



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 03:52 PM UTC

PDB ID : 7V9K / pdb_00007v9k
EMDB ID : EMD-31823
Title : Telomeric tetranucleosome
Authors : Soman, A.
Deposited on : 2021-08-25
Resolution : 8.10 Å(reported)
Based on initial model : 6KE9

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

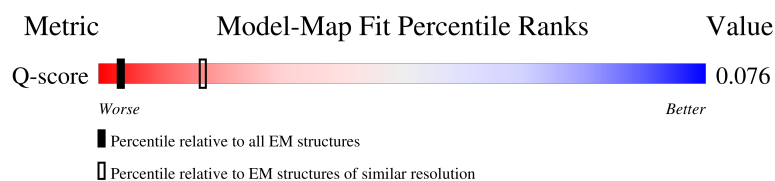
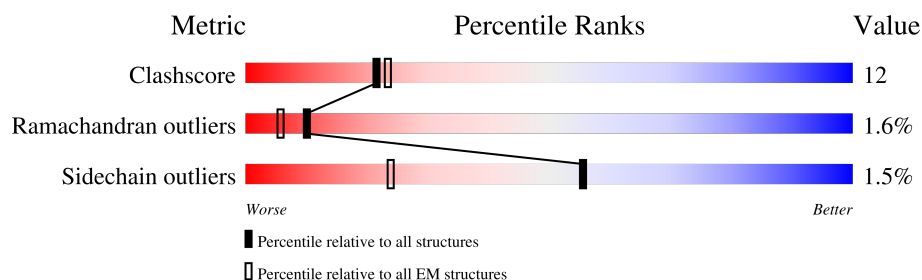
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 8.10 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.



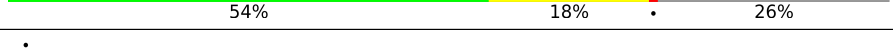
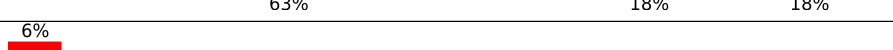
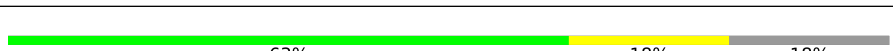
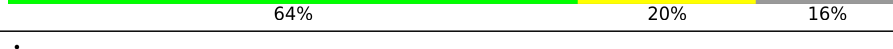
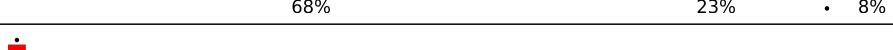
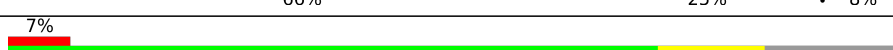
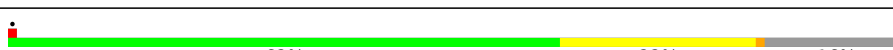
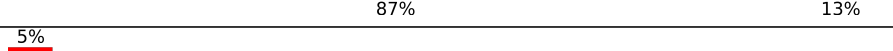
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

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	136	
1	E	136	
1	K	136	
1	O	136	

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Mol	Chain	Length	Quality of chain
1	S	136	
1	W	136	
1	a	136	
1	e	136	
2	B	103	
2	F	103	
2	L	103	
2	P	103	
2	T	103	
2	X	103	
2	b	103	
2	f	103	
3	C	130	
3	G	130	
3	M	130	
3	Q	130	
3	U	130	
3	Y	130	
3	c	130	
3	g	130	
4	D	99	
4	H	99	
4	N	99	
4	R	99	
4	V	99	

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Mol	Chain	Length	Quality of chain
4	Z	99	82%17%
4	d	99	7% 86%14%
4	h	99	8% 82%17%
5	I	539	40%60%
6	J	539	37%63%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 47361 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	100	Total	C	N	O	S	0	0
			824	520	160	140	4		
1	E	100	Total	C	N	O	S	0	0
			825	520	160	141	4		
1	K	100	Total	C	N	O	S	0	0
			824	520	160	140	4		
1	O	100	Total	C	N	O	S	0	0
			825	520	160	141	4		
1	S	100	Total	C	N	O	S	0	0
			824	520	160	140	4		
1	W	100	Total	C	N	O	S	0	0
			825	520	160	141	4		
1	a	100	Total	C	N	O	S	0	0
			824	520	160	140	4		
1	e	100	Total	C	N	O	S	0	0
			825	520	160	141	4		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	S	0	0
			673	424	133	115	1		
2	F	87	Total	C	N	O	S	0	0
			703	442	142	118	1		
2	L	87	Total	C	N	O	S	0	0
			703	442	142	118	1		
2	P	84	Total	C	N	O	S	0	0
			673	424	133	115	1		
2	T	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	X	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	b	84	Total	C	N	O	S	0	0
			673	424	133	115	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	f	87	Total	C	N	O	S	0	0
			703	442	142	118	1		

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	109	Total	C	N	O		0	0
			840	529	166	145			
3	G	120	Total	C	N	O		0	0
			927	582	185	160			
3	M	119	Total	C	N	O		0	0
			921	579	184	158			
3	Q	110	Total	C	N	O		0	0
			849	535	168	146			
3	U	109	Total	C	N	O		0	0
			840	529	166	145			
3	Y	110	Total	C	N	O		0	0
			849	535	168	146			
3	c	109	Total	C	N	O		0	0
			840	529	166	145			
3	g	120	Total	C	N	O		0	0
			927	582	185	160			

- Molecule 4 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	99	Total	C	N	O	S	0	0
			783	491	146	144	2		
4	H	98	Total	C	N	O	S	0	0
			773	485	144	142	2		
4	N	99	Total	C	N	O	S	0	0
			783	491	146	144	2		
4	R	98	Total	C	N	O	S	0	0
			773	485	144	142	2		
4	V	99	Total	C	N	O	S	0	0
			783	491	146	144	2		
4	Z	98	Total	C	N	O	S	0	0
			773	485	144	142	2		
4	d	99	Total	C	N	O	S	0	0
			783	491	146	144	2		
4	h	98	Total	C	N	O	S	0	0
			773	485	144	142	2		

- Molecule 5 is a DNA chain called DNA (539-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	539	Total	C	N	O	P	0	0
			11406	5390	2155	3323	538		

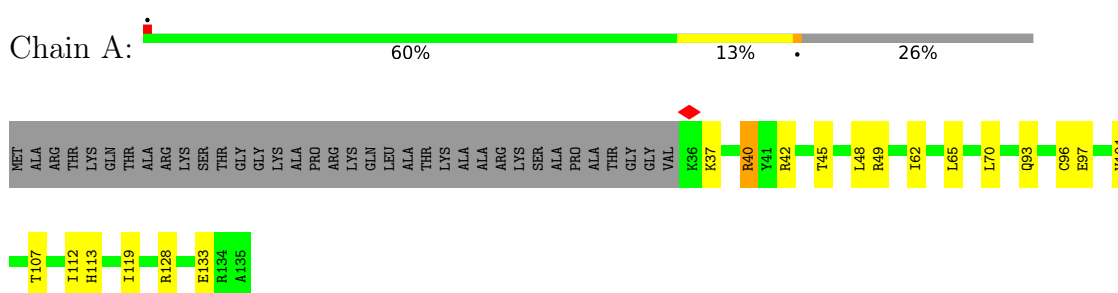
- Molecule 6 is a DNA chain called DNA (539-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	539	Total	C	N	O	P	0	0
			10690	5120	1888	3143	539		

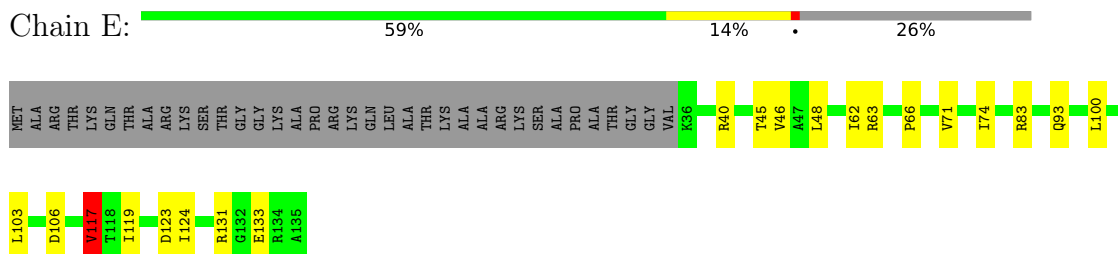
3 Residue-property plots [i](#)

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

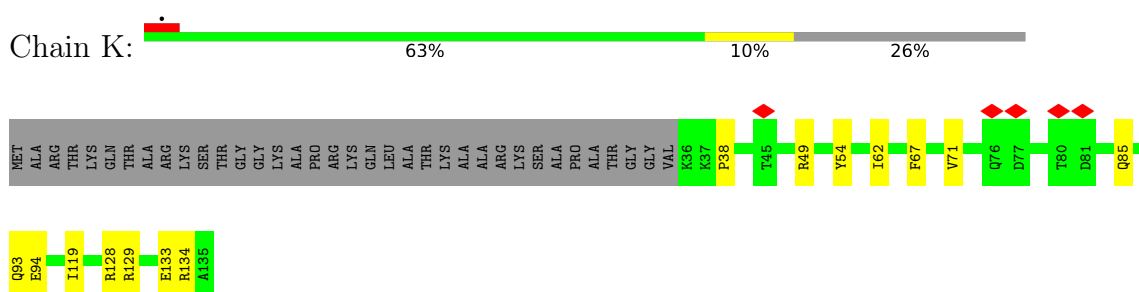
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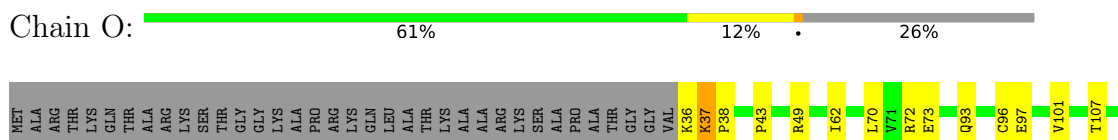
- Molecule 1: Histone H3.1



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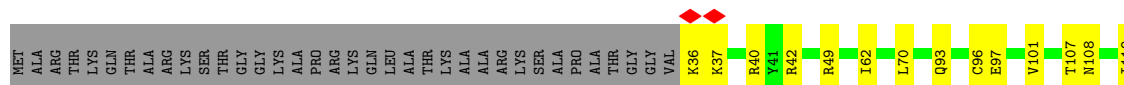


- Molecule 1: Histone H3.1

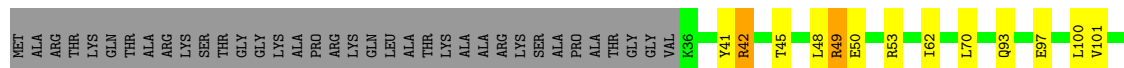




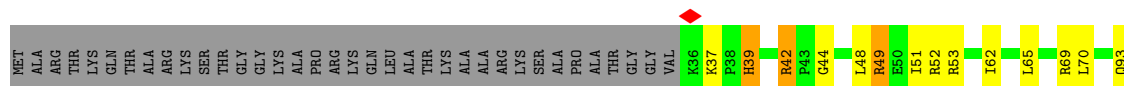
- Molecule 1: Histone H3.1



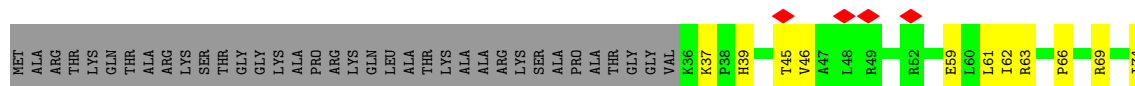
- Molecule 1: Histone H3.1



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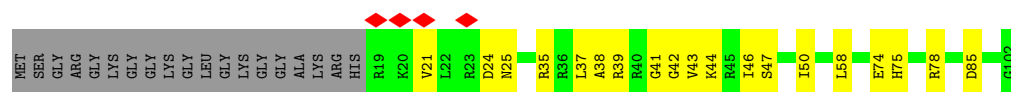


- Molecule 1: Histone H3.1

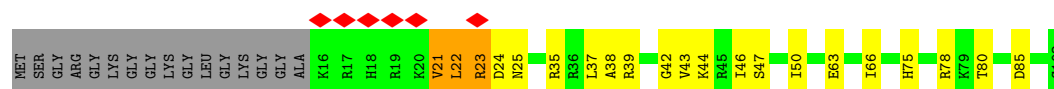


- Molecule 2: Histone H4

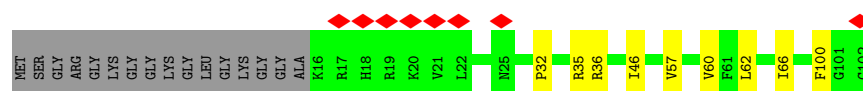
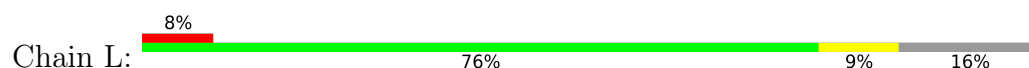




• Molecule 2: Histone H4



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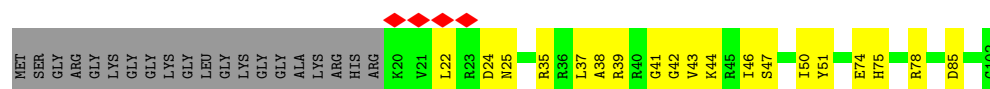
• Molecule 2: Histone H4



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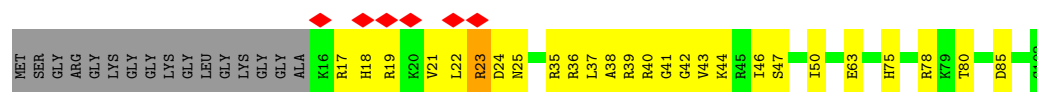


• Molecule 2: Histone H4

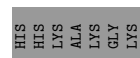


• Molecule 2: Histone H4

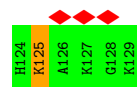




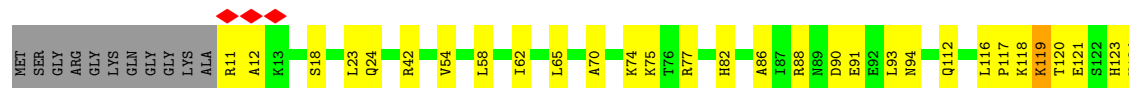
- Molecule 3: Histone H2A type 1-B/E



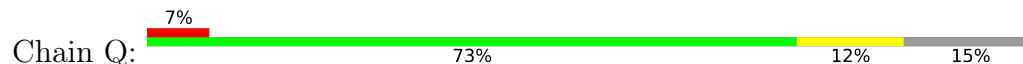
- Molecule 3: Histone H2A type 1-B/E



- Molecule 3: Histone H2A type 1-B/E



- Molecule 3: Histone H2A type 1-B/E



- Molecule 3: Histone H2A type 1-B/E



LYS
THR
GLU
SER
SER
HIS
HIS
LYS
LYS
ALA
GLY
LYS

• Molecule 3: Histone H2A type 1-B/E

Chain Y:  66% 18% 15%

MET SER GLY ARG GLY LYS GLN GLY LYS A10 A11 A12 A13 A14 S18 L23 Q24 R42 Y50 V54 I62 L65 A70 K74 K75 H82 A86 I87 R88 N89 D90 L93 N94 Q112 L116 P117 K118 K119 THR GLU SER HIS HIS LYS LYS ALA

LYS GLY LYS

• Molecule 3: Histone H2A type 1-B/E

Chain c:  9% 65% 18% 16%

MET SER GLY ARG GLY LYS GLN GLY LYS A10 A11 A12 A13 A14 K15 S18 L23 R35 V54 L58 I62 L65 N68 A69 A70 R71 D72 N73 K74 K75 H82 A86 I87 R88 N89 D90 E91 E92 L93 N94 L108 Q112 L115 L116 P117 K118

LYS THR GLU SER ARG GLY LYS GLN GLY LYS

• Molecule 3: Histone H2A type 1-B/E

Chain g:  15% 65% 25% 8%

MET SER GLY ARG GLY LYS GLN GLY LYS A10 A11 A12 A13 A14 K15 S18 L23 Q24 R32 N38 Y50 V54 L55 E61 I62 L63 E64 L65 N68 A69 A70 R71 K74 K75 H82 L85 A86 I87 R88 N89 D90 E91 E92 L93 N94 L108 P109

N110 I111 Q112 A113 V114 L115 L116 P117 K118 T120 E121 S122 H123 H124 K125 A126 K127 G128 K129

• Molecule 4: Histone H2B type 1-K

Chain D:  78% 21%

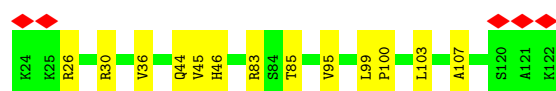
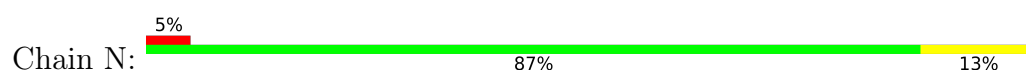
K24 K25 K26 K27 R28 S29 E32 S33 K43 T49 G50 I51 K54 A55 M56 L77 R83 S84 T85 I86 R89 E90 V95 L99 P100 L103 A107 K122

• Molecule 4: Histone H2B type 1-K

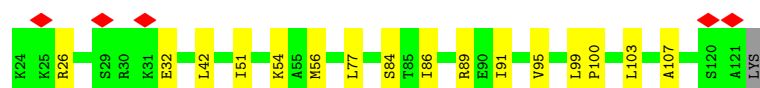
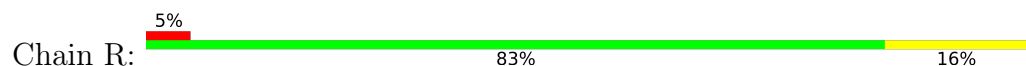
Chain H:  82% 16%

K24 K25 K26 K27 R30 Y37 V41 Q44 V45 H46 P47 D48 L77 E90 V95 L99 P100 L103 A107 A121 LYS

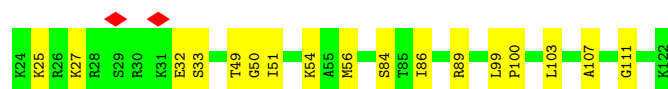
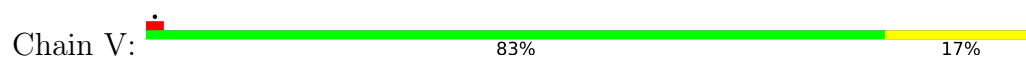
• Molecule 4: Histone H2B type 1-K



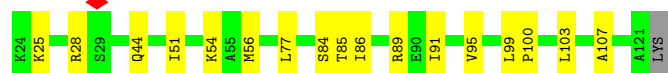
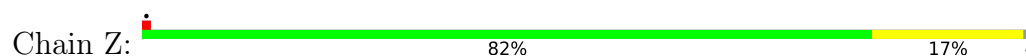
- Molecule 4: Histone H2B type 1-K



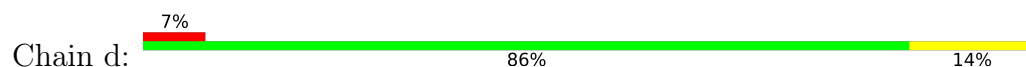
- Molecule 4: Histone H2B type 1-K



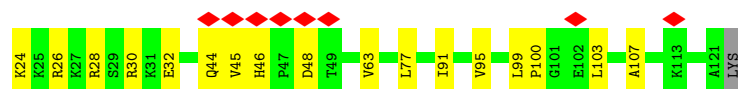
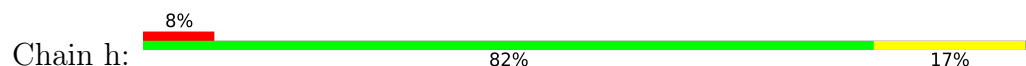
- Molecule 4: Histone H2B type 1-K



