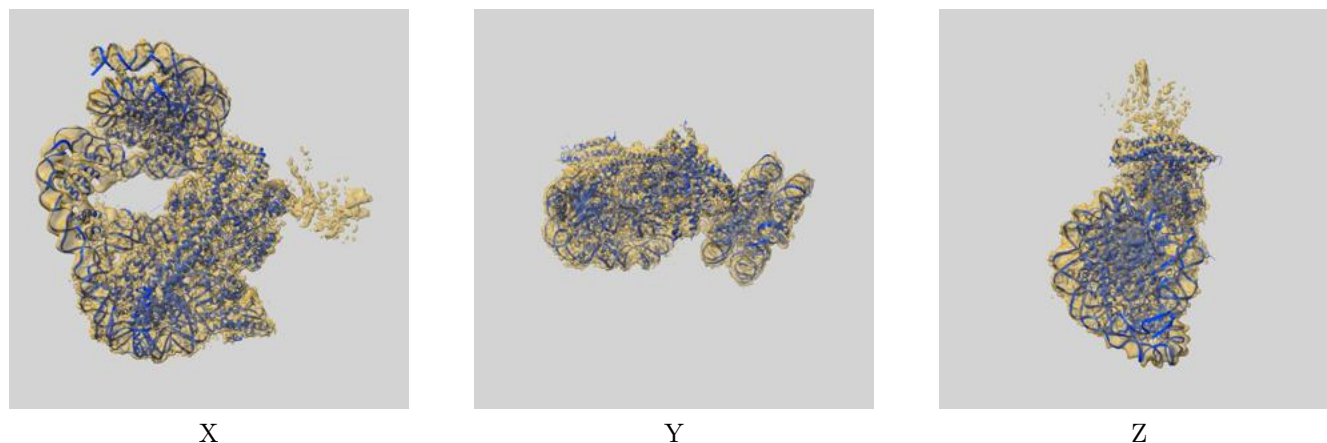
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.12	6.67	3.16
Unmasked-calculated*	9.91	20.12	14.64

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

9 Map-model fit [i](#)

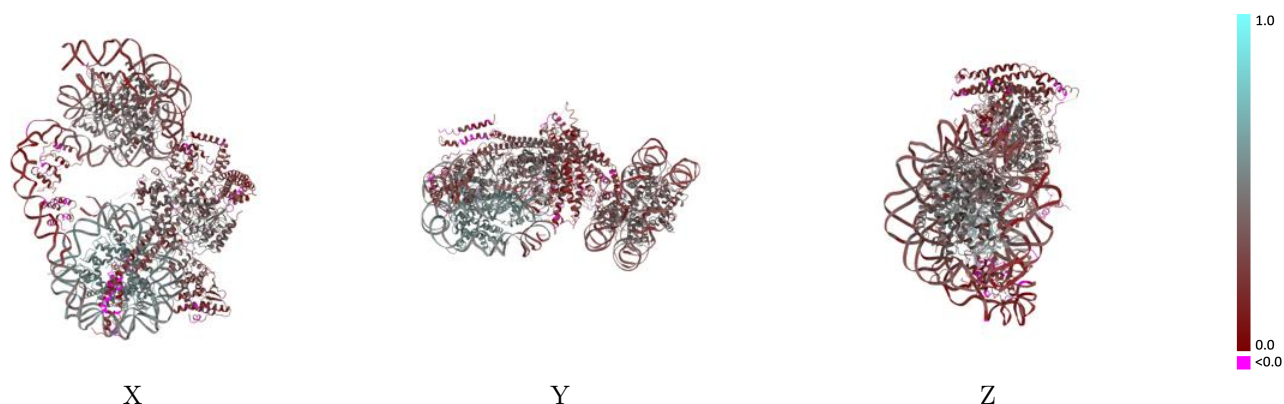
This section contains information regarding the fit between EMDB map EMD-64742 and PDB model 9V2W. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



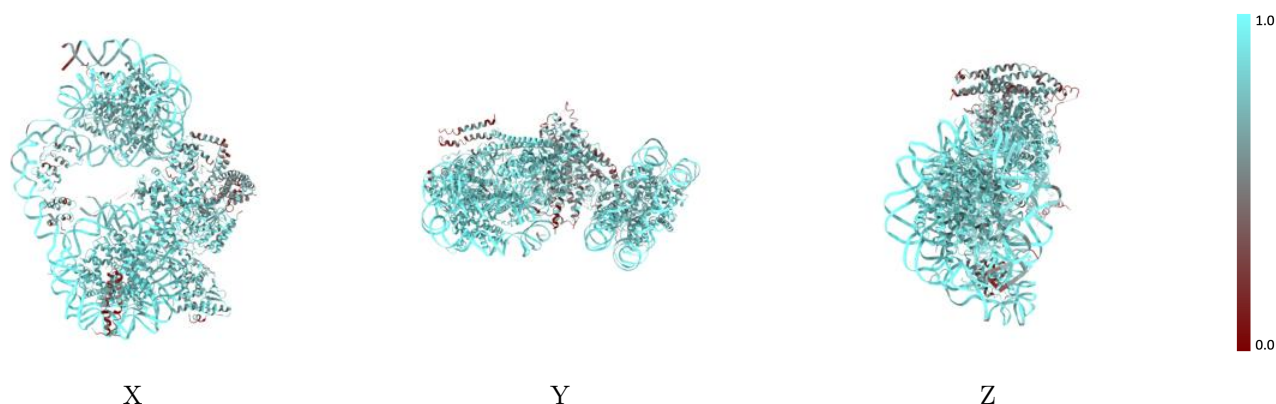
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



