



# wwPDB EM Validation Summary Report ⓘ

Jan 28, 2023 – 01:00 PM EST

PDB ID : 7UQI  
EMDB ID : EMD-26695  
Title : Cryo-EM structure of the *S. cerevisiae* chromatin remodeler Yta7 hexamer bound to ADP  
Authors : Wang, F.; Feng, X.; Li, H.  
Deposited on : 2022-04-19  
Resolution : 3.80 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](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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

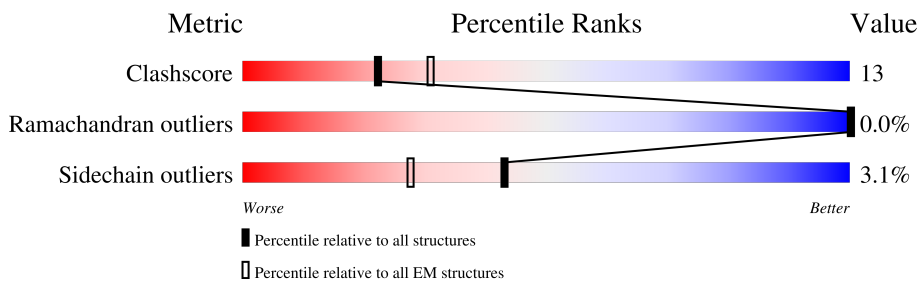
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 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.



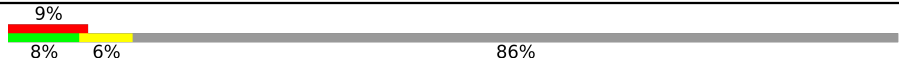
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	1416	
1	B	1416	
1	C	1416	
1	D	1416	
1	E	1416	
1	F	1416	
1	G	1416	
1	H	1416	

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Mol	Chain	Length	Quality of chain
1	I	1416	 <p>9% 8% 6% 86%</p>

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 32424 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 ATPase histone chaperone YTA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	576	4591	2945	780	850	16	0	0
1	B	579	4612	2957	783	855	17	0	0
1	C	578	4607	2954	782	854	17	0	0
1	D	576	4586	2940	780	849	17	0	0
1	E	558	4448	2855	752	824	17	0	0
1	F	567	4519	2903	763	836	17	0	0
1	G	197	1642	1046	288	301	7	0	0
1	H	197	1642	1046	288	301	7	0	0
1	I	197	1642	1046	288	301	7	0	0

There are 333 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	HIS	-	expression tag	UNP P40340
A	-34	HIS	-	expression tag	UNP P40340
A	-33	HIS	-	expression tag	UNP P40340
A	-32	HIS	-	expression tag	UNP P40340
A	-31	HIS	-	expression tag	UNP P40340
A	-30	HIS	-	expression tag	UNP P40340
A	-29	HIS	-	expression tag	UNP P40340
A	-28	HIS	-	expression tag	UNP P40340
A	-27	HIS	-	expression tag	UNP P40340
A	-26	HIS	-	expression tag	UNP P40340
A	-25	THR	-	expression tag	UNP P40340
A	-24	SER	-	expression tag	UNP P40340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	GLY	-	expression tag	UNP P40340
A	-22	SER	-	expression tag	UNP P40340
A	-21	MET	-	expression tag	UNP P40340
A	-20	ASP	-	expression tag	UNP P40340
A	-19	TYR	-	expression tag	UNP P40340
A	-18	LYS	-	expression tag	UNP P40340
A	-17	ASP	-	expression tag	UNP P40340
A	-16	HIS	-	expression tag	UNP P40340
A	-15	ASP	-	expression tag	UNP P40340
A	-14	GLY	-	expression tag	UNP P40340
A	-13	ASP	-	expression tag	UNP P40340
A	-12	TYR	-	expression tag	UNP P40340
A	-11	LYS	-	expression tag	UNP P40340
A	-10	ASP	-	expression tag	UNP P40340
A	-9	HIS	-	expression tag	UNP P40340
A	-8	ASP	-	expression tag	UNP P40340
A	-7	ILE	-	expression tag	UNP P40340
A	-6	ASP	-	expression tag	UNP P40340
A	-5	TYR	-	expression tag	UNP P40340
A	-4	LYS	-	expression tag	UNP P40340
A	-3	ASP	-	expression tag	UNP P40340
A	-2	ASP	-	expression tag	UNP P40340
A	-1	ASP	-	expression tag	UNP P40340
A	0	ASP	-	expression tag	UNP P40340
A	1	LYS	-	expression tag	UNP P40340
B	-36	HIS	-	expression tag	UNP P40340
B	-35	HIS	-	expression tag	UNP P40340
B	-34	HIS	-	expression tag	UNP P40340
B	-33	HIS	-	expression tag	UNP P40340
B	-32	HIS	-	expression tag	UNP P40340
B	-31	HIS	-	expression tag	UNP P40340
B	-30	HIS	-	expression tag	UNP P40340
B	-29	HIS	-	expression tag	UNP P40340
B	-28	HIS	-	expression tag	UNP P40340
B	-27	HIS	-	expression tag	UNP P40340
B	-26	THR	-	expression tag	UNP P40340
B	-25	SER	-	expression tag	UNP P40340
B	-24	GLY	-	expression tag	UNP P40340
B	-23	SER	-	expression tag	UNP P40340
B	-22	MET	-	expression tag	UNP P40340
B	-21	ASP	-	expression tag	UNP P40340
B	-20	TYR	-	expression tag	UNP P40340

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	LYS	-	expression tag	UNP P40340
B	-18	ASP	-	expression tag	UNP P40340
B	-17	HIS	-	expression tag	UNP P40340
B	-16	ASP	-	expression tag	UNP P40340
B	-15	GLY	-	expression tag	UNP P40340
B	-14	ASP	-	expression tag	UNP P40340
B	-13	TYR	-	expression tag	UNP P40340
B	-12	LYS	-	expression tag	UNP P40340
B	-11	ASP	-	expression tag	UNP P40340
B	-10	HIS	-	expression tag	UNP P40340
B	-9	ASP	-	expression tag	UNP P40340
B	-8	ILE	-	expression tag	UNP P40340
B	-7	ASP	-	expression tag	UNP P40340
B	-6	TYR	-	expression tag	UNP P40340
B	-5	LYS	-	expression tag	UNP P40340
B	-4	ASP	-	expression tag	UNP P40340
B	-3	ASP	-	expression tag	UNP P40340
B	-2	ASP	-	expression tag	UNP P40340
B	-1	ASP	-	expression tag	UNP P40340
B	0	LYS	-	expression tag	UNP P40340
C	-36	HIS	-	expression tag	UNP P40340
C	-35	HIS	-	expression tag	UNP P40340
C	-34	HIS	-	expression tag	UNP P40340
C	-33	HIS	-	expression tag	UNP P40340
C	-32	HIS	-	expression tag	UNP P40340
C	-31	HIS	-	expression tag	UNP P40340
C	-30	HIS	-	expression tag	UNP P40340
C	-29	HIS	-	expression tag	UNP P40340
C	-28	HIS	-	expression tag	UNP P40340
C	-27	HIS	-	expression tag	UNP P40340
C	-26	THR	-	expression tag	UNP P40340
C	-25	SER	-	expression tag	UNP P40340
C	-24	GLY	-	expression tag	UNP P40340
C	-23	SER	-	expression tag	UNP P40340
C	-22	MET	-	expression tag	UNP P40340
C	-21	ASP	-	expression tag	UNP P40340
C	-20	TYR	-	expression tag	UNP P40340
C	-19	LYS	-	expression tag	UNP P40340
C	-18	ASP	-	expression tag	UNP P40340
C	-17	HIS	-	expression tag	UNP P40340
C	-16	ASP	-	expression tag	UNP P40340
C	-15	GLY	-	expression tag	UNP P40340

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP P40340
C	-13	TYR	-	expression tag	UNP P40340
C	-12	LYS	-	expression tag	UNP P40340
C	-11	ASP	-	expression tag	UNP P40340
C	-10	HIS	-	expression tag	UNP P40340
C	-9	ASP	-	expression tag	UNP P40340
C	-8	ILE	-	expression tag	UNP P40340
C	-7	ASP	-	expression tag	UNP P40340
C	-6	TYR	-	expression tag	UNP P40340
C	-5	LYS	-	expression tag	UNP P40340
C	-4	ASP	-	expression tag	UNP P40340
C	-3	ASP	-	expression tag	UNP P40340
C	-2	ASP	-	expression tag	UNP P40340
C	-1	ASP	-	expression tag	UNP P40340
C	0	LYS	-	expression tag	UNP P40340
D	-36	HIS	-	expression tag	UNP P40340
D	-35	HIS	-	expression tag	UNP P40340
D	-34	HIS	-	expression tag	UNP P40340
D	-33	HIS	-	expression tag	UNP P40340
D	-32	HIS	-	expression tag	UNP P40340
D	-31	HIS	-	expression tag	UNP P40340
D	-30	HIS	-	expression tag	UNP P40340
D	-29	HIS	-	expression tag	UNP P40340
D	-28	HIS	-	expression tag	UNP P40340
D	-27	HIS	-	expression tag	UNP P40340
D	-26	THR	-	expression tag	UNP P40340
D	-25	SER	-	expression tag	UNP P40340
D	-24	GLY	-	expression tag	UNP P40340
D	-23	SER	-	expression tag	UNP P40340
D	-22	MET	-	expression tag	UNP P40340
D	-21	ASP	-	expression tag	UNP P40340
D	-20	TYR	-	expression tag	UNP P40340
D	-19	LYS	-	expression tag	UNP P40340
D	-18	ASP	-	expression tag	UNP P40340
D	-17	HIS	-	expression tag	UNP P40340
D	-16	ASP	-	expression tag	UNP P40340
D	-15	GLY	-	expression tag	UNP P40340
D	-14	ASP	-	expression tag	UNP P40340
D	-13	TYR	-	expression tag	UNP P40340
D	-12	LYS	-	expression tag	UNP P40340
D	-11	ASP	-	expression tag	UNP P40340
D	-10	HIS	-	expression tag	UNP P40340