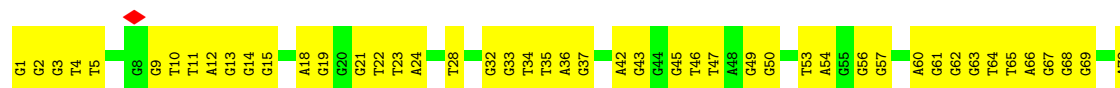
- Molecule 4: Histone H2B type 1-K

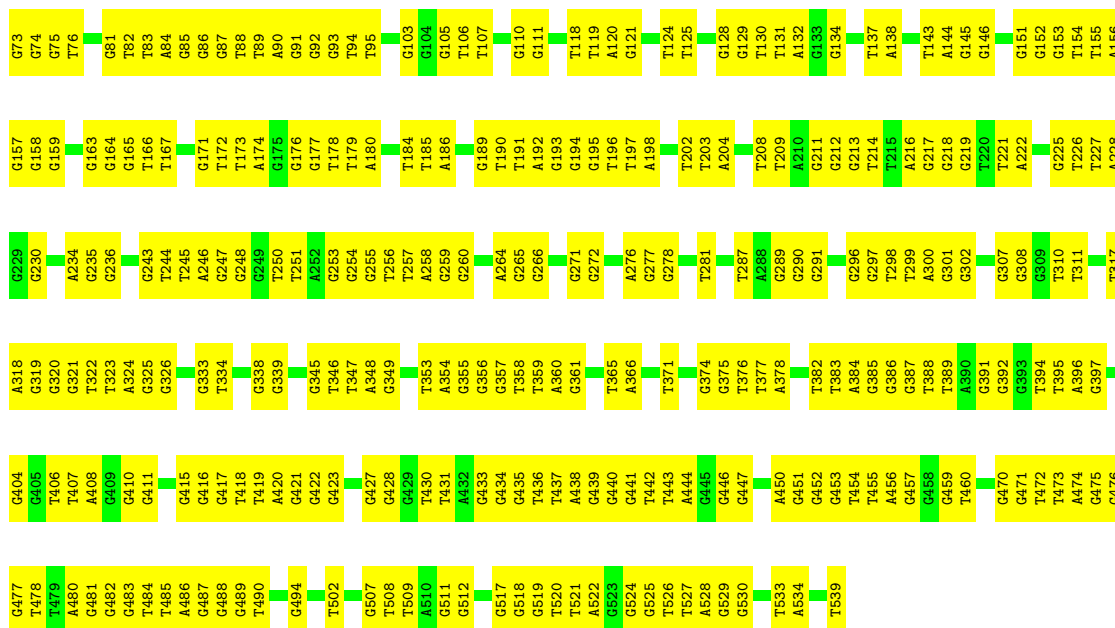


- Molecule 4: Histone H2B type 1-K

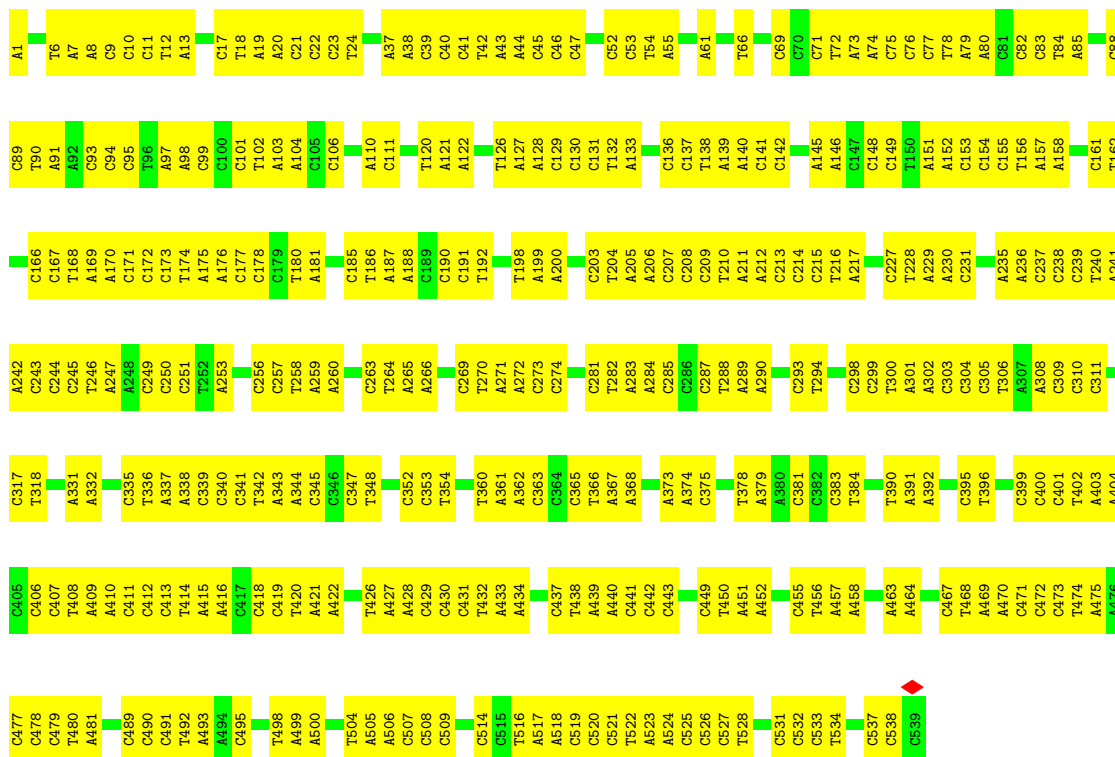


- Molecule 5: DNA (539-mer)





- Molecule 6: DNA (539-mer)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	26580	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0049	Depositor
Map size (Å)	358.4, 358.4, 358.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.06	0/836	0.19	0/1120
1	E	0.08	0/837	0.21	0/1120
1	K	0.07	0/836	0.19	0/1120
1	O	0.09	0/837	0.28	0/1120
1	S	0.07	0/836	0.24	0/1120
1	W	0.07	0/837	0.17	0/1120
1	a	0.16	0/836	0.36	1/1120 (0.1%)
1	e	0.07	0/837	0.20	0/1120
2	B	0.06	0/680	0.15	0/908
2	F	0.13	0/711	0.28	0/948
2	L	0.07	0/711	0.19	0/948
2	P	0.06	0/680	0.17	0/908
2	T	0.06	0/669	0.17	0/894
2	X	0.06	0/669	0.16	0/894
2	b	0.06	0/680	0.15	0/908
2	f	0.06	0/711	0.16	0/948
3	C	0.18	0/850	0.23	0/1146
3	G	0.18	0/939	0.26	0/1262
3	M	0.18	0/933	0.27	0/1253
3	Q	0.06	0/859	0.16	0/1157
3	U	0.18	0/850	0.21	0/1146
3	Y	0.19	0/859	0.24	0/1157
3	c	0.18	0/850	0.22	0/1146
3	g	0.18	0/939	0.27	0/1262
4	D	0.08	0/794	0.19	0/1061
4	H	0.07	0/784	0.14	0/1050
4	N	0.06	0/794	0.17	0/1061
4	R	0.07	0/784	0.17	0/1050
4	V	0.06	0/794	0.17	0/1061
4	Z	0.07	0/784	0.18	0/1050
4	d	0.07	0/794	0.18	0/1061
4	h	0.05	0/784	0.13	0/1050
5	I	0.20	0/12842	0.41	2/19935 (0.0%)
6	J	0.17	0/11947	0.34	0/18322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.15	0/50383	0.31	3/72546 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	42	ARG	O-C-N	-5.66	117.52	121.65
5	I	287	DT	C2'-C3'-O3'	5.52	119.78	111.50
5	I	28	DT	C2'-C3'-O3'	-5.46	103.31	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	824	0	869	14	0
1	E	825	0	869	15	0
1	K	824	0	869	10	0
1	O	825	0	869	16	0
1	S	824	0	869	16	0
1	W	825	0	869	17	0
1	a	824	0	869	28	0
1	e	825	0	869	20	0
2	B	673	0	722	18	0
2	F	703	0	755	17	0
2	L	703	0	755	7	0
2	P	673	0	722	17	0
2	T	662	0	709	18	0
2	X	662	0	709	18	0
2	b	673	0	722	19	0
2	f	703	0	755	20	0
3	C	840	0	902	19	0
3	G	927	0	994	26	0
3	M	921	0	989	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	849	0	915	13	0
3	U	840	0	902	34	0
3	Y	849	0	915	18	0
3	c	840	0	902	16	0
3	g	927	0	994	45	0
4	D	783	0	821	18	0
4	H	773	0	808	14	0
4	N	783	0	821	11	0
4	R	773	0	808	12	0
4	V	783	0	821	15	0
4	Z	773	0	808	14	0
4	d	783	0	821	12	0
4	h	773	0	808	14	0
5	I	11406	0	6111	311	0
6	J	10690	0	6019	342	0
All	All	47361	0	38960	968	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 12.

