



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2025 – 05:25 PM EDT

PDB ID : 9C9S / pdb\_00009c9s  
EMDB ID : EMD-45369  
Title : S.c INO80 in complex with S.c 0/40 nucleosome, Class 1  
Authors : Wu, H.; Kaur, U.; Narlikar, G.J.; Cheng, Y.F.  
Deposited on : 2024-06-15  
Resolution : 3.09 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.44

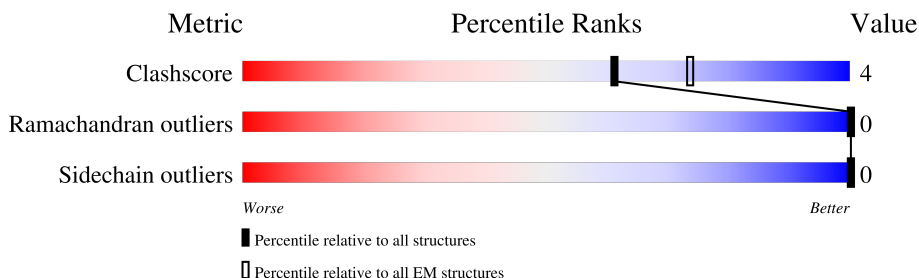
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.09 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.











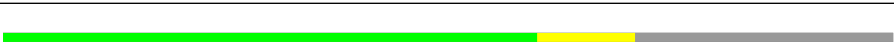

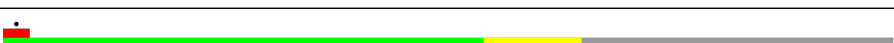

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	Q	1489	
2	R	755	
3	S	166	
4	T	463	
4	V	463	
4	X	463	
5	U	471	
5	W	471	

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Mol	Chain	Length	Quality of chain
5	Y	471	
6	Z	320	
7	A	136	
7	E	136	
8	B	103	
8	F	103	
9	C	132	
9	G	132	
10	D	131	
10	H	131	
11	I	227	
12	J	227	

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 43163 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 Chromatin-remodeling ATPase INO80.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	660	Total	C	N	O	S	0	0
			5277	3372	905	977	23		

- Molecule 2 is a protein called Actin-related protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	550	Total	C	N	O	S	0	0
			4067	2566	705	785	11		

- Molecule 3 is a protein called Chromatin-remodeling complex subunit IES6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	125	Total	C	N	O	S	0	0
			1014	647	189	176	2		

- Molecule 4 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	435	Total	C	N	O	S	0	0
			3339	2107	575	647	10		
4	V	442	Total	C	N	O	S	0	0
			3397	2144	584	659	10		
4	X	443	Total	C	N	O	S	0	0
			3404	2149	585	660	10		

- Molecule 5 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	445	Total	C	N	O	S	0	0
			3421	2138	594	677	12		
5	W	442	Total	C	N	O	S	0	0
			3394	2120	589	673	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	436	Total	C	N	O	S	0	0
			3350	2098	583	658	11		

- Molecule 6 is a protein called Ino eighty subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	52	Total	C	N	O	S	0	0
			367	229	69	67	2		

- Molecule 7 is a protein called Histone H3.

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

- Molecule 8 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	79	Total	C	N	O	S	0	0
			624	392	121	110	1		
8	F	79	Total	C	N	O	S	0	0
			620	389	120	110	1		

- Molecule 9 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	106	Total	C	N	O		0	0
			819	514	161	144			
9	G	108	Total	C	N	O		0	0
			827	517	164	146			

- Molecule 10 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	93	Total	C	N	O	S	0	0
			726	456	127	142	1		
10	H	93	Total	C	N	O	S	0	0
			726	456	127	142	1		

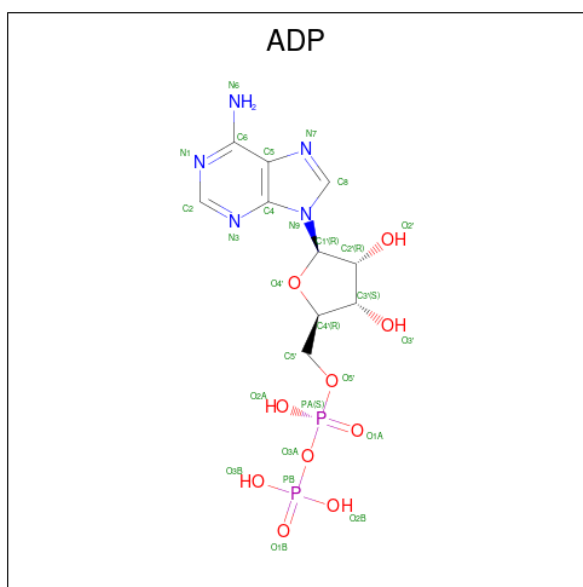
- Molecule 11 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	147	Total	C	N	O	P	0	0
			3030	1434	567	882	147		

- Molecule 12 is a DNA chain called DNA (227-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	147	Total	C	N	O	P	0	0
			2997	1423	545	882	147		

- Molecule 13 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

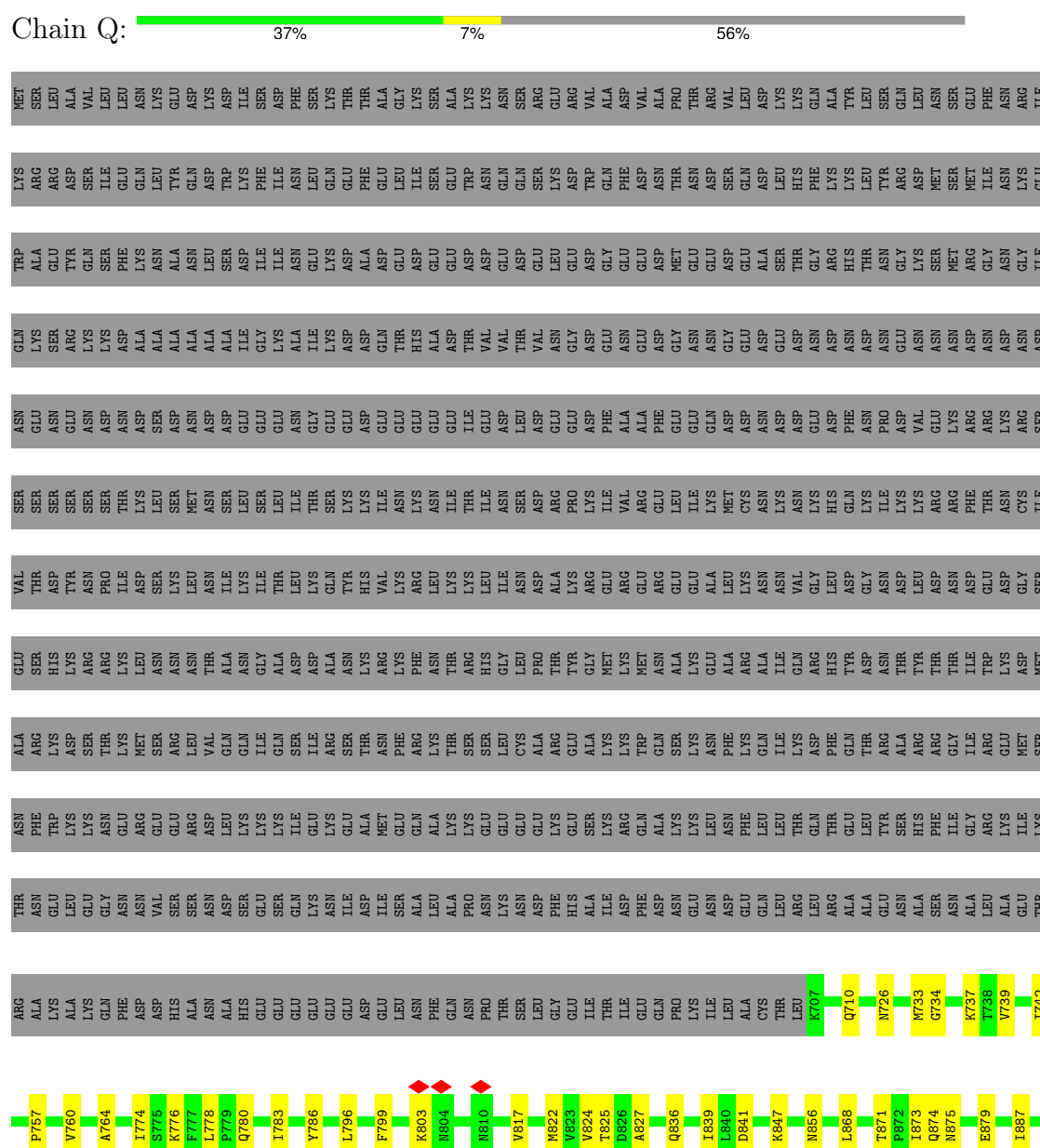


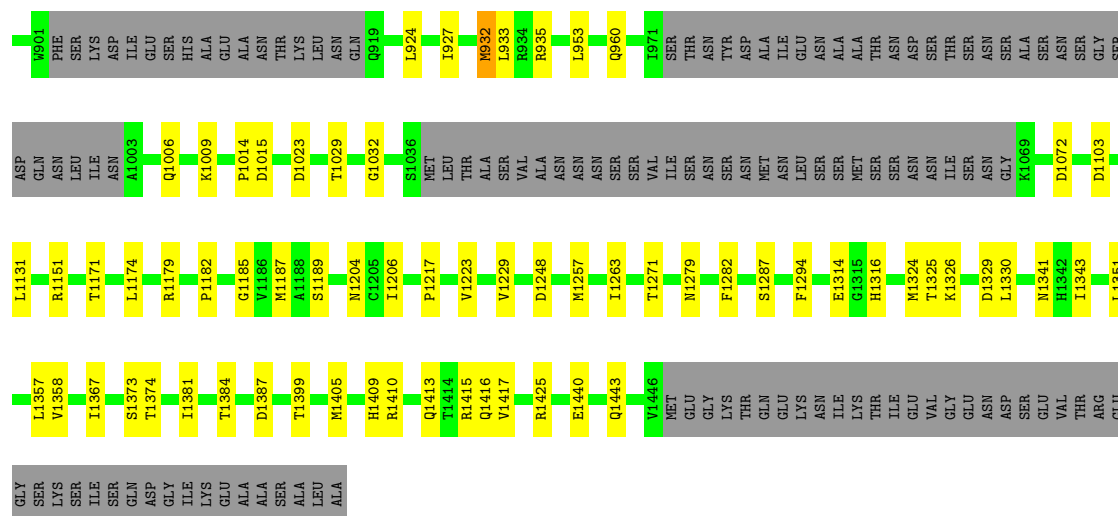
Mol	Chain	Residues	Atoms					AltConf
13	T	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	U	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	V	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
13	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	

### 3 Residue-property plots

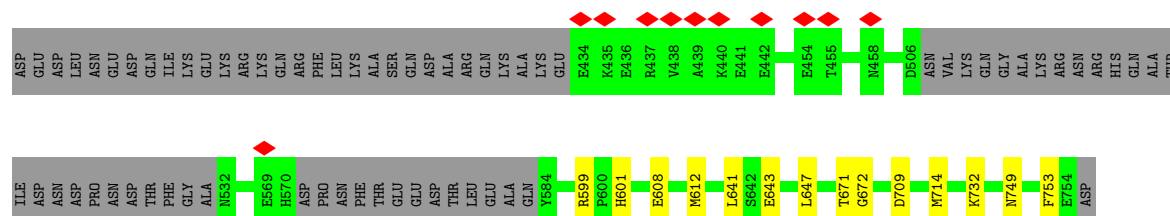
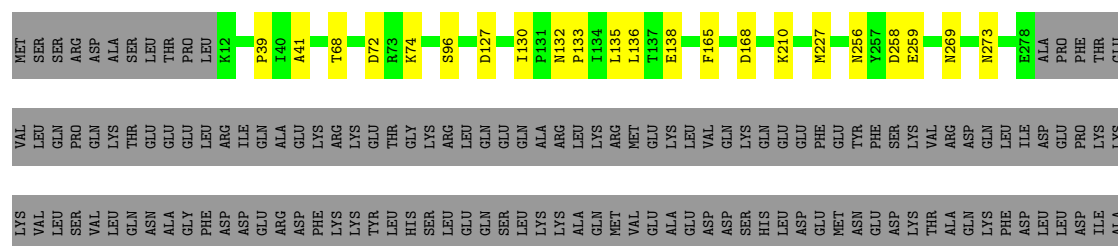
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: Chromatin-remodeling ATPase INO80

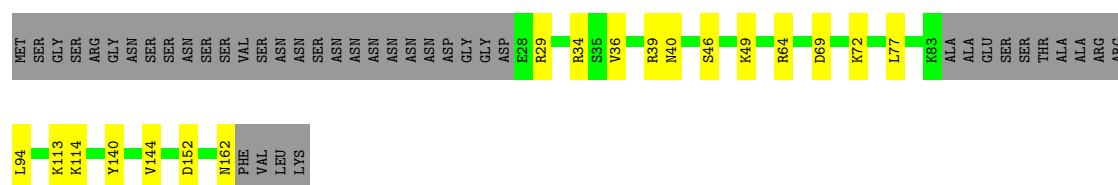




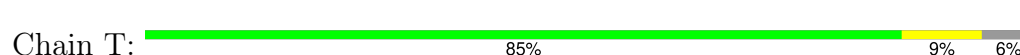
- Molecule 2: Actin-related protein 5



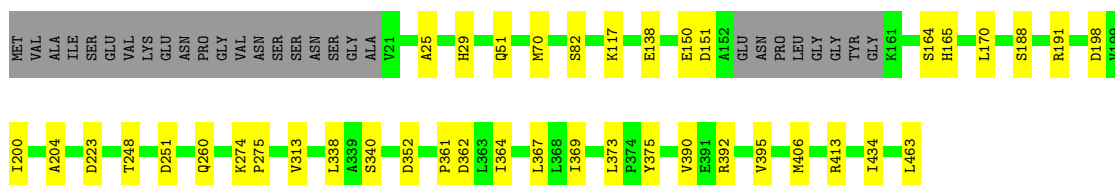
- Molecule 3: Chromatin-remodeling complex subunit IES6



- Molecule 4: RuvB-like protein 1

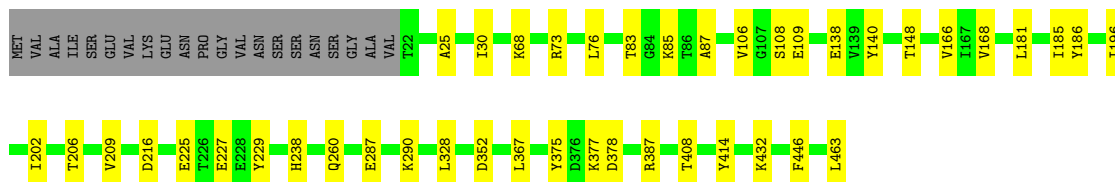






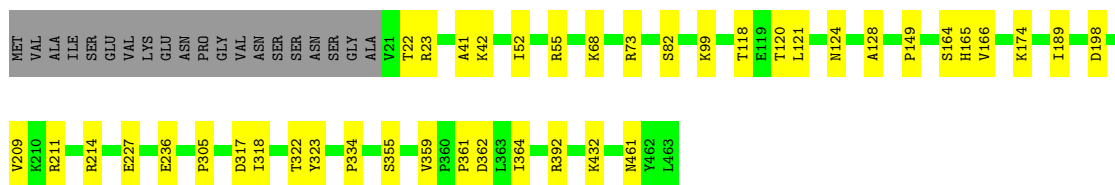
• Molecule 4: RuvB-like protein 1

Chain V: 86% 9% 5%



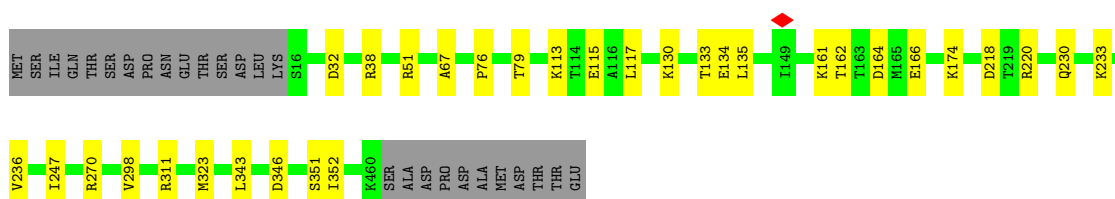
• Molecule 4: RuvB-like protein 1

Chain X: 87% 9% .



