



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:06 PM UTC

PDB ID : 8RHN / pdb_00008rhn
EMDB ID : EMD-19177
Title : Structure of the 55LCC ATPase complex
Authors : Foglizzo, M.; Degtjarik, O.; Zeqiraj, E.
Deposited on : 2023-12-15
Resolution : 4.50 Å(reported)
Based on initial model : .

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
MolProbity : 4-5-2 with Phenix2.0
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

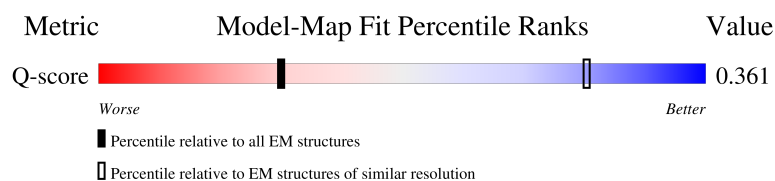
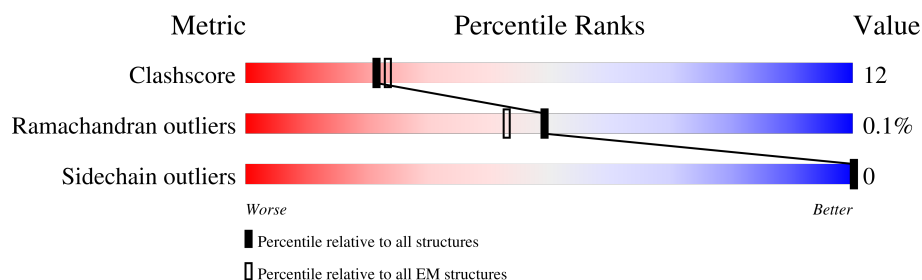
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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.



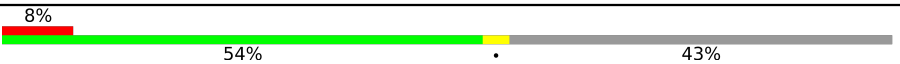
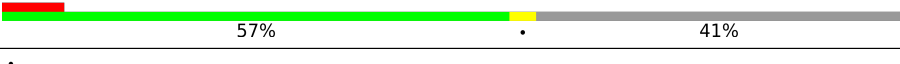
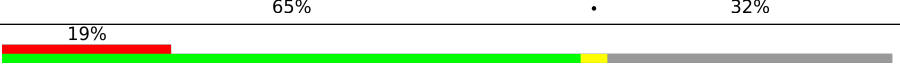
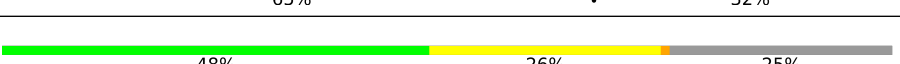
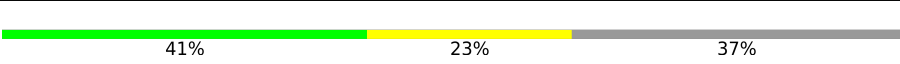
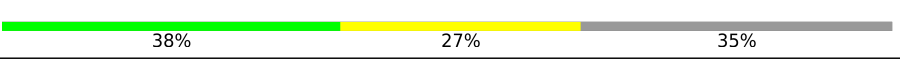
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	E	920	
1	F	920	
1	G	920	
1	H	920	

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Mol	Chain	Length	Quality of chain
1	K	920	
1	L	920	
1	M	920	
1	N	920	
2	I	777	
2	J	777	
2	O	777	
2	P	777	
3	A	264	
3	B	264	
4	C	237	
4	D	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 38368 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 family gene 2 protein homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	526	Total	C	N	O	S	0	0
			4056	2577	711	751	17		
1	L	545	Total	C	N	O	S	0	0
			4226	2686	741	782	17		
1	M	526	Total	C	N	O	S	0	0
			4056	2578	712	749	17		
1	N	546	Total	C	N	O	S	0	0
			4228	2686	742	783	17		
1	E	182	Total	C	N	O	S	0	0
			1392	886	233	263	10		
1	F	175	Total	C	N	O	S	0	0
			1346	858	225	253	10		
1	G	180	Total	C	N	O	S	0	0
			1379	879	231	259	10		
1	H	177	Total	C	N	O	S	0	0
			1358	866	227	255	10		

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-26	MET	-	initiating methionine	UNP Q8NB90
K	-25	SER	-	expression tag	UNP Q8NB90
K	-24	TYR	-	expression tag	UNP Q8NB90
K	-23	TYR	-	expression tag	UNP Q8NB90
K	-22	HIS	-	expression tag	UNP Q8NB90
K	-21	HIS	-	expression tag	UNP Q8NB90
K	-20	HIS	-	expression tag	UNP Q8NB90
K	-19	HIS	-	expression tag	UNP Q8NB90
K	-18	HIS	-	expression tag	UNP Q8NB90
K	-17	HIS	-	expression tag	UNP Q8NB90
K	-16	ASP	-	expression tag	UNP Q8NB90
K	-15	TYR	-	expression tag	UNP Q8NB90
K	-14	ASP	-	expression tag	UNP Q8NB90
K	-13	ILE	-	expression tag	UNP Q8NB90

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-12	PRO	-	expression tag	UNP Q8NB90
K	-11	THR	-	expression tag	UNP Q8NB90
K	-10	THR	-	expression tag	UNP Q8NB90
K	-9	GLU	-	expression tag	UNP Q8NB90
K	-8	ASN	-	expression tag	UNP Q8NB90
K	-7	LEU	-	expression tag	UNP Q8NB90
K	-6	TYR	-	expression tag	UNP Q8NB90
K	-5	PHE	-	expression tag	UNP Q8NB90
K	-4	GLN	-	expression tag	UNP Q8NB90
K	-3	GLY	-	expression tag	UNP Q8NB90
K	-2	ALA	-	expression tag	UNP Q8NB90
K	-1	MET	-	expression tag	UNP Q8NB90
K	0	GLY	-	expression tag	UNP Q8NB90
L	-26	MET	-	initiating methionine	UNP Q8NB90
L	-25	SER	-	expression tag	UNP Q8NB90
L	-24	TYR	-	expression tag	UNP Q8NB90
L	-23	TYR	-	expression tag	UNP Q8NB90
L	-22	HIS	-	expression tag	UNP Q8NB90
L	-21	HIS	-	expression tag	UNP Q8NB90
L	-20	HIS	-	expression tag	UNP Q8NB90
L	-19	HIS	-	expression tag	UNP Q8NB90
L	-18	HIS	-	expression tag	UNP Q8NB90
L	-17	HIS	-	expression tag	UNP Q8NB90
L	-16	ASP	-	expression tag	UNP Q8NB90
L	-15	TYR	-	expression tag	UNP Q8NB90
L	-14	ASP	-	expression tag	UNP Q8NB90
L	-13	ILE	-	expression tag	UNP Q8NB90
L	-12	PRO	-	expression tag	UNP Q8NB90
L	-11	THR	-	expression tag	UNP Q8NB90
L	-10	THR	-	expression tag	UNP Q8NB90
L	-9	GLU	-	expression tag	UNP Q8NB90
L	-8	ASN	-	expression tag	UNP Q8NB90
L	-7	LEU	-	expression tag	UNP Q8NB90
L	-6	TYR	-	expression tag	UNP Q8NB90
L	-5	PHE	-	expression tag	UNP Q8NB90
L	-4	GLN	-	expression tag	UNP Q8NB90
L	-3	GLY	-	expression tag	UNP Q8NB90
L	-2	ALA	-	expression tag	UNP Q8NB90
L	-1	MET	-	expression tag	UNP Q8NB90
L	0	GLY	-	expression tag	UNP Q8NB90
M	-26	MET	-	initiating methionine	UNP Q8NB90
M	-25	SER	-	expression tag	UNP Q8NB90

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-24	TYR	-	expression tag	UNP Q8NB90
M	-23	TYR	-	expression tag	UNP Q8NB90
M	-22	HIS	-	expression tag	UNP Q8NB90
M	-21	HIS	-	expression tag	UNP Q8NB90
M	-20	HIS	-	expression tag	UNP Q8NB90
M	-19	HIS	-	expression tag	UNP Q8NB90
M	-18	HIS	-	expression tag	UNP Q8NB90
M	-17	HIS	-	expression tag	UNP Q8NB90
M	-16	ASP	-	expression tag	UNP Q8NB90
M	-15	TYR	-	expression tag	UNP Q8NB90
M	-14	ASP	-	expression tag	UNP Q8NB90
M	-13	ILE	-	expression tag	UNP Q8NB90
M	-12	PRO	-	expression tag	UNP Q8NB90
M	-11	THR	-	expression tag	UNP Q8NB90
M	-10	THR	-	expression tag	UNP Q8NB90
M	-9	GLU	-	expression tag	UNP Q8NB90
M	-8	ASN	-	expression tag	UNP Q8NB90
M	-7	LEU	-	expression tag	UNP Q8NB90
M	-6	TYR	-	expression tag	UNP Q8NB90
M	-5	PHE	-	expression tag	UNP Q8NB90
M	-4	GLN	-	expression tag	UNP Q8NB90
M	-3	GLY	-	expression tag	UNP Q8NB90
M	-2	ALA	-	expression tag	UNP Q8NB90
M	-1	MET	-	expression tag	UNP Q8NB90
M	0	GLY	-	expression tag	UNP Q8NB90
N	-26	MET	-	initiating methionine	UNP Q8NB90
N	-25	SER	-	expression tag	UNP Q8NB90
N	-24	TYR	-	expression tag	UNP Q8NB90
N	-23	TYR	-	expression tag	UNP Q8NB90
N	-22	HIS	-	expression tag	UNP Q8NB90
N	-21	HIS	-	expression tag	UNP Q8NB90
N	-20	HIS	-	expression tag	UNP Q8NB90
N	-19	HIS	-	expression tag	UNP Q8NB90
N	-18	HIS	-	expression tag	UNP Q8NB90
N	-17	HIS	-	expression tag	UNP Q8NB90
N	-16	ASP	-	expression tag	UNP Q8NB90
N	-15	TYR	-	expression tag	UNP Q8NB90
N	-14	ASP	-	expression tag	UNP Q8NB90
N	-13	ILE	-	expression tag	UNP Q8NB90
N	-12	PRO	-	expression tag	UNP Q8NB90
N	-11	THR	-	expression tag	UNP Q8NB90
N	-10	THR	-	expression tag	UNP Q8NB90

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-9	GLU	-	expression tag	UNP Q8NB90
N	-8	ASN	-	expression tag	UNP Q8NB90
N	-7	LEU	-	expression tag	UNP Q8NB90
N	-6	TYR	-	expression tag	UNP Q8NB90
N	-5	PHE	-	expression tag	UNP Q8NB90
N	-4	GLN	-	expression tag	UNP Q8NB90
N	-3	GLY	-	expression tag	UNP Q8NB90
N	-2	ALA	-	expression tag	UNP Q8NB90
N	-1	MET	-	expression tag	UNP Q8NB90
N	0	GLY	-	expression tag	UNP Q8NB90
E	-26	MET	-	initiating methionine	UNP Q8NB90
E	-25	SER	-	expression tag	UNP Q8NB90
E	-24	TYR	-	expression tag	UNP Q8NB90
E	-23	TYR	-	expression tag	UNP Q8NB90
E	-22	HIS	-	expression tag	UNP Q8NB90
E	-21	HIS	-	expression tag	UNP Q8NB90
E	-20	HIS	-	expression tag	UNP Q8NB90
E	-19	HIS	-	expression tag	UNP Q8NB90
E	-18	HIS	-	expression tag	UNP Q8NB90
E	-17	HIS	-	expression tag	UNP Q8NB90
E	-16	ASP	-	expression tag	UNP Q8NB90
E	-15	TYR	-	expression tag	UNP Q8NB90
E	-14	ASP	-	expression tag	UNP Q8NB90
E	-13	ILE	-	expression tag	UNP Q8NB90
E	-12	PRO	-	expression tag	UNP Q8NB90
E	-11	THR	-	expression tag	UNP Q8NB90
E	-10	THR	-	expression tag	UNP Q8NB90
E	-9	GLU	-	expression tag	UNP Q8NB90
E	-8	ASN	-	expression tag	UNP Q8NB90
E	-7	LEU	-	expression tag	UNP Q8NB90
E	-6	TYR	-	expression tag	UNP Q8NB90
E	-5	PHE	-	expression tag	UNP Q8NB90
E	-4	GLN	-	expression tag	UNP Q8NB90
E	-3	GLY	-	expression tag	UNP Q8NB90
E	-2	ALA	-	expression tag	UNP Q8NB90
E	-1	MET	-	expression tag	UNP Q8NB90
E	0	GLY	-	expression tag	UNP Q8NB90
F	-26	MET	-	initiating methionine	UNP Q8NB90
F	-25	SER	-	expression tag	UNP Q8NB90
F	-24	TYR	-	expression tag	UNP Q8NB90
F	-23	TYR	-	expression tag	UNP Q8NB90
F	-22	HIS	-	expression tag	UNP Q8NB90