All (968) 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)
5:I:539:DT:O4	6:J:1:DA:C2	2.22	0.91
5:I:297:DG:H1	6:J:244:DC:H42	1.18	0.89
3:U:114:VAL:H	3:g:71:ARG:NH1	1.76	0.82
3:g:121:GLU:HG3	5:I:394:DT:H5'	1.63	0.81
3:U:114:VAL:H	3:g:71:ARG:HH11	1.25	0.81
4:h:30:ARG:HD3	6:J:120:DT:H2'	1.66	0.78
5:I:384:DA:H2'	5:I:385:DG:C8	2.20	0.77
1:O:43:PRO:HG3	6:J:475:DA:H3'	1.70	0.72
5:I:539:DT:O4	6:J:1:DA:N1	2.22	0.72
6:J:338:DA:H2''	6:J:339:DC:C4	2.25	0.71
5:I:378:DA:H61	6:J:162:DT:H3	1.37	0.71
6:J:365:DC:H2'	6:J:366:DT:C6	2.26	0.70
3:U:74:LYS:HB2	1:a:52:ARG:HH21	1.56	0.70
6:J:533:DC:H2'	6:J:534:DT:H71	1.74	0.70
3:g:120:THR:O	3:g:122:SER:N	2.25	0.70
5:I:93:DG:H2'	5:I:94:DT:H71	1.73	0.70
5:I:447:DG:N2	6:J:94:DC:O2	2.25	0.70
6:J:480:DT:H2''	6:J:481:DA:C5	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:384:DA:H61	6:J:156:DT:H3	1.40	0.69
1:a:49:ARG:NH2	6:J:140:DA:O4'	2.26	0.69
5:I:50:DG:N2	6:J:490:DC:O2	2.25	0.68
5:I:480:DA:H61	6:J:61:DA:H2	1.41	0.68
3:U:71:ARG:CZ	3:g:115:LEU:HB2	2.23	0.68
3:M:118:LYS:O	3:M:120:THR:N	2.27	0.67
3:U:74:LYS:HD3	1:a:48:LEU:HB3	1.75	0.67
5:I:64:DT:H2''	5:I:65:DT:C5	2.29	0.67
5:I:171:DG:H2'	5:I:172:DT:H71	1.77	0.66
5:I:85:DG:H2''	5:I:86:DG:C8	2.31	0.66
2:f:22:LEU:O	2:f:25:ASN:ND2	2.28	0.66
3:U:74:LYS:HZ3	1:a:51:ILE:HB	1.60	0.66
2:F:21:VAL:HG12	2:F:25:ASN:HD21	1.61	0.66
2:F:22:LEU:O	2:F:25:ASN:ND2	2.29	0.66
5:I:94:DT:H2''	5:I:95:DT:H5''	1.78	0.66
1:W:49:ARG:NH1	5:I:407:DT:OP1	2.23	0.66
3:Y:24:GLN:HG3	4:Z:44:GLN:HE22	1.62	0.65
6:J:203:DC:H2''	6:J:204:DT:H5''	1.79	0.65
5:I:158:DG:H2''	5:I:159:DG:N7	2.12	0.65
6:J:272:DA:H2'	6:J:273:DC:C6	2.32	0.65
3:U:70:ALA:O	3:U:74:LYS:N	2.30	0.65
4:N:45:VAL:HG12	4:N:46:HIS:HD2	1.62	0.65
4:d:26:ARG:HG2	6:J:101:DC:H5'	1.78	0.65
6:J:477:DC:H2'	6:J:478:DC:C6	2.31	0.65
6:J:491:DC:H2''	6:J:492:DT:C5	2.33	0.65
5:I:184:DT:H2''	5:I:185:DT:H5'	1.78	0.64
3:Y:70:ALA:O	3:Y:74:LYS:N	2.30	0.64
4:d:45:VAL:HG12	4:d:46:HIS:HD2	1.62	0.64
5:I:33:DG:H1	6:J:508:DC:H42	1.43	0.64
3:G:70:ALA:O	3:G:74:LYS:N	2.30	0.64
5:I:489:DG:N1	6:J:52:DC:N3	2.43	0.64
4:H:45:VAL:HG12	4:H:46:HIS:HD2	1.62	0.64
1:W:119:ILE:HD11	2:X:46:ILE:HG23	1.78	0.64
5:I:137:DT:H2''	5:I:138:DA:C8	2.32	0.64
6:J:213:DC:H2'	6:J:214:DC:C6	2.32	0.64
3:M:125:LYS:HE2	3:M:128:GLY:H	1.63	0.63
3:c:70:ALA:O	3:c:74:LYS:N	2.30	0.63
5:I:258:DA:H8	5:I:258:DA:H5''	1.63	0.63
1:S:119:ILE:HD11	2:T:46:ILE:HG23	1.79	0.63
6:J:229:DA:H2''	6:J:230:DA:N7	2.13	0.63
4:V:50:GLY:H	3:g:118:LYS:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:526:DT:H2'	5:I:527:DT:H71	1.79	0.63
5:I:333:DG:H2''	6:J:209:DC:H4'	1.81	0.63
6:J:8:DA:H2''	6:J:9:DC:H5''	1.79	0.63
4:h:45:VAL:HG12	4:h:46:HIS:HD2	1.62	0.63
5:I:33:DG:H22	6:J:508:DC:N4	1.97	0.62
2:b:21:VAL:O	2:b:25:ASN:ND2	2.32	0.62
5:I:10:DT:H2'	5:I:11:DT:H71	1.82	0.62
1:a:69:ARG:NH1	5:I:486:DA:OP2	2.32	0.62
6:J:339:DC:H2''	6:J:340:DC:C4	2.35	0.62
2:T:21:VAL:HG12	2:T:23:ARG:H	1.63	0.62
3:g:70:ALA:O	3:g:74:LYS:N	2.30	0.62
4:N:83:ARG:NH2	6:J:434:DA:OP2	2.33	0.62
2:f:21:VAL:HG12	2:f:25:ASN:HD21	1.65	0.61
5:I:323:DT:H2''	5:I:324:DA:C5	2.35	0.61
5:I:358:DT:H2'	5:I:359:DT:H71	1.82	0.61
5:I:355:DG:H2'	5:I:356:DG:H8	1.65	0.61
6:J:175:DA:H2''	6:J:176:DA:C8	2.35	0.61
6:J:521:DC:H2''	6:J:522:DT:C5	2.35	0.61
5:I:384:DA:H2'	5:I:385:DG:H8	1.66	0.61
6:J:151:DA:H2''	6:J:152:DA:N7	2.16	0.61
5:I:103:DG:H1	6:J:437:DC:H42	1.48	0.61
5:I:128:DG:H2'	5:I:129:DG:C8	2.35	0.61
5:I:290:DG:N2	6:J:251:DC:O2	2.33	0.61
1:A:40:ARG:HH22	5:I:213:DG:H21	1.49	0.60
1:a:122:LYS:NZ	6:J:69:DC:OP2	2.33	0.60
3:g:90:ASP:HB3	3:g:93:LEU:HB2	1.83	0.60
5:I:21:DG:H2'	5:I:22:DT:H71	1.83	0.60
6:J:44:DA:H2''	6:J:45:DC:C4	2.36	0.60
6:J:335:DC:H2'	6:J:336:DT:C6	2.36	0.60
3:M:70:ALA:O	3:M:74:LYS:N	2.30	0.60
1:O:37:LYS:HE2	6:J:399:DC:H4'	1.83	0.60
3:U:90:ASP:HB3	3:U:93:LEU:HB2	1.83	0.60
5:I:61:DG:H2'	5:I:62:DG:H8	1.66	0.60
5:I:419:DT:H2''	5:I:420:DA:N7	2.16	0.60
6:J:17:DC:H3'	6:J:18:DT:H72	1.84	0.60
3:C:90:ASP:HB3	3:C:93:LEU:HB2	1.83	0.60
5:I:325:DG:H2'	5:I:326:DG:C8	2.36	0.60
3:G:54:VAL:HG22	4:H:107:ALA:HB1	1.84	0.60
3:c:90:ASP:HB3	3:c:93:LEU:HB2	1.83	0.60
5:I:118:DT:H2''	5:I:119:DT:H5'	1.84	0.60
5:I:365:DT:H2''	5:I:366:DA:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:489:DC:H2''	6:J:490:DC:C5	2.37	0.59
1:a:119:ILE:HD11	2:b:46:ILE:HG23	1.83	0.59
5:I:128:DG:H2'	5:I:129:DG:H8	1.66	0.59
5:I:517:DG:H1	6:J:23:DC:H42	1.49	0.59
6:J:180:DT:H2''	6:J:181:DA:H5''	1.84	0.59
6:J:244:DC:H2''	6:J:245:DC:O2	2.02	0.59
3:C:70:ALA:O	3:C:74:LYS:N	2.30	0.59
3:M:90:ASP:HB3	3:M:93:LEU:HB2	1.83	0.59
3:Q:54:VAL:HG22	4:R:107:ALA:HB1	1.83	0.59
6:J:257:DC:H2''	6:J:258:DT:C5	2.37	0.59
5:I:472:DT:H2''	5:I:473:DT:C5	2.38	0.59
1:A:119:ILE:HD11	2:B:46:ILE:HG23	1.85	0.59
3:G:90:ASP:HB3	3:G:93:LEU:HB2	1.83	0.59
2:b:35:ARG:NH2	5:I:478:DT:OP1	2.36	0.58
6:J:71:DC:H2'	6:J:72:DT:C6	2.39	0.58
6:J:401:DC:H2'	6:J:402:DT:H71	1.85	0.58
5:I:155:DT:H2''	5:I:156:DA:N7	2.18	0.58
5:I:225:DG:H2''	5:I:226:DT:H5'	1.85	0.58
4:V:49:THR:O	3:g:120:THR:OG1	2.20	0.58
5:I:427:DG:H2''	5:I:428:DG:C8	2.39	0.58
6:J:410:DA:H1'	6:J:411:DC:N3	2.18	0.58
5:I:34:DT:H2''	5:I:35:DT:C5	2.39	0.58
6:J:360:DT:H2''	6:J:361:DA:N7	2.18	0.58
3:M:123:HIS:O	3:M:124:HIS:ND1	2.36	0.58
3:Q:90:ASP:HB3	3:Q:93:LEU:HB2	1.84	0.58
3:Y:90:ASP:HB3	3:Y:93:LEU:HB2	1.83	0.58
5:I:297:DG:C8	5:I:297:DG:H5'	2.39	0.58
6:J:317:DC:H2''	6:J:318:DT:C5	2.38	0.58
6:J:353:DC:H2''	6:J:354:DT:H5'	1.85	0.58
1:E:62:ILE:O	1:E:93:GLN:NE2	2.38	0.57
6:J:347:DC:H2''	6:J:348:DT:H5''	1.85	0.57
3:C:32:ARG:NH1	4:D:32:GLU:OE2	2.37	0.57
4:D:83:ARG:NH2	4:D:85:THR:OG1	2.38	0.57
6:J:390:DT:H2''	6:J:391:DA:C8	2.39	0.57
3:G:29:ARG:NH2	4:H:37:TYR:OH	2.37	0.57
6:J:75:DC:H2''	6:J:76:DC:C4	2.39	0.57
1:W:112:ILE:HD11	3:g:71:ARG:HH22	1.70	0.57
5:I:441:DG:H1	6:J:99:DC:H42	1.51	0.57
1:e:62:ILE:O	1:e:93:GLN:NE2	2.38	0.56
6:J:300:DT:H1'	6:J:301:DA:N7	2.20	0.56
4:H:99:LEU:HD22	4:H:103:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:99:LEU:HD22	4:N:103:LEU:HB3	1.87	0.56
1:S:40:ARG:HH21	5:I:347:DT:H5'	1.69	0.56
2:T:74:GLU:O	4:V:89:ARG:NH2	2.38	0.56
1:W:48:LEU:HD22	3:g:74:LYS:HD3	1.86	0.56
3:c:54:VAL:HG22	4:d:107:ALA:HB1	1.86	0.56
6:J:407:DC:H5'	6:J:407:DC:H6	1.69	0.56
3:Q:63:LEU:HB3	4:R:42:LEU:HD13	1.88	0.56
3:U:77:ARG:NH1	5:I:396:DA:OP2	2.38	0.56
4:D:28:ARG:HG3	4:D:29:SER:H	1.71	0.56
5:I:53:DT:H2'	5:I:54:DA:H8	1.71	0.56
2:P:75:HIS:HD2	4:R:77:LEU:HD22	1.70	0.56
5:I:43:DG:N2	6:J:498:DT:O2	2.38	0.56
6:J:136:DC:H2''	6:J:137:DC:C5	2.40	0.56
6:J:203:DC:H2'	6:J:204:DT:H71	1.87	0.56
6:J:361:DA:H2''	6:J:362:DA:N7	2.21	0.56
6:J:467:DC:H2''	6:J:468:DT:H5''	1.87	0.56
1:A:42:ARG:O	1:A:45:THR:OG1	2.23	0.56
4:d:99:LEU:HD22	4:d:103:LEU:HB3	1.87	0.56
6:J:414:DT:O4	6:J:415:DA:N6	2.39	0.56
4:h:99:LEU:HD22	4:h:103:LEU:HB3	1.87	0.56
5:I:407:DT:H2''	5:I:408:DA:C8	2.41	0.56
1:O:36:LYS:O	1:O:37:LYS:HB2	2.06	0.56
5:I:81:DG:H2''	5:I:82:DT:H5'	1.87	0.56
5:I:519:DG:H2'	5:I:520:DT:H71	1.87	0.56
6:J:216:DT:H2''	6:J:217:DA:C5	2.41	0.56
6:J:216:DT:H2''	6:J:217:DA:N7	2.21	0.56
1:e:106:ASP:OD2	1:e:131:ARG:NE	2.39	0.55
5:I:430:DT:H2'	5:I:431:DT:C4	2.41	0.55
6:J:6:DT:H2''	6:J:7:DA:C8	2.42	0.55
6:J:173:DC:H2'	6:J:174:DT:H71	1.88	0.55
3:G:11:ARG:HD3	5:I:163:DG:H5''	1.88	0.55
3:G:14:ALA:HB3	6:J:381:DC:H4'	1.88	0.55
1:W:62:ILE:O	1:W:93:GLN:NE2	2.39	0.55
1:e:61:LEU:O	2:f:36:ARG:NH2	2.39	0.55
6:J:148:DC:H2'	6:J:149:DC:C4	2.41	0.55
6:J:289:DA:H2''	6:J:290:DA:N7	2.21	0.55
1:K:62:ILE:O	1:K:93:GLN:NE2	2.39	0.55
1:O:62:ILE:O	1:O:93:GLN:NE2	2.39	0.55
6:J:187:DA:H2''	6:J:188:DA:C8	2.42	0.55
3:Y:54:VAL:HG22	4:Z:107:ALA:HB1	1.89	0.55
5:I:91:DG:H2'	5:I:92:DG:H8	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:378:DT:H2''	6:J:379:DA:H5'	1.87	0.55
6:J:432:DT:H2''	6:J:433:DA:N7	2.21	0.55
1:A:62:ILE:O	1:A:93:GLN:NE2	2.39	0.55
2:B:74:GLU:O	4:D:89:ARG:NH2	2.39	0.55
3:G:71:ARG:NE	3:M:119:LYS:HG3	2.21	0.55
1:O:119:ILE:HD11	2:P:46:ILE:HG23	1.88	0.55
3:c:54:VAL:HG21	4:d:95:VAL:HG21	1.89	0.55
5:I:62:DG:H2''	5:I:63:DG:H8	1.71	0.55
5:I:194:DG:H2'	5:I:195:DG:H8	1.71	0.55
5:I:482:DG:H2''	5:I:483:DG:C8	2.42	0.55
5:I:281:DT:H3	6:J:259:DA:H2	1.54	0.55
5:I:325:DG:H2'	5:I:326:DG:H8	1.72	0.55
3:Q:16:THR:O	3:Q:20:ARG:N	2.37	0.55
3:U:113:ALA:HA	3:g:71:ARG:HD3	1.89	0.55
1:a:62:ILE:O	1:a:93:GLN:NE2	2.39	0.55
4:h:28:ARG:HH21	6:J:122:DA:H5'	1.72	0.55
6:J:338:DA:H2''	6:J:339:DC:C5	2.42	0.55
6:J:495:DC:H6	6:J:495:DC:H5'	1.72	0.55
3:U:32:ARG:NH1	4:V:32:GLU:OE2	2.40	0.55
5:I:105:DG:H2'	5:I:106:DT:H73	1.89	0.55
5:I:418:DT:H2'	5:I:419:DT:H71	1.89	0.55
5:I:446:DG:N2	6:J:95:DC:O2	2.40	0.55
6:J:145:DA:H2''	6:J:146:DA:C8	2.42	0.55
3:G:71:ARG:HE	3:M:119:LYS:HG3	1.71	0.54
1:S:62:ILE:O	1:S:93:GLN:NE2	2.39	0.54
5:I:211:DG:H2''	5:I:212:DG:C8	2.42	0.54
5:I:427:DG:H2''	5:I:428:DG:H8	1.72	0.54
5:I:357:DG:H2'	5:I:358:DT:H71	1.88	0.54
6:J:211:DA:H3'	6:J:212:DA:H8	1.71	0.54
6:J:437:DC:H2'	6:J:438:DT:H71	1.90	0.54
2:X:51:TYR:OH	6:J:210:DT:OP1	2.20	0.54
3:U:112:GLN:HB2	3:g:71:ARG:NH1	2.21	0.54
5:I:472:DT:H2''	5:I:473:DT:C4	2.43	0.54
6:J:23:DC:H2''	6:J:24:DT:C5	2.42	0.54
6:J:516:DT:H2''	6:J:517:DA:H5'	1.89	0.54
3:Y:54:VAL:HG21	4:Z:95:VAL:HG21	1.90	0.54
5:I:276:DA:H2''	5:I:277:DG:C8	2.42	0.54
4:N:85:THR:HG21	6:J:433:DA:H4'	1.88	0.54
5:I:12:DA:H2''	5:I:13:DG:H5'	1.90	0.54
5:I:321:DG:H2''	5:I:322:DT:C5	2.43	0.54
6:J:20:DA:H4'	6:J:21:DC:OP1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:255:DG:H2'	5:I:256:DT:H71	1.89	0.54
6:J:42:DT:H2''	6:J:43:DA:N7	2.23	0.54
6:J:281:DC:H3'	6:J:282:DT:H72	1.90	0.54
3:M:42:ARG:HH22	6:J:431:DC:H1'	1.73	0.54
5:I:91:DG:H2'	5:I:92:DG:C8	2.43	0.54
1:O:97:GLU:HG2	2:P:37:LEU:HD21	1.90	0.53
5:I:106:DT:O2	5:I:107:DT:N3	2.41	0.53
5:I:310:DT:H2''	5:I:311:DT:C5	2.43	0.53
5:I:420:DA:H2''	5:I:421:DG:N7	2.23	0.53
6:J:166:DC:H1'	6:J:167:DC:C5	2.43	0.53
6:J:395:DC:H2''	6:J:396:DT:H5''	1.89	0.53
1:a:53:ARG:HH11	5:I:404:DG:H5''	1.73	0.53
2:b:75:HIS:HD2	4:d:77:LEU:HD22	1.73	0.53
5:I:248:DG:N2	6:J:293:DC:O2	2.41	0.53
5:I:517:DG:H2''	5:I:518:DG:H8	1.73	0.53
2:T:32:PRO:HG2	6:J:190:DC:OP2	2.08	0.53
3:U:114:VAL:N	3:g:71:ARG:HH11	2.02	0.53
5:I:164:DG:C2	5:I:165:DG:C6	2.97	0.53
1:A:112:ILE:HG23	3:G:114:VAL:HG21	1.90	0.53
5:I:21:DG:H2''	5:I:22:DT:H5'	1.91	0.53
5:I:218:DG:H2''	5:I:219:DG:C8	2.43	0.53
5:I:307:DG:H2'	5:I:308:DG:C8	2.43	0.53
6:J:37:DA:H2''	6:J:38:DA:N7	2.23	0.53
6:J:44:DA:H2''	6:J:45:DC:C5	2.43	0.53
6:J:284:DA:H4'	6:J:285:DC:OP1	2.07	0.53
5:I:264:DA:H2''	5:I:265:DG:C8	2.43	0.53
3:C:11:ARG:HH21	6:J:294:DT:H72	1.73	0.53
5:I:277:DG:H2''	5:I:278:DG:C8	2.43	0.53
1:E:83:ARG:HB2	2:F:80:THR:HG22	1.90	0.53
1:e:101:VAL:HG13	2:f:41:GLY:HA2	1.89	0.53
3:C:115:LEU:CD2	1:E:117:VAL:HG22	2.38	0.53
4:N:36:VAL:HG21	5:I:121:DG:H5''	1.91	0.53
3:U:65:LEU:HB3	3:U:86:ALA:HB1	1.91	0.53
3:Y:65:LEU:HB3	3:Y:86:ALA:HB1	1.91	0.53
5:I:355:DG:H2'	5:I:356:DG:C8	2.44	0.53
5:I:442:DT:H2''	5:I:443:DT:C5	2.43	0.53
6:J:155:DC:H2''	6:J:156:DT:C5	2.44	0.53
6:J:474:DT:H2''	6:J:475:DA:C8	2.44	0.53
6:J:508:DC:H2''	6:J:509:DC:O2	2.09	0.53
2:L:32:PRO:HA	2:L:35:ARG:HB2	1.91	0.53
3:U:116:LEU:HD23	3:U:117:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:65:LEU:HB3	3:g:86:ALA:HB1	1.91	0.52
6:J:127:DA:H2''	6:J:128:DA:C8	2.45	0.52
6:J:287:DC:H1'	6:J:288:DT:C4	2.44	0.52
1:W:53:ARG:NH2	6:J:212:DA:OP1	2.42	0.52
5:I:359:DT:H2''	5:I:360:DA:H2'	1.91	0.52
3:Q:32:ARG:NH1	4:R:32:GLU:OE2	2.41	0.52
5:I:226:DT:H2''	5:I:227:DT:H5''	1.91	0.52
6:J:102:DT:H4'	6:J:103:DA:OP1	2.09	0.52
3:M:116:LEU:HD23	3:M:117:PRO:HD2	1.91	0.52
5:I:42:DA:H2'	5:I:43:DG:C8	2.45	0.52
5:I:235:DG:H2''	5:I:236:DG:H8	1.75	0.52
6:J:41:DC:H2'	6:J:42:DT:H71	1.91	0.52
6:J:407:DC:H5'	6:J:407:DC:C6	2.45	0.52
5:I:256:DT:H2'	5:I:257:DT:H71	1.92	0.52
5:I:299:DT:H2''	5:I:300:DA:C5	2.44	0.52
5:I:450:DA:H2''	5:I:451:DG:H5'	1.92	0.52
5:I:508:DT:H2'	5:I:509:DT:H71	1.91	0.52
1:A:97:GLU:HG2	2:B:37:LEU:HD21	1.92	0.52
5:I:298:DT:H2''	5:I:299:DT:C5	2.45	0.52
6:J:199:DA:H2''	6:J:200:DA:C8	2.45	0.52
3:G:65:LEU:HB3	3:G:86:ALA:HB1	1.91	0.52
5:I:131:DT:H2''	5:I:132:DA:C8	2.45	0.52
6:J:411:DC:H2''	6:J:412:DC:O4'	2.09	0.52
3:G:116:LEU:HD23	3:G:117:PRO:HD2	1.91	0.52
3:U:62:ILE:HG12	3:U:93:LEU:HD11	1.92	0.52
3:g:62:ILE:HG12	3:g:93:LEU:HD11	1.92	0.52
5:I:74:DG:H1	6:J:467:DC:N4	2.07	0.52
1:E:106:ASP:OD2	1:E:131:ARG:NE	2.39	0.52
2:F:75:HIS:HD2	4:H:77:LEU:HD22	1.75	0.52
3:Y:116:LEU:HD23	3:Y:117:PRO:HD2	1.91	0.52
1:e:119:ILE:HD11	2:f:46:ILE:HG23	1.92	0.52
3:g:116:LEU:HD23	3:g:117:PRO:HD2	1.91	0.52
5:I:68:DG:H2''	5:I:69:DG:N7	2.25	0.51
5:I:348:DA:H4'	5:I:349:DG:OP1	2.09	0.51
6:J:265:DA:H2''	6:J:266:DA:C8	2.45	0.51
3:Q:65:LEU:HB3	3:Q:86:ALA:HB1	1.91	0.51
3:c:65:LEU:HB3	3:c:86:ALA:HB1	1.91	0.51
3:c:116:LEU:HD23	3:c:117:PRO:HD2	1.91	0.51
5:I:439:DG:H22	6:J:101:DC:N4	2.09	0.51
4:V:49:THR:HA	3:g:118:LYS:HB3	1.93	0.51
5:I:94:DT:H2'	5:I:95:DT:H71	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:77:DC:H2''	6:J:78:DT:C4	2.45	0.51
6:J:169:DA:H2''	6:J:170:DA:C8	2.45	0.51
2:F:78:ARG:NH2	2:F:85:ASP:OD2	2.44	0.51
2:P:78:ARG:NH2	2:P:85:ASP:OD2	2.44	0.51
5:I:289:DG:H2''	5:I:290:DG:N7	2.26	0.51
6:J:399:DC:H2''	6:J:400:DC:H5'	1.91	0.51
3:C:65:LEU:HB3	3:C:86:ALA:HB1	1.91	0.51
1:S:70:LEU:HD13	2:T:25:ASN:HB3	1.92	0.51
2:T:78:ARG:NH2	2:T:85:ASP:OD2	2.44	0.51
3:g:55:LEU:HD22	4:h:63:VAL:HG13	1.92	0.51
5:I:153:DG:H2'	5:I:154:DT:H71	1.92	0.51
5:I:265:DG:H2''	5:I:266:DG:C8	2.45	0.51
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.44	0.51
3:Y:62:ILE:HG12	3:Y:93:LEU:HD11	1.92	0.51
6:J:213:DC:H2'	6:J:214:DC:H6	1.75	0.51
6:J:467:DC:H2'	6:J:468:DT:H71	1.91	0.51
3:C:116:LEU:HD23	3:C:117:PRO:HD2	1.91	0.51
3:M:62:ILE:HG12	3:M:93:LEU:HD11	1.92	0.51
3:M:65:LEU:HB3	3:M:86:ALA:HB1	1.91	0.51
2:b:78:ARG:NH2	2:b:85:ASP:OD2	2.44	0.51
3:g:123:HIS:O	3:g:125:LYS:N	2.44	0.51
5:I:111:DG:H22	6:J:428:DA:H2	1.57	0.51
5:I:345:DG:H2''	5:I:346:DT:H5'	1.90	0.51
3:G:62:ILE:HG12	3:G:93:LEU:HD11	1.92	0.51
5:I:302:DG:N2	6:J:239:DC:N3	2.58	0.51
5:I:406:DT:H2''	5:I:407:DT:H71	1.92	0.51
6:J:45:DC:H2''	6:J:46:DC:C5	2.46	0.51
1:K:94:GLU:HG3	2:L:100:PHE:HE2	1.76	0.51
5:I:92:DG:H2'	5:I:93:DG:H8	1.76	0.51
5:I:163:DG:H2''	5:I:164:DG:H8	1.76	0.51