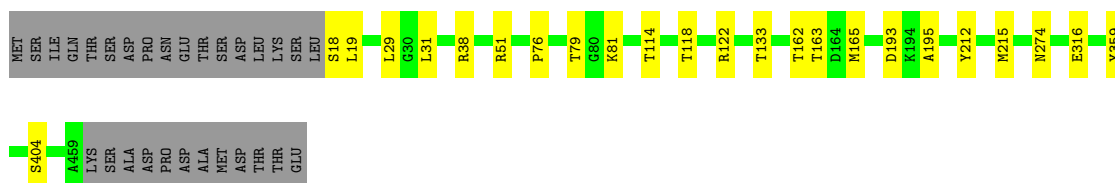
• Molecule 5: RuvB-like protein 2

Chain U: 88% 7% 6%



• Molecule 5: RuvB-like protein 2

Chain W: 89% 5% 6%



• Molecule 5: RuvB-like protein 2

MET	ASP	GLN	THR	SER	ASP	PRO	ASN	GLU	THR	SER	ASP	LEU	K15	A21	S24	Q36	P37	A67	G75	T79	G80	K81	E105	S108	L109	T114	T118	R122	K130	Q144	H145	D146	T150	E182	K183	D193	S196	R208	
ARG	ASP	TYR	ALA	MET	GLY	ALA	ASP	THR	R220	F221	V236	D245	T259	G260	D261	R327	S330	K331	Y359	I364	V392	D422	K460	SER	ALA	ASP	PRO	ASP	ALA	MET	ASP	THR	GLU						

- Chain Z:  14% 84%

ARG	ARG	SER	ASP	ASP	ILE	MET
ARG	ALA	GLU	ILE	ASP	ASP	ASP
ALA	GLU	LEU	GLY	GLY	GLU	GLU
ASN	ASN	VAL	GLU	LEU	ASP	SER
ALA	ARG	VAL	GLU	SER	ASP	ASP
ARG	LYS	VAL	GLU	VAL	ILE	ASP
ARG	LYS	ASN	SER	GLU	GLU	GLU
LYS	LYS	GLY	LEU	VAL	VAL	ALA
ASN	ASN	ASN	GLU	ASP	ASP	GLU
LEU	LEU	GLY	LYS	GLU	GLU	LEU
SER	SER	ASN	GLU	ASP	SER	SER
E254		GLU	LEU	TYR	ASP	ASP
		GLU	ASN	ASP	SER	ASP
S276		ASP	ARG	GLU	VAL	VAL
R277		ASP	GLY	GLU	SER	SER
SER		GLU	GLY	GLU	ALA	ALA
HIS		VAL	GLY	ASP	GLY	GLY
LEU		GLU	LYS	VAL	VAL	GLY
PRO		THR	GLU	LEU	LEU	GLU
ASN		ALA	VAL	SER	SER	GLU
ASP		LYS	GLU	PRO	TYR	GLU
ASP		GLU	LYS	SER	ILE	GLY
GLU		ASN	SER	LYS	ASP	GLY
LYS		THR	GLU	LYS	ASP	GLY
ASN		ASP	SER	HIS	ASP	GLY
ASP		SER	TYR	LEU	ASP	GLY
GLY		THR	TYR	HIS	THR	THR
SER		ARG	ALA	THR	GLU	GLU
SER		SER	GLN	ARG	ASP	ASP
SER		THR	ASN	SER	ILE	ASP
F293		THR	ASP	MET	ASP	ASP
S302		THR	VAL	ASP	ASP	ASP
		ARG	GLY	LYS	GLN	GLN
R307		SER	GLN	ARG	ILE	ILE
		LYS	LYS	VAL	VAL	VAL
R310		MET	GLY	GLN	THR	THR
		LEU	GLU	ALA	ALA	LYS
D315		LEU	GLU	GLU	ALA	LYS
		ASP	GLU	THR	THR	SER
		LEU	GLN	ALA	ALA	SER
C318		LEU	ASP	SER	ARG	ARG
T319		GLU	GLY	VAL	VAL	SER
F320		ASP	GLU	ASP	PRO	PRO
		GLY	SER	LYS	LYS	LYS
		GLY	GLY	SER	ALA	ALA
		GLY	GLY	ASP	ARG	ARG
		SER	TYR	GLY	VAL	SER
		LYS	GLU	ASP	THR	THR
		LYS	ASN	SER	PRO	PRO
		LEU	ASN	LYS	LYS	LYS
		THR	GLU	GLY	VAL	VAL
		GLU	PRO	ASN	ARG	ARG
		ASP	SER	ASP	GLY	GLY
		GLU	ILE	GLU	THR	THR
		ILE	SER	GLY	SER	SER
		GLN	LYS	LYS	ILE	LYS
		VAL	THR	THR	THR	THR

- Chain A: 

Sequence logo for the 100th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows amino acids: MET, ALA, ARG, THR, LYS, GLN, THR, ALA, ARG, LYS, LYS, SER, THR, GLY, LYS, LYS, ALA, PRO, ARG, LYS, GLN, LEU, ALA, SER, LYS, ALA, ALA, ARG, LYS, SER, ALA, PRO, SER, THR, GLY, GLY, VAL, LYS, LYS, P38, A47, L48, R49, R52, S57, T58, Q68, R69, L70, V71, R83, L100, F104. The 'P38' position is highlighted with a red diamond. The 'L70' position is highlighted with a green bar.

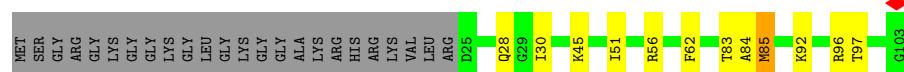
- Chain E:  54% 16% 29%

T107	T108	N108	L109	V117	T118	I119	Q120	K121	K122	K125	L126	R129	L130	R131	G132	E133	R134	SER	MET	ARG	THR	LYS	GLN	THR	ALA	ARG	LYS	SER	THR	GLY	LYS	ALA	PRO	ARG	LYS	GLN	LEU	ALA	SER	LYS	ALA	ALA	ARG	LYS	SER	PRO	SER	THR	GLY	VAL	LYS	LYS	P38	V46	R49	R52	R53	F54	G55	K56	S57	V71	I74	V96	L100	T101
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------

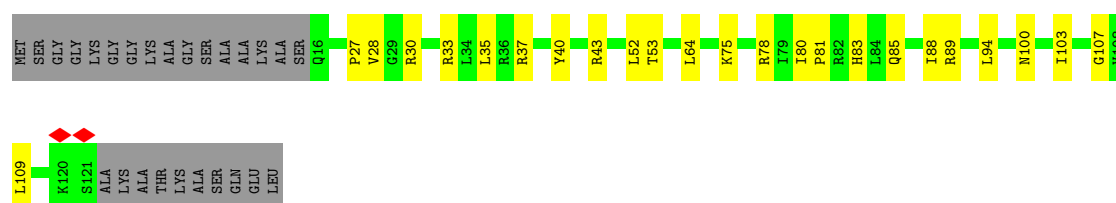
- Chain B:  61% 16% 23%



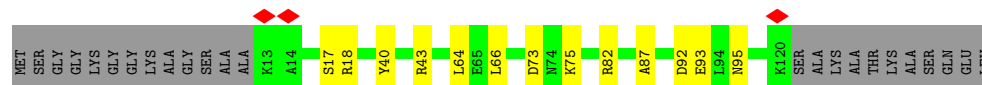
- Molecule 8: Histone H4



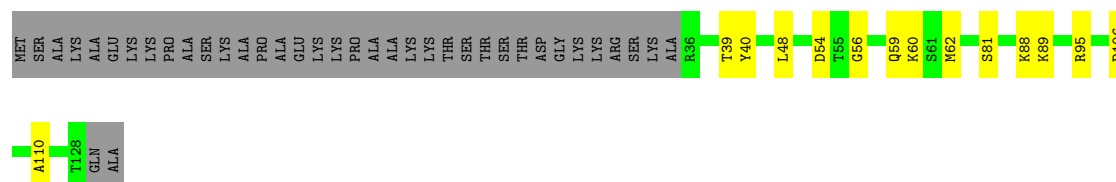
- Molecule 9: Histone H2A



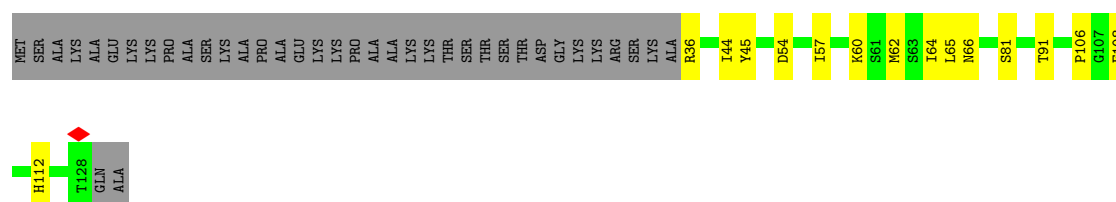
- Molecule 9: Histone H2A



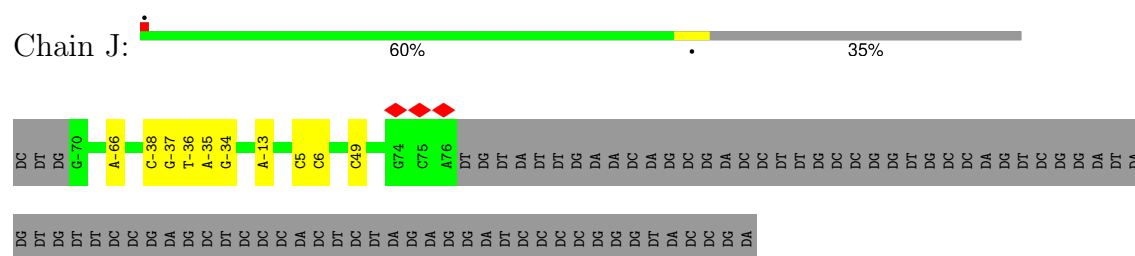
- Molecule 10: Histone H2B



- Molecule 10: Histone H2B



- Molecule 11: DNA (227-MER)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74790	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 ( $e^-/\text{\AA}^2$ )	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.170	Depositor
Minimum map value	-0.357	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	374.08, 374.08, 374.08	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835, 0.835, 0.835	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	Q	0.21	0/5395	0.48	1/7323 (0.0%)
2	R	0.16	0/4153	0.39	0/5667
3	S	0.20	0/1036	0.49	0/1392
4	T	0.18	0/3378	0.40	0/4569
4	V	0.18	0/3439	0.44	0/4652
4	X	0.19	0/3446	0.44	1/4662 (0.0%)
5	U	0.17	0/3459	0.39	0/4662
5	W	0.18	0/3432	0.40	0/4628
5	Y	0.17	0/3386	0.40	0/4561
6	Z	0.14	0/372	0.29	0/501
7	A	0.29	0/812	0.73	3/1086 (0.3%)
7	E	0.23	0/812	0.61	2/1086 (0.2%)
8	B	0.30	0/631	0.80	0/844
8	F	0.28	0/627	0.78	1/840 (0.1%)
9	C	0.24	0/830	0.61	1/1121 (0.1%)
9	G	0.28	0/838	0.68	0/1131
10	D	0.28	0/736	0.75	1/991 (0.1%)
10	H	0.29	0/736	0.76	0/991
11	I	0.21	0/3402	0.46	0/5253
12	J	0.19	0/3358	0.41	0/5176
All	All	0.20	0/44278	0.47	10/61136 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	F	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	105	GLU	CA-CB-CG	7.13	128.36	114.10
7	E	56	LYS	CA-CB-CG	6.26	126.62	114.10
7	A	105	GLU	N-CA-CB	6.02	120.22	110.40
8	F	85	MET	CB-CG-SD	5.91	130.43	112.70
10	D	88	LYS	CA-CB-CG	5.63	125.35	114.10
7	A	100	LEU	CA-CB-CG	5.51	135.60	116.30
1	Q	932	MET	CB-CG-SD	5.43	129.00	112.70
9	C	75	LYS	CA-CB-CG	5.40	124.89	114.10
4	X	99	LYS	CB-CG-CD	5.30	123.49	111.30
7	E	122	LYS	CA-CB-CG	5.08	124.25	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	F	96	ARG	Sidechain

## 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	Q	5277	0	5172	64	0
2	R	4067	0	3636	24	0
3	S	1014	0	1050	14	0
4	T	3339	0	3468	30	0
4	V	3397	0	3533	40	0
4	X	3404	0	3542	24	0
5	U	3421	0	3499	31	0
5	W	3394	0	3459	17	0
5	Y	3350	0	3444	26	0
6	Z	367	0	293	4	0
7	A	801	0	851	16	0
7	E	801	0	851	18	0
8	B	624	0	654	12	0
8	F	620	0	643	9	0
9	C	819	0	865	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	G	827	0	865	9	0
10	D	726	0	748	10	0
10	H	726	0	748	11	0
11	I	3030	0	1650	18	0
12	J	2997	0	1650	8	0
13	T	27	0	12	2	0
13	U	27	0	12	0	0
13	V	27	0	12	2	0
13	W	27	0	12	2	0
13	X	27	0	12	0	0
13	Y	27	0	12	2	0
All	All	43163	0	40693	343	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 4.