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-21	HIS	-	expression tag	UNP Q8NB90
F	-20	HIS	-	expression tag	UNP Q8NB90
F	-19	HIS	-	expression tag	UNP Q8NB90
F	-18	HIS	-	expression tag	UNP Q8NB90
F	-17	HIS	-	expression tag	UNP Q8NB90
F	-16	ASP	-	expression tag	UNP Q8NB90
F	-15	TYR	-	expression tag	UNP Q8NB90
F	-14	ASP	-	expression tag	UNP Q8NB90
F	-13	ILE	-	expression tag	UNP Q8NB90
F	-12	PRO	-	expression tag	UNP Q8NB90
F	-11	THR	-	expression tag	UNP Q8NB90
F	-10	THR	-	expression tag	UNP Q8NB90
F	-9	GLU	-	expression tag	UNP Q8NB90
F	-8	ASN	-	expression tag	UNP Q8NB90
F	-7	LEU	-	expression tag	UNP Q8NB90
F	-6	TYR	-	expression tag	UNP Q8NB90
F	-5	PHE	-	expression tag	UNP Q8NB90
F	-4	GLN	-	expression tag	UNP Q8NB90
F	-3	GLY	-	expression tag	UNP Q8NB90
F	-2	ALA	-	expression tag	UNP Q8NB90
F	-1	MET	-	expression tag	UNP Q8NB90
F	0	GLY	-	expression tag	UNP Q8NB90
G	-26	MET	-	initiating methionine	UNP Q8NB90
G	-25	SER	-	expression tag	UNP Q8NB90
G	-24	TYR	-	expression tag	UNP Q8NB90
G	-23	TYR	-	expression tag	UNP Q8NB90
G	-22	HIS	-	expression tag	UNP Q8NB90
G	-21	HIS	-	expression tag	UNP Q8NB90
G	-20	HIS	-	expression tag	UNP Q8NB90
G	-19	HIS	-	expression tag	UNP Q8NB90
G	-18	HIS	-	expression tag	UNP Q8NB90
G	-17	HIS	-	expression tag	UNP Q8NB90
G	-16	ASP	-	expression tag	UNP Q8NB90
G	-15	TYR	-	expression tag	UNP Q8NB90
G	-14	ASP	-	expression tag	UNP Q8NB90
G	-13	ILE	-	expression tag	UNP Q8NB90
G	-12	PRO	-	expression tag	UNP Q8NB90
G	-11	THR	-	expression tag	UNP Q8NB90
G	-10	THR	-	expression tag	UNP Q8NB90
G	-9	GLU	-	expression tag	UNP Q8NB90
G	-8	ASN	-	expression tag	UNP Q8NB90
G	-7	LEU	-	expression tag	UNP Q8NB90

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	TYR	-	expression tag	UNP Q8NB90
G	-5	PHE	-	expression tag	UNP Q8NB90
G	-4	GLN	-	expression tag	UNP Q8NB90
G	-3	GLY	-	expression tag	UNP Q8NB90
G	-2	ALA	-	expression tag	UNP Q8NB90
G	-1	MET	-	expression tag	UNP Q8NB90
G	0	GLY	-	expression tag	UNP Q8NB90
H	-26	MET	-	initiating methionine	UNP Q8NB90
H	-25	SER	-	expression tag	UNP Q8NB90
H	-24	TYR	-	expression tag	UNP Q8NB90
H	-23	TYR	-	expression tag	UNP Q8NB90
H	-22	HIS	-	expression tag	UNP Q8NB90
H	-21	HIS	-	expression tag	UNP Q8NB90
H	-20	HIS	-	expression tag	UNP Q8NB90
H	-19	HIS	-	expression tag	UNP Q8NB90
H	-18	HIS	-	expression tag	UNP Q8NB90
H	-17	HIS	-	expression tag	UNP Q8NB90
H	-16	ASP	-	expression tag	UNP Q8NB90
H	-15	TYR	-	expression tag	UNP Q8NB90
H	-14	ASP	-	expression tag	UNP Q8NB90
H	-13	ILE	-	expression tag	UNP Q8NB90
H	-12	PRO	-	expression tag	UNP Q8NB90
H	-11	THR	-	expression tag	UNP Q8NB90
H	-10	THR	-	expression tag	UNP Q8NB90
H	-9	GLU	-	expression tag	UNP Q8NB90
H	-8	ASN	-	expression tag	UNP Q8NB90
H	-7	LEU	-	expression tag	UNP Q8NB90
H	-6	TYR	-	expression tag	UNP Q8NB90
H	-5	PHE	-	expression tag	UNP Q8NB90
H	-4	GLN	-	expression tag	UNP Q8NB90
H	-3	GLY	-	expression tag	UNP Q8NB90
H	-2	ALA	-	expression tag	UNP Q8NB90
H	-1	MET	-	expression tag	UNP Q8NB90
H	0	GLY	-	expression tag	UNP Q8NB90

- Molecule 2 is a protein called ATPase family gene 2 protein homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	527	Total	C	N	O	S	0	0
			4016	2541	705	753	17		
2	P	529	Total	C	N	O	S	0	0
			4027	2549	707	753	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	183	Total	C	N	O	S	0	0
			1320	825	259	231	5		
2	J	181	Total	C	N	O	S	0	0
			1306	817	257	227	5		

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-23	MET	-	initiating methionine	UNP Q9BVQ7
O	-22	ASP	-	expression tag	UNP Q9BVQ7
O	-21	TYR	-	expression tag	UNP Q9BVQ7
O	-20	LYS	-	expression tag	UNP Q9BVQ7
O	-19	ASP	-	expression tag	UNP Q9BVQ7
O	-18	ASP	-	expression tag	UNP Q9BVQ7
O	-17	ASP	-	expression tag	UNP Q9BVQ7
O	-16	ASP	-	expression tag	UNP Q9BVQ7
O	-15	LYS	-	expression tag	UNP Q9BVQ7
O	-14	GLY	-	expression tag	UNP Q9BVQ7
O	-13	GLY	-	expression tag	UNP Q9BVQ7
O	-12	GLY	-	expression tag	UNP Q9BVQ7
O	-11	SER	-	expression tag	UNP Q9BVQ7
O	-10	GLU	-	expression tag	UNP Q9BVQ7
O	-9	ASN	-	expression tag	UNP Q9BVQ7
O	-8	LEU	-	expression tag	UNP Q9BVQ7
O	-7	TYR	-	expression tag	UNP Q9BVQ7
O	-6	PHE	-	expression tag	UNP Q9BVQ7
O	-5	GLN	-	expression tag	UNP Q9BVQ7
O	-4	GLY	-	expression tag	UNP Q9BVQ7
O	-3	ALA	-	expression tag	UNP Q9BVQ7
O	-2	GLY	-	expression tag	UNP Q9BVQ7
O	-1	SER	-	expression tag	UNP Q9BVQ7
O	0	THR	-	expression tag	UNP Q9BVQ7
P	-23	MET	-	initiating methionine	UNP Q9BVQ7
P	-22	ASP	-	expression tag	UNP Q9BVQ7
P	-21	TYR	-	expression tag	UNP Q9BVQ7
P	-20	LYS	-	expression tag	UNP Q9BVQ7
P	-19	ASP	-	expression tag	UNP Q9BVQ7
P	-18	ASP	-	expression tag	UNP Q9BVQ7
P	-17	ASP	-	expression tag	UNP Q9BVQ7
P	-16	ASP	-	expression tag	UNP Q9BVQ7
P	-15	LYS	-	expression tag	UNP Q9BVQ7
P	-14	GLY	-	expression tag	UNP Q9BVQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-13	GLY	-	expression tag	UNP Q9BVQ7
P	-12	GLY	-	expression tag	UNP Q9BVQ7
P	-11	SER	-	expression tag	UNP Q9BVQ7
P	-10	GLU	-	expression tag	UNP Q9BVQ7
P	-9	ASN	-	expression tag	UNP Q9BVQ7
P	-8	LEU	-	expression tag	UNP Q9BVQ7
P	-7	TYR	-	expression tag	UNP Q9BVQ7
P	-6	PHE	-	expression tag	UNP Q9BVQ7
P	-5	GLN	-	expression tag	UNP Q9BVQ7
P	-4	GLY	-	expression tag	UNP Q9BVQ7
P	-3	ALA	-	expression tag	UNP Q9BVQ7
P	-2	GLY	-	expression tag	UNP Q9BVQ7
P	-1	SER	-	expression tag	UNP Q9BVQ7
P	0	THR	-	expression tag	UNP Q9BVQ7
I	-23	MET	-	initiating methionine	UNP Q9BVQ7
I	-22	ASP	-	expression tag	UNP Q9BVQ7
I	-21	TYR	-	expression tag	UNP Q9BVQ7
I	-20	LYS	-	expression tag	UNP Q9BVQ7
I	-19	ASP	-	expression tag	UNP Q9BVQ7
I	-18	ASP	-	expression tag	UNP Q9BVQ7
I	-17	ASP	-	expression tag	UNP Q9BVQ7
I	-16	ASP	-	expression tag	UNP Q9BVQ7
I	-15	LYS	-	expression tag	UNP Q9BVQ7
I	-14	GLY	-	expression tag	UNP Q9BVQ7
I	-13	GLY	-	expression tag	UNP Q9BVQ7
I	-12	GLY	-	expression tag	UNP Q9BVQ7
I	-11	SER	-	expression tag	UNP Q9BVQ7
I	-10	GLU	-	expression tag	UNP Q9BVQ7
I	-9	ASN	-	expression tag	UNP Q9BVQ7
I	-8	LEU	-	expression tag	UNP Q9BVQ7
I	-7	TYR	-	expression tag	UNP Q9BVQ7
I	-6	PHE	-	expression tag	UNP Q9BVQ7
I	-5	GLN	-	expression tag	UNP Q9BVQ7
I	-4	GLY	-	expression tag	UNP Q9BVQ7
I	-3	ALA	-	expression tag	UNP Q9BVQ7
I	-2	GLY	-	expression tag	UNP Q9BVQ7
I	-1	SER	-	expression tag	UNP Q9BVQ7
I	0	THR	-	expression tag	UNP Q9BVQ7
J	-23	MET	-	initiating methionine	UNP Q9BVQ7
J	-22	ASP	-	expression tag	UNP Q9BVQ7
J	-21	TYR	-	expression tag	UNP Q9BVQ7
J	-20	LYS	-	expression tag	UNP Q9BVQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-19	ASP	-	expression tag	UNP Q9BVQ7
J	-18	ASP	-	expression tag	UNP Q9BVQ7
J	-17	ASP	-	expression tag	UNP Q9BVQ7
J	-16	ASP	-	expression tag	UNP Q9BVQ7
J	-15	LYS	-	expression tag	UNP Q9BVQ7
J	-14	GLY	-	expression tag	UNP Q9BVQ7
J	-13	GLY	-	expression tag	UNP Q9BVQ7
J	-12	GLY	-	expression tag	UNP Q9BVQ7
J	-11	SER	-	expression tag	UNP Q9BVQ7
J	-10	GLU	-	expression tag	UNP Q9BVQ7
J	-9	ASN	-	expression tag	UNP Q9BVQ7
J	-8	LEU	-	expression tag	UNP Q9BVQ7
J	-7	TYR	-	expression tag	UNP Q9BVQ7
J	-6	PHE	-	expression tag	UNP Q9BVQ7
J	-5	GLN	-	expression tag	UNP Q9BVQ7
J	-4	GLY	-	expression tag	UNP Q9BVQ7
J	-3	ALA	-	expression tag	UNP Q9BVQ7
J	-2	GLY	-	expression tag	UNP Q9BVQ7
J	-1	SER	-	expression tag	UNP Q9BVQ7
J	0	THR	-	expression tag	UNP Q9BVQ7

- Molecule 3 is a protein called cDNA FLJ55172.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	198	Total	C	N	O	S	0	0
			1604	1022	284	294	4		
3	B	196	Total	C	N	O	S	0	0
			1585	1012	279	290	4		

