



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:33 AM UTC

PDB ID : 7UQJ / pdb_00007uqj
EMDB ID : EMD-26696
Title : Cryo-EM structure of the *S. cerevisiae* chromatin remodeler Yta7 hexamer bound to ATPgS and histone H3 tail in state II
Authors : Wang, F.; Feng, X.; Li, H.
Deposited on : 2022-04-19
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

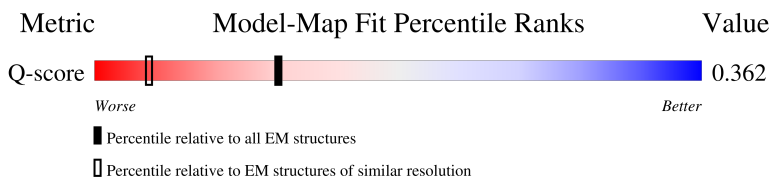
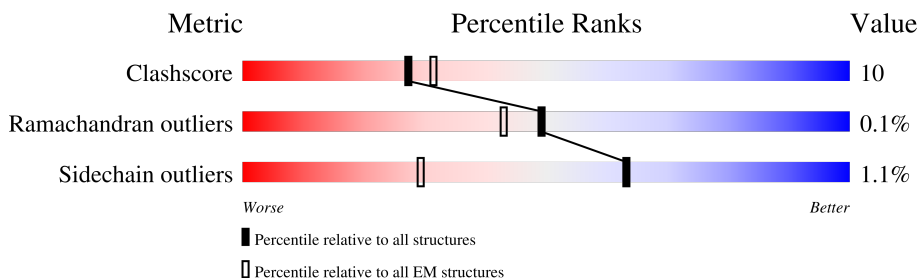
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	1416	 32% 9% 59%
1	B	1416	 33% 8% 59%
1	C	1416	 33% 8% 59%
1	D	1416	 35% 6% 59%

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Mol	Chain	Length	Quality of chain
1	E	1416	34% 7% 59%
1	F	1416	33% 7% 59%
2	G	25	28% 48% 8% • 40%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27983 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
1	A	585	Total	C	N	O	S	0	0
			4646	2978	785	866	17		
1	B	574	Total	C	N	O	S	0	0
			4573	2933	775	848	17		
1	C	581	Total	C	N	O	S	0	0
			4622	2965	782	858	17		
1	D	581	Total	C	N	O	S	0	0
			4622	2965	782	858	17		
1	E	578	Total	C	N	O	S	0	0
			4598	2949	779	853	17		
1	F	581	Total	C	N	O	S	0	0
			4628	2965	785	861	17		

There are 222 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	HIS	-	expression tag	UNP P40340
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	THR	-	expression tag	UNP P40340
A	-25	SER	-	expression tag	UNP P40340
A	-24	GLY	-	expression tag	UNP P40340
A	-23	SER	-	expression tag	UNP P40340
A	-22	MET	-	expression tag	UNP P40340
A	-21	ASP	-	expression tag	UNP P40340
A	-20	TYR	-	expression tag	UNP P40340
A	-19	LYS	-	expression tag	UNP P40340

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	ASP	-	expression tag	UNP P40340
A	-17	HIS	-	expression tag	UNP P40340
A	-16	ASP	-	expression tag	UNP P40340
A	-15	GLY	-	expression tag	UNP P40340
A	-14	ASP	-	expression tag	UNP P40340
A	-13	TYR	-	expression tag	UNP P40340
A	-12	LYS	-	expression tag	UNP P40340
A	-11	ASP	-	expression tag	UNP P40340
A	-10	HIS	-	expression tag	UNP P40340
A	-9	ASP	-	expression tag	UNP P40340
A	-8	ILE	-	expression tag	UNP P40340
A	-7	ASP	-	expression tag	UNP P40340
A	-6	TYR	-	expression tag	UNP P40340
A	-5	LYS	-	expression tag	UNP P40340
A	-4	ASP	-	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	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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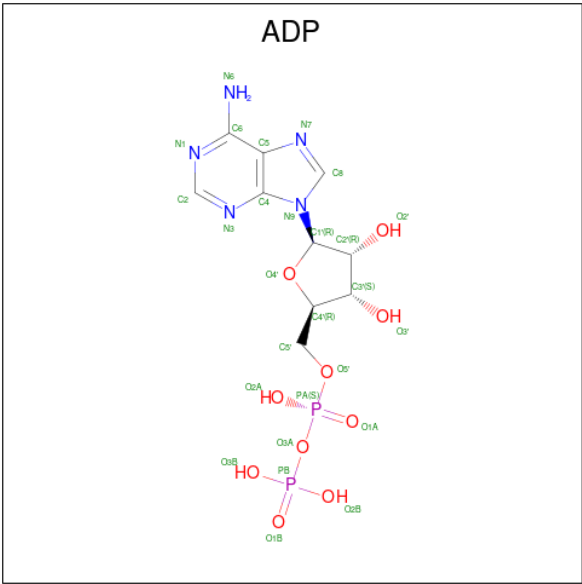
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-35	HIS	-	expression tag	UNP P40340
F	-34	HIS	-	expression tag	UNP P40340
F	-33	HIS	-	expression tag	UNP P40340
F	-32	HIS	-	expression tag	UNP P40340
F	-31	HIS	-	expression tag	UNP P40340
F	-30	HIS	-	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

- Molecule 2 is a protein called Histone H3.

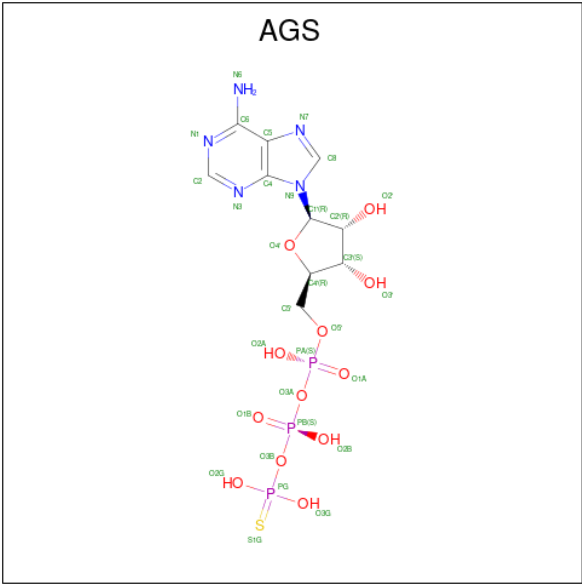
Mol	Chain	Residues	Atoms				AltConf	Trace
2	G	15	Total	C	N	O	0	0
			108	66	23	19		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
4	B	1	31	10	5	12	3	1	0

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Mol	Chain	Residues	Atoms						AltConf
4	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
4	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

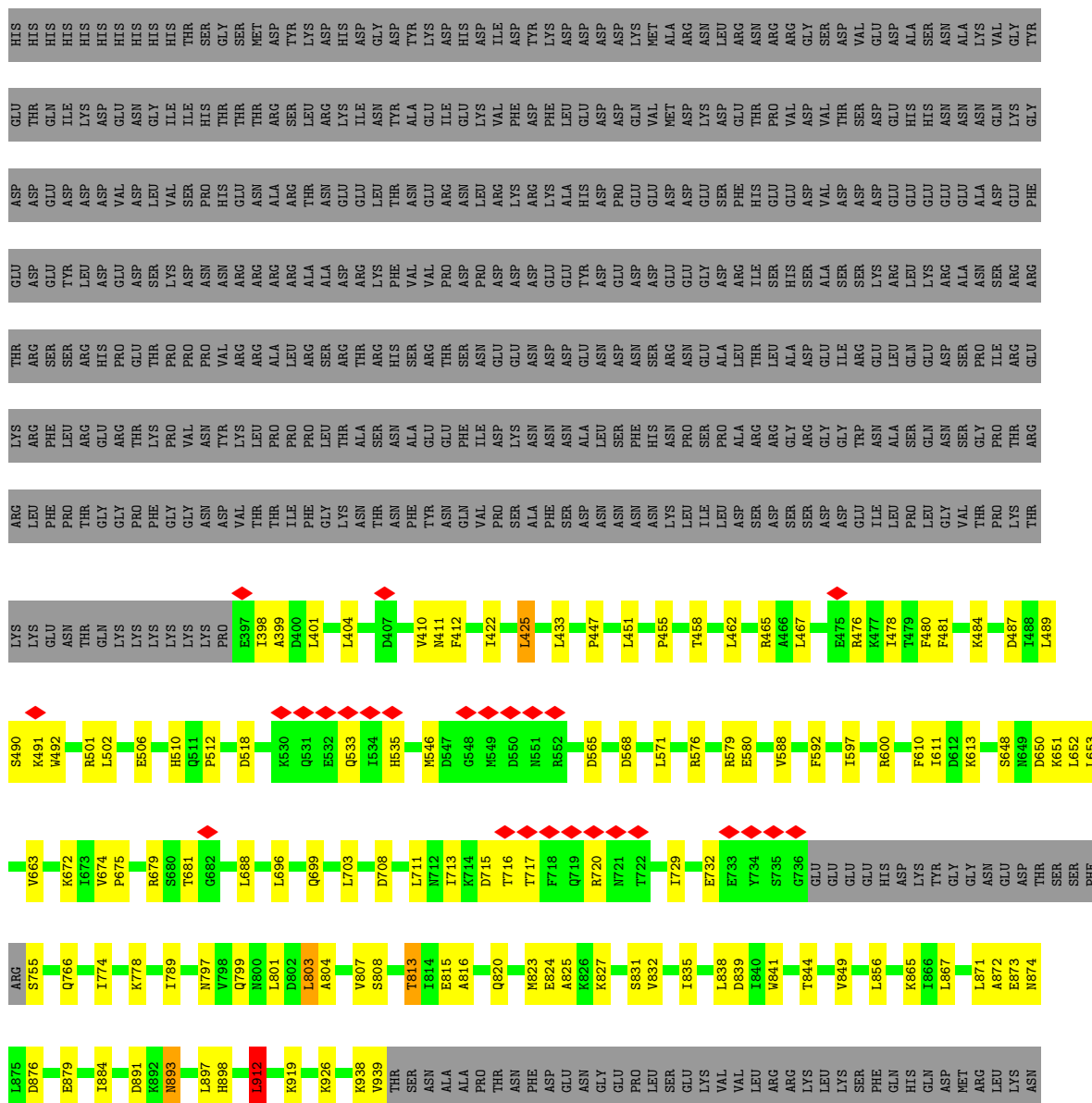
Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Mg	0
			1	1	
5	D	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	
5	F	1	Total	Mg	0
			1	1	

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: ATPase histone chaperone YTA7

Chain A: 



- Molecule 1: ATPase histone chaperone YTA7



I845	L696	F481	LYS	ARG	LYS	THR	GLU	ASP	THR	GLU	HIS
V849	A697	D487	LYS	LEU	PHE	ARG	GLU	ASP	THR	GLU	HIS
S854	L700		ASN	PRO	PHE	LEU	GLU	GLU	TYR	ILE	HIS
G855	L703	K491	THR	THR	THR	ARG	LEU	ASP	ASP	LYS	HIS
L856		W492	GLN	GLY	GLY	GLU	GLU	ASP	ASP	ASP	HIS
	Q719	W493	LYS	PRO	PRO	THR	THR	VAL	VAL	GLU	HIS
			LYS	PHE	GLY	ARG	LYS	ASP	THR	ILE	THR
S859	R720	E497	LYS	GLY	GLY	VAL	PRO	SER	SER	ASP	GLY
L860	N721	K509	LYS	ASN	ASN	ASN	ASN	PRO	ASN	ASN	SER
	T722	H510	LYS	THR	THR	THR	TYR	ASN	ASN	PRO	GLY
I866		Q511	PRO	ASP	ASP	VAL	VAL	ARG	GLU	HIS	GLY
L867	Y734	P512	ILE	VAL	VAL	LEU	ARG	ARG	THR	THR	SER
L868	S735	S513	ILE	THR	THR	LEU	ALA	ALA	ALA	ARG	THR
			ALA	THR	THR	PRO	PRO	ARG	ARG	ARG	THR
L871	GLY	R527	ASP	ILE	PHE	PRO	PRO	ARG	ALA	THR	LYS
A872	GLU		LEU	GLY	GLY	LEU	LEU	SER	ALA	THR	LYS
	GLU	L543	ASP	GLY	GLY	THR	THR	ARG	ASP	ARG	LYS
L875	GLU		PRO	LYS	LYS	THR	THR	ASP	GLU	GLU	HIS
E879	HIS	M546	LEU	ASN	ASN	ALA	ALA	ARG	GLU	ILE	ASP
V880	ASP	D547	GLY	THR	THR	SER	SER	LYS	LEU	ASN	GLY
	LYS	D550	VAL	ASN	PHE	ASN	ASN	HIS	THR	TYR	THR
G883	TYR		D407	THR	THR	GLU	GLU	SER	VAL	GLU	LYS
I884	GLY	I566	M408	ASN	TYR	THR	THR	ARG	GLU	ILE	ASP
D887	GLY	V557		GLN	ASN	GLU	GLU	ASP	PRO	PRO	HIS
	ASN		M411	VAL	VAL	ILE	ILE	LEU	ASP	ASP	LYS
L891	GLU	R576		PRO	PRO	ASP	GLU	GLU	ASP	VAL	ILE
D891	ASP	F577	D414	SER	SER	LYS	GLU	GLU	LYS	PHE	ASP
I894	THR	D578		PHE	ALA	ASN	ASN	ASN	ARG	ASP	TYR
	SER	R579	Q424	THR	THR	ASN	ASN	ASP	GLU	LEU	LYS
	SER			ASN	ASN	LEU	ASN	ASN	ASP	ASP	ASP
S901	PHE	R600	E427	SER	ASP	ASN	LEU	ASN	PRO	GLN	LYS
N904	ARG	T608	M428	ASN	ASN	SER	SER	GLU	GLU	VAL	ALA
	SER		V429	ASN	ASN	ASN	ASN	GLU	GLU	MET	ALA
E914	Y756		A430	ASN	ASN	PHE	SER	GLY	GLU	ASP	ASN
		I611	L431	ASN	ASN	THR	THR	ASP	GLU	ASP	ASN
K917	M762	E632	L438	LYS	LYS	ASN	ASN	ASP	GLU	LYS	ASN
T918	S765	Y439	Y439	LEU	LEU	PRO	PRO	SER	GLY	ASP	LEU
K919	R771	Q644	Q440	ILE	LEU	SER	PRO	ALA	ASP	ASP	LEU
P920			N441	LEU	ASP	ALA	ALA	LEU	SER	PHE	ARG
M925	I774	D655		ASP	SER	ALA	ALA	LEU	PHE	GLU	ARG
R929	S656	S657	T444	ASP	ASP	ARG	ARG	ILE	GLU	THR	ASN
	I789	S657	T445	SER	SER	GLY	GLY	ALA	GLU	PRO	ARG
		I673	P447	SER	SER	ARG	ARG	ALA	ASP	VAL	GLY
L933	L801		R448	ASP	ASP	GLY	GLY	GLU	VAL	THR	SER
		S676	Q449	GLU	GLU	TRP	TRP	ARG	SER	ASP	ASP
L936	S810			ILE	ILE	ASN	ASN	GLU	ASP	SER	VAL
W939	I814	R679	K460	PRO	PRO	ALA	ALA	LEU	GLU	GLU	ALA
THR	E815	L868	L462	LEU	LEU	GLN	GLN	LEU	GLU	HIS	ALA
SER	F822	P689	M463	GLY	GLY	ASN	ASN	ARG	GLU	ASN	ASN
ASN	M823	E590		THR	THR	GLY	GLY	SER	GLU	ALA	ALA
ALA		I691	A466			PRO	PRO	ILE	ASP	ASN	VAL
PRO	K826	I692	S470	LYS	LYS	THR	THR	ARG	GLU	GLN	GLY
THR		K693	C471	THR	THR	ARG	ARG	GLU	THR	ARG	THR

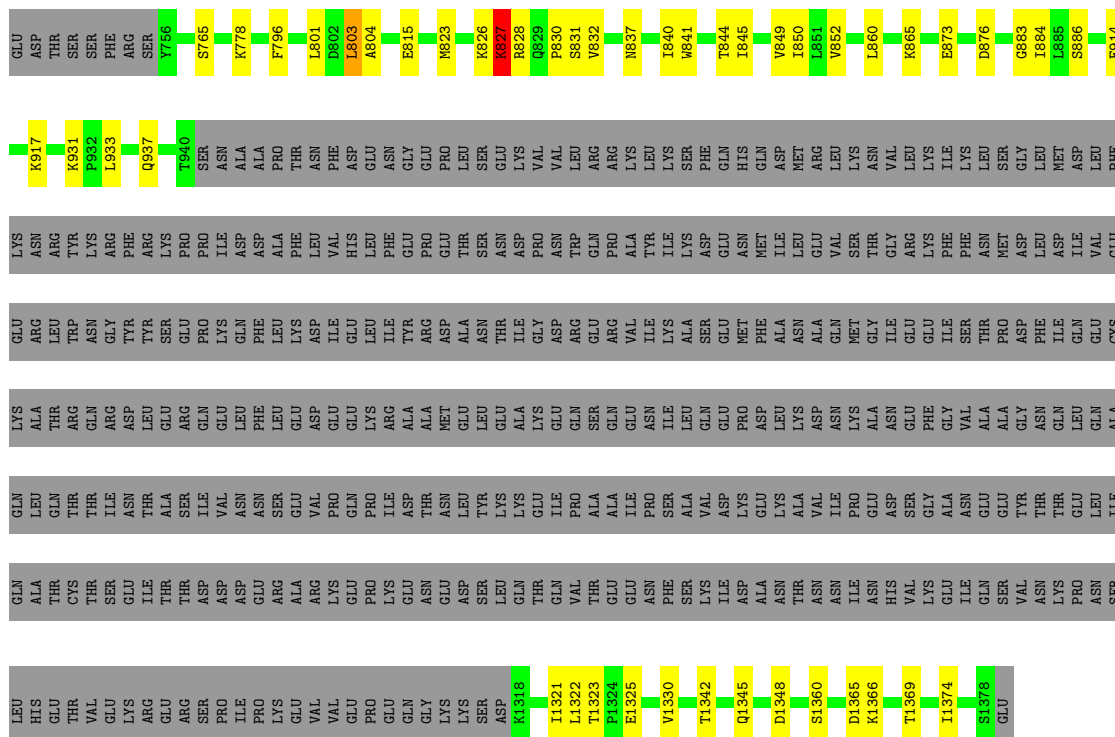
VAL	VAL	ARG	VAL	ASP	ASP	LEU	ASN
VAL	GLU	LYS	PRO	GLU	ILE	VAL	PHE
PRO	GLU	GLU	GLN	GLU	GLU	HIS	ASP
GLU	GLU	PRO	PRO	LYS	LEU	LEU	GLU
GLN	GLU	LYS	ILE	ARG	ILE	PHE	GLY
GLY	ASN	GLU	THR	ALA	ARG	GLU	GLU
LYS	GLU	GLU	ASN	MET	ARG	PRO	PRO
LYS	ASP	GLU	THR	LEU	ALA	GLU	LEU
SER	ASP	ASP	LYS	GLU	ALA	THR	SER
ASP	LEU	SER	LEU	GLU	ASN	SER	GLU
K1318	GLN	GLN	LYS	ALA	ILE	ASP	LYS
E1319	THR	THR	GLU	LYS	GLY	PRO	VAL
L1320	GLN	ILE	GLN	ASP	ASP	ASN	VAL
T1323	THR	VAL	PRO	ARG	TRP	ASN	VAL
P1324	GLU	ALA	ALA	GLU	GLN	ARG	ARG
F1325	GLU	ILE	ILE	VAL	VAL	ALA	LYS
Q1326	ASN	PRO	PRO	ASN	ILE	THR	LEU
K1355	PHE	SER	SER	ILE	LYS	ILE	LYS
K1361	LYS	SER	VAL	LEU	ALA	ASP	SER
S1362	ASP	ILE	ASP	GLU	GLU	GLU	PHE
V1370	ASN	ASN	LYS	PRO	MET	ASN	HIS
S1378	ILE	ASN	ILE	LYS	GLN	VAL	GLN
GLU	ASN	ASN	GLU	ALA	GLY	SER	LYS
	HIS	HIS	ASP	ASN	ILE	THR	ASN
	VAL	VAL	SER	GLU	GLU	GLY	VAL
	LYS	LYS	GLY	PHE	GLU	LYS	LYS
	GLU	GLU	ALA	GLY	ILE	PHE	ILE
	ILE	ILE	ASN	VAL	SER	PHE	LYS
	GLN	GLN	GLU	ALA	ASN	ASN	LEU
	SER	SER	GLU	ALA	PRO	MET	SER
	THR	THR	TYR	GLY	ASP	GLY	GLY
	ASN	ASN	THR	ASN	PHE	LEU	LEU
	LYS	LYS	THR	GLN	ILE	ASP	MET
	PRO	PRO	GLU	LEU	GLN	ILE	ASP
	ASN	ASN	ILE	GLN	VAL	LEU	LEU
	SER	SER	ILE	ALA	CYS	GLU	PHE
	LEU	LEU	GLN	GLN	LYS	GLU	LYS
	HIS	HIS	ALA	LEU	ALA	ARG	ASN
	GLU	GLU	THR	GLN	THR	LEU	ARG
	THR	THR	CYS	THR	ARG	TRP	TYR
	VAL	VAL	THR	THR	GLN	ASN	LYS
	GLU	GLU	SER	ILE	ARG	GLY	ARG
	ARG	ARG	GLU	THR	LEU	TYR	PHE
	GLU	GLU	THR	ALA	GLU	SER	LYS
	ARG	ARG	THR	SER	ARG	GLU	PRO
	SER	SER	ASP	ILE	GLN	PRO	PRO
	PRO	PRO	ASP	VAL	GLU	PRO	PRO
	ILE	ILE	LYS	THR	ILE	GLN	ASN
	PRO	PRO	GLU	ASN	PHE	PHE	ASP
	LYS	LYS	ALA	SER	LEU	ALA	ASP
	GLU	GLU	THR	GLU	GLU	LYS	THR

