



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 09:08 AM JST

PDB ID : 23FU / pdb_000023fu
EMDB ID : EMD-68935
Title : Cryo-EM structure of Chaetomium thermophilum RSC bound to a nucleosome
Authors : Ma, S.S.; Liu, M.D.; Shen, Q.T.; Chen, Y.
Deposited on : 2026-02-05
Resolution : 4.45 Å(reported)

This is a wwPDB EM Validation Summary 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

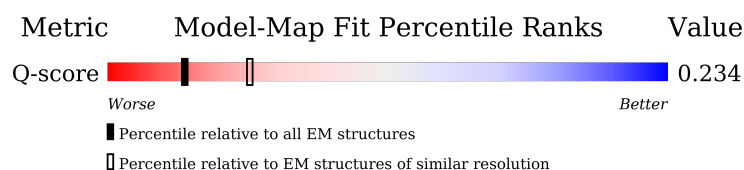
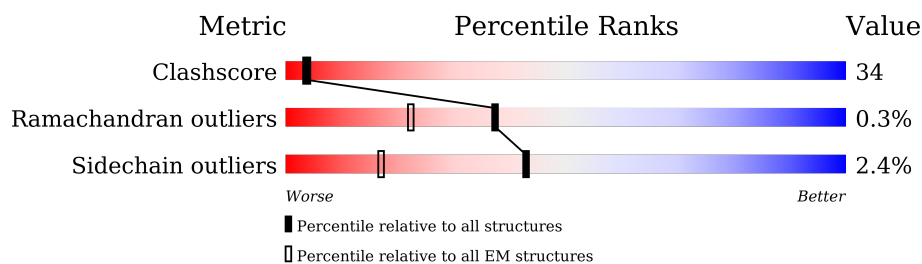
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.45 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3027 (3.95 - 4.95)

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

Mol	Chain	Length	Quality of chain
1	A	135	
1	E	135	
2	B	102	
2	F	102	

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Mol	Chain	Length	Quality of chain
3	C	129	
3	G	129	
4	D	125	
4	H	125	
5	I	167	
6	J	167	
7	K	1595	
8	L	733	
9	M	476	
10	N	694	
10	O	694	
11	P	547	
12	Q	769	
13	R	763	
14	S	607	
15	T	534	
16	U	991	
17	V	990	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 46373 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	91	Total	C	N	O	S	0	0
			744	469	141	131	3		
1	E	91	Total	C	N	O	S	0	0
			744	469	141	131	3		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			648	410	126	111	1		
2	F	77	Total	C	N	O	S	0	0
			614	389	119	105	1		

- Molecule 3 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	95	Total	C	N	O	0	0
			733	459	145	129		
3	G	95	Total	C	N	O	0	0
			734	461	145	128		

- Molecule 4 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	88	Total	C	N	O	S	0	0
			685	433	121	129	2		
4	H	90	Total	C	N	O	S	0	0
			703	444	124	133	2		

- Molecule 5 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	132	Total	C	N	O	P	0	0
			2694	1277	493	792	132		

- Molecule 6 is a DNA chain called DNA (167-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	132	Total	C	N	O	P	0	0
			2718	1285	509	792	132		

- Molecule 7 is a protein called WD40 repeat-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	826	Total	C	N	O	S	0	0
			6825	4307	1254	1229	35		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-60	GLY	-	expression tag	UNP G0SHD8
K	-59	SER	-	expression tag	UNP G0SHD8
K	-58	PRO	-	expression tag	UNP G0SHD8
K	-57	GLN	-	expression tag	UNP G0SHD8
K	-56	GLN	-	expression tag	UNP G0SHD8
K	-55	ASN	-	expression tag	UNP G0SHD8
K	-54	LYS	-	expression tag	UNP G0SHD8
K	-53	THR	-	expression tag	UNP G0SHD8
K	-52	ALA	-	expression tag	UNP G0SHD8
K	-51	ALA	-	expression tag	UNP G0SHD8
K	-50	LEU	-	expression tag	UNP G0SHD8
K	-49	ALA	-	expression tag	UNP G0SHD8
K	-48	GLN	-	expression tag	UNP G0SHD8
K	-47	HIS	-	expression tag	UNP G0SHD8
K	-46	ASP	-	expression tag	UNP G0SHD8
K	-45	GLU	-	expression tag	UNP G0SHD8
K	-44	ALA	-	expression tag	UNP G0SHD8
K	-43	ASP	-	expression tag	UNP G0SHD8
K	-42	TYR	-	expression tag	UNP G0SHD8
K	-41	LYS	-	expression tag	UNP G0SHD8
K	-40	ASP	-	expression tag	UNP G0SHD8
K	-39	HIS	-	expression tag	UNP G0SHD8
K	-38	ASP	-	expression tag	UNP G0SHD8
K	-37	GLY	-	expression tag	UNP G0SHD8
K	-36	ASP	-	expression tag	UNP G0SHD8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-35	TYR	-	expression tag	UNP G0SHD8
K	-34	LYS	-	expression tag	UNP G0SHD8
K	-33	ASP	-	expression tag	UNP G0SHD8
K	-32	HIS	-	expression tag	UNP G0SHD8
K	-31	ASP	-	expression tag	UNP G0SHD8
K	-30	ILE	-	expression tag	UNP G0SHD8
K	-29	ASP	-	expression tag	UNP G0SHD8
K	-28	TYR	-	expression tag	UNP G0SHD8
K	-27	LYS	-	expression tag	UNP G0SHD8
K	-26	ASP	-	expression tag	UNP G0SHD8
K	-25	ASP	-	expression tag	UNP G0SHD8
K	-24	ASP	-	expression tag	UNP G0SHD8
K	-23	ASP	-	expression tag	UNP G0SHD8
K	-22	LYS	-	expression tag	UNP G0SHD8
K	-21	GLY	-	expression tag	UNP G0SHD8
K	-20	GLY	-	expression tag	UNP G0SHD8
K	-19	SER	-	expression tag	UNP G0SHD8
K	-18	GLY	-	expression tag	UNP G0SHD8
K	-17	GLY	-	expression tag	UNP G0SHD8
K	-16	SER	-	expression tag	UNP G0SHD8
K	-15	LEU	-	expression tag	UNP G0SHD8
K	-14	GLU	-	expression tag	UNP G0SHD8
K	-13	VAL	-	expression tag	UNP G0SHD8
K	-12	LEU	-	expression tag	UNP G0SHD8
K	-11	PHE	-	expression tag	UNP G0SHD8
K	-10	GLN	-	expression tag	UNP G0SHD8
K	-9	GLY	-	expression tag	UNP G0SHD8
K	-8	PRO	-	expression tag	UNP G0SHD8
K	-7	GLY	-	expression tag	UNP G0SHD8
K	-6	GLY	-	expression tag	UNP G0SHD8
K	-5	SER	-	expression tag	UNP G0SHD8
K	-4	GLY	-	expression tag	UNP G0SHD8
K	-3	GLY	-	expression tag	UNP G0SHD8
K	-2	SER	-	expression tag	UNP G0SHD8
K	-1	GLY	-	expression tag	UNP G0SHD8
K	0	THR	-	expression tag	UNP G0SHD8
K	112	VAL	ILE	conflict	UNP G0SHD8
K	280	ILE	VAL	conflict	UNP G0SHD8
K	1511	THR	ALA	conflict	UNP G0SHD8

- Molecule 8 is a protein called Putative chromatin structure remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	415	Total	C	N	O	S	0	0
			3340	2121	587	614	18		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	374	PRO	ALA	conflict	UNP G0S882
L	375	ALA	THR	conflict	UNP G0S882
L	415	LYS	ARG	conflict	UNP G0S882
L	428	SER	PRO	conflict	UNP G0S882
L	712	GLU	-	expression tag	UNP G0S882
L	713	LEU	-	expression tag	UNP G0S882
L	714	GLY	-	expression tag	UNP G0S882
L	715	PRO	-	expression tag	UNP G0S882
L	716	LYS	-	expression tag	UNP G0S882
L	717	GLY	-	expression tag	UNP G0S882
L	718	ILE	-	expression tag	UNP G0S882
L	719	ARG	-	expression tag	UNP G0S882
L	720	SER	-	expression tag	UNP G0S882
L	721	HIS	-	expression tag	UNP G0S882
L	722	SER	-	expression tag	UNP G0S882
L	723	MET	-	expression tag	UNP G0S882
L	724	LEU	-	expression tag	UNP G0S882
L	725	ALA	-	expression tag	UNP G0S882
L	726	LEU	-	expression tag	UNP G0S882
L	727	GLU	-	expression tag	UNP G0S882
L	728	HIS	-	expression tag	UNP G0S882
L	729	HIS	-	expression tag	UNP G0S882
L	730	HIS	-	expression tag	UNP G0S882
L	731	HIS	-	expression tag	UNP G0S882
L	732	HIS	-	expression tag	UNP G0S882
L	733	HIS	-	expression tag	UNP G0S882

- Molecule 9 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	431	Total	C	N	O	S	0	0
			3371	2141	590	625	15		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	469	LEU	-	expression tag	UNP G0SBW4

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Chain	Residue	Modelled	Actual	Comment	Reference
M	470	GLU	-	expression tag	UNP G0SBW4
M	471	HIS	-	expression tag	UNP G0SBW4
M	472	HIS	-	expression tag	UNP G0SBW4
M	473	HIS	-	expression tag	UNP G0SBW4
M	474	HIS	-	expression tag	UNP G0SBW4
M	475	HIS	-	expression tag	UNP G0SBW4
M	476	HIS	-	expression tag	UNP G0SBW4