5:I:511:DG:H2'	5:I:512:DG:C8	2.46	0.51
6:J:455:DC:H2''	6:J:456:DT:H5'	1.93	0.51
1:A:65:LEU:HD22	5:I:222:DA:P	2.51	0.51
3:c:62:ILE:HG12	3:c:93:LEU:HD11	1.92	0.51
2:f:75:HIS:HD2	4:h:77:LEU:HD22	1.75	0.51
5:I:144:DA:H2''	5:I:145:DG:C8	2.46	0.51
5:I:320:DG:H2''	5:I:321:DG:C8	2.46	0.51
5:I:489:DG:H2''	5:I:490:DT:H5'	1.93	0.51
3:C:62:ILE:HG12	3:C:93:LEU:HD11	1.92	0.50
4:D:83:ARG:NH2	4:D:85:THR:HG1	2.09	0.50
2:X:78:ARG:NH2	2:X:85:ASP:OD2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:110:DA:H2''	6:J:111:DC:H5'	1.93	0.50
1:a:97:GLU:HG2	2:b:37:LEU:HD21	1.92	0.50
2:b:21:VAL:HB	2:b:24:ASP:HB2	1.91	0.50
5:I:184:DT:H2'	5:I:185:DT:H71	1.93	0.50
5:I:195:DG:H2'	5:I:196:DT:C6	2.46	0.50
5:I:417:DG:H2'	5:I:418:DT:H71	1.93	0.50
6:J:166:DC:H1'	6:J:167:DC:H5	1.76	0.50
6:J:269:DC:H2'	6:J:270:DT:H71	1.92	0.50
4:N:95:VAL:HG13	4:N:99:LEU:HD12	1.94	0.50
1:S:119:ILE:HD13	2:T:43:VAL:HG11	1.92	0.50
1:W:119:ILE:HG13	2:X:50:ILE:HG13	1.92	0.50
6:J:74:DA:H5'	6:J:74:DA:C8	2.46	0.50
2:X:74:GLU:O	4:Z:89:ARG:NH2	2.44	0.50
5:I:489:DG:H2'	5:I:490:DT:H71	1.93	0.50
6:J:73:DA:H2''	6:J:74:DA:N7	2.26	0.50
2:B:21:VAL:HB	2:B:24:ASP:HB2	1.93	0.50
6:J:391:DA:H2''	6:J:392:DA:C8	2.47	0.50
4:H:30:ARG:HH12	6:J:384:DT:H1'	1.77	0.50
1:e:83:ARG:HB2	2:f:80:THR:HG22	1.93	0.50
2:f:78:ARG:NH2	2:f:85:ASP:OD2	2.44	0.50
3:G:54:VAL:HG21	4:H:95:VAL:HG21	1.93	0.50
1:W:97:GLU:HG2	2:X:37:LEU:HD21	1.94	0.50
5:I:125:DT:O4	6:J:416:DA:N6	2.44	0.50
1:a:42:ARG:HD3	6:J:142:DC:OP2	2.12	0.50
5:I:32:DG:H2''	5:I:33:DG:C8	2.47	0.50
5:I:189:DG:H2''	5:I:190:DT:C5	2.47	0.50
5:I:388:DT:H2''	5:I:389:DT:C6	2.47	0.50
5:I:533:DT:H2'	5:I:534:DA:O4'	2.11	0.50
6:J:126:DT:H2''	6:J:127:DA:C8	2.47	0.50
4:H:95:VAL:HG13	4:H:99:LEU:HD12	1.94	0.50
2:T:30:THR:HB	6:J:190:DC:H5'	1.94	0.50
6:J:305:DC:H2'	6:J:306:DT:H71	1.94	0.50
5:I:435:DG:H2'	5:I:436:DT:H71	1.94	0.49
5:I:476:DG:H2''	5:I:477:DG:N7	2.27	0.49
5:I:494:DG:H22	6:J:47:DC:H1'	1.77	0.49
6:J:130:DC:H2''	6:J:131:DC:H5''	1.94	0.49
6:J:457:DA:H2''	6:J:458:DA:C8	2.47	0.49
1:A:70:LEU:HD13	2:B:25:ASN:HB3	1.92	0.49
1:A:119:ILE:HD13	2:B:43:VAL:HG11	1.94	0.49
5:I:81:DG:H2'	5:I:82:DT:H71	1.94	0.49
5:I:297:DG:H1	6:J:244:DC:N4	1.97	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:480:DA:H2''	5:I:481:DG:C8	2.47	0.49
1:S:97:GLU:HG2	2:T:37:LEU:HD21	1.95	0.49
6:J:41:DC:H2''	6:J:42:DT:H5'	1.94	0.49
6:J:42:DT:H2''	6:J:43:DA:C5	2.47	0.49
6:J:406:DC:H2'	6:J:407:DC:C5	2.47	0.49
1:a:37:LYS:HG3	1:a:39:HIS:H	1.77	0.49
3:c:58:LEU:HD21	4:d:99:LEU:HD21	1.94	0.49
1:e:69:ARG:NH1	6:J:88:DC:OP1	2.44	0.49
1:e:83:ARG:HH22	5:I:444:DA:H4'	1.77	0.49
5:I:348:DA:H2''	5:I:349:DG:N7	2.27	0.49
6:J:79:DA:H2'	6:J:80:DA:C8	2.47	0.49
6:J:78:DT:H2''	6:J:79:DA:C8	2.48	0.49
1:W:70:LEU:HD13	2:X:25:ASN:HB3	1.95	0.49
1:a:123:ASP:OD1	1:e:113:HIS:NE2	2.42	0.49
5:I:61:DG:H2'	5:I:62:DG:C8	2.45	0.49
6:J:440:DA:H2''	6:J:441:DC:C5	2.47	0.49
2:X:22:LEU:O	2:X:25:ASN:ND2	2.46	0.49
5:I:45:DG:H1	6:J:495:DC:H42	1.59	0.49
5:I:386:DG:C2	5:I:387:DG:C6	3.01	0.49
6:J:205:DA:H2''	6:J:206:DA:C8	2.48	0.49
3:Y:50:TYR:HB3	4:Z:91:ILE:HG21	1.94	0.49
5:I:256:DT:H2''	5:I:257:DT:H5'	1.94	0.49
6:J:367:DA:H2''	6:J:368:DA:C8	2.47	0.49
1:E:119:ILE:HD11	2:F:46:ILE:HG23	1.95	0.49
2:F:47:SER:HA	6:J:342:DT:H5''	1.95	0.49
3:M:123:HIS:C	3:M:125:LYS:H	2.21	0.49
1:W:101:VAL:HG13	2:X:41:GLY:HA2	1.94	0.49
4:d:95:VAL:HG13	4:d:99:LEU:HD12	1.94	0.49
1:e:74:ILE:HD13	2:f:63:GLU:HG3	1.94	0.49
5:I:204:DA:N1	6:J:337:DA:N6	2.61	0.49
5:I:339:DG:C8	5:I:339:DG:H5'	2.48	0.49
5:I:446:DG:H2''	5:I:447:DG:C8	2.48	0.49
2:B:75:HIS:HD2	4:D:77:LEU:HD22	1.78	0.49
2:T:75:HIS:O	4:V:89:ARG:NH1	2.45	0.49
3:c:88:ARG:NH1	3:c:94:ASN:OD1	2.46	0.49
5:I:60:DA:H2''	5:I:61:DG:C8	2.48	0.49
5:I:195:DG:H3'	5:I:196:DT:H71	1.93	0.49
5:I:507:DG:H2'	5:I:508:DT:C6	2.48	0.49
3:M:125:LYS:HG3	3:M:127:LYS:H	1.78	0.48
1:O:70:LEU:HD13	2:P:25:ASN:HB3	1.94	0.48
3:U:68:ASN:HA	3:g:112:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:14:DG:H2''	5:I:15:DG:C8	2.48	0.48
5:I:92:DG:H2'	5:I:93:DG:C8	2.48	0.48
6:J:420:DT:H2''	6:J:421:DA:N7	2.28	0.48
6:J:521:DC:H2''	6:J:522:DT:C4	2.47	0.48
5:I:166:DT:H2''	5:I:167:DT:C5	2.48	0.48
5:I:439:DG:H1	6:J:101:DC:H42	1.59	0.48
3:C:88:ARG:NH1	3:C:94:ASN:OD1	2.46	0.48
1:S:37:LYS:NZ	6:J:274:DC:OP1	2.39	0.48
1:a:70:LEU:HD13	2:b:25:ASN:HB3	1.94	0.48
5:I:53:DT:H2'	5:I:54:DA:C8	2.49	0.48
6:J:258:DT:H2''	6:J:259:DA:N7	2.28	0.48
6:J:336:DT:H2'	6:J:337:DA:C8	2.48	0.48
6:J:381:DC:H5'	6:J:381:DC:C6	2.48	0.48
6:J:409:DA:C5	6:J:410:DA:N6	2.81	0.48
6:J:504:DT:H2''	6:J:505:DA:N7	2.29	0.48
2:X:75:HIS:O	4:Z:89:ARG:NH1	2.46	0.48
1:a:119:ILE:HG13	2:b:50:ILE:HG13	1.94	0.48
3:c:35:ARG:NH1	5:I:508:DT:OP2	2.46	0.48
4:h:95:VAL:HG13	4:h:99:LEU:HD12	1.94	0.48
5:I:528:DA:H2''	5:I:529:DG:C8	2.48	0.48
6:J:231:DC:H5'	6:J:231:DC:C6	2.49	0.48
1:a:113:HIS:NE2	1:e:123:ASP:OD1	2.35	0.48
2:b:48:GLY:H	5:I:476:DG:H3'	1.79	0.48
3:g:88:ARG:NH1	3:g:94:ASN:OD1	2.46	0.48
5:I:35:DT:H2''	5:I:36:DA:C5	2.49	0.48
5:I:145:DG:H2''	5:I:146:DG:N7	2.27	0.48
6:J:429:DC:H2''	6:J:430:DC:C5	2.48	0.48
3:U:68:ASN:OD1	3:g:113:ALA:HB2	2.13	0.48
3:Y:88:ARG:NH1	3:Y:94:ASN:OD1	2.46	0.48
1:a:69:ARG:HH12	5:I:486:DA:H5'	1.77	0.48
6:J:340:DC:H2''	6:J:341:DC:C4	2.49	0.48
6:J:495:DC:H5'	6:J:495:DC:C6	2.48	0.48
3:G:88:ARG:NH1	3:G:94:ASN:OD1	2.46	0.48
3:M:88:ARG:NH1	3:M:94:ASN:OD1	2.46	0.48
1:a:96:CYS:HB3	2:b:58:LEU:HD11	1.95	0.48
3:U:67:GLY:O	3:g:116:LEU:HD11	2.13	0.48
2:b:31:LYS:HZ1	5:I:478:DT:H2'	1.78	0.48
5:I:296:DG:H2''	5:I:297:DG:C8	2.49	0.48
2:P:47:SER:HB3	2:P:50:ILE:HG12	1.96	0.48
3:Q:54:VAL:HG21	4:R:95:VAL:HG21	1.95	0.48
2:b:47:SER:HB3	2:b:50:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:75:HIS:CE1	4:d:90:GLU:HG2	2.48	0.48
2:f:47:SER:HB3	2:f:50:ILE:HG12	1.96	0.48
5:I:33:DG:H22	6:J:508:DC:H42	1.60	0.48
5:I:436:DT:H2'	5:I:437:DT:H71	1.95	0.48
6:J:301:DA:H2''	6:J:302:DA:C8	2.49	0.48
1:A:48:LEU:CD1	3:G:117:PRO:HD3	2.44	0.48
1:A:128:ARG:NH2	1:A:133:GLU:O	2.47	0.48
3:U:88:ARG:NH1	3:U:94:ASN:OD1	2.46	0.48
3:U:113:ALA:N	3:g:71:ARG:HH11	2.11	0.48
5:I:179:DT:H2''	5:I:180:DA:C8	2.49	0.48
6:J:77:DC:H2''	6:J:78:DT:C5	2.49	0.48
6:J:191:DC:H2''	6:J:192:DT:H5'	1.95	0.48
3:G:18:SER:OG	3:G:23:LEU:O	2.32	0.47
1:S:128:ARG:NH1	1:S:135:ALA:HB3	2.29	0.47
2:X:47:SER:HB3	2:X:50:ILE:HG12	1.96	0.47
2:f:18:HIS:O	2:f:19:ARG:NE	2.46	0.47
5:I:360:DA:H2''	5:I:361:DG:N7	2.28	0.47
5:I:524:DG:H2''	5:I:525:DG:C8	2.49	0.47
6:J:54:DT:H1'	6:J:55:DA:C5	2.49	0.47
1:O:36:LYS:C	1:O:38:PRO:HD2	2.39	0.47
1:O:37:LYS:HD2	1:O:37:LYS:HA	1.57	0.47
5:I:72:DA:H2'	5:I:73:DG:C8	2.49	0.47
5:I:318:DA:H2''	5:I:319:DG:C8	2.49	0.47
6:J:410:DA:H1'	6:J:411:DC:C2	2.48	0.47
1:a:128:ARG:NH2	1:a:133:GLU:O	2.47	0.47
5:I:374:DG:H2''	5:I:375:DG:C8	2.50	0.47
6:J:45:DC:H2''	6:J:46:DC:C4	2.49	0.47
6:J:337:DA:H2''	6:J:338:DA:C8	2.49	0.47
5:I:155:DT:H2''	5:I:156:DA:C5	2.48	0.47
6:J:305:DC:H2''	6:J:306:DT:H5'	1.96	0.47
5:I:259:DG:H1'	5:I:260:DG:C8	2.49	0.47
5:I:382:DT:H2''	5:I:383:DT:C5	2.49	0.47
5:I:382:DT:H2''	5:I:383:DT:C4	2.49	0.47
5:I:422:DG:H2''	5:I:423:DG:N7	2.29	0.47
6:J:523:DA:H2''	6:J:524:DA:C5	2.50	0.47
3:G:121:GLU:O	3:G:123:HIS:N	2.42	0.47
1:K:128:ARG:NH2	1:K:133:GLU:O	2.47	0.47
1:a:44:GLY:HA2	2:b:44:LYS:HD3	1.96	0.47
5:I:193:DG:H1	6:J:347:DC:H42	1.62	0.47
6:J:168:DT:H2''	6:J:169:DA:C5	2.49	0.47
6:J:257:DC:H1'	6:J:258:DT:C2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:302:DA:H2''	6:J:303:DC:C6	2.50	0.47
6:J:441:DC:H2''	6:J:442:DC:C5	2.49	0.47
6:J:522:DT:H2''	6:J:523:DA:N7	2.29	0.47
3:G:123:HIS:C	3:G:125:LYS:H	2.22	0.47
2:T:47:SER:HB3	2:T:50:ILE:HG12	1.96	0.47
4:Z:54:LYS:HA	4:Z:54:LYS:HD3	1.75	0.47
3:g:18:SER:OG	3:g:23:LEU:O	2.32	0.47
5:I:321:DG:H2''	5:I:322:DT:C4	2.50	0.47
6:J:129:DC:H2''	6:J:130:DC:O2	2.15	0.47
6:J:167:DC:H2''	6:J:168:DT:C6	2.49	0.47
6:J:469:DA:H2''	6:J:470:DA:C8	2.49	0.47
1:O:128:ARG:NH2	1:O:133:GLU:O	2.47	0.47
1:W:128:ARG:NH2	1:W:133:GLU:O	2.47	0.47
3:Y:18:SER:OG	3:Y:23:LEU:O	2.32	0.47
1:a:65:LEU:HD22	5:I:487:DG:OP2	2.15	0.47
5:I:56:DG:H2''	5:I:57:DG:C8	2.50	0.47
5:I:129:DG:N2	6:J:415:DA:OP1	2.48	0.47
6:J:148:DC:H2'	6:J:149:DC:C5	2.49	0.47
3:U:74:LYS:NZ	1:a:48:LEU:O	2.47	0.47
5:I:196:DT:H3	6:J:345:DC:N4	2.13	0.47
6:J:341:DC:H1'	6:J:342:DT:C2	2.50	0.47
4:h:24:LYS:N	6:J:45:DC:OP1	2.48	0.47
6:J:303:DC:H2''	6:J:304:DC:C5	2.50	0.47
4:d:79:HIS:CE1	3:g:38:ASN:HB2	2.50	0.46
2:F:47:SER:HB3	2:F:50:ILE:HG12	1.96	0.46
3:g:24:GLN:HG3	4:h:44:GLN:HE22	1.81	0.46
1:E:74:ILE:HD13	2:F:63:GLU:HG3	1.96	0.46
1:S:128:ARG:NH2	1:S:133:GLU:O	2.47	0.46
5:I:212:DG:H2''	5:I:213:DG:H8	1.81	0.46
6:J:72:DT:H2''	6:J:73:DA:N7	2.31	0.46
6:J:137:DC:H2''	6:J:138:DT:C5	2.50	0.46
5:I:66:DA:H2''	5:I:67:DG:C8	2.51	0.46
6:J:288:DT:H6	6:J:288:DT:H2'	1.63	0.46
3:Q:50:TYR:HB3	4:R:91:ILE:HG21	1.97	0.46
3:U:18:SER:OG	3:U:23:LEU:O	2.32	0.46
5:I:75:DG:H2''	5:I:76:DT:C6	2.51	0.46
5:I:338:DG:H1	6:J:203:DC:N4	2.13	0.46
6:J:185:DC:H2''	6:J:186:DT:C6	2.51	0.46
6:J:409:DA:C4	6:J:410:DA:C6	3.02	0.46
3:M:24:GLN:HG3	4:N:44:GLN:HE22	1.81	0.46
5:I:243:DG:H2'	5:I:244:DT:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:SER:HB3	2:B:50:ILE:HG12	1.96	0.46
3:C:54:VAL:HG22	4:D:107:ALA:HB1	1.98	0.46
4:V:54:LYS:HA	4:V:54:LYS:HD3	1.74	0.46
6:J:230:DA:H2''	6:J:231:DC:C5	2.50	0.46
3:C:29:ARG:NH1	4:D:33:SER:O	2.49	0.46
2:P:74:GLU:O	4:R:89:ARG:NH2	2.49	0.46
3:U:112:GLN:C	3:g:71:ARG:HD3	2.41	0.46
1:e:108:ASN:HB2	2:f:43:VAL:HG22	1.97	0.46
5:I:323:DT:H2''	5:I:324:DA:N7	2.30	0.46
4:D:27:LYS:HE3	4:D:27:LYS:HB2	1.76	0.46
3:M:54:VAL:HG22	4:N:107:ALA:HB1	1.97	0.46
6:J:39:DC:H2''	6:J:40:DC:C5	2.51	0.46
6:J:227:DC:H2''	6:J:228:DT:C7	2.46	0.46
6:J:419:DC:H2''	6:J:420:DT:C5	2.51	0.46
1:O:73:GLU:OE2	2:P:25:ASN:ND2	2.49	0.46
5:I:19:DG:H22	6:J:521:DC:H42	1.63	0.46
5:I:134:DG:N2	6:J:407:DC:H42	2.14	0.45
5:I:216:DA:H2''	5:I:217:DG:C8	2.50	0.45
6:J:449:DC:H2''	6:J:450:DT:C5	2.51	0.45
1:a:101:VAL:HG13	2:b:41:GLY:HA2	1.98	0.45
5:I:9:DG:H2'	5:I:10:DT:H71	1.98	0.45
5:I:324:DA:H2''	5:I:325:DG:C8	2.50	0.45
6:J:204:DT:H2''	6:J:205:DA:C8	2.52	0.45
2:B:39:ARG:NH1	2:B:44:LYS:O	2.50	0.45
4:H:41:VAL:HA	4:H:44:GLN:HE21	1.81	0.45
6:J:132:DT:C2	6:J:133:DA:N7	2.85	0.45
6:J:140:DA:H2''	6:J:141:DC:C4	2.52	0.45
6:J:506:DA:H2''	6:J:507:DC:C6	2.51	0.45
2:B:75:HIS:CE1	4:D:90:GLU:HG3	2.51	0.45
3:M:18:SER:OG	3:M:23:LEU:O	2.32	0.45
4:R:26:ARG:HB3	6:J:440:DA:H5''	1.98	0.45
6:J:256:DC:H2''	6:J:257:DC:C6	2.51	0.45
1:A:96:CYS:HB3	2:B:58:LEU:HD11	1.98	0.45
2:F:39:ARG:NH1	2:F:44:LYS:O	2.50	0.45
3:M:42:ARG:NH2	6:J:432:DT:O5'	2.37	0.45
3:U:116:LEU:HG	3:g:71:ARG:HG3	1.99	0.45
1:W:42:ARG:O	1:W:45:THR:OG1	2.33	0.45
5:I:119:DT:H2''	5:I:120:DA:C8	2.52	0.45
5:I:354:DA:H2''	5:I:355:DG:C8	2.52	0.45
6:J:438:DT:H2''	6:J:439:DA:N7	2.31	0.45
3:G:11:ARG:HH22	6:J:379:DA:H4'	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:75:HIS:HD2	4:Z:77:LEU:HD22	1.82	0.45
3:g:54:VAL:HG21	4:h:95:VAL:HG21	1.97	0.45
4:h:48:ASP:OD1	4:h:48:ASP:N	2.49	0.45
5:I:137:DT:H3	6:J:403:DA:H61	1.65	0.45
5:I:415:DG:H2''	5:I:416:DG:H8	1.82	0.45
6:J:331:DA:H2''	6:J:332:DA:N7	2.32	0.45
4:Z:28:ARG:NH1	6:J:253:DA:OP1	2.48	0.45
5:I:176:DG:H2''	5:I:177:DG:C8	2.51	0.45
5:I:247:DG:H2'	5:I:248:DG:C8	2.51	0.45
5:I:404:DG:N2	6:J:137:DC:N3	2.64	0.45
5:I:438:DA:H2''	5:I:439:DG:C8	2.52	0.45
6:J:129:DC:H2''	6:J:130:DC:C2	2.51	0.45
5:I:193:DG:H1	6:J:347:DC:N4	2.14	0.45
5:I:376:DT:H2''	5:I:377:DT:C6	2.52	0.45
6:J:373:DA:H2'	6:J:374:DA:H8	1.81	0.45
3:C:18:SER:OG	3:C:23:LEU:O	2.32	0.45
4:D:99:LEU:HD23	4:D:103:LEU:HB3	1.99	0.45
2:T:39:ARG:NH1	2:T:44:LYS:O	2.50	0.45
5:I:385:DG:H2''	5:I:386:DG:H8	1.82	0.45
6:J:198:DT:H2''	6:J:199:DA:H5''	1.99	0.45
6:J:340:DC:H1'	6:J:341:DC:N3	2.31	0.45
5:I:151:DG:H2''	5:I:152:DG:C8	2.52	0.45
5:I:173:DT:H2''	5:I:174:DA:H8	1.82	0.45
5:I:433:DG:H2''	5:I:434:DG:C8	2.51	0.45
5:I:485:DT:H1'	5:I:486:DA:H5''	1.98	0.45
6:J:282:DT:C2	6:J:283:DA:N7	2.85	0.45
6:J:411:DC:H6	6:J:411:DC:H2'	1.61	0.45
3:U:76:THR:HA	3:g:117:PRO:HG2	1.99	0.44
5:I:84:DA:H2''	5:I:85:DG:N7	2.32	0.44
5:I:184:DT:H2'	5:I:185:DT:C6	2.52	0.44
5:I:258:DA:H5''	5:I:258:DA:C8	2.48	0.44
5:I:475:DG:H2''	5:I:476:DG:C8	2.52	0.44
6:J:103:DA:H2''	6:J:104:DA:N7	2.31	0.44
2:X:39:ARG:NH1	2:X:44:LYS:O	2.50	0.44
2:b:39:ARG:NH1	2:b:44:LYS:O	2.50	0.44
2:P:39:ARG:NH1	2:P:44:LYS:O	2.50	0.44
1:S:101:VAL:HG13	2:T:41:GLY:HA2	1.98	0.44
3:U:50:TYR:CE1	4:V:111:GLY:HA3	2.53	0.44
1:a:52:ARG:NH1	6:J:139:DA:O5'	2.50	0.44
3:g:15:LYS:HE3	3:g:15:LYS:HB3	1.77	0.44
5:I:124:DT:H3	6:J:418:DC:H42	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:317:DT:H2'	5:I:318:DA:C8	2.52	0.44
5:I:410:DG:H2''	5:I:411:DG:C8	2.51	0.44
6:J:491:DC:H2''	6:J:492:DT:C4	2.52	0.44
3:c:18:SER:OG	3:c:23:LEU:O	2.32	0.44
5:I:456:DA:H2''	5:I:457:DG:H8	1.83	0.44
5:I:483:DG:C8	5:I:484:DT:C4	3.05	0.44
6:J:240:DT:C4	6:J:241:DA:N6	2.86	0.44
2:F:35:ARG:HG2	2:F:46:ILE:HD13	2.00	0.44
3:Q:88:ARG:NH1	3:Q:94:ASN:OD1	2.51	0.44
3:U:75:LYS:O	3:g:117:PRO:HG2	2.18	0.44
4:V:50:GLY:N	3:g:118:LYS:HD2	2.30	0.44
2:f:35:ARG:HG2	2:f:46:ILE:HD13	2.00	0.44
5:I:338:DG:H2''	5:I:339:DG:C8	2.53	0.44
5:I:455:DT:H2''	5:I:456:DA:H8	1.82	0.44
6:J:249:DC:H2''	6:J:250:DC:C5	2.53	0.44
6:J:449:DC:H2''	6:J:450:DT:C6	2.53	0.44
2:B:35:ARG:HG2	2:B:46:ILE:HD13	2.00	0.44
3:Q:16:THR:HB	6:J:514:DC:H5''	1.99	0.44
1:S:96:CYS:HB3	2:T:58:LEU:HD11	1.98	0.44
2:T:35:ARG:HG2	2:T:46:ILE:HD13	2.00	0.44
4:V:99:LEU:HD23	4:V:103:LEU:HB3	1.99	0.44
5:I:129:DG:H22	6:J:414:DT:H2''	1.82	0.44
5:I:193:DG:C2	5:I:194:DG:C5	3.06	0.44
5:I:230:DG:N2	6:J:311:DC:O2	2.50	0.44
5:I:333:DG:N3	5:I:333:DG:H2'	2.33	0.44
5:I:415:DG:H2''	5:I:416:DG:C8	2.53	0.44
4:D:54:LYS:HA	4:D:54:LYS:HD3	1.74	0.44
1:E:103:LEU:HD21	1:E:124:ILE:HG23	2.00	0.44
1:O:101:VAL:HG13	2:P:41:GLY:HA2	2.00	0.44
3:g:32:ARG:NH1	4:h:32:GLU:OE2	2.51	0.44
5:I:208:DT:H2''	5:I:209:DT:C5	2.53	0.44
5:I:212:DG:H2''	5:I:213:DG:C8	2.51	0.44
6:J:478:DC:H2''	6:J:479:DC:C5	2.52	0.44
1:K:129:ARG:HE	1:K:134:ARG:HA	1.83	0.44
4:Z:99:LEU:HD23	4:Z:103:LEU:HB3	1.99	0.44
1:e:59:GLU:O	2:f:40:ARG:NH2	2.50	0.44
1:e:131:ARG:NH1	1:e:133:GLU:OE2	2.49	0.44
5:I:439:DG:H2''	5:I:440:DG:N7	2.32	0.44