- Molecule 1: ATPase histone chaperone YTA7

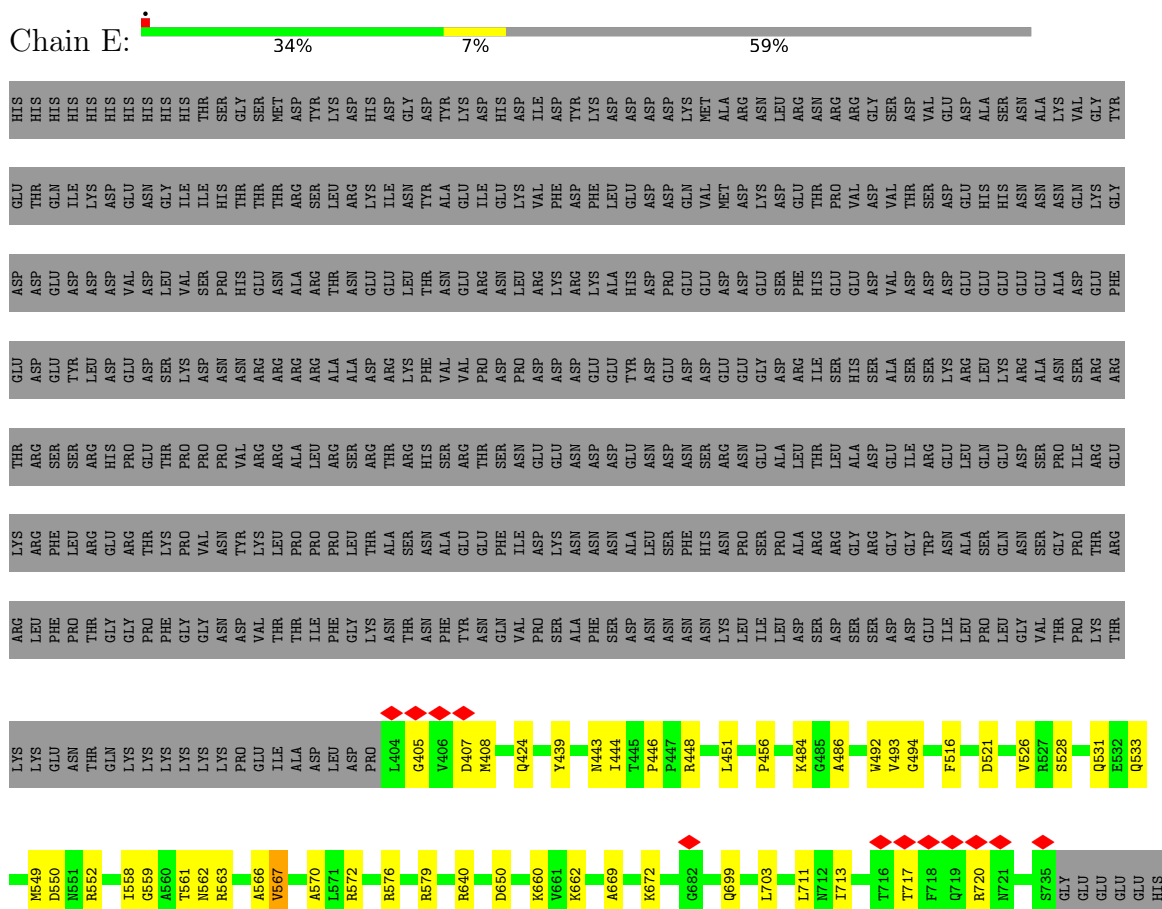


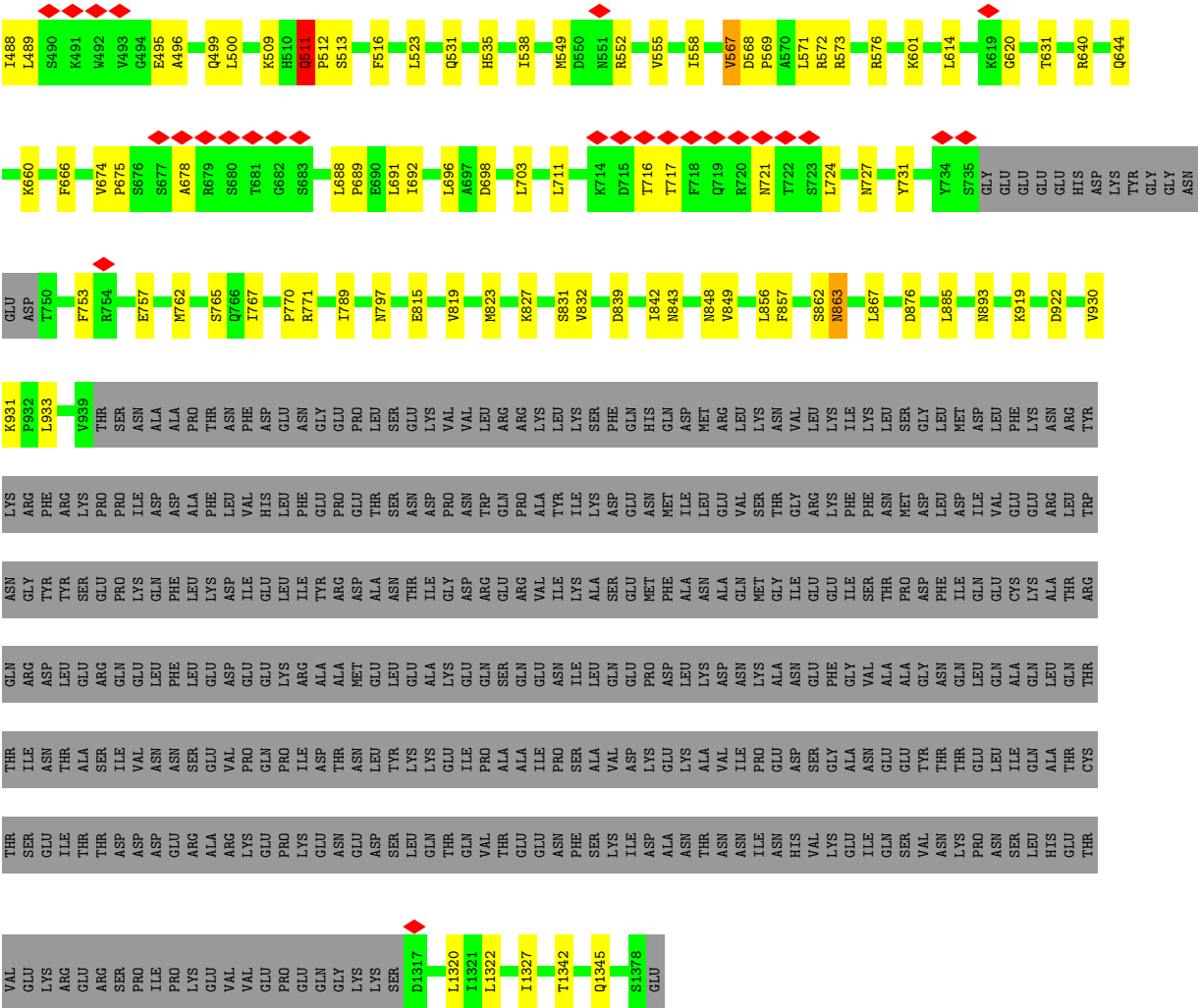
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	Q511	LYS	LEU	LEU	ARG	ASP	THR	GLN	HIS
		GLU	PHE	PHE	THR	GLU	GLU	GLU	HIS
	1520	ASN	PRO	PRO	LEU	TYR	ASP	ASP	LYS
A678		THR	THR	GLY	ARG	HIS	ASP	ASP	HIS
B679	S528	GLN	GLY	GLY	GLU	PRO	GLU	VAL	ASP
S680		LYS	PRO	GLY	ARG	THR	ASP	ASP	HIS
	Q531	LYS	GLY	GLY	THR	GLU	ASP	ASP	HIS
	S532	LYS	PHE	PHE	THR	LYS	SER	LEU	HIS
	Q533	LYS	GLY	GLY	PRO	PRO	VAL	VAL	HIS
S684		LYS	GLY	GLY	VAL	ASN	SER	SER	THR
	L542	LYS	ASN	ASN	PRO	ASN	PRO	HIS	SER
	L543	PRO	ASP	ASP	VAL	ASN	HIS	THR	GLY
P689		GLU	VAL	VAL	ARG	ARG	GLU	THR	SER
	M546	ILE	THR	THR	LYS	ARG	ARG	THR	THR
	Q547	ALA	THR	THR	PRO	ALA	ALA	ALA	MET
L696	Q548	ASP	ILE	ILE	PRO	ARG	ARG	ARG	ALA
	M549	ASP	PHE	PHE	PRO	LEU	THR	THR	TYR
L707	D550	LYS	GLY	GLY	LEU	ALA	ALA	LEU	LYS
D708		LYS	LYS	THR	THR	ALA	ASP	ARG	HIS
L711	1556	ASN	THR	THR	SER	PHE	LEU	ASN	GLY
	V557	ALA	PHE	THR	ALA	HIS	THR	TYR	ALA
T717	T561	D414	TYR	ASN	GLU	SER	VAL	ASN	LYS
F718	N562		ASN	ASN	THR	ARG	GLU	GLU	THR
Q719	L571	E427	GLN	PHE	SER	SER	PRO	ASP	ILE
R720	R572	V429	VAL	VAL	ILE	ASN	PRO	LEU	LYS
M721			PRO	PRO	ASP	GLU	ASP	ARG	VAL
	R576	E437	SER	SER	LYS	GLU	ASP	LYS	PHE
	F577		ALA	PHE	ASN	ASN	ASP	ARG	ASP
	S578	Q440	PHE	ASN	ASN	ASP	GLU	LYS	TYR
	R579		SER	SER	ALA	GLU	TYR	HIS	ASP
E580		Q449	ASN	ASN	ASP	ASN	ASP	ASP	ASP
			ASN	ASN	LEU	LEU	PRO	PRO	ASP
F583	P455		ASN	SER	ASP	ASN	GLU	GLN	LYS
	P456		ASN	PHE	ASN	ASN	GLU	GLN	LYS
R600	G457		ASN	ASN	SER	SER	ASP	VAL	MET
	T458		LYS	HIS	ARG	ARG	GLU	VAL	ALA
K613	Q459		LEU	LEU	PRO	ASP	GLY	LYS	ASP
HIS			ILE	ILE	SER	GLU	GLY	LYS	ASN
ASP			LEU	LEU	PRO	ALA	ASP	ASP	LEU
LYS	L617				ALA	THR	PHE	GLU	ASN
TYR			ASP	ASP	LEU	LEU	ILE	THR	ARG
GLY	R627	D474	SER	SER	THR	THR	ILE	THR	ASN
ASN		E475	ASP	ASP	LEU	LEU	SER	PRO	ARG
GLY	E632		SER	SER	ALA	ALA	GLY	VAL	ARG
ASN	K633		ASP	ASP	GLY	GLY	SER	ASP	GLY
GLU	L634		SER	SER	GLU	GLU	ALA	VAL	SER
ASP	L635	1478	ASP	ASP	ILE	ILE	VAL	THR	ASP
THR	L636		ASP	ASP	GLY	GLY	ASP	THR	GLY
SER			GLY	GLY	TRP	ARG	SER	ASP	VAL
SER	Q639	M482	ILE	ILE	GLU	GLU	LYS	ASP	SER
SER	R640	K483	LEU	LEU	LEU	LEU	ARG	ASP	GLU
PHE		K484	PRO	PRO	SER	GLN	LEU	GLY	ALA
ARG			LEU	LEU	GLN	GLU	LYS	HIS	ALA
SER	D650	D487	GLY	GLY	ASN	GLU	GLU	ASN	SER
		L488	VAL	VAL	SER	SER	ARG	ASN	ASN
Y756		L489	THR	THR	GLY	PRO	ALA	ALA	ALA
	V654	S490	PRO	PRO	THR	ILE	ASN	ASP	LYS
S765	D655		THR	THR	ARG	THR	SER	GLN	GLY
			LYS	LYS	THR	ARG	GLU	GLY	THR
P770		K508	THR	THR	ARG	GLU	THR	THR	GLY



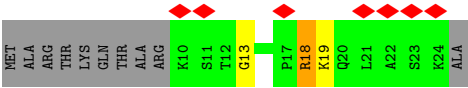


- Molecule 1: ATPase histone chaperone YTA7





● Molecule 2: Histone H3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	431065	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	2.228	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, 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	0.46	1/4735 (0.0%)	0.66	0/6401
1	B	0.47	0/4661	0.65	1/6298 (0.0%)
1	C	0.52	2/4711 (0.0%)	0.69	3/6368 (0.0%)
1	D	0.47	0/4711	0.63	2/6368 (0.0%)
1	E	0.46	0/4686	0.67	0/6332
1	F	0.45	0/4717	0.67	0/6373
2	G	0.65	0/108	1.04	0/140
All	All	0.48	3/28329 (0.0%)	0.66	6/38280 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	860	LEU	C-O	-6.28	1.15	1.23
1	A	912	LEU	C-O	-5.63	1.17	1.24
1	C	861	GLN	C-O	-5.17	1.17	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	831	SER	CA-C-N	-7.70	112.28	122.99
1	D	831	SER	C-N-CA	-7.70	112.28	122.99
1	C	861	GLN	CA-C-O	-7.09	112.77	120.92
1	C	510	HIS	N-CA-C	-6.43	100.37	109.96
1	B	512	PRO	N-CA-C	-5.84	101.04	110.74
1	C	510	HIS	CB-CA-C	5.39	117.92	110.16

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	4646	0	4756	115	0
1	B	4573	0	4690	95	0
1	C	4622	0	4741	110	0
1	D	4622	0	4741	78	0
1	E	4598	0	4717	92	0
1	F	4628	0	4737	114	0
2	G	108	0	123	13	0
3	A	27	0	12	1	0
4	B	31	0	12	2	0
4	C	31	0	12	7	0
4	D	31	0	12	1	0
4	E	31	0	12	1	0
4	F	31	0	12	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	27983	0	28577	552	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 10.