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-60	MET	-	initiating methionine	UNP B4DRQ5
A	-59	SER	-	expression tag	UNP B4DRQ5
A	-58	ALA	-	expression tag	UNP B4DRQ5
A	-57	TRP	-	expression tag	UNP B4DRQ5
A	-56	SER	-	expression tag	UNP B4DRQ5
A	-55	HIS	-	expression tag	UNP B4DRQ5
A	-54	PRO	-	expression tag	UNP B4DRQ5
A	-53	GLN	-	expression tag	UNP B4DRQ5
A	-52	PHE	-	expression tag	UNP B4DRQ5
A	-51	GLU	-	expression tag	UNP B4DRQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-50	LYS	-	expression tag	UNP B4DRQ5
A	-49	GLY	-	expression tag	UNP B4DRQ5
A	-48	GLY	-	expression tag	UNP B4DRQ5
A	-47	GLY	-	expression tag	UNP B4DRQ5
A	-46	SER	-	expression tag	UNP B4DRQ5
A	-45	GLY	-	expression tag	UNP B4DRQ5
A	-44	GLY	-	expression tag	UNP B4DRQ5
A	-43	GLY	-	expression tag	UNP B4DRQ5
A	-42	SER	-	expression tag	UNP B4DRQ5
A	-41	GLY	-	expression tag	UNP B4DRQ5
A	-40	GLY	-	expression tag	UNP B4DRQ5
A	-39	SER	-	expression tag	UNP B4DRQ5
A	-38	ALA	-	expression tag	UNP B4DRQ5
A	-37	TRP	-	expression tag	UNP B4DRQ5
A	-36	SER	-	expression tag	UNP B4DRQ5
A	-35	HIS	-	expression tag	UNP B4DRQ5
A	-34	PRO	-	expression tag	UNP B4DRQ5
A	-33	GLN	-	expression tag	UNP B4DRQ5
A	-32	PHE	-	expression tag	UNP B4DRQ5
A	-31	GLU	-	expression tag	UNP B4DRQ5
A	-30	LYS	-	expression tag	UNP B4DRQ5
A	-29	GLY	-	expression tag	UNP B4DRQ5
A	-28	ALA	-	expression tag	UNP B4DRQ5
A	-27	GLY	-	expression tag	UNP B4DRQ5
A	-26	SER	-	expression tag	UNP B4DRQ5
A	-25	GLU	-	expression tag	UNP B4DRQ5
A	-24	ASN	-	expression tag	UNP B4DRQ5
A	-23	LEU	-	expression tag	UNP B4DRQ5
A	-22	TYR	-	expression tag	UNP B4DRQ5
A	-21	PHE	-	expression tag	UNP B4DRQ5
A	-20	GLN	-	expression tag	UNP B4DRQ5
A	-19	GLY	-	expression tag	UNP B4DRQ5
A	-18	ALA	-	expression tag	UNP B4DRQ5
A	-17	GLY	-	expression tag	UNP B4DRQ5
A	-16	SER	-	expression tag	UNP B4DRQ5
A	-15	ASP	-	expression tag	UNP B4DRQ5
A	-14	SER	-	expression tag	UNP B4DRQ5
A	-13	LEU	-	expression tag	UNP B4DRQ5
A	-12	GLU	-	expression tag	UNP B4DRQ5
A	-11	PHE	-	expression tag	UNP B4DRQ5
A	-10	ILE	-	expression tag	UNP B4DRQ5
A	-9	ALA	-	expression tag	UNP B4DRQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	SER	-	expression tag	UNP B4DRQ5
A	-7	LYS	-	expression tag	UNP B4DRQ5
A	-6	LEU	-	expression tag	UNP B4DRQ5
A	-5	ALA	-	expression tag	UNP B4DRQ5
A	-4	GLY	-	expression tag	UNP B4DRQ5
A	-3	GLY	-	expression tag	UNP B4DRQ5
A	-2	GLY	-	expression tag	UNP B4DRQ5
A	-1	SER	-	expression tag	UNP B4DRQ5
A	0	THR	-	expression tag	UNP B4DRQ5
B	-60	MET	-	initiating methionine	UNP B4DRQ5
B	-59	SER	-	expression tag	UNP B4DRQ5
B	-58	ALA	-	expression tag	UNP B4DRQ5
B	-57	TRP	-	expression tag	UNP B4DRQ5
B	-56	SER	-	expression tag	UNP B4DRQ5
B	-55	HIS	-	expression tag	UNP B4DRQ5
B	-54	PRO	-	expression tag	UNP B4DRQ5
B	-53	GLN	-	expression tag	UNP B4DRQ5
B	-52	PHE	-	expression tag	UNP B4DRQ5
B	-51	GLU	-	expression tag	UNP B4DRQ5
B	-50	LYS	-	expression tag	UNP B4DRQ5
B	-49	GLY	-	expression tag	UNP B4DRQ5
B	-48	GLY	-	expression tag	UNP B4DRQ5
B	-47	GLY	-	expression tag	UNP B4DRQ5
B	-46	SER	-	expression tag	UNP B4DRQ5
B	-45	GLY	-	expression tag	UNP B4DRQ5
B	-44	GLY	-	expression tag	UNP B4DRQ5
B	-43	GLY	-	expression tag	UNP B4DRQ5
B	-42	SER	-	expression tag	UNP B4DRQ5
B	-41	GLY	-	expression tag	UNP B4DRQ5
B	-40	GLY	-	expression tag	UNP B4DRQ5
B	-39	SER	-	expression tag	UNP B4DRQ5
B	-38	ALA	-	expression tag	UNP B4DRQ5
B	-37	TRP	-	expression tag	UNP B4DRQ5
B	-36	SER	-	expression tag	UNP B4DRQ5
B	-35	HIS	-	expression tag	UNP B4DRQ5
B	-34	PRO	-	expression tag	UNP B4DRQ5
B	-33	GLN	-	expression tag	UNP B4DRQ5
B	-32	PHE	-	expression tag	UNP B4DRQ5
B	-31	GLU	-	expression tag	UNP B4DRQ5
B	-30	LYS	-	expression tag	UNP B4DRQ5
B	-29	GLY	-	expression tag	UNP B4DRQ5
B	-28	ALA	-	expression tag	UNP B4DRQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	GLY	-	expression tag	UNP B4DRQ5
B	-26	SER	-	expression tag	UNP B4DRQ5
B	-25	GLU	-	expression tag	UNP B4DRQ5
B	-24	ASN	-	expression tag	UNP B4DRQ5
B	-23	LEU	-	expression tag	UNP B4DRQ5
B	-22	TYR	-	expression tag	UNP B4DRQ5
B	-21	PHE	-	expression tag	UNP B4DRQ5
B	-20	GLN	-	expression tag	UNP B4DRQ5
B	-19	GLY	-	expression tag	UNP B4DRQ5
B	-18	ALA	-	expression tag	UNP B4DRQ5
B	-17	GLY	-	expression tag	UNP B4DRQ5
B	-16	SER	-	expression tag	UNP B4DRQ5
B	-15	ASP	-	expression tag	UNP B4DRQ5
B	-14	SER	-	expression tag	UNP B4DRQ5
B	-13	LEU	-	expression tag	UNP B4DRQ5
B	-12	GLU	-	expression tag	UNP B4DRQ5
B	-11	PHE	-	expression tag	UNP B4DRQ5
B	-10	ILE	-	expression tag	UNP B4DRQ5
B	-9	ALA	-	expression tag	UNP B4DRQ5
B	-8	SER	-	expression tag	UNP B4DRQ5
B	-7	LYS	-	expression tag	UNP B4DRQ5
B	-6	LEU	-	expression tag	UNP B4DRQ5
B	-5	ALA	-	expression tag	UNP B4DRQ5
B	-4	GLY	-	expression tag	UNP B4DRQ5
B	-3	GLY	-	expression tag	UNP B4DRQ5
B	-2	GLY	-	expression tag	UNP B4DRQ5
B	-1	SER	-	expression tag	UNP B4DRQ5
B	0	THR	-	expression tag	UNP B4DRQ5

- Molecule 4 is a protein called Cyclin-dependent kinase 2-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	150	Total	C	N	O	S	0	0
			1211	769	202	234	6		
4	D	155	Total	C	N	O	S	0	0
			1258	802	209	241	6		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-24	MET	-	initiating methionine	UNP Q9BW66
C	-23	SER	-	expression tag	UNP Q9BW66

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-22	TYR	-	expression tag	UNP Q9BW66
C	-21	TYR	-	expression tag	UNP Q9BW66
C	-20	HIS	-	expression tag	UNP Q9BW66
C	-19	HIS	-	expression tag	UNP Q9BW66
C	-18	HIS	-	expression tag	UNP Q9BW66
C	-17	HIS	-	expression tag	UNP Q9BW66
C	-16	HIS	-	expression tag	UNP Q9BW66
C	-15	HIS	-	expression tag	UNP Q9BW66
C	-14	ASP	-	expression tag	UNP Q9BW66
C	-13	TYR	-	expression tag	UNP Q9BW66
C	-12	ASP	-	expression tag	UNP Q9BW66
C	-11	ILE	-	expression tag	UNP Q9BW66
C	-10	PRO	-	expression tag	UNP Q9BW66
C	-9	THR	-	expression tag	UNP Q9BW66
C	-8	THR	-	expression tag	UNP Q9BW66
C	-7	GLU	-	expression tag	UNP Q9BW66
C	-6	ASN	-	expression tag	UNP Q9BW66
C	-5	LEU	-	expression tag	UNP Q9BW66
C	-4	TYR	-	expression tag	UNP Q9BW66
C	-3	PHE	-	expression tag	UNP Q9BW66
C	-2	GLN	-	expression tag	UNP Q9BW66
C	-1	GLY	-	expression tag	UNP Q9BW66
C	0	ALA	-	expression tag	UNP Q9BW66
D	-24	MET	-	initiating methionine	UNP Q9BW66
D	-23	SER	-	expression tag	UNP Q9BW66
D	-22	TYR	-	expression tag	UNP Q9BW66
D	-21	TYR	-	expression tag	UNP Q9BW66
D	-20	HIS	-	expression tag	UNP Q9BW66
D	-19	HIS	-	expression tag	UNP Q9BW66
D	-18	HIS	-	expression tag	UNP Q9BW66
D	-17	HIS	-	expression tag	UNP Q9BW66
D	-16	HIS	-	expression tag	UNP Q9BW66
D	-15	HIS	-	expression tag	UNP Q9BW66
D	-14	ASP	-	expression tag	UNP Q9BW66
D	-13	TYR	-	expression tag	UNP Q9BW66
D	-12	ASP	-	expression tag	UNP Q9BW66
D	-11	ILE	-	expression tag	UNP Q9BW66
D	-10	PRO	-	expression tag	UNP Q9BW66
D	-9	THR	-	expression tag	UNP Q9BW66
D	-8	THR	-	expression tag	UNP Q9BW66
D	-7	GLU	-	expression tag	UNP Q9BW66
D	-6	ASN	-	expression tag	UNP Q9BW66

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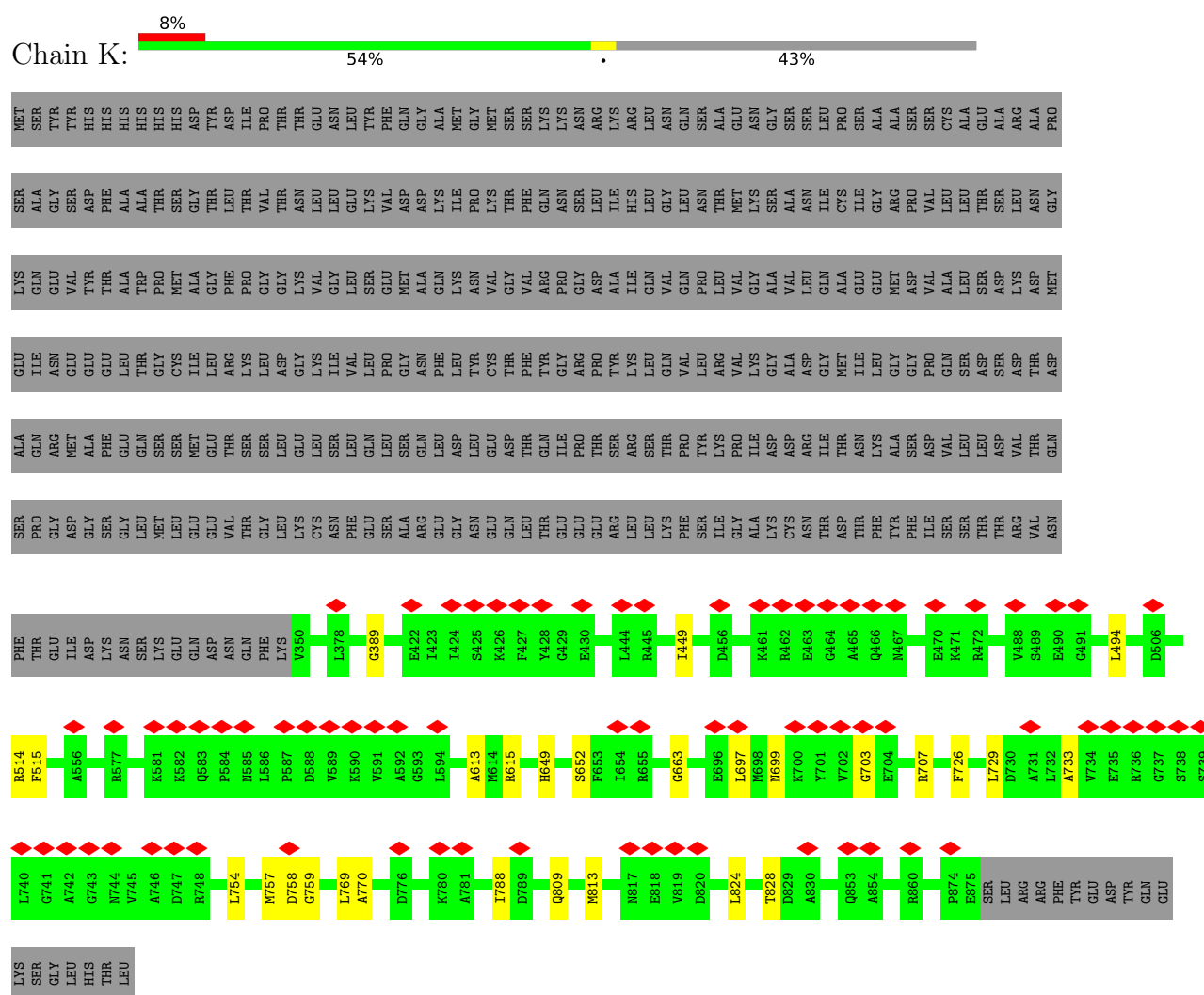
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	LEU	-	expression tag	UNP Q9BW66
D	-4	TYR	-	expression tag	UNP Q9BW66
D	-3	PHE	-	expression tag	UNP Q9BW66
D	-2	GLN	-	expression tag	UNP Q9BW66
D	-1	GLY	-	expression tag	UNP Q9BW66
D	0	ALA	-	expression tag	UNP Q9BW66

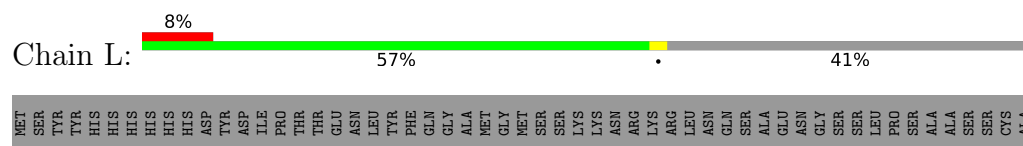
3 Residue-property plots

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 family gene 2 protein homolog A



- Molecule 1: ATPase family gene 2 protein homolog A



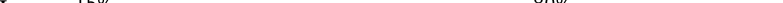
[illegible]

