



Full wwPDB EM Validation Report ⓘ

Mar 25, 2025 – 02:24 PM JST

PDB ID : 8X30
EMDB ID : EMD-38024
Title : Structure of piccolo NuA4 and H2A.Z nucleosome 2:1 complex
Authors : Wang, L.; Zhang, H.; Zhu, H.; Zhu, P.
Deposited on : 2023-11-10
Resolution : 4.30 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

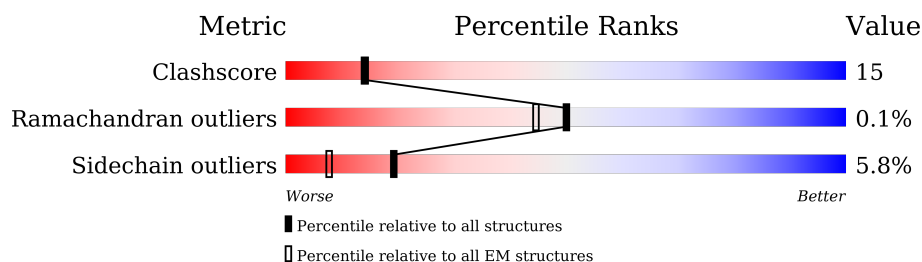
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.




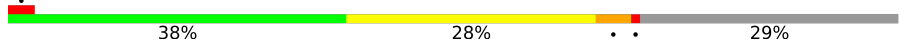
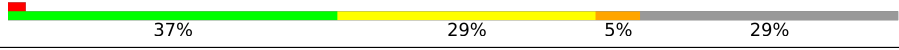
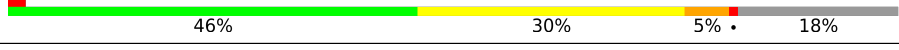
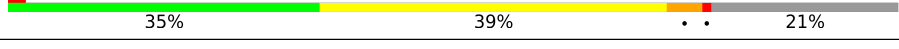
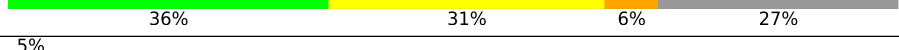

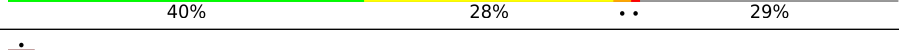
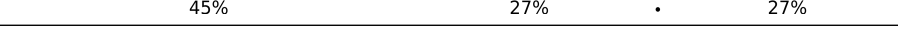
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	K	469	
1	O	469	
2	M	586	
2	Q	586	
3	N	120	
3	R	120	
4	P	537	
5	I	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	J	146	
6	A	136	
6	E	136	
7	B	102	
7	F	102	
8	C	134	
8	G	134	
9	D	131	
9	H	131	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21579 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 acetyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	272	Total	C	N	O	S	0	0
			2304	1487	388	419	10		
1	O	282	Total	C	N	O	S	0	0
			2380	1538	400	432	10		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-23	MET	-	initiating methionine	UNP A0A6A5Q414
K	-22	GLY	-	expression tag	UNP A0A6A5Q414
K	-21	SER	-	expression tag	UNP A0A6A5Q414
K	-20	SER	-	expression tag	UNP A0A6A5Q414
K	-19	HIS	-	expression tag	UNP A0A6A5Q414
K	-18	HIS	-	expression tag	UNP A0A6A5Q414
K	-17	HIS	-	expression tag	UNP A0A6A5Q414
K	-16	HIS	-	expression tag	UNP A0A6A5Q414
K	-15	HIS	-	expression tag	UNP A0A6A5Q414
K	-14	HIS	-	expression tag	UNP A0A6A5Q414
K	-13	SER	-	expression tag	UNP A0A6A5Q414
K	-12	GLN	-	expression tag	UNP A0A6A5Q414
K	-11	ASP	-	expression tag	UNP A0A6A5Q414
K	-10	HIS	-	expression tag	UNP A0A6A5Q414
K	-9	GLU	-	expression tag	UNP A0A6A5Q414
K	-8	ASN	-	expression tag	UNP A0A6A5Q414
K	-7	LEU	-	expression tag	UNP A0A6A5Q414
K	-6	TYR	-	expression tag	UNP A0A6A5Q414
K	-5	PHE	-	expression tag	UNP A0A6A5Q414
K	-4	GLN	-	expression tag	UNP A0A6A5Q414
K	-3	GLY	-	expression tag	UNP A0A6A5Q414
K	-2	ALA	-	expression tag	UNP A0A6A5Q414
K	-1	GLY	-	expression tag	UNP A0A6A5Q414
K	0	SER	-	expression tag	UNP A0A6A5Q414
O	-23	MET	-	initiating methionine	UNP A0A6A5Q414
O	-22	GLY	-	expression tag	UNP A0A6A5Q414

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
O	-21	SER	-	expression tag	UNP A0A6A5Q414
O	-20	SER	-	expression tag	UNP A0A6A5Q414
O	-19	HIS	-	expression tag	UNP A0A6A5Q414
O	-18	HIS	-	expression tag	UNP A0A6A5Q414
O	-17	HIS	-	expression tag	UNP A0A6A5Q414
O	-16	HIS	-	expression tag	UNP A0A6A5Q414
O	-15	HIS	-	expression tag	UNP A0A6A5Q414
O	-14	HIS	-	expression tag	UNP A0A6A5Q414
O	-13	SER	-	expression tag	UNP A0A6A5Q414
O	-12	GLN	-	expression tag	UNP A0A6A5Q414
O	-11	ASP	-	expression tag	UNP A0A6A5Q414
O	-10	HIS	-	expression tag	UNP A0A6A5Q414
O	-9	GLU	-	expression tag	UNP A0A6A5Q414
O	-8	ASN	-	expression tag	UNP A0A6A5Q414
O	-7	LEU	-	expression tag	UNP A0A6A5Q414
O	-6	TYR	-	expression tag	UNP A0A6A5Q414
O	-5	PHE	-	expression tag	UNP A0A6A5Q414
O	-4	GLN	-	expression tag	UNP A0A6A5Q414
O	-3	GLY	-	expression tag	UNP A0A6A5Q414
O	-2	ALA	-	expression tag	UNP A0A6A5Q414
O	-1	GLY	-	expression tag	UNP A0A6A5Q414
O	0	SER	-	expression tag	UNP A0A6A5Q414

- Molecule 2 is a protein called glutathione transferase,Enhancer of polycomb-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	180	Total	C	N	O	S	0	0
			1485	938	249	291	7		
2	Q	213	Total	C	N	O	S	0	0
			1777	1129	295	346	7		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	33	SER	-	linker	UNP Q540A3
M	34	ASP	-	linker	UNP Q540A3
M	35	LEU	-	linker	UNP Q540A3
M	36	VAL	-	linker	UNP Q540A3
M	37	PRO	-	linker	UNP Q540A3
M	38	ARG	-	linker	UNP Q540A3
M	39	GLY	-	linker	UNP Q540A3
M	40	SER	-	linker	UNP Q540A3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	41	GLU	-	linker	UNP Q540A3
M	42	ASN	-	linker	UNP Q540A3
M	43	LEU	-	linker	UNP Q540A3
M	44	TYR	-	linker	UNP Q540A3
M	45	PHE	-	linker	UNP Q540A3
M	46	GLN	-	linker	UNP Q540A3
M	47	GLY	-	linker	UNP Q540A3
M	48	HIS	-	linker	UNP Q540A3
M	49	MET	-	linker	UNP Q540A3
Q	33	SER	-	linker	UNP Q540A3
Q	34	ASP	-	linker	UNP Q540A3
Q	35	LEU	-	linker	UNP Q540A3
Q	36	VAL	-	linker	UNP Q540A3
Q	37	PRO	-	linker	UNP Q540A3
Q	38	ARG	-	linker	UNP Q540A3
Q	39	GLY	-	linker	UNP Q540A3
Q	40	SER	-	linker	UNP Q540A3
Q	41	GLU	-	linker	UNP Q540A3
Q	42	ASN	-	linker	UNP Q540A3
Q	43	LEU	-	linker	UNP Q540A3
Q	44	TYR	-	linker	UNP Q540A3
Q	45	PHE	-	linker	UNP Q540A3
Q	46	GLN	-	linker	UNP Q540A3
Q	47	GLY	-	linker	UNP Q540A3
Q	48	HIS	-	linker	UNP Q540A3
Q	49	MET	-	linker	UNP Q540A3

- Molecule 3 is a protein called Chromatin modification-related protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	71	Total	C	N	O	S	0	0
			576	366	99	109	2		
3	R	100	Total	C	N	O	S	0	0
			813	514	136	160	3		

- Molecule 4 is a protein called Maltose/maltodextrin-binding periplasmic protein,Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	P	32	Total	C	N	O	0	0
			283	174	46	63		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	-86	VAL	ALA	conflict	UNP P0AEX9
P	-31	ASN	-	linker	UNP P0AEX9
P	-30	SER	-	linker	UNP P0AEX9
P	-29	SER	-	linker	UNP P0AEX9
P	-28	SER	-	linker	UNP P0AEX9
P	-27	ASN	-	linker	UNP P0AEX9
P	-26	ASN	-	linker	UNP P0AEX9
P	-25	ASN	-	linker	UNP P0AEX9
P	-24	ASN	-	linker	UNP P0AEX9
P	-23	ASN	-	linker	UNP P0AEX9
P	-22	ASN	-	linker	UNP P0AEX9
P	-21	ASN	-	linker	UNP P0AEX9
P	-20	ASN	-	linker	UNP P0AEX9
P	-19	ASN	-	linker	UNP P0AEX9
P	-18	ASN	-	linker	UNP P0AEX9
P	-17	LEU	-	linker	UNP P0AEX9
P	-16	GLY	-	linker	UNP P0AEX9
P	-15	ILE	-	linker	UNP P0AEX9
P	-14	GLU	-	linker	UNP P0AEX9
P	-13	GLY	-	linker	UNP P0AEX9
P	-12	ARG	-	linker	UNP P0AEX9
P	-11	ILE	-	linker	UNP P0AEX9
P	-10	SER	-	linker	UNP P0AEX9
P	-9	GLU	-	linker	UNP P0AEX9
P	-8	PHE	-	linker	UNP P0AEX9
P	-7	GLU	-	linker	UNP P0AEX9
P	-6	ASN	-	linker	UNP P0AEX9
P	-5	LEU	-	linker	UNP P0AEX9
P	-4	TYR	-	linker	UNP P0AEX9
P	-3	PHE	-	linker	UNP P0AEX9
P	-2	GLN	-	linker	UNP P0AEX9
P	-1	GLY	-	linker	UNP P0AEX9
P	0	HIS	-	linker	UNP P0AEX9

- Molecule 5 is a DNA chain called DNA (146-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	146	Total	C	N	O	P	0	0
			2990	1430	541	874	145		
5	J	146	Total	C	N	O	P	0	0
			2990	1430	541	874	145		

- Molecule 6 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	97	Total	C	N	O	0	0
			801	508	155	138		
6	E	97	Total	C	N	O	0	0
			801	508	155	138		

- Molecule 7 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	84	Total	C	N	O	0	0
			679	429	134	116		
7	F	81	Total	C	N	O	0	0
			649	411	125	113		

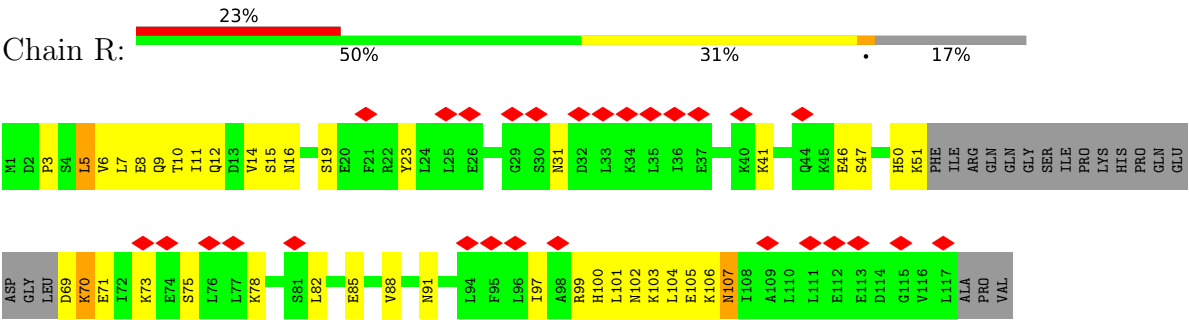
- Molecule 8 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	C	98	Total	C	N	O	0	0
			750	471	145	134		
8	G	108	Total	C	N	O	0	0
			829	524	160	145		

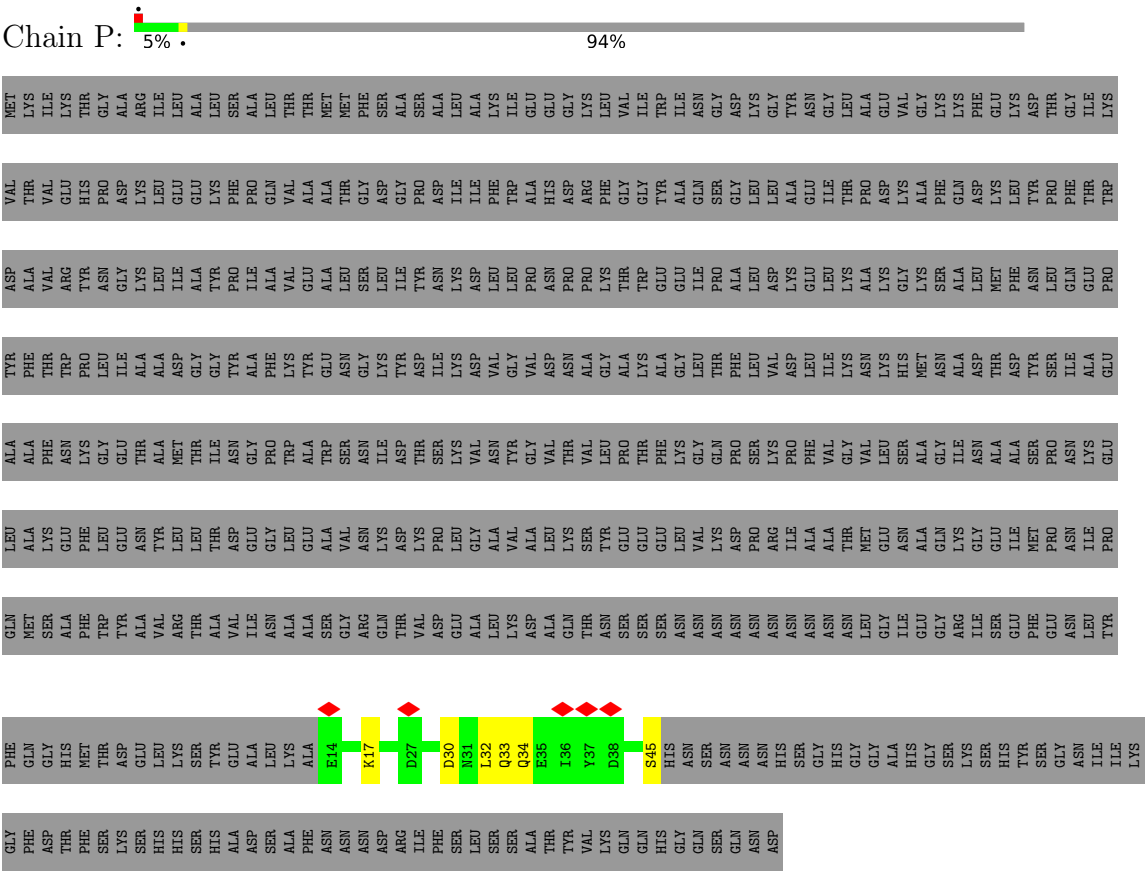
- Molecule 9 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	93	Total	C	N	O	S	0	0
			726	456	127	142	1		
9	H	96	Total	C	N	O	S	0	0
			746	467	131	147	1		

• Molecule 3: Chromatin modification-related protein



• Molecule 4: Maltose/maltodextrin-binding periplasmic protein,Chromatin modification-related protein EAF6