- Molecule 10 is a protein called Ssr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	471	Total	C	N	O	S	0	0
			3714	2319	662	713	20		
10	O	274	Total	C	N	O	S	0	0
			2245	1421	404	409	11		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	687	ASP	-	expression tag	UNP G0S647
N	688	TYR	-	expression tag	UNP G0S647
N	689	LYS	-	expression tag	UNP G0S647
N	690	ASP	-	expression tag	UNP G0S647
N	691	ASP	-	expression tag	UNP G0S647
N	692	ASP	-	expression tag	UNP G0S647
N	693	ASP	-	expression tag	UNP G0S647
N	694	LYS	-	expression tag	UNP G0S647
O	687	ASP	-	expression tag	UNP G0S647
O	688	TYR	-	expression tag	UNP G0S647
O	689	LYS	-	expression tag	UNP G0S647
O	690	ASP	-	expression tag	UNP G0S647
O	691	ASP	-	expression tag	UNP G0S647
O	692	ASP	-	expression tag	UNP G0S647
O	693	ASP	-	expression tag	UNP G0S647
O	694	LYS	-	expression tag	UNP G0S647

- Molecule 11 is a protein called DM2 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	377	Total	C	N	O	S	0	0
			3089	1944	553	583	9		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	191	ASP	ASN	conflict	UNP G0RYN3
P	540	ASP	-	expression tag	UNP G0RYN3
P	541	TYR	-	expression tag	UNP G0RYN3
P	542	LYS	-	expression tag	UNP G0RYN3
P	543	ASP	-	expression tag	UNP G0RYN3
P	544	ASP	-	expression tag	UNP G0RYN3
P	545	ASP	-	expression tag	UNP G0RYN3
P	546	ASP	-	expression tag	UNP G0RYN3
P	547	LYS	-	expression tag	UNP G0RYN3

- Molecule 12 is a protein called DUF1750-domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	319	Total	C	N	O	S	0	0
			2620	1679	466	465	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	763	ASP	-	expression tag	UNP G0SEZ9
Q	764	TYR	-	expression tag	UNP G0SEZ9
Q	765	LYS	-	expression tag	UNP G0SEZ9
Q	766	ASP	-	expression tag	UNP G0SEZ9
Q	767	ASP	-	expression tag	UNP G0SEZ9
Q	768	ASP	-	expression tag	UNP G0SEZ9
Q	769	ASP	-	expression tag	UNP G0SEZ9
Q	770	LYS	-	expression tag	UNP G0SEZ9

- Molecule 13 is a protein called Putative chromatin structure-remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	415	Total	C	N	O	S	0	0
			3307	2103	569	620	15		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	269	MET	-	initiating methionine	UNP G0S909
R	444	ILE	ASN	conflict	UNP G0S909
R	601	GLU	ASP	conflict	UNP G0S909
R	741	THR	SER	conflict	UNP G0S909

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Chain	Residue	Modelled	Actual	Comment	Reference
R	1026	HIS	-	expression tag	UNP G0S909
R	1027	HIS	-	expression tag	UNP G0S909
R	1028	HIS	-	expression tag	UNP G0S909
R	1029	HIS	-	expression tag	UNP G0S909
R	1030	HIS	-	expression tag	UNP G0S909
R	1031	HIS	-	expression tag	UNP G0S909

- Molecule 14 is a protein called Putative chromatin structure-remodeling complex protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	411	Total	C	N	O	S	0	0
			3276	2066	583	615	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	6	ASP	ASN	conflict	UNP G0S475
S	272	ILE	THR	conflict	UNP G0S475
S	600	ASP	-	expression tag	UNP G0S475
S	601	TYR	-	expression tag	UNP G0S475
S	602	LYS	-	expression tag	UNP G0S475
S	603	ASP	-	expression tag	UNP G0S475
S	604	ASP	-	expression tag	UNP G0S475
S	605	ASP	-	expression tag	UNP G0S475
S	606	ASP	-	expression tag	UNP G0S475
S	607	LYS	-	expression tag	UNP G0S475

- Molecule 15 is a protein called Rsc7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	197	Total	C	N	O	S	0	0
			1585	997	286	296	6		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	527	ASP	-	expression tag	UNP G0S6N5
T	528	TYR	-	expression tag	UNP G0S6N5
T	529	LYS	-	expression tag	UNP G0S6N5
T	530	ASP	-	expression tag	UNP G0S6N5
T	531	ASP	-	expression tag	UNP G0S6N5
T	532	ASP	-	expression tag	UNP G0S6N5

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Chain	Residue	Modelled	Actual	Comment	Reference
T	533	ASP	-	expression tag	UNP G0S6N5
T	534	LYS	-	expression tag	UNP G0S6N5

- Molecule 16 is a protein called Rsc1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	105	Total	C	N	O	S	0	0
			844	517	161	165	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	294	GLY	ASP	conflict	UNP G0SB54
U	300	ASP	ASN	conflict	UNP G0SB54
U	363	HIS	TYR	conflict	UNP G0SB54
U	984	ASP	-	expression tag	UNP G0SB54
U	985	TYR	-	expression tag	UNP G0SB54
U	986	LYS	-	expression tag	UNP G0SB54
U	987	ASP	-	expression tag	UNP G0SB54
U	988	ASP	-	expression tag	UNP G0SB54
U	989	ASP	-	expression tag	UNP G0SB54
U	990	ASP	-	expression tag	UNP G0SB54
U	991	LYS	-	expression tag	UNP G0SB54

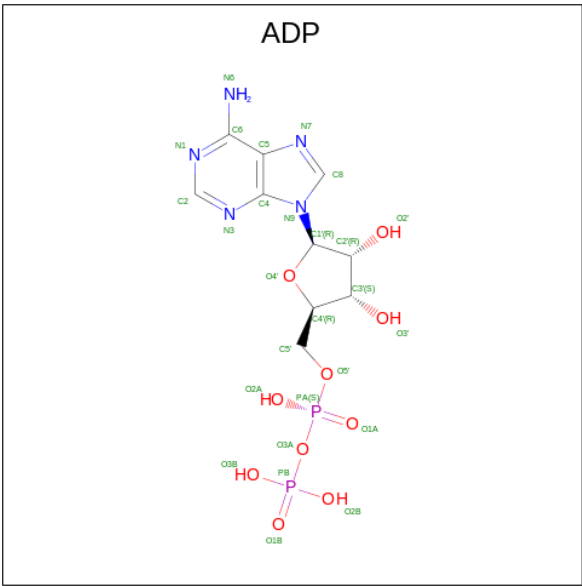
- Molecule 17 is a protein called Rsc58.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	143	Total	C	N	O	S	0	0
			1113	692	193	223	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	300	GLU	ASP	conflict	UNP G0S281
V	612	HIS	PRO	conflict	UNP G0S281
V	985	HIS	-	expression tag	UNP G0S281
V	986	HIS	-	expression tag	UNP G0S281
V	987	HIS	-	expression tag	UNP G0S281
V	988	HIS	-	expression tag	UNP G0S281
V	989	HIS	-	expression tag	UNP G0S281
V	990	HIS	-	expression tag	UNP G0S281

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

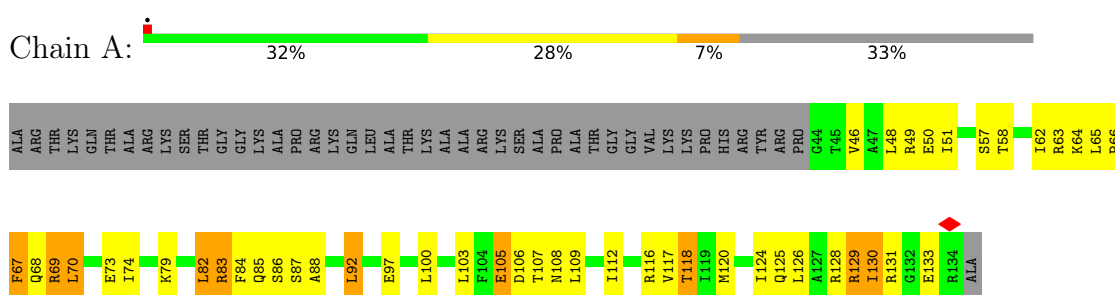


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	K	1	27	10	5	10	2	0

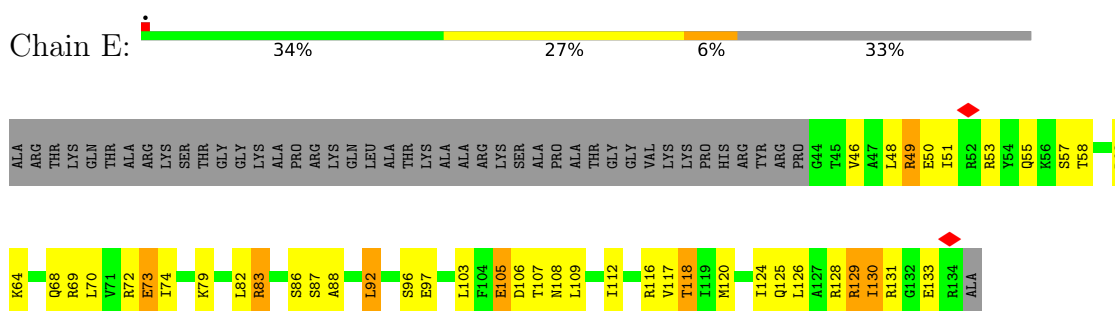
3 Residue-property plots [i](#)