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	ASP	-	expression tag	UNP P40340
D	-8	ILE	-	expression tag	UNP P40340
D	-7	ASP	-	expression tag	UNP P40340
D	-6	TYR	-	expression tag	UNP P40340
D	-5	LYS	-	expression tag	UNP P40340
D	-4	ASP	-	expression tag	UNP P40340
D	-3	ASP	-	expression tag	UNP P40340
D	-2	ASP	-	expression tag	UNP P40340
D	-1	ASP	-	expression tag	UNP P40340
D	0	LYS	-	expression tag	UNP P40340
E	-36	HIS	-	expression tag	UNP P40340
E	-35	HIS	-	expression tag	UNP P40340
E	-34	HIS	-	expression tag	UNP P40340
E	-33	HIS	-	expression tag	UNP P40340
E	-32	HIS	-	expression tag	UNP P40340
E	-31	HIS	-	expression tag	UNP P40340
E	-30	HIS	-	expression tag	UNP P40340
E	-29	HIS	-	expression tag	UNP P40340
E	-28	HIS	-	expression tag	UNP P40340
E	-27	HIS	-	expression tag	UNP P40340
E	-26	THR	-	expression tag	UNP P40340
E	-25	SER	-	expression tag	UNP P40340
E	-24	GLY	-	expression tag	UNP P40340
E	-23	SER	-	expression tag	UNP P40340
E	-22	MET	-	expression tag	UNP P40340
E	-21	ASP	-	expression tag	UNP P40340
E	-20	TYR	-	expression tag	UNP P40340
E	-19	LYS	-	expression tag	UNP P40340
E	-18	ASP	-	expression tag	UNP P40340
E	-17	HIS	-	expression tag	UNP P40340
E	-16	ASP	-	expression tag	UNP P40340
E	-15	GLY	-	expression tag	UNP P40340
E	-14	ASP	-	expression tag	UNP P40340
E	-13	TYR	-	expression tag	UNP P40340
E	-12	LYS	-	expression tag	UNP P40340
E	-11	ASP	-	expression tag	UNP P40340
E	-10	HIS	-	expression tag	UNP P40340
E	-9	ASP	-	expression tag	UNP P40340
E	-8	ILE	-	expression tag	UNP P40340
E	-7	ASP	-	expression tag	UNP P40340
E	-6	TYR	-	expression tag	UNP P40340
E	-5	LYS	-	expression tag	UNP P40340

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	ASP	-	expression tag	UNP P40340
E	-3	ASP	-	expression tag	UNP P40340
E	-2	ASP	-	expression tag	UNP P40340
E	-1	ASP	-	expression tag	UNP P40340
E	0	LYS	-	expression tag	UNP P40340
F	-36	HIS	-	expression tag	UNP P40340
F	-35	HIS	-	expression tag	UNP P40340
F	-34	HIS	-	expression tag	UNP P40340
F	-33	HIS	-	expression tag	UNP P40340
F	-32	HIS	-	expression tag	UNP P40340
F	-31	HIS	-	expression tag	UNP P40340
F	-30	HIS	-	expression tag	UNP P40340
F	-29	HIS	-	expression tag	UNP P40340
F	-28	HIS	-	expression tag	UNP P40340
F	-27	HIS	-	expression tag	UNP P40340
F	-26	THR	-	expression tag	UNP P40340
F	-25	SER	-	expression tag	UNP P40340
F	-24	GLY	-	expression tag	UNP P40340
F	-23	SER	-	expression tag	UNP P40340
F	-22	MET	-	expression tag	UNP P40340
F	-21	ASP	-	expression tag	UNP P40340
F	-20	TYR	-	expression tag	UNP P40340
F	-19	LYS	-	expression tag	UNP P40340
F	-18	ASP	-	expression tag	UNP P40340
F	-17	HIS	-	expression tag	UNP P40340
F	-16	ASP	-	expression tag	UNP P40340
F	-15	GLY	-	expression tag	UNP P40340
F	-14	ASP	-	expression tag	UNP P40340
F	-13	TYR	-	expression tag	UNP P40340
F	-12	LYS	-	expression tag	UNP P40340
F	-11	ASP	-	expression tag	UNP P40340
F	-10	HIS	-	expression tag	UNP P40340
F	-9	ASP	-	expression tag	UNP P40340
F	-8	ILE	-	expression tag	UNP P40340
F	-7	ASP	-	expression tag	UNP P40340
F	-6	TYR	-	expression tag	UNP P40340
F	-5	LYS	-	expression tag	UNP P40340
F	-4	ASP	-	expression tag	UNP P40340
F	-3	ASP	-	expression tag	UNP P40340
F	-2	ASP	-	expression tag	UNP P40340
F	-1	ASP	-	expression tag	UNP P40340
F	0	LYS	-	expression tag	UNP P40340

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-36	HIS	-	expression tag	UNP P40340
G	-35	HIS	-	expression tag	UNP P40340
G	-34	HIS	-	expression tag	UNP P40340
G	-33	HIS	-	expression tag	UNP P40340
G	-32	HIS	-	expression tag	UNP P40340
G	-31	HIS	-	expression tag	UNP P40340
G	-30	HIS	-	expression tag	UNP P40340
G	-29	HIS	-	expression tag	UNP P40340
G	-28	HIS	-	expression tag	UNP P40340
G	-27	HIS	-	expression tag	UNP P40340
G	-26	THR	-	expression tag	UNP P40340
G	-25	SER	-	expression tag	UNP P40340
G	-24	GLY	-	expression tag	UNP P40340
G	-23	SER	-	expression tag	UNP P40340
G	-22	MET	-	expression tag	UNP P40340
G	-21	ASP	-	expression tag	UNP P40340
G	-20	TYR	-	expression tag	UNP P40340
G	-19	LYS	-	expression tag	UNP P40340
G	-18	ASP	-	expression tag	UNP P40340
G	-17	HIS	-	expression tag	UNP P40340
G	-16	ASP	-	expression tag	UNP P40340
G	-15	GLY	-	expression tag	UNP P40340
G	-14	ASP	-	expression tag	UNP P40340
G	-13	TYR	-	expression tag	UNP P40340
G	-12	LYS	-	expression tag	UNP P40340
G	-11	ASP	-	expression tag	UNP P40340
G	-10	HIS	-	expression tag	UNP P40340
G	-9	ASP	-	expression tag	UNP P40340
G	-8	ILE	-	expression tag	UNP P40340
G	-7	ASP	-	expression tag	UNP P40340
G	-6	TYR	-	expression tag	UNP P40340
G	-5	LYS	-	expression tag	UNP P40340
G	-4	ASP	-	expression tag	UNP P40340
G	-3	ASP	-	expression tag	UNP P40340
G	-2	ASP	-	expression tag	UNP P40340
G	-1	ASP	-	expression tag	UNP P40340
G	0	LYS	-	expression tag	UNP P40340
H	-36	HIS	-	expression tag	UNP P40340
H	-35	HIS	-	expression tag	UNP P40340
H	-34	HIS	-	expression tag	UNP P40340
H	-33	HIS	-	expression tag	UNP P40340
H	-32	HIS	-	expression tag	UNP P40340

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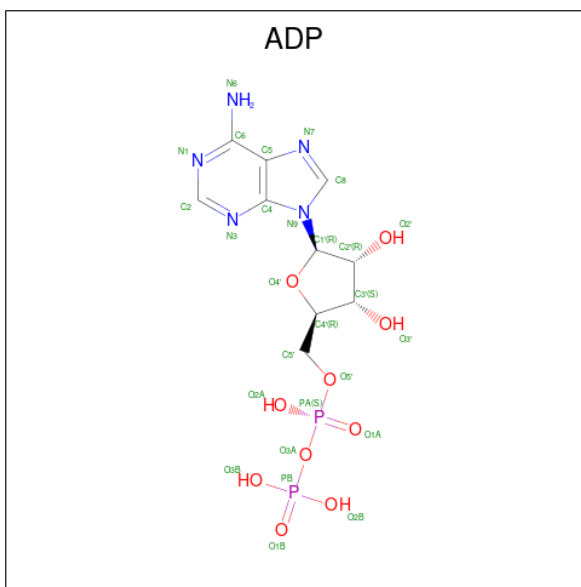
Chain	Residue	Modelled	Actual	Comment	Reference
H	-31	HIS	-	expression tag	UNP P40340
H	-30	HIS	-	expression tag	UNP P40340
H	-29	HIS	-	expression tag	UNP P40340
H	-28	HIS	-	expression tag	UNP P40340
H	-27	HIS	-	expression tag	UNP P40340
H	-26	THR	-	expression tag	UNP P40340
H	-25	SER	-	expression tag	UNP P40340
H	-24	GLY	-	expression tag	UNP P40340
H	-23	SER	-	expression tag	UNP P40340
H	-22	MET	-	expression tag	UNP P40340
H	-21	ASP	-	expression tag	UNP P40340
H	-20	TYR	-	expression tag	UNP P40340
H	-19	LYS	-	expression tag	UNP P40340
H	-18	ASP	-	expression tag	UNP P40340
H	-17	HIS	-	expression tag	UNP P40340
H	-16	ASP	-	expression tag	UNP P40340
H	-15	GLY	-	expression tag	UNP P40340
H	-14	ASP	-	expression tag	UNP P40340
H	-13	TYR	-	expression tag	UNP P40340
H	-12	LYS	-	expression tag	UNP P40340
H	-11	ASP	-	expression tag	UNP P40340
H	-10	HIS	-	expression tag	UNP P40340
H	-9	ASP	-	expression tag	UNP P40340
H	-8	ILE	-	expression tag	UNP P40340
H	-7	ASP	-	expression tag	UNP P40340
H	-6	TYR	-	expression tag	UNP P40340
H	-5	LYS	-	expression tag	UNP P40340
H	-4	ASP	-	expression tag	UNP P40340
H	-3	ASP	-	expression tag	UNP P40340
H	-2	ASP	-	expression tag	UNP P40340
H	-1	ASP	-	expression tag	UNP P40340
H	0	LYS	-	expression tag	UNP P40340
I	-36	HIS	-	expression tag	UNP P40340
I	-35	HIS	-	expression tag	UNP P40340
I	-34	HIS	-	expression tag	UNP P40340
I	-33	HIS	-	expression tag	UNP P40340
I	-32	HIS	-	expression tag	UNP P40340
I	-31	HIS	-	expression tag	UNP P40340
I	-30	HIS	-	expression tag	UNP P40340
I	-29	HIS	-	expression tag	UNP P40340
I	-28	HIS	-	expression tag	UNP P40340
I	-27	HIS	-	expression tag	UNP P40340