- Molecule 1: ATPase family gene 2 protein homolog A

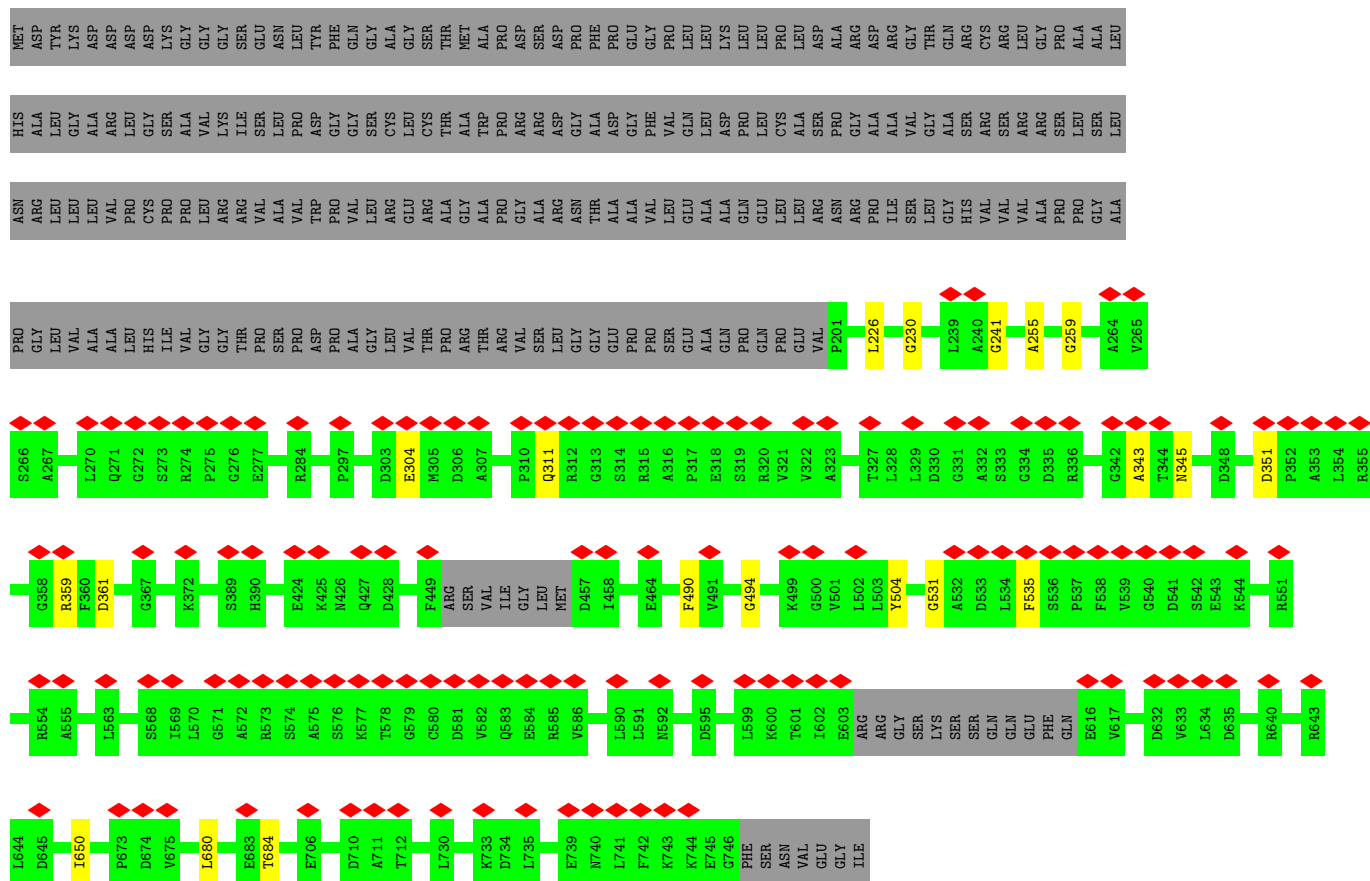
[illegible]

VAL	GLN	VAL	PHE	ILE	ASN	LEU
THR	PHE	LEU	LEU	GLY	GLU	ARG
PRO	HIS	ALA	ALA	GLY	ALA	ARG
ARG	SER	GLN	ILE	LEU	GLY	PRO
ILE	MET	LEU	LYS	GLU	LEU	GLY
PRO	PRO	LEU	GLY	SER	CYS	ARG
GLU	VAL	THR	PRO	ILE	ALA	PHE
SER	SER	THR	GLU	LYS	LEU	ASP
SER	ASN	MET	GLU	LEU	LEU	ASP
LEU	GLU	ASP	MET	LEU	ARG	LYS
ARG	VAL	ASP	ASN	GLY	ILE	ILE
PHE	ASP	ILE	LYS	LEU	LEU	GLU
TYR	LEU	GLU	TYR	GLN	LYS	ILE
ASP	GLU	GLN	VAL	ALA	GLY	GLY
GLU	GLU	LEU	GLY	VAL	GLN	VAL
TYR	LEU	LEU	GLU	GLU	PRO	PRO
GLN	ILE	ASP	SER	TRP	ASN	ASN
GLY	LEU	VAL	GLU	PRO	LEU	ALA
LYS	GLN	THR	ARG	LEU	PRO	GLN
SER	THR	ILE	ALA	LYS	ASP	ASP
GLY	ASP	LEU	VAL	HIS	VAL	ARG
LEU	ALA	LEU	ARG	PRO	LYS	LEU
HIS	TYR	ALA	GLU	GLU	VAL	ASP
THR	SER	THR	THR	SER	ALA	ILE
LEU	GLY	ASN	PHE	PHE	GLY	LEU
	ALA	PRO	ARG	ILE	LEU	GLN
	GLU	PRO	LYS	ARG	VAL	LYS
	ILE	ARG	ALA	MET	ASP	LEU
	VAL	ASP	ARG	GLY	ILE	LEU
	ALA	ILE	ALA	ILE	THR	ARG
	VAL	ASP	VAL	GLN	LEU	ARG
	CYS	LYS	ALA	PRO	LYS	VAL
	ARG	ALA	PRO	PRO	ASP	PRO
	GLU	LEU	SER	LYS	PHE	HIS
	ALA	MET	ILE	GLY	LEU	LEU
	ALA	ARG	ILE	VAL	GLN	LEU
	LEU	PRO	PHE	LEU	ALA	THR
	GLU	ASP	ASP	PRO	ILE	LEU
	GLU	ARG	ALA	PRO	ARG	LEU
	ILE	ILE	ASP	CYS	PRO	GLN
	ILE	TYR	GLN	SER	ALA	LEU
	ALA	VAL	VAL	LYS	MET	ASN
	ASN	PRO	GLU	THR	ARG	SER
	LEU	LEU	ARG	MET	GLU	ALA
	ILE	PRO	GLY	ILE	ILE	HIS
	MET	ASP	SER	ALA	GLY	TYR
	LYS	ALA	SER	LYS	ASP	VAL
	ARG	THR	GLY	ALA	VAL	GLY
	HIS	ARG	GLY	ALA	PRO	ALA
	PHE	ARG	GLY	ALA	ASN	ASP
	THR	ARG	GLN	ASN	VAL	VAL
	GLN	GLU	ASN	GLU	VAL	LYS
	ALA	ILE	VAL	SER	TRP	VAL
	LEU	PHE	ALA	GLY	LEU	LEU
	THR	LYS	ARG	ASN	SER	CYS

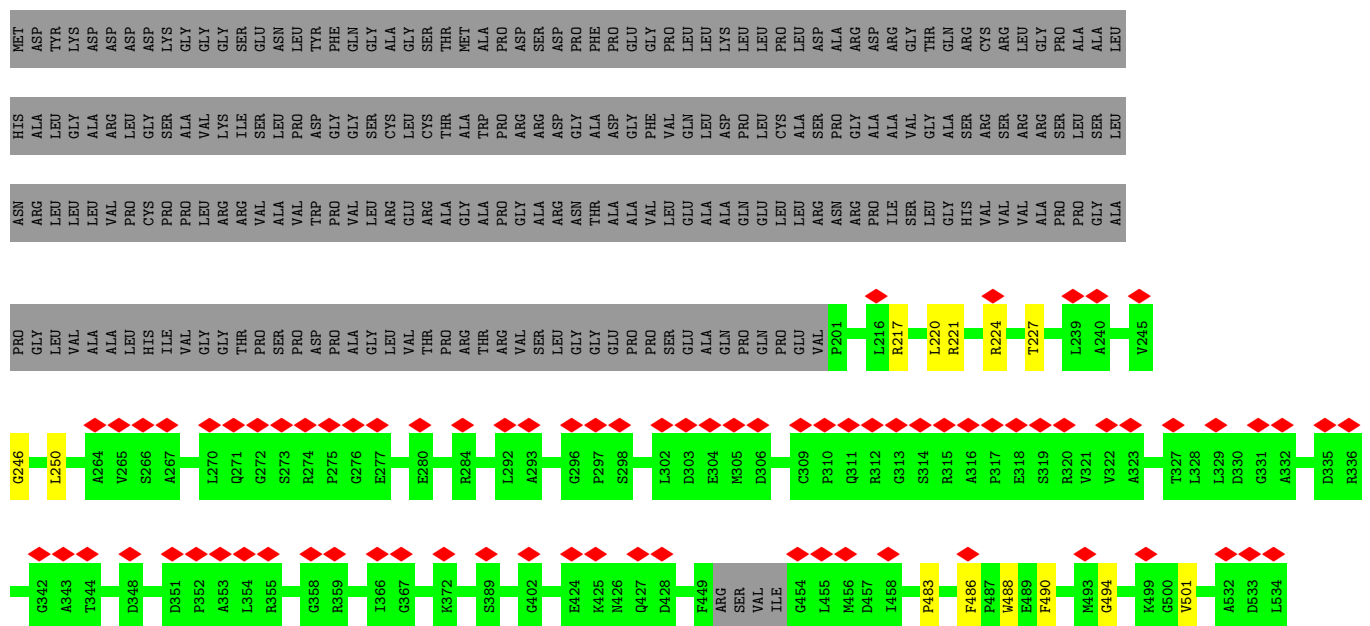
- Molecule 1: ATPase family gene 2 protein homolog A

Chain G:  15% 80%

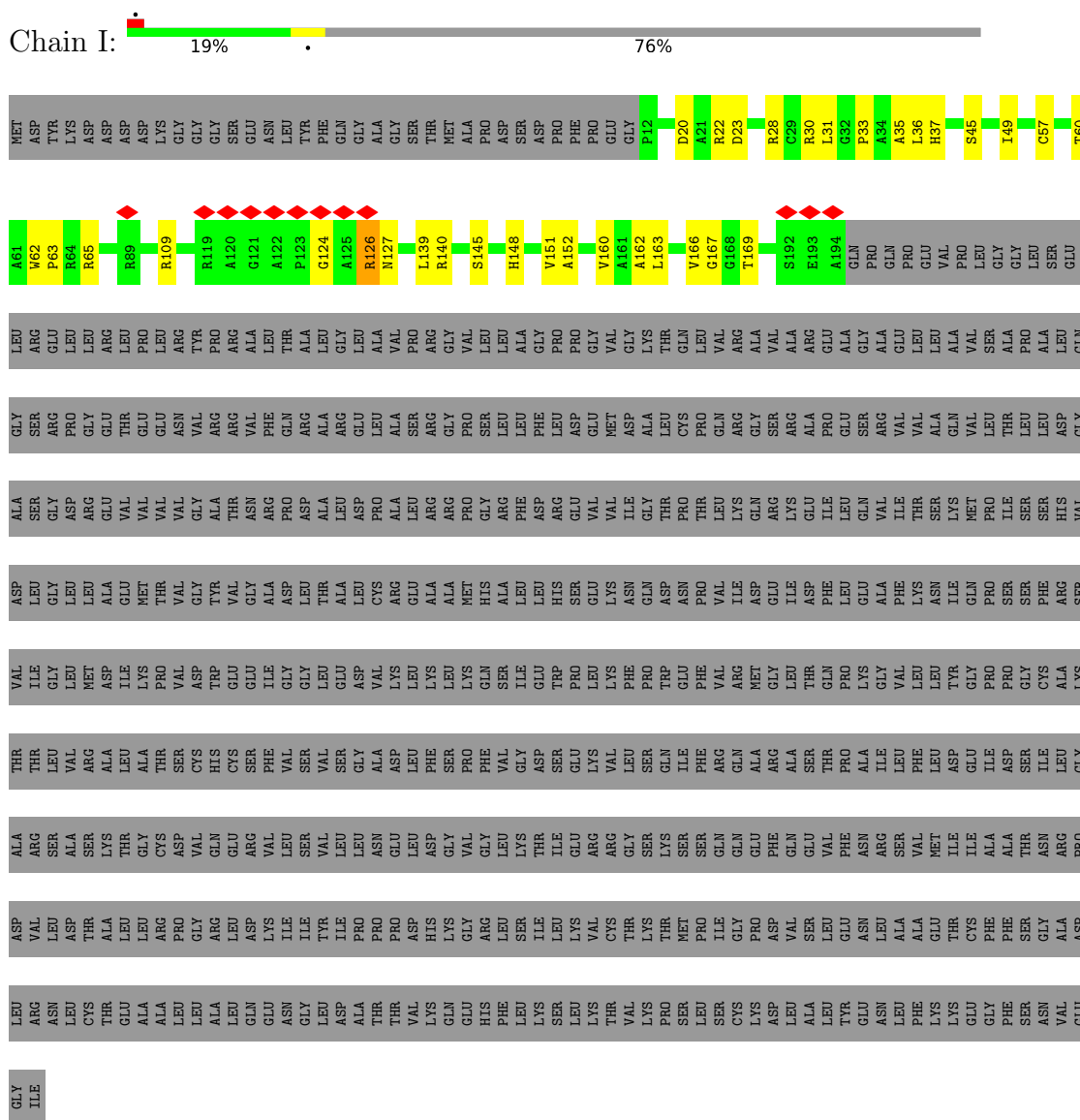
[illegible]