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

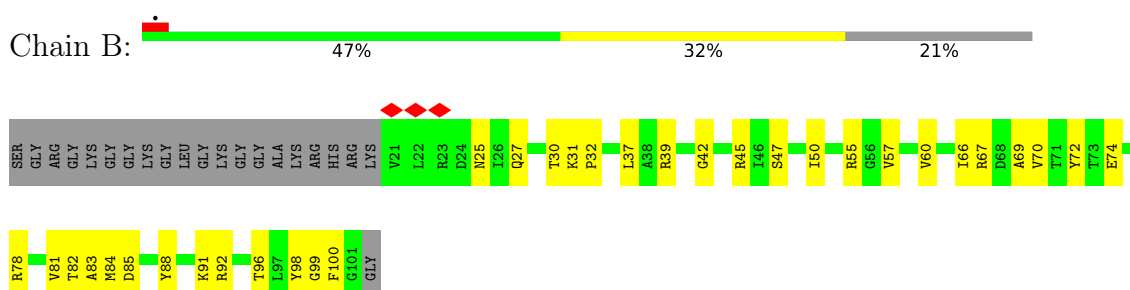
• Molecule 1: Histone H3



• Molecule 1: Histone H3



• Molecule 2: Histone H4

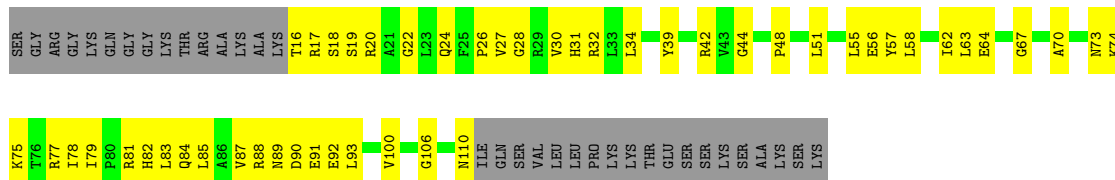


• Molecule 2: Histone H4

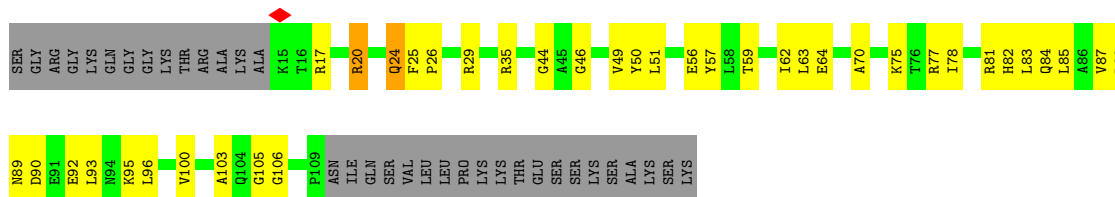




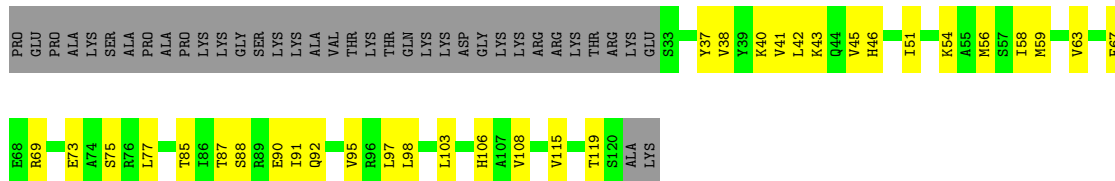
- Molecule 3: Histone H2A



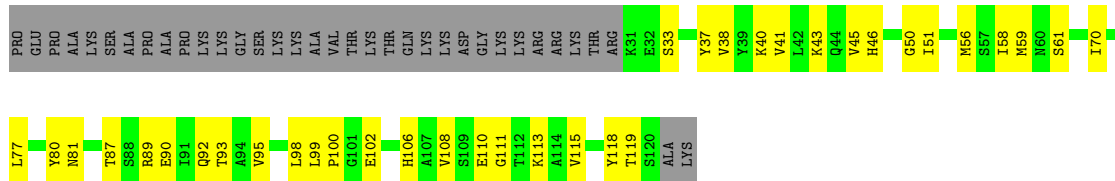
- Molecule 3: Histone H2A



- Molecule 4: Histone H2B



- Molecule 4: Histone H2B

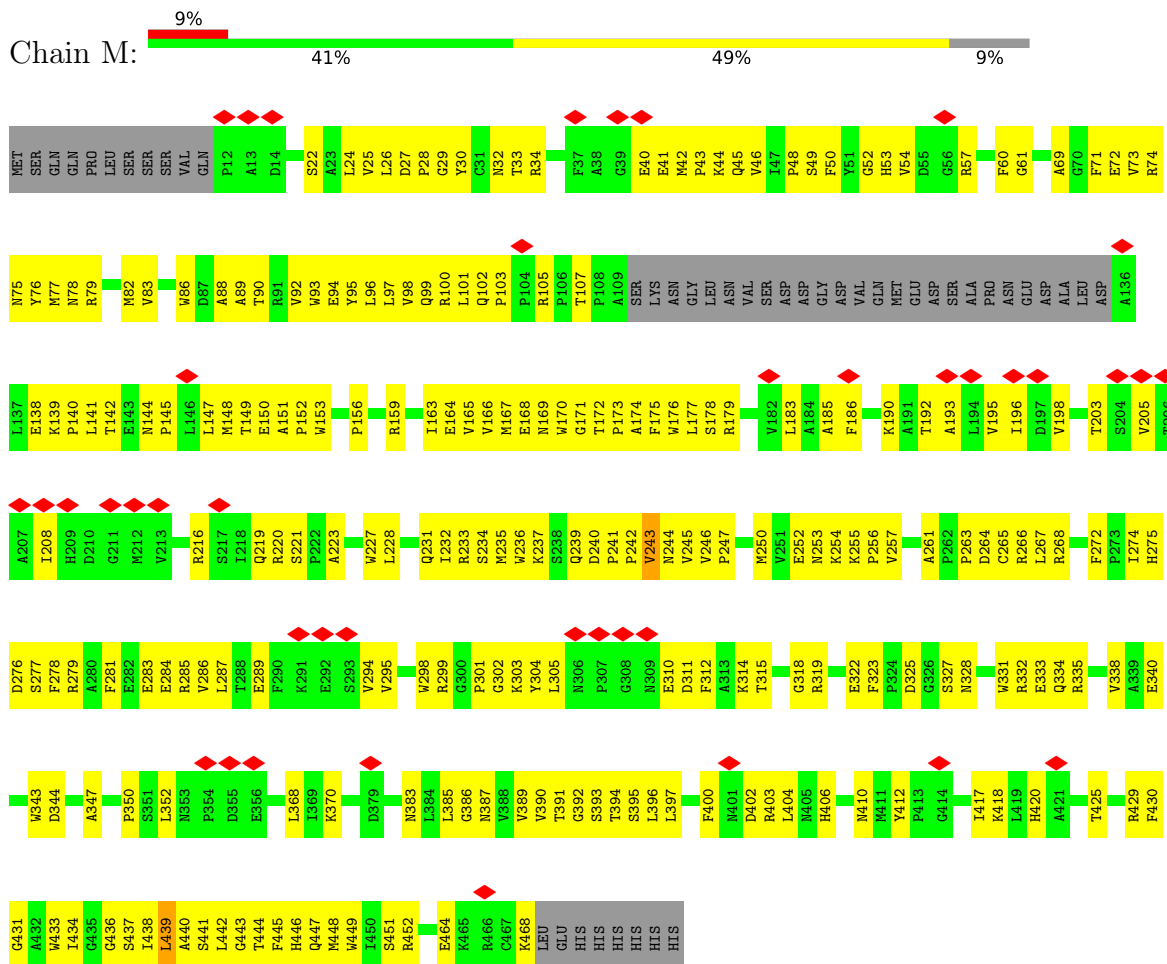


- Molecule 5: DNA (167-MER)