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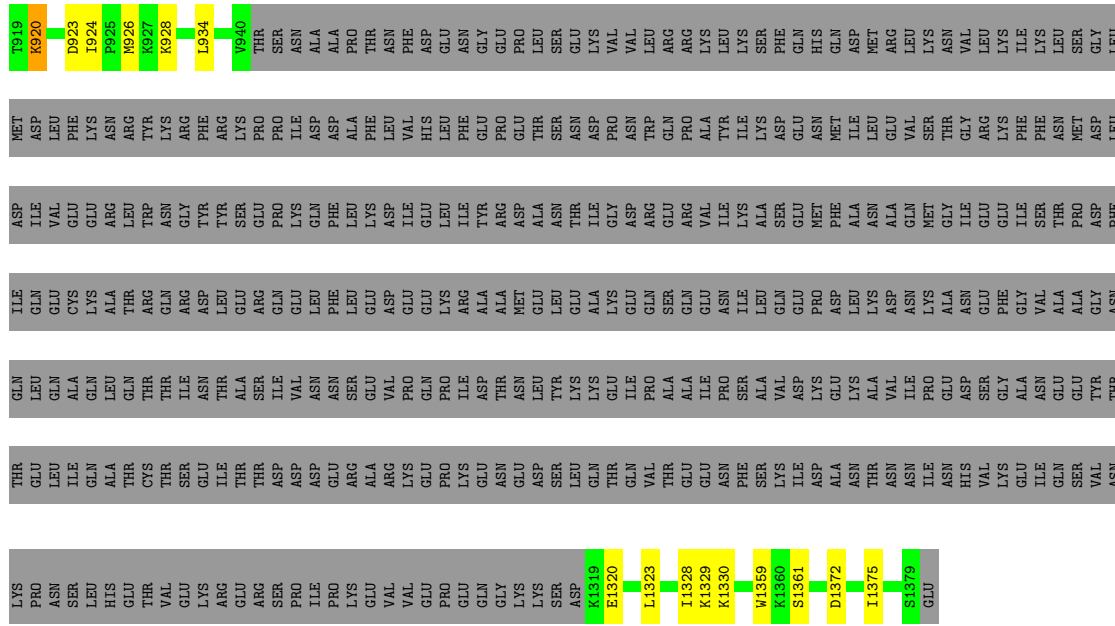
Chain	Residue	Modelled	Actual	Comment	Reference
I	-26	THR	-	expression tag	UNP P40340
I	-25	SER	-	expression tag	UNP P40340
I	-24	GLY	-	expression tag	UNP P40340
I	-23	SER	-	expression tag	UNP P40340
I	-22	MET	-	expression tag	UNP P40340
I	-21	ASP	-	expression tag	UNP P40340
I	-20	TYR	-	expression tag	UNP P40340
I	-19	LYS	-	expression tag	UNP P40340
I	-18	ASP	-	expression tag	UNP P40340
I	-17	HIS	-	expression tag	UNP P40340
I	-16	ASP	-	expression tag	UNP P40340
I	-15	GLY	-	expression tag	UNP P40340
I	-14	ASP	-	expression tag	UNP P40340
I	-13	TYR	-	expression tag	UNP P40340
I	-12	LYS	-	expression tag	UNP P40340
I	-11	ASP	-	expression tag	UNP P40340
I	-10	HIS	-	expression tag	UNP P40340
I	-9	ASP	-	expression tag	UNP P40340
I	-8	ILE	-	expression tag	UNP P40340
I	-7	ASP	-	expression tag	UNP P40340
I	-6	TYR	-	expression tag	UNP P40340
I	-5	LYS	-	expression tag	UNP P40340
I	-4	ASP	-	expression tag	UNP P40340
I	-3	ASP	-	expression tag	UNP P40340
I	-2	ASP	-	expression tag	UNP P40340
I	-1	ASP	-	expression tag	UNP P40340
I	0	LYS	-	expression tag	UNP P40340

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

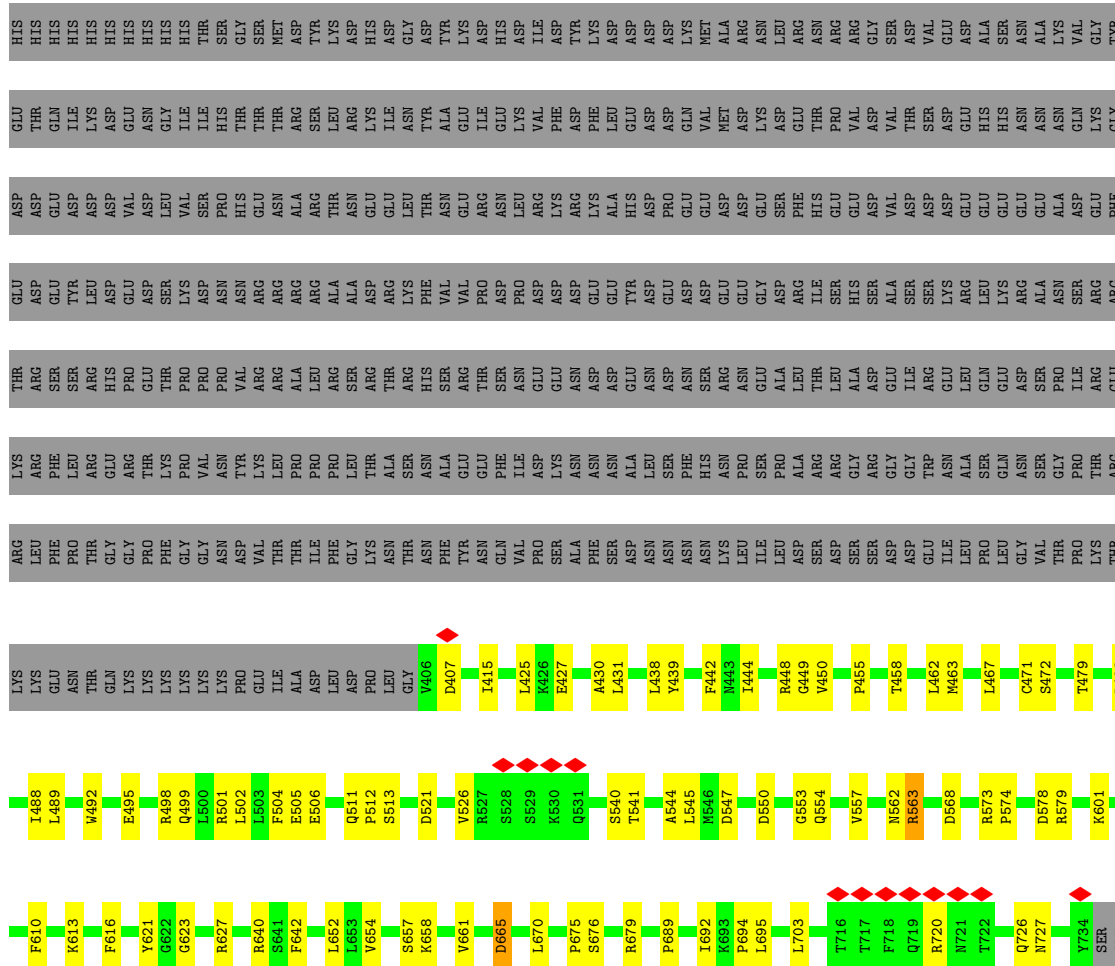


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	





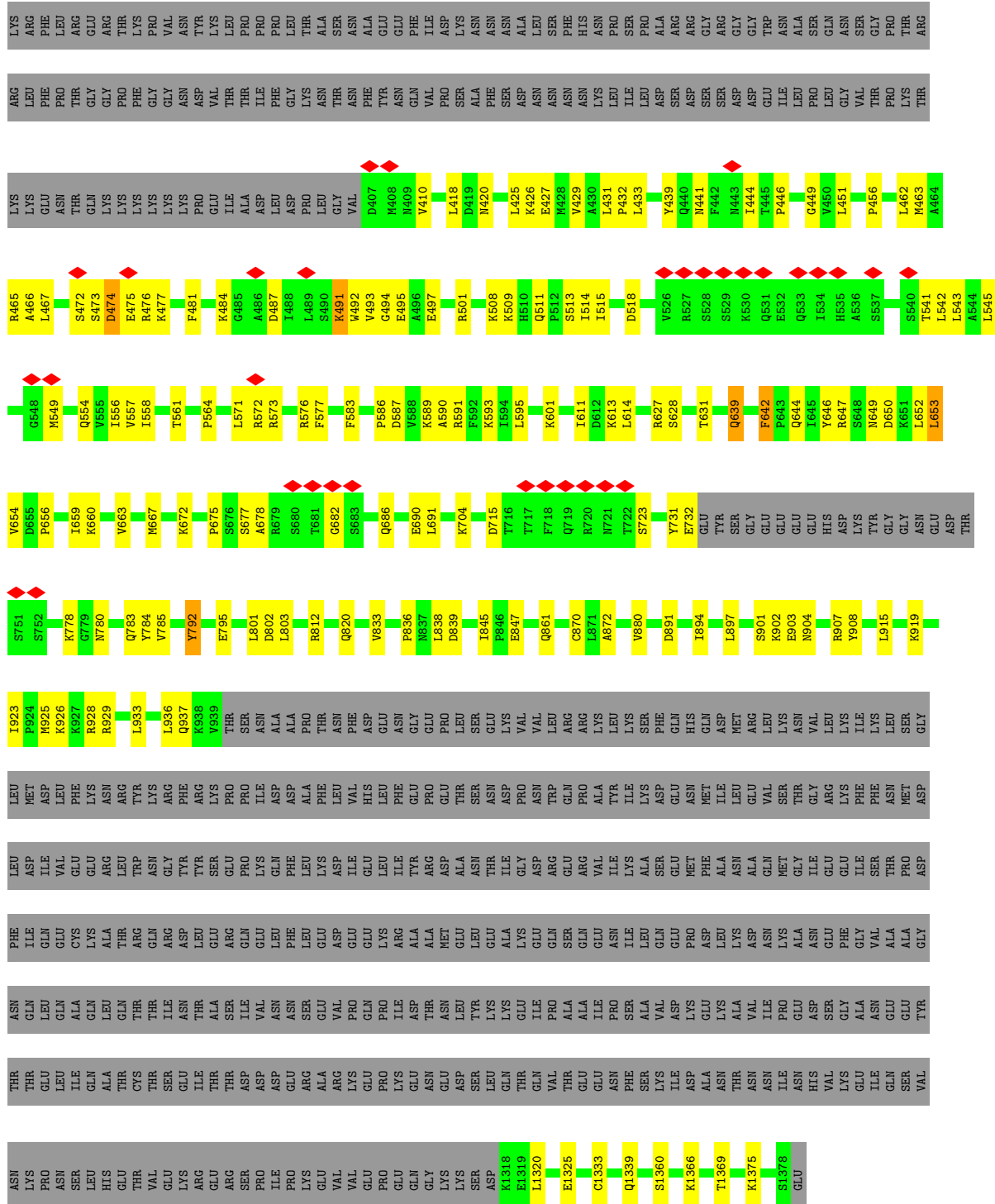
• Molecule 1: ATPase histone chaperone YTA7