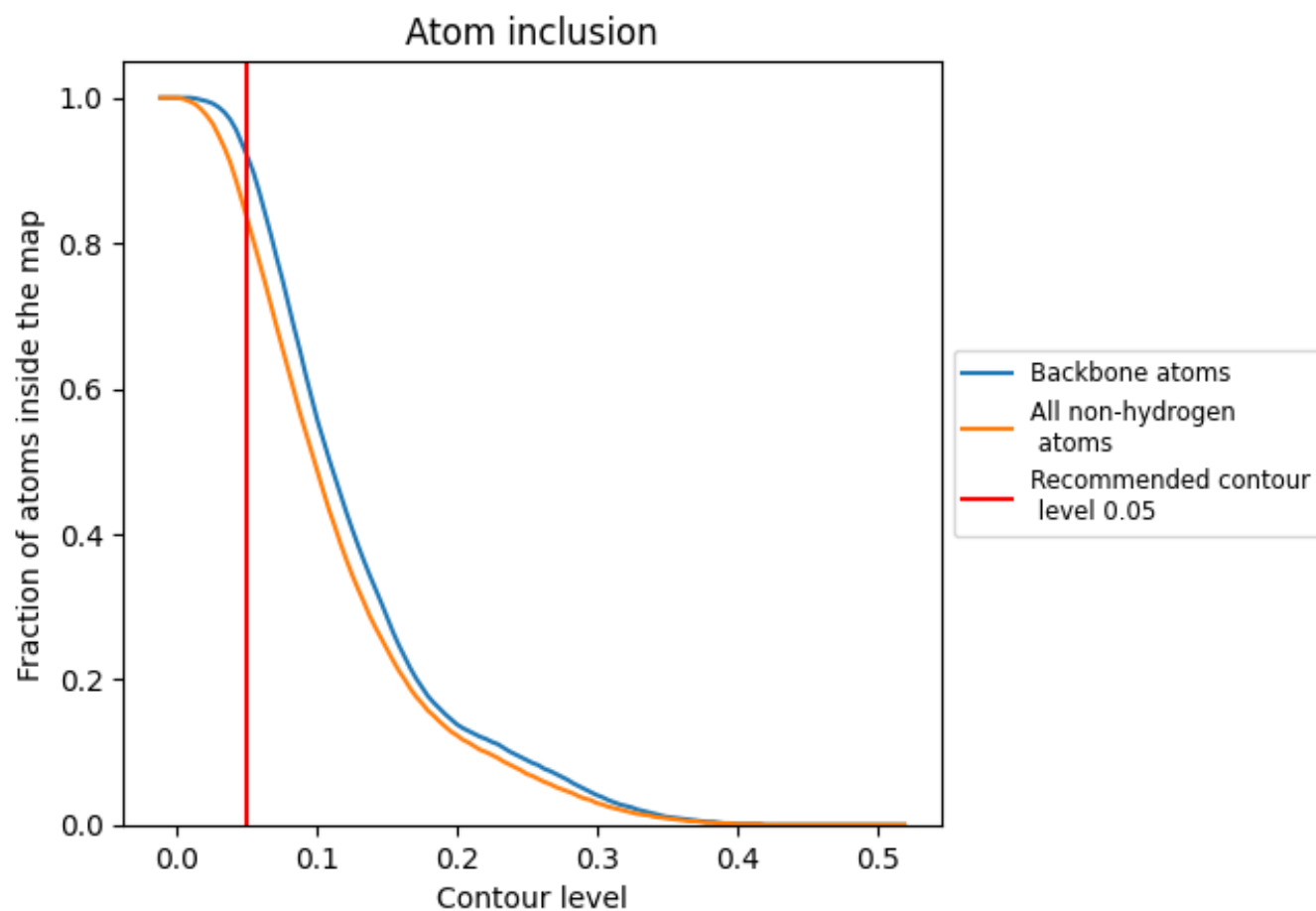
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 92% of all backbone atoms, 83% 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	 0.8330	 0.3620
A	 0.7270	 0.2410
B	 0.8250	 0.4100
C	 0.8340	 0.3960
D	 0.8110	 0.3930
E	 0.6490	 0.2280
F	 0.6780	 0.2680
G	 0.7230	 0.2900
H	 0.7690	 0.3630
I	 0.5430	 0.1780
J	 0.5420	 0.2220
K	 0.4080	 0.1080
L	 0.8350	 0.3860
M	 0.8310	 0.3920
N	 0.8260	 0.3900
O	 0.9490	 0.5340
P	 0.9550	 0.5260
Q	 0.9330	 0.5510
R	 0.9390	 0.5640
S	 0.9390	 0.5510
T	 0.9590	 0.5550
U	 0.9480	 0.5740
V	 0.9740	 0.5800
W	 0.8400	 0.4040
X	 0.9210	 0.3640
Y	 0.9180	 0.3590
Z	 0.9050	 0.4210