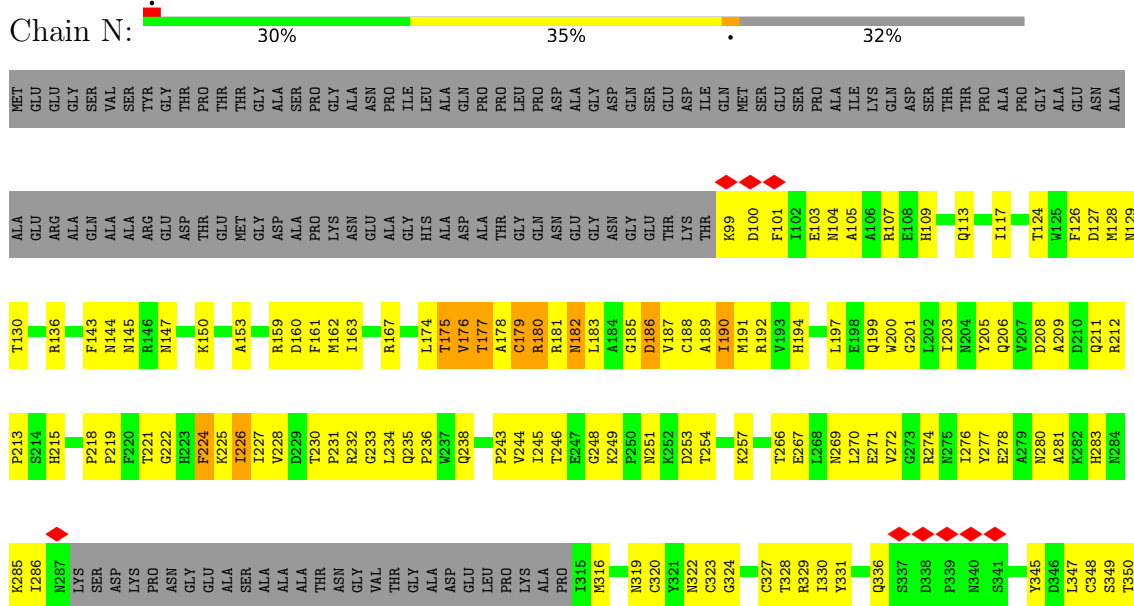




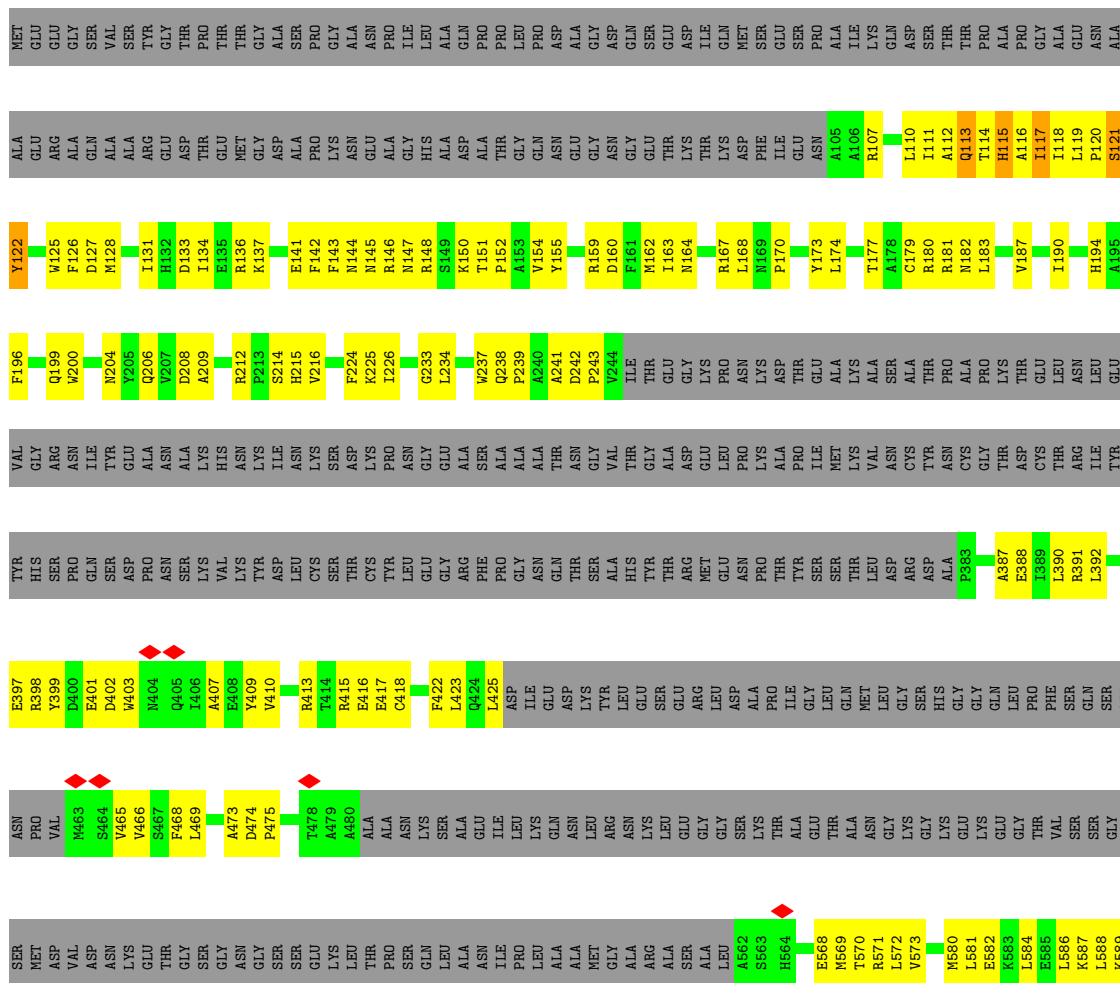
Chain M:



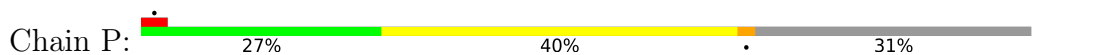
Chain N:



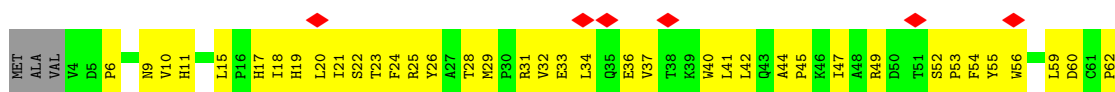
- Molecule 10: Ssr1

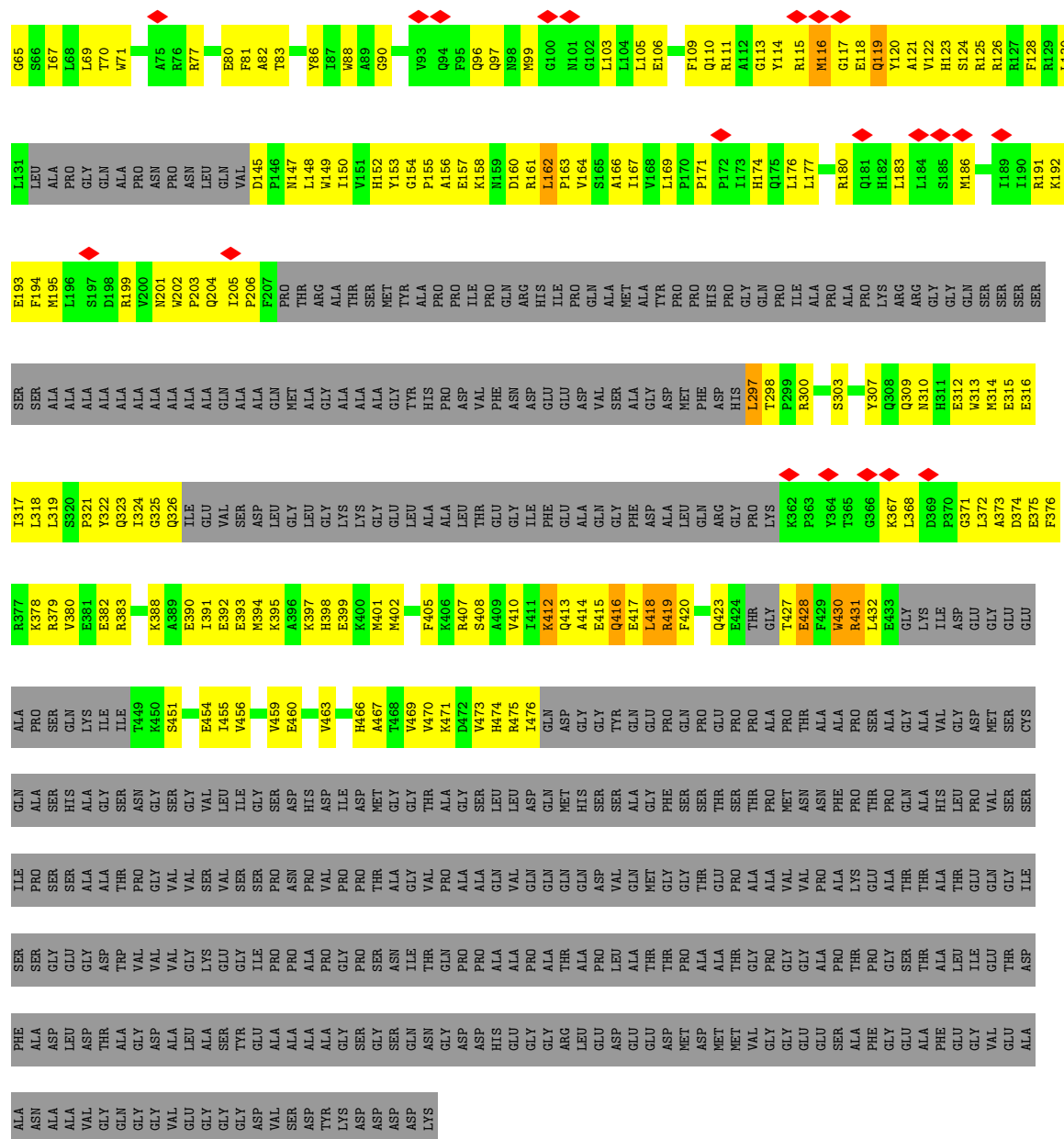


- Molecule 11: DM2 domain-containing protein

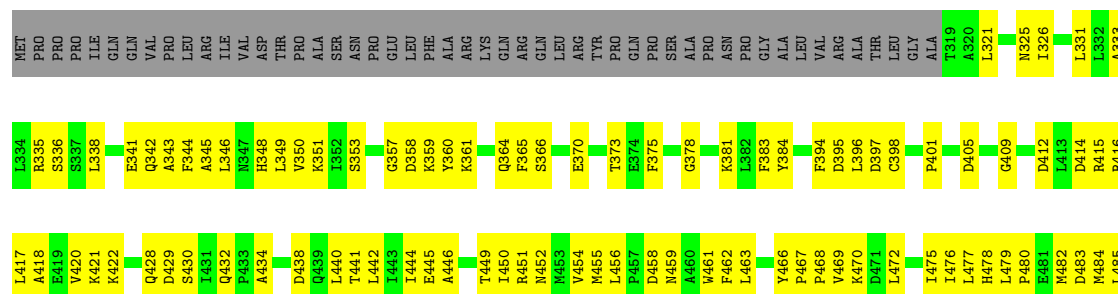
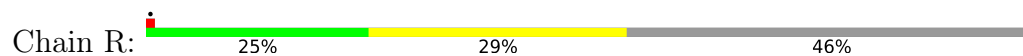