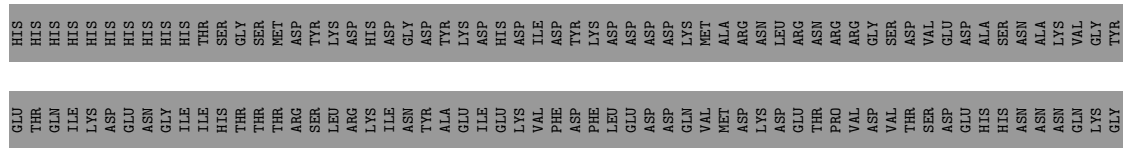




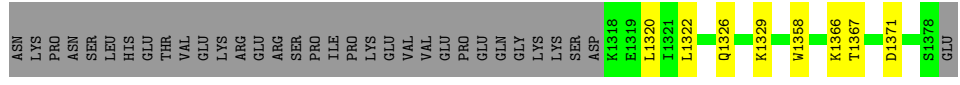




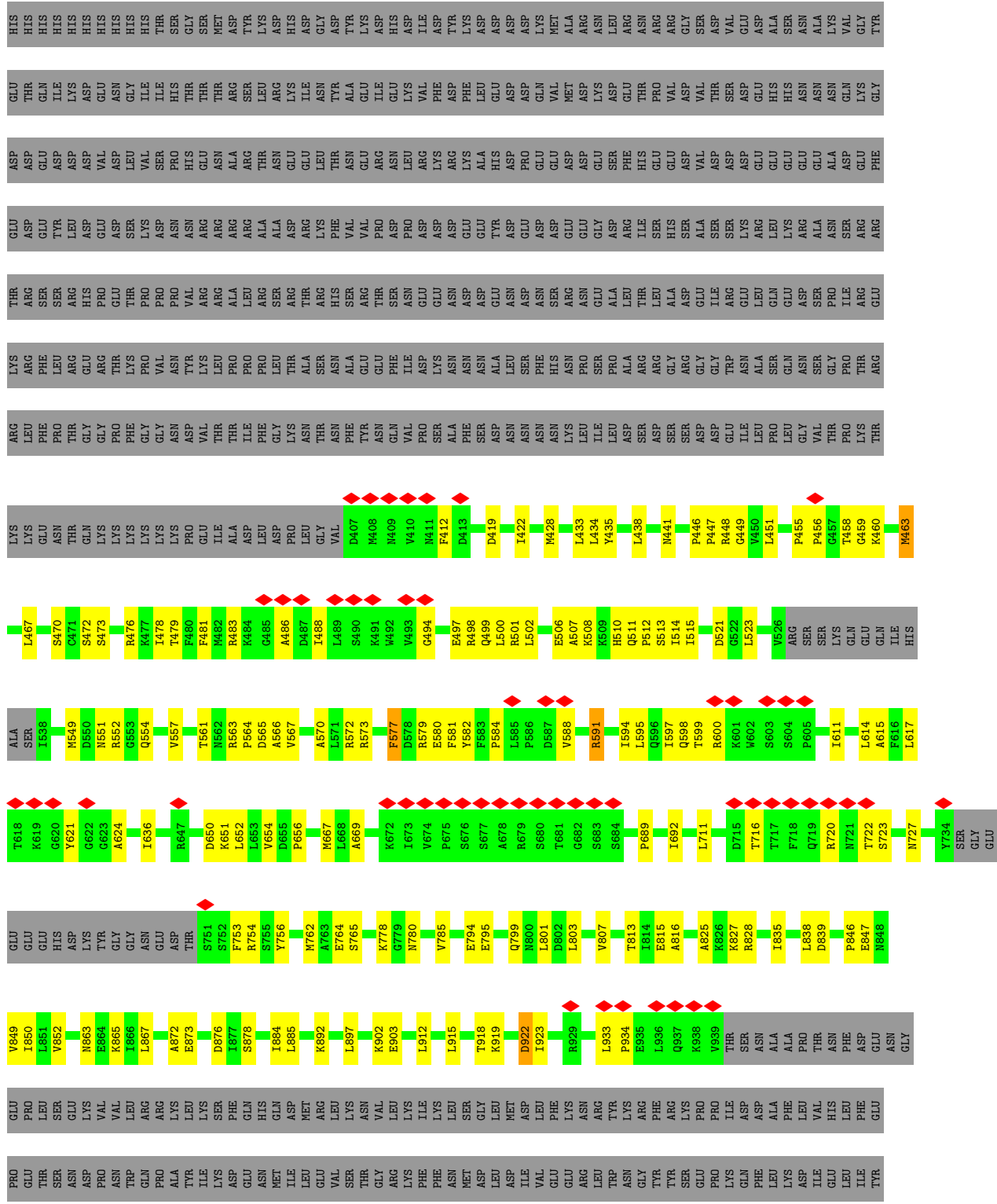
● Molecule 1: ATPase histone chaperone YTA7





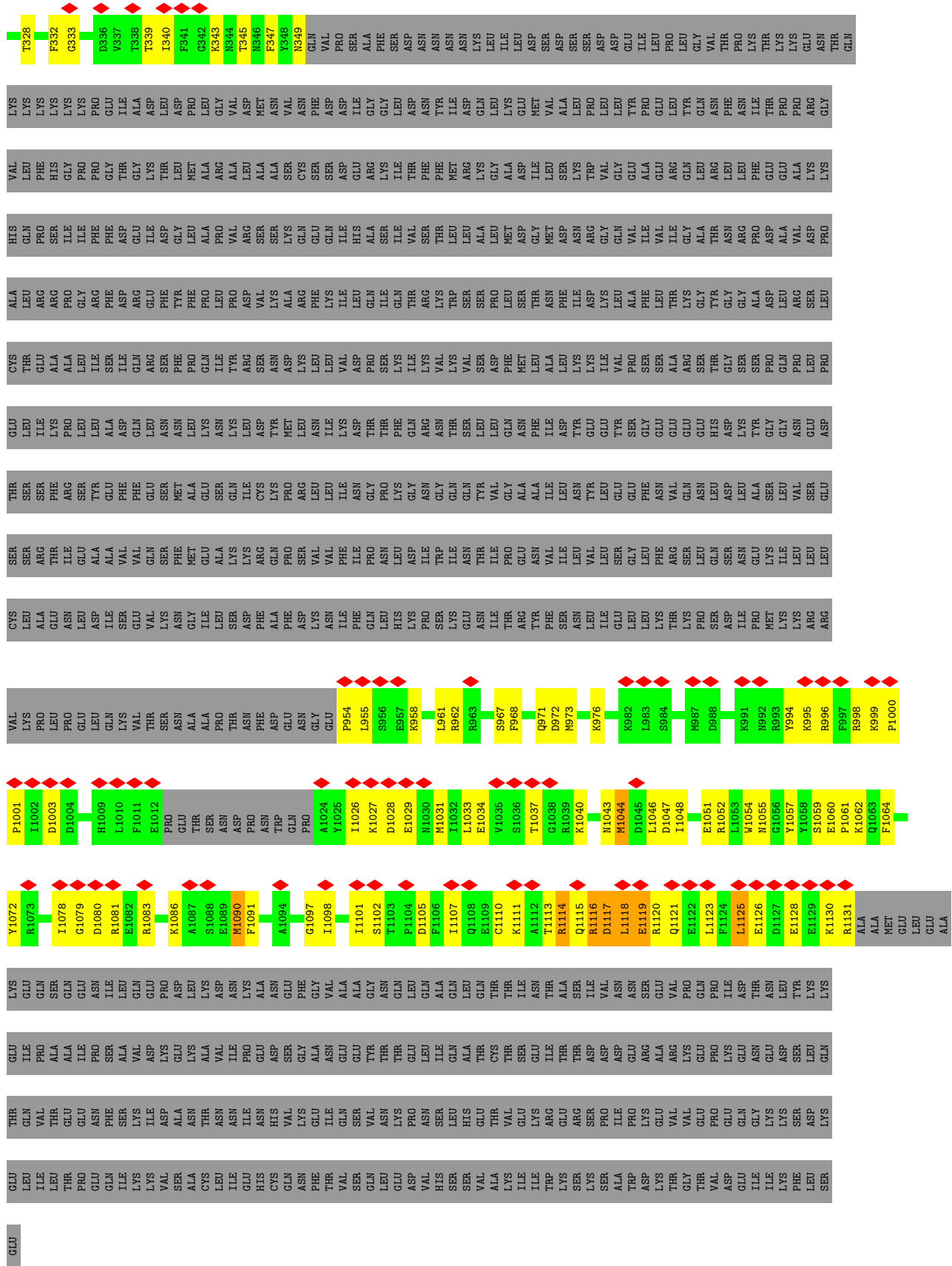


● Molecule 1: ATPase histone chaperone YTA7









• Molecule 1: ATPase histone chaperone YTA7







E1050	E1051	R1052	L1053	M1054	N1055	G1056	T1057	Y1058	S1059	E1060	P1061	K1062	Q1063	F1064	L1065	K1066	D1067	I1068	E1069	L1070	I1071	Y1072	R1073	D1074	A1075	N1076	T1077	I1078	G1079	D1080	R1081	E1082	R1083	V1084	I1085	K1086	A1087	S1088	E1089	M1090	F1091	A1092	N1093	A1094	Q1095	M1096	G1097	I1098	E1099	E1100	I1101	S1102	T1103	P1104	D1105	F1106	I1107	C1110																									
K1111	A1112	T1113	R1114	Q1115	R1116	D1117	L1118	E1119	R1120	Q1121	E1122	L1123	F1124	L1125	E1126	D1127	E1128	E1129	K1130	R1131	ALA	ALA	MET	GLU	LEU	GLU	ALA	ALA	LYS	GLU	GLN	PRO	SER	ALA	VAL	ASP	ASN	ILE	ASP	ASN	LYS	LEU	LEU	GLN	GLY	ASP	LEU	LYS	ASP	ASP	ASN	LYS	GLY	ASN	ALA	ASN	GLU	GLU	GLN	GLU	GLY	PHE	GLY	VAL	ALA	ALA	ASN	ASN	GLN	GLN	ALA												
GLN	LEU	GLN	THR	THR	ILE	ASN	THR	ALA	SER	ILE	VAL	ASN	SER	GLU	ARG	ALA	ARG	VAL	GLN	PRO	PRO	ILE	ASP	ASN	LEU	TYR	ALA	LYS	GLN	GLU	ALA	ALA	PRO	SER	ALA	VAL	ASP	ASN	ILE	ASP	ASN	LYS	LEU	LEU	GLN	GLY	ASP	ASN	LYS	GLY	ASN	ALA	ASN	GLU	GLU	GLN	GLU	GLY	PHE	GLY	VAL	ALA	ALA	ASN	ASN	GLN	GLN	ALA															
GLN	ALA	THR	THR	VAL	GLU	ILE	THR	THR	ASP	THR	ASP	GLU	ARG	ALA	ARG	VAL	GLU	PRO	PRO	LYS	GLU	GLN	THR	THR	VAL	THR	GLU	GLU	GLN	GLU	GLY	ILE	LYS	SER	SER	LEU	ASP	GLU	GLU	GLN	LEU	ILE	LEU	LEU	VAL	SER	ALA	ALA	THR	THR	GLU	GLN	GLN	GLY	ILE	LYS	VAL	GLU	GLU	GLN	GLY	PHE	THR	THR	GLU	VAL	ILE	GLU	GLU	GLN	GLY	GLN	GLY	GLN	GLU	GLU	GLY	ASN	ASN	GLU	GLU	GLN	ALA
SER	SER	ALA	ALA	ILE	ILE	TRP	SER	SER	SER	SER	ALA	TRP	ASP	LYS	VAL	THR	GLY	THR	VAL	VAL	ASP	GLU	ILE	ILE	PHE	LEU	SER	SER	GLU	ILE	LYS	VAL	SER	SER	ALA	ALA	CYS	LEU	ILE	GLU	CYS	HIS	GLN	ASN	PHE	THR	VAL	VAL	GLN	SER	GLN	LEU	GLU	VAL	VAL	ASP	VAL	HIS																									

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	514878	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.895	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.0237	Depositor
Map size ( $\text{\AA}$ )	331.2, 331.2, 331.2	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.29375, 1.29375, 1.29375	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	A	0.28	0/4680	0.52	1/6323 (0.0%)
1	B	0.28	0/4701	0.51	0/6351
1	C	0.30	0/4696	0.55	2/6344 (0.0%)
1	D	0.29	0/4674	0.53	0/6314
1	E	0.26	0/4532	0.51	0/6120
1	F	0.28	0/4606	0.52	0/6223
1	G	0.26	0/1672	0.59	2/2237 (0.1%)
1	H	0.25	0/1672	0.56	1/2237 (0.0%)
1	I	0.25	0/1672	0.57	0/2237
All	All	0.28	0/32905	0.53	6/44386 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1125	LEU	CA-CB-CG	7.23	131.94	115.30
1	C	414	ASP	CB-CG-OD1	6.22	123.90	118.30
1	H	1125	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	1372	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	655	ASP	CB-CG-OD1	5.19	122.97	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4591	0	4709	114	0
1	B	4612	0	4724	98	0
1	C	4607	0	4722	133	0
1	D	4586	0	4707	130	0
1	E	4448	0	4559	114	0
1	F	4519	0	4635	112	0
1	G	1642	0	1644	62	0
1	H	1642	0	1644	74	0
1	I	1642	0	1644	63	0
2	A	27	0	12	0	0
2	B	27	0	12	2	0
2	C	27	0	12	0	0
2	D	27	0	12	1	0
2	E	27	0	12	0	0
All	All	32424	0	33048	828	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 13.