5:I:476:DG:H2''	5:I:477:DG:C8	2.52	0.44
6:J:186:DT:H2''	6:J:187:DA:C4	2.53	0.44
6:J:521:DC:H2''	6:J:522:DT:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:15:LYS:HB3	3:G:15:LYS:HE3	1.77	0.44
3:M:77:ARG:HH21	6:J:415:DA:H5''	1.82	0.44
3:Q:74:LYS:HA	3:Q:74:LYS:HD2	1.84	0.44
3:U:74:LYS:HB2	1:a:52:ARG:NH2	2.29	0.44
2:X:35:ARG:HG2	2:X:46:ILE:HD13	2.00	0.44
2:f:39:ARG:NH1	2:f:44:LYS:O	2.50	0.44
5:I:86:DG:H1'	5:I:87:DG:C4	2.53	0.44
5:I:221:DT:H2''	5:I:222:DA:N7	2.32	0.44
5:I:246:DA:H2''	5:I:247:DG:C8	2.53	0.44
6:J:154:DC:H2''	6:J:155:DC:C6	2.53	0.44
3:c:11:ARG:O	3:c:13:LYS:N	2.51	0.43
5:I:83:DT:H4'	5:I:84:DA:OP1	2.15	0.43
5:I:197:DT:H1'	5:I:198:DA:C4	2.53	0.43
4:R:99:LEU:HD23	4:R:103:LEU:HB3	1.99	0.43
1:S:128:ARG:HH12	1:S:135:ALA:HB3	1.84	0.43
3:U:29:ARG:NH1	4:V:33:SER:O	2.52	0.43
3:c:93:LEU:HD23	3:c:93:LEU:HA	1.88	0.43
5:I:81:DG:H1	6:J:458:DA:H2	1.66	0.43
6:J:185:DC:H2''	6:J:186:DT:C5	2.53	0.43
6:J:420:DT:H2''	6:J:421:DA:C5	2.54	0.43
2:P:35:ARG:HG2	2:P:46:ILE:HD13	2.00	0.43
3:U:74:LYS:NZ	1:a:52:ARG:N	2.66	0.43
6:J:82:DC:H2''	6:J:83:DC:C5	2.53	0.43
6:J:161:DC:H2'	6:J:162:DT:H71	2.00	0.43
2:B:21:VAL:O	2:B:25:ASN:ND2	2.51	0.43
1:O:119:ILE:HD13	2:P:43:VAL:HG11	1.99	0.43
4:Z:25:LYS:HB2	4:Z:25:LYS:HE2	1.83	0.43
2:b:35:ARG:HG2	2:b:46:ILE:HD13	2.00	0.43
1:e:63:ARG:HB3	1:e:66:PRO:HD2	2.00	0.43
5:I:177:DG:H1'	5:I:178:DT:H5'	2.00	0.43
5:I:395:DT:H2''	5:I:396:DA:C8	2.53	0.43
6:J:211:DA:H2'	6:J:211:DA:N3	2.33	0.43
6:J:383:DC:H6	6:J:383:DC:H2'	1.69	0.43
1:W:42:ARG:H	1:W:42:ARG:HD3	1.83	0.43
3:g:117:PRO:O	3:g:118:LYS:HG3	2.18	0.43
5:I:234:DA:H2''	5:I:235:DG:C8	2.53	0.43
5:I:452:DG:H1'	5:I:453:DG:C4	2.53	0.43
6:J:366:DT:H2''	6:J:367:DA:H8	1.83	0.43
6:J:403:DA:H2''	6:J:404:DA:H5'	2.00	0.43
2:B:44:LYS:HB3	3:G:115:LEU:HD22	2.01	0.43
1:E:63:ARG:HB3	1:E:66:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:GLN:NE2	6:J:443:DC:OP1	2.52	0.43
2:L:57:VAL:HA	2:L:60:VAL:HG22	2.00	0.43
3:Q:40:SER:OG	4:R:84:SER:O	2.36	0.43
2:f:23:ARG:C	2:f:25:ASN:H	2.26	0.43
3:g:119:LYS:H	3:g:119:LYS:HG2	1.49	0.43
5:I:320:DG:H2''	5:I:321:DG:C5	2.53	0.43
6:J:153:DC:H2'	6:J:154:DC:C5	2.53	0.43
6:J:167:DC:H1'	6:J:168:DT:H5'	2.00	0.43
4:Z:84:SER:O	4:Z:84:SER:OG	2.37	0.43
5:I:487:DG:H2'	5:I:488:DG:O4'	2.19	0.43
5:I:507:DG:H2'	5:I:508:DT:H6	1.84	0.43
6:J:287:DC:H2''	6:J:288:DT:H73	2.00	0.43
6:J:374:DA:H2'	6:J:375:DC:C6	2.54	0.43
6:J:451:DA:H2''	6:J:452:DA:C8	2.54	0.43
6:J:504:DT:H2''	6:J:505:DA:C8	2.53	0.43
6:J:525:DC:H2''	6:J:526:DC:C6	2.54	0.43
1:O:96:CYS:HB3	2:P:58:LEU:HD11	2.00	0.43
1:S:108:ASN:HB2	2:T:43:VAL:HG22	2.01	0.43
1:W:108:ASN:HB2	2:X:43:VAL:HG22	2.01	0.43
5:I:259:DG:H4'	5:I:260:DG:OP1	2.17	0.43
5:I:347:DT:H2''	5:I:348:DA:H2'	2.00	0.43
6:J:407:DC:H2'	6:J:408:DT:C7	2.49	0.43
6:J:242:DA:H2'	6:J:243:DC:C6	2.54	0.43
6:J:533:DC:H2''	6:J:534:DT:O5'	2.18	0.43
3:G:24:GLN:HG3	4:H:44:GLN:HE22	1.82	0.43
3:M:127:LYS:HA	3:M:127:LYS:HD3	1.74	0.43
3:Y:118:LYS:HB3	3:Y:119:LYS:H	1.61	0.43
4:d:28:ARG:HB3	4:d:29:SER:H	1.61	0.43
3:g:54:VAL:HG22	4:h:107:ALA:HB1	1.99	0.43
5:I:529:DG:H2''	5:I:530:DG:H5'	2.01	0.43
3:C:117:PRO:HG3	1:E:48:LEU:CD1	2.48	0.42
3:c:115:LEU:CD2	1:e:117:VAL:HG22	2.48	0.42
5:I:213:DG:H2''	5:I:214:DT:H72	2.01	0.42
5:I:473:DT:H2''	5:I:474:DA:N7	2.33	0.42
1:E:100:LEU:HD12	2:F:37:LEU:HD13	2.01	0.42
4:H:26:ARG:HB2	4:H:27:LYS:H	1.61	0.42
1:K:71:VAL:HB	2:L:66:ILE:HD11	2.00	0.42
2:f:23:ARG:O	2:f:25:ASN:N	2.45	0.42
5:I:143:DT:H2''	5:I:144:DA:C8	2.54	0.42
5:I:227:DT:H2''	5:I:228:DA:H5'	2.00	0.42
5:I:257:DT:H2''	5:I:258:DA:N7	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:18:DT:C2	6:J:19:DA:N7	2.87	0.42
6:J:171:DC:H2''	6:J:172:DC:H5'	2.00	0.42
6:J:317:DC:H2''	6:J:318:DT:C4	2.54	0.42
6:J:450:DT:H6	6:J:450:DT:H2'	1.68	0.42
3:C:42:ARG:NH2	6:J:300:DT:O5'	2.51	0.42
1:E:119:ILE:HD13	2:F:43:VAL:HG11	2.01	0.42
4:V:84:SER:O	4:V:84:SER:OG	2.37	0.42
2:b:38:ALA:HB1	2:b:43:VAL:HB	2.01	0.42
5:I:18:DA:H2''	5:I:19:DG:C8	2.53	0.42
5:I:62:DG:H2''	5:I:63:DG:C8	2.52	0.42
5:I:334:DT:H6	5:I:334:DT:H2'	1.57	0.42
6:J:23:DC:H2''	6:J:24:DT:C6	2.54	0.42
6:J:132:DT:H2''	6:J:133:DA:H8	1.84	0.42
6:J:157:DA:H2''	6:J:158:DA:N7	2.34	0.42
1:A:113:HIS:NE2	1:E:123:ASP:OD1	2.44	0.42
4:D:83:ARG:NH1	4:D:90:GLU:OE2	2.53	0.42
1:E:40:ARG:HD3	1:E:40:ARG:HA	1.76	0.42
1:S:42:ARG:HH12	3:Y:119:LYS:HD2	1.83	0.42
3:U:75:LYS:HB2	3:U:82:HIS:HE1	1.85	0.42
4:Z:51:ILE:HG21	4:Z:56:MET:HE2	2.02	0.42
1:e:103:LEU:HD21	1:e:124:ILE:HG23	2.00	0.42
2:f:38:ALA:HB1	2:f:43:VAL:HB	2.02	0.42
6:J:177:DC:H2''	6:J:178:DC:C5	2.54	0.42
6:J:366:DT:H2''	6:J:367:DA:C8	2.54	0.42
6:J:407:DC:H2'	6:J:408:DT:H71	2.01	0.42
3:Q:16:THR:N	3:Q:19:SER:OG	2.52	0.42
3:g:75:LYS:HB2	3:g:82:HIS:HE1	1.85	0.42
3:g:121:GLU:HG2	3:g:122:SER:H	1.83	0.42
5:I:225:DG:H2'	5:I:226:DT:H71	2.00	0.42
5:I:271:DG:H2''	5:I:272:DG:H5''	2.00	0.42
5:I:290:DG:H2''	5:I:291:DG:C8	2.55	0.42
5:I:459:DG:C8	5:I:460:DT:H72	2.53	0.42
6:J:10:DC:H2''	6:J:11:DC:C5	2.54	0.42
6:J:259:DA:H2''	6:J:260:DA:C5	2.55	0.42
6:J:537:DC:OP2	6:J:538:DC:N4	2.52	0.42
3:C:15:LYS:HE3	3:C:15:LYS:HB3	1.77	0.42
4:H:48:ASP:OD1	4:H:48:ASP:N	2.49	0.42
1:e:100:LEU:HD12	2:f:37:LEU:HD13	2.01	0.42
5:I:130:DT:H5''	5:I:131:DT:H71	2.01	0.42
5:I:443:DT:H2''	5:I:444:DA:C8	2.54	0.42
5:I:454:DT:O4	6:J:85:DA:N6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:83:DC:H2''	6:J:84:DT:C6	2.55	0.42
6:J:343:DA:H2'	6:J:344:DA:N7	2.34	0.42
3:M:75:LYS:HB2	3:M:82:HIS:HE1	1.85	0.42
4:R:51:ILE:HG21	4:R:56:MET:HE2	2.02	0.42
3:Y:75:LYS:HB2	3:Y:82:HIS:HE1	1.85	0.42
3:g:50:TYR:HB3	4:h:91:ILE:HG21	2.02	0.42
5:I:23:DT:C2	5:I:24:DA:N7	2.88	0.42
5:I:374:DG:C2	5:I:375:DG:C6	3.06	0.42
5:I:440:DG:H2''	5:I:441:DG:N7	2.35	0.42
6:J:53:DC:H2''	6:J:54:DT:C4	2.55	0.42
6:J:170:DA:N7	6:J:171:DC:N4	2.67	0.42
3:G:121:GLU:C	3:G:123:HIS:H	2.25	0.42
5:I:3:DG:H5''	5:I:3:DG:C8	2.54	0.42
5:I:396:DA:H2''	5:I:397:DG:OP1	2.19	0.42
6:J:75:DC:H2''	6:J:76:DC:C5	2.54	0.42
6:J:174:DT:H2''	6:J:175:DA:N7	2.34	0.42
6:J:207:DC:H2''	6:J:208:DC:C5	2.54	0.42
3:C:88:ARG:HA	3:C:88:ARG:HD3	1.89	0.42
4:N:30:ARG:HD3	6:J:422:DA:H4'	2.02	0.42
1:S:36:LYS:HB3	1:S:36:LYS:HE3	1.81	0.42
4:d:26:ARG:HD2	4:d:26:ARG:HA	1.64	0.42
5:I:36:DA:H2''	5:I:37:DG:N7	2.35	0.42
6:J:73:DA:H2''	6:J:74:DA:C8	2.54	0.42
6:J:508:DC:H2''	6:J:509:DC:C2	2.55	0.42
6:J:531:DC:H2''	6:J:532:DC:C5	2.54	0.42
1:A:101:VAL:HG13	2:B:41:GLY:HA2	2.01	0.42
2:B:75:HIS:O	4:D:89:ARG:NH1	2.53	0.42
4:D:51:ILE:HG21	4:D:56:MET:HE2	2.01	0.42
1:E:71:VAL:HG13	2:F:66:ILE:HD11	2.01	0.42
1:S:119:ILE:HG13	2:T:50:ILE:HG13	2.01	0.42
3:c:75:LYS:HB2	3:c:82:HIS:HE1	1.85	0.42
6:J:362:DA:H1'	6:J:363:DC:H5'	2.02	0.42
6:J:426:DT:H1'	6:J:427:DA:N7	2.35	0.42
2:P:38:ALA:HB1	2:P:43:VAL:HB	2.02	0.41
4:R:54:LYS:HA	4:R:54:LYS:HD3	1.74	0.41
5:I:89:DT:H2''	5:I:90:DA:C8	2.55	0.41
5:I:347:DT:H4'	5:I:348:DA:OP1	2.20	0.41
5:I:486:DA:N3	5:I:487:DG:N1	2.67	0.41
6:J:427:DA:H2''	6:J:428:DA:C8	2.54	0.41
6:J:472:DC:H2''	6:J:473:DC:C5	2.55	0.41
3:C:75:LYS:HB2	3:C:82:HIS:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:75:LYS:HB2	3:G:82:HIS:HE1	1.85	0.41
3:M:54:VAL:HG21	4:N:95:VAL:HG21	2.01	0.41
5:I:4:DT:H2'	5:I:5:DT:C4	2.56	0.41
5:I:202:DT:C6	5:I:203:DT:H72	2.56	0.41
5:I:245:DT:H2''	5:I:246:DA:C8	2.55	0.41
5:I:338:DG:H2''	5:I:339:DG:N7	2.35	0.41
5:I:433:DG:O6	6:J:106:DC:N4	2.53	0.41
6:J:270:DT:C2	6:J:271:DA:C8	3.08	0.41
6:J:299:DC:H1'	6:J:300:DT:C2	2.55	0.41
6:J:343:DA:H2'	6:J:344:DA:C8	2.56	0.41
1:O:72:ARG:NH1	5:I:49:DG:OP1	2.53	0.41
5:I:88:DT:H2''	5:I:89:DT:H5'	2.01	0.41
5:I:416:DG:C2	5:I:417:DG:C5	3.08	0.41
5:I:438:DA:H2''	5:I:439:DG:H8	1.84	0.41
6:J:97:DA:H2''	6:J:98:DA:C8	2.55	0.41
6:J:211:DA:H3'	6:J:212:DA:C8	2.52	0.41
6:J:215:DC:H5'	6:J:215:DC:C6	2.56	0.41
6:J:242:DA:H2'	6:J:243:DC:C5	2.55	0.41
1:a:99:TYR:OH	1:a:133:GLU:OE1	2.31	0.41
6:J:22:DC:N3	6:J:23:DC:N4	2.68	0.41
6:J:46:DC:H2''	6:J:47:DC:C6	2.54	0.41
6:J:88:DC:H2''	6:J:89:DC:H5'	2.02	0.41
6:J:102:DT:C2	6:J:103:DA:N7	2.89	0.41
6:J:149:DC:H6	6:J:149:DC:H2'	1.72	0.41
6:J:246:DT:H2''	6:J:247:DA:N7	2.35	0.41
3:Y:93:LEU:HD23	3:Y:93:LEU:HA	1.88	0.41
1:a:128:ARG:HE	1:a:133:GLU:HB2	1.86	0.41
5:I:388:DT:H3	6:J:153:DC:H42	1.68	0.41
6:J:157:DA:H2''	6:J:158:DA:C8	2.55	0.41
6:J:256:DC:H2''	6:J:257:DC:H5'	2.03	0.41
2:B:38:ALA:HB1	2:B:43:VAL:HB	2.02	0.41
2:T:38:ALA:HB1	2:T:43:VAL:HB	2.02	0.41
3:U:54:VAL:HG22	4:V:107:ALA:HB1	2.02	0.41
1:W:50:GLU:OE2	6:J:211:DA:H2''	2.20	0.41
3:g:93:LEU:HD23	3:g:93:LEU:HA	1.88	0.41
5:I:194:DG:H2'	5:I:195:DG:C8	2.53	0.41
5:I:302:DG:H1	6:J:238:DC:H42	1.67	0.41
5:I:452:DG:H4'	5:I:453:DG:H5'	2.02	0.41
6:J:235:DA:H2''	6:J:236:DA:C8	2.55	0.41
6:J:407:DC:H2'	6:J:408:DT:C5	2.56	0.41
6:J:408:DT:H2''	6:J:409:DA:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:471:DC:H2''	6:J:472:DC:C5	2.56	0.41
6:J:499:DA:H1'	6:J:500:DA:H5'	2.01	0.41
3:C:71:ARG:HH21	3:Y:118:LYS:NZ	2.19	0.41
2:F:38:ALA:HB1	2:F:43:VAL:HB	2.02	0.41
3:M:58:LEU:HD21	4:N:99:LEU:HD21	2.02	0.41
3:g:88:ARG:HA	3:g:88:ARG:HD3	1.89	0.41
5:I:37:DG:H22	6:J:504:DT:H3	1.69	0.41
5:I:46:DT:H2''	5:I:47:DT:H71	2.02	0.41
5:I:474:DA:H1'	5:I:475:DG:H5'	2.03	0.41
6:J:76:DC:H6	6:J:76:DC:H2'	1.71	0.41
6:J:242:DA:H8	6:J:242:DA:H5''	1.85	0.41
6:J:298:DC:H6	6:J:298:DC:H2'	1.63	0.41
6:J:463:DA:H2''	6:J:464:DA:C8	2.56	0.41
6:J:492:DT:H2''	6:J:493:DA:N7	2.35	0.41
4:D:24:LYS:HA	4:D:24:LYS:HD3	1.90	0.41
3:U:112:GLN:O	3:g:71:ARG:HD3	2.21	0.41
5:I:185:DT:C2	5:I:186:DA:N7	2.88	0.41
5:I:189:DG:N2	6:J:352:DC:O2	2.54	0.41
5:I:191:DT:C2	5:I:192:DA:C8	3.09	0.41
5:I:301:DG:H22	6:J:240:DT:H3	1.69	0.41
5:I:419:DT:H3	6:J:121:DA:H2	1.68	0.41
6:J:93:DC:H2''	6:J:94:DC:C6	2.55	0.41
6:J:101:DC:H2''	6:J:102:DT:H5'	2.02	0.41
6:J:331:DA:H2''	6:J:332:DA:C8	2.56	0.41
1:K:119:ILE:HD11	2:L:46:ILE:HG23	2.02	0.41
1:K:128:ARG:HE	1:K:133:GLU:HB2	1.86	0.41
4:V:27:LYS:HE2	4:V:27:LYS:HB2	1.84	0.41
2:X:38:ALA:HB1	2:X:43:VAL:HB	2.02	0.41
3:c:15:LYS:HB3	3:c:15:LYS:HE3	1.77	0.41
1:e:37:LYS:HB2	1:e:39:HIS:CE1	2.55	0.41
1:e:116:ARG:NH2	1:e:123:ASP:OD2	2.49	0.41
5:I:1:DG:H2'	5:I:2:DG:C8	2.55	0.41
5:I:37:DG:N2	6:J:504:DT:H3	2.19	0.41
5:I:250:DT:H2''	5:I:251:DT:C5	2.55	0.41
5:I:253:DG:H2''	5:I:254:DG:C8	2.56	0.41
5:I:323:DT:H6	5:I:323:DT:H2'	1.75	0.41
5:I:353:DT:H2''	5:I:354:DA:C8	2.56	0.41
5:I:517:DG:H2''	5:I:518:DG:C8	2.53	0.41
6:J:90:DT:C2	6:J:91:DA:N7	2.88	0.41
6:J:203:DC:H5''	6:J:203:DC:H6	1.85	0.41
6:J:299:DC:H2''	6:J:300:DT:C5	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:478:DC:C2	6:J:479:DC:C4	3.09	0.41
3:C:54:VAL:HG21	4:D:95:VAL:HG21	2.03	0.41
3:G:13:LYS:HE2	3:G:13:LYS:HB2	1.83	0.41
3:Y:88:ARG:HA	3:Y:88:ARG:HD3	1.89	0.41
2:f:17:ARG:HH21	5:I:447:DG:H3'	1.85	0.41
6:J:236:DA:H1'	6:J:237:DC:C2	2.56	0.41
6:J:518:DA:C5	6:J:519:DC:C4	3.09	0.41
6:J:519:DC:C2	6:J:520:DC:C4	3.09	0.41
6:J:527:DC:H2''	6:J:528:DT:H5'	2.02	0.41
1:K:54:TYR:CZ	2:L:36:ARG:HG2	2.55	0.40
2:P:45:ARG:NH1	6:J:475:DA:OP2	2.40	0.40
1:W:119:ILE:HD13	2:X:43:VAL:HG11	2.03	0.40
5:I:235:DG:H2''	5:I:236:DG:C8	2.55	0.40
5:I:298:DT:H6	5:I:298:DT:H2'	1.74	0.40
6:J:12:DT:H2''	6:J:13:DA:C8	2.56	0.40
6:J:38:DA:H2''	6:J:39:DC:C6	2.55	0.40
6:J:412:DC:H1'	6:J:413:DC:C2	2.56	0.40
4:H:24:LYS:N	6:J:308:DA:H5''	2.37	0.40
1:O:119:ILE:HG13	2:P:50:ILE:HG13	2.03	0.40
4:V:51:ILE:HG21	4:V:56:MET:HE2	2.02	0.40
5:I:194:DG:C2	5:I:195:DG:C5	3.09	0.40
5:I:360:DA:H2''	5:I:361:DG:C8	2.56	0.40
5:I:502:DT:H6	5:I:502:DT:H2'	1.71	0.40
6:J:153:DC:H2'	6:J:154:DC:C6	2.57	0.40
6:J:263:DC:H2''	6:J:264:DT:H5'	2.01	0.40
6:J:412:DC:H6	6:J:412:DC:H2'	1.69	0.40
4:D:43:LYS:HD3	4:D:49:THR:HG22	2.03	0.40
1:K:67:PHE:CZ	2:L:62:LEU:HD11	2.56	0.40
3:Y:42:ARG:HD2	4:Z:85:THR:HG22	2.03	0.40
5:I:74:DG:H2''	5:I:75:DG:C8	2.56	0.40
5:I:157:DG:H2''	5:I:158:DG:C8	2.56	0.40
6:J:271:DA:H2''	6:J:272:DA:C8	2.57	0.40
6:J:381:DC:H6	6:J:381:DC:H2'	1.79	0.40
1:E:131:ARG:NH1	1:E:133:GLU:OE2	2.49	0.40
2:F:22:LEU:HB3	2:F:23:ARG:H	1.65	0.40
2:F:75:HIS:CE1	4:H:90:GLU:HG2	2.56	0.40
3:M:42:ARG:HB3	5:I:110:DG:H5''	2.03	0.40
2:P:19:ARG:NH2	5:I:49:DG:OP2	2.51	0.40
5:I:13:DG:H2''	5:I:14:DG:C8	2.56	0.40
5:I:475:DG:H21	6:J:66:DT:H3	1.69	0.40
3:G:119:LYS:HE3	6:J:331:DA:P	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:100:LEU:HD12	2:X:37:LEU:HD13	2.03	0.40
5:I:371:DT:H6	5:I:371:DT:H2'	1.75	0.40
5:I:391:DG:H2''	5:I:392:DG:O4'	2.21	0.40
5:I:470:DG:H2''	5:I:471:DG:C8	2.56	0.40
5:I:521:DT:H2''	5:I:522:DA:N7	2.36	0.40
6:J:309:DC:H2''	6:J:310:DC:C5	2.57	0.40
6:J:433:DA:H8	6:J:433:DA:H5''	1.86	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	98/136 (72%)	95 (97%)	3 (3%)	0	100	100
1	E	98/136 (72%)	92 (94%)	5 (5%)	1 (1%)	12	49
1	K	98/136 (72%)	94 (96%)	3 (3%)	1 (1%)	12	49
1	O	98/136 (72%)	91 (93%)	6 (6%)	1 (1%)	12	49
1	S	98/136 (72%)	95 (97%)	2 (2%)	1 (1%)	12	49
1	W	98/136 (72%)	95 (97%)	3 (3%)	0	100	100
1	a	98/136 (72%)	93 (95%)	4 (4%)	1 (1%)	12	49
1	e	98/136 (72%)	92 (94%)	5 (5%)	1 (1%)	12	49
2	B	82/103 (80%)	75 (92%)	6 (7%)	1 (1%)	10	44
2	F	85/103 (82%)	76 (89%)	7 (8%)	2 (2%)	4	27
2	L	85/103 (82%)	77 (91%)	8 (9%)	0	100	100
2	P	82/103 (80%)	73 (89%)	8 (10%)	1 (1%)	10	44
2	T	81/103 (79%)	74 (91%)	6 (7%)	1 (1%)	10	44
2	X	81/103 (79%)	73 (90%)	6 (7%)	2 (2%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	82/103 (80%)	75 (92%)	6 (7%)	1 (1%)	10	44
2	f	85/103 (82%)	76 (89%)	7 (8%)	2 (2%)	4	27
3	C	107/130 (82%)	99 (92%)	6 (6%)	2 (2%)	6	32
3	G	118/130 (91%)	105 (89%)	10 (8%)	3 (2%)	4	26
3	M	117/130 (90%)	101 (86%)	12 (10%)	4 (3%)	3	21
3	Q	108/130 (83%)	100 (93%)	8 (7%)	0	100	100
3	U	107/130 (82%)	98 (92%)	7 (6%)	2 (2%)	6	32
3	Y	108/130 (83%)	97 (90%)	7 (6%)	4 (4%)	2	20
3	c	107/130 (82%)	98 (92%)	7 (6%)	2 (2%)	6	32
3	g	118/130 (91%)	101 (86%)	13 (11%)	4 (3%)	3	21
4	D	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	12	49
4	H	96/99 (97%)	89 (93%)	5 (5%)	2 (2%)	5	30
4	N	97/99 (98%)	89 (92%)	6 (6%)	2 (2%)	5	30
4	R	96/99 (97%)	92 (96%)	3 (3%)	1 (1%)	12	49
4	V	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	12	49
4	Z	96/99 (97%)	91 (95%)	4 (4%)	1 (1%)	12	49
4	d	97/99 (98%)	87 (90%)	8 (8%)	2 (2%)	5	30
4	h	96/99 (97%)	88 (92%)	6 (6%)	2 (2%)	5	30
All	All	3109/3744 (83%)	2863 (92%)	197 (6%)	49 (2%)	10	38