• Molecule 2: ATPase family gene 2 protein homolog B

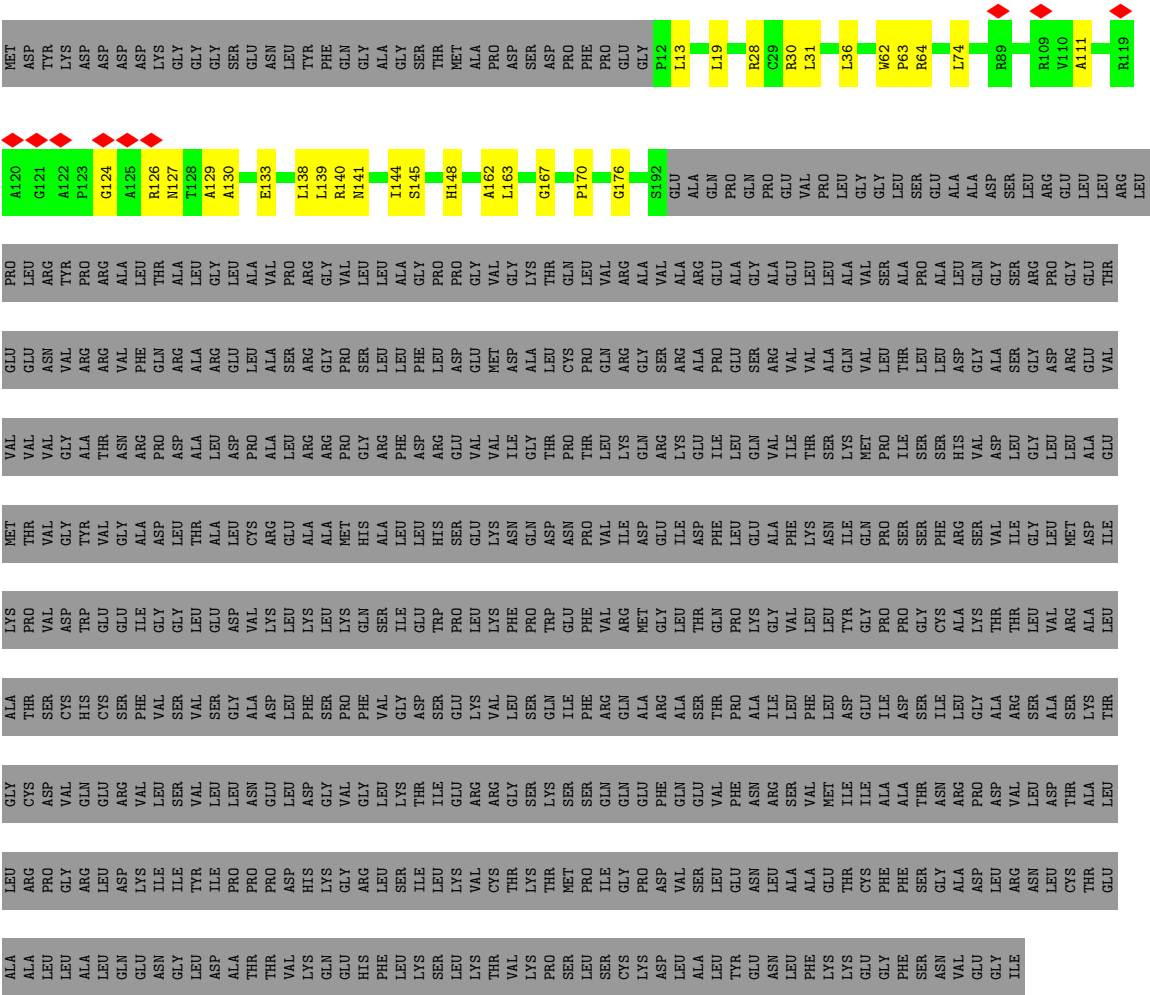


- Molecule 2: ATPase family gene 2 protein homolog B

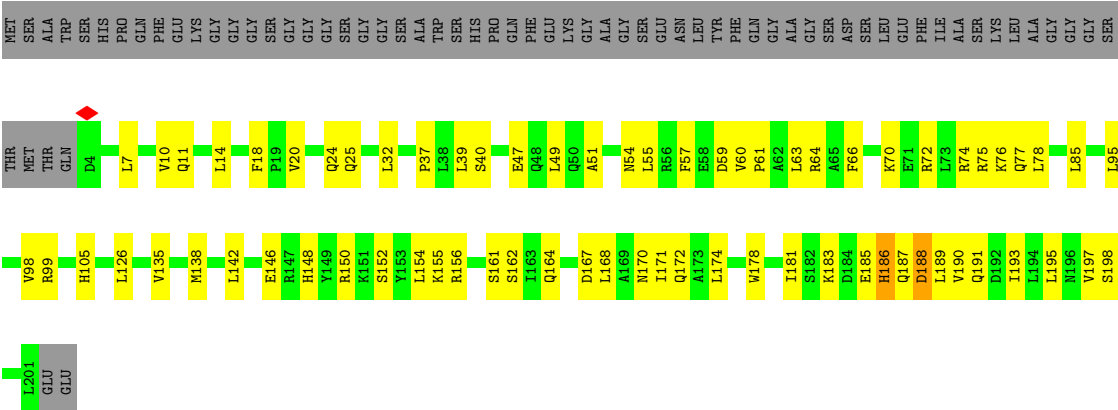


- Molecule 2: ATPase family gene 2 protein homolog B





● Molecule 3: cDNA FLJ55172

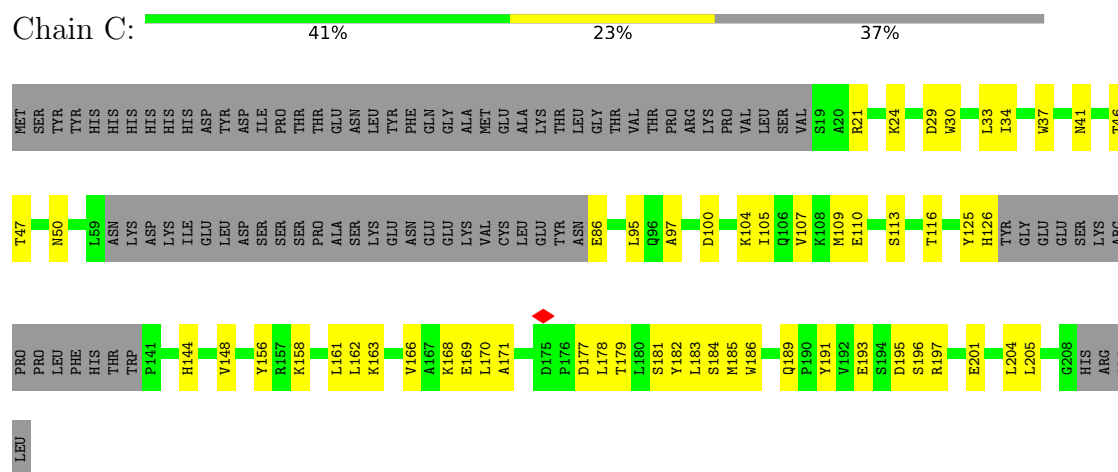


● Molecule 3: cDNA FLJ55172

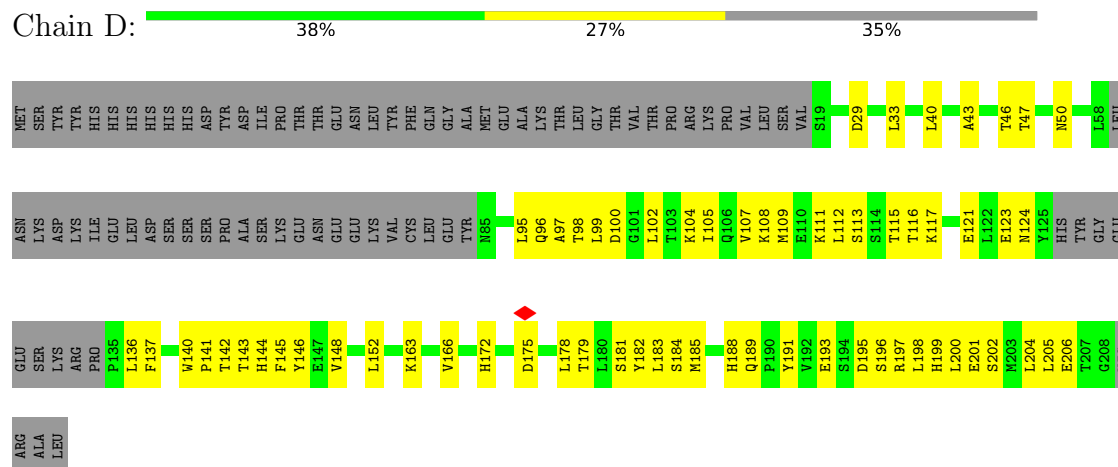




● Molecule 4: Cyclin-dependent kinase 2-interacting protein



● Molecule 4: Cyclin-dependent kinase 2-interacting protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	165778	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37.6	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.785	Depositor
Minimum map value	-0.413	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.131	Depositor
Map size (Å)	281.2, 281.2, 281.2	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.74, 0.74, 0.74	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	0.39	0/1413	0.48	0/1909
1	F	0.22	0/1367	0.37	0/1848
1	G	0.43	0/1400	0.61	1/1892 (0.1%)
1	H	0.22	0/1379	0.35	0/1864
1	K	0.24	0/4122	0.46	0/5582
1	L	0.24	0/4297	0.42	0/5815
1	M	0.23	0/4122	0.43	0/5581
1	N	0.24	0/4298	0.42	0/5817
2	I	0.38	0/1349	0.57	0/1844
2	J	0.38	0/1335	0.55	0/1825
2	O	0.20	0/4082	0.41	0/5532
2	P	0.26	1/4093 (0.0%)	0.42	0/5546
3	A	0.50	0/1633	0.64	1/2211 (0.0%)
3	B	0.47	0/1614	0.59	0/2185
4	C	0.35	0/1231	0.43	0/1660
4	D	0.34	0/1282	0.44	0/1732
All	All	0.30	1/39017 (0.0%)	0.46	2/52843 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	483	PRO	N-CD	-10.26	1.33	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	186	HIS	CB-CA-C	8.62	125.39	109.54
1	G	59	ILE	C-N-CD	-5.29	103.32	125.00

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	E	1392	0	1424	37	0
1	F	1346	0	1377	10	0
1	G	1379	0	1416	33	0
1	H	1358	0	1391	13	0
1	K	4056	0	4210	15	0
1	L	4226	0	4371	11	0
1	M	4056	0	4217	18	0
1	N	4228	0	4373	13	0
2	I	1320	0	1383	32	0
2	J	1306	0	1372	25	0
2	O	4016	0	4144	10	0
2	P	4027	0	4161	12	0
3	A	1604	0	1634	74	0
3	B	1585	0	1618	81	0
4	C	1211	0	1218	53	0
4	D	1258	0	1257	52	0
All	All	38368	0	39566	469	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 12.