The worst 5 of 828 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1073:ARG:O	1:I:1077:THR:HG22	1.46	1.14
1:C:494:GLY:H	1:D:491:LYS:HG2	1.14	1.11
1:D:449:GLY:HA2	1:D:557:VAL:O	1.54	1.05
1:H:1060:GLU:CD	1:H:1114:ARG:HD3	1.79	1.03
1:B:449:GLY:HA2	1:B:557:VAL:O	1.58	1.02

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	570/1416 (40%)	527 (92%)	43 (8%)	0	100	100
1	B	573/1416 (40%)	551 (96%)	22 (4%)	0	100	100
1	C	572/1416 (40%)	534 (93%)	38 (7%)	0	100	100
1	D	570/1416 (40%)	522 (92%)	48 (8%)	0	100	100
1	E	548/1416 (39%)	508 (93%)	40 (7%)	0	100	100
1	F	559/1416 (40%)	524 (94%)	35 (6%)	0	100	100
1	G	191/1416 (14%)	184 (96%)	7 (4%)	0	100	100
1	H	191/1416 (14%)	185 (97%)	5 (3%)	1 (0%)	29	66
1	I	191/1416 (14%)	184 (96%)	7 (4%)	0	100	100
All	All	3965/12744 (31%)	3719 (94%)	245 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1081	ARG

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	518/1281 (40%)	505 (98%)	13 (2%)	47	70
1	B	520/1281 (41%)	512 (98%)	8 (2%)	65	81
1	C	520/1281 (41%)	499 (96%)	21 (4%)	31	59
1	D	518/1281 (40%)	499 (96%)	19 (4%)	34	62
1	E	502/1281 (39%)	487 (97%)	15 (3%)	41	66
1	F	510/1281 (40%)	498 (98%)	12 (2%)	49	71
1	G	179/1281 (14%)	169 (94%)	10 (6%)	21	52
1	H	179/1281 (14%)	170 (95%)	9 (5%)	24	55
1	I	179/1281 (14%)	172 (96%)	7 (4%)	32	60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3625/11529 (31%)	3511 (97%)	114 (3%)	43 65

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	792	TYR
1	I	1064	PHE
1	E	792	TYR
1	I	1045	ASP
1	H	1044	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	531	GLN
1	C	896	GLN
1	I	1043	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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$
2	ADP	B	1401	-	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
2	ADP	C	1401	-	24,29,29	0.92	1 (4%)	29,45,45	1.54	4 (13%)
2	ADP	A	1401	-	24,29,29	0.93	1 (4%)	29,45,45	1.52	4 (13%)
2	ADP	D	1401	-	24,29,29	0.94	1 (4%)	29,45,45	1.55	4 (13%)
2	ADP	E	1401	-	24,29,29	0.96	1 (4%)	29,45,45	1.34	3 (10%)

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
2	ADP	B	1401	-	-	2/12/32/32	0/3/3/3
2	ADP	C	1401	-	-	2/12/32/32	0/3/3/3
2	ADP	A	1401	-	-	5/12/32/32	0/3/3/3
2	ADP	D	1401	-	-	4/12/32/32	0/3/3/3
2	ADP	E	1401	-	-	4/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1401	ADP	C5-C4	2.45	1.47	1.40
2	D	1401	ADP	C5-C4	2.42	1.47	1.40
2	C	1401	ADP	C5-C4	2.33	1.47	1.40
2	A	1401	ADP	C5-C4	2.32	1.47	1.40
2	B	1401	ADP	C5-C4	2.26	1.46	1.40

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1401	ADP	PA-O3A-PB	-4.38	117.80	132.83
2	D	1401	ADP	PA-O3A-PB	-4.32	117.99	132.83
2	A	1401	ADP	PA-O3A-PB	-3.93	119.33	132.83
2	D	1401	ADP	C3'-C2'-C1'	3.74	106.62	100.98
2	B	1401	ADP	C3'-C2'-C1'	3.68	106.52	100.98

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1401	ADP	C5'-O5'-PA-O1A
2	A	1401	ADP	C5'-O5'-PA-O2A
2	B	1401	ADP	C5'-O5'-PA-O3A
2	C	1401	ADP	C3'-C4'-C5'-O5'
2	D	1401	ADP	C5'-O5'-PA-O1A

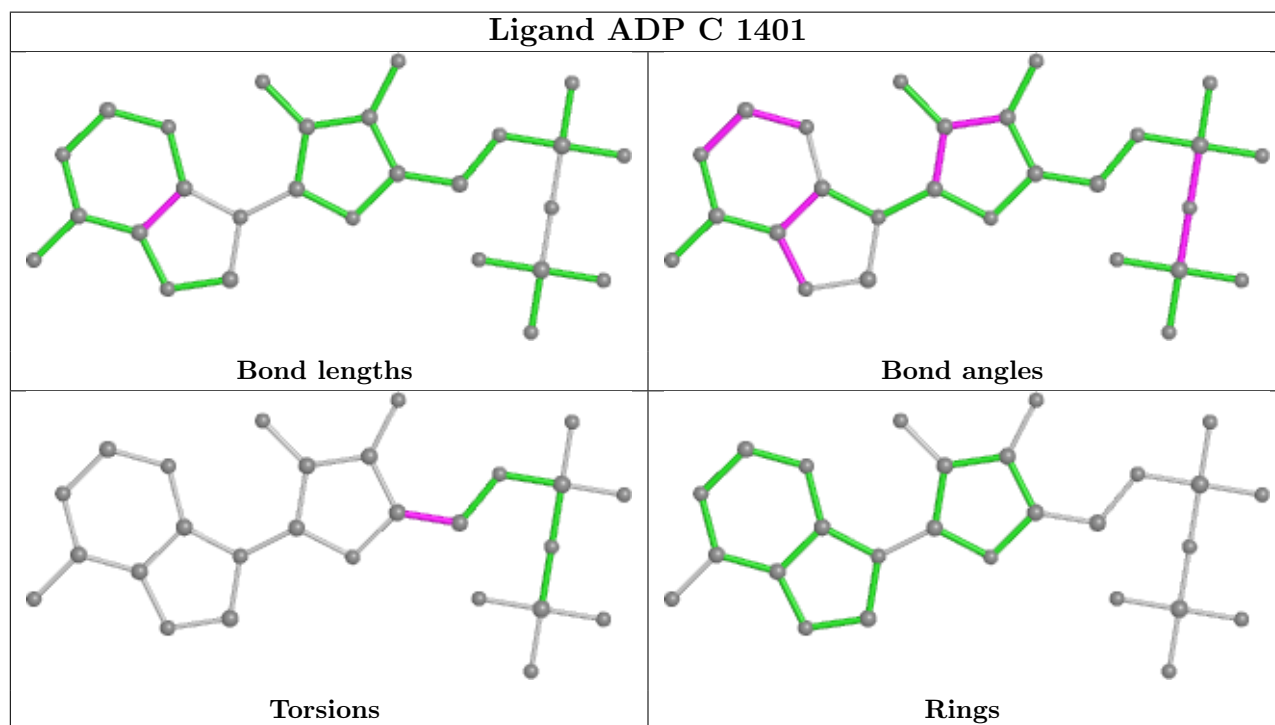
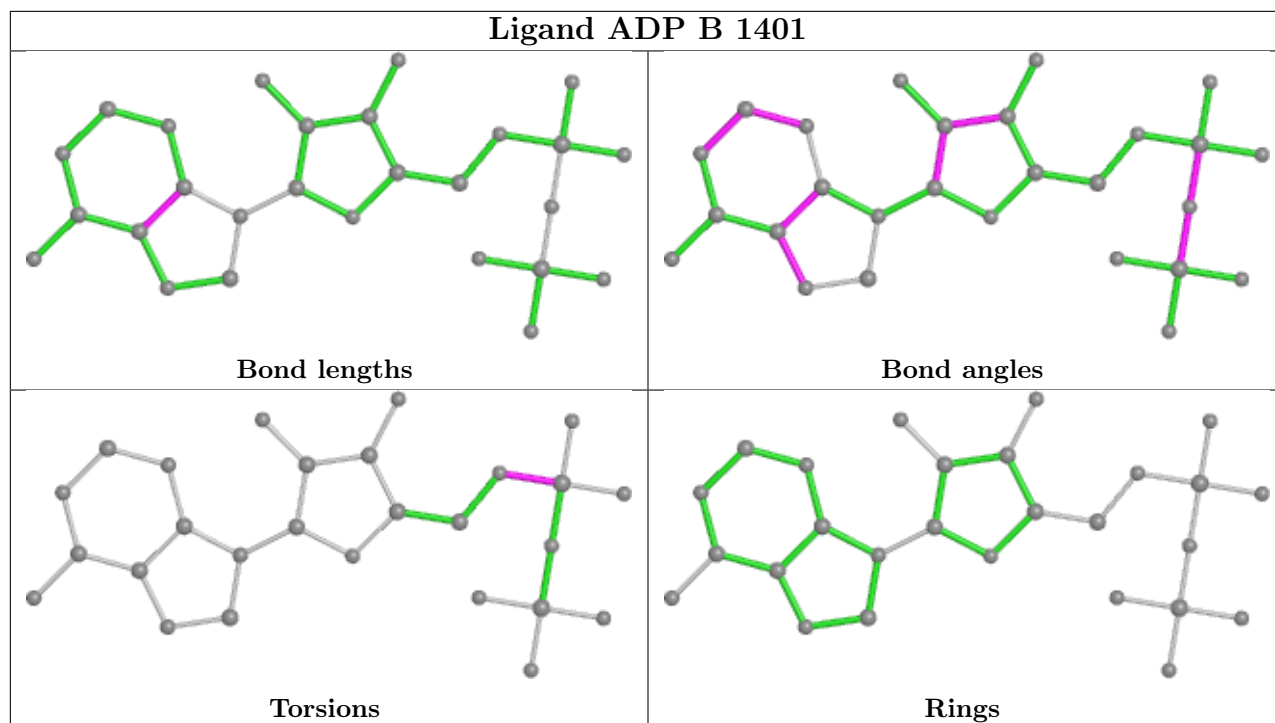
There are no ring outliers.