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	100	PRO
2	F	24	ASP
3	M	12	ALA
1	O	37	LYS
4	R	100	PRO
4	V	100	PRO
4	Z	100	PRO
2	f	24	ASP
3	g	118	LYS
3	g	121	GLU
4	H	26	ARG
4	H	100	PRO
3	M	119	LYS

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Mol	Chain	Res	Type
4	N	100	PRO
1	S	134	ARG
3	Y	14	ALA
3	Y	118	LYS
3	c	12	ALA
4	d	100	PRO
4	h	100	PRO
3	C	12	ALA
3	C	112	GLN
3	G	112	GLN
3	M	112	GLN
3	U	12	ALA
3	U	112	GLN
3	Y	112	GLN
3	c	112	GLN
4	d	27	LYS
3	g	112	GLN
4	h	26	ARG
2	B	42	GLY
2	F	42	GLY
3	G	118	LYS
3	G	125	LYS
2	P	42	GLY
2	T	42	GLY
2	X	24	ASP
2	X	42	GLY
3	Y	12	ALA
2	b	42	GLY
2	f	42	GLY
3	M	121	GLU
1	a	39	HIS
3	g	124	HIS
1	E	117	VAL
4	N	26	ARG
1	e	117	VAL
1	K	38	PRO

5.3.2 Protein sidechains [i](#)

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	87/111 (78%)	83 (95%)	4 (5%)	24	45
1	E	87/111 (78%)	84 (97%)	3 (3%)	32	54
1	K	87/111 (78%)	86 (99%)	1 (1%)	65	76
1	O	87/111 (78%)	85 (98%)	2 (2%)	44	64
1	S	87/111 (78%)	85 (98%)	2 (2%)	44	64
1	W	87/111 (78%)	83 (95%)	4 (5%)	24	45
1	a	87/111 (78%)	85 (98%)	2 (2%)	44	64
1	e	87/111 (78%)	84 (97%)	3 (3%)	32	54
2	B	69/79 (87%)	69 (100%)	0	100	100
2	F	72/79 (91%)	69 (96%)	3 (4%)	26	48
2	L	72/79 (91%)	72 (100%)	0	100	100
2	P	69/79 (87%)	69 (100%)	0	100	100
2	T	68/79 (86%)	68 (100%)	0	100	100
2	X	68/79 (86%)	68 (100%)	0	100	100
2	b	69/79 (87%)	68 (99%)	1 (1%)	59	72
2	f	72/79 (91%)	71 (99%)	1 (1%)	59	72
3	C	85/100 (85%)	84 (99%)	1 (1%)	63	75
3	G	94/100 (94%)	92 (98%)	2 (2%)	47	65
3	M	94/100 (94%)	92 (98%)	2 (2%)	47	65
3	Q	86/100 (86%)	86 (100%)	0	100	100
3	U	85/100 (85%)	84 (99%)	1 (1%)	63	75
3	Y	86/100 (86%)	86 (100%)	0	100	100
3	c	85/100 (85%)	85 (100%)	0	100	100
3	g	94/100 (94%)	92 (98%)	2 (2%)	47	65
4	D	85/85 (100%)	83 (98%)	2 (2%)	43	64
4	H	84/85 (99%)	84 (100%)	0	100	100
4	N	85/85 (100%)	85 (100%)	0	100	100
4	R	84/85 (99%)	83 (99%)	1 (1%)	63	75
4	V	85/85 (100%)	83 (98%)	2 (2%)	43	64
4	Z	84/85 (99%)	83 (99%)	1 (1%)	63	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	85/85 (100%)	85 (100%)	0	100	100
4	h	84/85 (99%)	84 (100%)	0	100	100
All	All	2640/3000 (88%)	2600 (98%)	40 (2%)	55	72

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	40	ARG
1	A	49	ARG
1	A	107	THR
3	C	91	GLU
4	D	28	ARG
4	D	86	ILE
1	E	45	THR
1	E	46	VAL
1	E	117	VAL
2	F	21	VAL
2	F	22	LEU
2	F	23	ARG
3	G	91	GLU
3	G	118	LYS
1	K	49	ARG
3	M	11	ARG
3	M	91	GLU
1	O	49	ARG
1	O	107	THR
4	R	86	ILE
1	S	49	ARG
1	S	107	THR
3	U	91	GLU
4	V	25	LYS
4	V	86	ILE
1	W	41	TYR
1	W	42	ARG
1	W	49	ARG
1	W	107	THR
4	Z	86	ILE
1	a	49	ARG
1	a	107	THR
2	b	22	LEU

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Mol	Chain	Res	Type
1	e	45	THR
1	e	46	VAL
1	e	117	VAL
2	f	23	ARG
3	g	91	GLU
3	g	118	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	108	ASN
2	B	75	HIS
3	C	24	GLN
3	C	84	GLN
3	C	104	GLN
3	C	110	ASN
4	D	60	ASN
4	D	92	GLN
4	D	106	HIS
1	E	68	GLN
1	E	108	ASN
2	F	25	ASN
2	F	75	HIS
3	G	24	GLN
3	G	84	GLN
3	G	110	ASN
3	G	124	HIS
4	H	44	GLN
4	H	46	HIS
1	K	68	GLN
1	K	76	GLN
2	L	27	GLN
3	M	84	GLN
3	M	104	GLN
3	M	110	ASN
4	N	44	GLN
4	N	46	HIS
1	O	68	GLN
2	P	75	HIS
3	Q	84	GLN
3	Q	110	ASN

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Mol	Chain	Res	Type
4	R	60	ASN
4	R	92	GLN
1	S	68	GLN
1	S	76	GLN
1	S	108	ASN
2	T	75	HIS
3	U	24	GLN
3	U	84	GLN
3	U	110	ASN
4	V	44	GLN
4	V	60	ASN
4	V	92	GLN
4	V	106	HIS
1	W	39	HIS
1	W	68	GLN
2	X	75	HIS
3	Y	24	GLN
3	Y	84	GLN
3	Y	104	GLN
3	Y	110	ASN
4	Z	44	GLN
4	Z	60	ASN
4	Z	92	GLN
4	Z	106	HIS
1	a	68	GLN
1	a	108	ASN
2	b	75	HIS
3	c	84	GLN
3	c	110	ASN
4	d	46	HIS
1	e	39	HIS
1	e	68	GLN
1	e	108	ASN
2	f	25	ASN
2	f	75	HIS
3	g	84	GLN
3	g	104	GLN
3	g	110	ASN
3	g	123	HIS
4	h	44	GLN
4	h	46	HIS

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

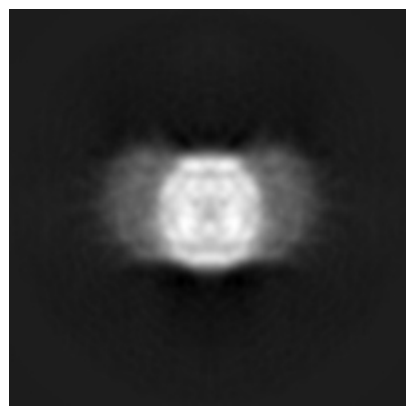
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31823. These allow visual inspection of the internal detail of the map and identification of artifacts.

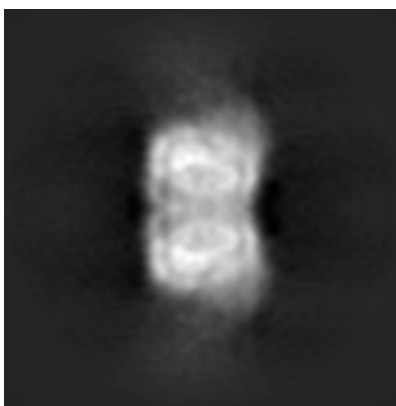
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

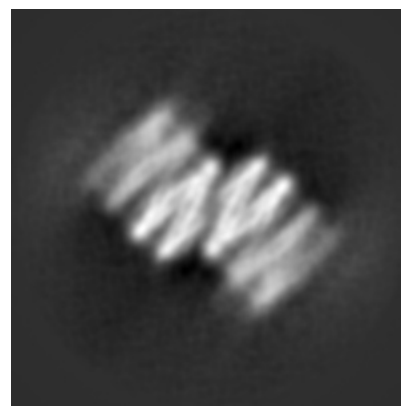
6.1.1 Primary map



X

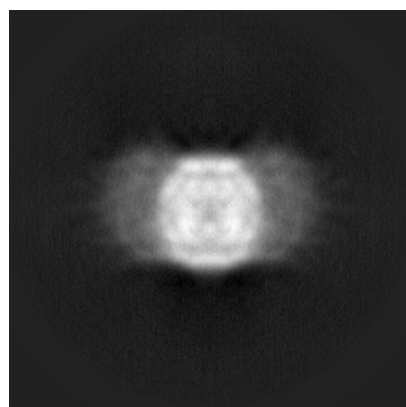


Y

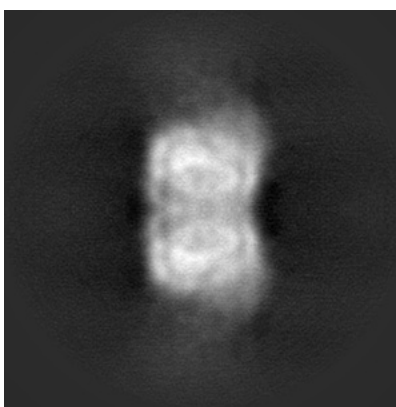


Z

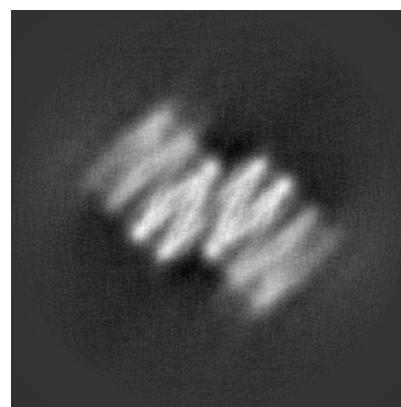
6.1.2 Raw map



X



Y

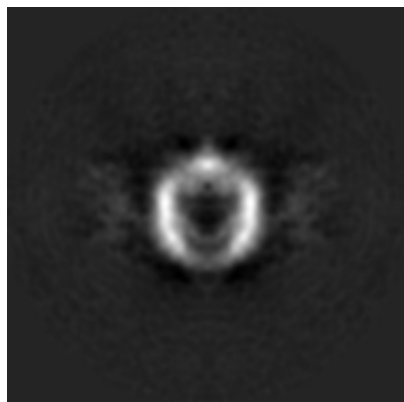


Z

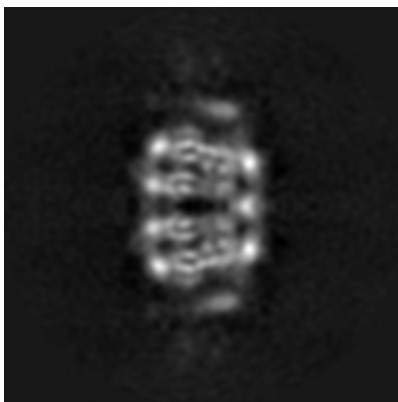
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