All (343) 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:U:352:ILE:CG2	4:V:446:PHE:HB3	1.79	1.13
5:U:352:ILE:HG21	4:V:446:PHE:HB3	1.58	0.84
1:Q:760:VAL:HG22	1:Q:839:ILE:HB	1.79	0.65
1:Q:1174:LEU:HD23	1:Q:1187:MET:HE1	1.79	0.64
5:W:212:TYR:HB2	5:W:215:MET:HE1	1.80	0.64
9:G:66:LEU:HB3	9:G:87:ALA:HB1	1.80	0.62
1:Q:1182:PRO:HD3	4:V:206:THR:HG22	1.81	0.62
4:V:30:ILE:CD1	4:V:87:ALA:HB1	2.30	0.62
1:Q:1440:GLU:HA	1:Q:1443:GLN:HE21	1.65	0.62
4:X:68:LYS:HG2	4:X:305:PRO:HD2	1.83	0.61
8:F:30:ILE:O	8:F:56:ARG:NH2	2.34	0.61
1:Q:822:MET:HA	1:Q:825:THR:HG22	1.83	0.60
5:U:162:THR:HG23	5:U:164:ASP:H	1.66	0.60
1:Q:1179:ARG:HH12	4:V:260:GLN:HB3	1.65	0.60
1:Q:1223:VAL:HB	1:Q:1229:VAL:HG11	1.84	0.60
5:U:352:ILE:HG21	4:V:446:PHE:CB	2.30	0.59
7:E:54:PHE:HA	7:E:57:SER:HB3	1.84	0.59
9:C:28:VAL:HG22	9:C:53:THR:HG21	1.84	0.59
9:G:64:LEU:HD11	10:H:44:ILE:HG13	1.85	0.59
4:T:367:LEU:HD11	4:T:369:ILE:HG12	1.85	0.59
5:W:215:MET:HE3	5:W:215:MET:H	1.68	0.58
7:E:96:VAL:O	7:E:100:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1103:ASP:N	1:Q:1103:ASP:OD1	2.37	0.58
4:X:362:ASP:OD1	4:X:362:ASP:N	2.37	0.57
1:Q:1204:ASN:ND2	5:W:195:ALA:O	2.36	0.57
10:H:36:ARG:HH22	12:J:49:DC:H4'	1.69	0.57
4:V:106:VAL:HG12	4:V:108:SER:H	1.70	0.57
5:U:352:ILE:HG22	4:V:446:PHE:HB3	1.80	0.57
1:Q:757:PRO:HD2	1:Q:836:GLN:HE22	1.68	0.57
5:U:352:ILE:HD12	4:V:414:TYR:CE1	2.40	0.57
5:U:352:ILE:HG23	4:V:446:PHE:HB3	1.81	0.56
11:I:37:DC:H41	12:J:-37:DG:H1	1.50	0.56
7:A:120:GLN:OE1	7:A:122:LYS:NZ	2.38	0.56
9:C:40:TYR:HB3	10:D:81:SER:HB2	1.87	0.56
1:Q:847:LYS:HD2	1:Q:879:GLU:HG3	1.88	0.55
7:A:57:SER:O	8:B:41:ARG:NH2	2.39	0.55
3:S:36:VAL:O	3:S:40:ASN:ND2	2.39	0.55
7:A:100:LEU:O	7:A:104:PHE:HB2	2.07	0.55
4:V:138:GLU:OE1	4:V:238:HIS:NE2	2.40	0.55
1:Q:778:LEU:HD22	1:Q:780:GLN:HE22	1.72	0.55
5:Y:208:ARG:O	5:Y:208:ARG:NH1	2.39	0.55
6:Z:310:ARG:NH1	6:Z:315:ASP:OD2	2.40	0.55
7:E:46:VAL:HG23	7:E:49:ARG:HH21	1.71	0.55
1:Q:1294:PHE:HZ	1:Q:1330:LEU:HB3	1.73	0.54
1:Q:1324:MET:HA	11:I:-61:DT:H4'	1.90	0.54
5:U:115:GLU:OE2	5:U:270:ARG:NH2	2.40	0.54
9:C:85:GLN:NE2	9:C:107:GLY:O	2.41	0.54
2:R:72:ASP:OD1	2:R:72:ASP:N	2.41	0.54
5:U:346:ASP:OD1	5:U:346:ASP:N	2.40	0.54
7:A:48:LEU:HB3	7:A:52:ARG:HH21	1.73	0.54
8:B:58:VAL:HA	8:B:61:VAL:HG22	1.90	0.54
5:W:18:SER:OG	5:W:19:LEU:N	2.40	0.54
1:Q:1294:PHE:CZ	1:Q:1330:LEU:HB3	2.43	0.53
2:R:168:ASP:OD1	2:R:168:ASP:N	2.41	0.53
5:W:316:GLU:O	4:X:23:ARG:NH2	2.41	0.53
7:A:49:ARG:HA	7:A:52:ARG:HE	1.73	0.53
1:Q:1171:THR:HA	1:Q:1174:LEU:HD12	1.91	0.53
1:Q:1257:MET:HB3	1:Q:1263:ILE:HD12	1.90	0.53
9:C:100:ASN:OD1	9:C:100:ASN:N	2.41	0.53
1:Q:827:ALA:HB2	1:Q:856:ASN:HD22	1.73	0.53
4:V:216:ASP:N	4:V:216:ASP:OD1	2.40	0.53
2:R:135:LEU:HD12	2:R:714:MET:HB3	1.91	0.52
1:Q:764:ALA:HB1	1:Q:1351:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:227:MET:HE2	2:R:612:MET:HE3	1.89	0.52
9:C:81:PRO:HG2	10:D:60:LYS:HE2	1.91	0.52
1:Q:710:GLN:OE1	1:Q:935:ARG:NH1	2.43	0.52
9:C:78:ARG:HE	10:D:56:GLY:HA3	1.75	0.52
1:Q:796:LEU:HD23	1:Q:799:PHE:HD2	1.75	0.52
2:R:127:ASP:OD1	2:R:127:ASP:N	2.41	0.52
4:T:188:SER:OG	4:T:191:ARG:NH1	2.41	0.52
4:V:181:LEU:HD23	4:V:185:ILE:HG21	1.92	0.52
5:W:81:LYS:H	13:W:1001:ADP:PB	2.33	0.51
4:V:166:VAL:HG12	4:V:168:VAL:HG23	1.92	0.51
8:F:83:THR:OG1	8:F:84:ALA:N	2.43	0.51
5:W:122:ARG:NH2	5:W:274:ASN:OD1	2.41	0.51
1:Q:932:MET:HE3	1:Q:933:LEU:H	1.74	0.51
2:R:138:GLU:OE2	2:R:749:ASN:ND2	2.42	0.51
6:Z:319:THR:OG1	6:Z:320:PHE:N	2.44	0.51
10:H:45:TYR:HE1	10:H:57:ILE:HG21	1.76	0.51
5:W:162:THR:HG23	5:W:165:MET:H	1.76	0.51
10:H:108:GLU:O	10:H:112:HIS:ND1	2.44	0.51
7:E:49:ARG:HH12	12:J:-66:DA:H4'	1.76	0.51
12:J:5:DC:H4'	12:J:6:DC:H5'	1.93	0.51
1:Q:1341:ASN:HB3	1:Q:1367:ILE:HD12	1.93	0.50
8:B:37:ARG:NH2	12:J:-13:DA:OP1	2.44	0.50
4:T:170:LEU:HD11	4:T:200:ILE:HD11	1.93	0.50
1:Q:1387:ASP:HB2	1:Q:1417:VAL:HA	1.94	0.50
10:D:89:LYS:HE2	12:J:-34:DG:H3'	1.93	0.50
4:T:362:ASP:OD1	4:T:362:ASP:N	2.45	0.50
4:X:461:ASN:OD1	4:X:461:ASN:N	2.43	0.50
10:H:62:MET:O	10:H:66:ASN:HB2	2.12	0.50
4:X:198:ASP:OD1	4:X:214:ARG:NH1	2.45	0.50
11:I:-23:DT:H2''	11:I:-22:DG:H5''	1.92	0.50
1:Q:1325:THR:HG23	11:I:-61:DT:H5'	1.93	0.50
2:R:601:HIS:ND1	2:R:608:GLU:OE2	2.43	0.50
3:S:39:ARG:O	3:S:39:ARG:NH1	2.40	0.50
7:A:127:ALA:O	7:A:131:ARG:HB2	2.11	0.50
3:S:29:ARG:O	3:S:29:ARG:NH1	2.43	0.50
4:V:30:ILE:HD13	4:V:87:ALA:HB1	1.92	0.50
1:Q:824:VAL:HA	1:Q:856:ASN:HD21	1.77	0.50
1:Q:1326:LYS:HA	1:Q:1329:ASP:HB2	1.94	0.50
5:Y:359:TYR:OH	13:Y:1001:ADP:N7	2.42	0.50
10:D:59:GLN:HA	10:D:62:MET:HG2	1.93	0.50
1:Q:726:ASN:ND2	1:Q:887:ILE:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:873:ILE:O	1:Q:875:ASN:ND2	2.43	0.49
1:Q:1032:GLY:HA3	5:Y:182:GLU:HA	1.94	0.49
2:R:671:THR:OG1	2:R:672:GLY:N	2.44	0.49
4:V:140:TYR:HB2	4:V:202:ILE:HB	1.92	0.49
4:V:73:ARG:NH2	5:W:404:SER:OG	2.45	0.49
3:S:114:LYS:NZ	4:T:223:ASP:OD1	2.46	0.49
7:E:52:ARG:HB3	7:E:56:LYS:HZ1	1.78	0.49
4:V:85:LYS:NZ	13:V:1001:ADP:O2B	2.39	0.49
4:X:120:THR:O	4:X:124:ASN:ND2	2.44	0.49
7:A:69:ARG:NH2	11:I:17:DA:OP2	2.43	0.49
5:Y:122:ARG:NE	5:Y:245:ASP:OD2	2.41	0.49
8:B:61:VAL:O	8:B:65:ASN:ND2	2.45	0.49
10:H:44:ILE:HD11	10:H:65:LEU:HD23	1.95	0.49
1:Q:1384:THR:O	1:Q:1413:GLN:NE2	2.45	0.49
4:T:361:PRO:HA	4:T:364:ILE:HB	1.93	0.49
8:F:28:GLN:HA	8:F:56:ARG:HH22	1.78	0.49
2:R:258:ASP:OD2	3:S:113:LYS:NZ	2.45	0.49
1:Q:1416:GLN:NE2	1:Q:1417:VAL:O	2.44	0.49
3:S:69:ASP:HA	3:S:72:LYS:HG2	1.95	0.49
5:U:134:GLU:OE1	5:U:230:GLN:NE2	2.46	0.49
4:V:352:ASP:N	4:V:352:ASP:OD1	2.45	0.49
1:Q:739:VAL:HA	1:Q:742:ILE:HG22	1.94	0.49
1:Q:1343:ILE:HD12	1:Q:1357:LEU:HD22	1.95	0.49
4:X:174:LYS:NZ	4:X:236:GLU:OE2	2.46	0.49
8:B:56:ARG:HA	8:B:59:LEU:HG	1.94	0.49
9:G:93:GLU:HB2	10:H:106:PRO:HG2	1.94	0.49
4:X:42:LYS:O	4:X:55:ARG:NH2	2.46	0.48
9:C:80:ILE:HG13	9:C:83:HIS:H	1.77	0.48
1:Q:1131:LEU:HG	5:U:247:ILE:HG13	1.95	0.48
4:X:211:ARG:NH1	4:X:227:GLU:OE1	2.42	0.48
5:W:38:ARG:O	5:W:51:ARG:NH2	2.40	0.48
4:V:148:THR:O	4:V:148:THR:OG1	2.31	0.48
3:S:162:ASN:OD1	3:S:162:ASN:N	2.43	0.48
3:S:140:TYR:HA	3:S:144:VAL:HB	1.95	0.48
5:U:67:ALA:HB3	4:V:25:ALA:HB2	1.95	0.48
4:V:377:LYS:HD2	4:V:408:THR:HG21	1.95	0.48
7:A:130:LEU:HD12	7:E:130:LEU:HD12	1.96	0.48
9:G:73:ASP:O	9:G:75:LYS:NZ	2.47	0.48
1:Q:1029:THR:HG22	1:Q:1217:PRO:HD3	1.95	0.48
7:E:104:PHE:HA	7:E:107:THR:HG22	1.95	0.48
8:B:83:THR:HG23	8:B:85:MET:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:352:ASP:N	4:T:352:ASP:OD1	2.46	0.48
4:X:149:PRO:HB3	4:X:166:VAL:HG22	1.96	0.47
1:Q:786:TYR:H	1:Q:817:VAL:HG22	1.79	0.47
4:T:313:VAL:HG21	4:T:338:LEU:HD13	1.97	0.47
4:T:367:LEU:HD11	4:T:369:ILE:CG1	2.45	0.47
7:A:119:ILE:O	8:B:48:SER:OG	2.31	0.47
5:W:162:THR:OG1	5:W:163:THR:N	2.46	0.47
7:E:46:VAL:HA	7:E:49:ARG:HE	1.79	0.47
1:Q:803:LYS:HA	1:Q:803:LYS:HD3	1.79	0.47
1:Q:1373:SER:OG	1:Q:1374:THR:N	2.47	0.47
4:X:361:PRO:HA	4:X:364:ILE:HB	1.95	0.47
9:G:40:TYR:HB3	10:H:81:SER:HB2	1.97	0.47
1:Q:1023:ASP:HB3	1:Q:1287:SER:HB2	1.97	0.47
7:A:47:ALA:HB1	8:B:40:ARG:HH22	1.79	0.47
7:E:117:VAL:HG21	8:F:45:LYS:HE3	1.96	0.47
11:I:-59:DT:H2''	11:I:-58:DC:H2'	1.96	0.47
1:Q:1358:VAL:HG11	1:Q:1381:ILE:HD11	1.97	0.47
2:R:256:ASN:ND2	2:R:259:GLU:OE2	2.47	0.47
1:Q:1151:ARG:NH2	4:T:260:GLN:O	2.48	0.47
1:Q:1405:MET:O	1:Q:1409:HIS:N	2.44	0.47
4:T:313:VAL:HG12	4:T:340:SER:HB2	1.98	0.46
5:U:351:SER:O	5:U:352:ILE:HD13	2.15	0.46
5:W:79:THR:O	5:W:359:TYR:OH	2.33	0.46
3:S:152:ASP:OD1	3:S:152:ASP:N	2.47	0.46
4:T:151:ASP:OD1	4:T:151:ASP:N	2.46	0.46
5:U:311:ARG:HD2	5:U:311:ARG:HA	1.78	0.46
4:X:22:THR:OG1	4:X:392:ARG:NH2	2.41	0.46
7:E:96:VAL:HG12	8:F:62:PHE:HE2	1.80	0.46
2:R:41:ALA:HA	2:R:135:LEU:HB2	1.97	0.46
4:T:117:LYS:H	4:T:117:LYS:HG2	1.50	0.46
7:E:121:LYS:O	7:E:125:LYS:NZ	2.44	0.46
12:J:-36:DT:H2''	12:J:-35:DA:C8	2.50	0.46
1:Q:1006:GLN:HA	1:Q:1009:LYS:HG2	1.96	0.46
1:Q:1248:ASP:HA	1:Q:1271:THR:HB	1.97	0.46
1:Q:1387:ASP:OD1	1:Q:1387:ASP:N	2.48	0.46
9:C:30:ARG:NH2	11:I:49:DC:OP1	2.46	0.46
9:C:33:ARG:HA	9:C:37:ARG:HH21	1.80	0.46
5:Y:259:THR:OG1	5:Y:261:ASP:OD1	2.30	0.46
1:Q:874:GLN:HG3	1:Q:1399:THR:HG21	1.98	0.46
4:T:375:TYR:OH	13:T:1001:ADP:N7	2.44	0.46
5:U:352:ILE:CD1	4:V:414:TYR:CD1	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:52:TYR:HB3	8:B:56:ARG:HH12	1.81	0.46
9:G:92:ASP:HA	9:G:95:ASN:HB2	1.98	0.46
10:D:106:PRO:O	10:D:110:ALA:N	2.48	0.46
1:Q:733:MET:HE1	1:Q:737:LYS:H	1.81	0.46
7:E:129:ARG:O	7:E:129:ARG:NH1	2.45	0.46
4:X:317:ASP:OD1	4:X:317:ASP:N	2.42	0.45
7:E:119:ILE:HG13	8:F:51:ILE:HG13	1.97	0.45
2:R:753:PHE:HB3	3:S:94:LEU:HD11	1.98	0.45
5:Y:81:LYS:N	13:Y:1001:ADP:O2A	2.50	0.45
5:Y:327:ARG:HA	5:Y:327:ARG:HD3	1.81	0.45
5:Y:193:ASP:OD2	5:Y:196:SER:OG	2.33	0.45
5:Y:108:SER:OG	5:Y:109:LEU:N	2.50	0.45
2:R:269:ASN:OD1	2:R:273:ASN:ND2	2.40	0.45
4:T:29:HIS:HB3	4:T:390:VAL:HG21	1.99	0.45
4:T:392:ARG:HE	4:T:392:ARG:HB2	1.58	0.45
7:A:118:THR:HA	8:B:46:ARG:HB3	1.99	0.45
4:T:406:MET:HE3	4:T:406:MET:HB2	1.79	0.45
8:F:83:THR:HG23	8:F:85:MET:H	1.81	0.45
1:Q:734:GLY:HA2	1:Q:1410:ARG:HG3	1.98	0.45
2:R:136:LEU:HD23	2:R:165:PHE:HE1	1.82	0.45
1:Q:1185:GLY:O	1:Q:1189:SER:OG	2.28	0.45
4:V:196:ILE:HD12	4:V:196:ILE:HA	1.88	0.45
1:Q:1072:ASP:O	5:Y:183:LYS:NZ	2.38	0.44
4:V:202:ILE:HG12	4:V:209:VAL:HG12	1.99	0.44
4:V:375:TYR:OH	13:V:1001:ADP:N7	2.39	0.44
9:C:64:LEU:HD22	10:D:48:LEU:HD13	1.99	0.44
4:V:76:LEU:HB3	4:V:367:LEU:HD13	1.99	0.44
7:A:68:GLN:HA	7:A:71:VAL:HG22	2.00	0.44
9:C:88:ILE:HD12	9:C:94:LEU:HB3	1.99	0.44
1:Q:742:ILE:HD12	1:Q:774:ILE:HD13	1.98	0.44
9:C:27:PRO:HB2	9:C:30:ARG:HB2	1.99	0.44
4:X:432:LYS:HB2	4:X:432:LYS:HE2	1.69	0.44
2:R:210:LYS:HG3	2:R:641:LEU:HD22	1.98	0.44
2:R:643:GLU:HG2	2:R:647:LEU:HD12	1.99	0.44
5:U:133:THR:OG1	5:U:233:LYS:O	2.32	0.44
9:C:43:ARG:HD2	11:I:39:DA:H5'	1.99	0.44
5:U:323:MET:HE3	5:U:323:MET:HB2	1.93	0.44
3:S:77:LEU:HD23	3:S:77:LEU:HA	1.89	0.44
4:V:83:THR:O	4:V:375:TYR:OH	2.36	0.44
4:V:166:VAL:HG21	4:V:186:TYR:HB2	2.00	0.44
4:T:150:GLU:O	4:T:164:SER:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:76:PRO:O	5:W:79:THR:OG1	2.34	0.43
10:D:54:ASP:N	10:D:54:ASP:OD1	2.47	0.43
2:R:39:PRO:HB3	2:R:133:PRO:HG2	2.00	0.43
4:V:225:GLU:OE1	4:V:229:TYR:OH	2.36	0.43
5:Y:144:GLN:NE2	5:Y:146:ASP:OD1	2.46	0.43
4:T:138:GLU:HB3	4:T:204:ALA:HB3	2.00	0.43
5:U:218:ASP:O	5:U:220:ARG:NH1	2.52	0.43
10:D:39:THR:OG1	10:D:40:TYR:N	2.51	0.43
5:U:76:PRO:O	5:U:79:THR:OG1	2.33	0.43
4:X:41:ALA:HB3	4:X:52:ILE:HG23	2.00	0.43
4:X:82:SER:O	4:X:82:SER:OG	2.34	0.43
11:I:-61:DT:H2'	11:I:-60:DA:C8	2.54	0.43
5:Y:76:PRO:O	5:Y:79:THR:OG1	2.34	0.43
8:F:92:LYS:HA	8:F:97:THR:HG22	2.00	0.43
5:U:352:ILE:CG2	4:V:446:PHE:CB	2.72	0.43
4:X:318:ILE:O	4:X:322:THR:OG1	2.33	0.43
9:C:35:LEU:HD11	9:C:52:LEU:HD23	2.01	0.43
8:F:28:GLN:HA	8:F:56:ARG:HH12	1.84	0.43
11:I:-20:DC:N4	11:I:-19:DG:O6	2.51	0.43
7:E:71:VAL:HA	7:E:74:ILE:HG22	2.01	0.43
5:U:233:LYS:HB2	5:U:233:LYS:HE2	1.85	0.43
5:Y:220:ARG:HB3	5:Y:221:PHE:H	1.71	0.43
1:Q:1279:ASN:HB2	1:Q:1282:PHE:HD1	1.83	0.43
2:R:269:ASN:O	2:R:273:ASN:ND2	2.52	0.43
4:T:25:ALA:HB2	5:Y:67:ALA:HB3	2.00	0.43
10:H:60:LYS:O	10:H:64:ILE:HG13	2.19	0.43
4:T:164:SER:OG	4:T:165:HIS:ND1	2.46	0.42
6:Z:307:ARG:HB3	6:Z:318:CYS:HB2	2.01	0.42
1:Q:960:GLN:HG2	1:Q:1014:PRO:HG3	2.00	0.42
1:Q:1314:GLU:OE1	1:Q:1316:HIS:ND1	2.52	0.42
4:T:198:ASP:OD1	4:T:198:ASP:N	2.53	0.42
8:B:60:LYS:O	8:B:64:GLU:HG2	2.19	0.42
4:T:463:LEU:HD22	5:Y:75:GLY:HA2	2.02	0.42
4:V:432:LYS:HE2	4:V:432:LYS:HB2	1.85	0.42
2:R:709:ASP:OD1	2:R:709:ASP:N	2.51	0.42
6:Z:302:SER:O	6:Z:302:SER:OG	2.35	0.42
7:E:119:ILE:H	7:E:119:ILE:HG12	1.70	0.42
7:E:132:GLY:HA2	7:E:134:ARG:HH12	1.84	0.42
11:I:16:DA:H1'	11:I:17:DA:N7	2.34	0.42
1:Q:776:LYS:HA	1:Q:776:LYS:HD3	1.73	0.42
4:T:274:LYS:NZ	4:T:275:PRO:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:73:ARG:HE	4:X:73:ARG:HB3	1.60	0.42
3:S:46:SER:HB2	3:S:49:LYS:HG2	2.02	0.42
4:T:413:ARG:NH2	13:T:1001:ADP:O3A	2.53	0.42
4:X:118:THR:HG21	5:Y:105:GLU:HG2	2.00	0.42
4:X:164:SER:O	4:X:165:HIS:ND1	2.51	0.42
4:V:378:ASP:OD1	4:V:378:ASP:N	2.52	0.42
5:Y:76:PRO:O	5:Y:81:LYS:NZ	2.53	0.42
8:B:76:HIS:O	10:D:95:ARG:NH2	2.39	0.42
1:Q:783:ILE:HD13	1:Q:783:ILE:HA	1.88	0.42
1:Q:1316:HIS:CE1	1:Q:1415:ARG:HE	2.38	0.42
2:R:599:ARG:HA	2:R:599:ARG:HD3	1.84	0.42
7:A:113:HIS:CD2	7:E:126:LEU:HG	2.55	0.42
4:T:248:THR:OG1	4:T:251:ASP:OD1	2.37	0.41
10:H:54:ASP:OD1	10:H:54:ASP:N	2.41	0.41
2:R:68:THR:HB	2:R:96:SER:HA	2.02	0.41
5:U:113:LYS:H	5:U:113:LYS:HG3	1.68	0.41
4:V:68:LYS:HB2	4:V:68:LYS:HE3	1.85	0.41
4:X:128:ALA:HB3	4:X:334:PRO:HG3	2.02	0.41
1:Q:871:THR:HG22	1:Q:873:ILE:HG22	2.01	0.41
2:R:74:LYS:HE3	3:S:34:ARG:HE	1.84	0.41
2:R:732:LYS:HE2	2:R:732:LYS:HB2	1.90	0.41
3:S:64:ARG:NH2	11:I:-32:DT:O3'	2.53	0.41
5:U:32:ASP:OD1	5:U:38:ARG:NE	2.53	0.41
4:V:328:LEU:HD23	4:V:328:LEU:HA	1.94	0.41
5:Y:114:THR:O	5:Y:118:THR:OG1	2.37	0.41
5:Y:330:SER:OG	5:Y:331:LYS:N	2.53	0.41
11:I:-54:DC:H2'	11:I:-53:DA:C8	2.55	0.41
1:Q:1015:ASP:OD1	1:Q:1015:ASP:N	2.53	0.41
4:X:121:LEU:HD23	4:X:323:TYR:HD2	1.85	0.41
4:X:355:SER:OG	4:X:359:VAL:O	2.33	0.41
9:C:89:ARG:HG2	9:C:109:LEU:HG	2.02	0.41
1:Q:953:LEU:HD13	1:Q:1425:ARG:HD3	2.01	0.41
4:T:395:VAL:HA	4:T:434:ILE:HB	2.02	0.41
5:Y:130:LYS:HG2	5:Y:236:VAL:HG22	2.03	0.41
9:G:43:ARG:HG2	10:H:91:THR:HG23	2.02	0.41
11:I:14:DT:H2''	11:I:15:DT:H5'	2.01	0.41
12:J:-38:DC:H2''	12:J:-37:DG:C8	2.55	0.41
5:U:76:PRO:HD3	4:V:463:LEU:HD13	2.02	0.41
5:U:130:LYS:HB2	5:U:236:VAL:HG22	2.03	0.41
5:U:298:VAL:HG13	5:U:343:LEU:HD21	2.03	0.41
5:Y:331:LYS:HB2	5:Y:331:LYS:HE3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:103:ILE:HD12	9:C:103:ILE:HA	1.84	0.41
11:I:-52:DC:H2"	11:I:-51:DG:C8	2.56	0.41
4:T:70:MET:HE3	4:T:70:MET:HB3	1.92	0.41
5:U:135:LEU:HD23	5:U:135:LEU:HA	1.95	0.41
5:Y:109:LEU:HD23	5:Y:109:LEU:HA	1.94	0.41
5:Y:364:ILE:HD12	5:Y:392:VAL:HG12	2.03	0.41
7:A:109:LEU:HD23	7:A:109:LEU:HA	1.93	0.41
5:U:38:ARG:O	5:U:51:ARG:NH2	2.54	0.41
5:U:117:LEU:HD23	5:U:117:LEU:HA	1.94	0.41
4:V:287:GLU:HA	4:V:290:LYS:HG2	2.02	0.41
5:W:29:LEU:HB3	5:W:31:LEU:HD13	2.03	0.41
5:W:114:THR:O	5:W:118:THR:OG1	2.33	0.41
5:W:359:TYR:OH	13:W:1001:ADP:N7	2.38	0.41
5:Y:422:ASP:OD1	5:Y:422:ASP:N	2.52	0.41
7:A:83:ARG:HD2	11:I:27:DG:H5"	2.03	0.41
11:I:-5:DG:H2"	11:I:-4:DG:C8	2.56	0.41
4:T:51:GLN:NE2	4:T:373:LEU:O	2.54	0.41
4:T:82:SER:O	4:T:82:SER:OG	2.34	0.41
5:U:174:LYS:HD2	4:V:227:GLU:HB2	2.03	0.41
1:Q:841:ASP:HA	1:Q:868:LEU:HB2	2.03	0.40
1:Q:924:LEU:HD13	1:Q:927:ILE:HD12	2.03	0.40
4:X:189:ILE:HD13	4:X:209:VAL:HG11	2.03	0.40
7:A:58:THR:HG22	9:G:82:ARG:HH21	1.85	0.40
11:I:-74:DC:H2"	11:I:-73:DA:C8	2.56	0.40
4:V:106:VAL:HB	4:V:109:GLU:HG3	2.02	0.40
4:V:387:ARG:HA	4:V:387:ARG:HD2	1.91	0.40
5:W:133:THR:OG1	5:W:193:ASP:OD1	2.34	0.40
5:Y:21:ALA:H	5:Y:24:SER:HB3	1.86	0.40
7:E:109:LEU:HD23	7:E:109:LEU:HA	1.91	0.40
2:R:130:ILE:HG22	2:R:132:ASN:H	1.85	0.40
5:Y:36:GLN:HA	5:Y:37:PRO:HD3	1.96	0.40
1:Q:1206:ILE:O	1:Q:1279:ASN:ND2	2.53	0.40
5:U:161:LYS:HB2	5:U:166:GLU:HB2	2.04	0.40
9:G:17:SER:OG	9:G:18:ARG:N	2.54	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	652/1489 (44%)	618 (95%)	34 (5%)	0	100	100
2	R	542/755 (72%)	531 (98%)	11 (2%)	0	100	100
3	S	121/166 (73%)	116 (96%)	5 (4%)	0	100	100
4	T	431/463 (93%)	418 (97%)	13 (3%)	0	100	100
4	V	440/463 (95%)	426 (97%)	14 (3%)	0	100	100
4	X	441/463 (95%)	427 (97%)	14 (3%)	0	100	100
5	U	443/471 (94%)	424 (96%)	19 (4%)	0	100	100
5	W	440/471 (93%)	422 (96%)	18 (4%)	0	100	100
5	Y	432/471 (92%)	412 (95%)	20 (5%)	0	100	100
6	Z	48/320 (15%)	48 (100%)	0	0	100	100
7	A	95/136 (70%)	93 (98%)	2 (2%)	0	100	100
7	E	95/136 (70%)	92 (97%)	3 (3%)	0	100	100
8	B	77/103 (75%)	73 (95%)	4 (5%)	0	100	100
8	F	77/103 (75%)	73 (95%)	4 (5%)	0	100	100
9	C	104/132 (79%)	99 (95%)	5 (5%)	0	100	100
9	G	106/132 (80%)	103 (97%)	3 (3%)	0	100	100
10	D	91/131 (70%)	91 (100%)	0	0	100	100
10	H	91/131 (70%)	89 (98%)	2 (2%)	0	100	100
All	All	4726/6536 (72%)	4555 (96%)	171 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	Q	579/1350 (43%)	579 (100%)	0	100	100
2	R	389/682 (57%)	389 (100%)	0	100	100
3	S	109/142 (77%)	109 (100%)	0	100	100
4	T	367/391 (94%)	367 (100%)	0	100	100
4	V	374/391 (96%)	374 (100%)	0	100	100
4	X	375/391 (96%)	375 (100%)	0	100	100
5	U	378/403 (94%)	378 (100%)	0	100	100
5	W	374/403 (93%)	374 (100%)	0	100	100
5	Y	371/403 (92%)	371 (100%)	0	100	100
6	Z	27/285 (10%)	27 (100%)	0	100	100
7	A	85/113 (75%)	85 (100%)	0	100	100
7	E	85/113 (75%)	85 (100%)	0	100	100
8	B	63/79 (80%)	63 (100%)	0	100	100
8	F	62/79 (78%)	62 (100%)	0	100	100
9	C	85/99 (86%)	85 (100%)	0	100	100
9	G	84/99 (85%)	84 (100%)	0	100	100
10	D	81/109 (74%)	81 (100%)	0	100	100
10	H	81/109 (74%)	81 (100%)	0	100	100
All	All	3969/5641 (70%)	3969 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	740	GLN
1	Q	856	ASN
1	Q	960	GLN
1	Q	1117	ASN
1	Q	1281	ASN
1	Q	1359	HIS
1	Q	1382	ASN
1	Q	1409	HIS
1	Q	1413	GLN