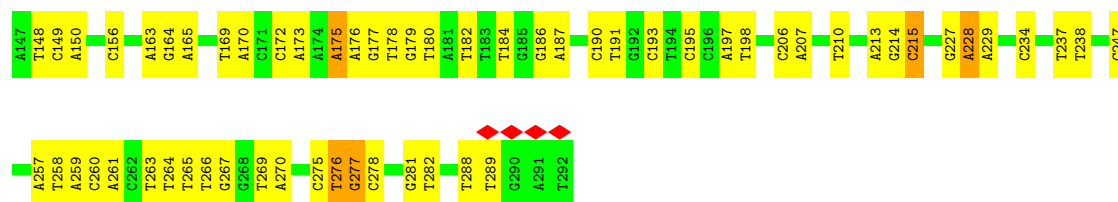


• Molecule 5: DNA (146-MER)



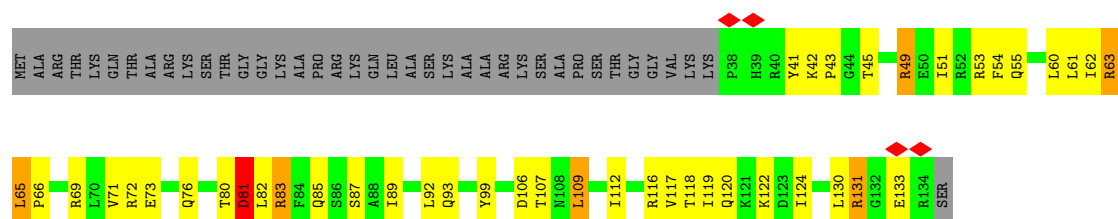
- Molecule 5: DNA (146-MER)

Chain J:  59% 38%



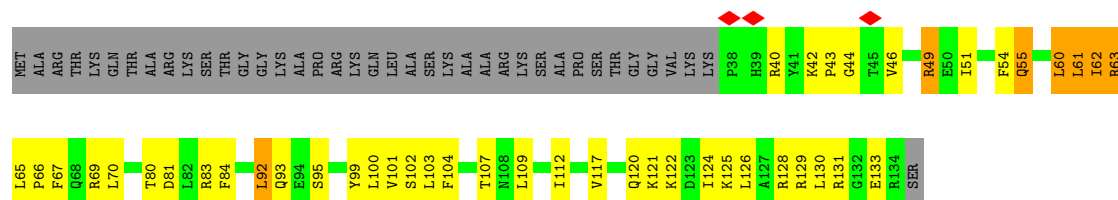
- Molecule 6: Histone H3

Chain A:  38% 28% 29%



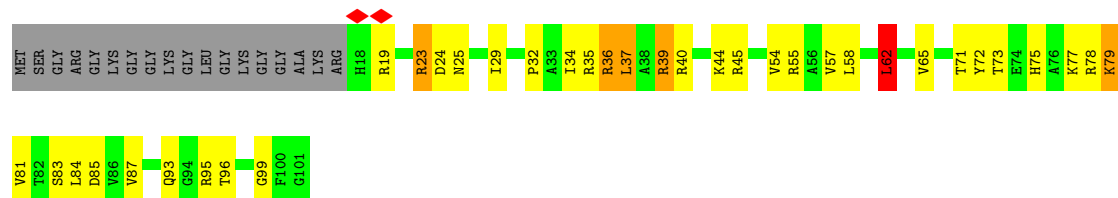
- Molecule 6: Histone H3

Chain E:  37% 29% 5% 29%




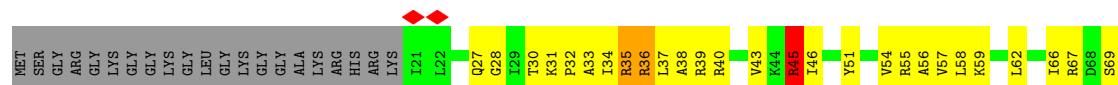
- Molecule 7: Histone H4

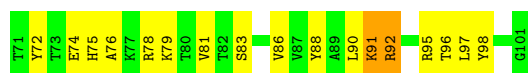
Chain B:  46% 30% 5% 18%



- Molecule 7: Histone H4

Chain F:  35% 39% 21%

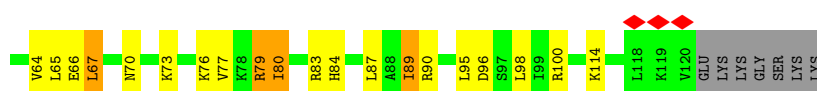
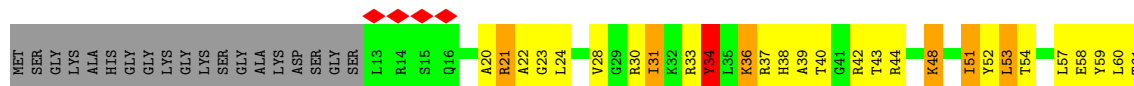




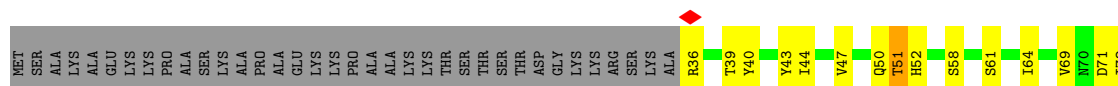
- Molecule 8: Histone H2A



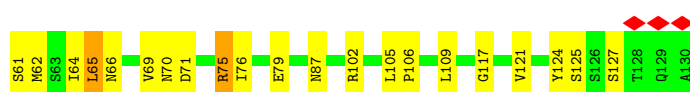
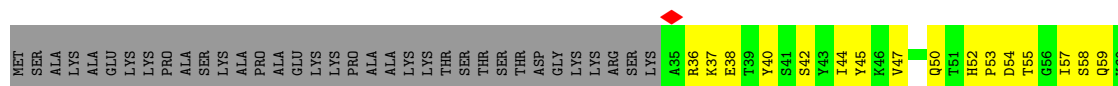
- Molecule 8: Histone H2A



- Molecule 9: Histone H2B



- Molecule 9: Histone H2B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10982	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	15.171	Depositor
Minimum map value	-0.139	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.431	Depositor
Recommended contour level	0.905	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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	K	0.48	0/2362	0.82	2/3189 (0.1%)
1	O	0.44	0/2441	0.76	4/3298 (0.1%)
2	M	0.38	0/1514	0.72	2/2040 (0.1%)
2	Q	0.40	0/1815	0.70	1/2449 (0.0%)
3	N	0.37	0/579	0.69	0/774
3	R	0.44	0/819	0.66	1/1095 (0.1%)
4	P	0.33	0/286	0.65	0/381
5	I	1.52	11/3354 (0.3%)	1.24	6/5175 (0.1%)
5	J	1.55	12/3354 (0.4%)	1.22	6/5175 (0.1%)
6	A	0.58	0/812	0.99	3/1086 (0.3%)
6	E	0.54	0/812	0.92	3/1086 (0.3%)
7	B	0.58	0/687	0.94	3/919 (0.3%)
7	F	0.63	0/656	0.97	0/879
8	C	0.51	0/759	0.91	1/1023 (0.1%)
8	G	0.54	0/838	1.04	4/1128 (0.4%)
9	D	0.54	0/736	0.93	3/991 (0.3%)
9	H	0.57	0/756	0.86	1/1017 (0.1%)
All	All	0.93	23/22580 (0.1%)	0.98	40/31705 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	8
1	O	0	7
6	A	0	1
6	E	0	1
7	B	0	1
7	F	0	2
8	G	0	3
9	D	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
9	H	0	1
All	All	0	25

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	61	DA	C3'-O3'	-6.84	1.35	1.44
5	J	277	DG	C3'-O3'	-6.53	1.35	1.44
5	I	48	DT	C3'-O3'	-6.36	1.35	1.44
5	J	276	DT	C3'-O3'	-6.33	1.35	1.44
5	I	129	DC	C3'-O3'	-6.12	1.35	1.44
5	I	20	DT	C3'-O3'	-5.88	1.36	1.44
5	J	206	DC	C3'-O3'	-5.80	1.36	1.44
5	J	182	DT	C3'-O3'	-5.79	1.36	1.44
5	I	62	DT	C3'-O3'	-5.75	1.36	1.44
5	I	72	DA	C3'-O3'	-5.69	1.36	1.44
5	J	213	DA	C3'-O3'	-5.47	1.36	1.44
5	I	92	DT	C3'-O3'	-5.45	1.36	1.44
5	J	215	DC	C3'-O3'	-5.40	1.36	1.44
5	J	156	DC	C3'-O3'	-5.32	1.37	1.44
5	J	195	DC	C3'-O3'	-5.32	1.37	1.44
5	I	64	DT	C3'-O3'	-5.28	1.37	1.44
5	I	56	DA	N7-C5	-5.28	1.36	1.39
5	I	51	DA	C3'-O3'	-5.18	1.37	1.44
5	J	228	DA	C3'-O3'	-5.07	1.37	1.44
5	I	41	DA	C3'-O3'	-5.06	1.37	1.44
5	J	175	DA	C3'-O3'	-5.05	1.37	1.44
5	J	173	DA	C3'-O3'	-5.04	1.37	1.44
5	J	198	DT	C3'-O3'	-5.04	1.37	1.44

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	106	ASP	CB-CG-OD1	8.09	125.58	118.30
5	I	80	DT	O4'-C4'-C3'	-7.88	101.27	106.00
6	A	65	LEU	CA-CB-CG	7.88	133.42	115.30
5	I	19	DA	O4'-C4'-C3'	-7.55	101.47	106.00
8	G	67	LEU	CA-CB-CG	7.52	132.59	115.30
8	G	34	TYR	CA-CB-CG	6.62	125.99	113.40
2	M	346	ASP	CB-CG-OD1	6.56	124.20	118.30
5	I	58	DG	O4'-C4'-C3'	-6.53	101.89	104.50
2	Q	329	LEU	CA-CB-CG	6.52	130.29	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	184	DT	O4'-C4'-C3'	-6.48	101.91	104.50
8	G	89	ILE	CG1-CB-CG2	-6.39	97.34	111.40
8	G	53	LEU	CA-CB-CG	6.29	129.78	115.30
1	O	394	LEU	CA-CB-CG	6.14	129.42	115.30
3	R	5	LEU	CA-CB-CG	6.13	129.39	115.30
1	K	286	LEU	CA-CB-CG	6.03	129.17	115.30
1	O	357	LEU	CA-CB-CG	5.78	128.58	115.30
1	O	361	LEU	CA-CB-CG	5.74	128.50	115.30
6	A	81	ASP	CB-CG-OD1	5.70	123.42	118.30
9	D	83	LEU	CA-CB-CG	5.67	128.35	115.30
5	J	207	DA	OP2-P-O3'	5.56	117.42	105.20
7	B	62	LEU	CA-CB-CG	5.53	128.01	115.30
5	J	184	DT	C4'-C3'-C2'	-5.52	98.13	103.10
7	B	62	LEU	CB-CG-CD2	5.50	120.34	111.00
5	J	193	DC	C1'-O4'-C4'	-5.47	104.63	110.10
9	H	71	ASP	CB-CG-OD1	5.45	123.21	118.30
7	B	37	LEU	CA-CB-CG	5.43	127.78	115.30
2	M	341	LEU	CA-CB-CG	5.37	127.66	115.30
9	D	103	LEU	CA-CB-CG	5.34	127.58	115.30
5	J	207	DA	P-O3'-C3'	5.32	126.08	119.70
9	D	71	ASP	CB-CG-OD1	5.31	123.08	118.30
1	K	397	TYR	CA-CB-CG	5.29	123.44	113.40
6	E	103	LEU	CA-CB-CG	5.25	127.37	115.30
6	E	92	LEU	CA-CB-CG	5.19	127.24	115.30
1	O	320	LEU	CA-CB-CG	5.17	127.18	115.30
8	C	74	ASP	CB-CG-OD1	5.17	122.95	118.30
5	I	54	DA	O4'-C1'-N9	5.08	111.55	108.00
5	I	54	DA	C1'-O4'-C4'	-5.07	105.03	110.10
6	E	63	ARG	NE-CZ-NH1	5.04	122.82	120.30
5	I	119	DT	O4'-C4'-C3'	-5.03	102.49	104.50
5	J	210	DT	O4'-C4'-C3'	-5.02	102.49	104.50

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	41	TYR	Peptide
7	B	23	ARG	Peptide
9	D	51	THR	Peptide
6	E	60	LEU	Peptide
7	F	35	ARG	Peptide
7	F	45	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	G	38	HIS	Peptide
8	G	59	TYR	Peptide
8	G	76	LYS	Peptide
9	H	106	PRO	Peptide
1	K	185	TYR	Peptide
1	K	194	PHE	Peptide
1	K	260	ASP	Peptide
1	K	269	ASP	Peptide
1	K	279	ARG	Peptide
1	K	305	ILE	Peptide
1	K	390	THR	Peptide
1	K	391	LEU	Peptide
1	O	266	TYR	Peptide
1	O	295	GLU	Peptide
1	O	299	GLY	Peptide
1	O	330	LYS	Peptide
1	O	331	GLU	Peptide
1	O	361	LEU	Peptide
1	O	391	LEU	Peptide

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	K	2304	0	2288	101	0
1	O	2380	0	2369	90	0
2	M	1485	0	1438	51	0
2	Q	1777	0	1710	66	0
3	N	576	0	609	12	0
3	R	813	0	847	35	0
4	P	283	0	258	4	0
5	I	2990	0	1651	34	0
5	J	2990	0	1651	40	0
6	A	801	0	851	44	0
6	E	801	0	851	41	0
7	B	679	0	729	34	0
7	F	649	0	696	32	0
8	C	750	0	796	42	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	G	829	0	898	45	0
9	D	726	0	748	29	0
9	H	746	0	766	32	0
All	All	21579	0	19156	622	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 15.