- Molecule 12: DUF1750-domain-containing protein





- Molecule 13: Putative chromatin structure-remodeling complex protein







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.472	Depositor
Minimum map value	-0.067	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.47	0/752	0.92	4/1008 (0.4%)
1	E	0.42	0/752	0.75	2/1008 (0.2%)
2	B	0.37	0/655	0.58	0/878
2	F	0.38	0/621	0.59	0/832
3	C	0.32	0/742	0.56	0/1002
3	G	0.37	0/743	0.62	0/1002
4	D	0.34	0/696	0.44	0/939
4	H	0.33	0/714	0.48	0/962
5	I	0.35	0/3019	0.43	0/4654
6	J	0.36	0/3051	0.44	0/4710
7	K	0.25	0/6936	0.57	6/9302 (0.1%)
8	L	0.23	0/3418	0.51	0/4633
9	M	0.25	0/3459	0.48	1/4704 (0.0%)
10	N	0.33	0/3789	0.67	4/5135 (0.1%)
10	O	0.35	0/2292	0.70	3/3103 (0.1%)
11	P	0.32	0/3148	0.61	0/4244
12	Q	0.45	0/2683	0.69	0/3628
13	R	0.32	0/3369	0.56	0/4573
14	S	0.35	0/3363	0.61	2/4578 (0.0%)
15	T	0.33	0/1627	0.64	1/2214 (0.0%)
16	U	0.20	0/851	0.56	0/1140
17	V	0.29	0/1126	0.62	0/1515
All	All	0.33	0/47806	0.58	23/65764 (0.0%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	1016	ILE	N-CA-C	-10.25	94.88	109.63
7	K	620	ILE	N-CA-C	10.00	120.82	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	618	GLN	N-CA-C	-7.38	103.38	112.38
14	S	455	ARG	N-CA-C	6.35	119.02	111.33
10	N	427	ILE	N-CA-C	-6.19	107.26	113.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	744	0	784	49	0
1	E	744	0	784	43	0
2	B	648	0	693	32	0
2	F	614	0	656	42	0
3	C	733	0	771	51	0
3	G	734	0	778	46	0
4	D	685	0	703	33	0
4	H	703	0	722	43	0
5	I	2694	0	1480	117	0
6	J	2718	0	1480	134	0
7	K	6825	0	6974	499	0
8	L	3340	0	3316	252	0
9	M	3371	0	3303	228	0
10	N	3714	0	3619	391	0
10	O	2245	0	2217	225	0
11	P	3089	0	3054	288	0
12	Q	2620	0	2607	232	0
13	R	3307	0	3325	226	0
14	S	3276	0	3189	216	0
15	T	1585	0	1542	125	0
16	U	844	0	836	48	0
17	V	1113	0	1081	98	0
18	K	27	0	12	7	0
All	All	46373	0	43926	2974	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 34.

The worst 5 of 2974 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)
7:K:1018:GLN:NE2	7:K:1020:ASN:HD22	1.31	1.24
10:N:320:CYS:SG	10:N:348:CYS:CB	2.29	1.21
7:K:1018:GLN:HE21	7:K:1020:ASN:ND2	1.41	1.17
10:N:320:CYS:SG	10:N:348:CYS:HB2	1.84	1.17
11:P:426:LEU:HD21	17:V:360:LEU:CB	1.76	1.15

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	89/135 (66%)	85 (96%)	4 (4%)	0	100	100
1	E	89/135 (66%)	85 (96%)	4 (4%)	0	100	100
2	B	79/102 (78%)	72 (91%)	7 (9%)	0	100	100
2	F	75/102 (74%)	70 (93%)	5 (7%)	0	100	100
3	C	93/129 (72%)	87 (94%)	6 (6%)	0	100	100
3	G	93/129 (72%)	88 (95%)	5 (5%)	0	100	100
4	D	86/125 (69%)	81 (94%)	5 (6%)	0	100	100
4	H	88/125 (70%)	83 (94%)	5 (6%)	0	100	100
7	K	810/1595 (51%)	735 (91%)	75 (9%)	0	100	100
8	L	405/733 (55%)	364 (90%)	41 (10%)	0	100	100
9	M	427/476 (90%)	394 (92%)	33 (8%)	0	100	100
10	N	463/694 (67%)	392 (85%)	65 (14%)	6 (1%)	9	41
10	O	266/694 (38%)	239 (90%)	26 (10%)	1 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	P	363/547 (66%)	318 (88%)	43 (12%)	2 (1%)	21	59
12	Q	307/769 (40%)	287 (94%)	19 (6%)	1 (0%)	36	71
13	R	409/763 (54%)	385 (94%)	22 (5%)	2 (0%)	24	63
14	S	401/607 (66%)	356 (89%)	44 (11%)	1 (0%)	43	77
15	T	195/534 (36%)	177 (91%)	18 (9%)	0	100	100
16	U	99/991 (10%)	87 (88%)	12 (12%)	0	100	100
17	V	135/990 (14%)	125 (93%)	10 (7%)	0	100	100
All	All	4972/10375 (48%)	4510 (91%)	449 (9%)	13 (0%)	37	71

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	Q	419	ARG
10	N	180	ARG
10	N	610	GLN
13	R	1009	SER
14	S	415	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	79/110 (72%)	66 (84%)	13 (16%)	2	12
1	E	79/110 (72%)	66 (84%)	13 (16%)	2	12
2	B	67/78 (86%)	67 (100%)	0	100	100
2	F	63/78 (81%)	63 (100%)	0	100	100
3	C	74/101 (73%)	74 (100%)	0	100	100
3	G	74/101 (73%)	72 (97%)	2 (3%)	39	59
4	D	75/105 (71%)	75 (100%)	0	100	100
4	H	77/105 (73%)	77 (100%)	0	100	100
7	K	736/1356 (54%)	718 (98%)	18 (2%)	43	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	L	363/605 (60%)	362 (100%)	1 (0%)	86	84
9	M	354/395 (90%)	352 (99%)	2 (1%)	78	80
10	N	393/562 (70%)	381 (97%)	12 (3%)	35	56
10	O	238/562 (42%)	231 (97%)	7 (3%)	37	58
11	P	337/462 (73%)	324 (96%)	13 (4%)	28	50
12	Q	279/598 (47%)	264 (95%)	15 (5%)	20	42
13	R	360/655 (55%)	357 (99%)	3 (1%)	73	77
14	S	353/493 (72%)	348 (99%)	5 (1%)	59	71
15	T	173/457 (38%)	171 (99%)	2 (1%)	63	73
16	U	85/861 (10%)	85 (100%)	0	100	100
17	V	121/836 (14%)	121 (100%)	0	100	100
All	All	4380/8630 (51%)	4274 (98%)	106 (2%)	43	63

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	N	424	GLN
11	P	327	LEU
14	S	123	TYR
10	N	614	LEU
10	O	611	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
14	S	24	ASN
17	V	390	GLN
14	S	122	ASN
15	T	376	HIS
7	K	1018	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	$\# Z > 2$
18	ADP	K	1601	-	27,29,29	1.36	4 (14%)	42,45,45	2.10	15 (35%)

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
18	ADP	K	1601	-	-	7/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	1601	ADP	C5-C4	3.99	1.46	1.39
18	K	1601	ADP	C4-N9	-2.52	1.32	1.37
18	K	1601	ADP	C5-N7	-2.47	1.34	1.39
18	K	1601	ADP	C5-C6	2.44	1.47	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	1601	ADP	C5-C4-N3	-5.55	119.50	126.75
18	K	1601	ADP	N3-C4-N9	4.60	134.66	127.08
18	K	1601	ADP	PA-O3A-PB	-4.56	117.19	132.83
18	K	1601	ADP	C2-N3-C4	3.73	120.56	111.75
18	K	1601	ADP	N3-C2-N1	-3.20	123.60	128.60