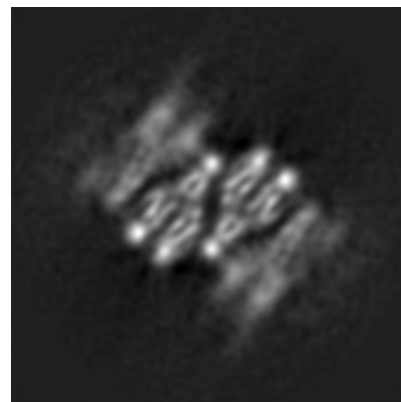
6.2.1 Primary map



X Index: 128

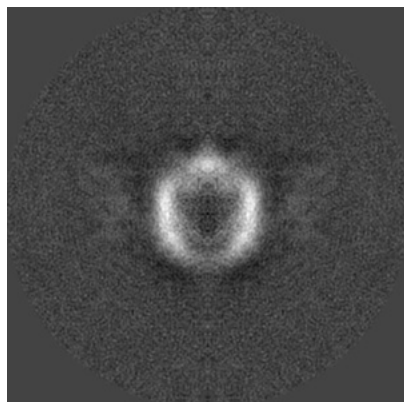


Y Index: 128

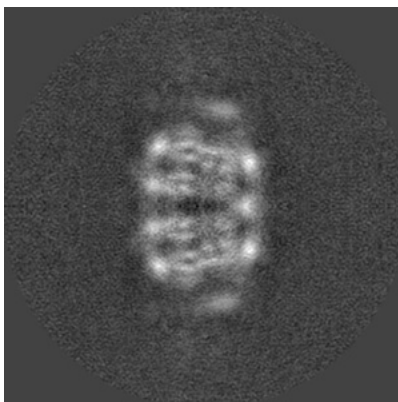


Z Index: 128

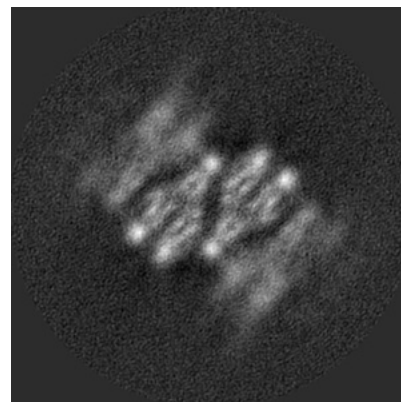
6.2.2 Raw map



X Index: 128



Y Index: 128

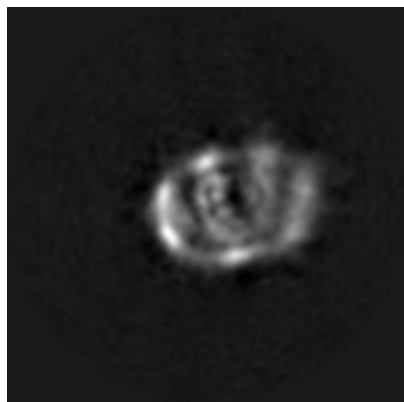


Z Index: 128

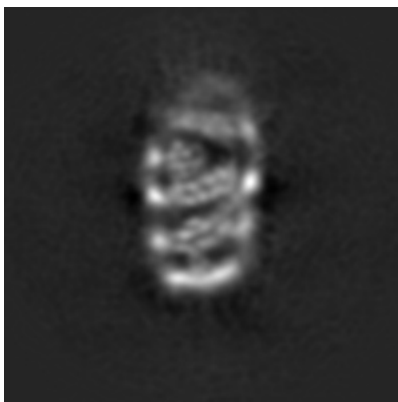
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

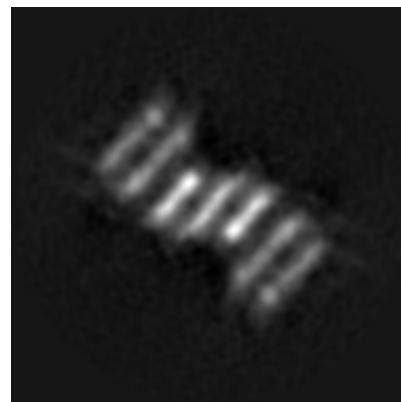
6.3.1 Primary map



X Index: 99

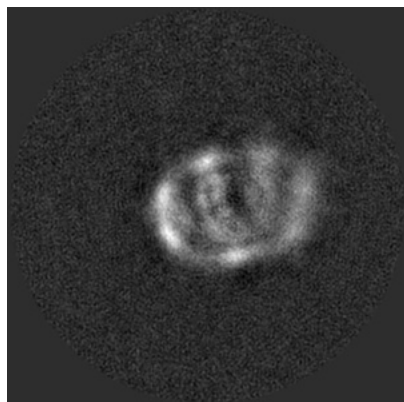


Y Index: 114

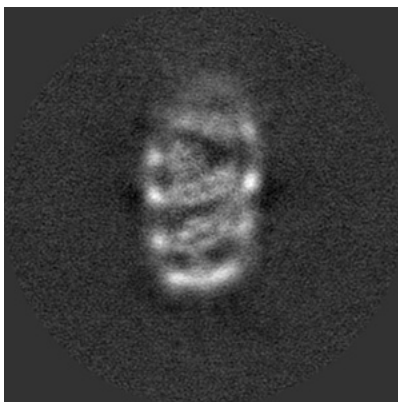


Z Index: 156

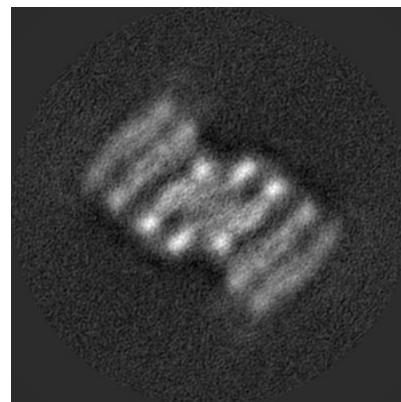
6.3.2 Raw map



X Index: 99



Y Index: 114

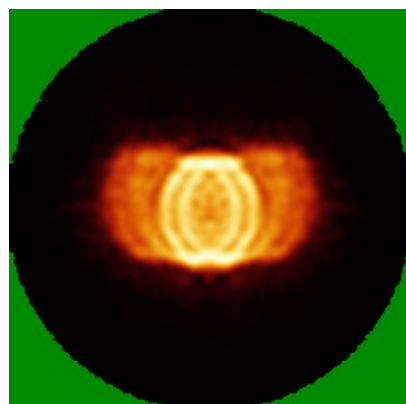


Z Index: 145

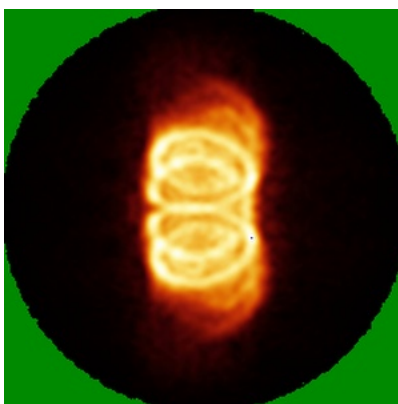
The images above show the largest variance slices of the map in three orthogonal directions.

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

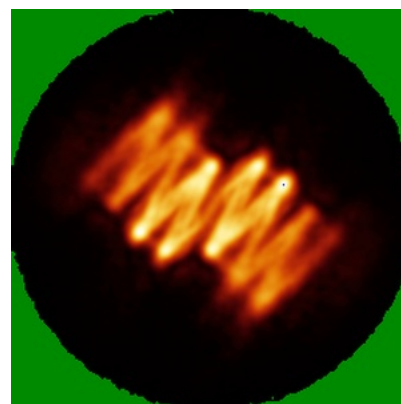
6.4.1 Primary map



X

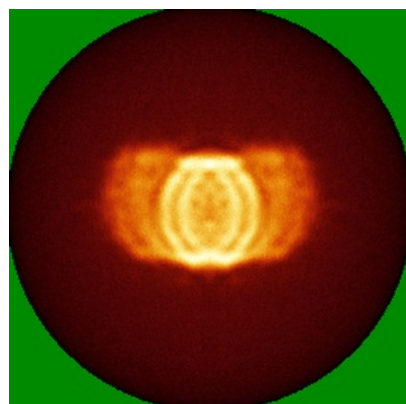


Y

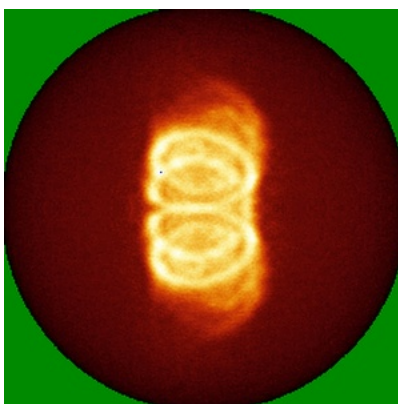


Z

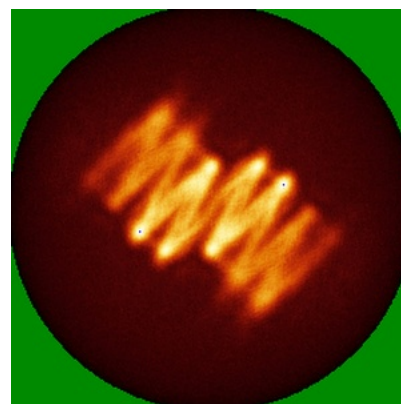
6.4.2 Raw map



X



Y

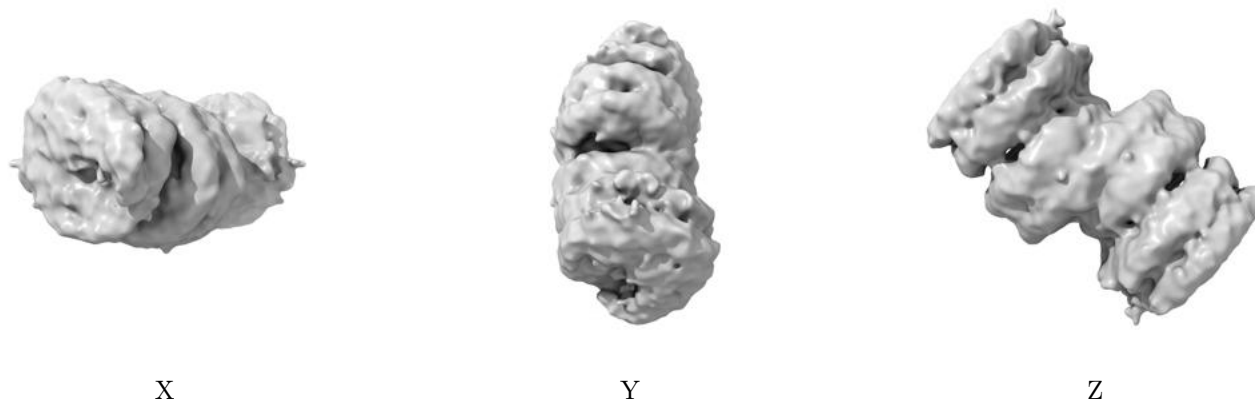


Z

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.

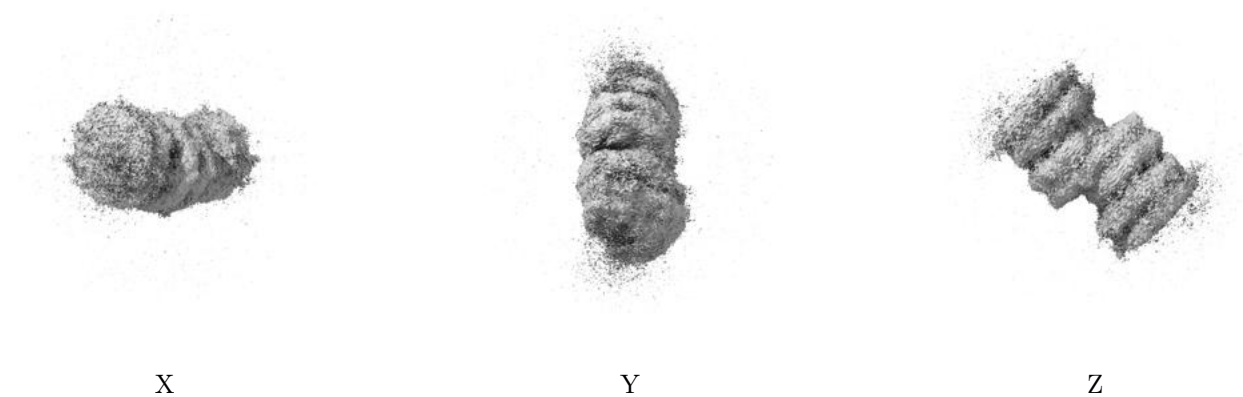
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0049. 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.

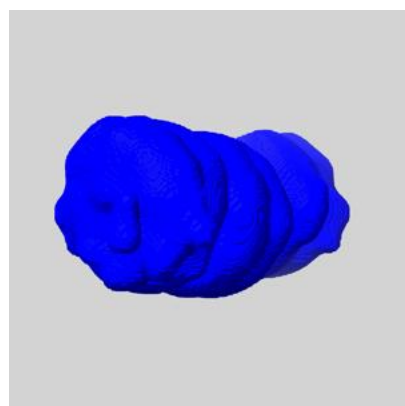
6.6 Mask visualisation [i](#)

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

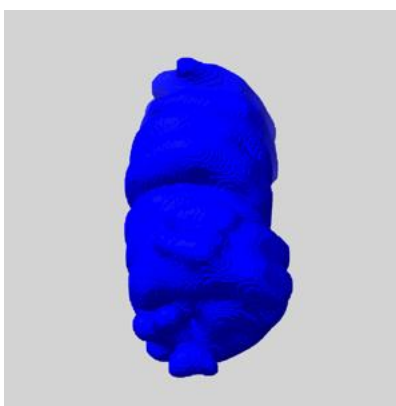
A mask typically either:

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

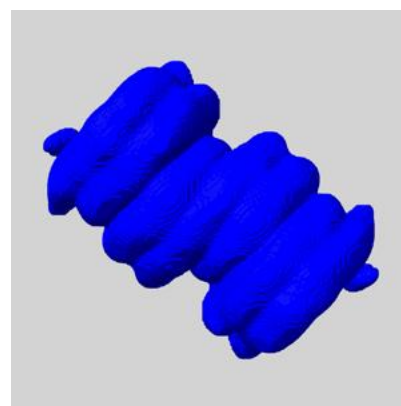
6.6.1 emd_31823_msk_1.map [i](#)



X



Y

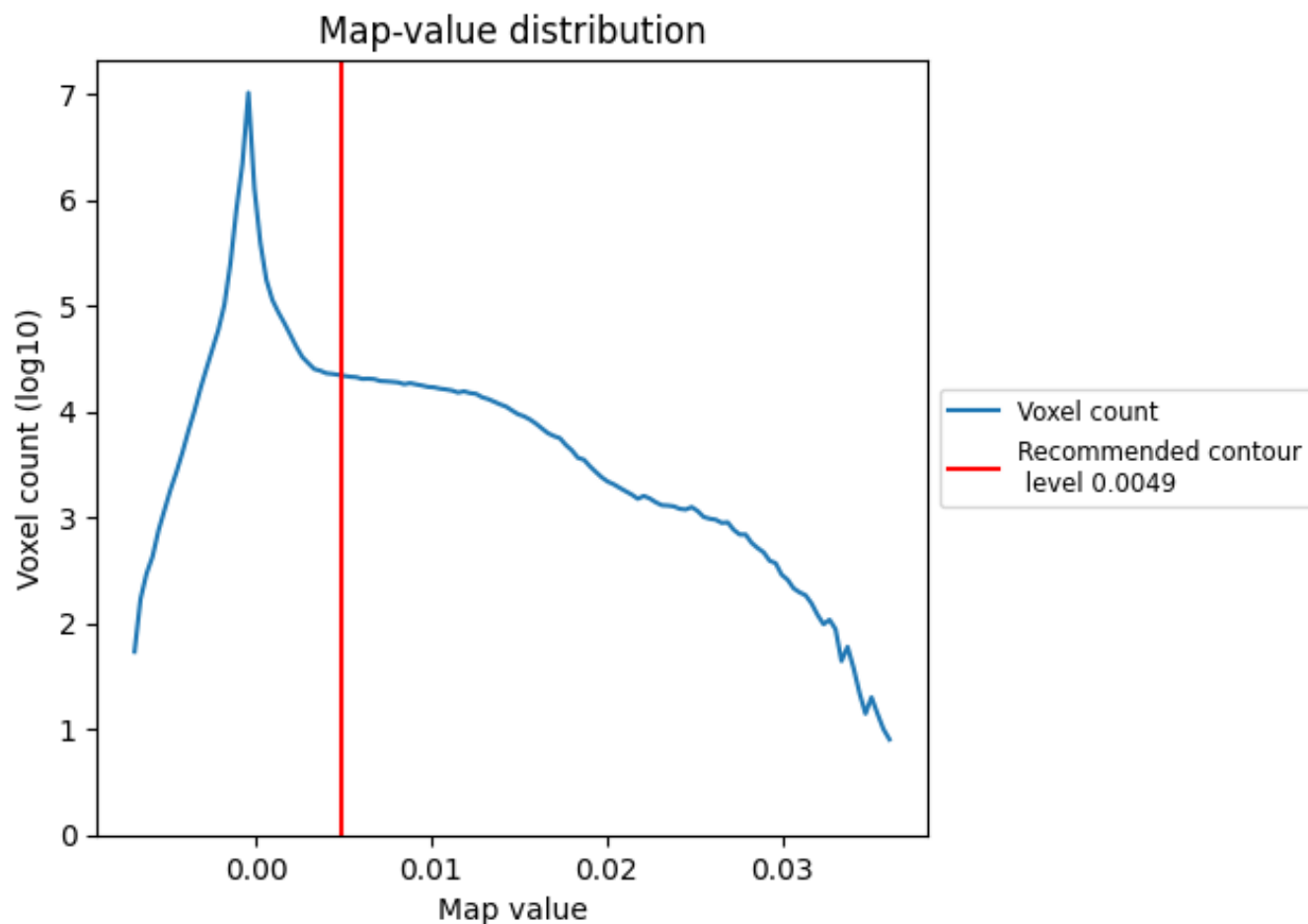


Z

7 Map analysis [i](#)

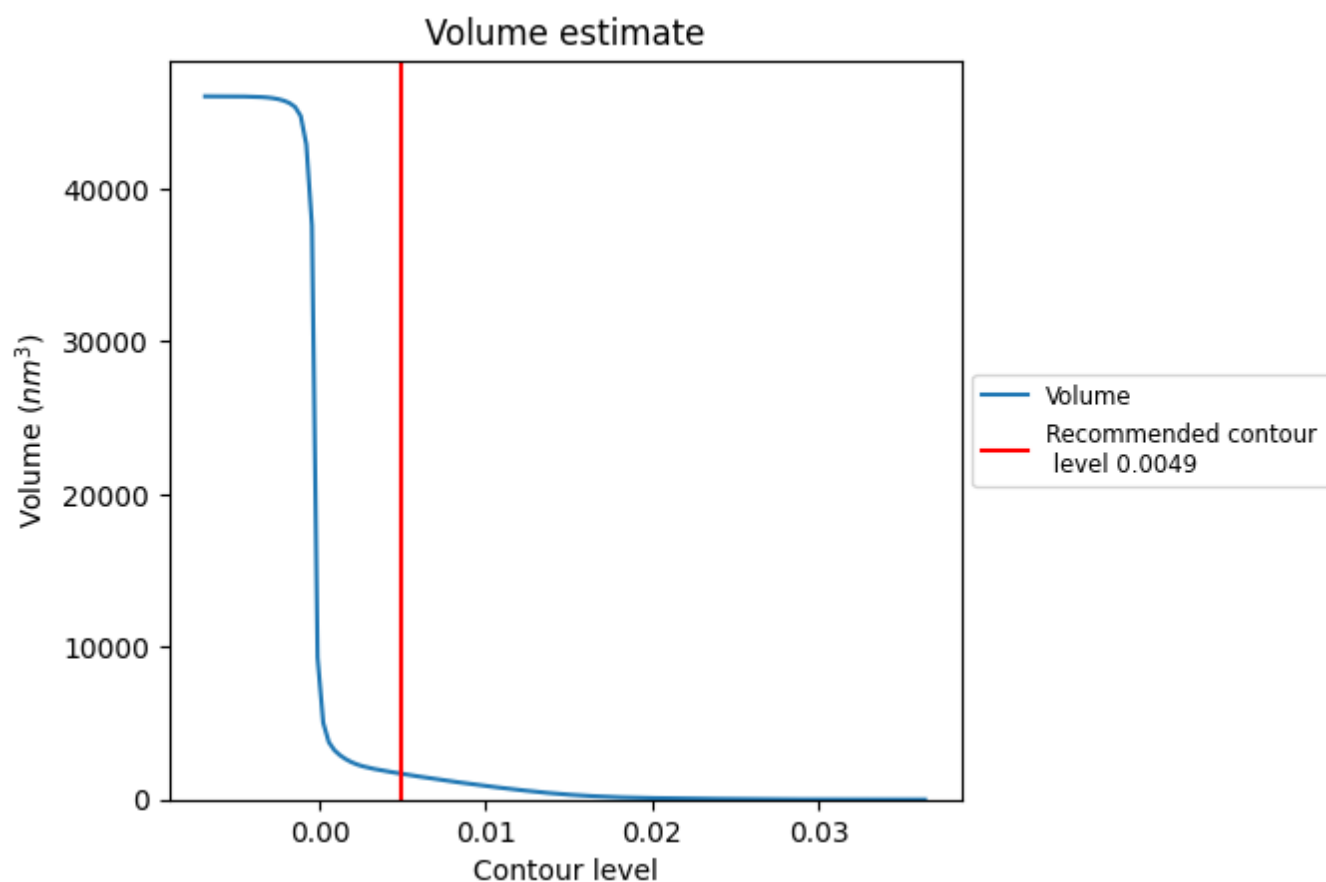
This section contains the results of statistical analysis of the map.