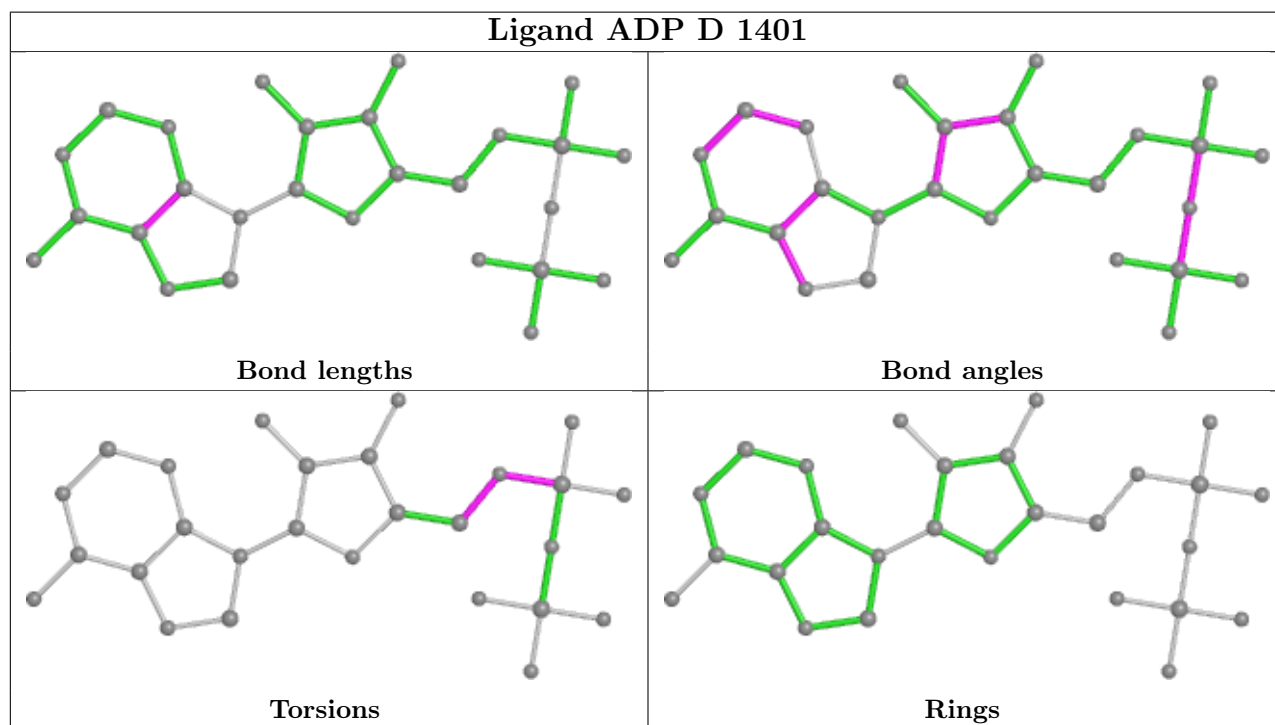
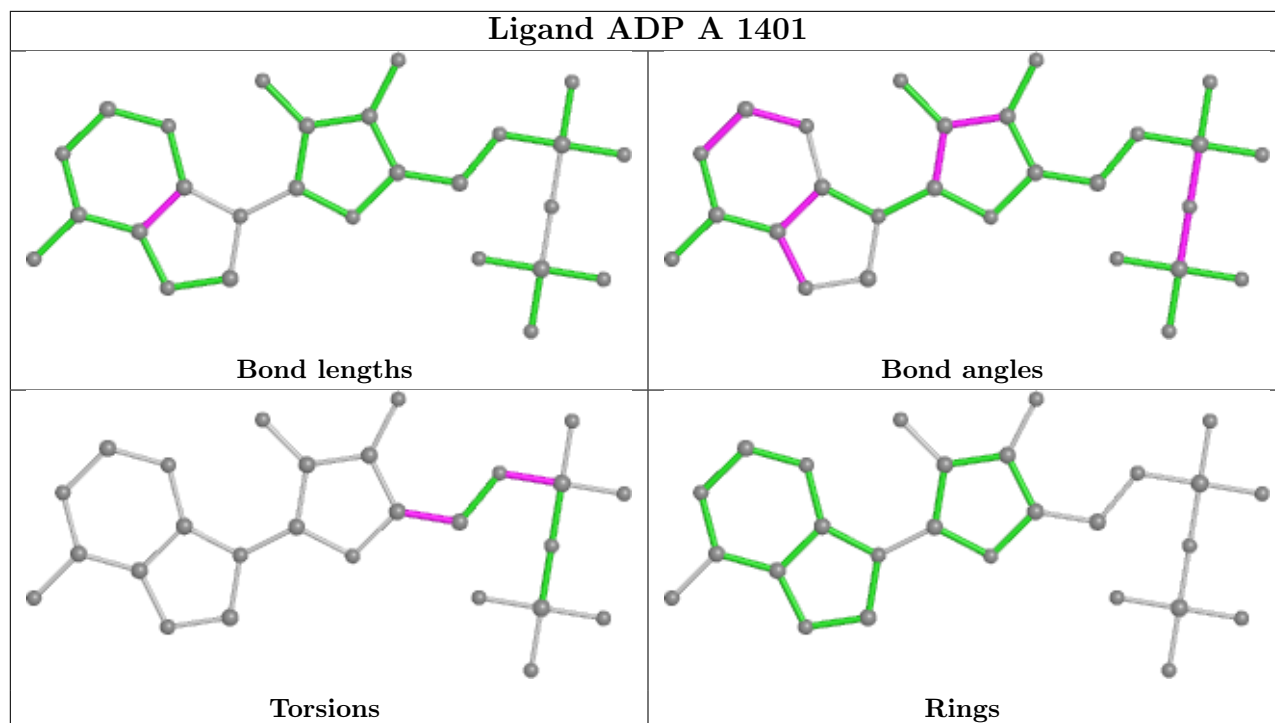
2 monomers are involved in 3 short contacts:

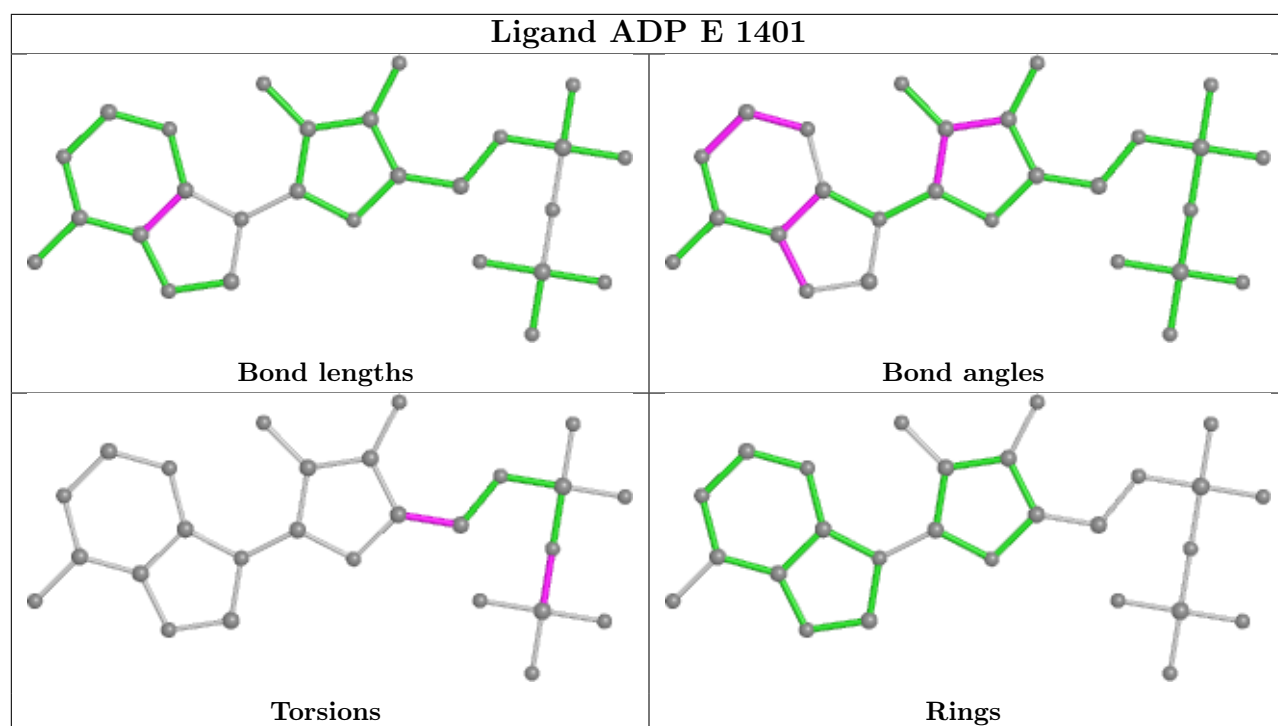
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1401	ADP	2	0
2	D	1401	ADP	1	0

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.

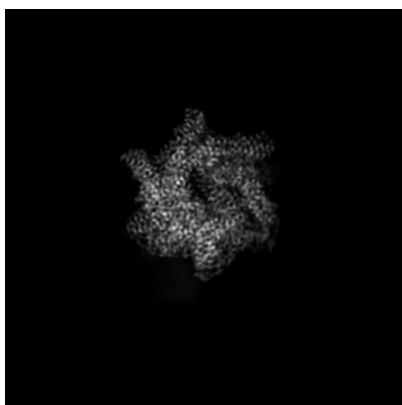
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26695. These allow visual inspection of the internal detail of the map and identification of artifacts.

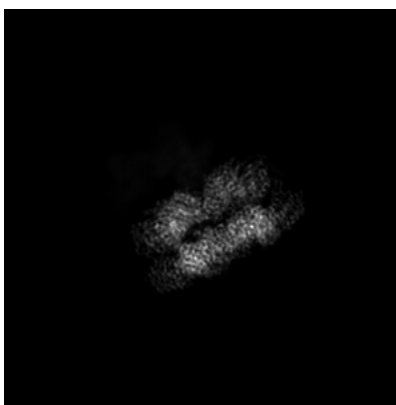
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

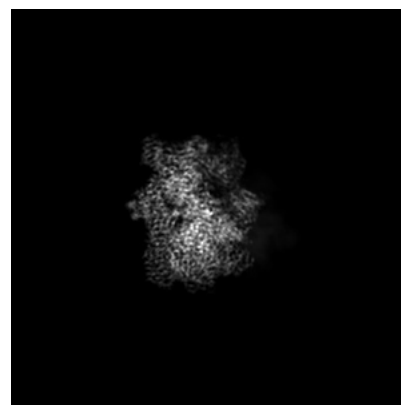
#### 6.1.1 Primary map



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: 128



Y Index: 128



Z Index: 128

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

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

### 6.3.1 Primary map



X Index: 113



Y Index: 108

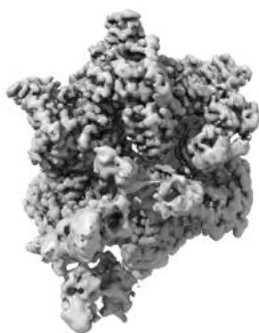


Z Index: 128

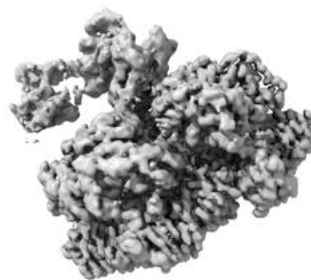
The images above show the largest variance slices of the map in three orthogonal directions.