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

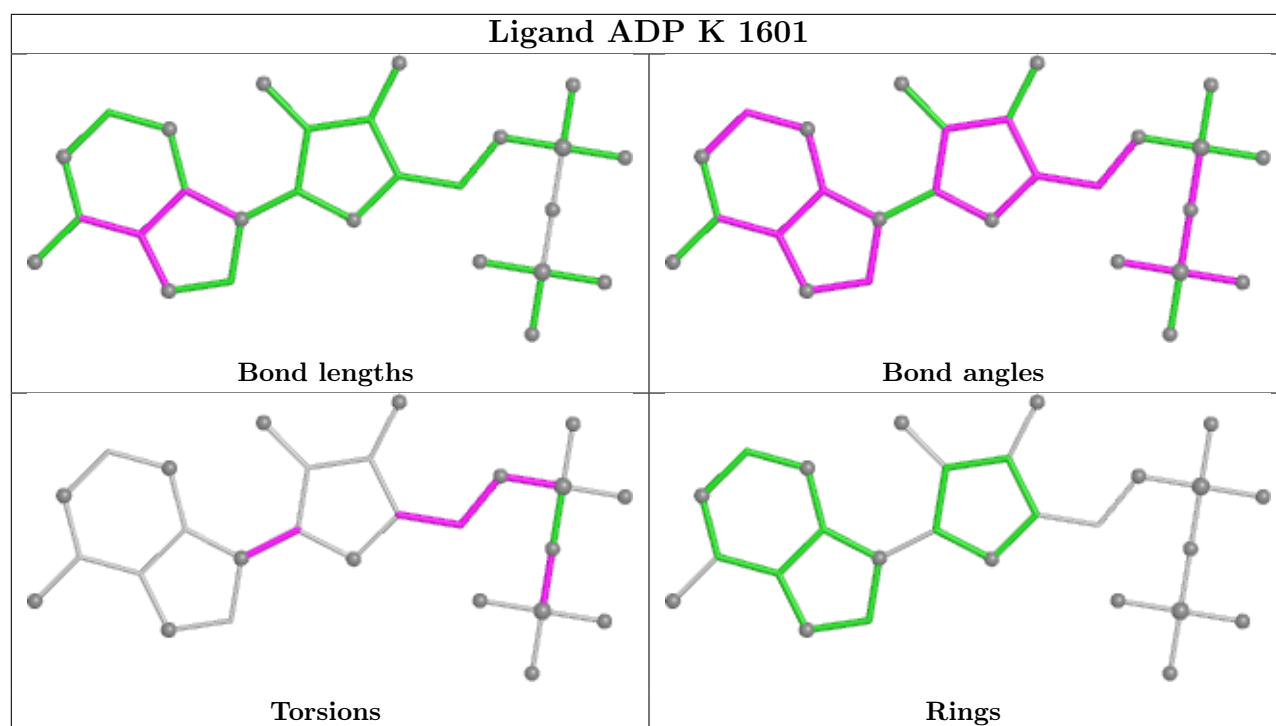
Mol	Chain	Res	Type	Atoms
18	K	1601	ADP	PA-O3A-PB-O3B
18	K	1601	ADP	C5'-O5'-PA-O2A
18	K	1601	ADP	C5'-O5'-PA-O3A
18	K	1601	ADP	C4'-C5'-O5'-PA
18	K	1601	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	K	1601	ADP	7	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.

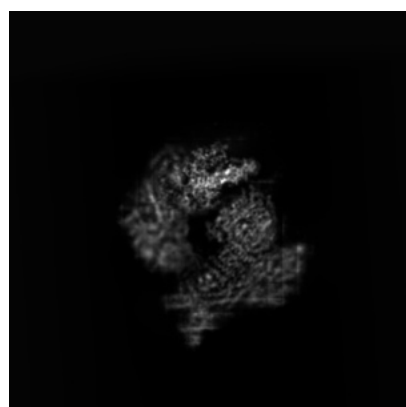
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68935. These allow visual inspection of the internal detail of the map and identification of artifacts.

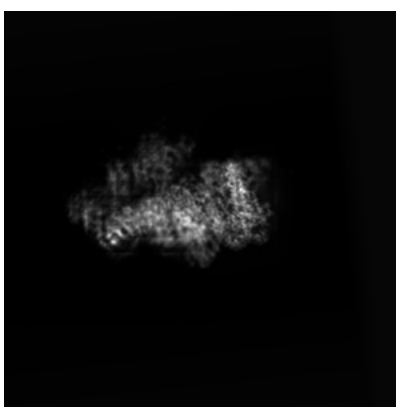
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

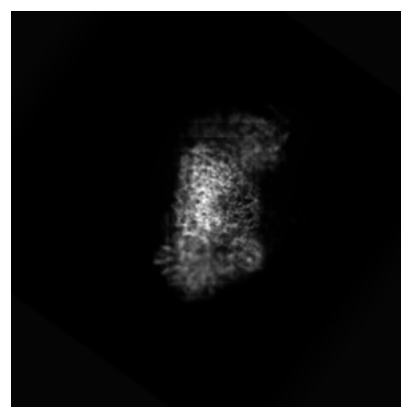
6.1.1 Primary map



X



Y



Z

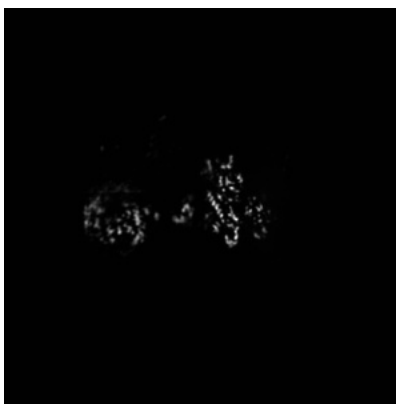
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

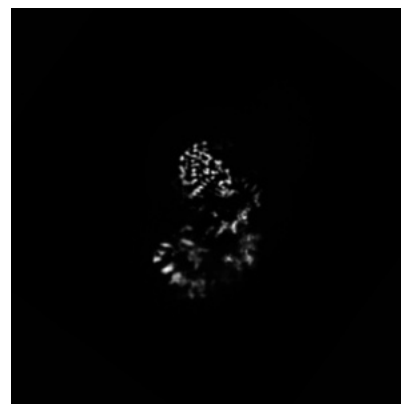
6.2.1 Primary map



X Index: 210



Y Index: 210

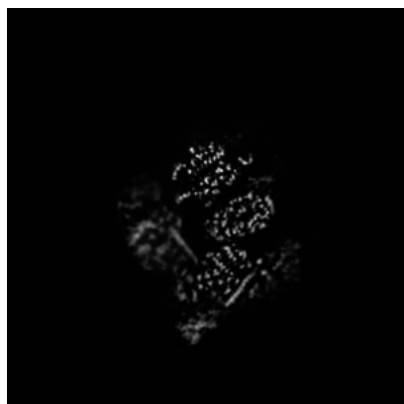


Z Index: 210

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

6.3 Largest variance slices [i](#)

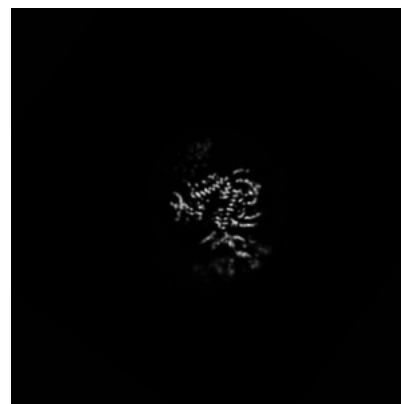
6.3.1 Primary map



X Index: 202



Y Index: 208



Z Index: 242

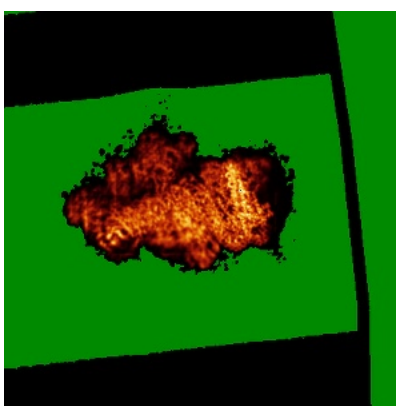
The images above show the largest variance slices of the map in three orthogonal directions.

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

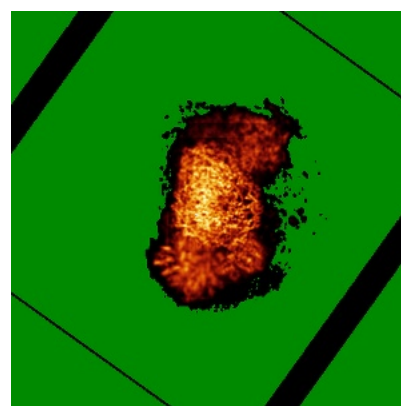
6.4.1 Primary map



X



Y



Z

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 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

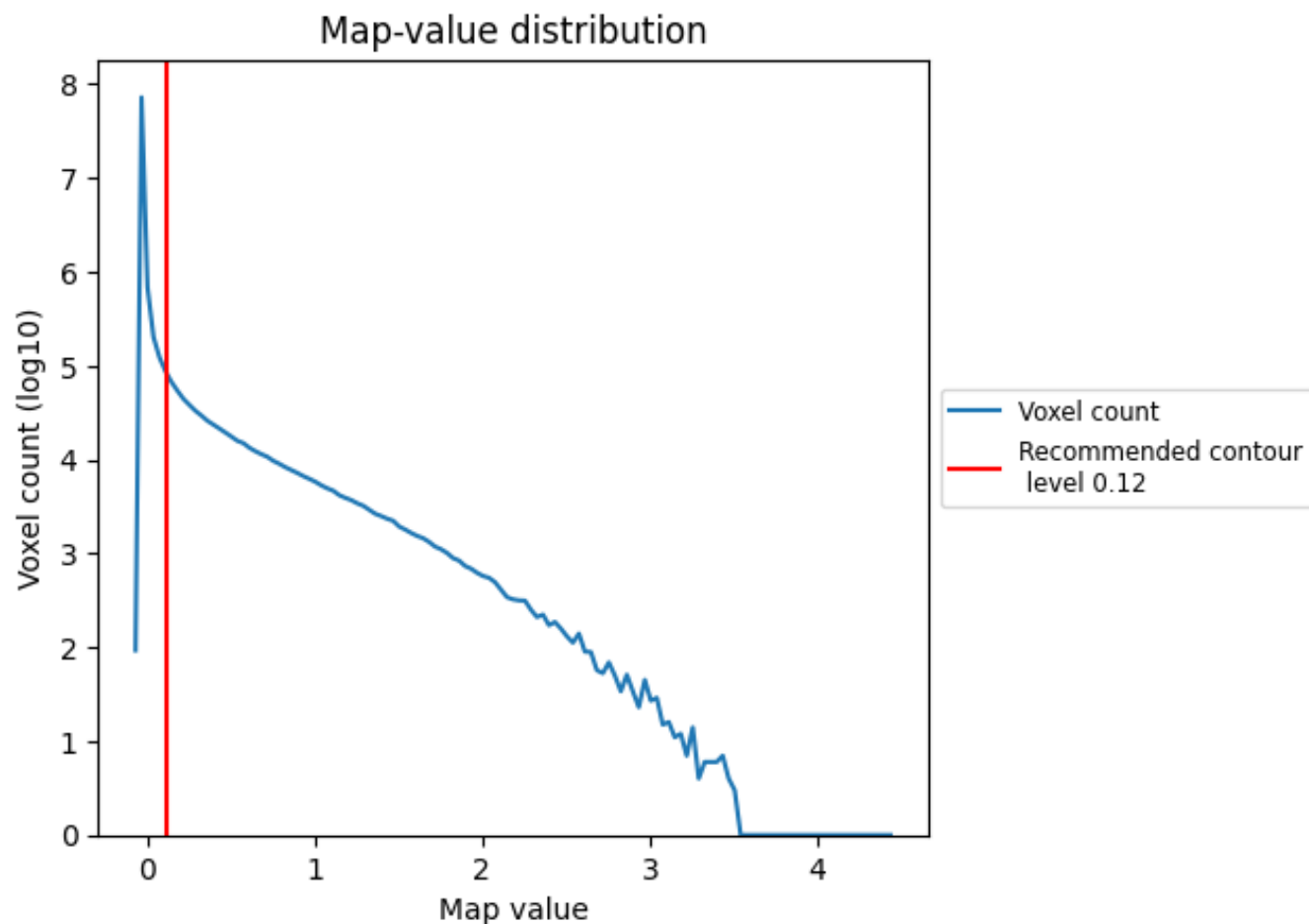
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