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.

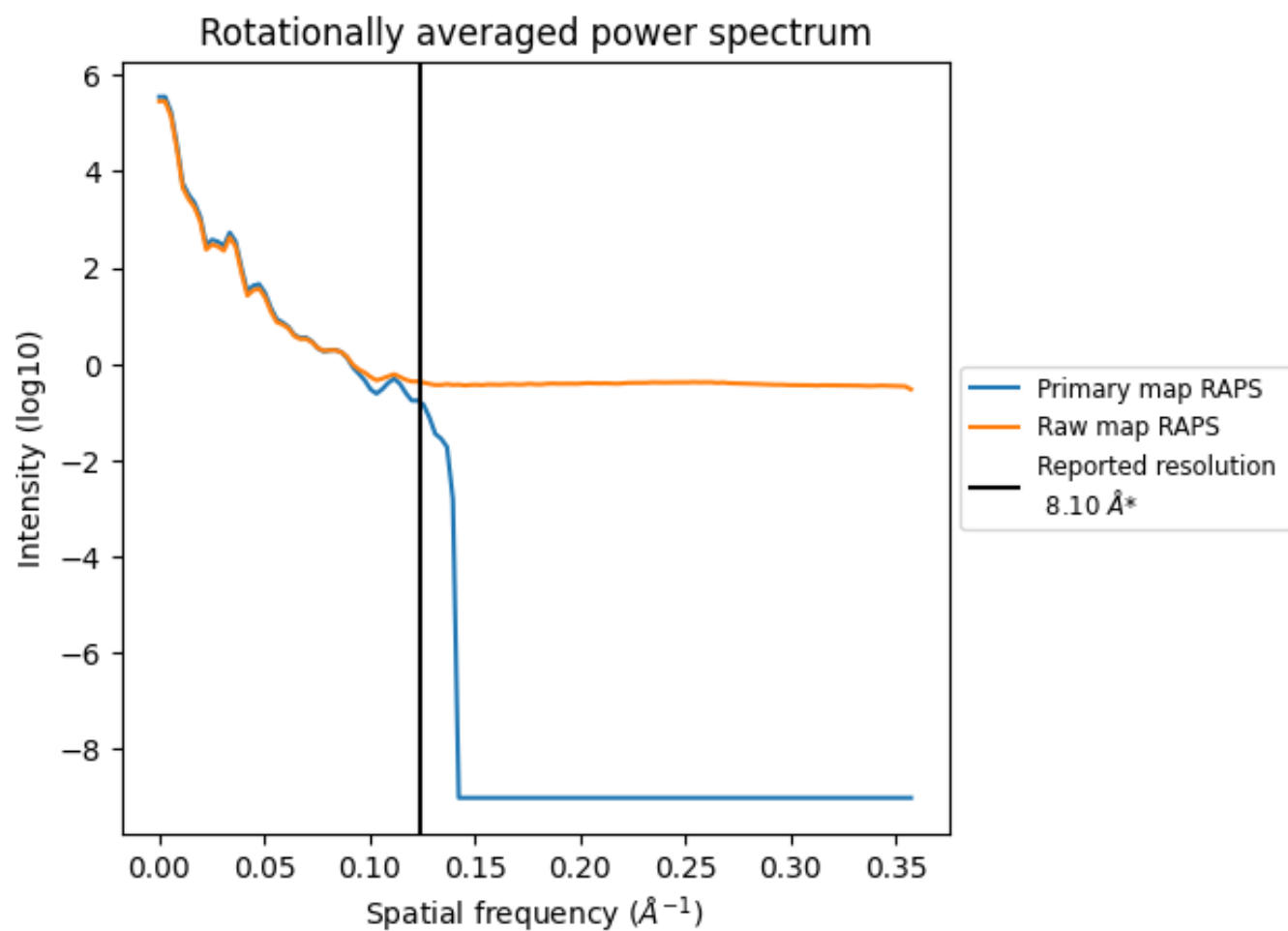
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1696 nm³; this corresponds to an approximate mass of 1532 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 ⓘ

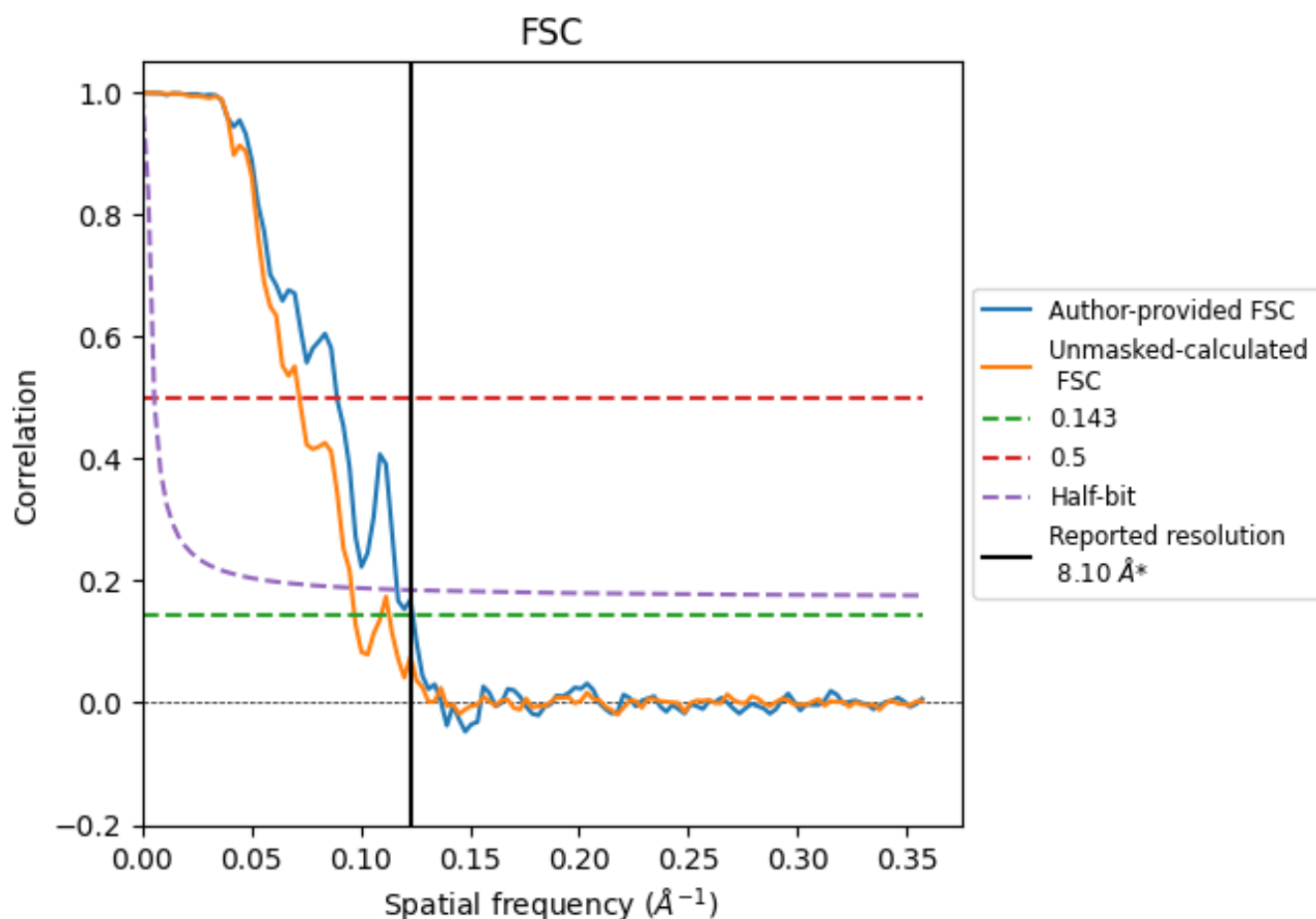


*Reported resolution corresponds to spatial frequency of 0.123 Å⁻¹

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 0.123 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

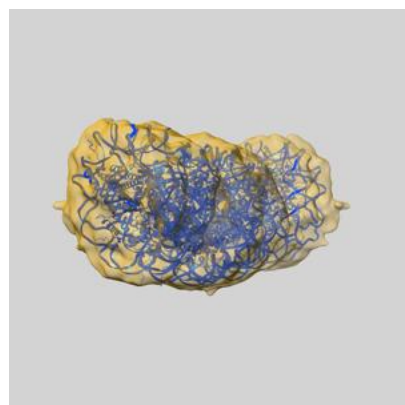
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.10	-	-
Author-provided FSC curve	8.08	11.21	8.57
Unmasked-calculated*	10.29	13.89	10.44

*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 10.29 differs from the reported value 8.1 by more than 10 %

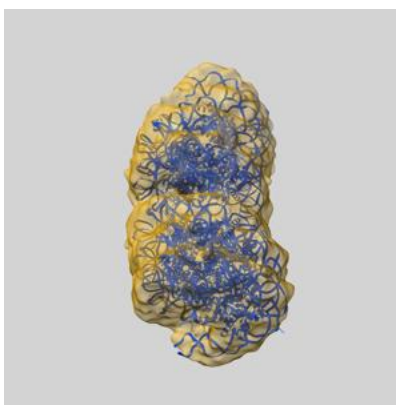
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31823 and PDB model 7V9K. Per-residue inclusion information can be found in section [3](#) on page [8](#).

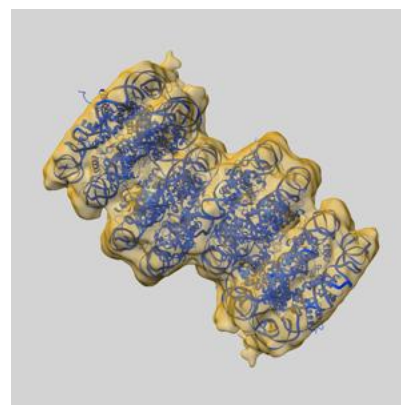
9.1 Map-model overlay [i](#)



X



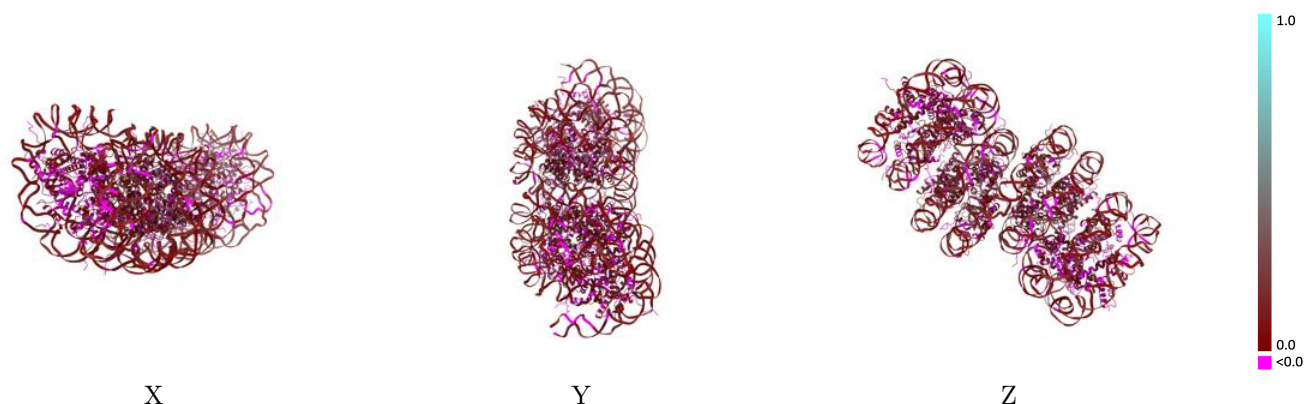
Y



Z

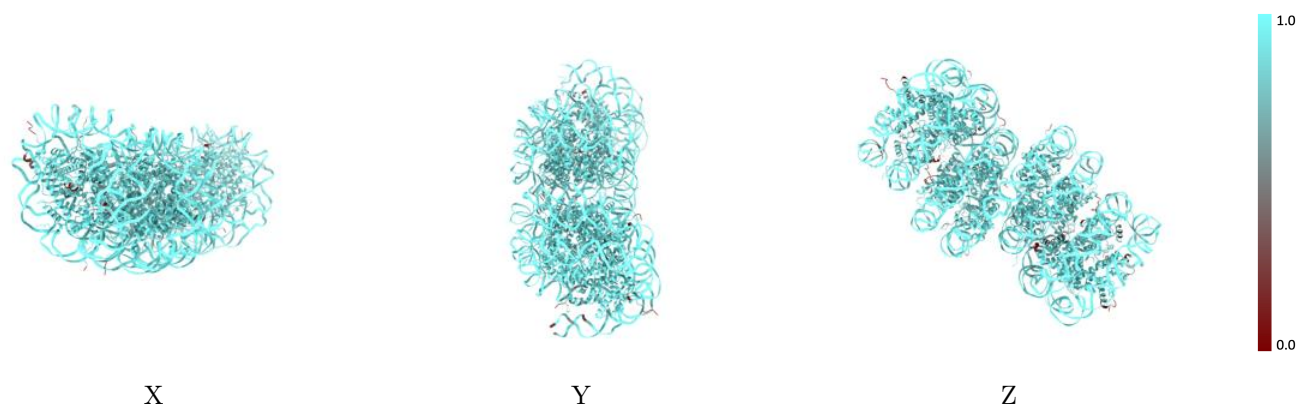
The images above show the 3D surface view of the map at the recommended contour level 0.0049 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



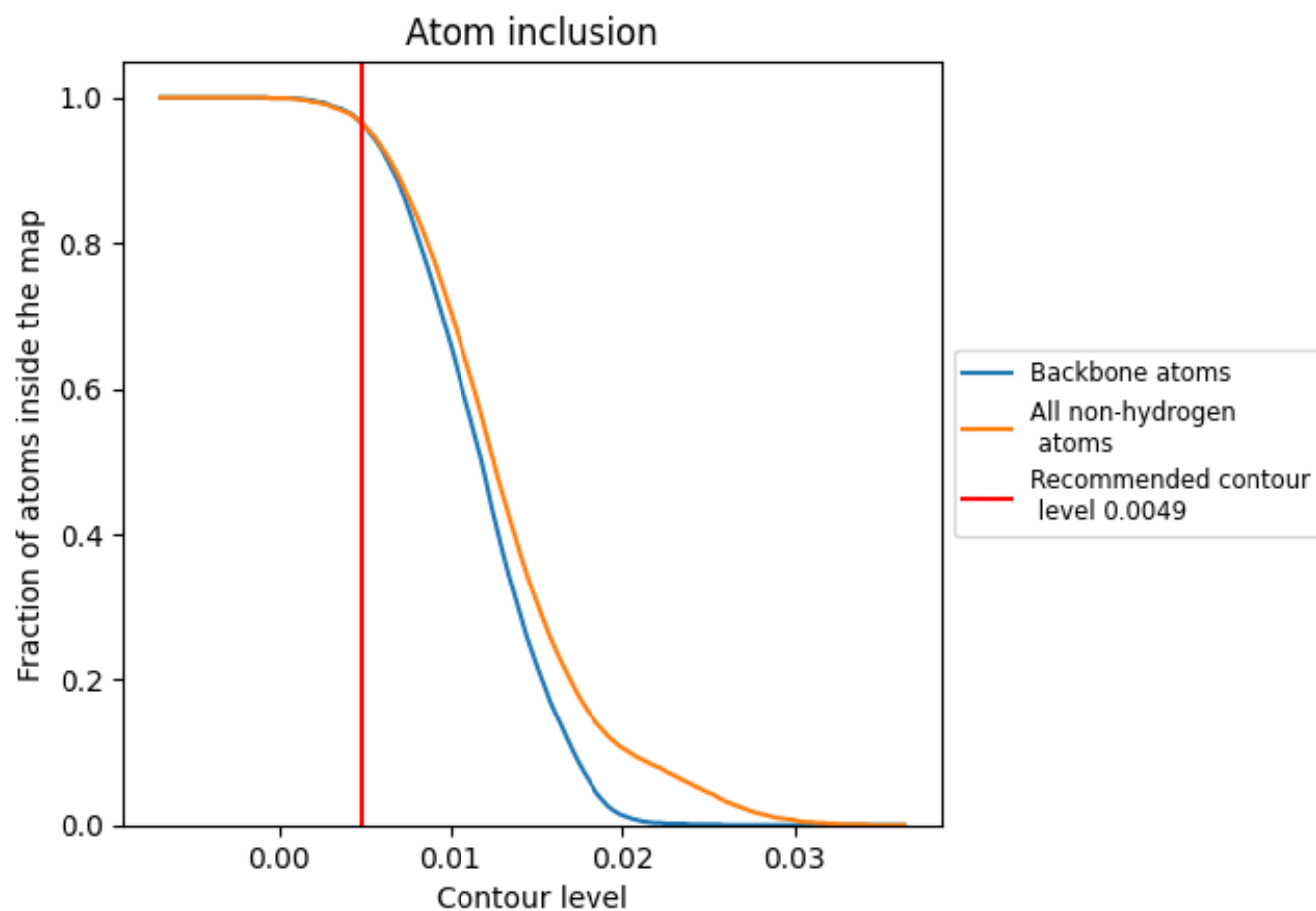
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0049).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.0049) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.0760
A	 0.9850	 0.1100
B	 0.9460	 0.0920
C	 0.9900	 0.0550
D	 0.9580	 0.1150
E	 0.9950	 0.0960
F	 0.9140	 0.0850
G	 0.9660	 0.0780
H	 0.9840	 0.1080
I	 0.9840	 0.0980
J	 0.9810	 0.0890
K	 0.9290	 0.0570
L	 0.8690	 0.0420
M	 0.9680	 0.0300
N	 0.9190	 0.0630
O	 0.9990	 0.0370
P	 1.0000	 0.0340
Q	 0.8980	 0.0350
R	 0.9270	 0.0490
S	 0.9770	 0.1000
T	 0.9750	 0.0870
U	 0.9720	 0.0560
V	 0.9620	 0.0930
W	 0.9950	 0.1040
X	 0.9590	 0.0920
Y	 0.9840	 0.0810
Z	 0.9590	 0.1000
a	 0.9860	 -0.0020
b	 1.0000	 0.0050
c	 0.8680	 0.0010
d	 0.8990	 0.0200
e	 0.9290	 0.0520
f	 0.8970	 0.0470
g	 0.8530	 0.0200
h	 0.8620	 0.0060