All (552) 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:F:412:PHE:CD1	1:F:422:ILE:HD13	1.76	1.20
1:B:546:MET:HB2	1:B:576:ARG:HD2	1.23	1.19
1:E:493:VAL:HG23	2:G:18:ARG:HB3	1.25	1.13
1:C:456:PRO:HB3	4:C:1401:AGS:S1G	1.90	1.11
1:A:823:MET:HA	1:A:823:MET:HE2	1.27	1.10
1:B:823:MET:HE2	1:B:823:MET:HA	1.34	1.09
1:F:422:ILE:HG12	1:F:463:MET:HE1	1.12	1.09
1:F:511:GLN:HB3	1:F:512:PRO:CD	1.83	1.08
1:E:493:VAL:CG2	2:G:18:ARG:HB3	1.83	1.08
1:A:613:LYS:HE2	1:F:753:PHE:CB	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:LEU:H	1:A:803:LEU:HD12	1.21	1.02
1:F:568:ASP:OD1	1:F:569:PRO:HD2	1.60	1.01
1:A:613:LYS:HE2	1:F:753:PHE:HB3	1.01	0.99
1:A:681:THR:HG21	1:A:804:ALA:HB3	1.43	0.98
1:F:511:GLN:CB	1:F:512:PRO:HD2	1.94	0.98
1:A:613:LYS:CE	1:F:753:PHE:HB3	1.93	0.97
1:B:546:MET:HB2	1:B:576:ARG:CD	1.94	0.97
1:D:477:LYS:O	1:D:512:PRO:HB2	1.64	0.97
1:C:557:VAL:HG12	1:C:577:PHE:CE1	2.03	0.94
1:E:567:VAL:CG2	1:E:572:ARG:HD2	1.98	0.94
1:F:771:ARG:NH2	1:F:857:PHE:HD1	1.67	0.93
1:C:458:THR:CG2	1:C:583:PHE:HB3	1.98	0.93
1:F:422:ILE:HG12	1:F:463:MET:CE	1.98	0.92
1:F:771:ARG:HH22	1:F:857:PHE:HD1	1.17	0.92
1:E:526:VAL:HG23	1:E:566:ALA:O	1.68	0.92
1:F:422:ILE:CG1	1:F:463:MET:HE1	2.00	0.91
1:F:771:ARG:NH2	1:F:857:PHE:CD1	2.39	0.91
1:D:803:LEU:HD22	1:D:803:LEU:H	1.36	0.90
1:B:546:MET:CB	1:B:576:ARG:HD2	2.01	0.90
1:D:823:MET:O	1:D:827:LYS:HG3	1.72	0.89
1:F:412:PHE:HD1	1:F:422:ILE:HD13	1.27	0.88
1:F:511:GLN:CB	1:F:512:PRO:CD	2.46	0.87
1:C:458:THR:HG21	1:C:583:PHE:HB3	1.56	0.86
1:E:567:VAL:HG22	1:E:572:ARG:HD2	1.56	0.85
1:F:567:VAL:CG1	1:F:571:LEU:HD21	2.06	0.85
1:A:613:LYS:HG2	1:F:753:PHE:CG	2.12	0.84
1:C:576:ARG:NH1	4:D:1401:AGS:S1G	2.50	0.84
1:F:567:VAL:HG12	1:F:571:LEU:HD21	1.57	0.84
1:D:644:GLN:NE2	1:D:933:LEU:HD22	1.93	0.83
1:C:856:LEU:HD21	1:D:804:ALA:HB2	1.59	0.83
1:C:543:LEU:HD22	1:C:576:ARG:NH1	1.95	0.82
1:F:511:GLN:HB3	1:F:512:PRO:HD3	1.61	0.82
1:D:827:LYS:NZ	1:D:827:LYS:HB3	1.96	0.81
1:A:803:LEU:HD23	1:A:844:THR:CG2	2.11	0.81
1:F:511:GLN:HB2	1:F:512:PRO:HD2	1.63	0.81
1:A:823:MET:HA	1:A:823:MET:CE	2.10	0.81
1:B:546:MET:HE2	1:B:576:ARG:HB3	1.62	0.81
1:A:803:LEU:HD21	1:A:844:THR:HB	1.63	0.80
1:E:818:VAL:HG21	1:E:849:VAL:HG11	1.61	0.80
1:C:542:LEU:HD23	1:C:571:LEU:HD11	1.63	0.79
1:F:425:LEU:HD21	1:F:467:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:568:ASP:OD1	1:F:569:PRO:CD	2.30	0.79
1:C:826:LYS:HE3	1:C:860:LEU:HD23	1.63	0.79
1:E:493:VAL:CG2	2:G:18:ARG:CB	2.61	0.78
1:C:557:VAL:HG12	1:C:577:PHE:HE1	1.48	0.78
1:A:803:LEU:H	1:A:803:LEU:CD1	1.97	0.77
1:A:823:MET:HE2	1:A:823:MET:CA	2.13	0.77
1:B:814:ILE:HD11	1:B:845:ILE:HD13	1.68	0.76
1:A:653:LEU:HD12	1:A:653:LEU:O	1.86	0.76
1:F:511:GLN:HA	1:F:511:GLN:OE1	1.85	0.76
1:A:613:LYS:HG2	1:F:753:PHE:CD1	2.20	0.76
1:B:547:ASP:N	1:B:576:ARG:HD3	2.00	0.75
1:C:546:MET:HE2	1:C:576:ARG:HB3	1.69	0.75
1:A:1321:ILE:HD12	1:A:1365:ASP:HB2	1.69	0.75
1:E:818:VAL:HG21	1:E:849:VAL:CG1	2.16	0.74
1:A:592:PHE:CD1	1:A:611:ILE:HG22	2.23	0.74
1:E:494:GLY:H	2:G:18:ARG:NH2	1.86	0.74
1:C:822:PHE:HE1	1:C:857:PHE:CZ	2.04	0.74
1:E:443:ASN:HD21	1:F:601:LYS:HD3	1.53	0.73
1:A:803:LEU:HD12	1:A:803:LEU:N	2.01	0.73
1:A:803:LEU:CD2	1:A:844:THR:CG2	2.66	0.73
1:D:481:PHE:HE2	1:D:513:SER:HB2	1.52	0.73
1:B:547:ASP:H	1:B:576:ARG:HD3	1.53	0.72
1:D:644:GLN:HE21	1:D:933:LEU:HD22	1.52	0.72
1:C:458:THR:HG22	1:C:583:PHE:HB3	1.70	0.72
1:B:823:MET:HE2	1:B:823:MET:CA	2.16	0.72
1:E:493:VAL:HG22	2:G:18:ARG:CB	2.20	0.71
1:B:823:MET:HA	1:B:823:MET:CE	2.15	0.71
1:A:653:LEU:HD12	1:A:653:LEU:C	2.16	0.71
1:F:412:PHE:HD1	1:F:422:ILE:CD1	2.03	0.71
1:D:803:LEU:HD22	1:D:803:LEU:N	2.05	0.70
1:C:892:LYS:NZ	1:D:1348:ASP:OD1	2.24	0.70
1:A:1323:THR:HG22	1:A:1325:GLU:H	1.56	0.70
1:F:495:GLU:O	1:F:499:GLN:HB2	1.91	0.70
1:E:1339:GLN:OE1	1:E:1339:GLN:HA	1.92	0.70
1:C:856:LEU:HD21	1:D:804:ALA:CB	2.21	0.69
1:B:815:GLU:HG3	1:B:849:VAL:HG22	1.74	0.69
1:B:546:MET:CB	1:B:576:ARG:CD	2.65	0.69
1:D:576:ARG:NH2	4:E:1401:AGS:S1G	2.65	0.69
1:A:592:PHE:HD1	1:A:611:ILE:HG22	1.58	0.69
1:E:840:ILE:O	1:E:844:THR:HG23	1.94	0.67
1:B:814:ILE:HD11	1:B:845:ILE:CD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:PHE:HE1	1:C:857:PHE:CE2	2.13	0.67
1:D:486:ALA:HB1	1:D:489:LEU:HD13	1.77	0.67
1:D:778:LYS:HA	1:D:873:GLU:HG2	1.78	0.66
1:C:508:LYS:O	1:C:511:GLN:NE2	2.29	0.66
1:A:803:LEU:CD2	1:A:844:THR:HG21	2.26	0.66
1:C:578:ASP:OD1	1:C:578:ASP:N	2.28	0.66
1:C:826:LYS:HE3	1:C:860:LEU:CD2	2.26	0.65
1:F:721:ASN:HD21	1:F:727:ASN:HD22	1.45	0.65
1:A:648:SER:OG	1:A:652:LEU:HD11	1.96	0.65
1:A:803:LEU:HD23	1:A:844:THR:HG22	1.79	0.65
1:E:1323:THR:HG22	1:E:1325:GLU:H	1.61	0.65
1:F:1342:THR:H	1:F:1345:GLN:HE21	1.45	0.65
1:F:448:ARG:NH2	1:F:549:MET:O	2.30	0.64
1:B:676:SER:HA	1:B:679:ARG:HG2	1.79	0.64
1:A:681:THR:HG21	1:A:804:ALA:CB	2.23	0.64
1:D:830:PRO:HB3	1:D:865:LYS:HE3	1.80	0.64
1:C:822:PHE:CE1	1:C:857:PHE:CE2	2.86	0.63
1:A:803:LEU:CD2	1:A:844:THR:HB	2.27	0.63
1:D:827:LYS:HB3	1:D:827:LYS:HZ1	1.63	0.63
1:C:861:GLN:O	1:C:864:GLU:HG2	1.99	0.63
1:C:858:ARG:NH2	1:D:837:ASN:HB3	2.13	0.62
1:F:412:PHE:CD1	1:F:422:ILE:CD1	2.69	0.62
1:F:815:GLU:HG3	1:F:849:VAL:HG22	1.80	0.62
1:A:844:THR:HG23	1:F:848:ASN:HB2	1.82	0.62
1:F:571:LEU:HD12	1:F:571:LEU:C	2.24	0.62
1:B:1326:GLN:HG2	1:B:1370:VAL:HG11	1.81	0.62
1:D:803:LEU:H	1:D:803:LEU:CD2	2.12	0.62
1:A:816:ALA:O	1:A:820:GLN:HG3	1.98	0.62
1:F:471:CYS:C	1:F:473:SER:H	2.07	0.61
1:C:474:ASP:OD1	1:C:474:ASP:N	2.32	0.61
1:C:640:ARG:NH2	1:C:660:LYS:O	2.32	0.61
1:A:650:ASP:HB3	1:A:938:LYS:HG2	1.83	0.61
1:D:796:PHE:HB3	1:D:832:VAL:HG23	1.83	0.61
1:F:569:PRO:O	1:F:573:ARG:NH2	2.34	0.61
1:C:777:PRO:HD2	1:C:780:ASN:HD22	1.66	0.60
1:C:858:ARG:HH21	1:D:837:ASN:HB3	1.66	0.60
1:C:894:ILE:HG23	1:C:894:ILE:O	2.01	0.60
1:E:492:TRP:C	2:G:18:ARG:HG2	2.27	0.60
1:A:717:THR:HG22	1:A:717:THR:O	2.02	0.60
1:B:644:GLN:HE22	1:B:933:LEU:HD23	1.67	0.60
1:E:456:PRO:HG3	1:E:562:ASN:HD21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ASP:OD1	1:B:578:ASP:N	2.35	0.60
1:D:803:LEU:N	1:D:803:LEU:HD13	2.17	0.60
1:F:425:LEU:CD2	1:F:467:LEU:HD21	2.33	0.59
1:F:770:PRO:HB2	1:F:867:LEU:HA	1.85	0.59
1:A:613:LYS:HG2	1:F:753:PHE:CD2	2.38	0.59
1:A:716:THR:HG22	1:A:716:THR:O	2.02	0.59
1:E:815:GLU:HA	1:E:815:GLU:OE2	2.02	0.59
1:A:717:THR:OG1	1:A:865:LYS:NZ	2.36	0.58
1:A:876:ASP:OD1	1:A:879:GLU:HB2	2.03	0.58
1:D:1342:THR:H	1:D:1345:GLN:HE21	1.50	0.58
1:E:567:VAL:CG2	1:E:572:ARG:CD	2.79	0.58
1:B:557:VAL:HG12	1:B:577:PHE:CE1	2.39	0.58
1:C:919:LYS:NZ	1:C:921:SER:OG	2.35	0.58
1:A:766:GLN:O	1:B:1355:LYS:NZ	2.35	0.58
1:A:815:GLU:HG3	1:A:849:VAL:HG22	1.85	0.57
1:A:838:LEU:HB3	1:A:872:ALA:HB2	1.86	0.57
1:C:822:PHE:HE1	1:C:857:PHE:CE1	2.22	0.57
1:F:478:ILE:HG22	1:F:478:ILE:O	2.04	0.57
1:C:414:ASP:OD1	1:C:600:ARG:NH2	2.38	0.57
1:B:546:MET:CE	1:B:576:ARG:HB3	2.33	0.57
1:D:1321:ILE:HB	1:D:1365:ASP:HA	1.87	0.57
1:E:521:ASP:OD2	1:E:561:THR:O	2.23	0.57
1:F:425:LEU:HD21	1:F:467:LEU:HD21	1.86	0.57
1:F:620:GLY:HA3	1:F:678:ALA:HA	1.87	0.57
1:C:809:GLU:HG2	1:C:812:ARG:HE	1.70	0.56
1:A:610:PHE:CE2	1:A:663:VAL:HG22	2.40	0.56
1:A:650:ASP:CG	1:A:938:LYS:HE2	2.30	0.56
1:B:492:TRP:NE1	1:C:490:SER:O	2.37	0.56
1:B:925:MET:HE1	1:B:1361:LYS:HE2	1.88	0.56
1:C:456:PRO:CB	4:C:1401:AGS:S1G	2.82	0.56
1:B:693:LYS:O	1:B:697:ALA:HB2	2.05	0.56
1:E:443:ASN:ND2	1:F:601:LYS:HD3	2.19	0.56
1:F:688:LEU:HD21	1:F:696:LEU:HB2	1.87	0.56
1:D:511:GLN:HE21	1:D:511:GLN:CA	2.18	0.56
1:B:880:VAL:HG11	1:B:894:ILE:HD11	1.87	0.56
1:C:822:PHE:CE1	1:C:857:PHE:CZ	2.91	0.55
1:F:412:PHE:CE1	1:F:422:ILE:CG2	2.89	0.55
1:A:401:LEU:HD21	1:A:502:LEU:HB3	1.87	0.55
1:C:856:LEU:CD2	1:D:804:ALA:HB2	2.34	0.55
1:B:492:TRP:HB2	2:G:13:GLY:HA3	1.88	0.55
1:C:892:LYS:NZ	1:D:1348:ASP:CG	2.64	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:818:VAL:HG11	1:E:849:VAL:HG12	1.88	0.55
1:B:527:ARG:HH22	1:C:562:ASN:HD21	1.54	0.55
1:A:926:LYS:HD2	1:F:731:TYR:HB3	1.88	0.55
1:B:703:LEU:HD13	1:B:789:ILE:HD11	1.89	0.55
1:C:572:ARG:NE	1:C:580:GLU:OE2	2.33	0.55
1:E:720:ARG:NH1	1:E:794:GLU:OE2	2.38	0.55
1:F:711:LEU:HD11	1:F:867:LEU:HD22	1.88	0.55
1:B:547:ASP:HB3	1:B:576:ARG:NH1	2.21	0.55
1:B:632:GLU:HG3	1:B:673:ILE:HD11	1.88	0.55
1:C:557:VAL:HG12	1:C:577:PHE:CZ	2.41	0.55
1:E:850:ILE:HG21	1:E:884:ILE:HG22	1.87	0.55
1:A:703:LEU:HD13	1:A:789:ILE:HD11	1.89	0.54
1:A:729:ILE:O	1:B:929:ARG:NH1	2.40	0.54
1:D:828:ARG:O	1:D:828:ARG:HG3	2.07	0.54
1:E:561:THR:C	1:E:563:ARG:H	2.15	0.54
1:B:891:ASP:OD1	1:B:891:ASP:N	2.37	0.54
1:D:1323:THR:HG22	1:D:1325:GLU:H	1.71	0.54
1:F:698:ASP:OD1	1:F:698:ASP:N	2.40	0.54
1:D:823:MET:O	1:D:827:LYS:CG	2.50	0.54
1:F:571:LEU:O	1:F:576:ARG:HB3	2.08	0.54
1:B:444:ILE:HD13	1:C:634:ALA:HB3	1.89	0.54
1:F:424:GLN:O	1:F:428:MET:HB2	2.08	0.54
1:D:734:TYR:O	1:E:662:LYS:NZ	2.40	0.54
1:E:841:TRP:CE2	1:E:845:ILE:HG13	2.43	0.54
1:F:412:PHE:CE1	1:F:422:ILE:HD13	2.38	0.54
1:E:780:ASN:ND2	1:E:897:LEU:O	2.41	0.54
1:A:824:GLU:OE2	1:A:824:GLU:HA	2.08	0.53
1:E:1360:SER:O	1:E:1366:LYS:NZ	2.40	0.53
1:C:455:PRO:HD2	1:C:583:PHE:O	2.08	0.53
1:F:513:SER:O	1:F:555:VAL:HA	2.08	0.53
1:D:451:LEU:HB3	1:D:580:GLU:HG2	1.90	0.53
1:E:841:TRP:O	1:E:845:ILE:HB	2.08	0.53
1:A:803:LEU:CD2	1:A:844:THR:CB	2.87	0.53
1:D:551:ASN:HD21	1:E:405:GLY:HA3	1.74	0.53
1:F:919:LYS:HG3	1:F:922:ASP:HB2	1.90	0.53
1:A:398:ILE:HD11	1:F:531:GLN:HB3	1.90	0.53
1:C:892:LYS:NZ	1:D:1348:ASP:OD2	2.40	0.53
1:C:471:CYS:HB3	1:C:478:ILE:HB	1.91	0.53
1:C:1323:THR:HG22	1:C:1325:GLU:H	1.73	0.53
1:E:550:ASP:O	1:E:552:ARG:NH2	2.42	0.53
1:F:644:GLN:HE21	1:F:933:LEU:HD12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:LYS:HE3	1:B:679:ARG:HB2	1.90	0.53
1:C:632:GLU:HG3	1:C:673:ILE:HD11	1.90	0.53
1:A:732:GLU:HB2	1:B:929:ARG:HG3	1.91	0.52
1:A:711:LEU:HD11	1:A:867:LEU:HD22	1.89	0.52
1:D:1360:SER:OG	1:D:1369:THR:OG1	2.24	0.52
1:A:803:LEU:HD23	1:A:844:THR:HG21	1.85	0.52
1:F:428:MET:HE3	1:F:447:PRO:HG3	1.90	0.52
1:F:640:ARG:NH2	1:F:660:LYS:O	2.43	0.52
1:E:818:VAL:HG11	1:E:849:VAL:CG1	2.40	0.52
1:D:826:LYS:HE2	1:D:860:LEU:HD23	1.90	0.52
1:A:919:LYS:HG2	1:A:1320:LEU:HB2	1.92	0.52
1:F:485:GLY:HA2	1:F:523:LEU:HB2	1.92	0.52
1:A:425:LEU:HD23	1:A:467:LEU:HD13	1.92	0.52
1:A:613:LYS:HE2	1:F:753:PHE:CG	2.43	0.52
1:D:481:PHE:CE2	1:D:513:SER:HB2	2.39	0.52
1:E:424:GLN:OE1	1:E:579:ARG:NH1	2.41	0.52
1:E:774:ILE:HB	1:E:871:LEU:HD23	1.92	0.52
1:F:1322:LEU:HD21	1:F:1327:ILE:HD11	1.91	0.52
1:E:650:ASP:OD1	1:E:650:ASP:N	2.41	0.52
1:E:880:VAL:HG12	1:E:885:LEU:HD12	1.92	0.52
1:A:447:PRO:HG2	1:A:579:ARG:HE	1.75	0.51
1:C:429:VAL:HG12	1:C:556:ILE:HD13	1.91	0.51
1:A:804:ALA:O	1:A:808:SER:HB2	2.11	0.51
1:D:511:GLN:CA	1:D:511:GLN:NE2	2.73	0.51
1:B:860:LEU:HD21	1:B:866:ILE:HD12	1.93	0.51
1:C:876:ASP:OD1	1:C:876:ASP:N	2.43	0.51
1:D:1360:SER:OG	1:D:1360:SER:O	2.28	0.51
1:E:493:VAL:HA	2:G:18:ARG:CZ	2.41	0.51
1:E:640:ARG:NH2	1:E:660:LYS:O	2.44	0.51
1:A:433:LEU:HD23	1:A:476:ARG:HD2	1.91	0.51
1:E:533:GLN:HG2	1:F:531:GLN:HE22	1.75	0.51
1:D:1322:LEU:HD13	1:D:1366:LYS:HB2	1.91	0.51
1:A:592:PHE:CD1	1:A:611:ILE:CG2	2.94	0.51
1:F:425:LEU:HD12	1:F:452:PHE:HZ	1.76	0.51
1:F:425:LEU:CD1	1:F:452:PHE:HZ	2.24	0.51
1:A:568:ASP:HB3	1:A:571:LEU:HD23	1.93	0.50
1:B:576:ARG:NH2	4:C:1401:AGS:S1G	2.84	0.50
1:E:925:MET:SD	1:E:1361:LYS:NZ	2.84	0.50
1:B:511:GLN:OE1	1:C:401:LEU:N	2.44	0.50
1:C:546:MET:HE2	1:C:576:ARG:CB	2.38	0.50
1:D:596:GLN:HE21	1:D:611:ILE:HD12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:822:PHE:HB3	1:C:856:LEU:HD13	1.93	0.50
1:F:832:VAL:HG12	1:F:867:LEU:HB3	1.92	0.50
1:A:410:VAL:HG21	1:A:465:ARG:HE	1.77	0.50
1:D:479:THR:O	1:D:514:ILE:N	2.39	0.50
1:C:822:PHE:CD2	1:C:856:LEU:HB3	2.46	0.50
1:C:550:ASP:OD1	1:D:484:LYS:NZ	2.31	0.50
1:D:420:ASN:HB3	1:D:723:SER:HA	1.93	0.50
1:F:489:LEU:HD13	1:F:535:HIS:CE1	2.46	0.50
1:F:412:PHE:CE1	1:F:422:ILE:HG21	2.47	0.50
1:F:489:LEU:HD13	1:F:535:HIS:NE2	2.26	0.50
1:C:458:THR:HG22	1:C:458:THR:O	2.11	0.50
1:D:504:PHE:O	1:D:507:ALA:HB3	2.10	0.50
1:E:451:LEU:HD12	1:E:559:GLY:O	2.11	0.50
1:F:425:LEU:HD23	1:F:425:LEU:C	2.37	0.50
1:F:425:LEU:HD11	1:F:467:LEU:HD11	1.93	0.50
1:B:427:GLU:O	1:B:439:TYR:OH	2.30	0.49
1:A:451:LEU:HB3	1:A:580:GLU:HG3	1.93	0.49
1:E:810:SER:C	1:E:812:ARG:H	2.20	0.49
1:C:449:GLY:HA3	1:C:576:ARG:O	2.12	0.49
1:C:457:GLY:O	4:C:1401:AGS:H8	2.13	0.49
1:C:459:GLY:HA2	4:C:1401:AGS:O1A	2.12	0.49
1:D:546:MET:HB3	1:D:576:ARG:HB3	1.94	0.49
1:A:681:THR:CG2	1:A:804:ALA:HB3	2.28	0.49
1:B:481:PHE:HE1	1:B:513:SER:OG	1.95	0.49