All (469) 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)
4:C:158:LYS:HE2	4:C:191:TYR:CZ	1.35	1.62
4:C:158:LYS:CE	4:C:191:TYR:CE1	2.14	1.30
3:A:148:HIS:CE1	3:A:185:GLU:OE1	1.83	1.29
4:C:158:LYS:CE	4:C:191:TYR:CZ	2.18	1.27
3:A:148:HIS:HE1	3:A:185:GLU:OE1	1.00	1.27
3:A:148:HIS:HE1	3:A:185:GLU:CD	1.49	1.20
4:C:29:ASP:O	4:C:33:LEU:HD23	1.43	1.18
4:C:158:LYS:NZ	4:C:191:TYR:CE1	2.13	1.17
4:C:158:LYS:HE2	4:C:191:TYR:CE1	1.78	1.16
3:A:60:VAL:O	3:A:64:ARG:HG3	1.47	1.13
4:C:158:LYS:NZ	4:C:191:TYR:HE1	1.48	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:61:PRO:HA	3:A:64:ARG:HE	1.18	1.08
3:B:106:VAL:CG1	3:B:110:PHE:HE2	1.68	1.07
3:B:106:VAL:HG12	3:B:110:PHE:HE2	1.21	1.05
3:A:148:HIS:CE1	3:A:185:GLU:CD	2.30	1.05
3:B:50:GLN:OE1	3:B:168:LEU:HB2	1.58	1.03
3:B:106:VAL:HG12	3:B:110:PHE:CE2	1.94	1.01
3:A:10:VAL:O	3:A:14:LEU:HD23	1.61	1.01
3:A:178:TRP:O	3:A:181:ILE:HG22	1.59	1.01
3:B:50:GLN:OE1	3:B:168:LEU:CB	2.10	1.00
3:B:178:TRP:O	3:B:181:ILE:HG22	1.61	0.99
2:J:139:LEU:HD21	2:J:163:LEU:HD12	1.45	0.99
3:B:195:LEU:HG	1:G:59:ILE:HA	1.50	0.91
3:B:186:HIS:HB3	3:B:188:ASP:OD1	1.70	0.90
4:D:117:LYS:HB2	4:D:146:TYR:CE1	2.06	0.90
3:B:106:VAL:CG1	3:B:110:PHE:CE2	2.53	0.89
3:B:91:ARG:O	3:B:94:ILE:HG22	1.73	0.87
4:C:158:LYS:HE2	4:C:191:TYR:OH	1.72	0.87
1:E:141:ALA:HB2	1:E:324:TYR:HB3	1.58	0.84
1:G:141:ALA:HB2	1:G:324:TYR:HB3	1.59	0.84
3:A:152:SER:HB2	3:A:185:GLU:OE2	1.78	0.83
4:C:158:LYS:HZ3	4:C:191:TYR:HE1	0.83	0.83
1:E:65:ASN:HD21	1:E:168:LEU:HD23	1.44	0.82
1:M:663:GLY:HA3	1:M:788:ILE:HA	1.59	0.82
4:D:148:VAL:O	4:D:152:LEU:HD23	1.79	0.82
2:I:33:PRO:O	2:I:37:HIS:CD2	2.32	0.82
4:C:158:LYS:CD	4:C:191:TYR:CE1	2.63	0.80
4:C:158:LYS:CE	4:C:191:TYR:OH	2.28	0.79
4:C:179:THR:O	4:C:183:LEU:HD23	1.83	0.79
3:A:138:MET:O	3:A:142:LEU:HD23	1.85	0.77
3:A:186:HIS:HB3	3:A:189:LEU:HD21	1.65	0.77
1:E:140:GLN:NE2	1:E:327:SER:OG	2.16	0.76
2:J:31:LEU:HB2	2:J:36:LEU:HD21	1.67	0.75
3:A:150:ARG:HH22	2:I:140:ARG:HD2	1.52	0.75
2:I:33:PRO:O	2:I:37:HIS:HD2	1.69	0.75
1:G:87:LEU:HA	1:G:97:VAL:HG12	1.69	0.75
4:D:108:LYS:O	4:D:112:LEU:HD23	1.86	0.75
1:G:140:GLN:NE2	1:G:327:SER:OG	2.17	0.74
1:K:663:GLY:HA3	1:K:788:ILE:HA	1.70	0.74
2:O:490:PHE:O	2:O:494:GLY:N	2.22	0.73
1:E:140:GLN:NE2	1:E:329:THR:OG1	2.21	0.73
3:B:167:ASP:OD1	3:B:170:ASN:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:THR:O	4:D:102:LEU:HD23	1.89	0.73
2:I:31:LEU:HD21	2:I:35:ALA:HB3	1.69	0.72
1:L:663:GLY:HA3	1:L:788:ILE:HA	1.70	0.72
2:P:490:PHE:O	2:P:494:GLY:N	2.17	0.72
2:I:139:LEU:HD21	2:I:163:LEU:HG	1.70	0.72
3:A:7:LEU:O	3:A:11:GLN:HG2	1.89	0.72
3:B:50:GLN:OE1	3:B:168:LEU:HB3	1.88	0.71
4:C:158:LYS:HD3	4:C:191:TYR:CE1	2.24	0.71
2:I:162:ALA:O	2:I:163:LEU:HD22	1.89	0.71
1:E:141:ALA:O	1:E:330:THR:OG1	2.08	0.71
4:C:158:LYS:HD3	4:C:191:TYR:CD1	2.25	0.71
1:G:66:SER:OG	1:G:99:THR:N	2.21	0.71
2:J:111:ALA:N	2:J:167:GLY:O	2.24	0.70
3:A:72:ARG:HD2	3:A:75:ARG:HH21	1.57	0.70
4:D:179:THR:O	4:D:183:LEU:HD23	1.92	0.70
1:F:142:GLU:O	1:F:330:THR:HA	1.90	0.70
4:C:144:HIS:O	4:C:148:VAL:HG23	1.92	0.69
1:G:96:GLU:OE2	1:G:171:LYS:NZ	2.25	0.69
2:P:246:GLY:O	2:P:250:LEU:N	2.22	0.69
3:B:102:VAL:HG11	3:B:149:TYR:HD2	1.56	0.69
1:G:63:PHE:O	1:G:67:LEU:HG	1.93	0.68
4:C:29:ASP:O	4:C:33:LEU:CD2	2.32	0.68
3:B:125:VAL:HG13	3:B:135:VAL:HG23	1.75	0.68
1:G:62:THR:C	1:G:64:GLN:H	1.99	0.68
1:G:65:ASN:HD22	1:G:168:LEU:HD13	1.57	0.68
1:K:824:LEU:O	1:K:828:THR:N	2.27	0.68
3:A:191:GLN:O	3:A:195:LEU:HD23	1.94	0.68
4:D:181:SER:O	4:D:184:SER:OG	2.09	0.68
3:A:61:PRO:HA	3:A:64:ARG:NE	2.01	0.68
4:C:197:ARG:NH1	1:H:58:LYS:O	2.26	0.68
3:A:32:LEU:HD11	3:A:156:ARG:HH21	1.59	0.68
1:L:759:GLY:O	1:L:763:LEU:N	2.24	0.67
1:H:47:THR:HA	1:H:128:ALA:HA	1.77	0.67
1:N:561:GLY:O	1:N:564:LEU:N	2.28	0.66
3:A:95:LEU:O	3:A:98:VAL:HG12	1.96	0.66
4:C:21:ARG:HA	4:C:24:LYS:HD3	1.77	0.66
1:M:649:HIS:O	1:M:653:PHE:N	2.29	0.66
4:D:199:HIS:O	4:D:202:SER:OG	2.12	0.66
1:G:140:GLN:NE2	1:G:329:THR:OG1	2.28	0.66
3:B:193:ILE:O	3:B:197:VAL:HG12	1.96	0.65
1:K:754:LEU:O	1:K:758:ASP:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:186:HIS:HB2	3:B:189:LEU:HG	1.78	0.65
1:H:142:GLU:O	1:H:330:THR:HA	1.96	0.65
4:D:121:GLU:O	4:D:124:ASN:ND2	2.29	0.65
2:O:226:LEU:O	2:O:230:GLY:N	2.29	0.65
3:B:152:SER:OG	3:B:156:ARG:NH1	2.30	0.65
4:D:46:THR:O	4:D:50:ASN:ND2	2.30	0.65
1:L:561:GLY:O	1:L:564:LEU:N	2.30	0.65
4:D:102:LEU:HA	4:D:105:ILE:HD12	1.79	0.64
4:D:43:ALA:O	4:D:46:THR:OG1	2.15	0.64
1:E:65:ASN:ND2	1:E:168:LEU:HD23	2.11	0.64
4:C:181:SER:O	4:C:184:SER:OG	2.16	0.64
4:D:142:THR:HA	4:D:145:PHE:HD2	1.63	0.63
2:I:162:ALA:C	2:I:163:LEU:HD22	2.23	0.63
4:C:158:LYS:HE2	4:C:191:TYR:CE2	2.22	0.63
4:C:158:LYS:NZ	4:C:191:TYR:CZ	2.56	0.63
4:D:96:GLN:NE2	1:E:185:GLY:O	2.31	0.63
2:J:138:LEU:O	2:J:138:LEU:HD23	1.98	0.63
2:P:680:LEU:O	2:P:684:THR:N	2.27	0.63
3:B:143:GLN:O	3:B:146:GLU:HG2	1.99	0.63
1:E:322:THR:HG21	1:E:324:TYR:CZ	2.33	0.63
4:C:125:TYR:O	4:C:126:HIS:ND1	2.32	0.62
2:I:166:VAL:HG23	2:I:167:GLY:N	2.15	0.62
4:C:46:THR:O	4:C:50:ASN:ND2	2.33	0.62
1:E:197:GLY:HA3	1:E:324:TYR:CE1	2.35	0.62
1:F:165:LEU:HD21	1:F:328:SER:HA	1.81	0.61
1:G:167:LYS:C	1:G:168:LEU:HD22	2.25	0.61
3:B:186:HIS:O	3:B:189:LEU:N	2.23	0.61
4:C:29:ASP:C	4:C:33:LEU:HD23	2.22	0.61
3:A:99:ARG:HH21	3:A:150:ARG:NE	1.98	0.61
1:K:649:HIS:O	1:K:652:SER:N	2.32	0.61
1:G:197:GLY:HA3	1:G:324:TYR:CE1	2.35	0.61
3:B:143:GLN:HE22	3:B:147:ARG:NH2	1.99	0.61
3:A:66:PHE:HZ	4:C:161:LEU:HG	1.66	0.61
2:I:28:ARG:HB2	2:I:62:TRP:HD1	1.66	0.60
1:H:161:THR:HA	1:H:164:ILE:HD12	1.81	0.60
3:A:150:ARG:HH22	2:I:140:ARG:HH11	1.50	0.60
1:G:62:THR:C	1:G:64:GLN:N	2.60	0.60
1:E:144:MET:O	1:E:332:VAL:HA	2.01	0.59
3:A:55:LEU:HD12	3:A:57:PHE:HE1	1.65	0.59
1:M:824:LEU:O	1:M:828:THR:N	2.34	0.59
2:I:20:ASP:N	2:I:20:ASP:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:167:ASP:OD2	3:A:170:ASN:HB3	2.01	0.59
1:E:322:THR:HG22	1:E:323:PHE:N	2.17	0.59
2:J:139:LEU:HD21	2:J:163:LEU:CD1	2.29	0.59
3:B:191:GLN:O	3:B:195:LEU:HD23	2.04	0.58
2:I:166:VAL:HG23	2:I:167:GLY:H	1.68	0.58
4:C:97:ALA:HA	4:C:100:ASP:OD1	2.03	0.58
3:B:34:ASP:OD2	3:B:91:ARG:NE	2.36	0.58
1:E:95:GLN:NE2	1:E:317:LYS:O	2.32	0.58
1:N:454:GLU:N	1:N:498:ALA:O	2.37	0.58
4:D:123:GLU:O	4:D:123:GLU:HG2	2.03	0.58
2:I:145:SER:O	2:I:148:HIS:ND1	2.36	0.57
3:A:150:ARG:NH2	2:I:140:ARG:HD2	2.18	0.57
1:L:780:LYS:O	1:L:784:ARG:N	2.37	0.57
4:C:86:GLU:OE1	1:G:166:ARG:NH1	2.38	0.57
2:J:144:ILE:O	2:J:176:GLY:N	2.33	0.57
3:B:120:VAL:HG23	3:B:120:VAL:O	2.04	0.57
1:E:322:THR:HG21	1:E:324:TYR:OH	2.05	0.57
3:B:48:GLN:HE21	3:B:77:GLN:HE21	1.52	0.57
1:E:86:VAL:O	1:E:97:VAL:HG23	2.03	0.57
2:J:124:GLY:C	2:J:126:ARG:H	2.13	0.57
1:G:66:SER:HG	1:G:99:THR:H	1.51	0.57
3:B:187:GLN:OE1	3:B:187:GLN:N	2.31	0.56
2:O:304:GLU:N	2:O:343:ALA:O	2.37	0.56
4:C:105:ILE:HG22	4:C:109:MET:HE2	1.88	0.56
3:A:59:ASP:OD1	3:A:59:ASP:O	2.24	0.56
4:C:158:LYS:NZ	4:C:191:TYR:OH	2.39	0.56
1:E:146:VAL:O	1:E:334:PHE:HA	2.06	0.56
1:L:653:PHE:HA	1:L:657:GLY:HA2	1.87	0.56
3:B:42:LEU:HD12	3:B:84:VAL:HG13	1.88	0.56
1:M:525:ASN:O	1:M:529:ARG:N	2.33	0.56
2:I:49:ILE:O	2:I:57:CYS:N	2.35	0.55
4:D:117:LYS:HB2	4:D:146:TYR:HE1	1.64	0.55
1:N:525:ASN:O	1:N:529:ARG:N	2.26	0.55
1:M:726:PHE:N	1:M:769:LEU:O	2.36	0.55
1:N:663:GLY:HA3	1:N:788:ILE:HA	1.89	0.55
1:E:97:VAL:CG1	1:E:172:ILE:HB	2.36	0.55
2:O:531:GLY:O	2:O:535:PHE:N	2.34	0.54
4:C:201:GLU:HG3	4:C:205:LEU:HD23	1.89	0.54
4:D:33:LEU:HD12	4:D:105:ILE:HG23	1.88	0.54
1:N:653:PHE:O	1:N:657:GLY:N	2.40	0.54
4:D:201:GLU:O	4:D:205:LEU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:20:VAL:HG11	3:A:105:HIS:ND1	2.23	0.53
3:A:47:GLU:HB2	3:A:172:GLN:OE1	2.08	0.53
3:B:60:VAL:HG23	3:B:63:LEU:HB2	1.90	0.53
1:G:172:ILE:HG23	1:G:324:TYR:O	2.08	0.53
2:P:217:ARG:O	2:P:221:ARG:N	2.34	0.53
1:F:47:THR:HA	1:F:128:ALA:HA	1.89	0.53
4:D:195:ASP:OD1	4:D:195:ASP:N	2.39	0.53
4:D:40:LEU:HD12	4:D:105:ILE:HD11	1.90	0.53
2:P:565:GLU:HA	2:P:628:THR:HA	1.90	0.53
1:L:392:LEU:O	1:L:498:ALA:HA	2.09	0.53
3:B:106:VAL:HG22	3:B:142:LEU:HD12	1.89	0.53
3:A:25:GLN:CD	3:A:190:VAL:HG11	2.33	0.53
1:N:780:LYS:O	1:N:784:ARG:N	2.42	0.52
3:B:60:VAL:HG21	3:B:63:LEU:HD12	1.91	0.52
1:L:645:TRP:O	1:L:648:LYS:N	2.40	0.52
2:P:501:VAL:HA	2:P:646:LYS:O	2.10	0.52
4:C:34:ILE:HD12	4:C:156:TYR:CZ	2.44	0.52
1:G:88:LEU:HB2	1:G:96:GLU:O	2.08	0.52
3:A:85:LEU:C	3:A:85:LEU:HD23	2.34	0.52
3:A:72:ARG:CD	3:A:75:ARG:HH21	2.21	0.52
3:B:106:VAL:HG12	3:B:110:PHE:CD2	2.42	0.52
3:B:20:VAL:O	3:B:24:GLN:HG2	2.10	0.52
3:B:68:ASP:C	3:B:69:LEU:HD22	2.34	0.52
2:O:241:GLY:N	2:O:345:ASN:O	2.43	0.51
3:B:48:GLN:HE21	3:B:77:GLN:NE2	2.07	0.51
1:M:461:LYS:O	1:M:465:ALA:N	2.26	0.51
3:A:47:GLU:HA	3:A:172:GLN:OE1	2.11	0.51
2:I:28:ARG:CB	2:I:62:TRP:HD1	2.23	0.51
1:E:71:GLY:O	1:E:75:MET:N	2.33	0.51
1:L:429:GLY:O	1:L:433:ALA:N	2.41	0.51
1:N:392:LEU:O	1:N:498:ALA:HA	2.10	0.51
1:G:144:MET:O	1:G:332:VAL:HA	2.11	0.51
2:J:30:ARG:NH1	2:J:63:PRO:O	2.44	0.51
3:B:95:LEU:O	3:B:98:VAL:HG12	2.12	0.50
3:B:197:VAL:O	3:B:197:VAL:HG22	2.11	0.50
3:A:39:LEU:HD11	3:A:174:LEU:HB3	1.93	0.50
3:A:10:VAL:O	3:A:14:LEU:CD2	2.47	0.50
1:K:726:PHE:N	1:K:769:LEU:O	2.39	0.50
1:M:645:TRP:O	1:M:647:LEU:N	2.44	0.50
4:C:163:LYS:O	4:C:166:VAL:HG12	2.11	0.50
1:M:809:GLN:O	1:M:813:MET:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:195:LEU:HA	3:A:198:SER:OG	2.12	0.50
4:D:189:GLN:O	4:D:191:TYR:N	2.43	0.50
1:H:46:LEU:O	1:H:129:ILE:N	2.41	0.50
4:C:166:VAL:HG23	4:C:182:TYR:CD1	2.48	0.49
1:F:48:VAL:N	1:F:127:ASP:O	2.36	0.49
1:G:65:ASN:ND2	1:G:167:LYS:O	2.45	0.49
3:A:188:ASP:HB2	3:A:191:GLN:HB2	1.95	0.49
1:E:138:VAL:C	1:E:139:LEU:HD23	2.37	0.49
3:B:63:LEU:O	3:B:66:PHE:HB2	2.13	0.49
1:E:68:ILE:HG13	1:E:68:ILE:O	2.11	0.49
1:M:650:PRO:O	1:M:654:ILE:N	2.46	0.49
4:D:97:ALA:HA	4:D:100:ASP:OD1	2.12	0.49
3:A:161:SER:O	3:A:161:SER:OG	2.28	0.49
4:C:30:TRP:O	4:C:34:ILE:HG12	2.12	0.49
1:E:97:VAL:HG11	1:E:172:ILE:HB	1.94	0.49
1:N:370:GLU:O	1:N:374:LYS:N	2.46	0.49
3:B:68:ASP:N	3:B:68:ASP:OD1	2.44	0.49
4:D:196:SER:OG	4:D:197:ARG:N	2.46	0.49
3:B:48:GLN:HE22	4:D:188:HIS:CD2	2.31	0.48
3:A:168:LEU:HD13	3:A:171:ILE:HG21	1.95	0.48
3:A:162:SER:O	3:A:162:SER:OG	2.30	0.48
3:B:72:ARG:NH2	4:D:193:GLU:OE2	2.45	0.48
3:A:150:ARG:HH12	2:I:140:ARG:CZ	2.27	0.48
3:B:78:LEU:CD1	1:F:166:ARG:NH2	2.77	0.48
4:C:41:ASN:OD1	4:C:186:TRP:NE1	2.47	0.48
1:E:65:ASN:ND2	1:E:168:LEU:CD2	2.76	0.48
3:B:69:LEU:HD22	3:B:69:LEU:N	2.29	0.48
3:A:20:VAL:O	3:A:24:GLN:HG2	2.12	0.48
3:A:32:LEU:HD11	3:A:156:ARG:NH2	2.27	0.48
4:C:113:SER:O	4:C:116:THR:OG1	2.30	0.48
1:E:68:ILE:HD11	1:E:86:VAL:HG11	1.95	0.48
2:J:31:LEU:C	2:J:64:ARG:HG2	2.38	0.48
3:B:20:VAL:HG11	3:B:105:HIS:ND1	2.29	0.48
1:G:62:THR:O	1:G:64:GLN:N	2.47	0.48
3:B:118:ASP:OD1	3:B:119:THR:HG23	2.13	0.47
3:A:197:VAL:HG22	3:A:197:VAL:O	2.13	0.47
3:B:164:GLN:O	3:B:167:ASP:OD2	2.32	0.47
3:B:195:LEU:CG	1:G:59:ILE:HA	2.34	0.47
1:E:132:GLN:OE1	1:E:319:ASN:HB3	2.14	0.47
3:A:99:ARG:HE	3:A:150:ARG:HD2	1.79	0.47
1:K:389:GLY:HA3	1:K:515:PHE:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:224:ARG:O	2:P:227:THR:N	2.48	0.47
3:B:106:VAL:O	3:B:110:PHE:HD2	1.97	0.47
3:B:145:ILE:HD11	3:B:190:VAL:HG22	1.97	0.47
1:G:174:LEU:HB3	1:G:175:PRO:HD2	1.97	0.47
1:K:613:ALA:C	1:K:615:ARG:H	2.21	0.47
3:B:125:VAL:CG1	3:B:135:VAL:HG23	2.44	0.47
4:C:178:LEU:HD12	4:C:182:TYR:CE2	2.49	0.47
1:H:114:SER:O	1:H:118:GLN:N	2.39	0.47
2:I:22:ARG:HG3	2:I:23:ASP:H	1.79	0.47
2:I:36:LEU:HD23	2:I:36:LEU:HA	1.77	0.47
2:J:31:LEU:O	2:J:64:ARG:HG2	2.14	0.47
2:O:504:TYR:O	2:O:650:ILE:N	2.38	0.47
2:O:680:LEU:O	2:O:684:THR:N	2.48	0.47
4:C:47:THR:HG21	4:C:95:LEU:HB2	1.97	0.47
2:J:145:SER:O	2:J:148:HIS:ND1	2.48	0.47
1:M:389:GLY:HA3	1:M:514:ARG:O	2.14	0.47
4:D:172:HIS:CG	4:D:172:HIS:O	2.67	0.46
2:J:162:ALA:O	2:J:163:LEU:HD23	2.15	0.46
1:G:141:ALA:O	1:G:330:THR:HG23	2.15	0.46
2:I:30:ARG:NH1	2:I:63:PRO:O	2.48	0.46
3:B:161:SER:O	3:B:161:SER:OG	2.24	0.46
3:B:106:VAL:O	3:B:110:PHE:CD2	2.68	0.46
1:K:703:GLY:O	1:K:707:ARG:N	2.32	0.46
4:C:189:GLN:O	4:C:191:TYR:N	2.46	0.46
1:F:87:LEU:HD12	1:F:88:LEU:H	1.80	0.46
2:J:30:ARG:C	2:J:31:LEU:HD12	2.40	0.46
3:A:11:GLN:HE22	3:A:135:VAL:HG22	1.80	0.46
4:D:108:LYS:O	4:D:112:LEU:CD2	2.62	0.46
4:D:166:VAL:HG23	4:D:182:TYR:CD1	2.51	0.46
1:G:178:PHE:HA	1:G:190:LEU:O	2.16	0.46
4:D:29:ASP:O	4:D:33:LEU:HD23	2.15	0.46
4:D:136:LEU:HG	4:D:137:PHE:H	1.81	0.46
4:D:140:TRP:CE3	4:D:144:HIS:HD2	2.33	0.46
1:F:165:LEU:HD11	1:F:328:SER:HA	1.97	0.46
1:K:726:PHE:O	1:K:770:ALA:HA	2.16	0.46
3:A:193:ILE:O	3:A:197:VAL:HG12	2.16	0.46
4:D:99:LEU:HD23	4:D:99:LEU:HA	1.70	0.46
3:A:189:LEU:O	3:A:193:ILE:HG12	2.16	0.45
2:J:127:ASN:O	2:J:130:ALA:N	2.46	0.45
3:A:66:PHE:CZ	4:C:161:LEU:HG	2.49	0.45
3:A:155:LYS:HD2	3:A:181:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:61:PRO:O	3:B:64:ARG:HB3	2.15	0.45
3:B:78:LEU:HD13	1:F:166:ARG:NH2	2.32	0.45
1:E:169:ASP:OD1	1:E:169:ASP:N	2.50	0.45
1:M:666:LEU:HA	1:M:792:ILE:O	2.16	0.45
1:G:138:VAL:C	1:G:139:LEU:HD23	2.41	0.45
3:B:91:ARG:HD3	3:B:91:ARG:HA	1.70	0.45
4:C:169:GLU:HG2	4:C:182:TYR:OH	2.16	0.45
2:O:255:ALA:O	2:O:259:GLY:N	2.46	0.45
3:A:148:HIS:CE1	3:A:185:GLU:OE2	2.65	0.45
3:B:18:PHE:CE1	3:B:197:VAL:HG11	2.52	0.45
1:N:649:HIS:O	1:N:652:SER:N	2.44	0.45
2:P:217:ARG:O	2:P:220:LEU:N	2.49	0.45
3:A:39:LEU:HD21	3:A:174:LEU:HB3	1.98	0.45
3:B:69:LEU:O	3:B:70:LYS:C	2.60	0.45
4:C:204:LEU:C	4:C:204:LEU:HD23	2.42	0.45
3:A:49:LEU:HA	3:A:77:GLN:HE22	1.80	0.45
3:B:125:VAL:HG13	3:B:135:VAL:CG2	2.47	0.45
4:C:193:GLU:C	4:C:195:ASP:H	2.25	0.45
1:E:322:THR:CG2	1:E:324:TYR:CZ	2.99	0.45
3:A:195:LEU:O	3:A:198:SER:OG	2.35	0.44
3:B:69:LEU:HD13	3:B:69:LEU:HA	1.86	0.44
4:C:196:SER:OG	4:C:197:ARG:N	2.50	0.44
4:D:163:LYS:O	4:D:166:VAL:HG12	2.17	0.44
1:E:319:ASN:OD1	1:E:320:THR:HG23	2.18	0.44
2:I:31:LEU:HD22	2:I:36:LEU:HG	1.99	0.44
1:E:87:LEU:HD12	1:E:87:LEU:HA	1.85	0.44
1:G:86:VAL:HG13	1:G:132:GLN:O	2.17	0.44
3:B:39:LEU:C	3:B:39:LEU:HD23	2.43	0.44
4:C:104:LYS:O	4:C:107:VAL:HG12	2.17	0.44
4:C:185:MET:HB2	4:C:185:MET:HE3	1.80	0.44
4:D:172:HIS:O	4:D:172:HIS:CD2	2.70	0.44
1:E:322:THR:CG2	1:E:323:PHE:N	2.80	0.44
2:J:138:LEU:HD23	2:J:138:LEU:C	2.43	0.44
4:D:175:ASP:N	4:D:175:ASP:OD1	2.48	0.44
1:F:45:THR:HA	1:F:129:ILE:O	2.18	0.44
3:A:155:LYS:HB3	3:A:181:ILE:HD11	1.99	0.44
3:B:189:LEU:O	3:B:193:ILE:HG12	2.16	0.44
4:D:104:LYS:O	4:D:107:VAL:HG12	2.18	0.44
4:D:117:LYS:HB2	4:D:146:TYR:CD1	2.52	0.44
1:G:143:GLU:O	1:G:196:LYS:N	2.43	0.44
3:B:134:SER:HG	3:B:137:ASP:H	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:178:LEU:HD12	4:D:182:TYR:CE2	2.53	0.44
4:D:200:LEU:C	4:D:200:LEU:HD23	2.43	0.44
1:E:172:ILE:HG23	1:E:324:TYR:O	2.17	0.44
1:E:142:GLU:O	1:E:330:THR:HG23	2.18	0.43
1:K:809:GLN:O	1:K:813:MET:N	2.51	0.43
1:M:610:ARG:O	1:M:612:SER:N	2.47	0.43
4:C:162:LEU:HD11	4:C:185:MET:SD	2.58	0.43
2:I:28:ARG:HD3	2:I:62:TRP:CD1	2.53	0.43
2:J:19:LEU:HD11	2:J:74:LEU:O	2.17	0.43
3:A:187:GLN:NE2	3:A:187:GLN:N	2.66	0.43
4:C:110:GLU:O	4:C:113:SER:OG	2.30	0.43
2:I:126:ARG:O	2:I:127:ASN:C	2.62	0.43
1:G:68:ILE:O	1:G:68:ILE:HG13	2.18	0.43
3:A:51:ALA:HB1	4:C:177:ASP:OD2	2.18	0.43
3:A:183:LYS:HE2	3:A:183:LYS:HB3	1.64	0.43
2:J:28:ARG:HB3	2:J:62:TRP:CD1	2.53	0.43
3:B:34:ASP:O	3:B:37:PRO:HD2	2.19	0.43
4:C:170:LEU:O	4:C:171:ALA:C	2.61	0.43
1:F:164:ILE:HG23	1:F:168:LEU:HD12	2.01	0.43
2:I:124:GLY:C	2:I:126:ARG:H	2.27	0.43
2:P:704:LEU:O	2:P:708:GLY:C	2.62	0.42
4:D:142:THR:HG22	4:D:142:THR:O	2.17	0.42
1:M:394:GLY:HA3	1:M:521:ILE:O	2.19	0.42
2:P:565:GLU:N	2:P:627:ALA:O	2.52	0.42
3:A:37:PRO:O	3:A:40:SER:OG	2.30	0.42
3:A:54:ASN:O	3:A:55:LEU:HD23	2.18	0.42
1:E:70:LEU:HD23	1:E:70:LEU:HA	1.83	0.42
1:L:725:PHE:HA	1:L:769:LEU:O	2.19	0.42
4:D:108:LYS:HE3	4:D:108:LYS:HB2	1.87	0.42
4:D:113:SER:O	4:D:116:THR:OG1	2.31	0.42
3:A:60:VAL:HG11	3:A:63:LEU:HD12	2.00	0.42
4:D:184:SER:OG	4:D:185:MET:N	2.52	0.42
1:M:697:LEU:O	1:M:699:ASN:N	2.49	0.42
1:M:645:TRP:O	1:M:648:LYS:N	2.45	0.42
1:E:82:ILE:C	1:E:84:ARG:H	2.28	0.42
4:D:47:THR:HG21	4:D:95:LEU:HB2	2.01	0.42
4:D:140:TRP:CD2	4:D:206:GLU:OE1	2.73	0.42
1:E:84:ARG:NH1	2:I:65:ARG:HH21	2.16	0.42
2:J:13:LEU:HD12	2:J:13:LEU:HA	1.95	0.42
3:B:193:ILE:HD13	3:B:193:ILE:HA	1.82	0.42
4:D:111:LYS:O	4:D:115:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:ASP:O	4:D:198:LEU:HB3	2.20	0.42
1:G:86:VAL:HG21	1:G:100:ALA:HB2	2.02	0.42
3:A:47:GLU:CB	3:A:172:GLN:OE1	2.67	0.42
2:I:109:ARG:H	2:I:169:THR:HG1	1.67	0.42
3:A:47:GLU:CA	3:A:172:GLN:OE1	2.67	0.42
3:A:126:LEU:HD22	2:I:63:PRO:HB2	2.01	0.42
3:B:186:HIS:CB	3:B:188:ASP:OD1	2.56	0.42
1:H:69:HIS:C	1:H:70:LEU:HD23	2.45	0.42
1:K:389:GLY:HA3	1:K:514:ARG:O	2.20	0.41
1:L:400:LYS:O	1:L:403:ILE:N	2.53	0.41
1:M:703:GLY:O	1:M:707:ARG:N	2.47	0.41
1:N:561:GLY:O	1:N:562:ALA:C	2.63	0.41
2:O:359:ARG:O	2:O:361:ASP:N	2.53	0.41
3:A:49:LEU:HD11	3:A:74:ARG:NH1	2.34	0.41
3:A:146:GLU:OE1	3:A:146:GLU:C	2.63	0.41
1:H:179:LEU:N	1:H:190:LEU:O	2.52	0.41
2:P:486:PHE:O	2:P:488:TRP:N	2.53	0.41
4:C:37:TRP:CD1	4:C:37:TRP:C	2.98	0.41
2:I:45:SER:O	2:I:60:THR:HA	2.20	0.41
1:M:757:MET:O	1:M:759:GLY:N	2.53	0.41
1:N:665:LEU:O	1:N:791:ILE:HA	2.21	0.41
3:A:57:PHE:CD2	3:A:70:LYS:HB2	2.55	0.41
3:A:78:LEU:HB3	1:H:166:ARG:NH2	2.35	0.41
1:E:102:PRO:O	1:E:103:MET:C	2.63	0.41
1:G:63:PHE:O	1:G:67:LEU:CD2	2.68	0.41
4:D:141:PRO:C	4:D:143:THR:H	2.27	0.41
1:E:66:SER:O	1:E:99:THR:OG1	2.30	0.41
1:H:45:THR:HA	1:H:130:GLN:HA	2.02	0.41
2:J:31:LEU:HB2	2:J:36:LEU:CD2	2.44	0.41
3:B:106:VAL:HG13	3:B:110:PHE:CE2	2.52	0.41
2:I:65:ARG:HA	2:I:65:ARG:HD2	1.85	0.41
2:J:139:LEU:CD2	2:J:163:LEU:HD12	2.34	0.41
1:N:891:HIS:C	1:N:893:LEU:H	2.28	0.41
3:B:39:LEU:HD23	3:B:175:PRO:HG3	2.01	0.41
3:B:55:LEU:HD12	3:B:57:PHE:CE1	2.55	0.41
4:C:168:LYS:HB3	4:C:168:LYS:HE2	1.70	0.41
1:K:757:MET:O	1:K:759:GLY:N	2.54	0.41
3:A:154:LEU:C	3:A:154:LEU:HD23	2.45	0.41
3:B:178:TRP:CD1	3:B:178:TRP:C	2.98	0.41
3:B:186:HIS:CB	3:B:189:LEU:HG	2.48	0.41
3:B:194:LEU:HA	3:B:194:LEU:HD23	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:204:LEU:O	4:D:204:LEU:HD23	2.20	0.41
1:E:174:LEU:HD23	1:E:174:LEU:HA	1.79	0.41
1:E:198:ALA:C	1:E:200:GLY:H	2.28	0.41
3:B:54:ASN:O	3:B:55:LEU:HD23	2.21	0.41
3:B:135:VAL:O	3:B:139:LEU:HG	2.21	0.41
3:B:189:LEU:HA	3:B:189:LEU:HD23	1.66	0.41
4:D:105:ILE:O	4:D:109:MET:HG2	2.21	0.41
2:I:151:VAL:HG12	2:I:152:ALA:N	2.36	0.41
2:I:160:VAL:HG11	2:I:163:LEU:HD21	2.01	0.41
2:J:19:LEU:HD23	2:J:19:LEU:HA	1.93	0.41
3:A:74:ARG:C	3:A:76:LYS:N	2.79	0.41
3:B:195:LEU:HA	3:B:198:SER:HG	1.86	0.41
3:A:142:LEU:HD13	3:A:142:LEU:HA	1.87	0.40
3:B:66:PHE:HB3	3:B:69:LEU:CD2	2.51	0.40
3:B:69:LEU:N	3:B:69:LEU:CD2	2.83	0.40
1:K:449:ILE:HA	1:K:494:LEU:O	2.21	0.40
1:M:754:LEU:O	1:M:755:THR:C	2.65	0.40
3:A:54:ASN:C	3:A:55:LEU:HD23	2.47	0.40
4:D:198:LEU:O	4:D:199:HIS:C	2.64	0.40
1:G:319:ASN:OD1	1:G:320:THR:HG23	2.20	0.40
1:G:320:THR:O	1:G:320:THR:OG1	2.31	0.40
2:I:166:VAL:CG2	2:I:167:GLY:N	2.84	0.40
2:J:28:ARG:HB3	2:J:62:TRP:HD1	1.86	0.40
2:J:127:ASN:O	2:J:129:ALA:N	2.55	0.40
1:K:729:LEU:O	1:K:733:ALA:N	2.49	0.40
1:N:725:PHE:HA	1:N:769:LEU:O	2.21	0.40
3:A:20:VAL:HG21	3:A:105:HIS:CE1	2.55	0.40
3:A:164:GLN:O	3:A:167:ASP:OD1	2.39	0.40
3:A:171:ILE:HD12	3:A:174:LEU:CD2	2.51	0.40
4:C:37:TRP:CZ3	4:C:156:TYR:HD1	2.40	0.40
4:D:204:LEU:HD23	4:D:204:LEU:C	2.47	0.40
1:G:167:LYS:HE2	1:G:167:LYS:HB2	1.95	0.40
2:O:311:GLN:HA	2:O:351:ASP:HA	2.04	0.40
3:A:18:PHE:CZ	3:A:142:LEU:HD21	2.56	0.40
3:B:92:LEU:HA	3:B:92:LEU:HD12	1.83	0.40
3:B:142:LEU:O	3:B:145:ILE:HG22	2.22	0.40
3:B:155:LYS:HD2	3:B:181:ILE:HG13	2.03	0.40
3:B:168:LEU:HD13	3:B:168:LEU:HA	1.83	0.40
1:H:157:GLU:HA	1:H:160:LEU:HB3	2.03	0.40
1:H:168:LEU:HD23	1:H:168:LEU:HA	1.76	0.40
1:H:172:ILE:HA	1:H:325:PHE:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:140:ARG:HG2	2:J:141:ASN:OD1	2.21	0.40
1:K:697:LEU:O	1:K:699:ASN:N	2.49	0.40
1:L:720:ALA:O	1:L:722:SER:N	2.55	0.40
2:P:708:GLY:O	2:P:709:LEU:C	2.64	0.40
3:B:158:TYR:OH	2:J:133:GLU:OE2	2.30	0.40
3:B:195:LEU:HA	3:B:195:LEU:HD13	1.95	0.40
4:D:196:SER:O	4:D:199:HIS:HB2	2.21	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	E	178/920 (19%)	150 (84%)	28 (16%)	0	100	100
1	F	171/920 (19%)	150 (88%)	21 (12%)	0	100	100
1	G	176/920 (19%)	144 (82%)	29 (16%)	3 (2%)	7	35
1	H	173/920 (19%)	157 (91%)	16 (9%)	0	100	100
1	K	524/920 (57%)	458 (87%)	66 (13%)	0	100	100
1	L	543/920 (59%)	472 (87%)	71 (13%)	0	100	100
1	M	524/920 (57%)	461 (88%)	63 (12%)	0	100	100
1	N	544/920 (59%)	483 (89%)	60 (11%)	1 (0%)	43	77
2	I	181/777 (23%)	139 (77%)	41 (23%)	1 (1%)	21	58
2	J	179/777 (23%)	139 (78%)	39 (22%)	1 (1%)	21	58
2	O	521/777 (67%)	450 (86%)	71 (14%)	0	100	100
2	P	523/777 (67%)	452 (86%)	71 (14%)	0	100	100
3	A	196/264 (74%)	180 (92%)	15 (8%)	1 (0%)	24	63
3	B	194/264 (74%)	173 (89%)	21 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	144/237 (61%)	134 (93%)	10 (7%)	0	100	100
4	D	149/237 (63%)	137 (92%)	12 (8%)	0	100	100
All	All	4920/11470 (43%)	4279 (87%)	634 (13%)	7 (0%)	49	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	59	ILE
3	A	188	ASP
1	G	60	PRO
1	G	63	PHE
2	I	126	ARG
1	N	614	MET
2	J	170	PRO