All (622) 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:K:170:ILE:HB	1:K:177:ILE:O	1.65	0.96
8:G:79:ARG:HG3	9:H:57:ILE:HA	1.67	0.77
6:A:131:ARG:HG2	6:A:133:GLU:H	1.56	0.71
7:F:32:PRO:O	7:F:36:ARG:NH1	2.24	0.70
1:K:428:ARG:NH2	2:M:147:TYR:OH	2.25	0.70
1:O:228:ILE:HG13	1:O:428:ARG:HD2	1.73	0.69
2:M:199:ALA:O	2:M:203:ARG:HB2	1.93	0.69
1:O:316:TYR:O	1:O:320:LEU:HB2	1.94	0.68
2:M:279:TRP:HA	2:M:282:ARG:HD3	1.75	0.68
8:C:40:THR:O	8:C:42:ARG:NH1	2.26	0.68
6:A:83:ARG:HH11	7:B:80:THR:HB	1.59	0.67
8:G:80:ILE:H	8:G:83:ARG:HD3	1.60	0.67
1:O:234:VAL:HA	1:O:278:ARG:HH21	1.58	0.67
5:J:238:DT:OP2	6:A:63:ARG:NH2	2.28	0.67
1:O:301:ASN:H	1:O:336:SER:H	1.43	0.67
6:A:116:ARG:HH11	6:A:117:VAL:H	1.41	0.66
1:O:280:ASP:HB2	1:O:283:GLY:H	1.60	0.66
1:O:326:GLU:O	1:O:330:LYS:HB2	1.95	0.66
8:G:67:LEU:O	8:G:83:ARG:NH2	2.29	0.65
1:K:396:TYR:HB3	1:K:403:ILE:HB	1.78	0.65
5:I:51:DA:OP1	6:A:72:ARG:NH2	2.29	0.65
9:H:40:TYR:HE2	9:H:70:ASN:HB3	1.62	0.65
9:H:36:ARG:NH2	9:H:37:LYS:O	2.30	0.65
1:O:231:ASP:O	1:O:279:ARG:NH2	2.30	0.64
6:A:62:ILE:HG22	6:A:93:GLN:HE21	1.62	0.64
2:M:157:CYS:SG	2:M:158:CYS:N	2.70	0.64
1:K:168:ASN:ND2	1:K:192:GLU:O	2.28	0.64
3:N:105:GLU:HA	3:N:108:ILE:HD12	1.78	0.64
1:O:421:ARG:HG2	1:O:422:ARG:HG3	1.80	0.64
6:A:130:LEU:O	6:E:131:ARG:NH2	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:70:LYS:HD2	3:R:71:GLU:HB2	1.80	0.64
1:O:170:ILE:HB	1:O:177:ILE:HB	1.79	0.64
1:O:347:LEU:HA	1:O:350:ARG:HD2	1.80	0.64
2:Q:338:HIS:NE2	3:R:105:GLU:OE2	2.31	0.63
8:C:27:PRO:O	8:C:30:ARG:NH1	2.31	0.63
8:G:30:ARG:NH1	9:H:38:GLU:OE2	2.31	0.63
1:K:242:ARG:NH2	1:K:269:ASP:O	2.31	0.63
1:K:412:ARG:NH1	1:K:415:ARG:O	2.32	0.63
1:O:427:ASN:O	1:O:428:ARG:NH1	2.31	0.63
7:F:28:GLY:O	7:F:55:ARG:NH1	2.31	0.63
1:K:228:ILE:O	1:K:428:ARG:NH1	2.32	0.62
8:G:79:ARG:NH2	9:H:62:MET:SD	2.69	0.62
1:O:428:ARG:NH2	2:Q:147:TYR:OH	2.32	0.62
8:G:54:THR:HG21	9:H:117:GLY:HA2	1.81	0.62
1:K:318:LYS:HE2	1:K:420:LYS:HE3	1.81	0.62
1:O:221:ARG:NH1	2:Q:138:THR:O	2.32	0.62
2:Q:212:GLU:OE2	2:Q:280:ARG:NH2	2.32	0.62
1:O:256:LYS:HZ3	1:O:262:LYS:HG2	1.63	0.62
7:F:33:ALA:O	7:F:37:LEU:N	2.33	0.62
7:F:38:ALA:HB1	7:F:43:VAL:HG21	1.82	0.62
1:O:237:PHE:HB2	1:O:275:CYS:HB3	1.82	0.61
9:H:54:ASP:OD1	9:H:54:ASP:N	2.32	0.61
2:Q:283:LYS:HA	2:Q:286:VAL:HG22	1.81	0.61
2:Q:360:ASN:O	2:Q:364:ASP:HB2	2.00	0.61
1:K:353:TRP:O	1:K:357:LEU:HB2	2.00	0.61
1:O:198:ASP:HB2	1:O:203:GLN:HG3	1.83	0.61
8:C:86:GLN:O	8:C:90:ARG:NH1	2.34	0.61
8:G:33:ARG:HA	8:G:36:LYS:HD3	1.82	0.61
1:K:395:ARG:HH22	1:K:398:LYS:H	1.46	0.61
6:A:63:ARG:HH11	6:A:64:LYS:H	1.46	0.60
1:O:234:VAL:O	1:O:279:ARG:NH2	2.34	0.60
1:O:235:SER:HG	1:O:277:THR:HG1	1.44	0.60
3:N:80:GLN:OE1	3:N:83:GLN:NE2	2.34	0.60
1:K:230:ARG:NH1	1:K:279:ARG:O	2.31	0.60
2:M:276:TYR:O	2:M:280:ARG:NH1	2.33	0.60
8:G:48:LYS:HD2	8:G:51:ILE:HD11	1.83	0.60
8:C:110:PRO:HB3	6:E:55:GLN:HG3	1.82	0.60
8:C:48:LYS:HE2	9:D:94:ALA:HB2	1.83	0.60
8:G:34:TYR:HA	8:G:37:ARG:HG2	1.83	0.60
6:A:117:VAL:HG23	7:B:45:ARG:HG2	1.84	0.60
8:G:70:ASN:HA	8:G:73:LYS:HD3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:342:LYS:HD3	2:Q:345:LYS:HZ1	1.67	0.59
5:I:80:DT:H4'	7:F:45:ARG:HH12	1.66	0.59
7:F:30:THR:OG1	7:F:31:LYS:N	2.32	0.59
4:P:30:ASP:O	4:P:34:GLN:NE2	2.36	0.59
6:A:72:ARG:NH1	6:A:82:LEU:O	2.35	0.59
1:K:214:TYR:HA	1:K:217:LYS:HB3	1.84	0.59
7:B:75:HIS:O	9:D:95:ARG:NH1	2.36	0.59
1:K:255:SER:HB2	1:K:259:LEU:HD22	1.83	0.59
9:D:116:GLU:HB2	9:D:119:ARG:HH21	1.68	0.59
2:Q:214:ILE:O	2:Q:280:ARG:NH2	2.36	0.59
7:B:78:ARG:HH12	7:B:79:LYS:HG3	1.67	0.59
9:D:64:ILE:O	7:F:98:TYR:OH	2.18	0.59
5:I:122:DG:O3'	9:H:36:ARG:NH2	2.31	0.59
1:K:234:VAL:HG12	1:K:278:ARG:HB2	1.85	0.59
1:O:301:ASN:ND2	1:O:333:LYS:O	2.36	0.59
8:G:57:LEU:HA	8:G:60:LEU:HD23	1.85	0.59
2:M:215:LEU:O	2:M:276:TYR:OH	2.20	0.59
1:K:255:SER:O	1:K:259:LEU:N	2.35	0.58
7:B:99:GLY:HA3	9:H:64:ILE:HG22	1.84	0.58
2:Q:195:SER:HA	2:Q:229:MET:HG3	1.84	0.58
5:J:227:DG:O3'	7:B:45:ARG:NH2	2.36	0.58
8:C:33:ARG:HA	8:C:36:LYS:HB2	1.85	0.58
1:O:271:PHE:HB2	1:O:293:GLU:HA	1.83	0.58
4:P:45:SER:O	2:Q:339:GLN:NE2	2.36	0.58
2:Q:342:LYS:HZ3	3:R:101:LEU:HD11	1.69	0.58
1:O:244:GLN:HA	2:Q:153:THR:HG23	1.85	0.58
1:K:301:ASN:H	1:K:335:GLY:HA3	1.68	0.58
1:O:412:ARG:HA	1:O:415:ARG:HE	1.68	0.58
3:N:41:LYS:HE2	3:N:78:LYS:HD2	1.85	0.57
7:B:78:ARG:NH1	7:B:80:THR:OG1	2.34	0.57
6:E:42:LYS:NZ	6:E:43:PRO:O	2.37	0.57
7:F:74:GLU:OE2	9:H:102:ARG:NH1	2.36	0.57
1:O:299:GLY:O	1:O:333:LYS:NZ	2.37	0.57
1:K:279:ARG:NH2	2:M:143:GLU:OE1	2.38	0.57
7:B:29:ILE:O	7:B:55:ARG:NH2	2.37	0.57
1:K:291:SER:OG	1:K:292:LYS:N	2.36	0.57
1:O:329:LYS:O	1:O:332:ASN:ND2	2.37	0.57
3:R:46:GLU:O	3:R:50:HIS:HB2	2.04	0.57
8:C:67:LEU:HG	8:C:83:ARG:HH12	1.70	0.57
8:C:82:PRO:HA	8:C:106:GLY:HA2	1.86	0.57
1:K:244:GLN:OE1	1:K:246:THR:OG1	2.22	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:64:LYS:HA	6:E:67:PHE:CE1	2.40	0.57
1:K:160:GLU:HG3	1:K:161:VAL:HG23	1.87	0.57
5:J:229:DA:H5'	6:A:43:PRO:HA	1.86	0.57
2:M:195:SER:HB2	2:M:264:LEU:HD21	1.86	0.56
8:C:64:VAL:HA	8:C:67:LEU:HD13	1.85	0.56
1:K:212:GLU:HA	1:K:215:ARG:HB2	1.87	0.56
1:K:308:LEU:O	1:K:312:GLN:NE2	2.38	0.56
1:K:386:HIS:O	1:K:390:THR:OG1	2.20	0.56
3:R:41:LYS:NZ	3:R:75:SER:OG	2.37	0.56
8:C:109:LEU:HD22	8:C:110:PRO:HD2	1.87	0.56
8:G:87:LEU:HA	8:G:90:ARG:HG2	1.87	0.56
3:N:13:ASP:OD1	3:N:13:ASP:N	2.38	0.56
8:G:70:ASN:OD1	8:G:83:ARG:NH2	2.38	0.56
1:K:228:ILE:HG12	1:K:428:ARG:HH11	1.71	0.56
1:K:381:THR:HA	1:K:384:ILE:HG12	1.85	0.56
2:M:192:LEU:HD21	2:M:275:ILE:HG13	1.87	0.56
8:G:21:ARG:HG2	9:H:124:TYR:HB2	1.87	0.56
8:G:79:ARG:NH1	9:H:61:SER:OG	2.38	0.56
2:M:231:ASP:HB2	2:M:234:LEU:HB2	1.86	0.56
1:K:240:ASP:HA	1:K:272:LEU:HD22	1.87	0.56
6:E:128:ARG:NH1	6:E:133:GLU:O	2.39	0.56
1:K:278:ARG:NH2	1:K:316:TYR:OH	2.36	0.56
2:M:239:ASN:HB3	2:M:249:PHE:HB2	1.86	0.55
1:O:233:TYR:O	1:O:278:ARG:NE	2.39	0.55
1:O:327:LEU:O	1:O:331:GLU:N	2.37	0.55
2:Q:218:GLU:HA	2:Q:221:LYS:HG2	1.87	0.55
6:A:66:PRO:O	7:B:25:ASN:ND2	2.40	0.55
1:K:383:ASP:OD1	1:K:386:HIS:NE2	2.39	0.55
1:O:228:ILE:O	1:O:428:ARG:NE	2.40	0.55
1:O:229:TYR:HB2	1:O:428:ARG:HE	1.71	0.55
5:I:70:DG:OP1	6:A:116:ARG:NH1	2.40	0.55
1:K:241:GLY:HA2	1:K:244:GLN:HB3	1.87	0.55
8:C:21:ARG:NH1	9:D:124:TYR:O	2.37	0.55
9:H:37:LYS:NZ	9:H:38:GLU:O	2.37	0.55
1:K:372:GLU:O	1:K:375:SER:HB2	2.07	0.55
8:C:96:ASP:OD1	8:C:96:ASP:N	2.39	0.55
6:E:46:VAL:O	6:E:49:ARG:NH1	2.39	0.55
1:O:278:ARG:HG2	1:O:287:VAL:HG21	1.88	0.55
5:J:278:DC:OP1	8:C:77:VAL:N	2.35	0.55
2:M:229:MET:SD	2:M:229:MET:N	2.81	0.54
1:K:177:ILE:HG12	1:K:309:PRO:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:231:ASP:OD1	1:O:234:VAL:N	2.34	0.54
6:E:120:GLN:HE22	6:E:122:LYS:HB3	1.72	0.54
2:Q:149:LYS:HE3	3:R:23:TYR:HE2	1.72	0.54
7:F:92:ARG:O	7:F:92:ARG:NH1	2.40	0.54
1:K:275:CYS:SG	1:K:276:MET:N	2.80	0.54
9:D:39:THR:OG1	9:D:40:TYR:N	2.40	0.54
3:R:103:LYS:O	3:R:107:ASN:HB2	2.08	0.54
6:A:72:ARG:HH12	6:A:83:ARG:HA	1.73	0.54
6:A:120:GLN:HE22	6:A:122:LYS:HB3	1.72	0.54
9:H:61:SER:HA	9:H:64:ILE:HG12	1.90	0.54
1:K:237:PHE:HD2	1:K:275:CYS:HB3	1.72	0.54
2:Q:250:ILE:O	3:R:91:ASN:ND2	2.40	0.54
8:G:89:ILE:HG23	8:G:95:LEU:HD21	1.90	0.54
1:K:301:ASN:OD1	1:K:335:GLY:N	2.41	0.54
1:K:383:ASP:HA	1:K:386:HIS:CE1	2.42	0.54
2:M:162:TYR:HE2	2:M:164:MET:HB2	1.72	0.54
1:O:334:VAL:HA	1:O:378:SER:HA	1.89	0.54
1:K:245:ARG:HA	1:K:248:CYS:HB3	1.89	0.53
3:R:69:ASP:OD1	3:R:73:LYS:NZ	2.37	0.53
8:G:21:ARG:HH12	8:G:28:VAL:HG21	1.73	0.53
1:O:239:ILE:HB	1:O:273:PHE:HB2	1.89	0.53
4:P:32:LEU:O	2:Q:354:ARG:NH2	2.42	0.53
5:I:24:DA:H2''	5:I:25:DC:H2'	1.89	0.53
7:F:36:ARG:O	7:F:39:ARG:HB2	2.07	0.53
6:A:130:LEU:HD22	6:E:130:LEU:HD22	1.91	0.53
8:C:70:ASN:O	8:C:74:ASP:N	2.41	0.53
1:K:181:TYR:OH	1:K:259:LEU:O	2.22	0.53
1:O:236:PHE:HE2	1:O:424:ILE:HG21	1.72	0.53
2:Q:215:LEU:O	2:Q:276:TYR:OH	2.25	0.53
5:J:275:DC:H2''	5:J:276:DT:H2'	1.91	0.53
6:E:126:LEU:HD13	6:E:130:LEU:HD23	1.91	0.53
9:H:66:ASN:HA	9:H:69:VAL:HG22	1.89	0.53
8:C:32:LYS:NZ	8:C:46:GLY:O	2.41	0.53
1:K:214:TYR:O	1:K:218:CYS:N	2.42	0.53
5:I:54:DA:H2''	5:I:55:DA:C8	2.44	0.53
7:B:32:PRO:HA	7:B:35:ARG:HG2	1.90	0.53
7:F:69:SER:HA	7:F:72:TYR:CE1	2.44	0.53
1:K:221:ARG:HH12	1:K:284:HIS:HD2	1.57	0.53
1:O:410:LEU:HG	1:O:413:TYR:HB3	1.90	0.53
4:P:33:GLN:HA	2:Q:354:ARG:HH12	1.74	0.53
2:Q:356:ASN:HA	2:Q:359:LEU:HG	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:177:DG:OP1	8:G:21:ARG:NH2	2.36	0.53
1:K:374:SER:HB3	1:K:380:THR:HA	1.90	0.53
3:R:5:LEU:O	3:R:9:GLN:NE2	2.41	0.53
8:C:42:ARG:NH2	8:G:40:THR:O	2.42	0.53
2:M:233:ASN:OD1	2:M:233:ASN:N	2.42	0.52
8:C:42:ARG:NH1	8:G:39:ALA:O	2.35	0.52
5:J:264:DT:H2''	5:J:265:DT:C5	2.45	0.52
1:O:345:GLY:O	1:O:349:TYR:N	2.42	0.52
1:O:361:LEU:HD22	1:O:373:ILE:HG21	1.91	0.52
1:O:377:THR:HB	1:O:379:MET:HG3	1.91	0.52
6:A:61:LEU:HD13	7:B:37:LEU:HB3	1.90	0.52
6:E:60:LEU:HD21	6:E:93:GLN:HE21	1.74	0.52
1:K:229:TYR:O	1:K:236:PHE:N	2.33	0.52
3:R:103:LYS:HA	3:R:106:LYS:HG2	1.90	0.52
1:K:213:ARG:O	1:K:217:LYS:HB2	2.09	0.52
2:M:172:LEU:HD11	2:M:184:LEU:HB3	1.91	0.52
8:C:59:TYR:HE2	9:D:69:VAL:HG12	1.73	0.52
8:G:43:THR:O	8:G:44:ARG:NH1	2.36	0.52
3:N:34:LYS:HG3	3:N:82:LEU:HD21	1.91	0.52
2:Q:341:LEU:HD11	3:R:101:LEU:HD13	1.90	0.52
5:I:91:DT:O5'	6:E:63:ARG:NH2	2.40	0.52
2:M:198:HIS:O	2:M:201:HIS:ND1	2.37	0.52
3:N:94:LEU:HD13	3:N:97:ILE:HD12	1.92	0.52
5:I:120:DT:O4	5:J:172:DC:N4	2.42	0.52
1:K:202:LEU:O	1:K:250:ASN:ND2	2.40	0.52
6:A:55:GLN:HA	7:B:40:ARG:HH21	1.74	0.52
1:K:232:ASP:OD1	1:K:422:ARG:NH2	2.37	0.52
2:M:171:PHE:O	2:M:175:GLN:NE2	2.35	0.52
1:O:223:PRO:HD2	1:O:284:HIS:HB2	1.92	0.52
5:I:100:DG:H3'	7:F:79:LYS:HZ2	1.75	0.52
1:O:233:TYR:OH	1:O:421:ARG:NH2	2.42	0.51
2:Q:244:SER:O	2:Q:247:THR:OG1	2.25	0.51
3:R:85:GLU:HA	3:R:88:VAL:HG12	1.92	0.51
5:I:14:DT:H2''	5:I:15:DG:C8	2.45	0.51
1:K:358:ILE:HA	1:K:361:LEU:HD23	1.91	0.51
8:G:22:ALA:HB2	9:H:124:TYR:HB3	1.91	0.51
1:K:165:ARG:NH1	1:K:167:LEU:O	2.43	0.51
1:K:235:SER:OG	1:K:277:THR:OG1	2.28	0.51
8:C:17:SER:O	8:C:21:ARG:N	2.35	0.51
1:O:316:TYR:O	1:O:320:LEU:CB	2.58	0.51
6:A:85:GLN:OE1	7:B:83:SER:OG	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:130:LEU:HD13	6:E:130:LEU:HB2	1.92	0.51
7:B:23:ARG:HG3	7:B:24:ASP:H	1.76	0.51
2:M:244:SER:OG	2:M:247:THR:O	2.29	0.51
1:O:383:ASP:O	1:O:386:HIS:ND1	2.44	0.51
2:Q:267:LEU:HD23	2:Q:270:LYS:HD3	1.91	0.51
3:R:6:VAL:HG11	3:R:107:ASN:HD21	1.75	0.51
1:K:230:ARG:NH2	1:K:233:TYR:O	2.44	0.51
7:F:33:ALA:HA	7:F:36:ARG:HH11	1.76	0.51
2:Q:235:ARG:NH1	2:Q:236:ASN:OD1	2.44	0.51
7:B:36:ARG:O	7:B:39:ARG:NH1	2.44	0.51
5:J:175:DA:H2''	5:J:176:DA:C5	2.45	0.51
7:B:72:TYR:OH	7:B:85:ASP:O	2.16	0.51
2:M:272:GLY:HA2	2:M:275:ILE:HB	1.93	0.51
9:H:121:VAL:O	9:H:125:SER:CB	2.59	0.51
1:O:230:ARG:HE	1:O:279:ARG:HE	1.60	0.51
2:Q:193:CYS:HB2	2:Q:279:TRP:CD2	2.45	0.51
2:Q:203:ARG:NH2	2:Q:219:GLU:OE1	2.44	0.51
9:D:99:THR:HA	9:D:102:ARG:HG2	1.91	0.51
2:Q:234:LEU:HD22	2:Q:237:GLN:HB3	1.91	0.50
6:A:54:PHE:HB2	7:B:40:ARG:HE	1.76	0.50
9:D:100:ALA:HA	9:D:103:LEU:HD22	1.93	0.50
9:D:105:LEU:HD12	9:D:109:LEU:HG	1.94	0.50
1:O:245:ARG:HH11	1:O:249:ARG:HG2	1.76	0.50
2:Q:162:TYR:OH	2:Q:193:CYS:SG	2.61	0.50
8:C:89:ILE:HD13	8:C:95:LEU:HD21	1.94	0.50
8:C:103:ILE:HD13	8:C:106:GLY:H	1.75	0.50
2:M:167:ARG:NE	2:M:282:ARG:HE	2.10	0.50
7:B:72:TYR:HA	9:D:102:ARG:HH22	1.77	0.50
6:E:62:ILE:HD11	6:E:93:GLN:HG3	1.92	0.50
8:G:64:VAL:HA	8:G:67:LEU:HD13	1.93	0.50
1:O:330:LYS:HG2	1:O:426:PRO:HB3	1.94	0.50
5:I:29:DA:O5'	9:D:36:ARG:NH1	2.45	0.50
2:Q:363:ASN:HA	2:Q:366:LEU:HB2	1.94	0.50
5:J:258:DT:O4	5:J:259:DA:N6	2.44	0.50
6:E:42:LYS:HD2	6:E:43:PRO:HD2	1.94	0.50
6:E:63:ARG:HD2	6:E:64:LYS:H	1.77	0.50
2:M:202:GLU:OE2	2:M:203:ARG:NH1	2.45	0.50
2:Q:258:GLN:O	2:Q:261:THR:OG1	2.30	0.50
1:O:173:GLY:O	2:Q:130:TRP:N	2.44	0.49
1:O:272:LEU:HG	1:O:294:LYS:HA	1.93	0.49
3:N:17:LEU:HD21	3:N:96:LEU:HG	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:242:ARG:HH22	3:R:9:GLN:HA	1.76	0.49
5:I:112:DT:OP1	8:G:44:ARG:N	2.43	0.49
5:I:142:DT:O4	5:J:150:DA:N6	2.45	0.49
8:C:60:LEU:HD21	9:D:47:VAL:HG21	1.94	0.49
2:Q:276:TYR:OH	2:Q:280:ARG:NH1	2.46	0.49
8:C:80:ILE:HG23	8:C:82:PRO:HD2	1.93	0.49
1:O:214:TYR:HA	1:O:217:LYS:HG2	1.95	0.49
1:O:328:SER:HA	1:O:331:GLU:HG2	1.93	0.49
1:O:248:CYS:HA	1:O:251:LEU:HB2	1.95	0.49
3:N:7:LEU:HD12	3:N:11:ILE:HD13	1.95	0.49
1:O:209:LYS:NZ	2:Q:166:GLU:OE1	2.45	0.49
5:I:112:DT:H2''	5:I:113:DA:C8	2.47	0.49
6:E:99:TYR:O	6:E:102:SER:OG	2.28	0.49
2:M:239:ASN:N	2:M:239:ASN:OD1	2.43	0.49
5:J:176:DA:OP1	8:G:33:ARG:NH1	2.36	0.49
5:I:86:DT:H2''	5:I:87:DG:N7	2.28	0.49
5:I:93:DT:H2''	5:I:94:DG:H5''	1.93	0.49
5:J:237:DT:H3'	6:A:63:ARG:HH21	1.77	0.49
8:C:24:LEU:HB3	8:C:57:LEU:HD11	1.95	0.49
8:C:79:ARG:HG3	9:D:58:SER:H	1.78	0.49
7:F:75:HIS:HE1	9:H:87:ASN:HD22	1.60	0.49
2:Q:353:LYS:HD3	2:Q:356:ASN:HD21	1.78	0.48
6:E:80:THR:OG1	6:E:81:ASP:N	2.43	0.48
8:G:28:VAL:HG12	8:G:53:LEU:HD11	1.93	0.48
1:O:242:ARG:NH2	3:R:8:GLU:O	2.45	0.48
6:E:51:ILE:HD13	6:E:54:PHE:HZ	1.78	0.48
1:O:275:CYS:HA	1:O:289:TYR:HA	1.96	0.48
1:K:198:ASP:HB2	1:K:202:LEU:H	1.78	0.48
1:O:326:GLU:HA	1:O:329:LYS:HD3	1.95	0.48
2:Q:338:HIS:CD2	2:Q:342:LYS:HE2	2.48	0.48
3:R:100:HIS:HA	3:R:103:LYS:HG2	1.94	0.48
5:J:258:DT:H2'	5:J:259:DA:C8	2.49	0.48
6:A:80:THR:OG1	6:A:81:ASP:N	2.46	0.48
9:D:109:LEU:O	9:D:113:ALA:HB2	2.14	0.48
1:K:245:ARG:NH2	1:K:252:CYS:SG	2.80	0.48
2:M:207:LEU:HB3	2:M:213:SER:HB2	1.95	0.48
8:C:33:ARG:HA	8:C:36:LYS:HE2	1.95	0.48
1:K:370:ILE:O	1:K:374:SER:N	2.47	0.48
3:R:3:PRO:HA	3:R:6:VAL:HG22	1.95	0.48
2:Q:235:ARG:HD3	2:Q:249:PHE:HB2	1.94	0.48
8:C:84:HIS:CE1	9:D:64:ILE:HG21	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:356:THR:HB	1:K:377:THR:HG21	1.96	0.47
1:O:169:ARG:NH2	1:O:193:ASP:OD2	2.41	0.47
6:E:117:VAL:HG13	7:F:45:ARG:HD2	1.96	0.47
6:E:107:THR:HG21	6:E:124:ILE:HG13	1.96	0.47
1:K:259:LEU:HD11	1:K:306:LEU:HD21	1.96	0.47
6:E:101:VAL:HA	6:E:104:PHE:CE1	2.49	0.47
7:F:36:ARG:HA	7:F:39:ARG:HB2	1.95	0.47
1:K:344:LEU:HD13	1:K:348:SER:HB3	1.96	0.47
5:I:81:DG:OP1	7:F:46:ILE:N	2.47	0.47
1:K:413:TYR:HA	1:K:416:LEU:HD23	1.97	0.47
2:Q:246:LYS:NZ	2:Q:355:GLU:OE1	2.39	0.47
2:Q:347:LEU:HD13	2:Q:350:LEU:HD23	1.95	0.47