1:D:849:VAL:HA	1:D:852:VAL:HB	1.95	0.49
1:C:533:GLN:HG2	1:D:525:PRO:HG3	1.94	0.49
1:D:420:ASN:N	1:D:420:ASN:OD1	2.43	0.49
1:D:731:TYR:HE1	1:E:928:ARG:HD2	1.77	0.49
1:F:420:ASN:N	1:F:420:ASN:HD22	2.09	0.49
1:A:506:GLU:OE2	1:A:510:HIS:NE2	2.46	0.49
1:E:439:TYR:CZ	1:E:446:PRO:HB3	2.47	0.49
1:F:471:CYS:C	1:F:473:SER:N	2.70	0.49
1:A:801:LEU:HB2	1:A:835:ILE:HG12	1.94	0.49
1:C:919:LYS:HG3	1:C:921:SER:H	1.77	0.49
1:E:439:TYR:CE1	1:E:446:PRO:HB3	2.48	0.49
1:C:546:MET:CE	1:C:576:ARG:HB3	2.40	0.49
1:C:919:LYS:HA	1:C:1320:LEU:HD11	1.94	0.49
1:D:650:ASP:OD1	1:D:650:ASP:N	2.44	0.49
1:A:839:ASP:OD1	1:A:839:ASP:N	2.42	0.49
1:A:501:ARG:NH1	1:B:487:ASP:O	2.42	0.49
1:E:533:GLN:NE2	1:F:531:GLN:OE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:771:ARG:O	1:F:893:ASN:HB3	2.12	0.49
1:A:708:ASP:HB3	1:A:713:ILE:HB	1.94	0.48
1:C:427:GLU:HB3	1:D:646:TYR:HE2	1.78	0.48
1:C:692:ILE:HD12	1:C:696:LEU:HD12	1.94	0.48
1:D:533:GLN:O	1:D:537:SER:HB2	2.13	0.48
1:C:826:LYS:HG3	1:C:860:LEU:HD21	1.95	0.48
1:D:481:PHE:HE2	1:D:513:SER:CB	2.25	0.48
1:E:847:GLU:OE1	1:E:851:LEU:HG	2.14	0.48
1:A:484:LYS:HG3	1:A:518:ASP:HB3	1.93	0.48
1:C:546:MET:HE2	1:C:576:ARG:CA	2.43	0.48
1:C:822:PHE:CE1	1:C:857:PHE:CD2	3.01	0.48
1:C:844:THR:O	1:C:844:THR:OG1	2.26	0.48
1:A:404:LEU:HB3	1:A:480:PHE:HD2	1.79	0.48
1:B:801:LEU:HB2	1:B:835:ILE:HG12	1.95	0.48
1:A:462:LEU:HD22	3:A:1401:ADP:H2'	1.96	0.48
1:B:462:LEU:HD22	4:B:1401:AGS:H2'	1.96	0.48
1:F:573:ARG:O	1:F:576:ARG:HB2	2.13	0.48
1:A:774:ILE:HB	1:A:871:LEU:HG	1.96	0.48
1:D:477:LYS:O	1:D:512:PRO:CB	2.51	0.48
1:A:876:ASP:OD1	1:A:879:GLU:CB	2.62	0.47
1:C:458:THR:HG21	1:C:583:PHE:CB	2.36	0.47
1:D:827:LYS:NZ	1:D:827:LYS:CB	2.73	0.47
1:F:412:PHE:CE1	1:F:422:ILE:HG23	2.49	0.47
1:A:912:LEU:HD13	1:F:762:MET:HE1	1.97	0.47
1:D:511:GLN:NE2	1:D:511:GLN:HA	2.28	0.47
1:D:827:LYS:HB3	1:D:827:LYS:HZ2	1.79	0.47
1:B:854:SER:HB2	1:B:887:ASP:HB3	1.96	0.47
1:A:699:GLN:HE22	1:A:898:HIS:CD2	2.33	0.47
1:A:912:LEU:HD22	1:A:1350:HIS:CE1	2.50	0.47
1:E:484:LYS:HE3	1:E:486:ALA:HB3	1.95	0.47
1:E:713:ILE:O	1:E:717:THR:OG1	2.32	0.47
1:B:547:ASP:HB3	1:B:576:ARG:HH11	1.78	0.47
1:C:707:LEU:HD13	1:C:772:LEU:HD22	1.97	0.47
1:E:407:ASP:OD1	1:E:408:MET:N	2.48	0.47
1:E:570:ALA:O	1:E:576:ARG:NH1	2.46	0.47
1:C:528:SER:HB3	1:C:531:GLN:HB2	1.96	0.47
1:B:445:THR:HG23	1:C:404:LEU:O	2.15	0.47
1:E:915:LEU:HD21	1:E:1358:TRP:HE3	1.78	0.47
1:A:533:GLN:HE22	1:A:535:HIS:CD2	2.32	0.47
1:A:653:LEU:C	1:A:653:LEU:CD1	2.88	0.47
1:B:765:SER:O	1:B:765:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:567:VAL:HG23	1:E:572:ARG:HD2	1.93	0.47
1:A:565:ASP:OD2	1:A:824:GLU:HG3	2.15	0.47
1:C:708:ASP:OD2	1:C:792:TYR:OH	2.31	0.47
1:E:846:PRO:HD2	1:E:849:VAL:HG21	1.98	0.46
1:A:799:GLN:HG3	1:A:825:ALA:HB2	1.96	0.46
1:B:546:MET:HE2	1:B:576:ARG:CB	2.39	0.46
1:E:493:VAL:HA	2:G:18:ARG:NE	2.30	0.46
1:E:917:LYS:HD2	1:E:1327:ILE:HD11	1.96	0.46
1:F:876:ASP:OD1	1:F:876:ASP:N	2.48	0.46
1:A:778:LYS:HA	1:A:873:GLU:OE2	2.16	0.46
1:D:644:GLN:HE21	1:D:933:LEU:HD13	1.80	0.46
1:E:1336:GLU:O	1:E:1339:GLN:HG2	2.15	0.46
1:A:679:ARG:HD3	1:F:827:LYS:HD2	1.97	0.46
1:E:448:ARG:HG3	1:E:549:MET:HE1	1.97	0.46
1:C:457:GLY:H	4:C:1401:AGS:PB	2.38	0.46
1:B:428:MET:HB2	1:B:447:PRO:O	2.16	0.45
1:B:689:PRO:HD2	1:B:692:ILE:HD11	1.97	0.45
1:A:481:PHE:HZ	1:A:510:HIS:HD2	1.64	0.45
1:B:444:ILE:O	1:B:444:ILE:HG13	2.16	0.45
1:B:822:PHE:CD1	1:B:856:LEU:HD22	2.51	0.45
1:E:493:VAL:N	2:G:18:ARG:HG2	2.31	0.45
1:F:474:ASP:OD1	1:F:474:ASP:N	2.48	0.45
1:F:489:LEU:CD1	1:F:535:HIS:NE2	2.79	0.45
1:F:703:LEU:HD13	1:F:789:ILE:HD11	1.98	0.45
1:A:681:THR:CG2	1:A:804:ALA:CB	2.91	0.45
1:B:543:LEU:HD22	1:B:576:ARG:HH21	1.80	0.45
1:C:549:MET:HE2	1:C:549:MET:HB3	1.78	0.45
1:C:770:PRO:HB2	1:C:867:LEU:HA	1.98	0.45
1:B:466:ALA:O	1:B:470:SER:HB3	2.17	0.45
1:C:627:ARG:HE	1:C:627:ARG:HB3	1.46	0.45
1:E:528:SER:HB3	1:E:531:GLN:HG2	1.97	0.45
1:E:812:ARG:HH11	1:E:817:ALA:CB	2.29	0.45
1:A:688:LEU:HD21	1:A:696:LEU:HB2	1.98	0.45
1:A:813:THR:HG22	1:B:810:SER:OG	2.17	0.45
1:F:716:THR:OG1	1:F:717:THR:N	2.50	0.45
1:B:481:PHE:CE1	1:B:513:SER:OG	2.69	0.45
1:C:689:PRO:HG2	1:C:692:ILE:HG12	1.98	0.45
1:B:414:ASP:OD1	1:B:600:ARG:NH2	2.50	0.45
1:C:548:GLY:HA3	1:D:484:LYS:HE2	1.99	0.45
1:B:470:SER:OG	1:B:471:CYS:N	2.50	0.44
1:C:458:THR:HG21	1:C:583:PHE:C	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASP:OD1	1:A:938:LYS:HE2	2.17	0.44
1:A:893:ASN:OD1	1:A:893:ASN:N	2.50	0.44
1:C:655:ASP:OD1	1:C:655:ASP:N	2.42	0.44
1:C:765:SER:O	1:C:765:SER:OG	2.33	0.44
1:B:578:ASP:O	1:C:679:ARG:NH2	2.48	0.44
1:B:688:LEU:HD22	1:B:700:LEU:HD22	1.99	0.44
1:A:856:LEU:HD23	1:A:856:LEU:HA	1.87	0.44
1:C:520:ILE:HG22	1:C:561:THR:HG23	2.00	0.44
1:C:801:LEU:HD23	1:C:833:VAL:HG13	2.00	0.44
1:E:809:GLU:OE1	1:E:809:GLU:HA	2.17	0.44
1:E:846:PRO:HD2	1:E:849:VAL:CG2	2.48	0.44
1:A:597:ILE:HA	1:A:600:ARG:HD3	1.99	0.44
1:B:901:SER:OG	1:B:904:ASN:ND2	2.50	0.44
1:A:399:ALA:HB3	1:A:401:LEU:HG	2.00	0.44
1:D:488:ILE:HD13	1:D:500:LEU:HG	1.99	0.44
1:F:863:ASN:C	1:F:863:ASN:ND2	2.73	0.44
1:C:681:THR:OG1	1:C:682:GLY:N	2.49	0.44
1:C:858:ARG:HE	1:D:840:ILE:HD12	1.82	0.44
1:E:815:GLU:OE2	1:E:849:VAL:HG13	2.18	0.44
1:F:567:VAL:HG11	1:F:571:LEU:HD21	1.96	0.44
1:A:672:LYS:HD2	1:F:724:LEU:HD11	1.98	0.43
1:C:572:ARG:HH21	1:C:580:GLU:CD	2.26	0.43
1:C:822:PHE:CE2	1:C:856:LEU:HB3	2.53	0.43
1:A:489:LEU:HB2	1:A:492:TRP:HE3	1.83	0.43
1:B:427:GLU:HA	1:B:431:LEU:HB2	2.00	0.43
1:B:429:VAL:HG23	1:B:556:ILE:HD13	1.99	0.43
1:B:449:GLY:C	1:B:577:PHE:HA	2.42	0.43
1:D:850:ILE:HG21	1:D:884:ILE:HG12	1.99	0.43
1:E:699:GLN:HG2	1:E:897:LEU:HD23	2.00	0.43
1:A:410:VAL:HG21	1:A:465:ARG:HH21	1.83	0.43
1:A:613:LYS:HE3	1:F:757:GLU:CD	2.44	0.43
1:B:509:LYS:NZ	1:B:509:LYS:HB3	2.33	0.43
1:B:879:GLU:HA	1:B:883:GLY:HA3	2.00	0.43
1:E:773:LEU:HB3	1:E:894:ILE:HG12	2.00	0.43
1:E:803:LEU:HD21	1:E:844:THR:OG1	2.18	0.43
1:A:801:LEU:O	1:A:841:TRP:NE1	2.43	0.43
1:F:856:LEU:HD23	1:F:856:LEU:HA	1.87	0.43
1:B:438:LEU:HD21	1:C:654:VAL:HG11	2.00	0.43
1:E:812:ARG:HH11	1:E:817:ALA:HB1	1.83	0.43
1:A:651:LYS:O	1:A:651:LYS:HG3	2.19	0.43
1:B:762:MET:HE3	1:B:762:MET:HB3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:PRO:HB3	1:B:1362:SER:HA	1.99	0.43
1:C:711:LEU:HD11	1:C:867:LEU:HD22	2.00	0.43
1:E:493:VAL:HG22	2:G:18:ARG:HB2	1.96	0.43
1:F:425:LEU:O	1:F:429:VAL:N	2.47	0.43
1:A:412:PHE:HB3	1:A:422:ILE:HD13	2.01	0.43
1:C:457:GLY:N	4:C:1401:AGS:O3B	2.38	0.43
1:E:444:ILE:HD12	1:F:631:THR:HG23	2.01	0.43
1:F:839:ASP:OD1	1:F:839:ASP:N	2.51	0.43
1:A:699:GLN:HG2	1:A:897:LEU:HD23	2.00	0.43
1:A:716:THR:HG22	1:A:720:ARG:H	1.84	0.43
1:C:543:LEU:CD2	1:C:576:ARG:NH1	2.74	0.43
1:C:650:ASP:OD1	1:C:650:ASP:N	2.42	0.43
1:E:1370:VAL:O	1:E:1374:ILE:HG12	2.19	0.43
1:F:689:PRO:HD2	1:F:692:ILE:HD11	2.01	0.43
1:F:765:SER:O	1:F:765:SER:OG	2.36	0.43
1:A:912:LEU:HD22	1:A:1350:HIS:ND1	2.33	0.43
1:E:832:VAL:HG22	1:E:867:LEU:HB3	2.01	0.43
1:E:838:LEU:HB3	1:E:872:ALA:HB2	2.01	0.43
1:E:927:LYS:HB2	1:E:927:LYS:HE3	1.80	0.43
1:F:614:LEU:HD21	1:F:666:PHE:HB3	2.00	0.43
1:E:801:LEU:O	1:E:841:TRP:NE1	2.51	0.42
1:F:839:ASP:O	1:F:843:ASN:ND2	2.52	0.42
1:A:823:MET:CE	1:A:823:MET:CA	2.86	0.42
1:B:608:THR:HA	1:B:611:ILE:HG22	2.01	0.42
1:B:644:GLN:HB2	1:B:936:LEU:HD12	2.00	0.42
1:F:511:GLN:HE22	1:F:552:ARG:HH22	1.67	0.42
1:B:439:TYR:CD2	1:B:446:PRO:HG3	2.54	0.42
1:E:448:ARG:HG3	1:E:549:MET:CE	2.49	0.42
1:E:448:ARG:CD	1:E:549:MET:HE3	2.50	0.42
1:F:691:LEU:HD12	1:F:691:LEU:HA	1.93	0.42
1:A:411:ASN:OD1	1:A:411:ASN:N	2.52	0.42
1:B:1323:THR:HA	1:B:1324:PRO:HD3	1.90	0.42
1:D:636:ILE:HD11	1:D:672:LYS:HE3	2.02	0.42
1:E:561:THR:C	1:E:563:ARG:N	2.77	0.42
1:F:500:LEU:HD12	1:F:500:LEU:HA	1.89	0.42
1:A:455:PRO:HG2	1:A:458:THR:HG21	2.02	0.42
1:C:683:SER:OG	1:C:684:SER:N	2.51	0.42
1:D:521:ASP:OD2	1:D:561:THR:OG1	2.34	0.42
1:E:902:LYS:HB3	1:E:902:LYS:HE2	1.72	0.42
1:B:411:ASN:OD1	1:B:411:ASN:N	2.52	0.42
1:B:914:GLU:HA	1:B:917:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:774:ILE:HB	1:C:871:LEU:HD23	2.02	0.42
1:C:797:ASN:H	1:C:831:SER:HA	1.85	0.42
1:D:450:VAL:HG23	1:D:558:ILE:HG23	2.01	0.42
1:F:797:ASN:H	1:F:831:SER:HA	1.85	0.42
1:C:437:GLU:HA	1:C:440:GLN:HB2	2.00	0.42
1:E:839:ASP:OD1	1:E:839:ASP:N	2.52	0.42
1:B:550:ASP:OD1	1:B:550:ASP:N	2.53	0.42
1:E:516:PHE:HA	1:E:558:ILE:O	2.20	0.42
1:E:1360:SER:O	1:E:1360:SER:OG	2.30	0.42
1:B:774:ILE:HB	1:B:871:LEU:HG	2.01	0.42
1:C:482:MET:SD	1:C:484:LYS:NZ	2.92	0.42
1:D:914:GLU:HA	1:D:917:LYS:HG2	2.02	0.42
1:A:884:ILE:HD12	1:A:884:ILE:HA	1.89	0.42
1:B:493:VAL:O	1:B:497:GLU:HG2	2.20	0.42
1:C:860:LEU:CD1	1:C:866:ILE:HD12	2.50	0.42
1:D:593:LYS:HE3	1:D:597:ILE:HD11	2.02	0.42
1:F:571:LEU:HD12	1:F:572:ARG:N	2.34	0.42
1:F:930:VAL:HG23	1:F:931:LYS:HD3	2.01	0.42
1:A:674:VAL:HA	1:A:675:PRO:HD3	1.90	0.41
1:A:755:SER:O	1:A:755:SER:OG	2.28	0.41
1:C:636:ILE:HA	1:C:639:GLN:HG2	2.02	0.41
1:D:801:LEU:O	1:D:841:TRP:NE1	2.52	0.41
1:A:487:ASP:HB2	1:A:490:SER:HB3	2.02	0.41
1:B:463:MET:HE2	1:B:463:MET:HB2	1.78	0.41
1:B:655:ASP:OD2	1:B:657:SER:OG	2.37	0.41
1:C:919:LYS:NZ	1:C:1364:TRP:HE1	2.18	0.41
1:F:819:VAL:O	1:F:823:MET:HG2	2.20	0.41
1:A:797:ASN:H	1:A:831:SER:HA	1.86	0.41
1:B:449:GLY:HA3	1:B:577:PHE:H	1.85	0.41
1:C:1330:VAL:O	1:C:1334:LEU:HB2	2.21	0.41
1:D:653:LEU:HD23	1:D:937:GLN:HB3	2.00	0.41
1:F:674:VAL:HA	1:F:675:PRO:HD3	1.90	0.41
1:C:799:GLN:HG3	1:C:825:ALA:HB2	2.02	0.41
1:F:425:LEU:HD12	1:F:452:PHE:CZ	2.54	0.41
1:A:912:LEU:HD11	1:A:1354:ALA:HB2	2.02	0.41
1:B:692:ILE:HD12	1:B:696:LEU:HD12	2.02	0.41
1:B:771:ARG:HG3	1:B:868:LEU:HB3	2.01	0.41
1:B:826:LYS:HA	1:B:866:ILE:HD11	2.02	0.41
1:D:414:ASP:OD1	1:D:600:ARG:NH2	2.36	0.41
1:D:815:GLU:HG3	1:D:849:VAL:HB	2.03	0.41
1:E:444:ILE:HB	1:F:631:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:790:LEU:HD13	1:E:798:VAL:HG21	2.01	0.41
1:E:815:GLU:OE2	1:E:849:VAL:HG22	2.20	0.41
1:F:919:LYS:HA	1:F:1320:LEU:HD13	2.01	0.41
1:C:861:GLN:HB2	1:C:864:GLU:HG2	2.03	0.41
1:B:441:ASN:ND2	1:C:656:PRO:O	2.54	0.41
1:D:1330:VAL:HA	1:D:1374:ILE:HD11	2.02	0.41
1:E:669:ALA:HA	1:E:672:LYS:HG2	2.02	0.41
1:E:923:ILE:HB	1:E:925:MET:HG2	2.02	0.41
1:F:767:ILE:O	1:F:862:SER:O	2.39	0.41
1:A:491:LYS:O	1:A:535:HIS:NE2	2.53	0.41
1:B:460:LYS:N	4:B:1401:AGS:O2B	2.43	0.41
1:D:883:GLY:N	1:D:886:SER:OG	2.53	0.41
1:F:842:ILE:HD13	1:F:842:ILE:HA	1.85	0.41
1:A:717:THR:HB	1:A:720:ARG:HB3	2.02	0.41
1:B:872:ALA:HB1	1:B:875:LEU:HB2	2.01	0.41
1:C:487:ASP:OD1	1:C:487:ASP:N	2.54	0.41
1:C:802:ASP:OD1	1:C:802:ASP:N	2.47	0.41
1:D:549:MET:HE3	1:D:549:MET:HB3	1.88	0.41
1:D:931:LYS:HE2	1:D:931:LYS:HB2	1.90	0.41
1:E:492:TRP:HZ3	2:G:19:LYS:HD3	1.85	0.41
1:E:711:LEU:HD11	1:E:867:LEU:HD22	2.02	0.41
1:F:425:LEU:HD21	1:F:467:LEU:CD1	2.43	0.41
1:F:516:PHE:HD1	1:F:558:ILE:HB	1.85	0.41
1:A:891:ASP:OD1	1:A:891:ASP:N	2.47	0.41
1:B:543:LEU:HD22	1:B:576:ARG:NH2	2.36	0.41
1:B:691:LEU:HD23	1:B:691:LEU:HA	1.83	0.41
1:B:920:PRO:HD3	1:B:1320:LEU:HD13	2.03	0.41
1:C:613:LYS:HE2	1:C:617:LEU:HD11	2.03	0.41
1:C:678:ALA:HB1	1:C:683:SER:HA	2.03	0.41
1:E:803:LEU:O	1:E:807:VAL:HG22	2.21	0.41
1:F:842:ILE:HD11	1:F:885:LEU:HD21	2.02	0.41
1:A:478:ILE:HD13	1:A:512:PRO:HB2	2.02	0.40
1:D:765:SER:O	1:D:765:SER:OG	2.38	0.40
1:A:613:LYS:HG2	1:F:753:PHE:CE1	2.56	0.40
1:A:816:ALA:O	1:A:820:GLN:CG	2.66	0.40
1:B:771:ARG:HH21	1:B:857:PHE:HB3	1.85	0.40
1:B:919:LYS:HB2	1:B:919:LYS:HE2	1.84	0.40
1:F:692:ILE:HD12	1:F:696:LEU:HD12	2.03	0.40
1:B:424:GLN:O	1:B:579:ARG:NH2	2.55	0.40
1:D:876:ASP:OD1	1:D:876:ASP:N	2.48	0.40
1:B:497:GLU:HG3	1:C:489:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:854:SER:O	1:B:858:ARG:HB2	2.22	0.40
1:F:496:ALA:HB1	1:F:538:ILE:HD11	2.02	0.40
1:A:546:MET:HG3	1:A:576:ARG:HG3	2.04	0.40
1:B:491:LYS:HD2	2:G:13:GLY:HA2	2.02	0.40
1:C:919:LYS:HD2	1:C:920:PRO:HD2	2.02	0.40
1:D:844:THR:OG1	1:D:845:ILE:N	2.55	0.40
1:E:703:LEU:HD21	1:E:774:ILE:HG12	2.03	0.40
1:E:815:GLU:OE1	1:E:849:VAL:N	2.54	0.40
1:F:797:ASN:HB3	1:F:831:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/1416 (41%)	540 (93%)	39 (7%)	0	100	100
1	B	568/1416 (40%)	545 (96%)	23 (4%)	0	100	100
1	C	575/1416 (41%)	543 (94%)	31 (5%)	1 (0%)	43	76
1	D	575/1416 (41%)	551 (96%)	23 (4%)	1 (0%)	43	76
1	E	572/1416 (40%)	540 (94%)	32 (6%)	0	100	100
1	F	575/1416 (41%)	543 (94%)	30 (5%)	2 (0%)	36	70
2	G	13/25 (52%)	12 (92%)	1 (8%)	0	100	100
All	All	3457/8521 (41%)	3274 (95%)	179 (5%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	511	GLN
1	D	827	LYS