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

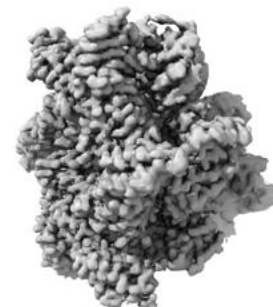
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0237. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

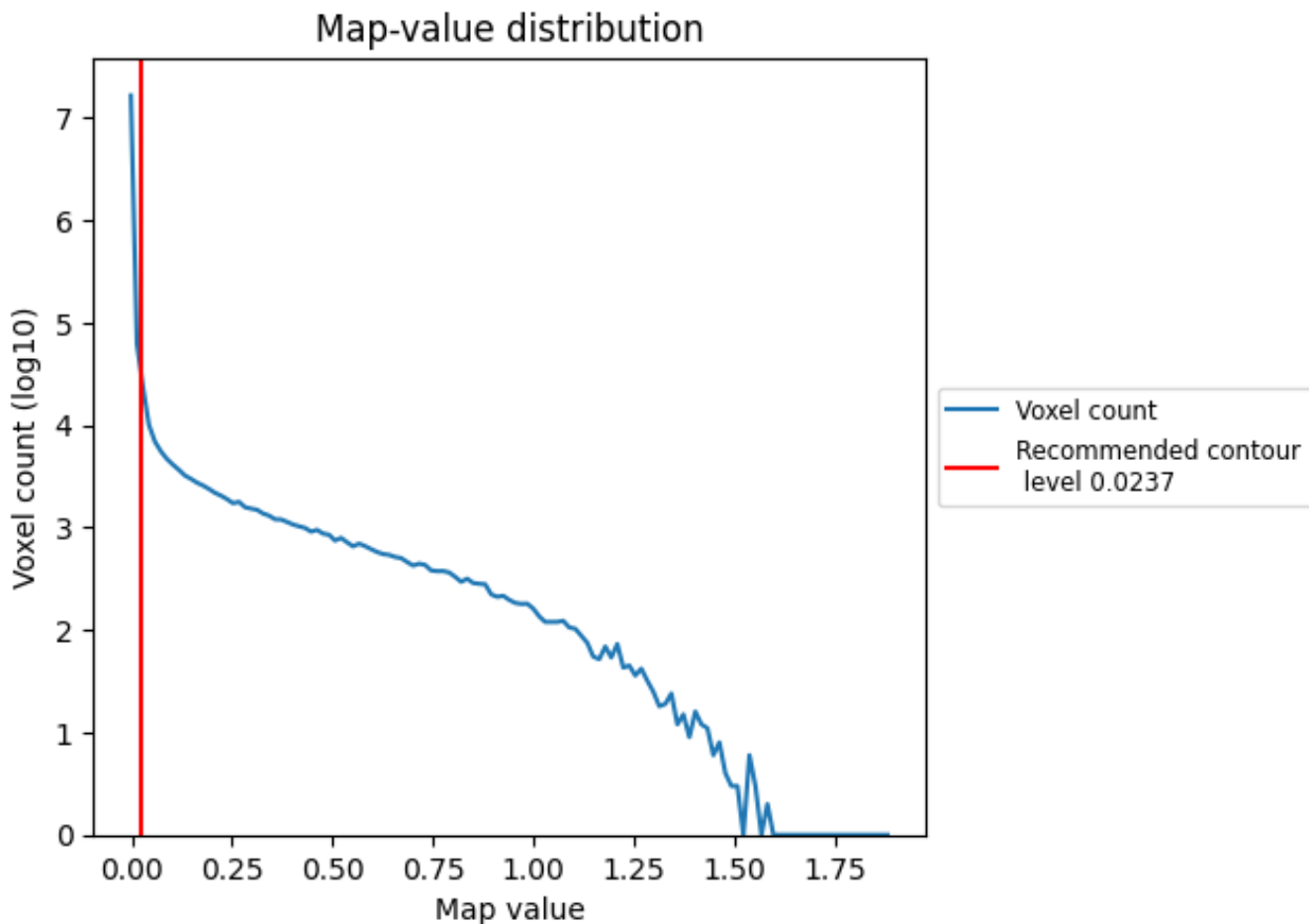
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

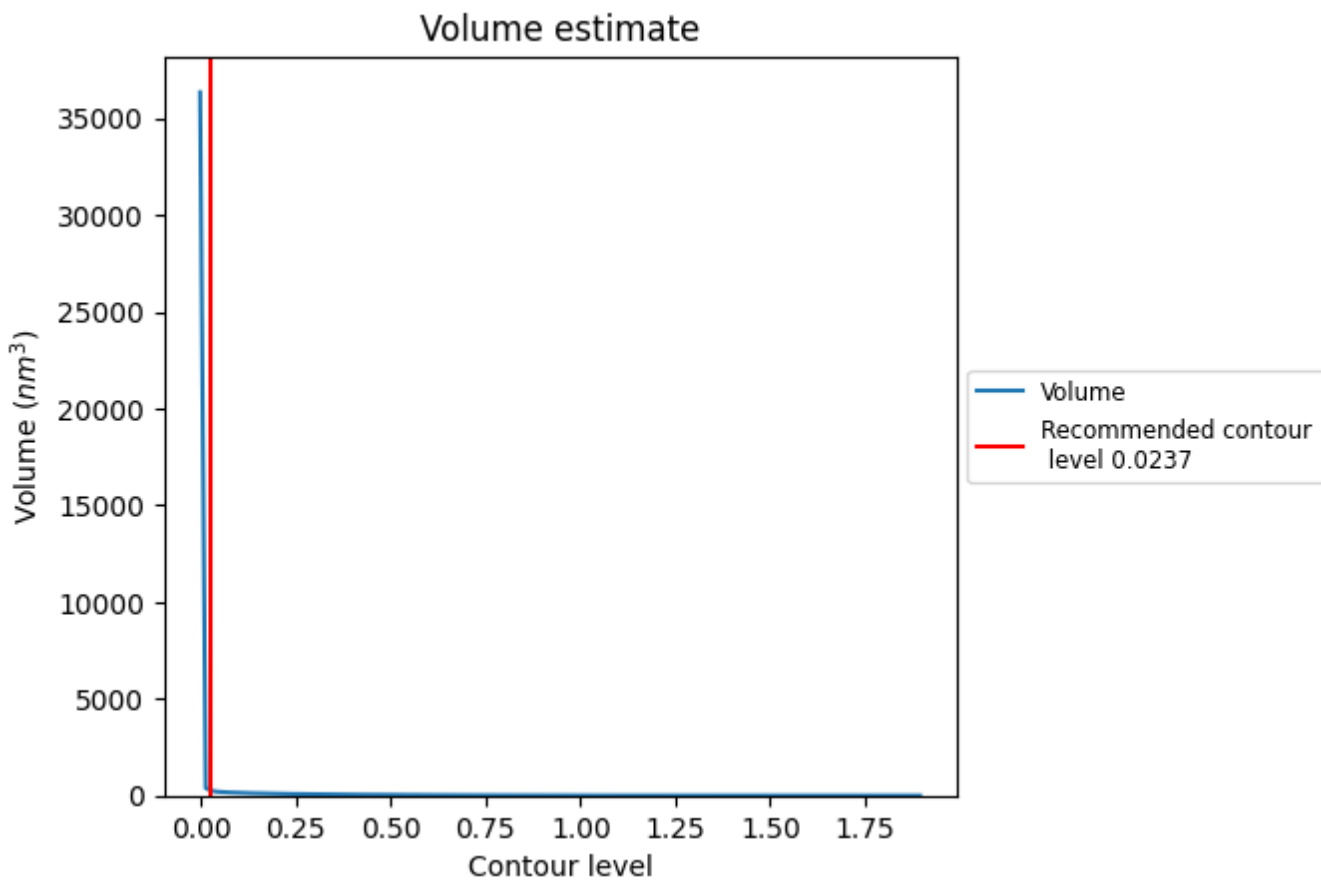
This section contains the results of statistical analysis of the map.

### 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](#)

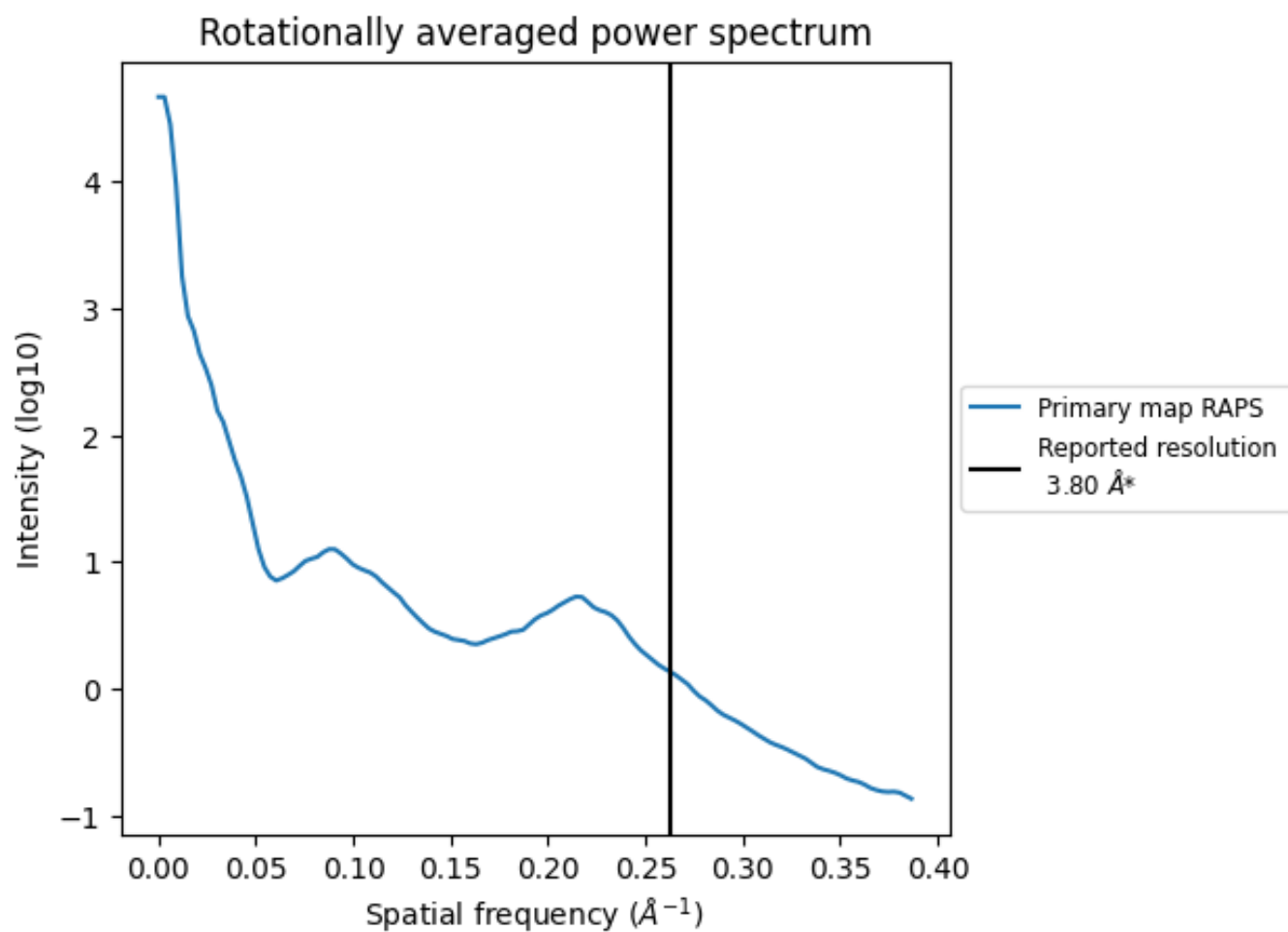


The volume at the recommended contour level is 288  $\text{nm}^3$ ; this corresponds to an approximate mass of 260 kDa.