3:R:11:ILE:HA	3:R:14:VAL:HG22	1.97	0.47
2:M:200:ILE:HB	2:M:204:GLN:HE21	1.79	0.47
8:G:84:HIS:CE1	9:H:61:SER:HB2	2.50	0.47
1:O:211:TYR:HB3	2:Q:136:PHE:HZ	1.79	0.47
1:O:271:PHE:HA	1:O:294:LYS:HB2	1.96	0.47
1:O:276:MET:O	1:O:288:GLY:N	2.48	0.47
1:O:293:GLU:HG3	1:O:297:ALA:HB2	1.95	0.47
2:Q:204:GLN:HG2	2:Q:206:PHE:HD2	1.79	0.47
9:D:47:VAL:HA	9:D:50:GLN:HG3	1.97	0.47
9:D:72:ILE:HA	9:D:75:ARG:HG2	1.97	0.47
3:N:95:PHE:HA	3:N:98:ALA:HB3	1.97	0.47
3:R:75:SER:HA	3:R:78:LYS:HG2	1.96	0.47
7:B:93:GLN:OE1	7:B:95:ARG:NE	2.40	0.47
6:E:70:LEU:HD11	7:F:62:LEU:HD22	1.96	0.47
8:G:20:ALA:O	8:G:23:GLY:N	2.47	0.47
1:O:301:ASN:HB2	1:O:335:GLY:HA3	1.97	0.47
5:J:276:DT:H4'	5:J:277:DG:H5'	1.97	0.47
2:M:243:ASN:O	2:M:246:LYS:NZ	2.36	0.47
1:O:369:THR:HG22	1:O:372:GLU:HG2	1.97	0.47
8:C:74:ASP:OD1	8:C:75:LEU:N	2.48	0.47
6:E:61:LEU:HD12	7:F:37:LEU:HD22	1.95	0.47
7:F:86:VAL:HG22	7:F:90:LEU:HD13	1.97	0.47
1:O:268:VAL:HA	1:O:271:PHE:HE1	1.80	0.46
2:Q:221:LYS:HA	2:Q:224:LEU:HB2	1.97	0.46
6:A:63:ARG:NH1	6:A:64:LYS:H	2.13	0.46
7:B:84:LEU:HA	7:B:87:VAL:HG12	1.96	0.46
1:O:320:LEU:HA	1:O:323:PHE:CZ	2.51	0.46
5:I:83:DA:OP1	6:E:40:ARG:NE	2.48	0.46
9:H:121:VAL:O	9:H:125:SER:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:230:ARG:HH11	1:K:279:ARG:HG3	1.80	0.46
2:M:167:ARG:HG3	2:M:282:ARG:HH21	1.81	0.46
1:O:277:THR:HG22	1:O:286:LEU:HA	1.97	0.46
3:R:16:ASN:O	3:R:19:SER:OG	2.29	0.46
1:K:411:ASP:HB2	1:K:415:ARG:HH22	1.81	0.46
2:M:262:ARG:HB3	2:M:266:GLN:NE2	2.30	0.46
9:D:93:SER:N	9:D:96:GLU:OE2	2.48	0.46
8:G:87:LEU:HA	8:G:90:ARG:HE	1.81	0.46
1:K:369:THR:OG1	1:K:372:GLU:OE1	2.27	0.46
3:R:11:ILE:O	3:R:15:SER:HB3	2.16	0.46
1:K:250:ASN:HA	1:K:253:LEU:HG	1.96	0.46
1:O:304:CYS:N	1:O:338:GLU:OE2	2.47	0.46
2:Q:221:LYS:O	2:Q:225:ILE:N	2.45	0.46
3:R:9:GLN:O	3:R:12:GLN:NE2	2.49	0.46
5:J:179:DG:H1'	5:J:180:DT:H5'	1.98	0.46
6:A:49:ARG:O	6:A:53:ARG:HB2	2.16	0.46
8:C:31:ILE:HA	8:C:34:TYR:HB2	1.98	0.46
2:Q:168:ASP:HA	2:Q:278:TYR:HE2	1.81	0.46
6:A:54:PHE:HE1	7:B:44:LYS:HZ1	1.62	0.46
6:A:89:ILE:HD13	6:A:92:LEU:HD21	1.97	0.46
6:E:69:ARG:HG3	7:F:27:GLN:HG2	1.97	0.46
8:G:58:GLU:O	8:G:61:THR:OG1	2.26	0.46
2:M:274:LYS:HA	2:M:277:ASP:HB2	1.97	0.46
3:R:31:ASN:HD22	3:R:82:LEU:HB3	1.80	0.46
7:B:62:LEU:HA	7:B:65:VAL:HG22	1.98	0.46
7:F:72:TYR:O	7:F:76:ALA:N	2.49	0.46
1:K:279:ARG:HA	1:K:284:HIS:HA	1.98	0.45
5:J:247:DC:OP2	7:B:78:ARG:NH1	2.48	0.45
2:M:286:VAL:HG22	2:M:289:TYR:HB2	1.98	0.45
5:J:263:DT:H6	5:J:263:DT:H2'	1.61	0.45
9:D:99:THR:O	9:D:103:LEU:HB3	2.17	0.45
6:E:109:LEU:HD22	6:E:112:ILE:HD11	1.98	0.45
2:Q:335:ARG:HE	2:Q:338:HIS:CE1	2.35	0.45
6:A:42:LYS:O	6:A:45:THR:OG1	2.27	0.45
1:K:231:ASP:OD2	1:K:422:ARG:NH2	2.50	0.45
3:R:5:LEU:HD22	3:R:9:GLN:HE22	1.81	0.45
8:G:70:ASN:HD21	8:G:87:LEU:HD23	1.81	0.45
1:K:201:THR:HB	1:K:203:GLN:HE22	1.80	0.45
1:K:245:ARG:O	1:K:249:ARG:N	2.47	0.45
1:O:371:ASP:OD1	1:O:381:THR:OG1	2.28	0.45
3:R:7:LEU:HA	3:R:10:THR:HG22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:275:ILE:O	2:M:279:TRP:HB2	2.16	0.45
2:Q:216:SER:OG	2:Q:217:PHE:N	2.49	0.45
2:Q:348:ALA:HA	2:Q:351:VAL:HG22	1.98	0.45
3:N:83:GLN:HA	3:N:86:LYS:HE2	1.99	0.45
1:K:343:ASP:OD1	1:K:343:ASP:N	2.49	0.45
5:I:63:DG:C8	5:I:64:DT:H72	2.52	0.45
1:K:228:ILE:HG12	1:K:428:ARG:HD3	1.99	0.45
1:O:428:ARG:HB3	1:O:431:TRP:HH2	1.81	0.45
5:I:82:DA:OP1	6:E:44:GLY:N	2.50	0.45
9:D:91:THR:OG1	9:D:92:ILE:N	2.50	0.45
1:K:328:SER:HA	1:K:331:GLU:HG2	1.98	0.45
8:C:45:VAL:HG13	8:C:47:SER:H	1.82	0.45
9:D:51:THR:OG1	9:D:52:HIS:O	2.35	0.45
2:M:176:VAL:O	2:M:180:SER:OG	2.30	0.44
2:Q:341:LEU:HD13	3:R:97:ILE:HG23	1.98	0.44
5:I:88:DC:H4'	5:I:89:DC:H5'	1.99	0.44
5:J:260:DC:H2'	5:J:261:DA:C8	2.52	0.44
8:C:79:ARG:HH11	9:D:61:SER:HB2	1.83	0.44
7:F:54:VAL:HA	7:F:57:VAL:HG22	1.99	0.44
8:G:61:THR:HA	8:G:64:VAL:HG22	1.99	0.44
8:G:64:VAL:HA	8:G:67:LEU:HB2	1.99	0.44
1:O:302:VAL:HG11	1:O:325:TYR:HD1	1.82	0.44
2:Q:217:PHE:HZ	2:Q:268:ILE:HG23	1.81	0.44
5:J:165:DA:OP2	9:H:59:GLN:NE2	2.49	0.44
7:F:34:ILE:HA	7:F:37:LEU:HB2	1.98	0.44
2:M:221:LYS:HZ2	2:M:224:LEU:HD12	1.81	0.44
2:Q:224:LEU:HD22	2:Q:268:ILE:HD11	2.00	0.44
6:E:81:ASP:N	6:E:81:ASP:OD1	2.49	0.44
8:G:84:HIS:ND1	9:H:64:ILE:HD11	2.33	0.44
2:M:221:LYS:HA	2:M:224:LEU:HB2	1.99	0.44
7:B:77:LYS:H	9:D:95:ARG:HH12	1.66	0.44
6:E:51:ILE:HA	6:E:54:PHE:CE1	2.52	0.44
1:K:386:HIS:HA	1:K:389:LYS:HG2	1.99	0.44
2:M:211:PRO:HA	2:M:287:ASN:HA	1.99	0.44
9:D:123:LYS:HA	9:D:126:SER:HB3	1.99	0.44
2:M:238:LEU:HB3	2:M:249:PHE:CE1	2.53	0.44
2:M:348:ALA:HA	2:M:351:VAL:HG22	2.00	0.44
2:Q:281:GLU:HA	2:Q:284:ILE:HD12	1.99	0.44
5:I:26:DC:N4	5:J:266:DT:O4	2.51	0.44
5:J:176:DA:P	8:G:33:ARG:HH12	2.40	0.44
6:A:69:ARG:HB2	7:B:25:ASN:HD22	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:411:ASP:OD1	1:K:411:ASP:N	2.49	0.44
1:O:219:THR:OG1	2:Q:253:PHE:O	2.35	0.44
5:I:50:DC:H2'	5:I:51:DA:C8	2.52	0.44
1:K:245:ARG:HE	1:K:248:CYS:HB3	1.83	0.44
2:M:214:ILE:HD11	2:M:220:LEU:HD21	2.00	0.44
6:A:109:LEU:HA	6:A:112:ILE:HG12	2.00	0.44
8:G:24:LEU:HD22	8:G:57:LEU:HD22	2.00	0.44
1:K:229:TYR:HA	2:M:147:TYR:CE1	2.52	0.43
1:O:198:ASP:HB3	1:O:202:LEU:H	1.83	0.43
1:O:219:THR:HA	1:O:221:ARG:HE	1.83	0.43
1:O:374:SER:O	1:O:377:THR:OG1	2.31	0.43
6:A:51:ILE:HA	6:A:54:PHE:CE1	2.53	0.43
7:F:66:ILE:HD13	7:F:66:ILE:HA	1.89	0.43
1:K:242:ARG:NE	1:K:269:ASP:OD2	2.51	0.43
1:K:349:TYR:HA	1:K:352:TYR:CD2	2.53	0.43
2:M:239:ASN:HD22	2:M:248:HIS:CD2	2.37	0.43
1:O:346:LEU:HA	1:O:349:TYR:HD2	1.83	0.43
8:C:53:LEU:HA	8:C:56:VAL:HG22	1.99	0.43
1:K:231:ASP:OD1	1:K:234:VAL:N	2.41	0.43
1:K:256:LYS:HA	1:K:256:LYS:HD3	1.65	0.43
2:M:154:VAL:HA	2:M:157:CYS:HB3	1.99	0.43
2:M:202:GLU:HA	2:M:205:PRO:HB3	2.00	0.43
5:I:66:DC:H2''	5:I:67:DA:C8	2.53	0.43
6:A:71:VAL:HG12	7:B:62:LEU:HD12	2.01	0.43
7:B:24:ASP:N	7:B:24:ASP:OD1	2.51	0.43
8:C:36:LYS:HD3	8:C:44:ARG:HD3	1.99	0.43
2:Q:214:ILE:HG21	2:Q:283:LYS:HD3	2.00	0.43
1:K:168:ASN:ND2	1:K:189:LEU:O	2.52	0.43
3:R:46:GLU:O	3:R:50:HIS:CB	2.65	0.43
5:I:53:DC:H2'	5:I:54:DA:C8	2.54	0.43
5:I:77:DC:H2''	5:I:78:DG:N7	2.33	0.43
1:K:349:TYR:HD1	1:K:352:TYR:HD2	1.66	0.43
1:O:221:ARG:HH11	1:O:282:LEU:HD12	1.84	0.43
1:O:226:ASN:OD1	2:Q:151:SER:OG	2.37	0.43
5:I:55:DA:H2''	5:I:56:DA:N7	2.34	0.43
5:I:90:DT:H5'	6:E:66:PRO:HD3	2.00	0.43
7:F:51:TYR:O	7:F:55:ARG:HB2	2.18	0.43
1:K:289:TYR:O	1:K:306:LEU:N	2.48	0.43
1:O:196:TYR:HB2	1:O:205:PHE:HZ	1.84	0.43
1:O:271:PHE:HE2	1:O:291:SER:HB3	1.82	0.43
7:B:96:THR:O	8:G:100:ARG:NH1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:51:ILE:HD13	6:E:54:PHE:CZ	2.53	0.43
6:E:84:PHE:HA	7:F:81:VAL:HG12	2.00	0.43
9:H:124:TYR:O	9:H:127:SER:OG	2.34	0.43
1:K:370:ILE:HG13	1:K:403:ILE:HG13	2.01	0.43
2:M:345:LYS:HA	2:M:348:ALA:HB3	2.00	0.43
5:J:186:DG:H1'	5:J:187:DA:H5'	1.99	0.43
8:C:67:LEU:HD12	8:C:87:LEU:HD11	2.00	0.43
1:K:394:LEU:HB3	1:K:396:TYR:CZ	2.54	0.43
2:Q:267:LEU:HA	2:Q:270:LYS:HG2	1.99	0.43
8:C:47:SER:OG	8:C:48:LYS:NZ	2.50	0.43
9:H:42:SER:HA	9:H:45:TYR:CE1	2.54	0.43
9:H:44:ILE:HG21	9:H:65:LEU:HD21	2.01	0.43
9:H:75:ARG:O	9:H:79:GLU:HG3	2.18	0.43
1:K:168:ASN:OD1	1:K:168:ASN:N	2.49	0.42
1:K:263:THR:HB	1:K:265:TYR:HD1	1.83	0.42
5:J:190:DC:H1'	5:J:191:DT:H5'	2.01	0.42
5:J:228:DA:P	7:B:45:ARG:HH21	2.42	0.42
6:A:119:ILE:H	6:A:119:ILE:HG13	1.55	0.42
7:B:73:THR:HG21	7:B:81:VAL:HG12	2.01	0.42
6:E:51:ILE:HA	6:E:54:PHE:CZ	2.54	0.42
2:M:338:HIS:O	2:M:342:LYS:HG2	2.18	0.42
6:E:92:LEU:O	6:E:95:SER:OG	2.26	0.42
8:G:84:HIS:HD2	8:G:87:LEU:HD21	1.83	0.42
1:K:165:ARG:NH2	1:K:168:ASN:O	2.53	0.42
1:K:342:SER:HB3	1:K:345:GLY:HA3	2.00	0.42
3:N:101:LEU:O	3:N:105:GLU:HG2	2.19	0.42
5:I:31:DG:H1'	5:I:32:DT:H5'	2.01	0.42
6:A:130:LEU:HB2	6:E:130:LEU:HD13	2.01	0.42
9:H:52:HIS:HA	9:H:53:PRO:HD3	1.92	0.42
2:Q:256:VAL:O	2:Q:258:GLN:N	2.53	0.42
5:I:134:DG:H1'	5:I:135:DG:H5'	2.01	0.42
8:C:54:THR:HG21	9:D:117:GLY:HA2	2.00	0.42
8:C:61:THR:HA	8:C:64:VAL:HG12	2.01	0.42
1:K:277:THR:HG22	1:K:286:LEU:HA	2.02	0.42
2:M:198:HIS:CE1	2:M:229:MET:HA	2.54	0.42
1:O:174:LYS:NZ	2:Q:134:ASP:OD1	2.48	0.42
7:B:54:VAL:HA	7:B:57:VAL:HG12	2.02	0.42
9:H:47:VAL:HA	9:H:50:GLN:HG3	2.01	0.42
1:K:260:ASP:OD1	1:K:260:ASP:N	2.53	0.42
1:O:213:ARG:HE	1:O:217:LYS:HZ3	1.68	0.42
2:Q:335:ARG:HA	2:Q:338:HIS:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:50:DC:H2'	5:I:51:DA:H8	1.85	0.42
6:E:121:LYS:HD2	6:E:125:LYS:HZ2	1.85	0.42
6:E:130:LEU:HD12	6:E:131:ARG:HG2	2.01	0.42
7:F:69:SER:OG	7:F:70:VAL:N	2.53	0.42
7:F:83:SER:HA	7:F:86:VAL:HG12	2.01	0.42
2:M:351:VAL:HA	2:M:354:ARG:HD2	2.01	0.42
2:Q:338:HIS:O	2:Q:342:LYS:HG2	2.20	0.42
5:J:267:DG:O5'	9:D:43:TYR:OH	2.38	0.42
1:K:200:PHE:HB3	1:K:221:ARG:HA	2.01	0.42
1:K:394:LEU:HD13	1:K:394:LEU:HA	1.83	0.42
2:M:217:PHE:O	2:M:221:LYS:NZ	2.47	0.42
1:O:230:ARG:HH21	1:O:279:ARG:HG3	1.84	0.42
1:O:235:SER:OG	1:O:277:THR:OG1	2.19	0.42
2:Q:192:LEU:HD21	2:Q:272:GLY:HA2	2.02	0.42
3:R:41:LYS:HZ1	3:R:78:LYS:NZ	2.18	0.42
5:J:197:DA:H5'	6:E:83:ARG:HD3	2.01	0.42
5:J:238:DT:H72	6:A:65:LEU:HD21	2.02	0.42
5:J:257:DA:P	8:C:46:GLY:H	2.43	0.42
2:M:229:MET:HB2	2:M:232:PHE:CD1	2.55	0.42
2:M:283:LYS:HE3	2:M:288:GLY:HA2	2.01	0.42
3:R:47:SER:O	3:R:51:LYS:N	2.45	0.42
3:R:101:LEU:HA	3:R:104:LEU:HB3	2.00	0.42
7:B:78:ARG:HG3	7:B:80:THR:H	1.85	0.42
6:E:63:ARG:HH11	6:E:64:LYS:N	2.18	0.42
1:K:318:LYS:HD2	1:K:352:TYR:CE1	2.55	0.41
1:K:350:ARG:HE	1:K:353:TRP:HE1	1.67	0.41
6:A:85:GLN:OE1	6:A:87:SER:OG	2.36	0.41
2:M:250:ILE:HG13	3:N:91:ASN:HD21	1.84	0.41
5:J:148:DT:H2''	5:J:149:DC:C4	2.55	0.41
5:J:288:DT:H2''	5:J:289:DT:C2	2.55	0.41
6:A:118:THR:OG1	6:A:119:ILE:N	2.53	0.41
7:F:88:TYR:HD1	7:F:91:LYS:HZ3	1.68	0.41
1:O:412:ARG:HA	1:O:415:ARG:HB2	2.03	0.41
5:I:139:DA:H2'	5:I:140:DT:H71	2.02	0.41
6:A:99:TYR:OH	6:A:133:GLU:OE2	2.34	0.41
1:K:169:ARG:NH1	1:K:176:GLU:OE1	2.53	0.41
1:K:255:SER:HA	1:K:259:LEU:HD13	2.03	0.41
1:K:271:PHE:HB3	1:K:273:PHE:HE1	1.85	0.41
5:J:234:DC:H6	5:J:234:DC:H2'	1.74	0.41
5:J:269:DT:H2''	5:J:270:DA:C8	2.55	0.41
6:A:109:LEU:HD11	6:E:129:ARG:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:81:THR:HA	8:C:84:HIS:CD2	2.55	0.41
8:C:83:ARG:HE	8:C:83:ARG:HB3	1.67	0.41
7:F:56:ALA:HA	7:F:59:LYS:HG2	2.02	0.41
8:G:77:VAL:HG22	9:H:55:THR:HA	2.02	0.41
1:O:376:MET:SD	1:O:376:MET:N	2.94	0.41
2:Q:238:LEU:O	2:Q:242:ILE:HG12	2.21	0.41
5:J:214:DG:H2''	5:J:215:DC:C6	2.55	0.41
8:C:80:ILE:HG13	8:C:81:THR:H	1.85	0.41
1:K:222:HIS:ND1	1:K:223:PRO:O	2.52	0.41
1:K:293:GLU:HG3	1:K:294:LYS:H	1.84	0.41
1:O:244:GLN:NE2	2:Q:152:ALA:H	2.18	0.41
1:O:259:LEU:HB2	1:O:306:LEU:HD21	2.03	0.41
1:O:288:GLY:HA3	1:O:320:LEU:HD11	2.03	0.41
7:F:55:ARG:HD3	7:F:55:ARG:HA	1.82	0.41
8:G:52:TYR:CZ	9:H:76:ILE:HG12	2.56	0.41
8:G:66:GLU:HG3	8:G:87:LEU:HB2	2.03	0.41
1:K:289:TYR:HB3	1:K:306:LEU:HB2	2.02	0.41
5:I:25:DC:N4	5:J:267:DG:O6	2.54	0.41
5:J:266:DT:H2''	5:J:267:DG:C8	2.55	0.41
6:A:60:LEU:HB2	6:A:93:GLN:HE22	1.85	0.41
6:A:107:THR:HG21	6:A:124:ILE:HG22	2.03	0.41
6:E:63:ARG:HH12	6:E:65:LEU:H	1.69	0.41
2:Q:282:ARG:HA	2:Q:285:GLU:HG3	2.02	0.41
5:J:169:DT:H1'	5:J:170:DA:H5'	2.02	0.41
1:K:196:TYR:CE2	1:K:208:LYS:HD3	2.56	0.41
1:K:212:GLU:HG3	1:K:215:ARG:HD2	2.02	0.41
1:K:371:ASP:HA	1:K:374:SER:HB2	2.01	0.41
1:K:406:ASN:N	1:K:406:ASN:OD1	2.53	0.41
1:O:410:LEU:HB3	1:O:415:ARG:HH22	1.86	0.41
2:Q:193:CYS:HA	2:Q:196:PHE:CD2	2.56	0.41
6:A:72:ARG:O	6:A:76:GLN:HB3	2.21	0.41
6:A:73:GLU:O	6:A:76:GLN:HG2	2.20	0.41
9:D:123:LYS:HE3	9:D:123:LYS:HB3	1.70	0.41
8:G:28:VAL:O	8:G:31:ILE:HG13	2.21	0.41
8:G:79:ARG:NH1	9:H:58:SER:H	2.19	0.41
2:Q:149:LYS:HB3	3:R:23:TYR:CE2	2.56	0.41
5:I:125:DG:H2''	5:I:126:DA:C8	2.56	0.41
3:R:41:LYS:HB3	3:R:41:LYS:HE3	1.87	0.40
3:R:99:ARG:HH21	3:R:102:ASN:HB3	1.86	0.40
5:J:163:DA:H2''	5:J:164:DG:C8	2.56	0.40
6:A:61:LEU:HD12	6:A:62:ILE:HB	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:71:THR:O	9:D:102:ARG:NH2	2.54	0.40
8:G:70:ASN:ND2	8:G:83:ARG:O	2.54	0.40
1:O:300:TYR:OH	1:O:338:GLU:OE2	2.31	0.40
8:C:51:ILE:H	8:C:51:ILE:HG13	1.66	0.40
2:M:262:ARG:HE	2:M:266:GLN:HE22	1.68	0.40
1:O:171:ILE:HG23	2:Q:130:TRP:HE1	1.86	0.40
3:R:85:GLU:H	3:R:85:GLU:HG3	1.77	0.40
5:J:178:DT:H2''	5:J:179:DG:C8	2.56	0.40
7:B:34:ILE:HA	7:B:37:LEU:HG	2.03	0.40
8:G:96:ASP:OD1	8:G:96:ASP:N	2.54	0.40
1:K:248:CYS:HA	1:K:251:LEU:HB2	2.03	0.40
2:M:244:SER:HA	2:M:246:LYS:HD2	2.02	0.40
2:Q:282:ARG:O	2:Q:286:VAL:N	2.49	0.40
2:Q:336:ALA:O	2:Q:339:GLN:NE2	2.55	0.40
9:H:105:LEU:HD13	9:H:109:LEU:HG	2.04	0.40
1:K:363:GLU:OE1	1:K:363:GLU:N	2.46	0.40
1:O:370:ILE:HD11	1:O:403:ILE:HB	2.03	0.40
5:J:281:DG:H2'	5:J:282:DT:C6	2.57	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	K	270/469 (58%)	216 (80%)	53 (20%)	1 (0%)	30	67
1	O	280/469 (60%)	230 (82%)	50 (18%)	0	100	100
2	M	176/586 (30%)	150 (85%)	26 (15%)	0	100	100
2	Q	209/586 (36%)	183 (88%)	26 (12%)	0	100	100
3	N	67/120 (56%)	65 (97%)	2 (3%)	0	100	100
3	R	96/120 (80%)	92 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	30/537 (6%)	29 (97%)	1 (3%)	0	100	100
6	A	95/136 (70%)	85 (90%)	9 (10%)	1 (1%)	12	46
6	E	95/136 (70%)	85 (90%)	10 (10%)	0	100	100
7	B	82/102 (80%)	72 (88%)	10 (12%)	0	100	100
7	F	79/102 (78%)	69 (87%)	10 (13%)	0	100	100
8	C	96/134 (72%)	78 (81%)	18 (19%)	0	100	100
8	G	106/134 (79%)	86 (81%)	20 (19%)	0	100	100
9	D	91/131 (70%)	84 (92%)	7 (8%)	0	100	100
9	H	94/131 (72%)	91 (97%)	3 (3%)	0	100	100
All	All	1866/3893 (48%)	1615 (86%)	249 (13%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	340	PRO
6	A	81	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	254/434 (58%)	243 (96%)	11 (4%)	25	48
1	O	263/434 (61%)	249 (95%)	14 (5%)	19	42
2	M	169/542 (31%)	162 (96%)	7 (4%)	26	49
2	Q	201/542 (37%)	197 (98%)	4 (2%)	50	69
3	N	66/111 (60%)	64 (97%)	2 (3%)	36	57
3	R	94/111 (85%)	92 (98%)	2 (2%)	48	67
4	P	32/442 (7%)	31 (97%)	1 (3%)	35	56
6	A	85/113 (75%)	80 (94%)	5 (6%)	16	39
6	E	85/113 (75%)	80 (94%)	5 (6%)	16	39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	B	72/81 (89%)	66 (92%)	6 (8%)	9	28
7	F	69/81 (85%)	57 (83%)	12 (17%)	1	10
8	C	77/103 (75%)	67 (87%)	10 (13%)	3	16
8	G	86/103 (84%)	74 (86%)	12 (14%)	3	15
9	D	81/109 (74%)	74 (91%)	7 (9%)	8	27
9	H	82/109 (75%)	80 (98%)	2 (2%)	44	64
All	All	1716/3428 (50%)	1616 (94%)	100 (6%)	19	39