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Mol	Chain	Res	Type
1	C	509	LYS
1	F	488	ILE

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	524/1281 (41%)	512 (98%)	12 (2%)	44	74
1	B	516/1281 (40%)	513 (99%)	3 (1%)	78	88
1	C	522/1281 (41%)	517 (99%)	5 (1%)	68	84
1	D	522/1281 (41%)	518 (99%)	4 (1%)	73	86
1	E	519/1281 (40%)	516 (99%)	3 (1%)	78	88
1	F	523/1281 (41%)	517 (99%)	6 (1%)	65	83
2	G	11/18 (61%)	10 (91%)	1 (9%)	9	33
All	All	3137/7704 (41%)	3103 (99%)	34 (1%)	63	83

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	425	LEU
1	A	588	VAL
1	A	715	ASP
1	A	803	LEU
1	A	807	VAL
1	A	813	THR
1	A	832	VAL
1	A	874	ASN
1	A	893	ASN
1	A	912	LEU
1	A	939	VAL
1	A	1321	ILE
1	B	509	LYS
1	B	578	ASP
1	B	884	ILE

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Mol	Chain	Res	Type
1	C	411	ASN
1	C	474	ASP
1	C	578	ASP
1	C	813	THR
1	C	844	THR
1	D	450	VAL
1	D	511	GLN
1	D	803	LEU
1	D	827	LYS
1	E	567	VAL
1	E	844	THR
1	E	847	GLU
1	F	420	ASN
1	F	450	VAL
1	F	509	LYS
1	F	511	GLN
1	F	567	VAL
1	F	863	ASN
2	G	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	ASN
1	A	699	GLN
1	A	726	GLN
1	A	766	GLN
1	A	780	ASN
1	A	799	GLN
1	A	829	GLN
1	A	863	ASN
1	A	874	ASN
1	A	896	GLN
1	A	898	HIS
1	A	1340	ASN
1	A	1345	GLN
1	B	441	ASN
1	B	511	GLN
1	B	562	ASN
1	B	644	GLN
1	B	712	ASN
1	B	721	ASN

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Mol	Chain	Res	Type
1	B	726	GLN
1	B	797	ASN
1	B	820	GLN
1	B	904	ASN
1	C	531	GLN
1	C	551	ASN
1	C	562	ASN
1	C	686	GLN
1	C	712	ASN
1	C	766	GLN
1	C	780	ASN
1	C	799	GLN
1	C	861	GLN
1	C	874	ASN
1	C	1350	HIS
1	D	424	GLN
1	D	453	HIS
1	D	510	HIS
1	D	511	GLN
1	D	551	ASN
1	D	562	ASN
1	D	596	GLN
1	D	639	GLN
1	D	644	GLN
1	D	719	GLN
1	D	791	ASN
1	D	896	GLN
1	D	1340	ASN
1	D	1345	GLN
1	D	1350	HIS
1	E	420	ASN
1	E	533	GLN
1	E	535	HIS
1	E	551	ASN
1	E	554	GLN
1	E	699	GLN
1	E	712	ASN
1	E	719	GLN
1	E	721	ASN
1	E	726	GLN
1	E	727	ASN
1	E	799	GLN

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Mol	Chain	Res	Type
1	E	800	ASN
1	E	820	GLN
1	E	848	ASN
1	E	896	GLN
1	E	1340	ASN
1	E	1350	HIS
1	F	420	ASN
1	F	443	ASN
1	F	531	GLN
1	F	554	GLN
1	F	644	GLN
1	F	702	ASN
1	F	721	ASN
1	F	775	ASN
1	F	800	ASN
1	F	843	ASN
1	F	863	ASN
1	F	893	ASN
1	F	896	GLN
1	F	911	ASN
1	F	1326	GLN
1	F	1345	GLN
1	F	1350	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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
4	AGS	B	1401	-	32,33,33	0.74	2 (6%)	45,52,52	0.72	1 (2%)
4	AGS	D	1401	5	32,33,33	0.89	4 (12%)	45,52,52	0.58	1 (2%)
4	AGS	E	1401	5	32,33,33	0.96	3 (9%)	45,52,52	0.67	2 (4%)
4	AGS	F	1401	5	32,33,33	0.92	2 (6%)	45,52,52	0.64	1 (2%)
3	ADP	A	1401	-	28,29,29	1.40	5 (17%)	43,45,45	1.86	11 (25%)
4	AGS	C	1401	5	32,33,33	1.02	3 (9%)	45,52,52	0.72	2 (4%)

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
4	AGS	B	1401	-	-	8/21/38/38	0/3/3/3
4	AGS	D	1401	5	-	3/21/38/38	0/3/3/3
4	AGS	E	1401	5	-	2/21/38/38	0/3/3/3
4	AGS	F	1401	5	-	0/21/38/38	0/3/3/3
3	ADP	A	1401	-	-	2/16/32/32	0/3/3/3
4	AGS	C	1401	5	-	4/21/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1401	ADP	C5-C4	4.32	1.46	1.39
4	C	1401	AGS	PB-O3B	-3.29	1.55	1.59
4	E	1401	AGS	PB-O3B	-3.22	1.56	1.59
4	F	1401	AGS	PA-O3A	-3.08	1.56	1.59
4	C	1401	AGS	PA-O3A	-2.84	1.56	1.59
3	A	1401	ADP	C5-N7	-2.62	1.34	1.39
3	A	1401	ADP	C5-C6	2.51	1.48	1.41
4	D	1401	AGS	PA-O1A	-2.39	1.42	1.50
4	C	1401	AGS	PA-O1A	-2.38	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1401	AGS	PA-O3A	-2.34	1.57	1.59
4	D	1401	AGS	PG-S1G	2.29	1.95	1.90
4	E	1401	AGS	PA-O1A	-2.27	1.43	1.50
4	D	1401	AGS	PA-O3A	-2.26	1.57	1.59
4	B	1401	AGS	PG-S1G	2.19	1.95	1.90
4	D	1401	AGS	PB-O3A	-2.17	1.57	1.59
3	A	1401	ADP	C4-N9	-2.14	1.33	1.37
4	B	1401	AGS	PA-O1A	-2.06	1.43	1.50
4	F	1401	AGS	PB-O3B	-2.03	1.57	1.59
3	A	1401	ADP	C8-N9	-2.03	1.34	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1401	ADP	C5-C4-N3	-5.84	118.67	126.72
3	A	1401	ADP	N3-C4-N9	4.69	135.14	127.17
3	A	1401	ADP	C2-N3-C4	3.74	120.95	111.83
3	A	1401	ADP	C4-C5-N7	-3.58	106.49	110.58
4	B	1401	AGS	PB-O3B-PG	-3.50	120.36	133.17
3	A	1401	ADP	N3-C2-N1	-3.36	123.49	128.58
4	C	1401	AGS	PB-O3B-PG	-3.13	121.71	133.17
3	A	1401	ADP	C4-N9-C8	2.80	108.68	105.74
4	E	1401	AGS	PB-O3B-PG	-2.67	123.40	133.17
4	F	1401	AGS	PB-O3B-PG	-2.65	123.45	133.17
3	A	1401	ADP	C5-N7-C8	2.63	107.59	103.45
4	D	1401	AGS	PB-O3B-PG	-2.49	124.05	133.17
3	A	1401	ADP	C2'-C1'-N9	-2.38	107.38	113.30
4	C	1401	AGS	O2B-PB-O3B	-2.26	101.17	107.27
3	A	1401	ADP	C6-C5-N7	2.14	136.21	132.09
4	E	1401	AGS	O2B-PB-O3B	-2.11	101.56	107.27
3	A	1401	ADP	C3'-C2'-C1'	2.11	105.44	101.46
3	A	1401	ADP	N9-C8-N7	-2.04	111.05	113.94

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1401	ADP	C5'-O5'-PA-O2A
3	A	1401	ADP	C5'-O5'-PA-O3A
4	B	1401	AGS	C5'-O5'-PA-O1A
4	B	1401	AGS	C5'-O5'-PA-O3A
4	C	1401	AGS	PB-O3B-PG-O2G

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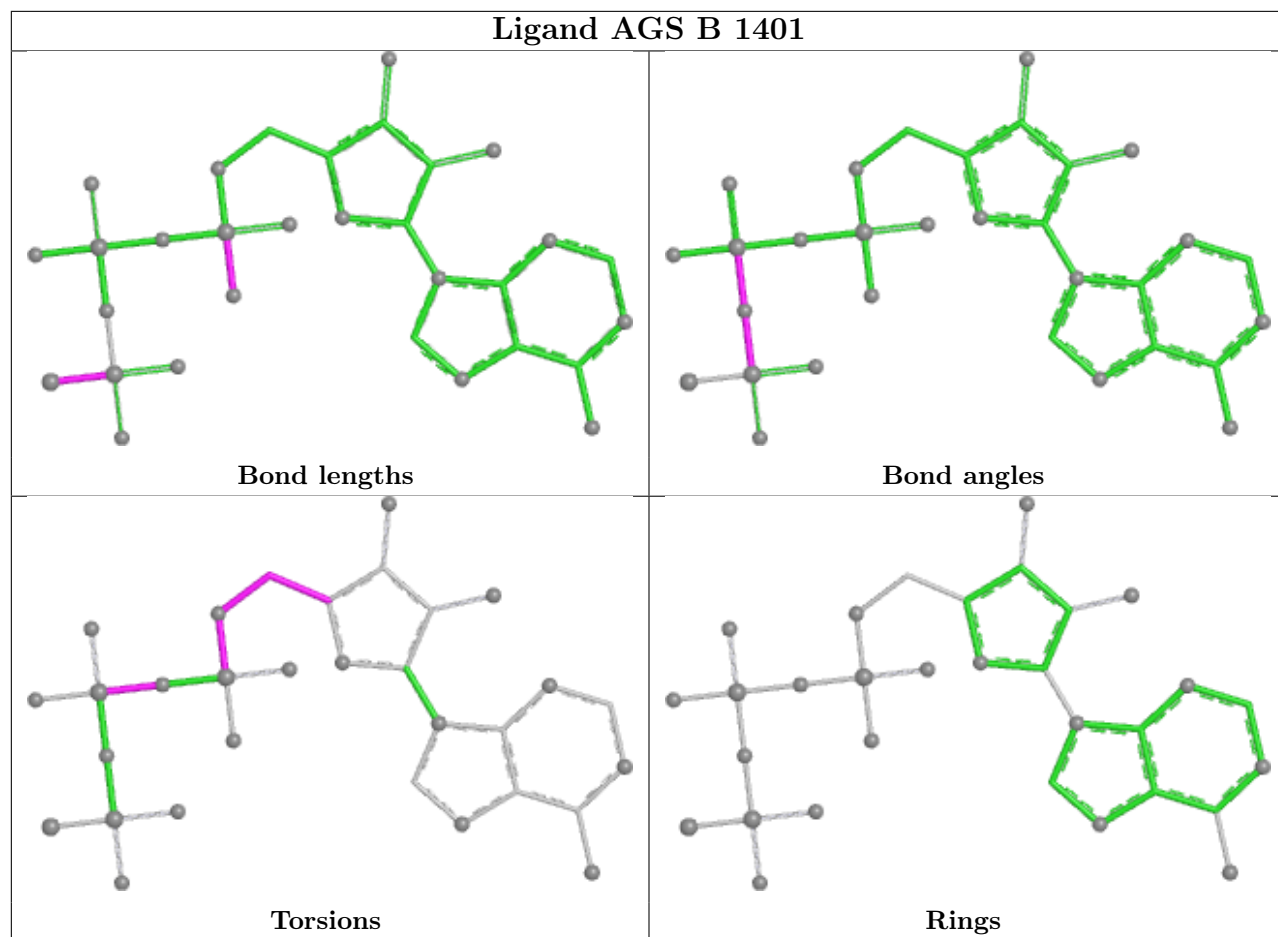
Mol	Chain	Res	Type	Atoms
4	D	1401	AGS	PB-O3B-PG-O3G
4	E	1401	AGS	PB-O3B-PG-O2G
4	E	1401	AGS	PB-O3B-PG-O3G
4	B	1401	AGS	O4'-C4'-C5'-O5'
4	C	1401	AGS	PG-O3B-PB-O1B
4	B	1401	AGS	C3'-C4'-C5'-O5'
4	B	1401	AGS	C5'-O5'-PA-O2A
4	B	1401	AGS	PA-O3A-PB-O2B
4	B	1401	AGS	C4'-C5'-O5'-PA
4	C	1401	AGS	PB-O3B-PG-O3G
4	C	1401	AGS	PG-O3B-PB-O2B
4	D	1401	AGS	PG-O3B-PB-O1B
4	D	1401	AGS	PG-O3B-PB-O2B
4	B	1401	AGS	PA-O3A-PB-O1B