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	E	154/776 (20%)	154 (100%)	0	100	100
1	F	150/776 (19%)	150 (100%)	0	100	100
1	G	153/776 (20%)	153 (100%)	0	100	100
1	H	151/776 (20%)	151 (100%)	0	100	100
1	K	436/776 (56%)	436 (100%)	0	100	100
1	L	454/776 (58%)	454 (100%)	0	100	100
1	M	436/776 (56%)	436 (100%)	0	100	100
1	N	454/776 (58%)	454 (100%)	0	100	100
2	I	137/633 (22%)	137 (100%)	0	100	100
2	J	136/633 (22%)	136 (100%)	0	100	100
2	O	440/633 (70%)	440 (100%)	0	100	100
2	P	441/633 (70%)	441 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	176/221 (80%)	176 (100%)	0	100	100
3	B	174/221 (79%)	174 (100%)	0	100	100
4	C	136/216 (63%)	136 (100%)	0	100	100
4	D	141/216 (65%)	141 (100%)	0	100	100
All	All	4169/9614 (43%)	4169 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	11	GLN
3	A	36	GLN
3	A	50	GLN
3	A	77	GLN
3	A	116	HIS
3	A	148	HIS
3	A	187	GLN
3	B	29	GLN
3	B	48	GLN
3	B	127	GLN
3	B	143	GLN
3	B	148	HIS
4	C	96	GLN
4	C	172	HIS
4	D	144	HIS
1	E	65	ASN
1	E	140	GLN
2	I	37	HIS
2	J	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