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Mol	Chain	Res	Type
1	Q	1441	GLN
2	R	23	GLN
2	R	61	HIS
2	R	132	ASN
2	R	144	GLN
2	R	195	ASN
3	S	153	GLN
4	T	245	GLN
4	T	331	ASN
5	U	408	GLN
4	V	154	ASN
4	V	263	GLN
4	V	430	ASN
5	W	173	ASN
5	W	237	HIS
5	W	242	HIS
5	W	362	GLN
4	X	357	HIS
5	Y	360	ASN
5	Y	408	GLN
5	Y	453	ASN
6	Z	301	ASN
8	B	65	ASN
9	C	74	ASN
9	C	85	GLN
9	G	105	GLN
10	H	70	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	ADP	W	1001	-	24,29,29	0.94	1 (4%)	29,45,45	1.29	3 (10%)
13	ADP	X	1001	-	24,29,29	0.87	0	29,45,45	1.20	2 (6%)
13	ADP	U	1001	-	24,29,29	0.85	0	29,45,45	1.23	2 (6%)
13	ADP	T	1001	-	24,29,29	0.87	0	29,45,45	1.24	2 (6%)
13	ADP	Y	1001	-	24,29,29	0.86	0	29,45,45	1.21	2 (6%)
13	ADP	V	1001	-	24,29,29	0.84	0	29,45,45	1.21	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	ADP	W	1001	-	-	3/12/32/32	0/3/3/3
13	ADP	X	1001	-	-	0/12/32/32	0/3/3/3
13	ADP	U	1001	-	-	3/12/32/32	0/3/3/3
13	ADP	T	1001	-	-	1/12/32/32	0/3/3/3
13	ADP	Y	1001	-	-	3/12/32/32	0/3/3/3
13	ADP	V	1001	-	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	W	1001	ADP	PA-O3A	2.14	1.61	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	U	1001	ADP	N3-C2-N1	-3.73	123.61	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	1001	ADP	N3-C2-N1	-3.69	123.67	128.67
13	V	1001	ADP	N3-C2-N1	-3.66	123.71	128.67
13	X	1001	ADP	N3-C2-N1	-3.59	123.80	128.67
13	Y	1001	ADP	N3-C2-N1	-3.55	123.85	128.67
13	W	1001	ADP	N3-C2-N1	-3.52	123.89	128.67
13	V	1001	ADP	C4-C5-N7	-2.54	106.66	109.34
13	U	1001	ADP	C4-C5-N7	-2.49	106.70	109.34
13	Y	1001	ADP	C4-C5-N7	-2.45	106.75	109.34
13	T	1001	ADP	C4-C5-N7	-2.43	106.77	109.34
13	X	1001	ADP	C4-C5-N7	-2.39	106.81	109.34
13	W	1001	ADP	C4'-O4'-C1'	2.25	111.99	109.92
13	W	1001	ADP	C4-C5-N7	-2.25	106.95	109.34