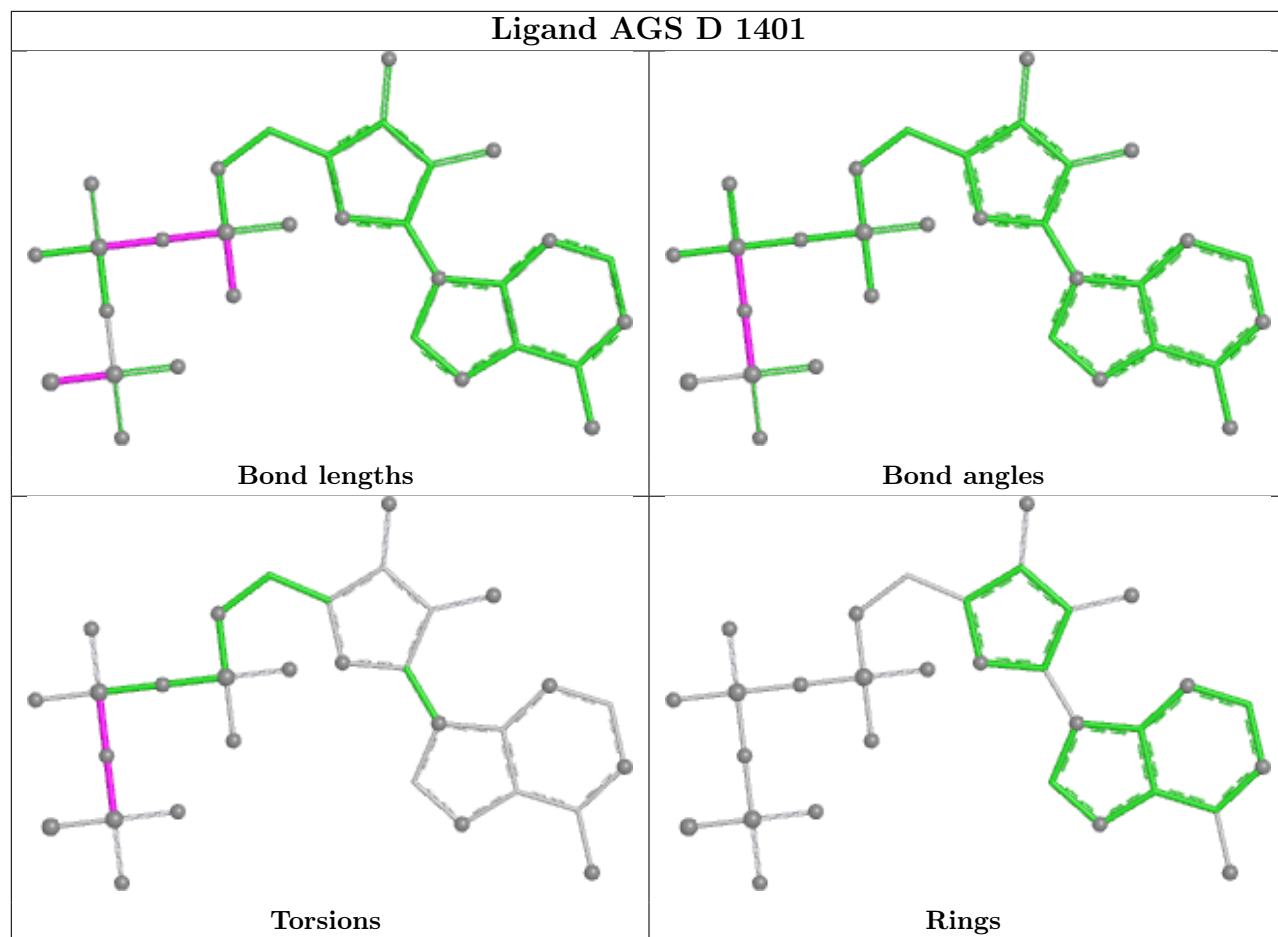
There are no ring outliers.

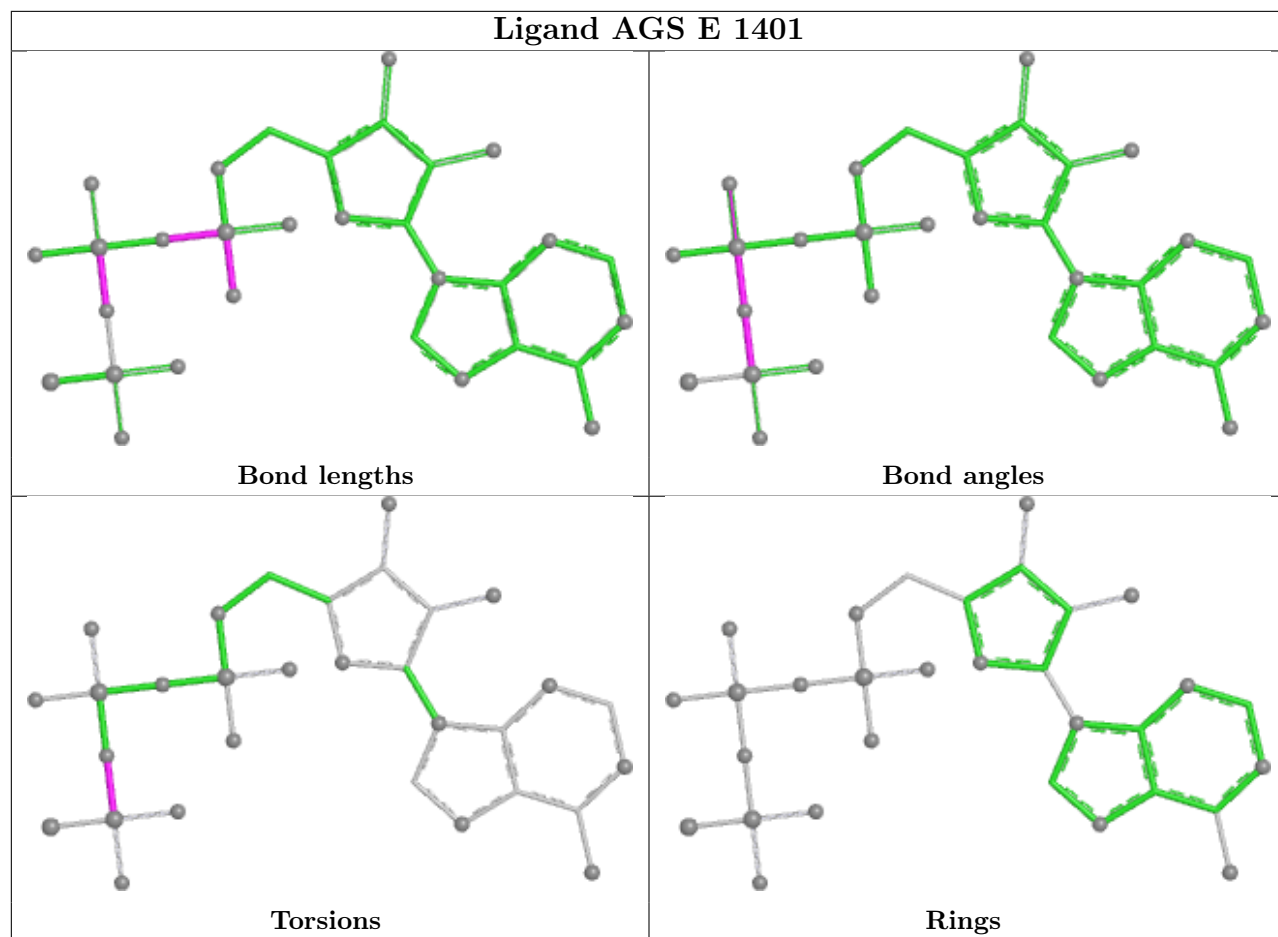
5 monomers are involved in 12 short contacts:

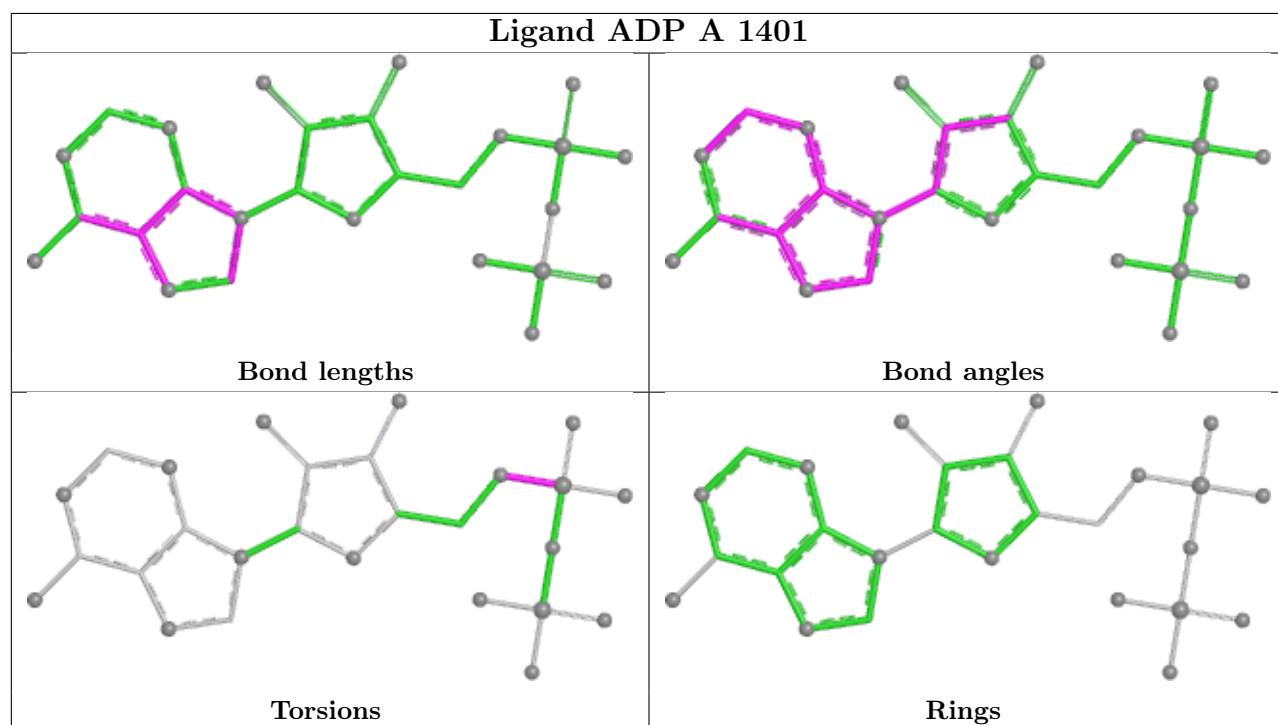
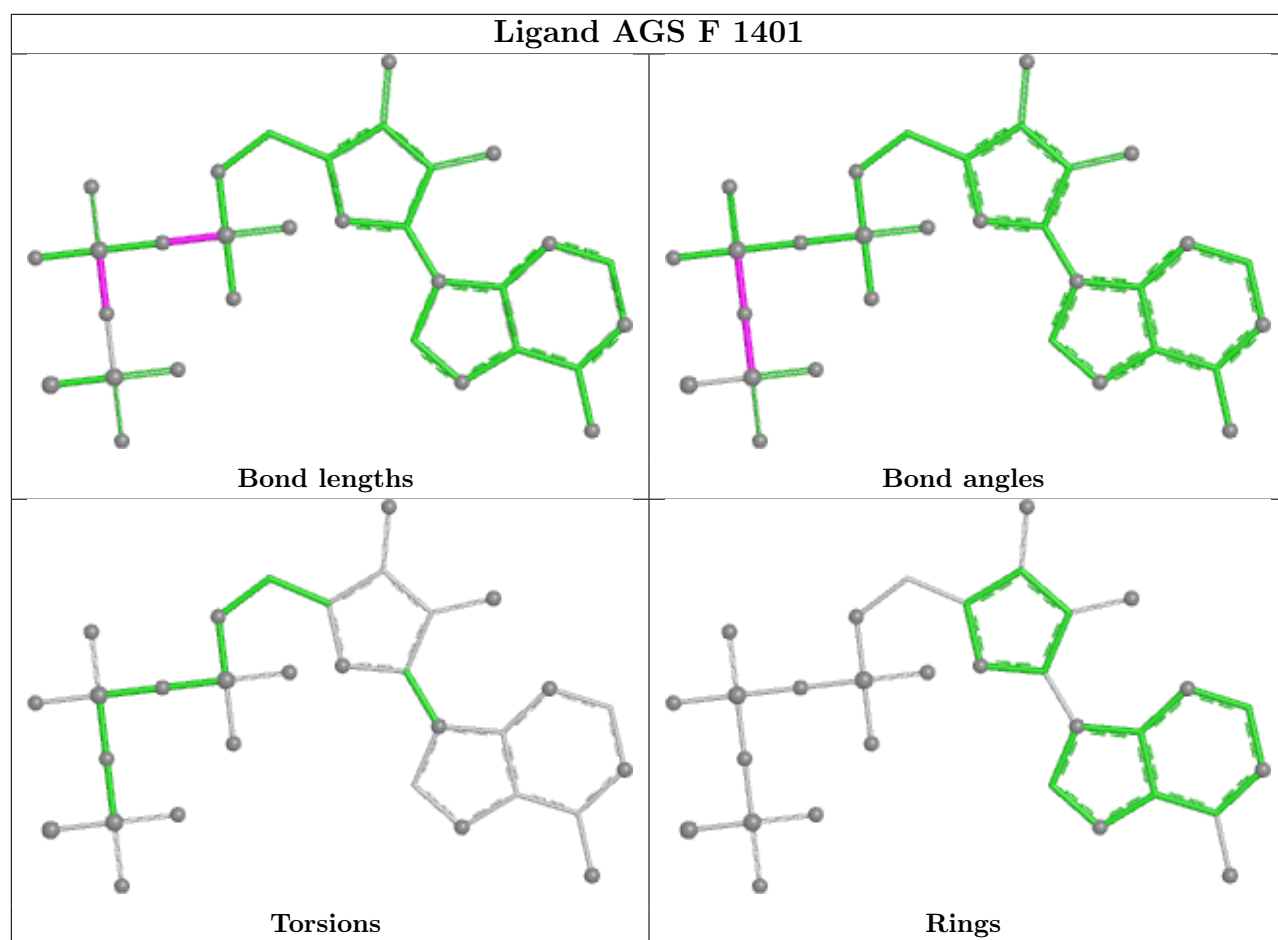
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1401	AGS	2	0
4	D	1401	AGS	1	0
4	E	1401	AGS	1	0
3	A	1401	ADP	1	0
4	C	1401	AGS	7	0

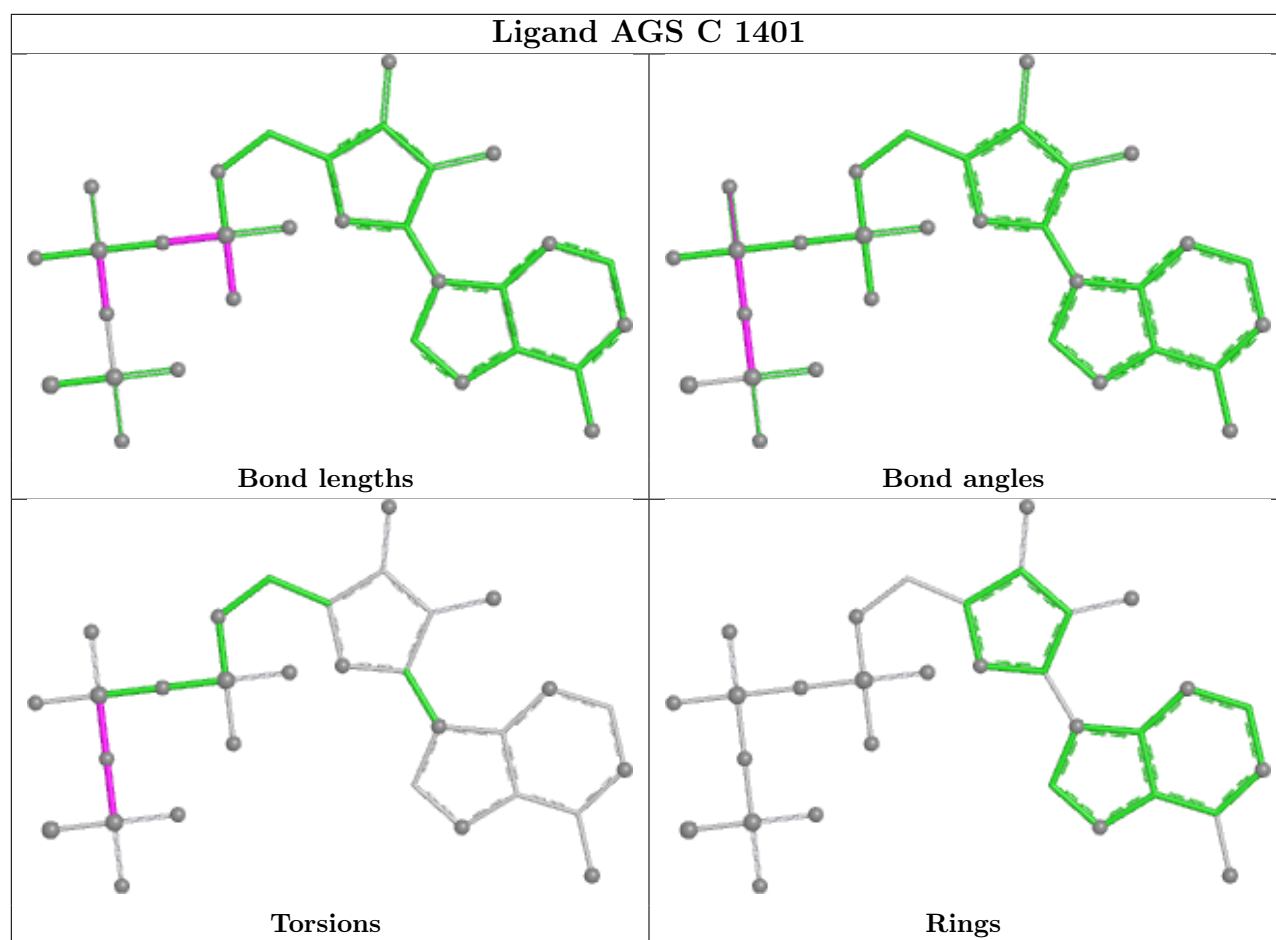
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

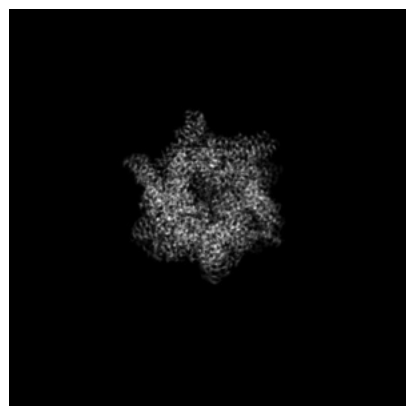
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26696. These allow visual inspection of the internal detail of the map and identification of artifacts.