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	165	ARG
1	K	169	ARG
1	K	221	ARG
1	K	262	LYS
1	K	279	ARG
1	K	313	ARG
1	K	361	LEU
1	K	379	MET
1	K	415	ARG
1	K	421	ARG
1	K	422	ARG
2	M	229	MET
2	M	246	LYS
2	M	258	GLN
2	M	259	MET
2	M	270	LYS
2	M	274	LYS
2	M	353	LYS
3	N	22	ARG
3	N	41	LYS
1	O	213	ARG
1	O	279	ARG
1	O	313	ARG
1	O	329	LYS
1	O	330	LYS
1	O	333	LYS
1	O	346	LEU
1	O	350	ARG
1	O	361	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	376	MET
1	O	384	ILE
1	O	405	LEU
1	O	415	ARG
1	O	421	ARG
4	P	17	LYS
2	Q	149	LYS
2	Q	226	LYS
2	Q	246	LYS
2	Q	347	LEU
3	R	70	LYS
3	R	107	ASN
6	A	49	ARG
6	A	63	ARG
6	A	83	ARG
6	A	109	LEU
6	A	131	ARG
7	B	19	ARG
7	B	36	ARG
7	B	39	ARG
7	B	58	LEU
7	B	62	LEU
7	B	79	LYS
8	C	21	ARG
8	C	30	ARG
8	C	33	ARG
8	C	53	LEU
8	C	60	LEU
8	C	78	LYS
8	C	79	ARG
8	C	85	LEU
8	C	90	ARG
8	C	98	LEU
9	D	44	ILE
9	D	79	GLU
9	D	82	LYS
9	D	98	GLN
9	D	103	LEU
9	D	105	LEU
9	D	111	LYS
6	E	49	ARG
6	E	55	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	E	61	LEU
6	E	62	ILE
6	E	100	LEU
7	F	35	ARG
7	F	36	ARG
7	F	40	ARG
7	F	45	ARG
7	F	58	LEU
7	F	67	ARG
7	F	78	ARG
7	F	91	LYS
7	F	92	ARG
7	F	95	ARG
7	F	96	THR
7	F	97	LEU
8	G	21	ARG
8	G	31	ILE
8	G	34	TYR
8	G	36	LYS
8	G	42	ARG
8	G	48	LYS
8	G	51	ILE
8	G	65	LEU
8	G	79	ARG
8	G	80	ILE
8	G	98	LEU
8	G	114	LYS
9	H	65	LEU
9	H	75	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	203	GLN
2	M	173	ASN
2	M	248	HIS
2	M	338	HIS
3	N	31	ASN
1	O	285	HIS
1	O	332	ASN
4	P	34	GLN
2	Q	339	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	363	ASN
3	R	9	GLN
3	R	31	ASN
3	R	107	ASN
6	A	93	GLN
6	A	113	HIS
6	E	113	HIS
7	F	27	GLN
7	F	75	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.