There are no chirality outliers.

All (14) torsion outliers are listed below:

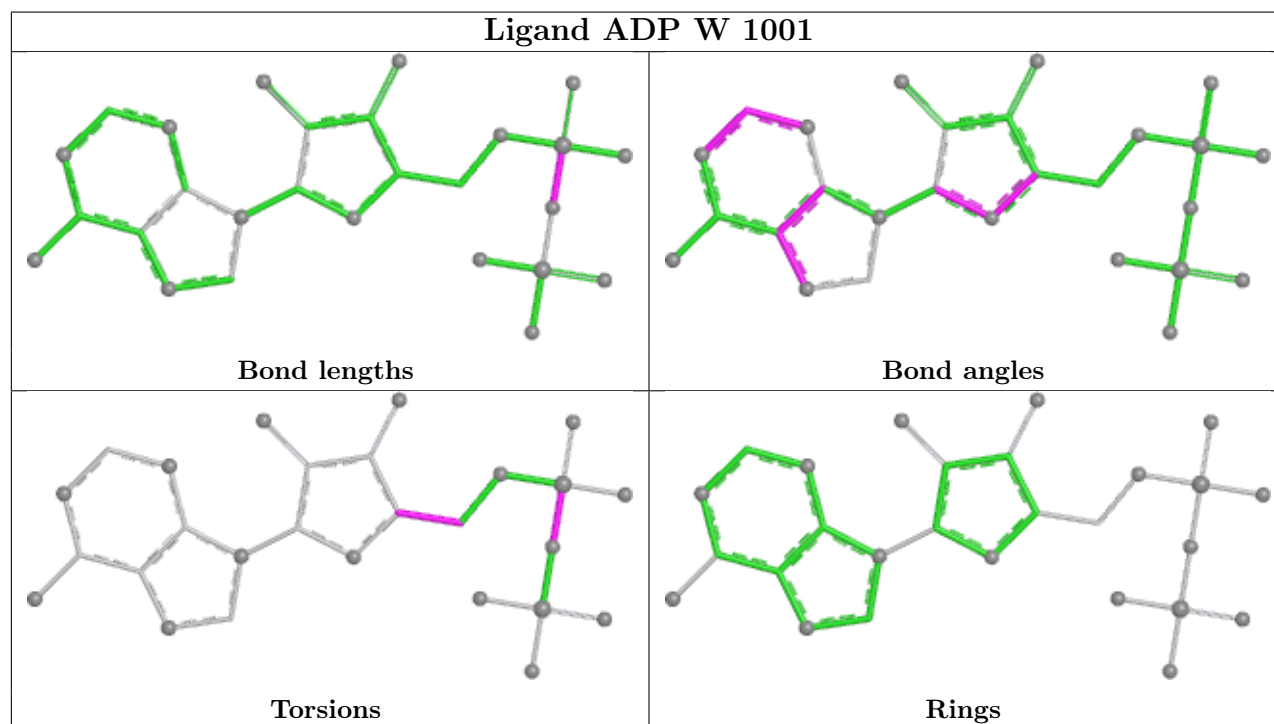
Mol	Chain	Res	Type	Atoms
13	U	1001	ADP	C5'-O5'-PA-O1A
13	U	1001	ADP	C5'-O5'-PA-O2A
13	U	1001	ADP	C5'-O5'-PA-O3A
13	V	1001	ADP	C5'-O5'-PA-O1A
13	V	1001	ADP	C5'-O5'-PA-O2A
13	V	1001	ADP	C5'-O5'-PA-O3A
13	Y	1001	ADP	C5'-O5'-PA-O1A
13	Y	1001	ADP	C5'-O5'-PA-O3A
13	W	1001	ADP	O4'-C4'-C5'-O5'
13	W	1001	ADP	C3'-C4'-C5'-O5'
13	W	1001	ADP	PB-O3A-PA-O5'
13	T	1001	ADP	O4'-C4'-C5'-O5'
13	V	1001	ADP	O4'-C4'-C5'-O5'
13	Y	1001	ADP	PB-O3A-PA-O1A

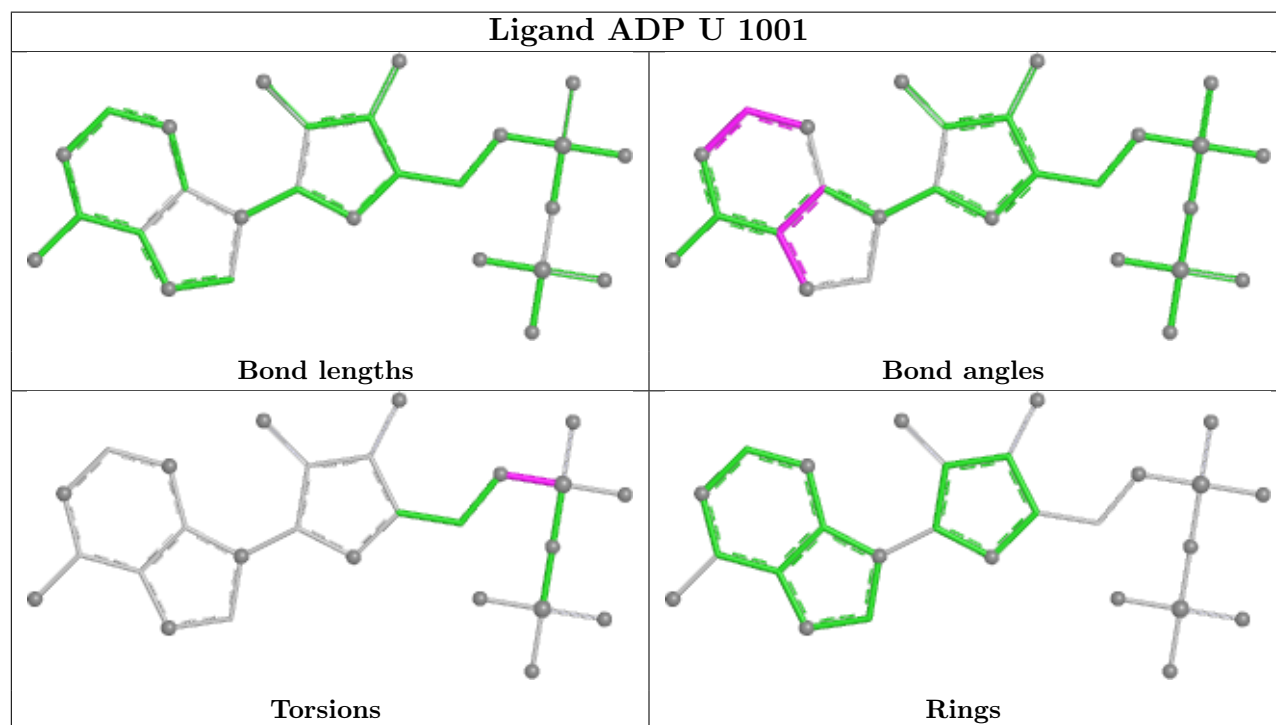
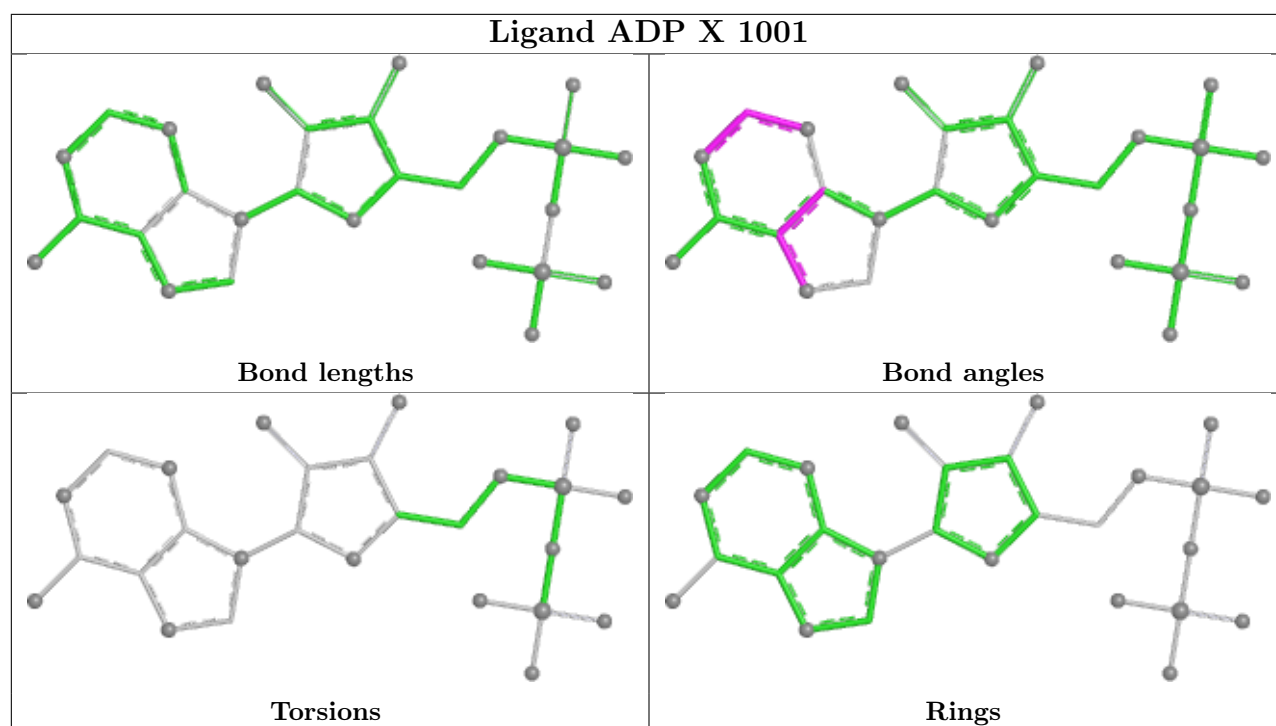
There are no ring outliers.

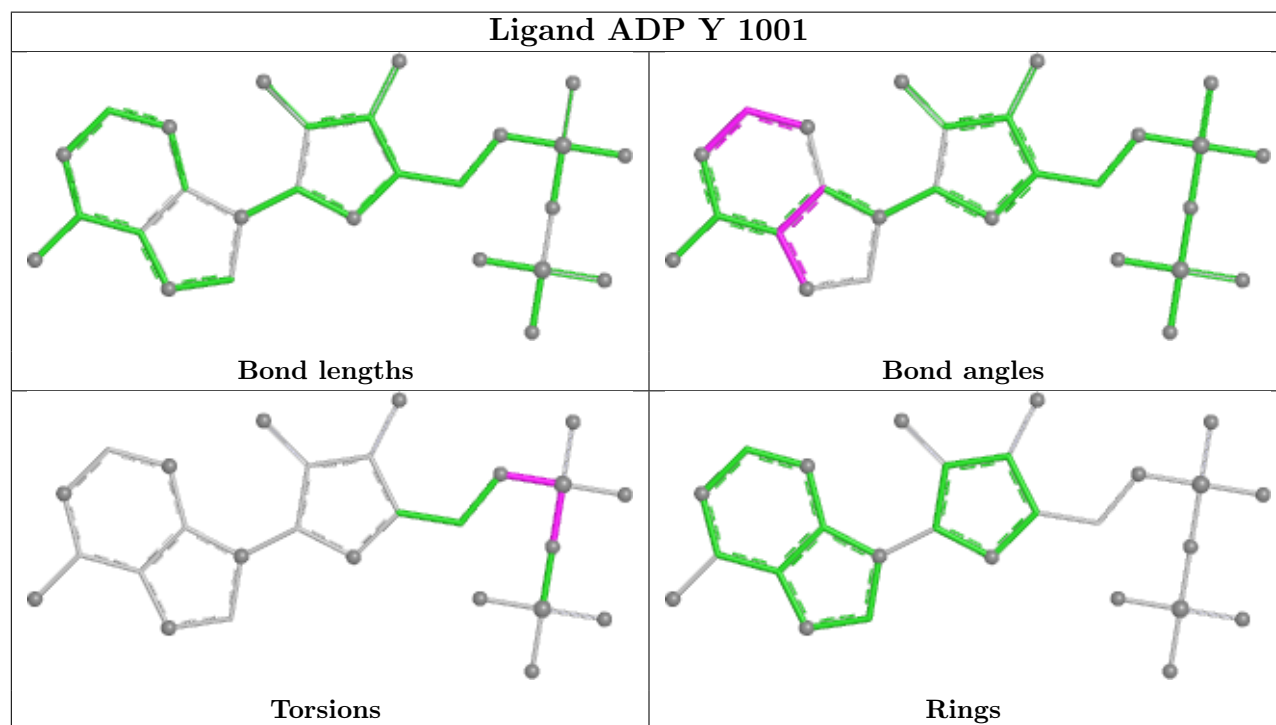
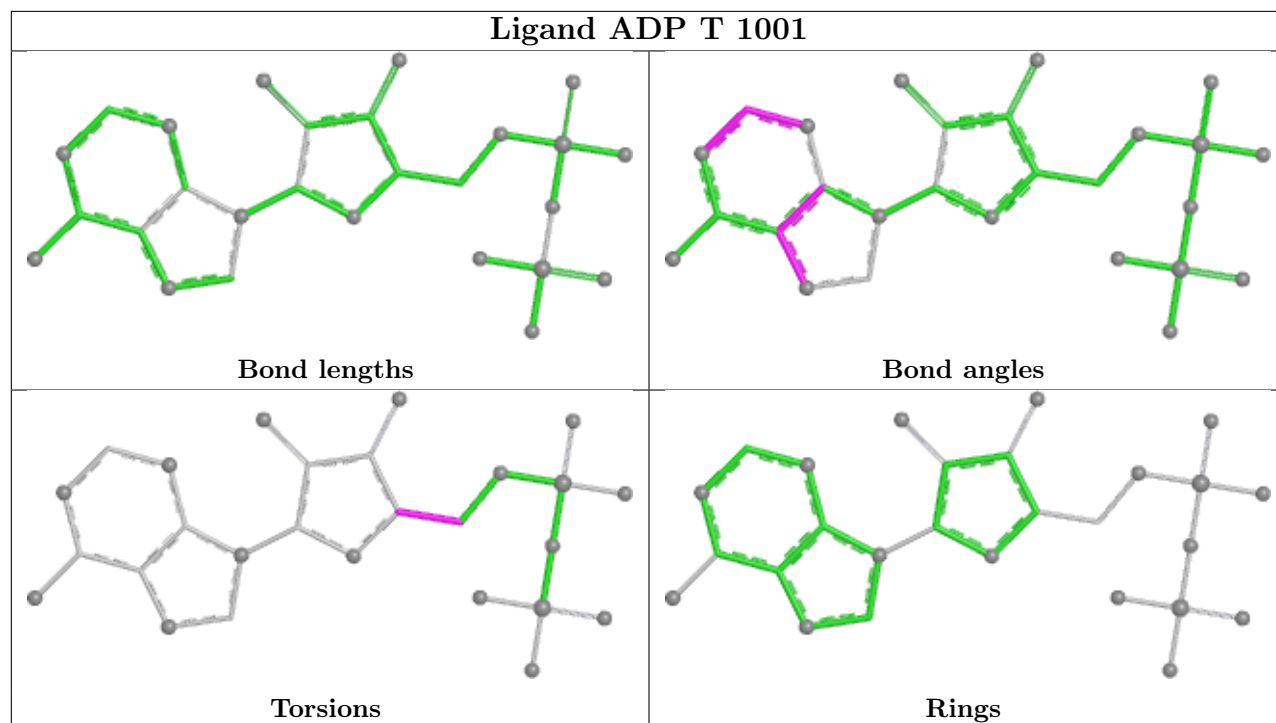
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	W	1001	ADP	2	0
13	T	1001	ADP	2	0
13	Y	1001	ADP	2	0
13	V	1001	ADP	2	0