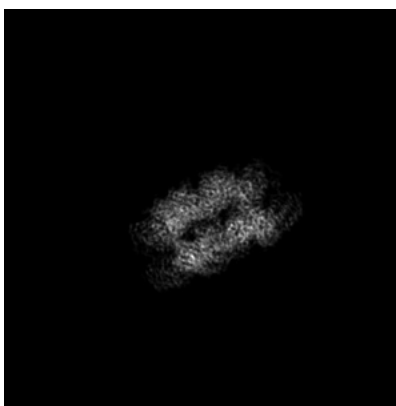
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

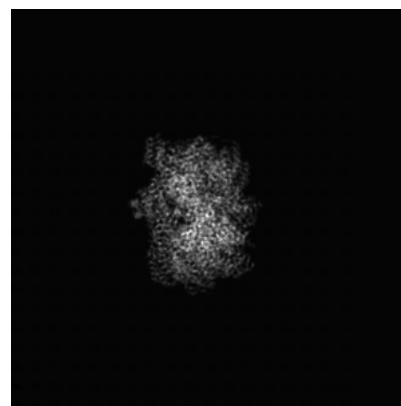
6.1.1 Primary map



X

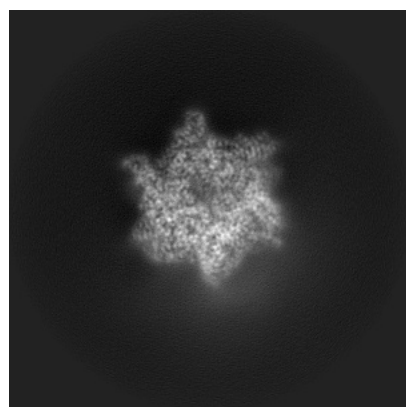


Y

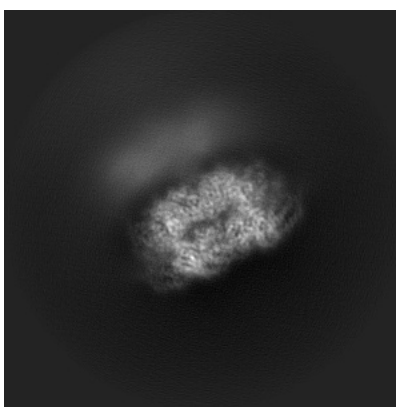


Z

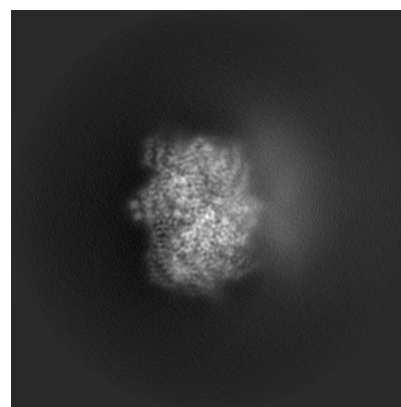
6.1.2 Raw map



X



Y

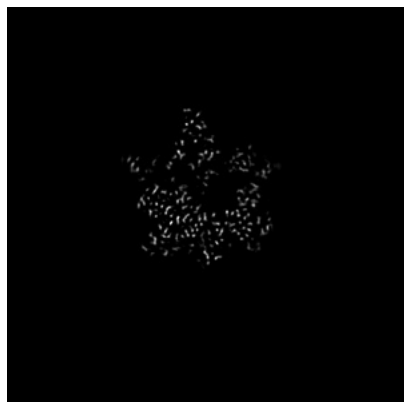


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200

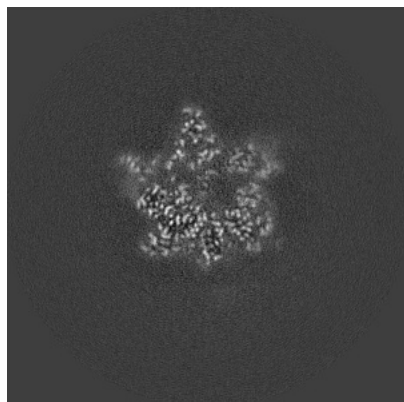


Y Index: 200

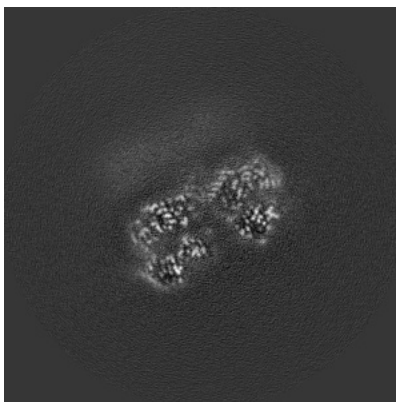


Z Index: 200

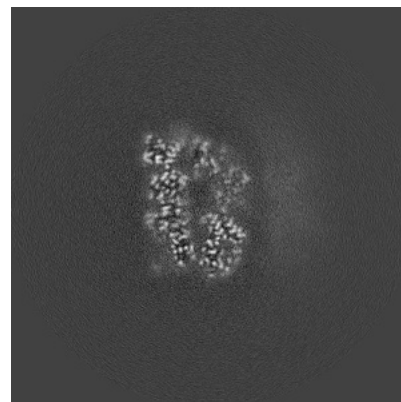
6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

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: 183

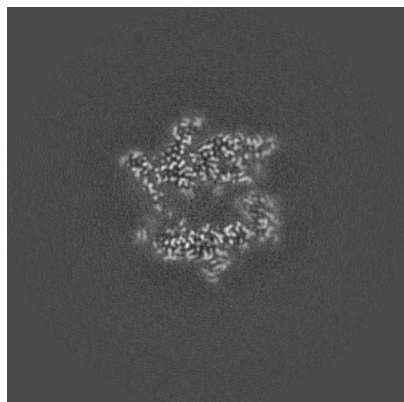


Y Index: 170

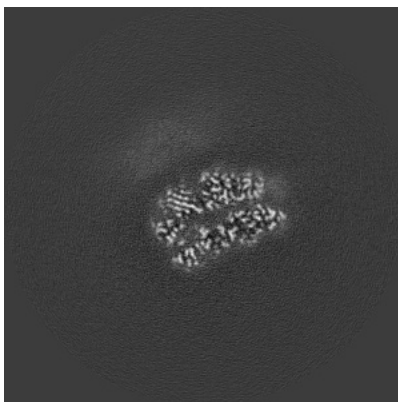


Z Index: 176

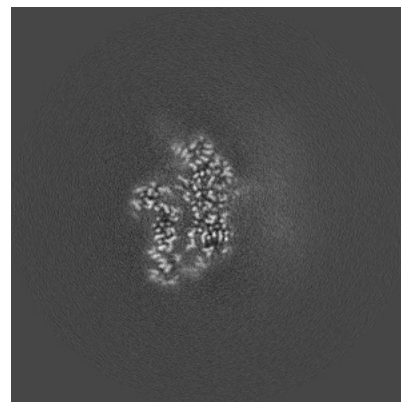
6.3.2 Raw map



X Index: 183



Y Index: 170

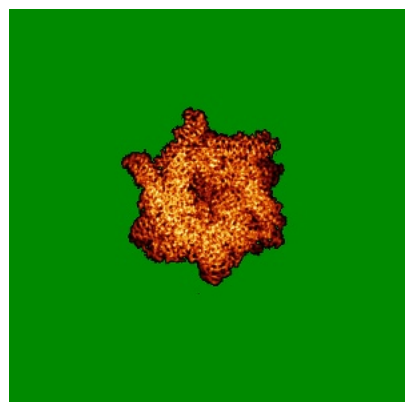


Z Index: 176

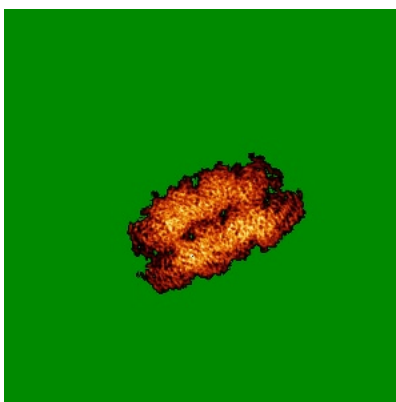
The images above show the largest variance slices of the map in three orthogonal directions.

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

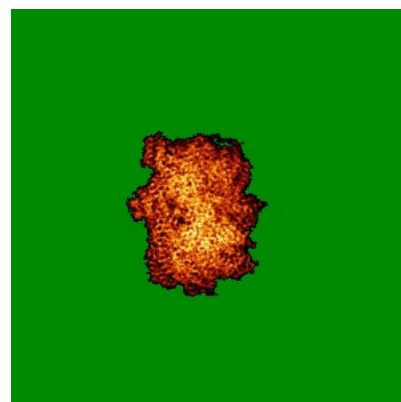
6.4.1 Primary map



X

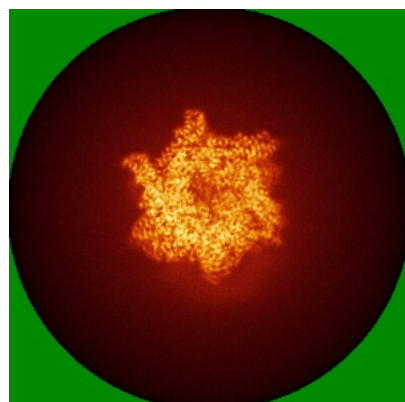


Y

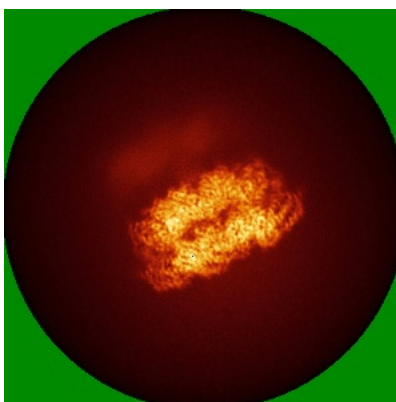


Z

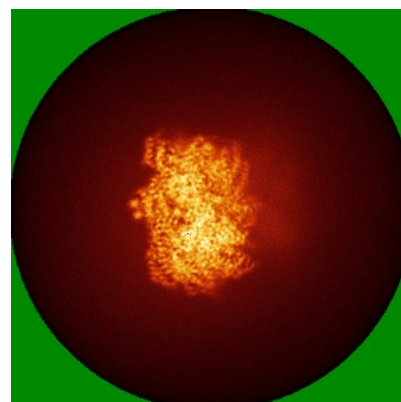
6.4.2 Raw map



X



Y

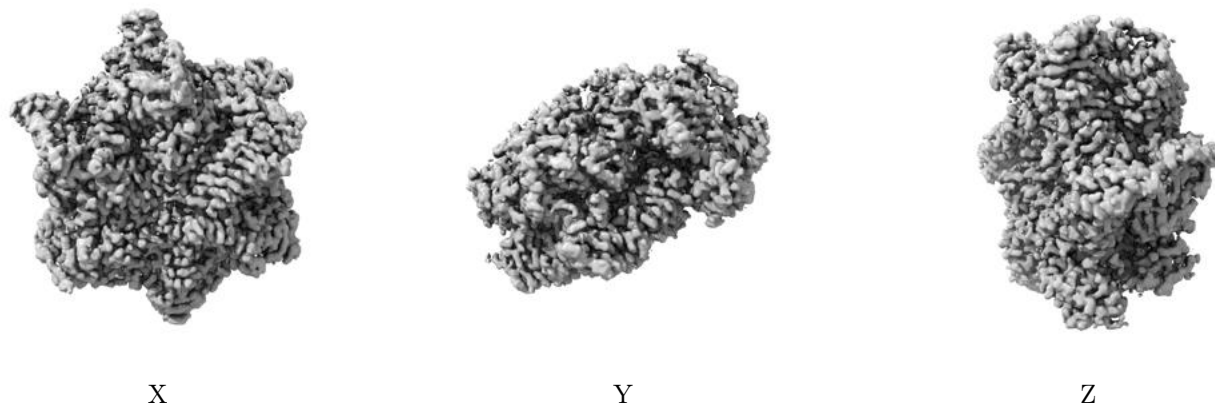


Z

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

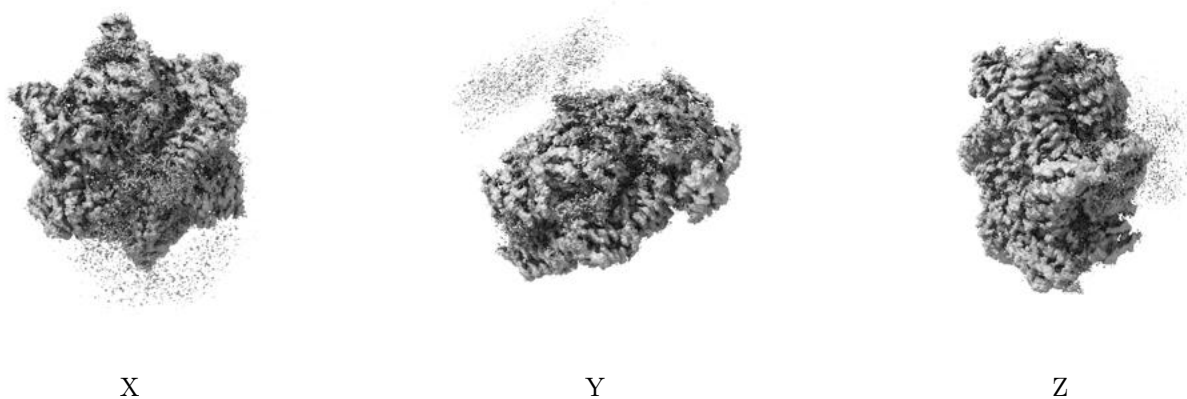
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

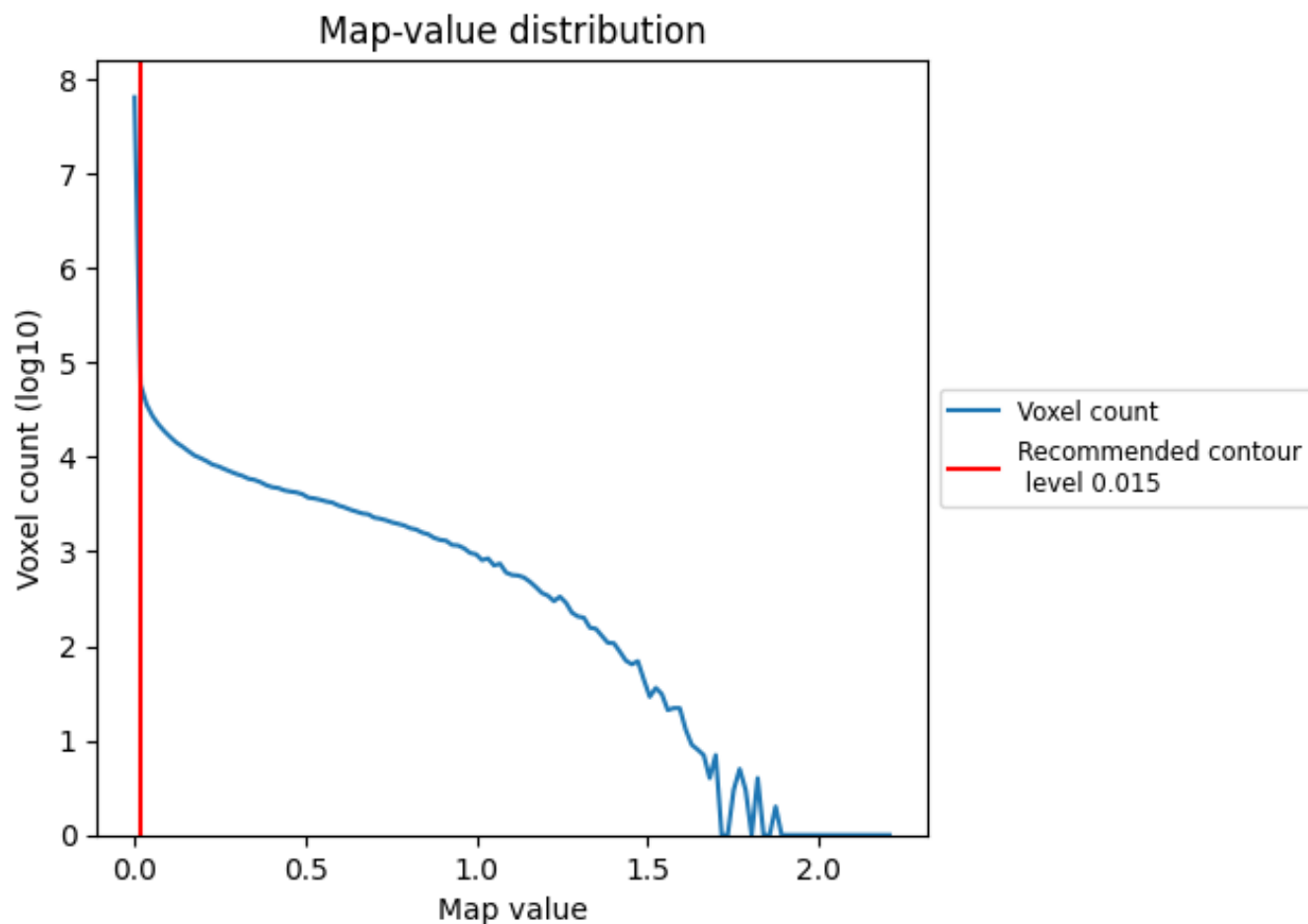
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

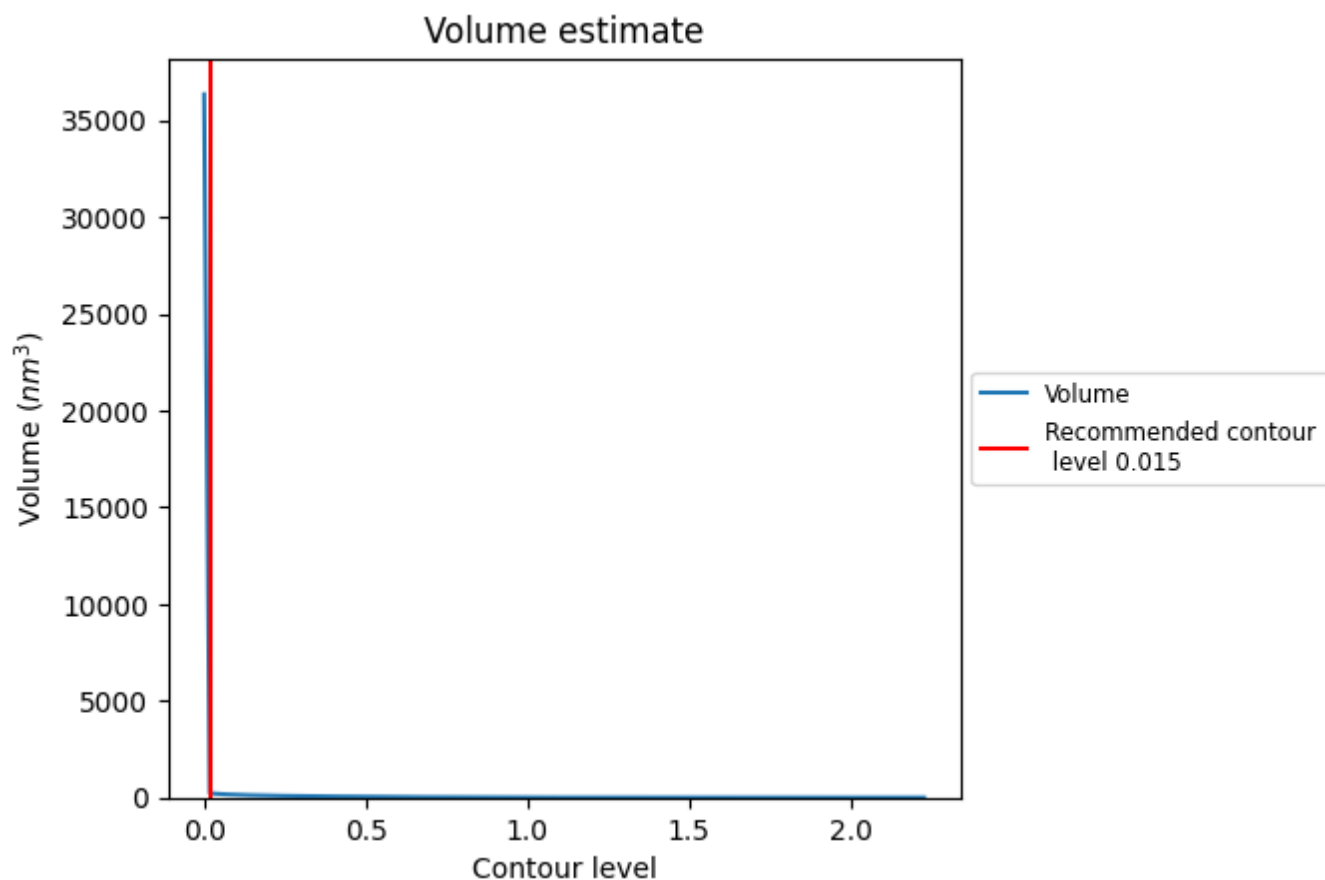
This section contains the results of statistical analysis of the map.