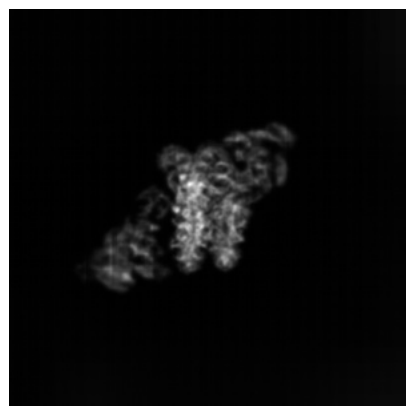
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38024. These allow visual inspection of the internal detail of the map and identification of artifacts.

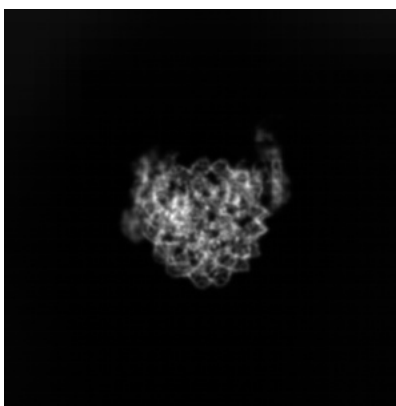
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

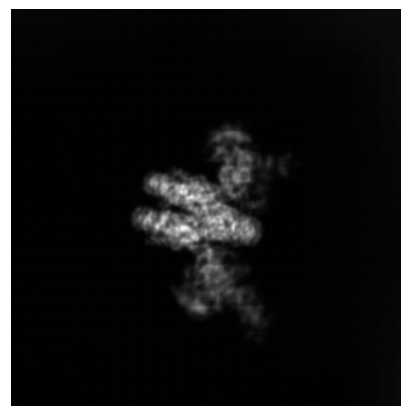
6.1.1 Primary map



X

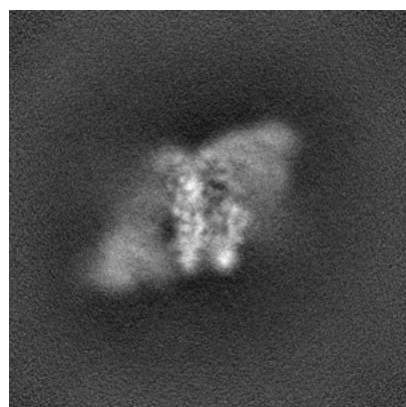


Y

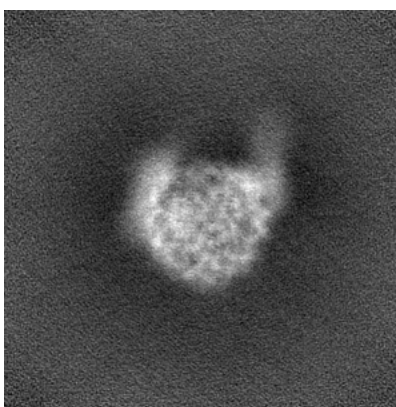


Z

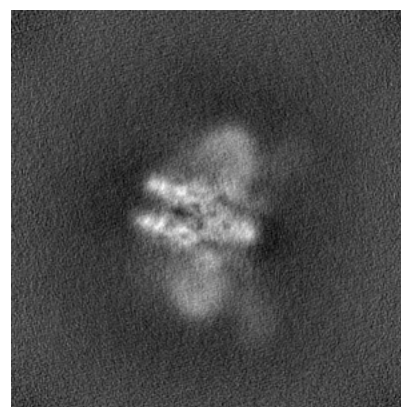
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

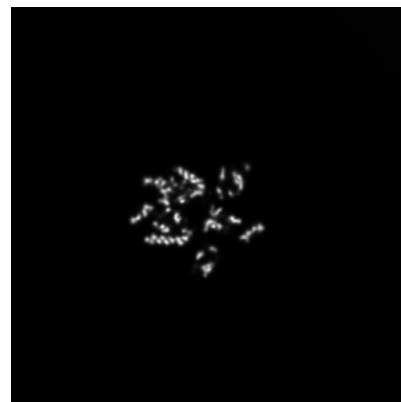
6.2.1 Primary map



X Index: 150

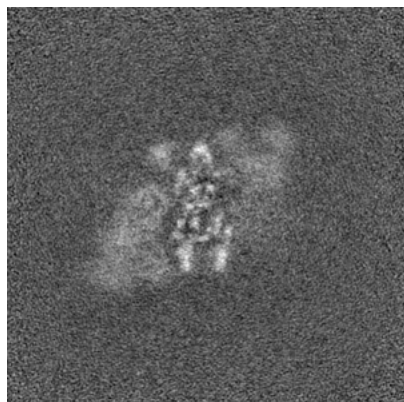


Y Index: 150

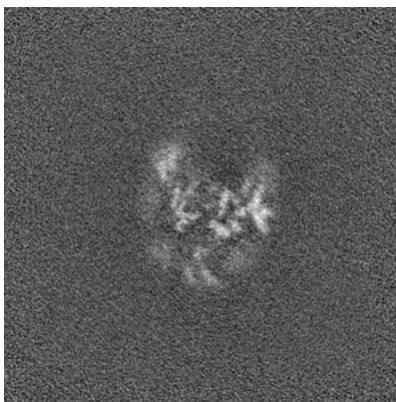


Z Index: 150

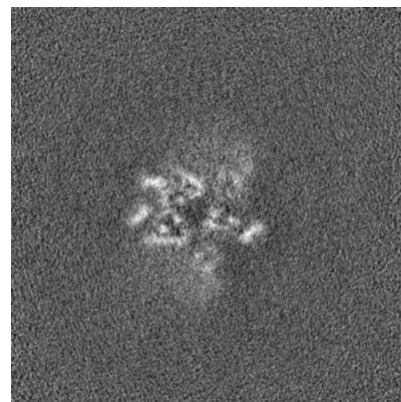
6.2.2 Raw map



X Index: 150



Y Index: 150

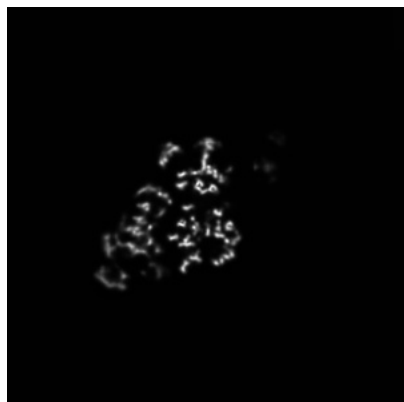


Z Index: 150

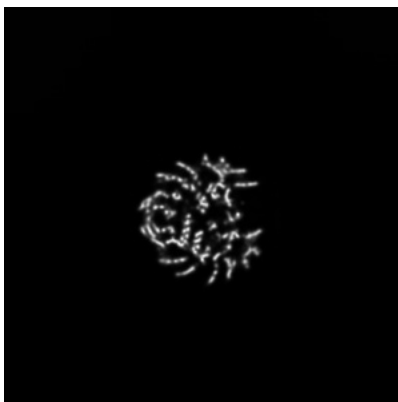
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 146

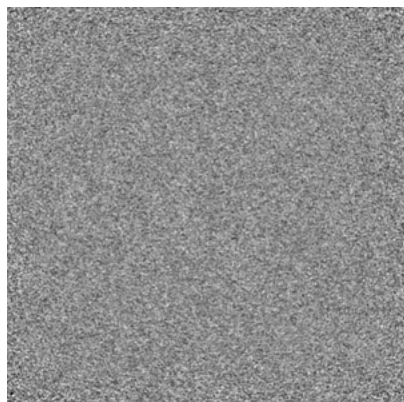


Y Index: 135

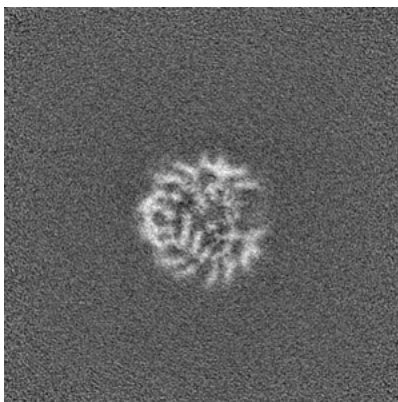


Z Index: 137

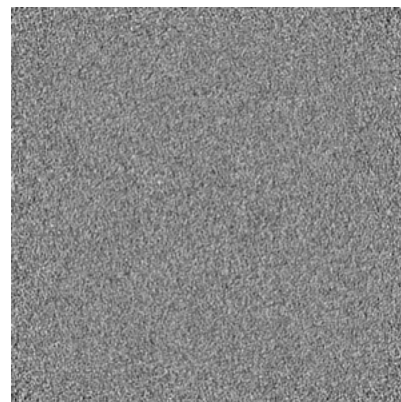
6.3.2 Raw map



X Index: 0



Y Index: 134

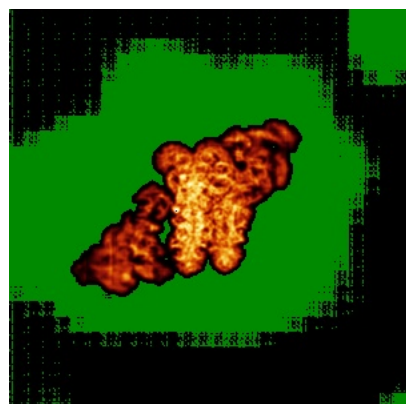


Z Index: 0

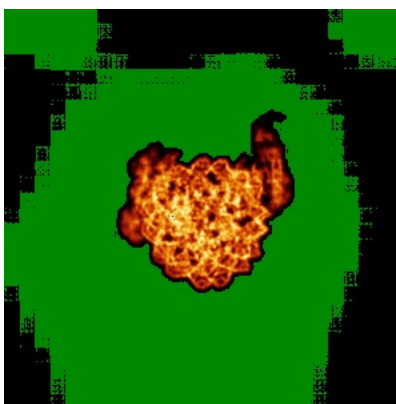
The images above show the largest variance slices of the map in three orthogonal directions.