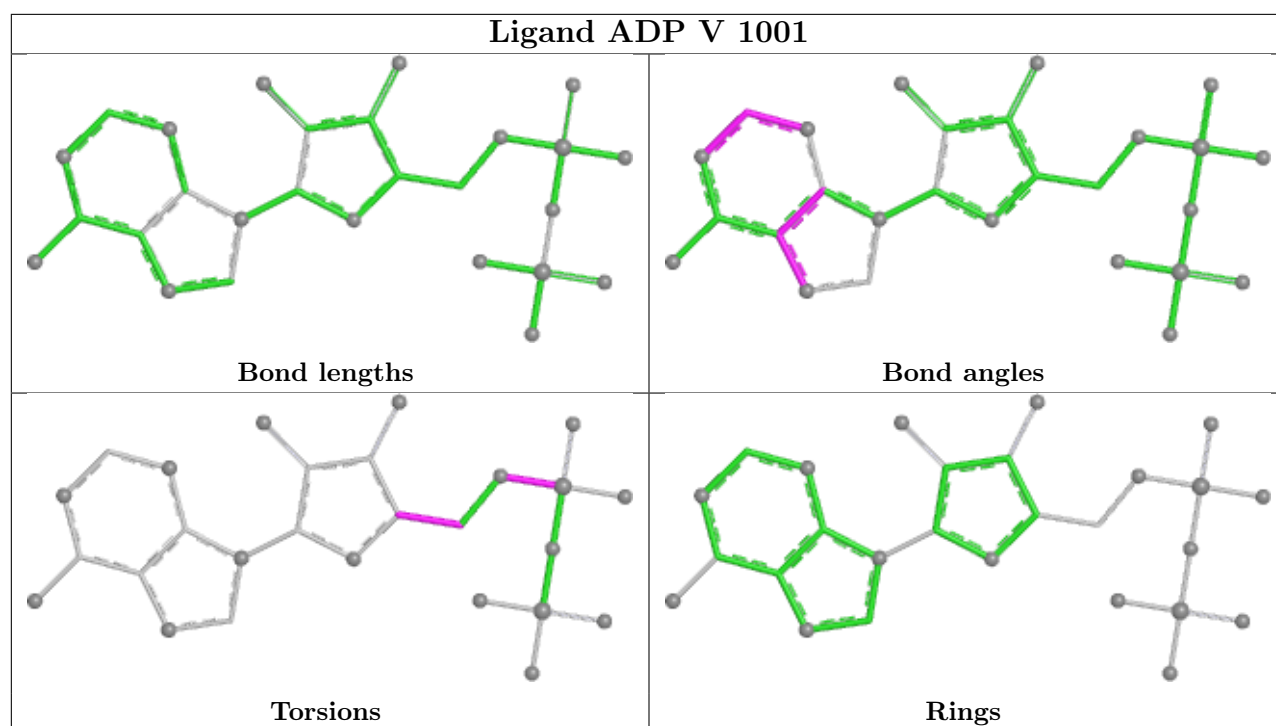
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 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.

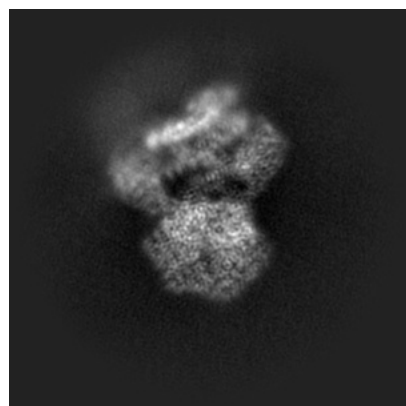
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45369. These allow visual inspection of the internal detail of the map and identification of artifacts.

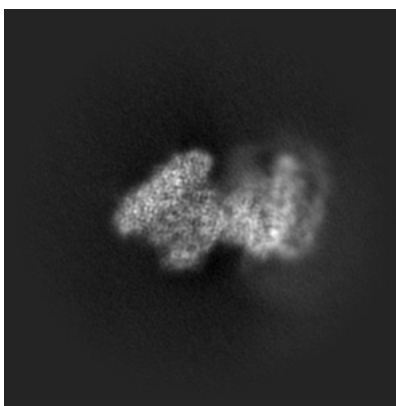
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

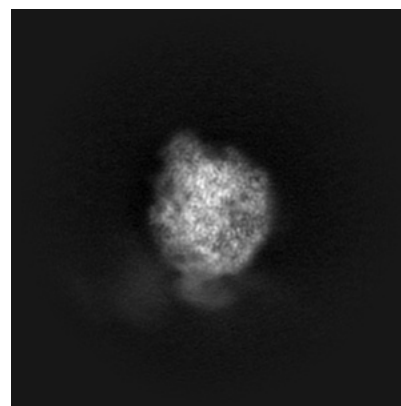
#### 6.1.1 Primary map



X

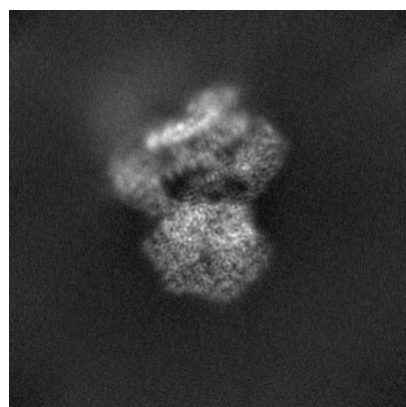


Y

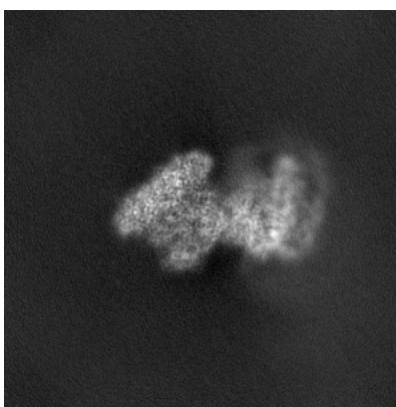


Z

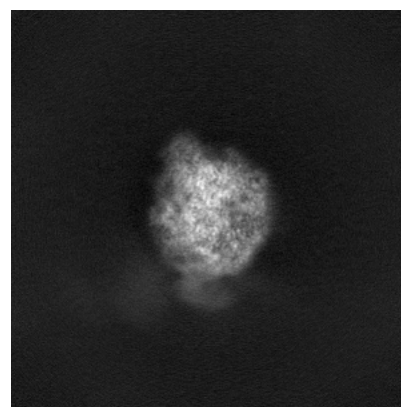
#### 6.1.2 Raw map



X



Y

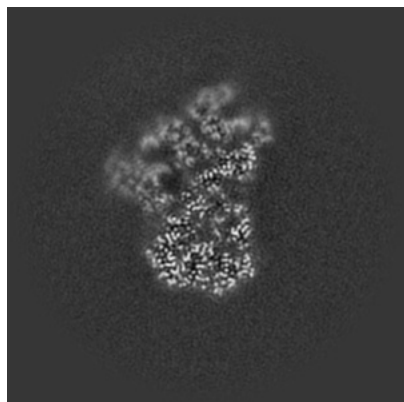


Z

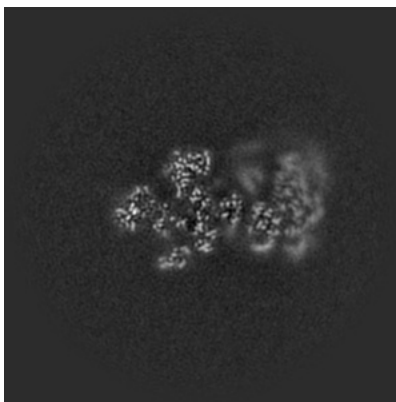
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

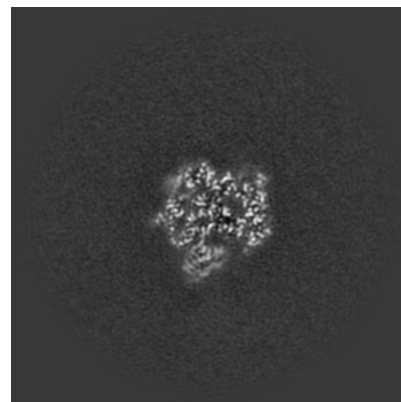
### 6.2.1 Primary map



X Index: 224

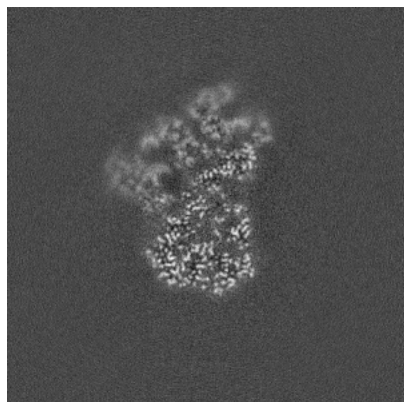


Y Index: 224

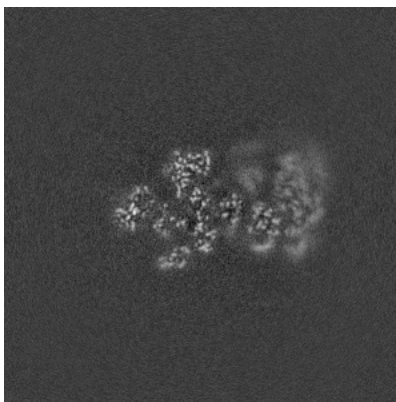


Z Index: 224

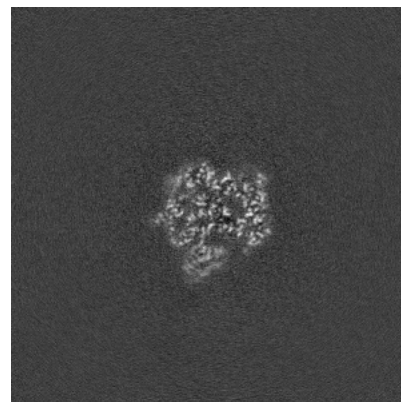
### 6.2.2 Raw map



X Index: 224



Y Index: 224

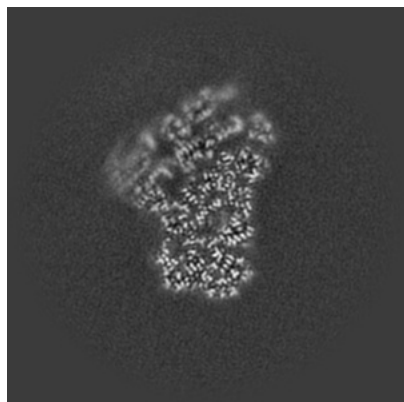


Z Index: 224

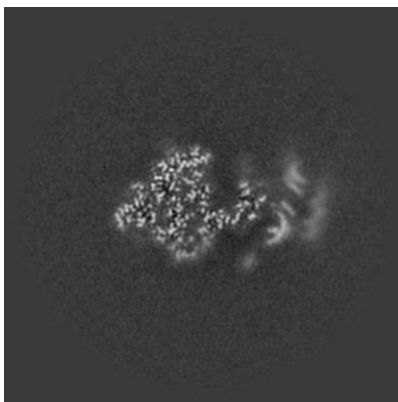
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

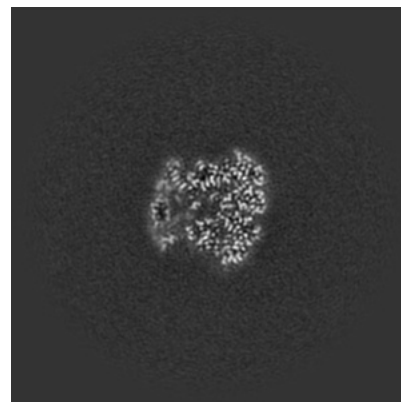
### 6.3.1 Primary map



X Index: 215

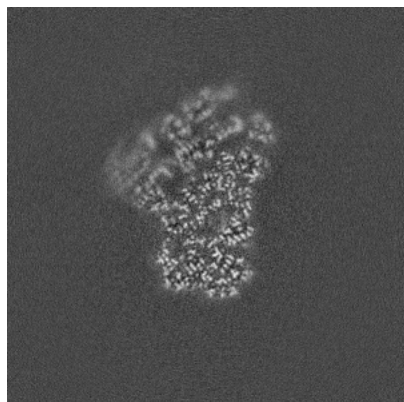


Y Index: 251

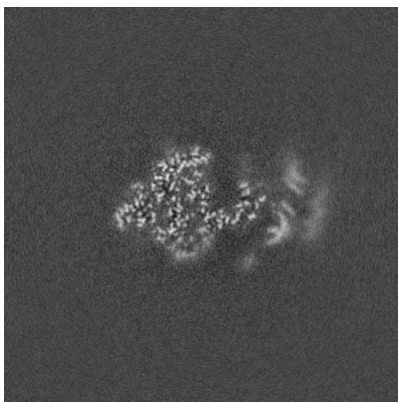


Z Index: 195

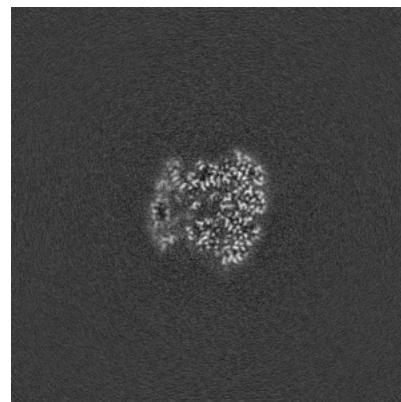
### 6.3.2 Raw map



X Index: 215



Y Index: 251

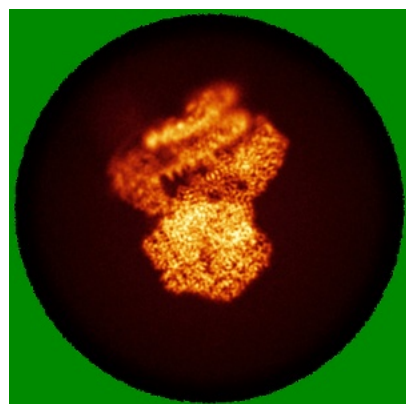


Z Index: 195

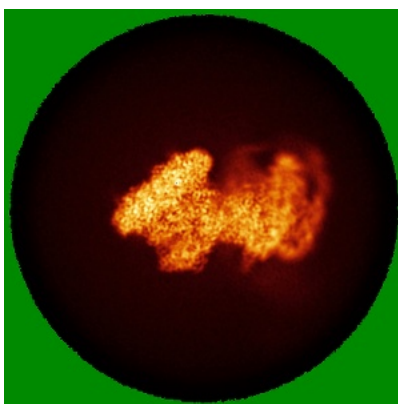
The images above show the largest variance slices of the map in three orthogonal directions.