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.

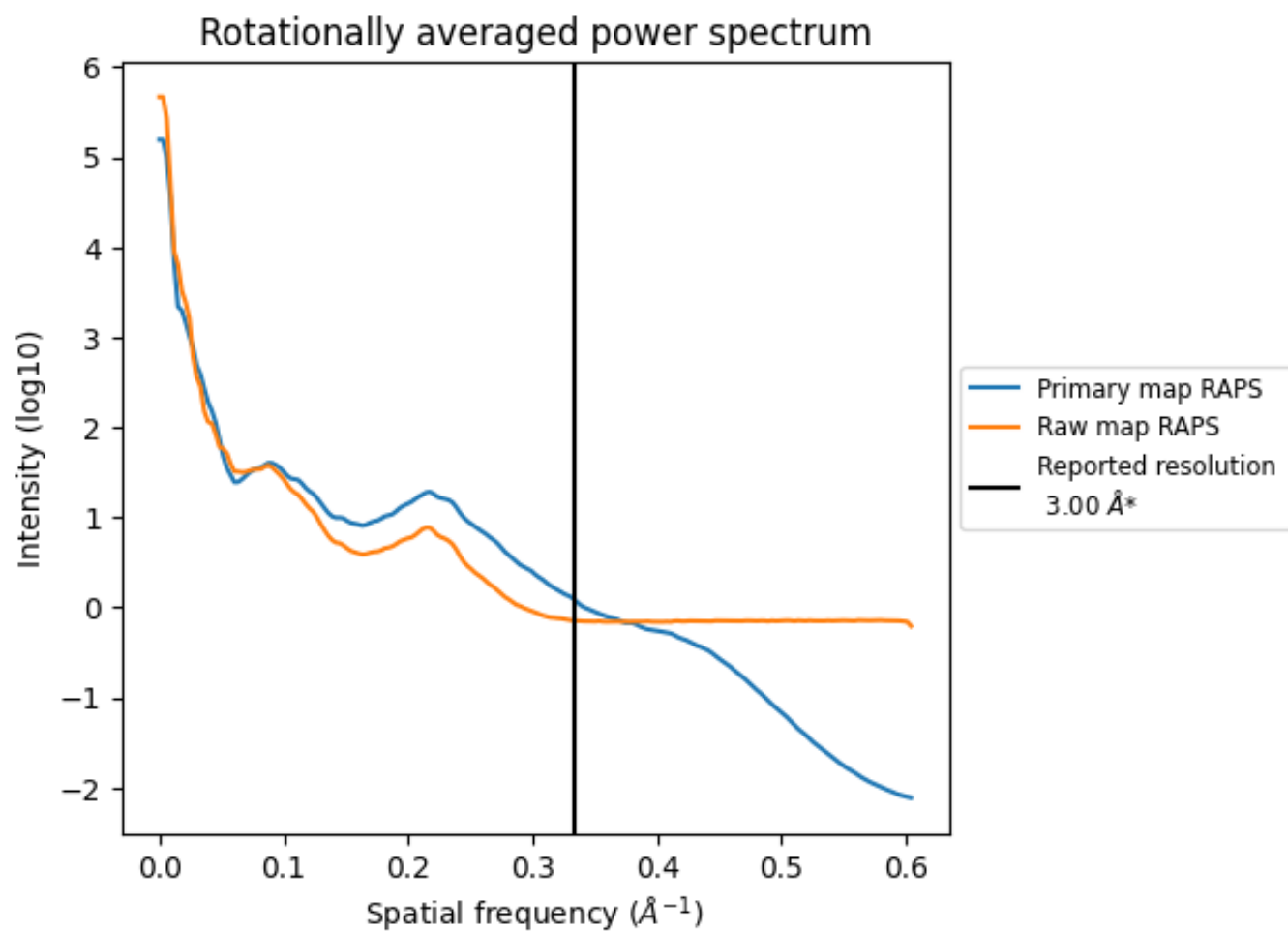
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1555 nm^3 ; this corresponds to an approximate mass of 1405 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 ⓘ

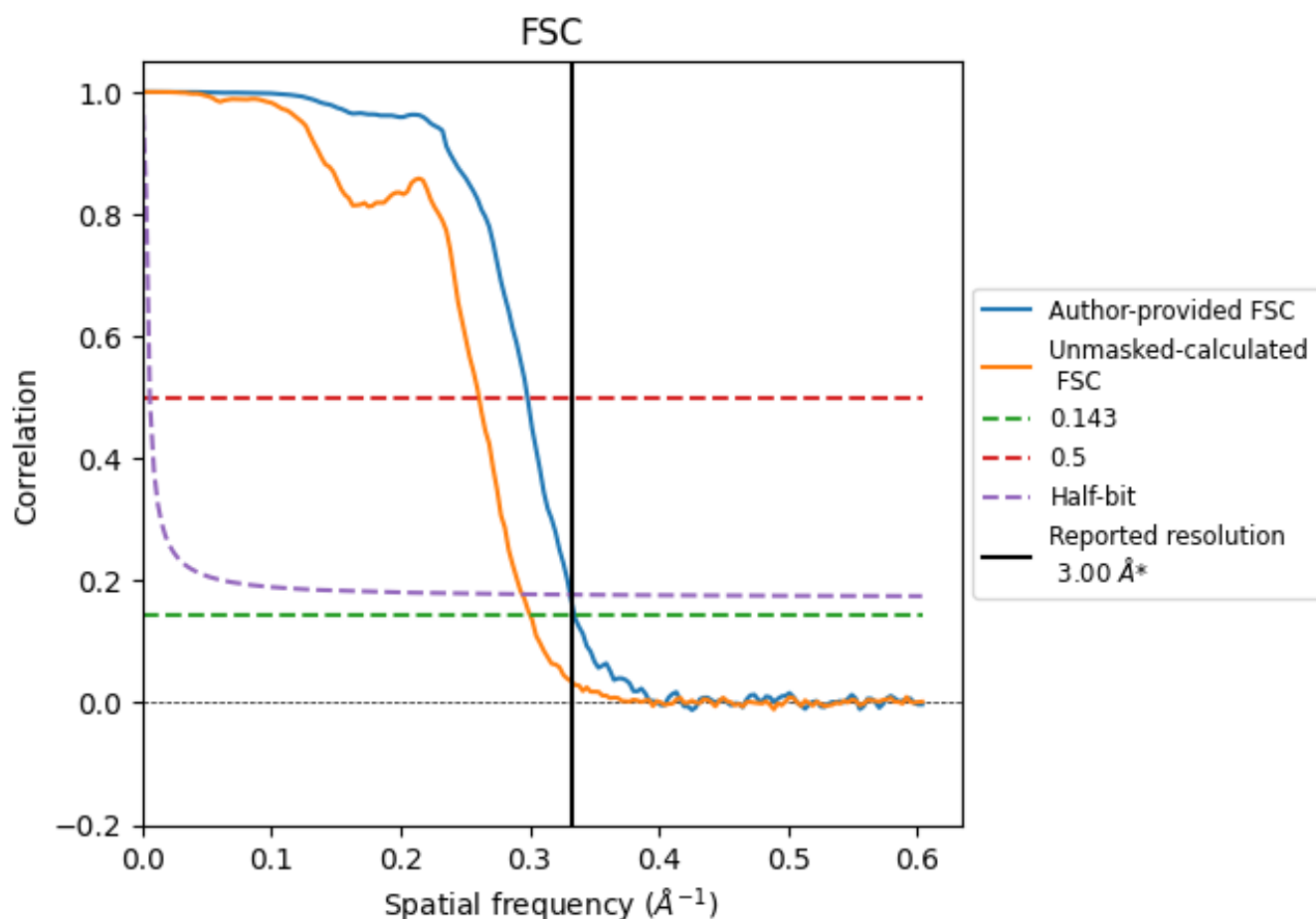


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

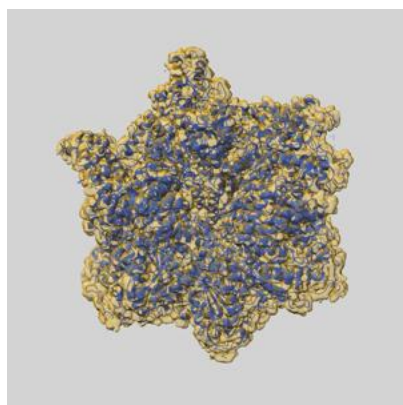
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.35	3.02
Unmasked-calculated*	3.33	3.84	3.40

*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 3.33 differs from the reported value 3.0 by more than 10 %

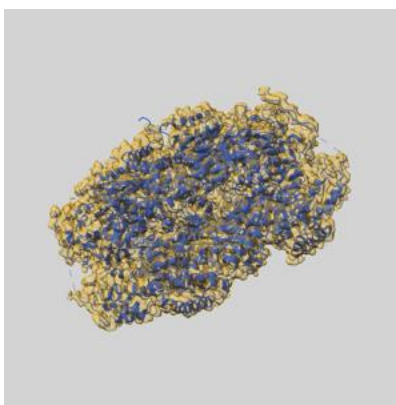
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26696 and PDB model 7UQJ. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

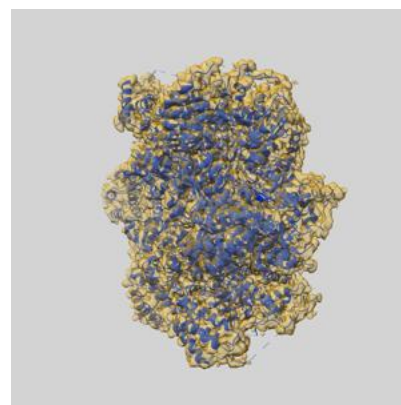
9.1 Map-model overlay [i](#)



X



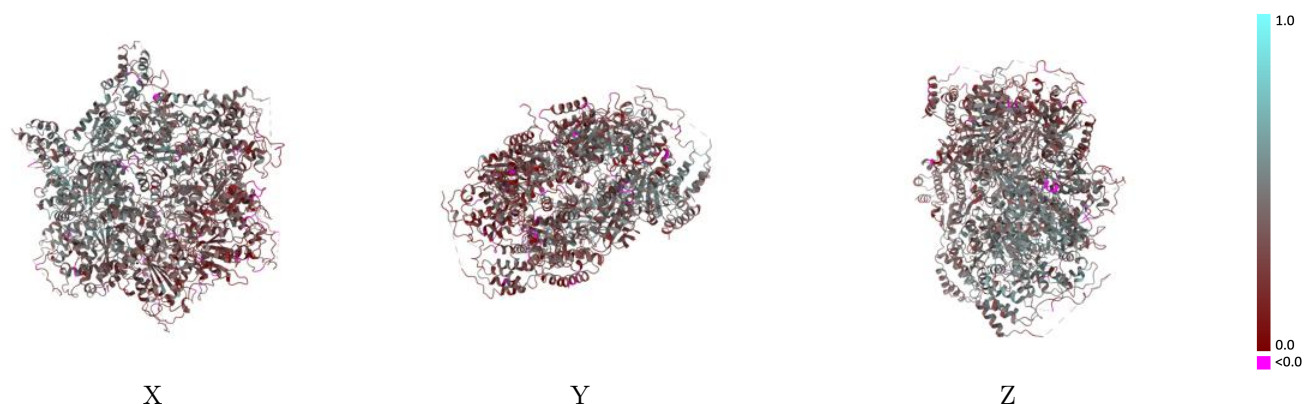
Y



Z

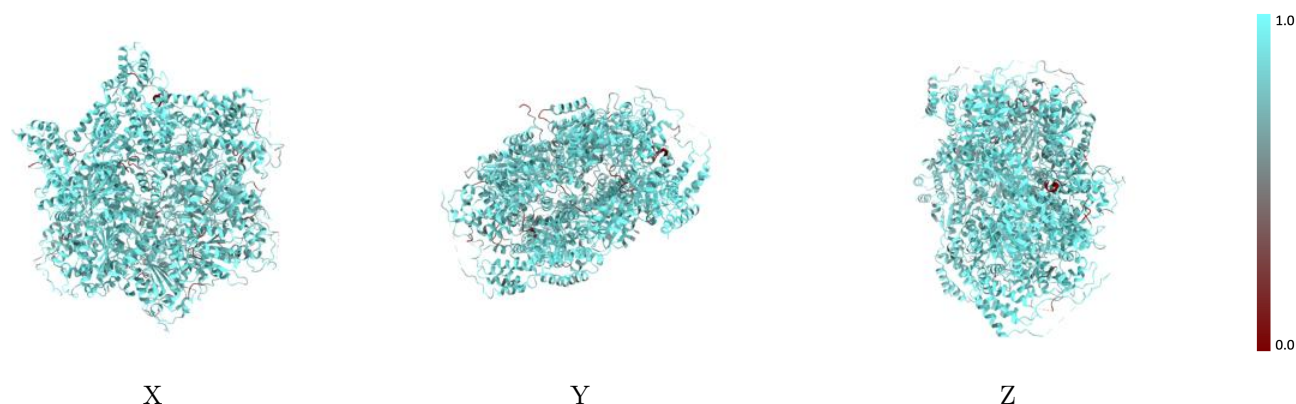
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



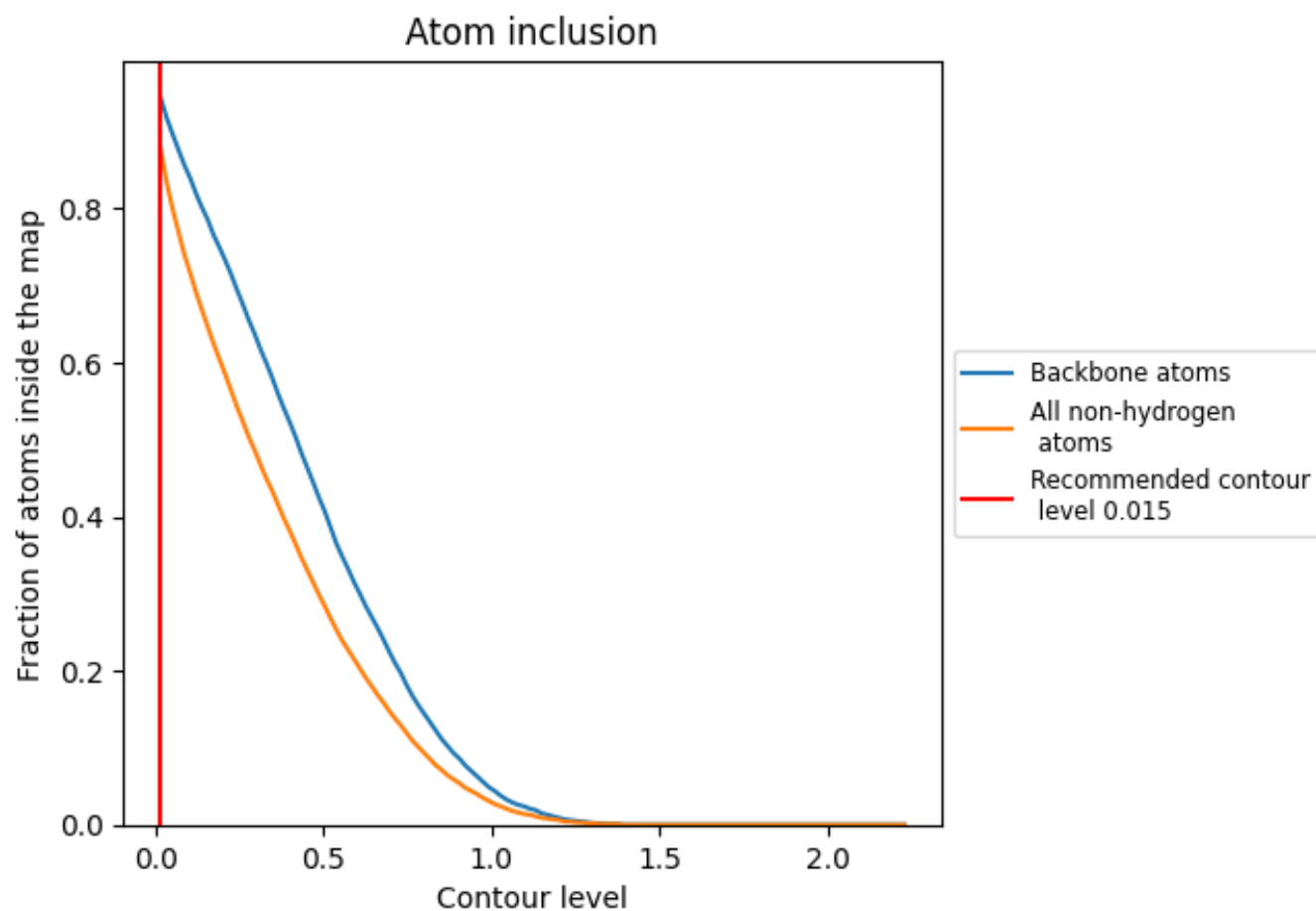
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.3620
A	0.8720	0.3920
B	0.9160	0.4480
C	0.9120	0.4320
D	0.8860	0.3390
E	0.8570	0.2710
F	0.8390	0.2940
G	0.3680	0.1090

1.0

0.0

<0.0