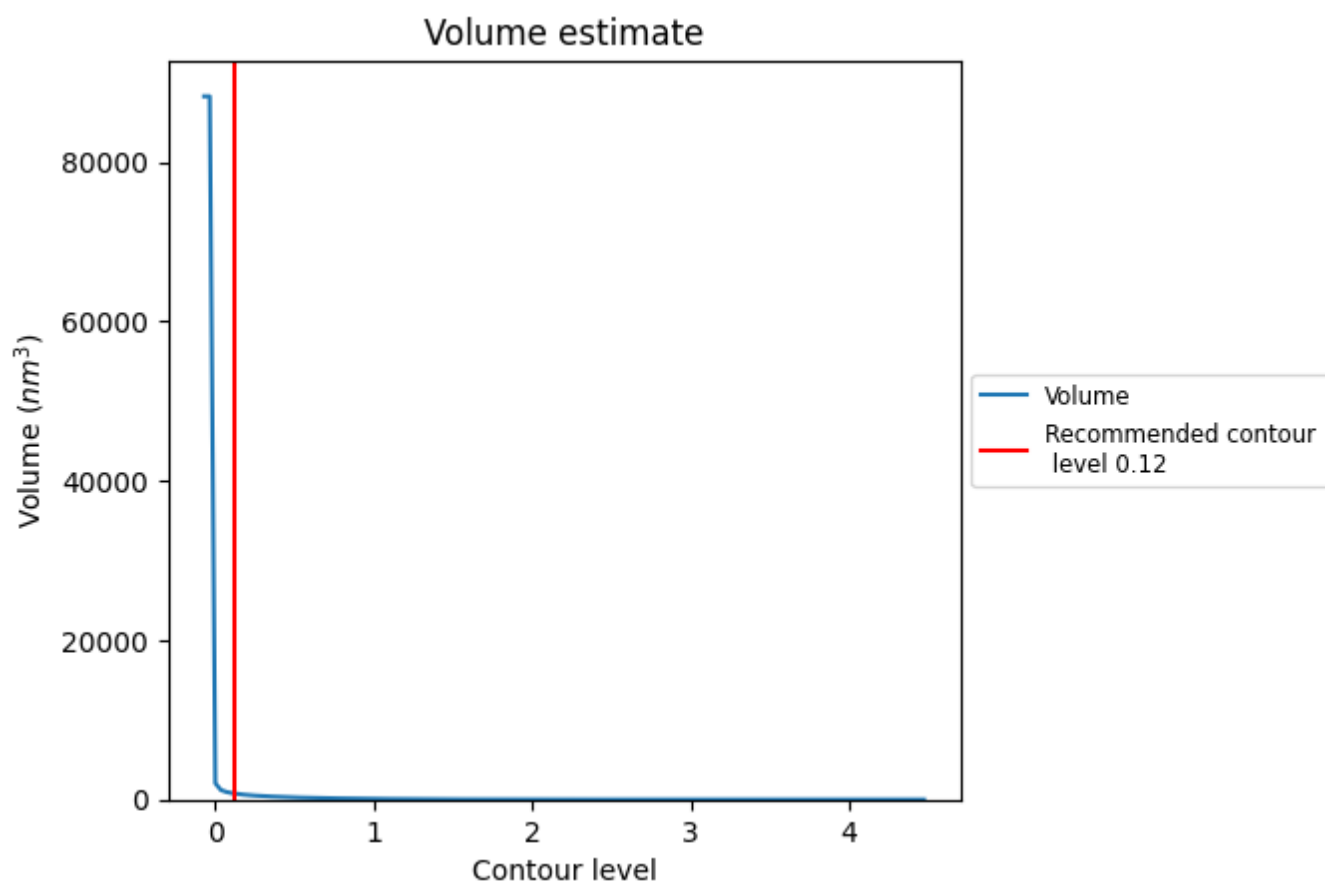
This section contains the results of statistical analysis of the map.

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.

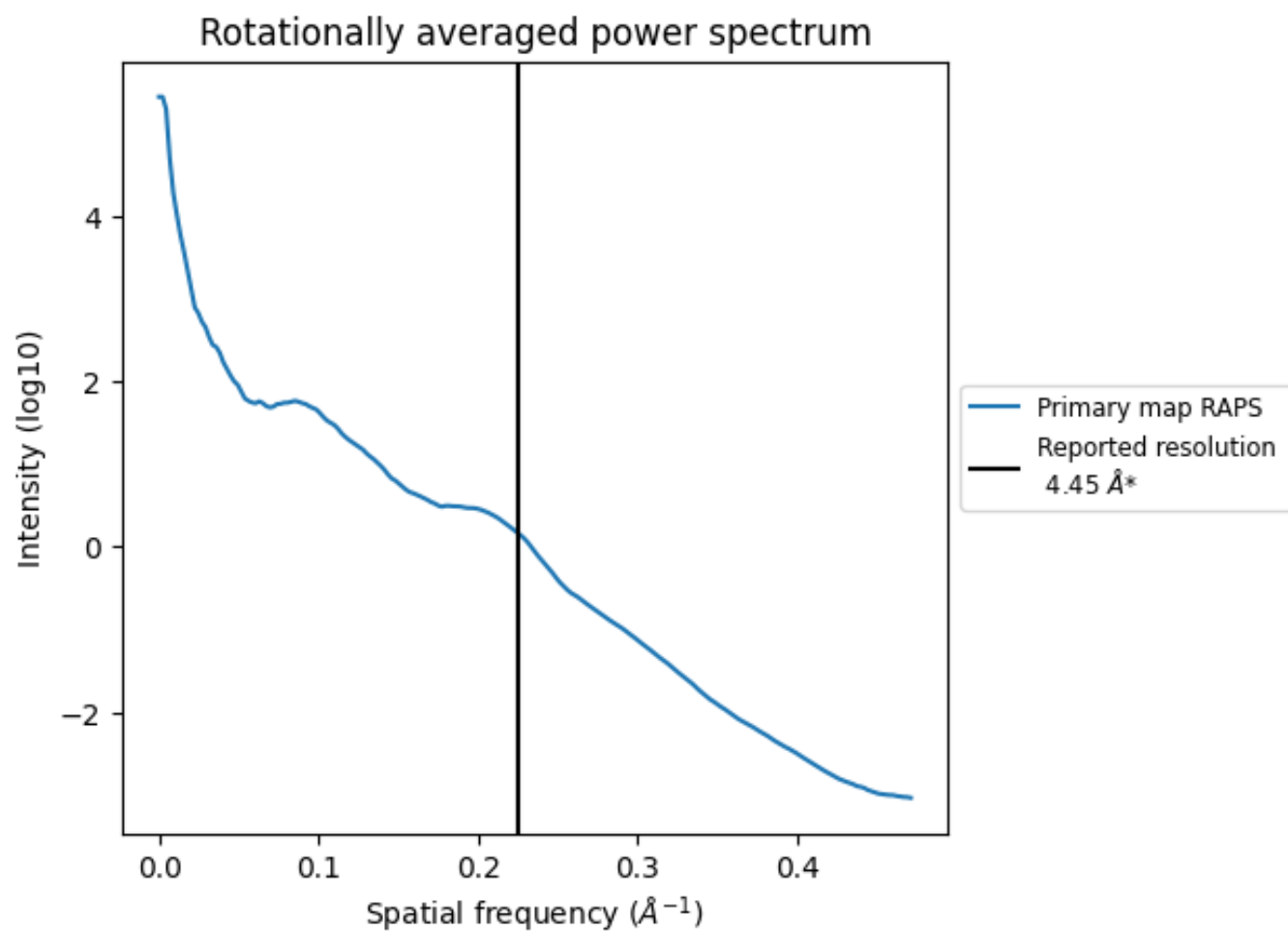
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 773 nm³; this corresponds to an approximate mass of 698 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 0.225 Å⁻¹

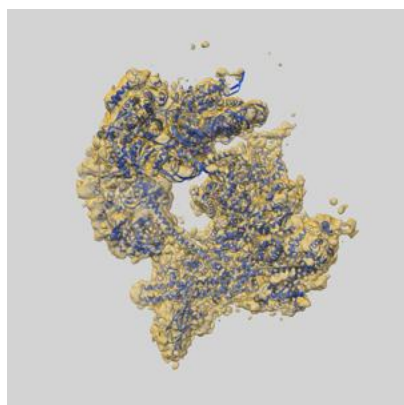
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

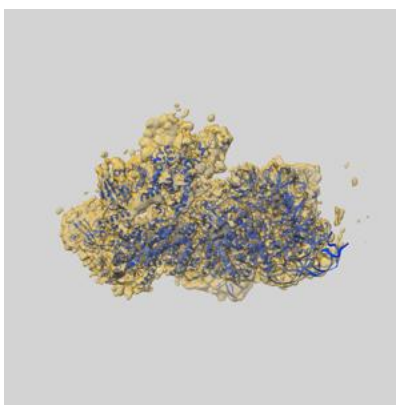
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68935 and PDB model 23FU. Per-residue inclusion information can be found in section [3](#) on page [13](#).