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

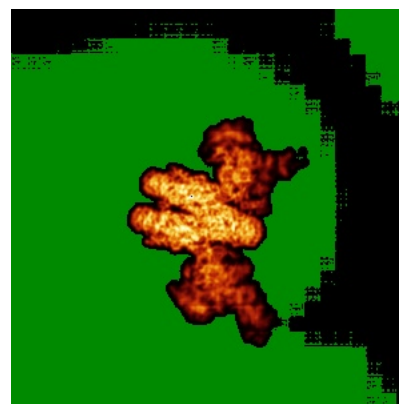
6.4.1 Primary map



X

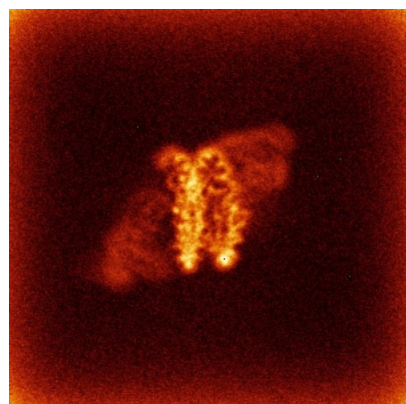


Y

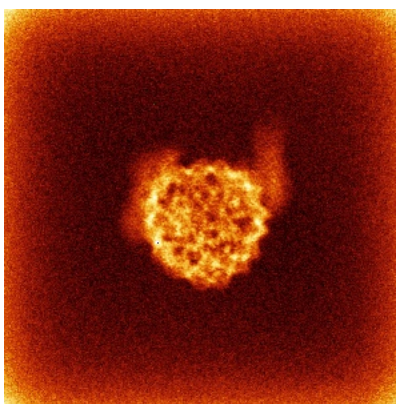


Z

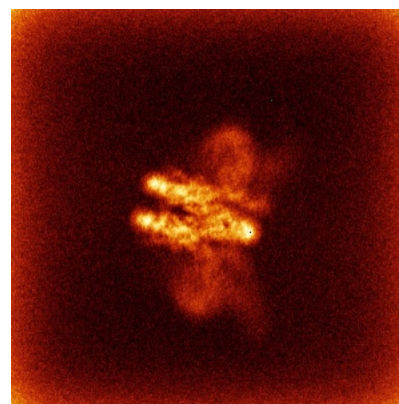
6.4.2 Raw map



X



Y

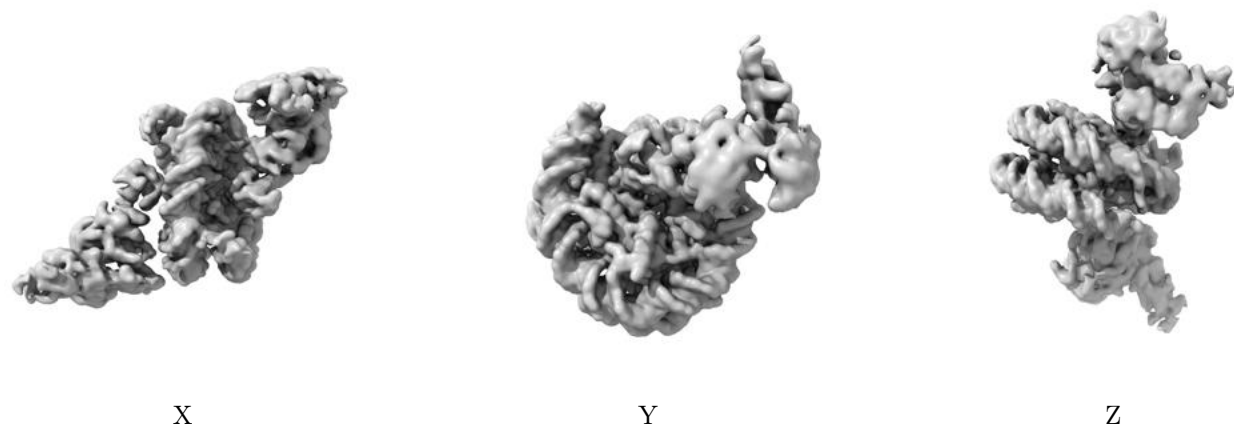


Z

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.

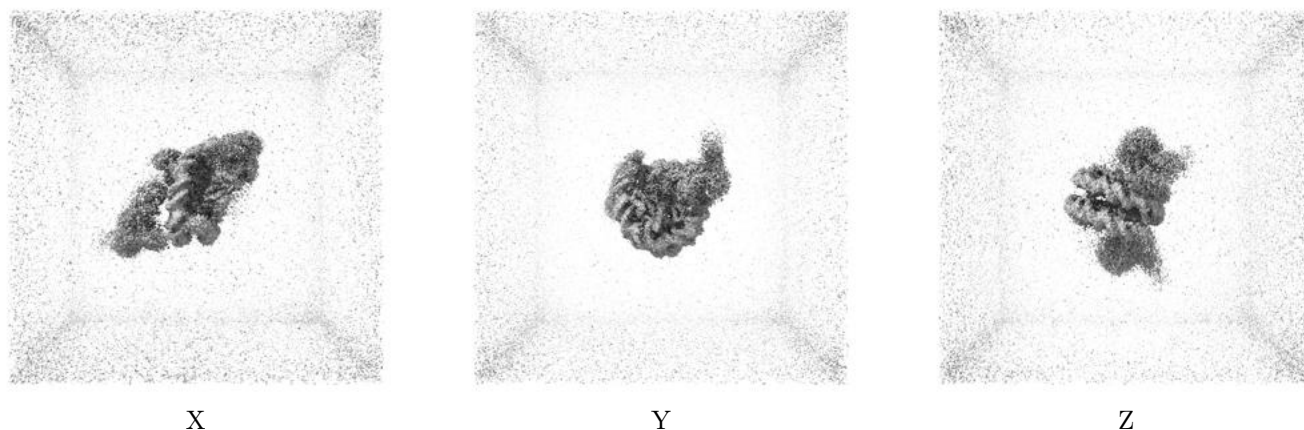
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.905. 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.

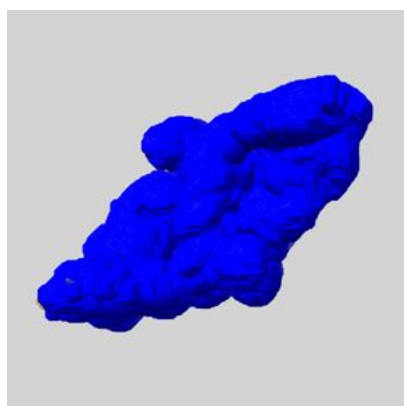
6.6 Mask visualisation [i](#)

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

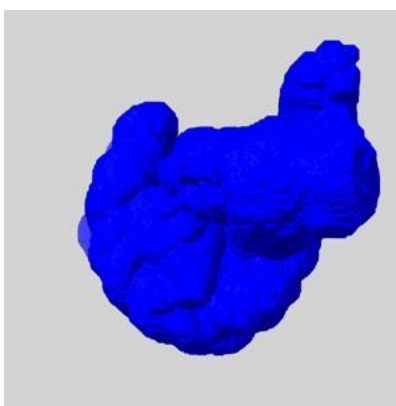
A mask typically either:

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

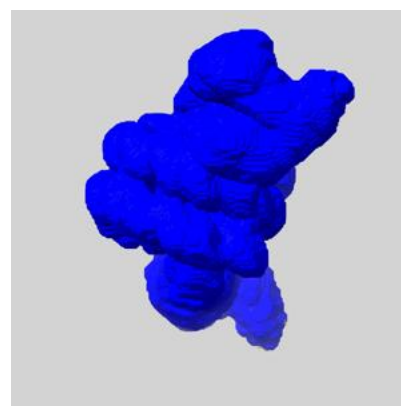
6.6.1 emd_38024_msk_1.map [i](#)



X



Y

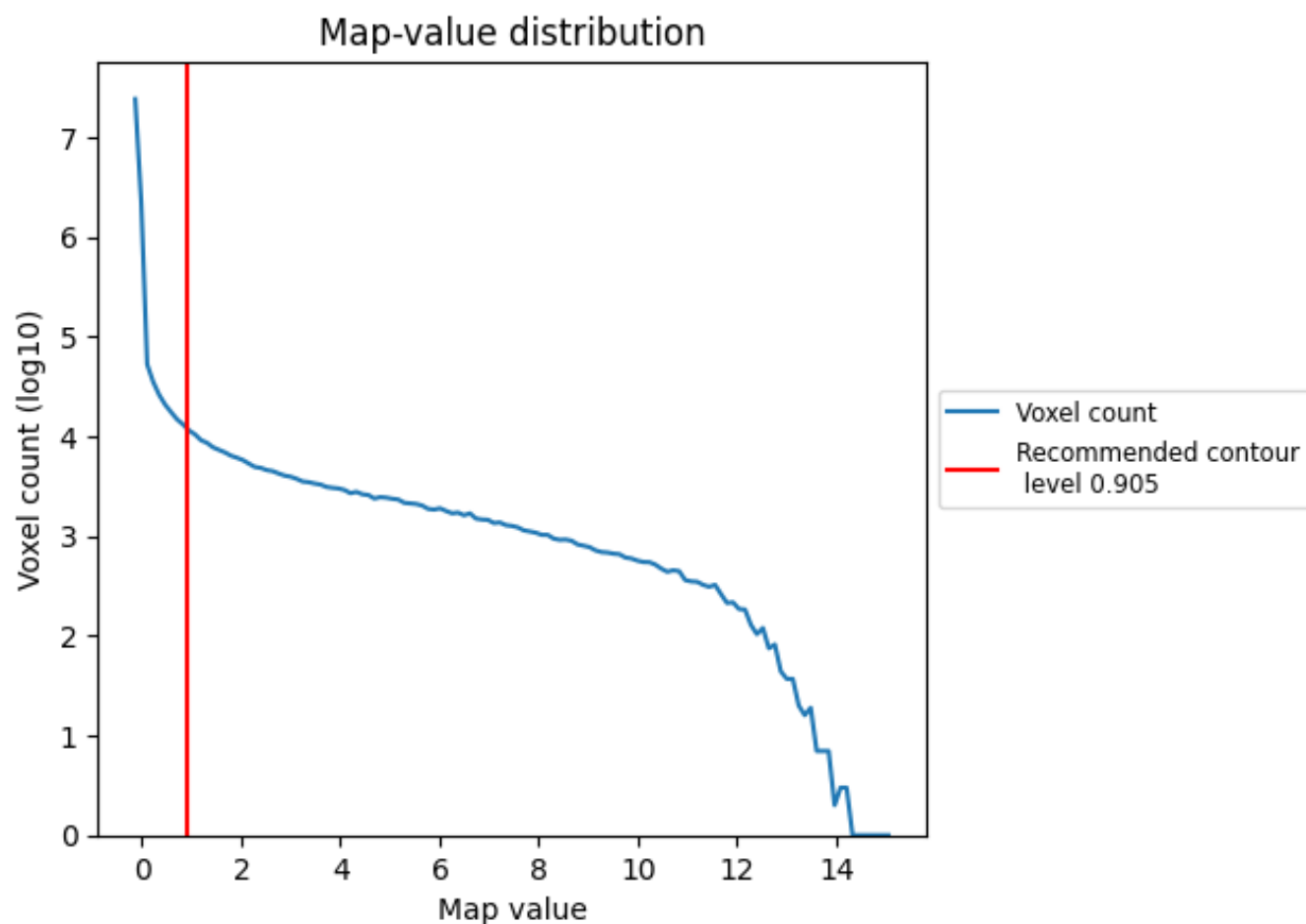


Z

7 Map analysis [i](#)

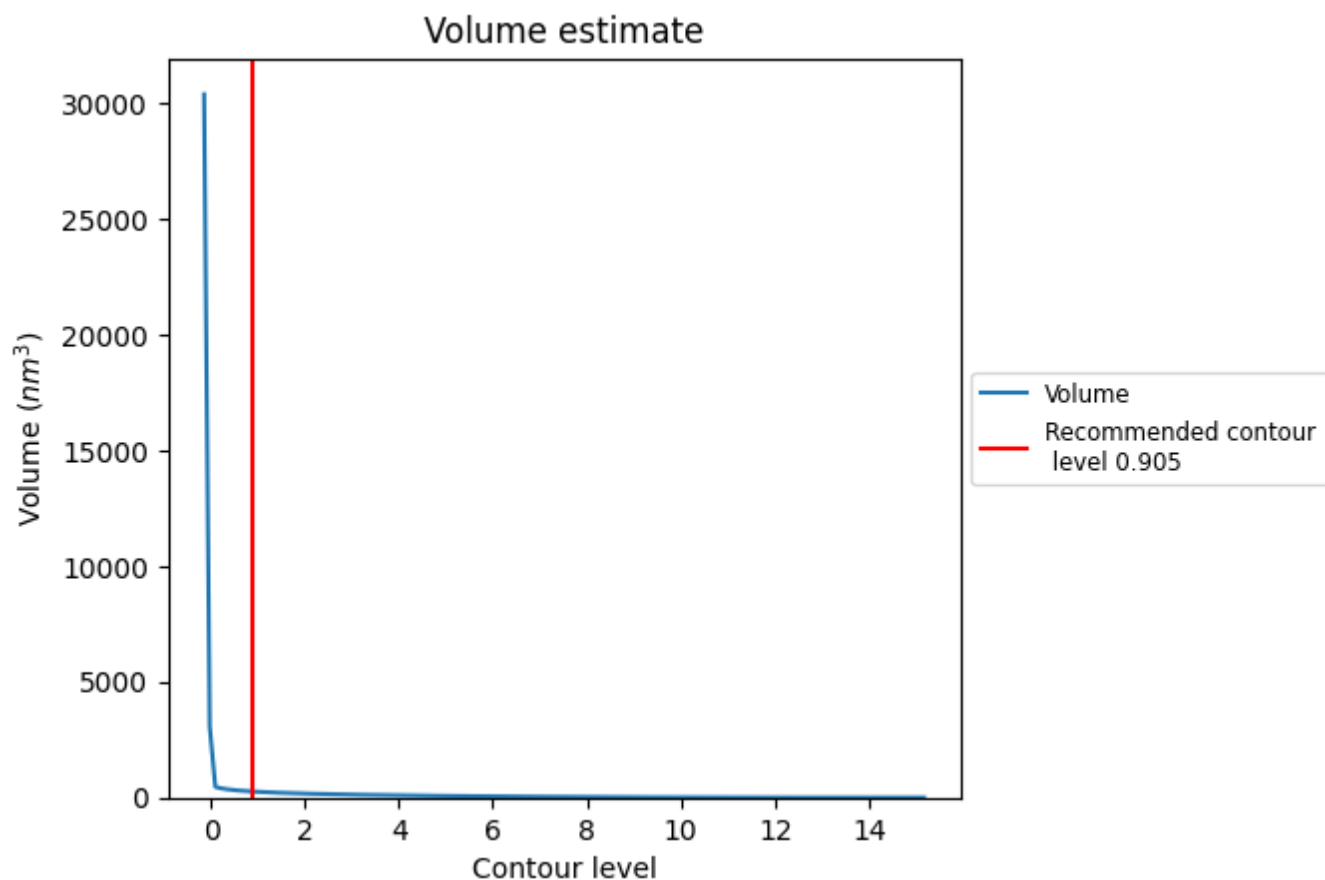
This section contains the results of statistical analysis of the map.

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.