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.263 Å<sup>-1</sup>

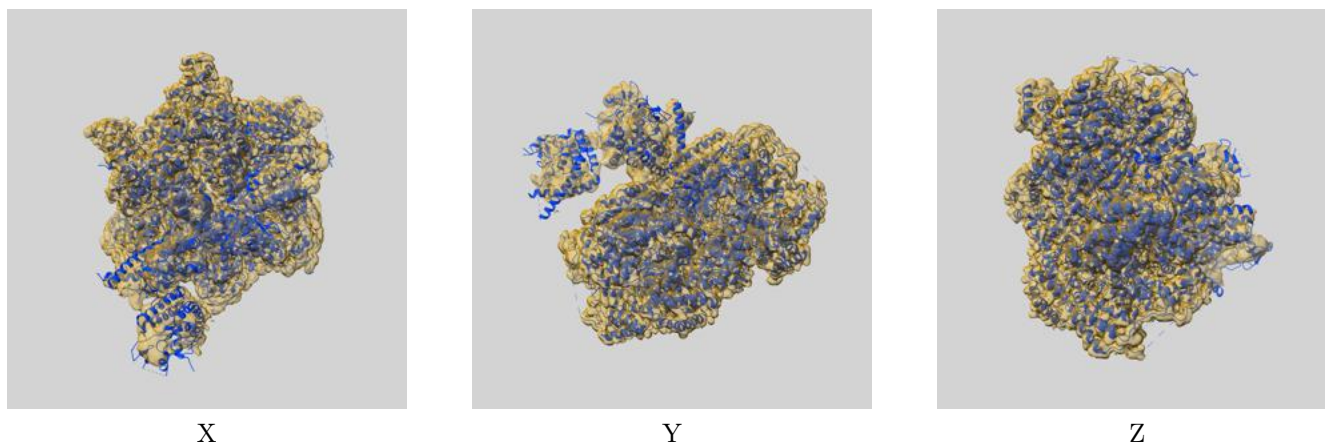
## 8 Fourier-Shell correlation

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

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

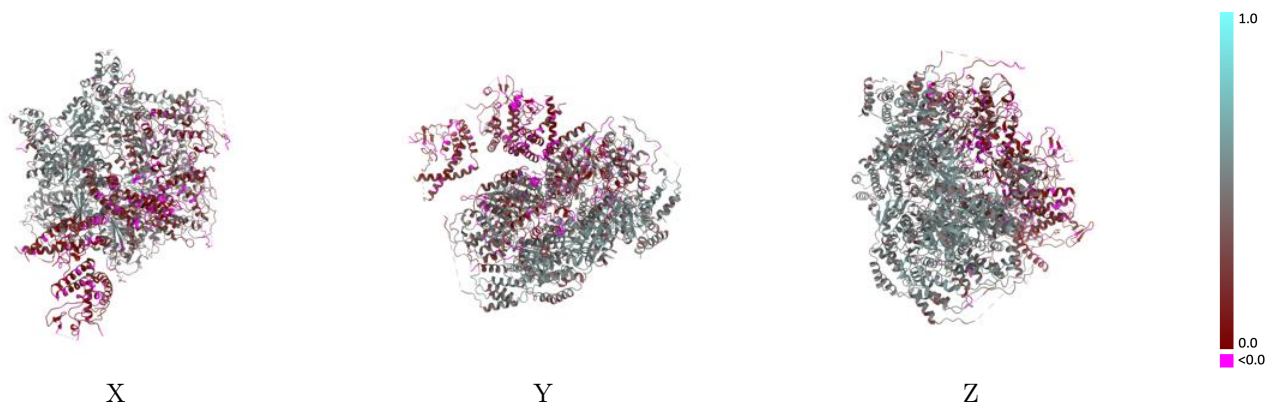
This section contains information regarding the fit between EMDB map EMD-26695 and PDB model 7UQI. Per-residue inclusion information can be found in section 3 on page 14.

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



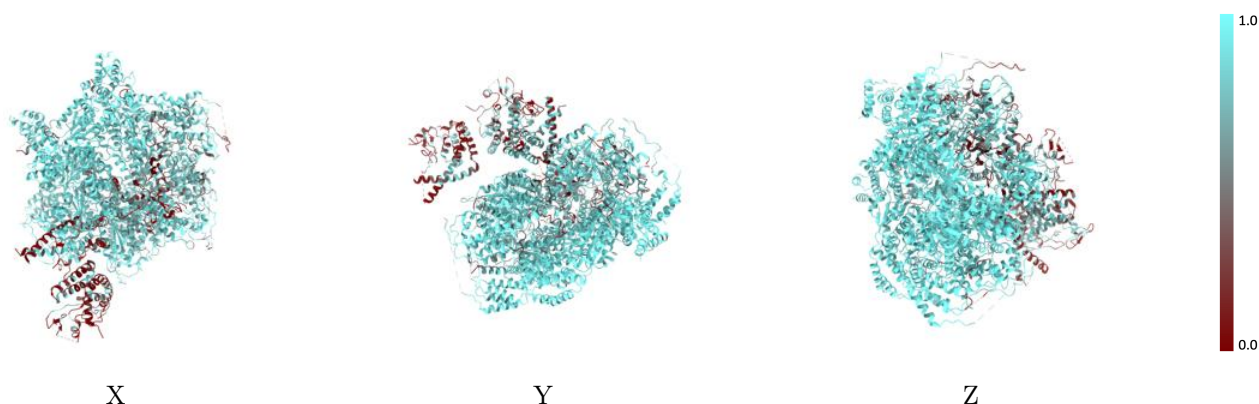
The images above show the 3D surface view of the map at the recommended contour level 0.0237 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



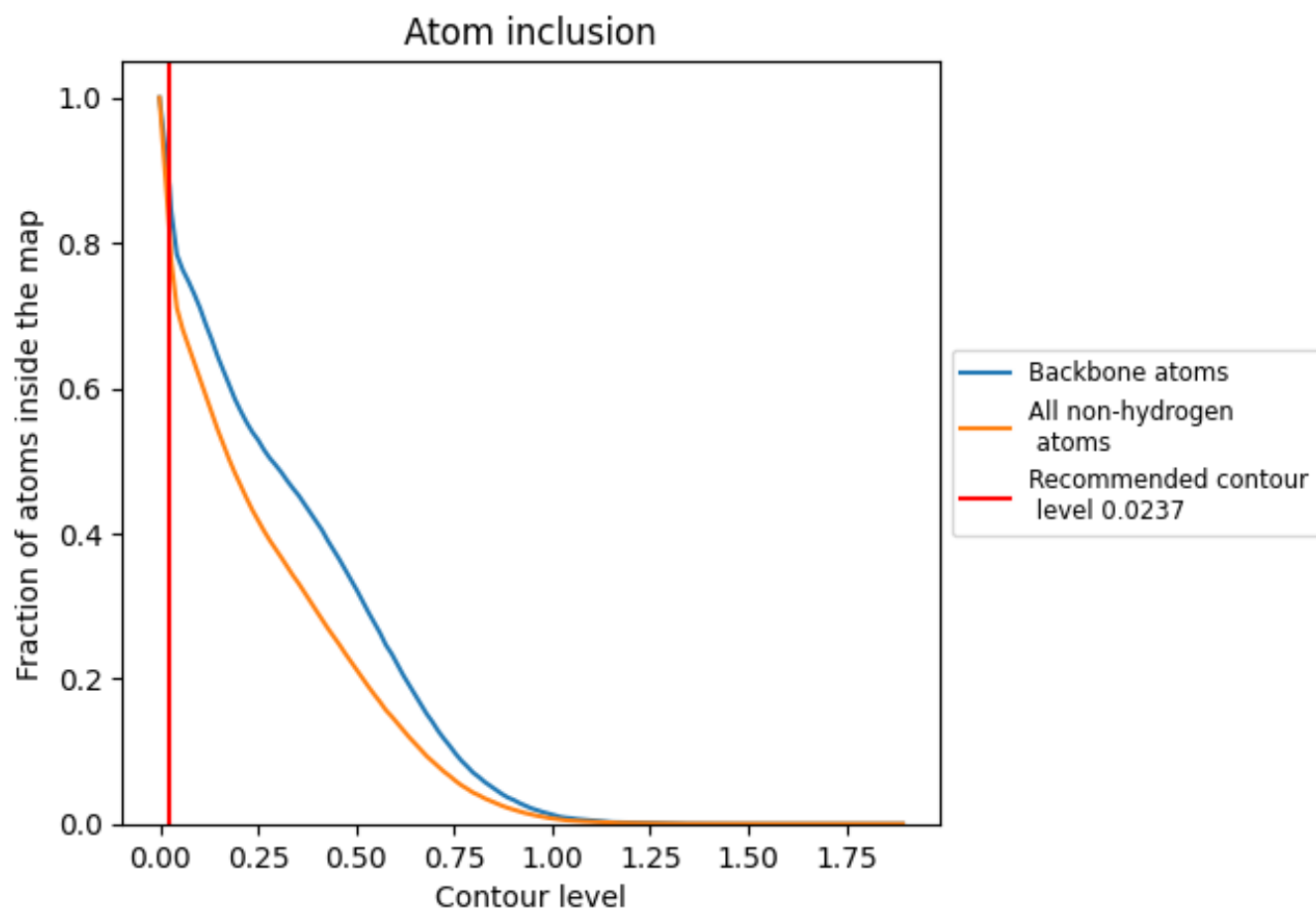
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0237).





















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 81% 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 (0.0237) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.3690
A	 0.9206	 0.4770
B	 0.9290	 0.4790
C	 0.9270	 0.4670
D	 0.8852	 0.3950
E	 0.7643	 0.3070
F	 0.8129	 0.3600
G	 0.5646	 0.0990
H	 0.5434	 0.1250
I	 0.3198	 0.1140