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

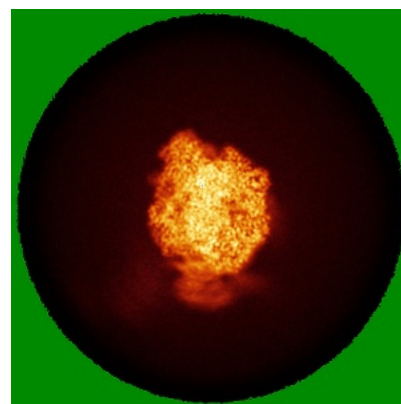
### 6.4.1 Primary map



X

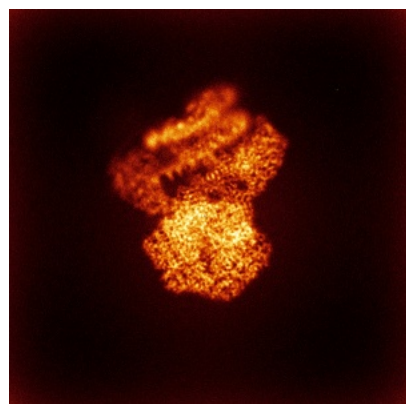


Y

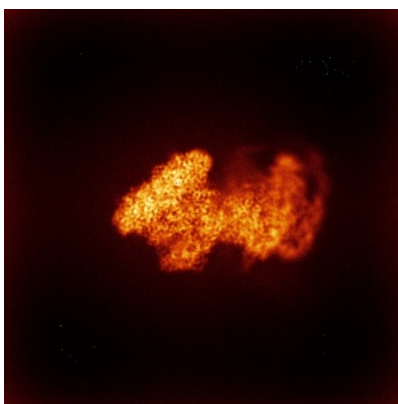


Z

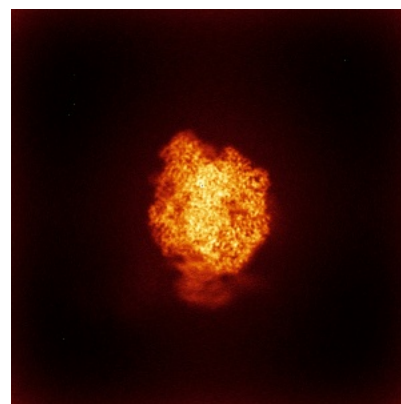
### 6.4.2 Raw map



X



Y



Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



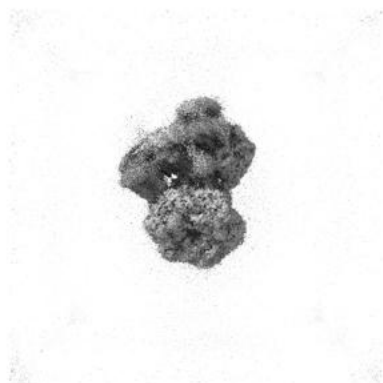
Y



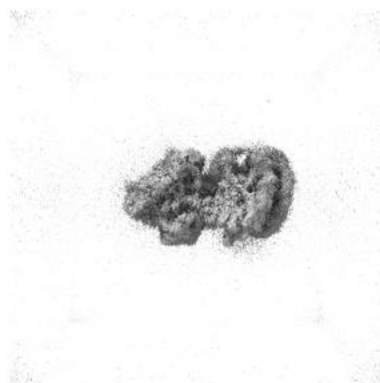
Z

The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

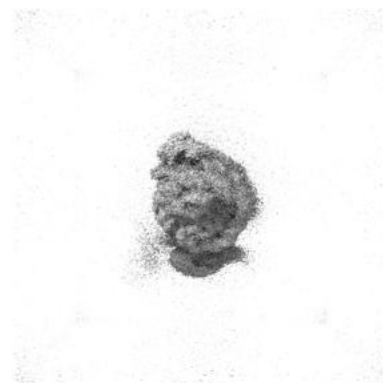
### 6.5.2 Raw map



X



Y



Z

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

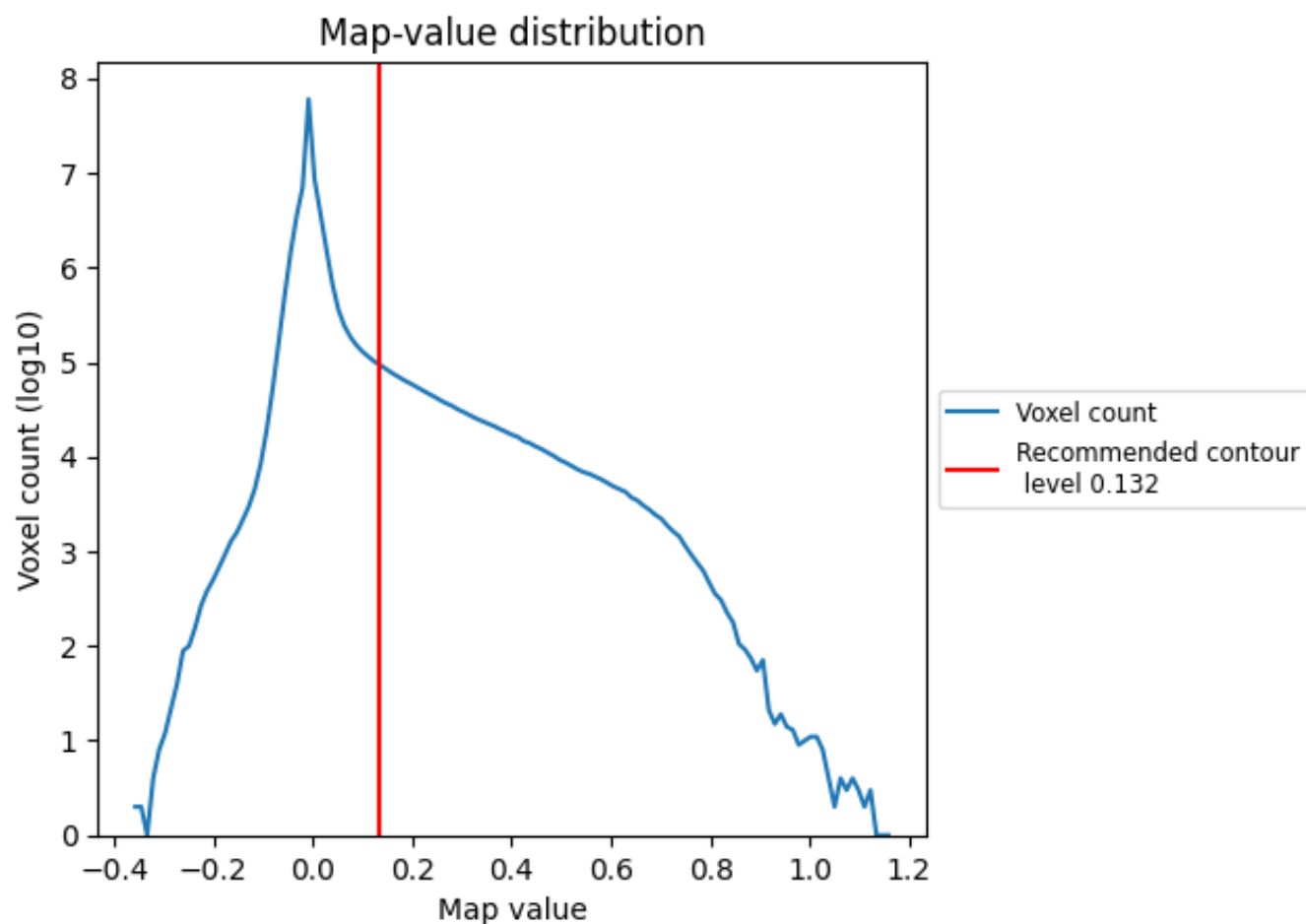
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

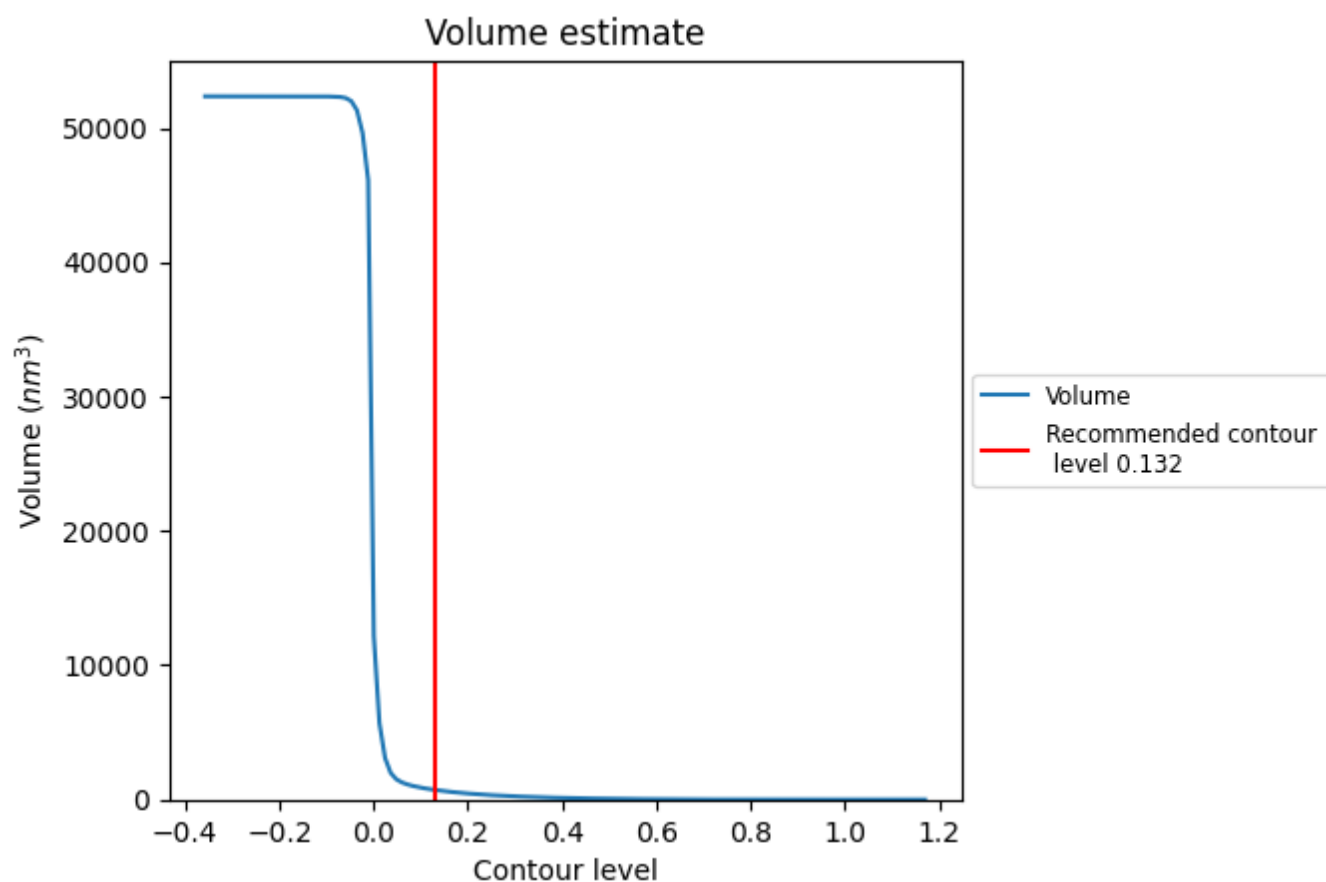
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

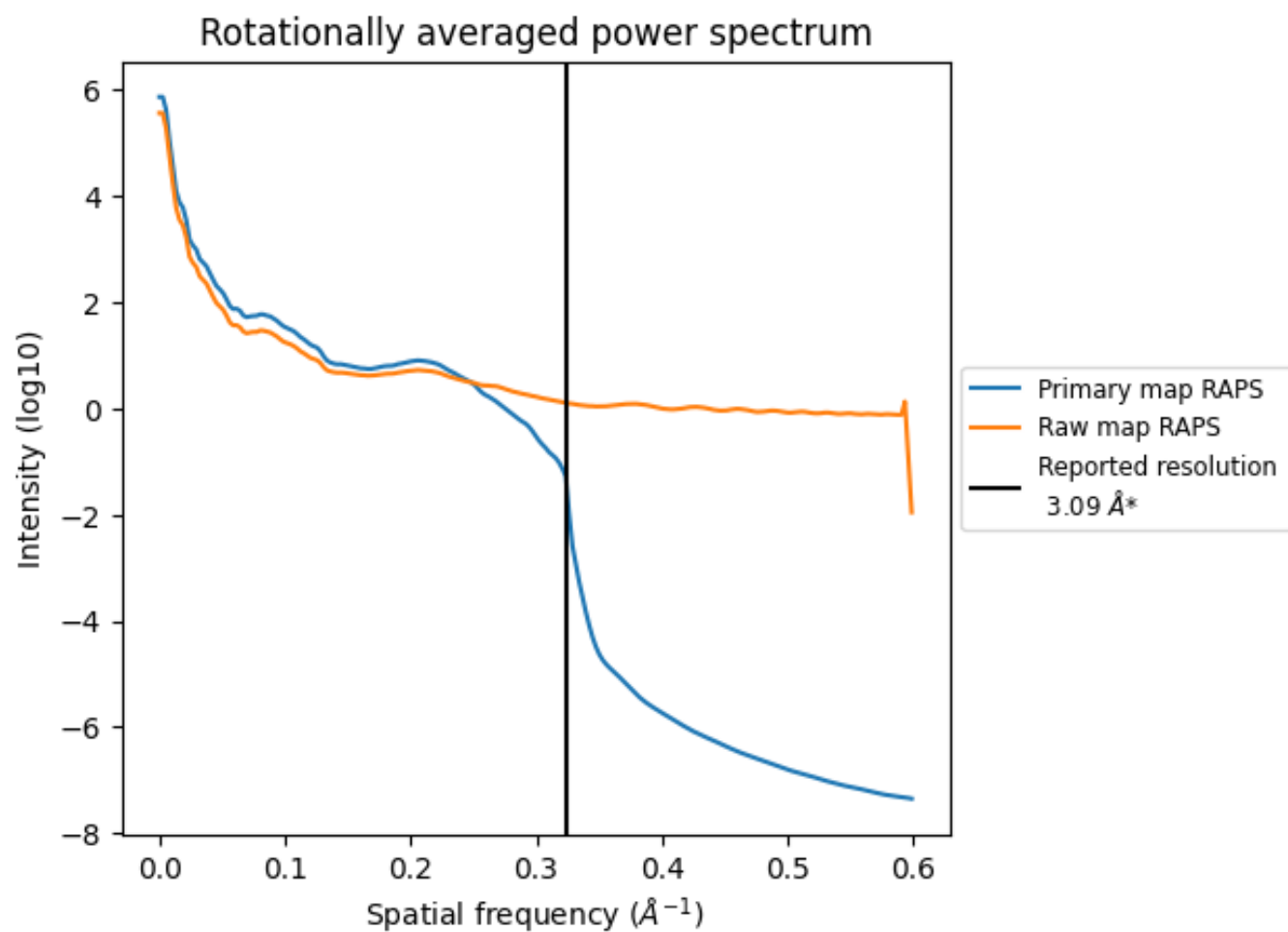


The volume at the recommended contour level is 709 nm<sup>3</sup>; this corresponds to an approximate mass of 640 kDa.