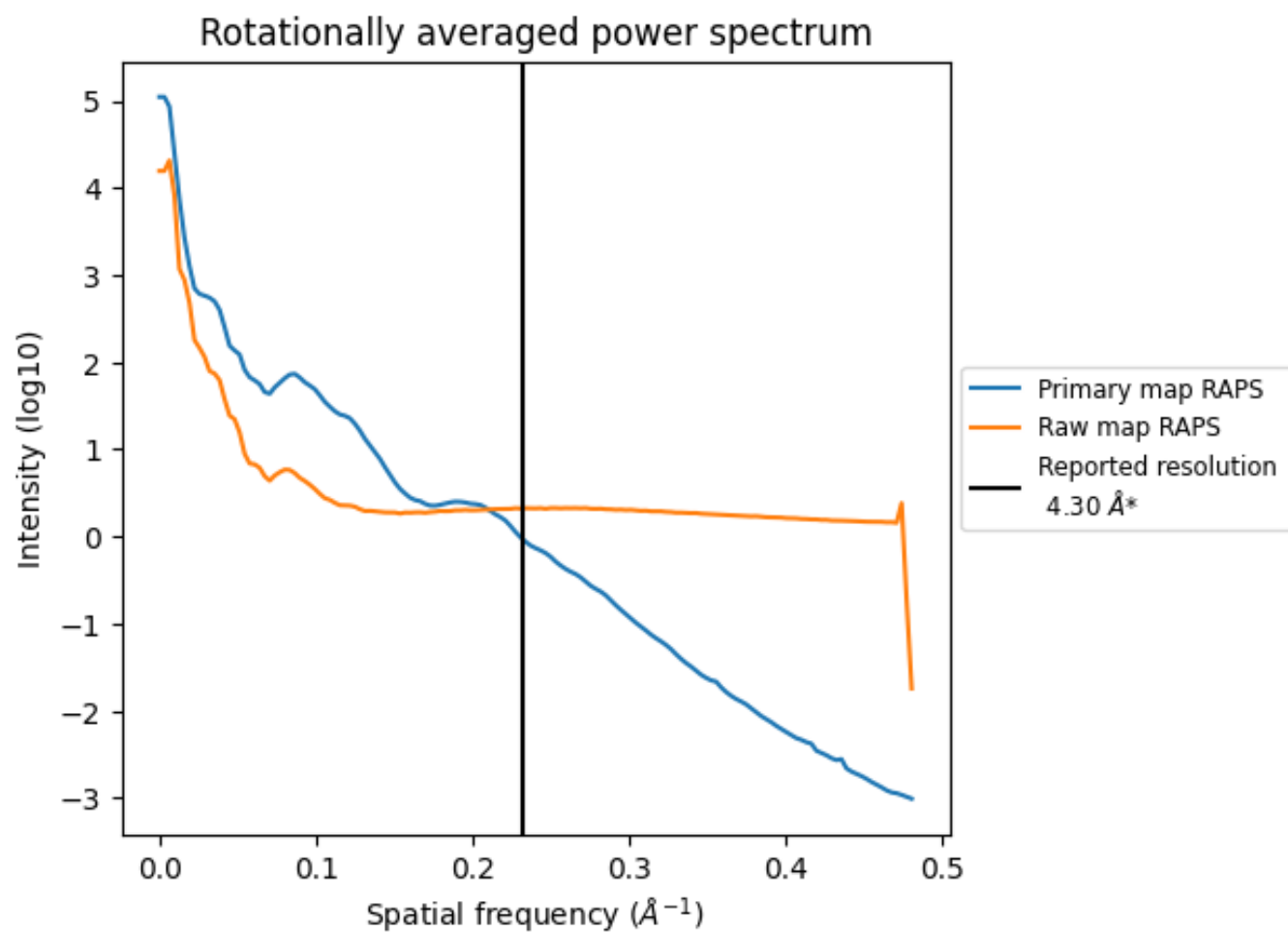
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 260 nm³; this corresponds to an approximate mass of 235 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 ⓘ

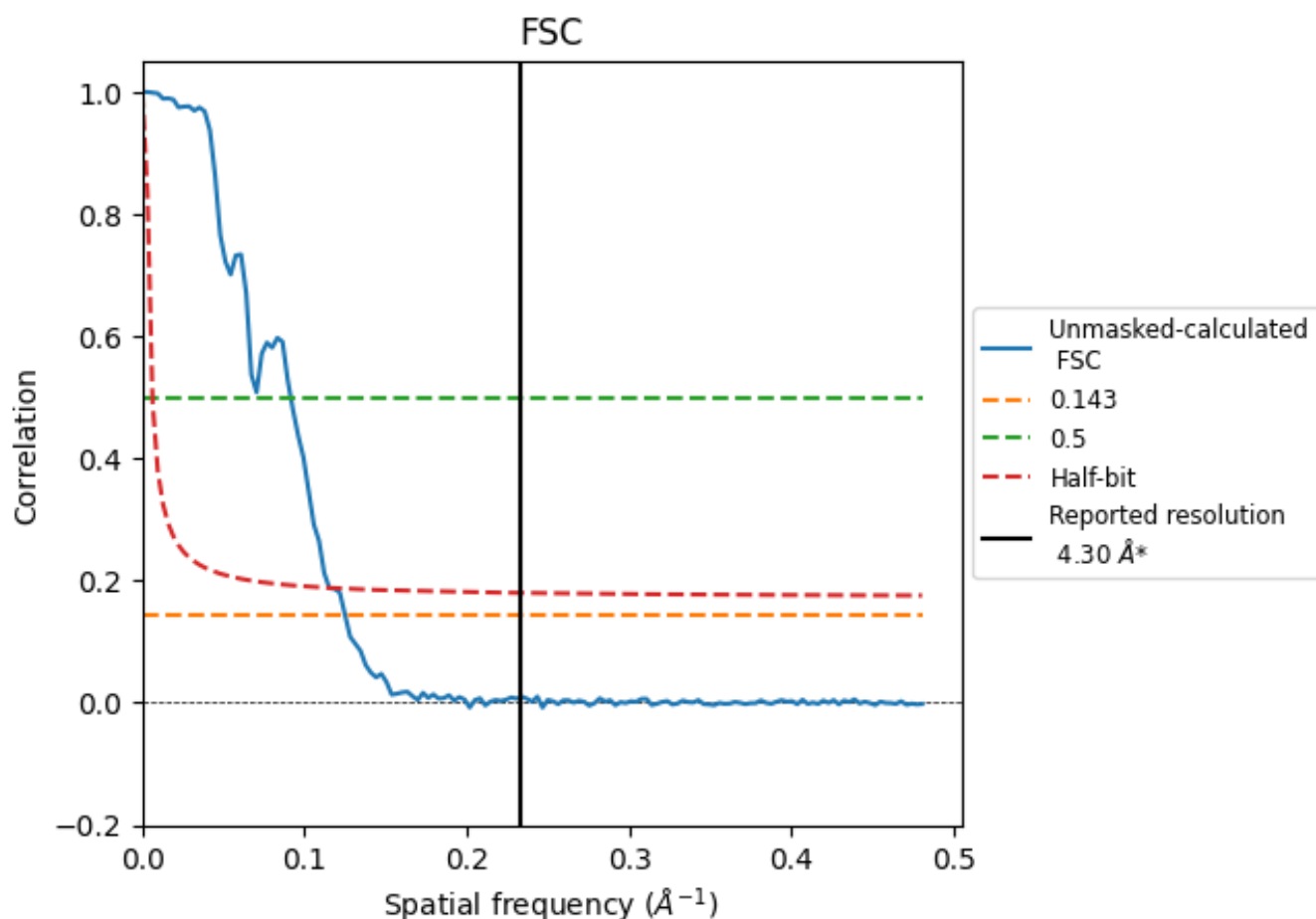


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

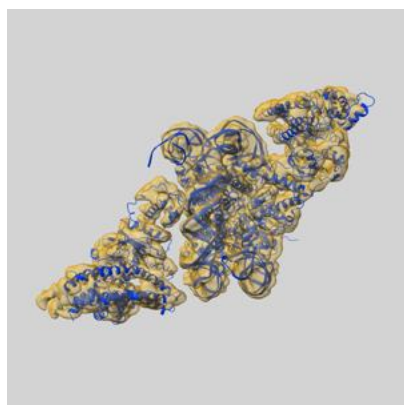
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.00	10.92	8.67

*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 8.00 differs from the reported value 4.3 by more than 10 %

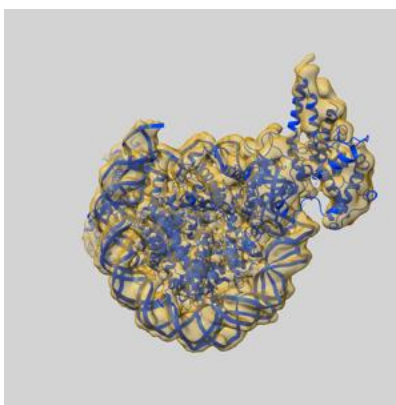
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38024 and PDB model 8X30. Per-residue inclusion information can be found in section [3](#) on page [9](#).

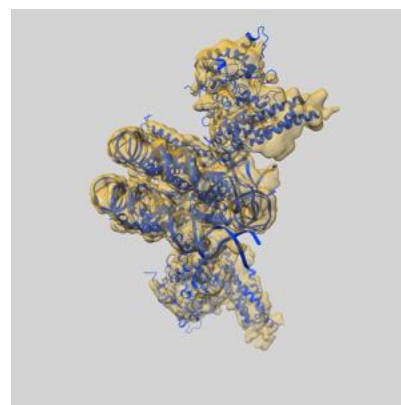
9.1 Map-model overlay [i](#)



X



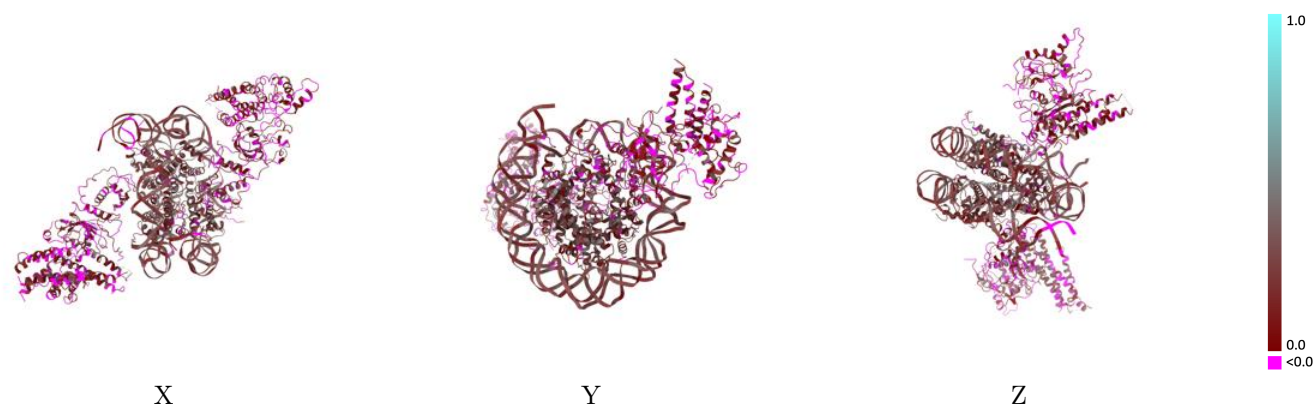
Y



Z

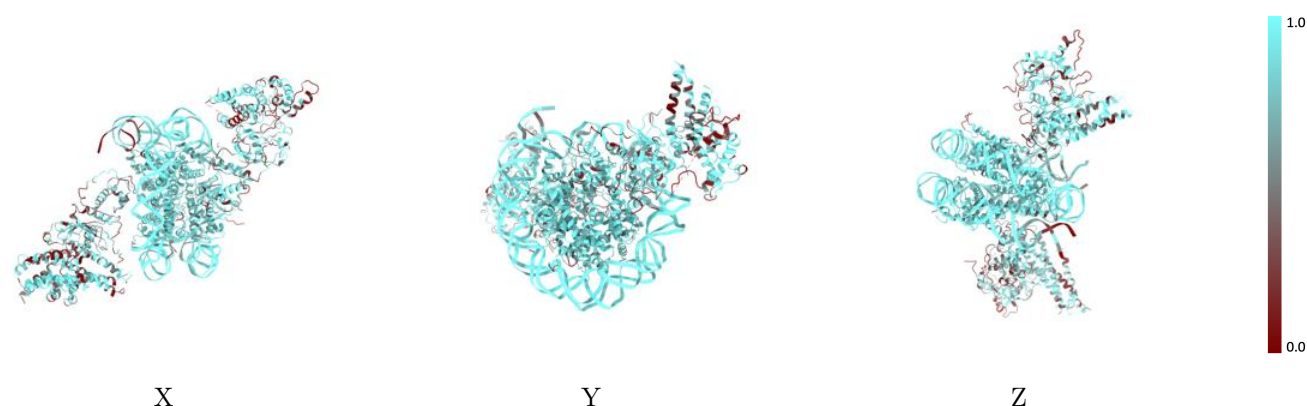
The images above show the 3D surface view of the map at the recommended contour level 0.905 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



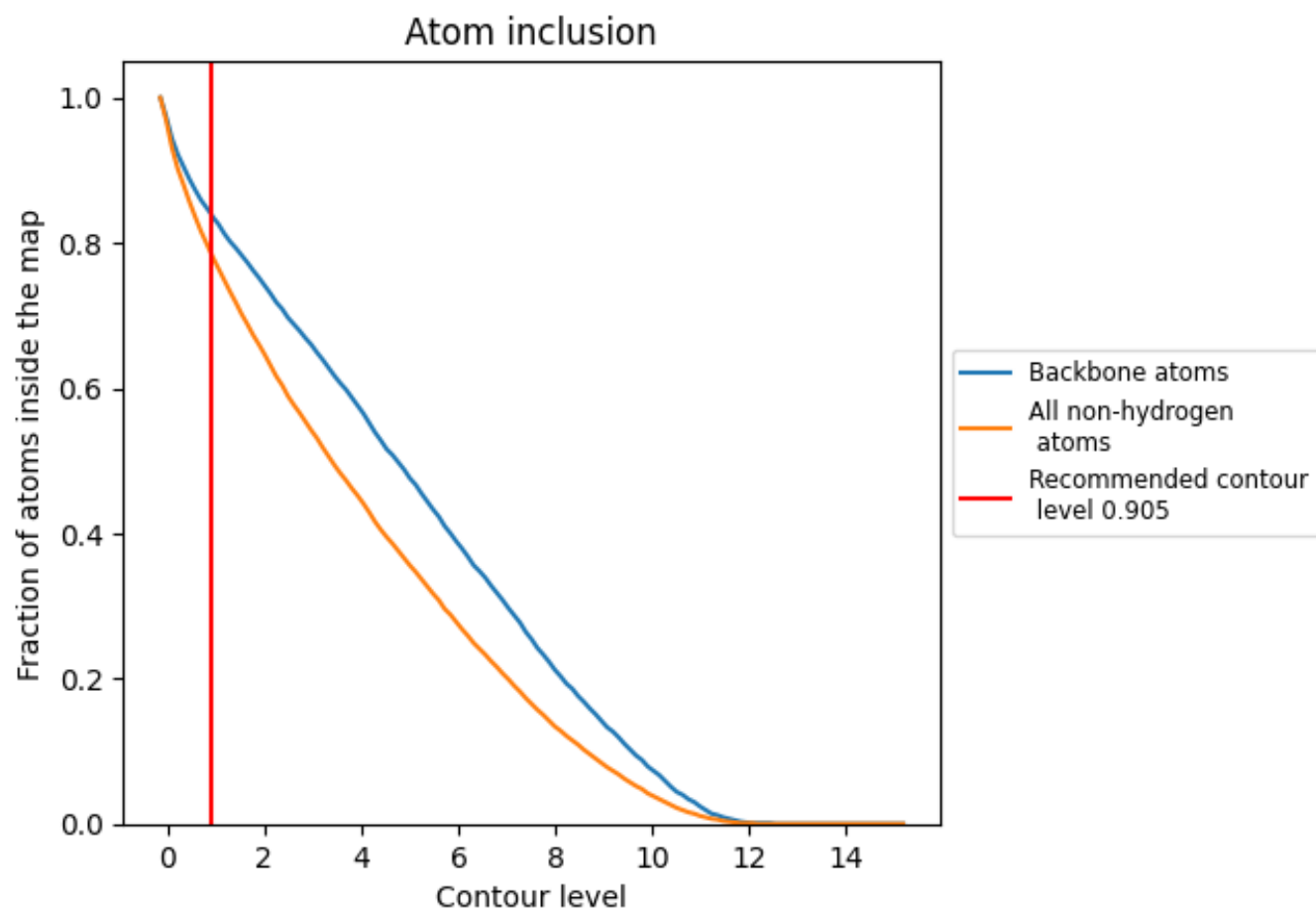
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.905).





































9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.905) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7860	 0.1650
A	 0.8770	 0.2170
B	 0.8920	 0.2430
C	 0.8860	 0.2230
D	 0.8820	 0.2440
E	 0.8510	 0.1990
F	 0.9040	 0.2280
G	 0.8360	 0.1930
H	 0.8740	 0.2400
I	 0.9180	 0.2510
J	 0.9310	 0.2510
K	 0.6680	 0.0820
M	 0.6160	 0.0690
N	 0.6710	 0.0960
O	 0.5900	 0.0720
P	 0.7260	 0.0940
Q	 0.6780	 0.0740
R	 0.6530	 0.0760