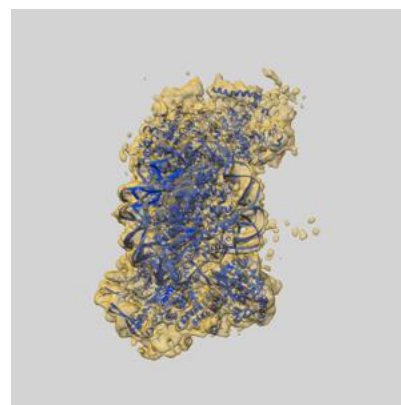
9.1 Map-model overlay [i](#)



X



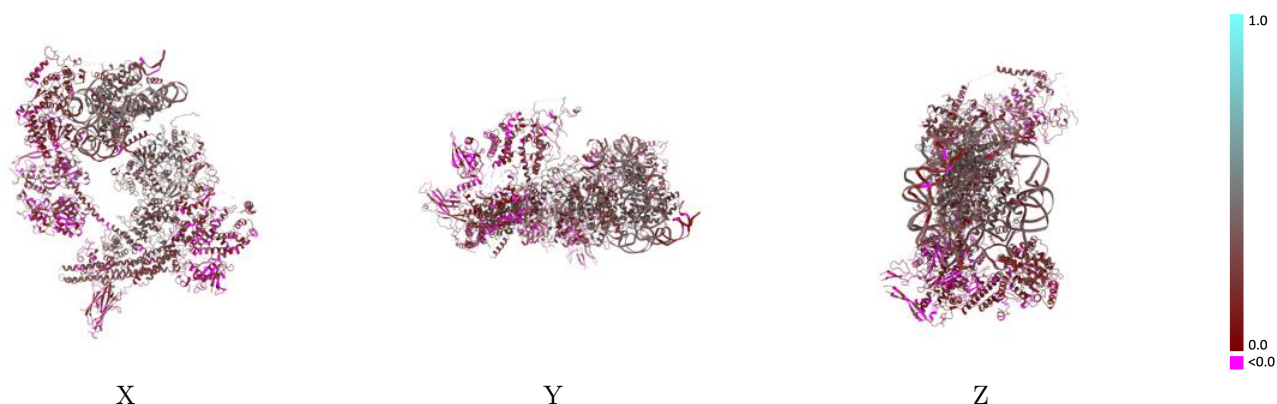
Y



Z

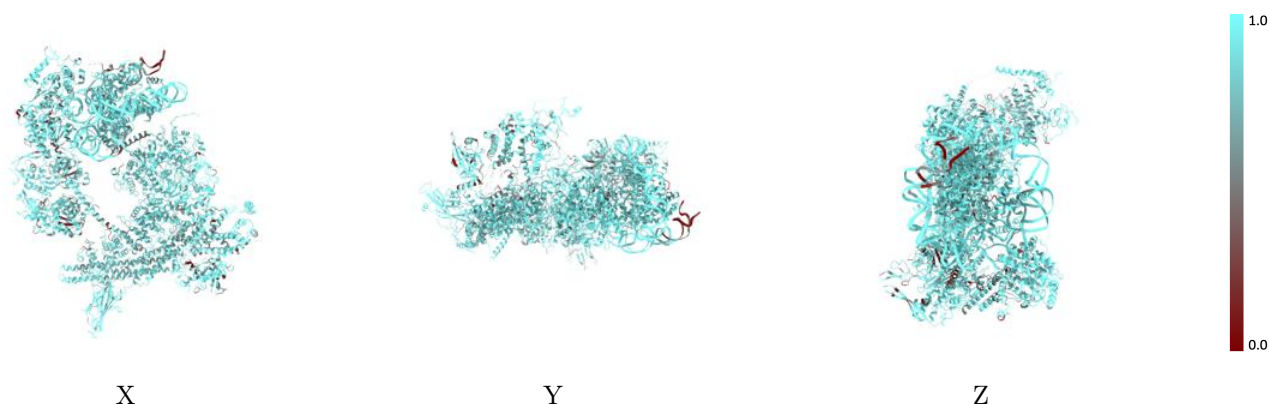
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



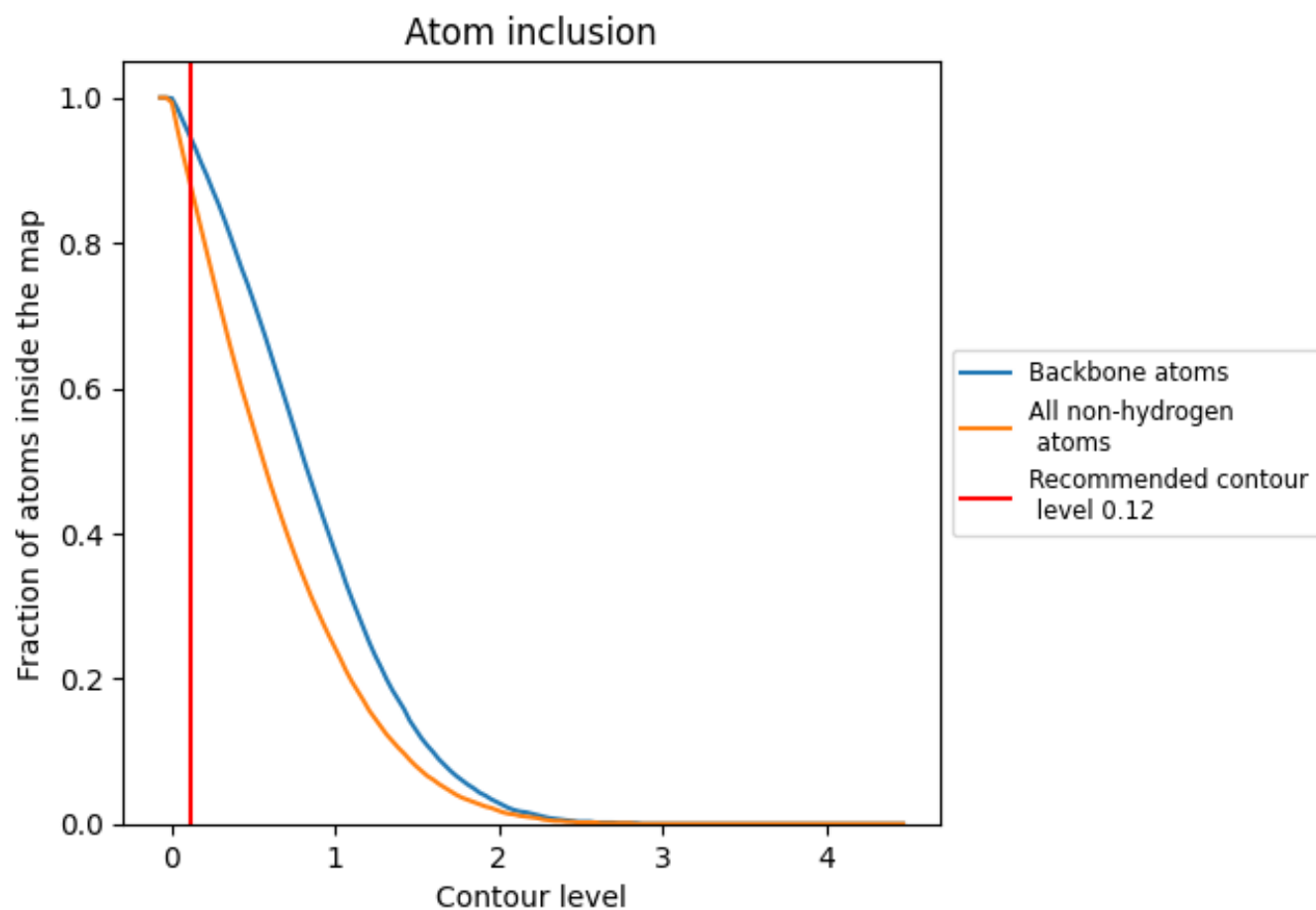
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.2340
A	 0.9050	 0.3230
B	 0.9000	 0.3850
C	 0.9280	 0.3570
D	 0.9370	 0.3670
E	 0.8900	 0.3340
F	 0.9320	 0.3960
G	 0.8930	 0.3440
H	 0.9110	 0.3510
I	 0.9160	 0.3150
J	 0.9100	 0.3050
K	 0.8070	 0.1630
L	 0.8730	 0.1100
M	 0.8710	 0.0770
N	 0.8890	 0.2610
O	 0.8990	 0.2570
P	 0.8610	 0.1840
Q	 0.8200	 0.1300
R	 0.9150	 0.3060
S	 0.8880	 0.3070
T	 0.9110	 0.3260
U	 0.9040	 0.2290
V	 0.8560	 0.2100