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 ⓘ

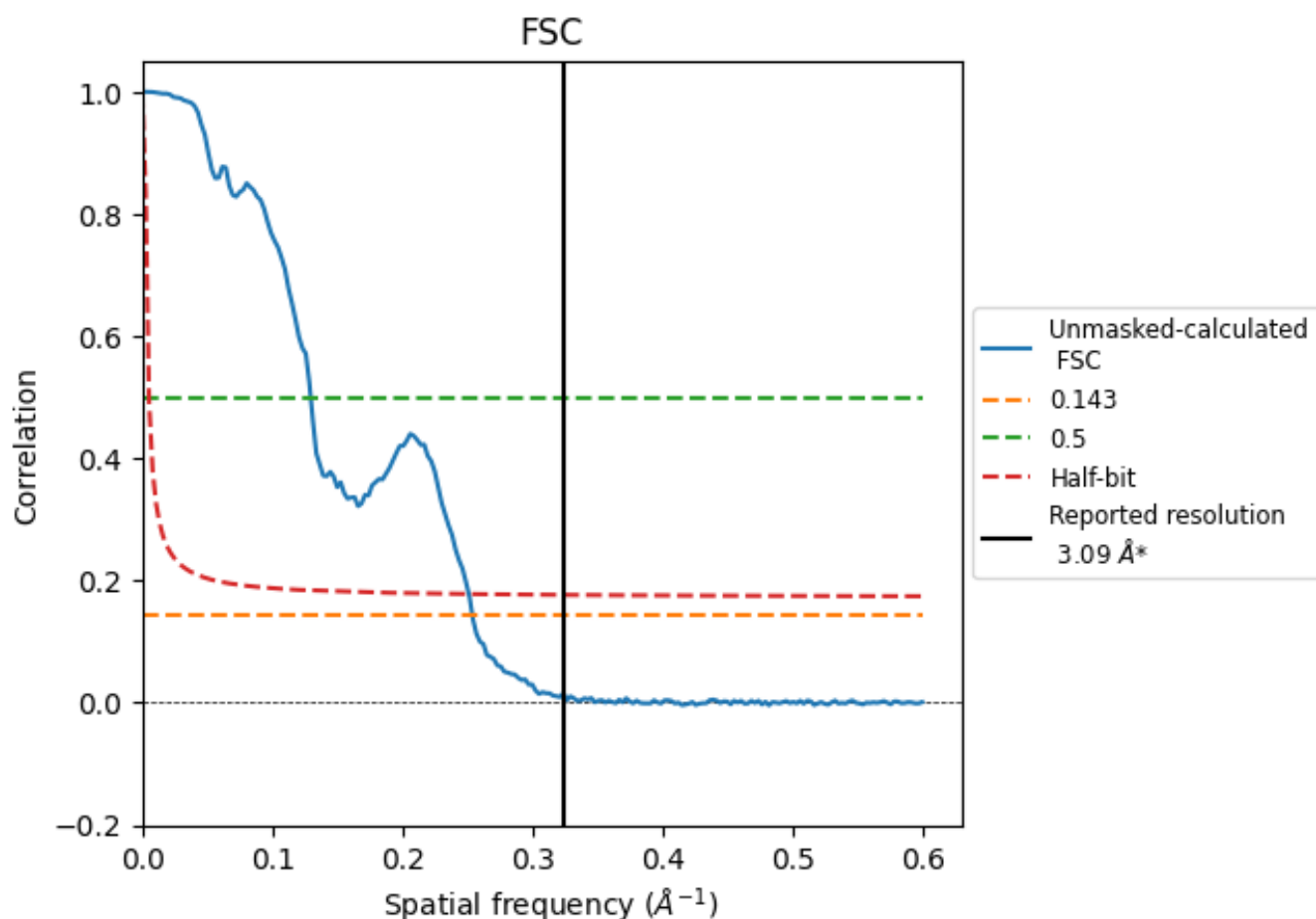


\*Reported resolution corresponds to spatial frequency of 0.324 Å<sup>-1</sup>

## 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  $0.324 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

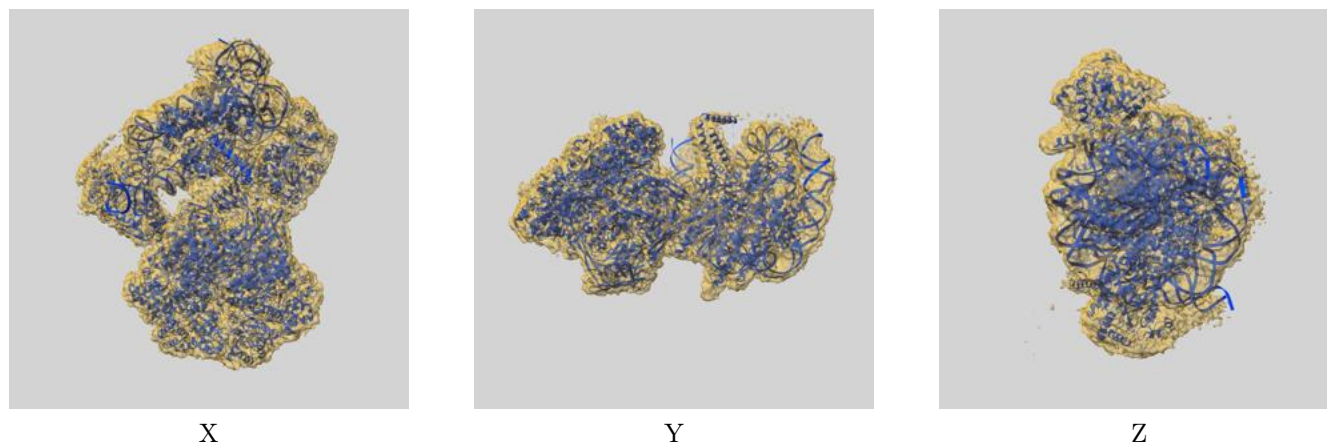
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.09	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	7.73	3.99

\*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 3.95 differs from the reported value 3.09 by more than 10 %

## 9 Map-model fit [i](#)

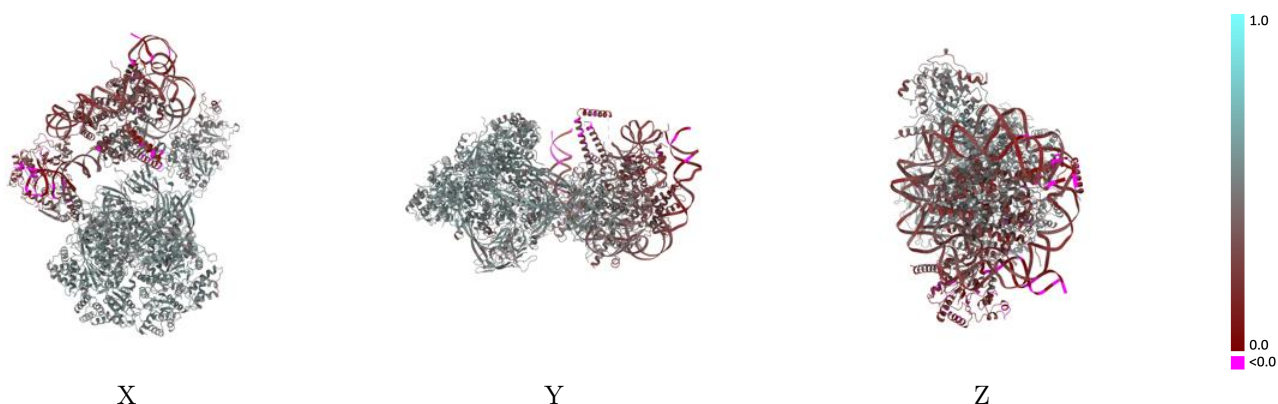
This section contains information regarding the fit between EMDB map EMD-45369 and PDB model 9C9S. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



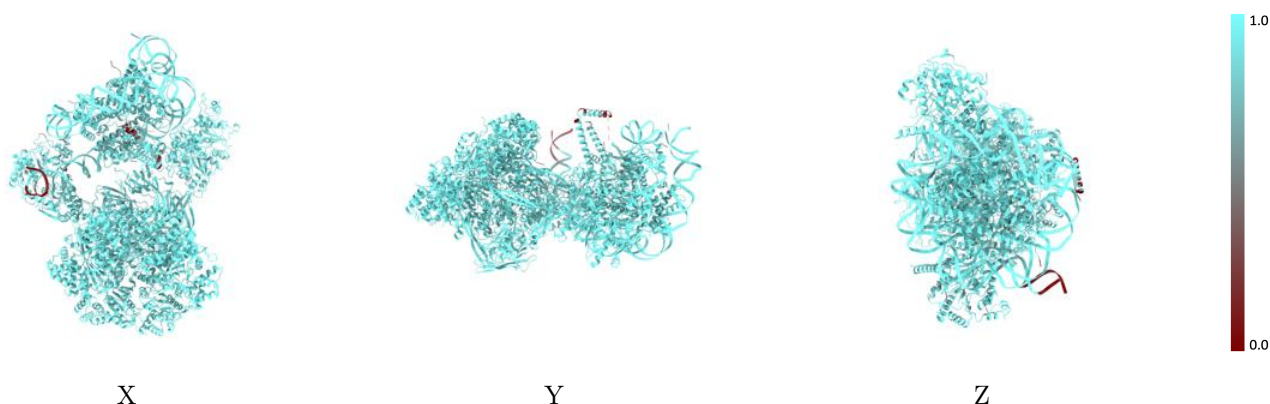
The images above show the 3D surface view of the map at the recommended contour level 0.132 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



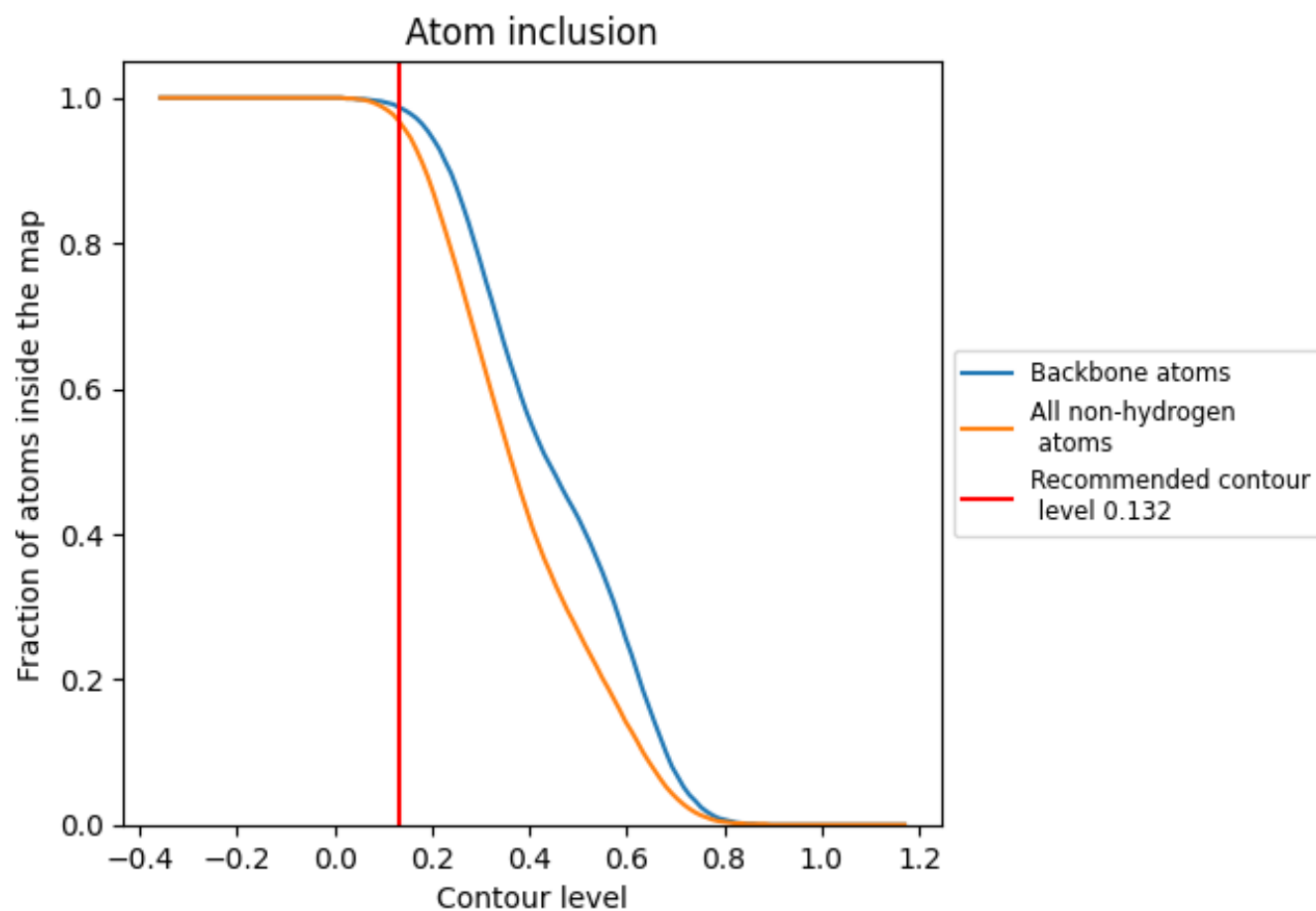
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.132).











































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9680	 0.4240
A	 0.9590	 0.2840
B	 0.9750	 0.2860
C	 0.9550	 0.3030
D	 0.9790	 0.2950
E	 0.9610	 0.2970
F	 0.9550	 0.3360
G	 0.9330	 0.4090
H	 0.9580	 0.4160
I	 0.9310	 0.2380
J	 0.9510	 0.2330
Q	 0.9460	 0.3580
R	 0.9690	 0.4390
S	 0.9870	 0.4550
T	 0.9860	 0.5260
U	 0.9880	 0.5140
V	 0.9830	 0.5070
W	 0.9890	 0.5210
X	 0.9800	 0.5270
Y	 0.9770	 0.5230
Z	 0.9610	 0.4350