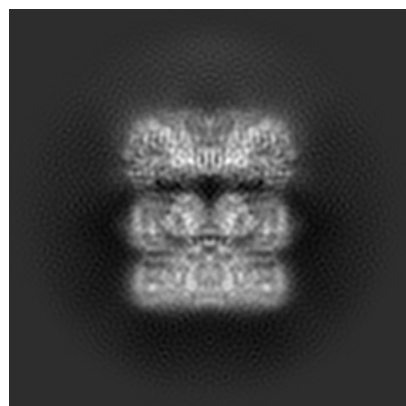
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19177. These allow visual inspection of the internal detail of the map and identification of artifacts.

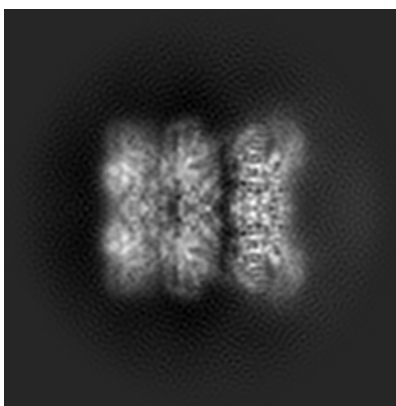
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

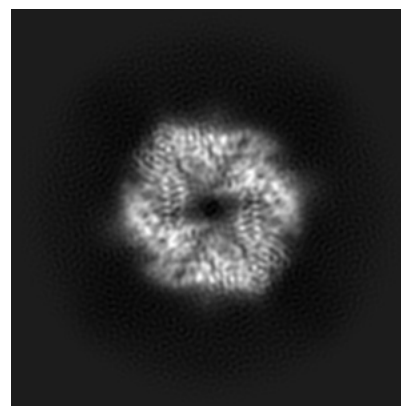
6.1.1 Primary map



X

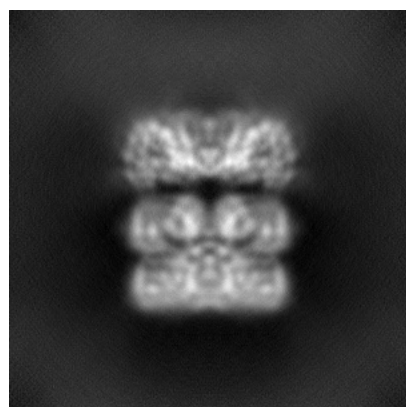


Y

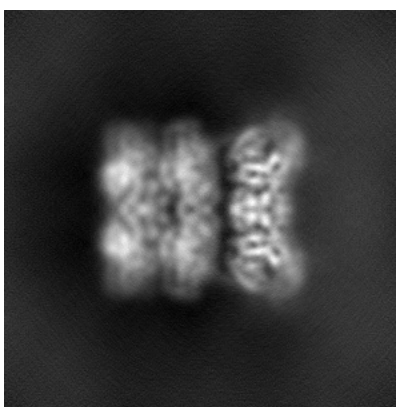


Z

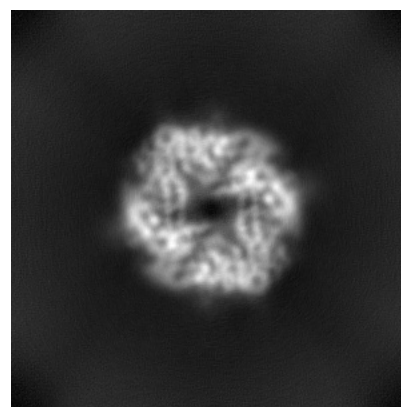
6.1.2 Raw map



X



Y

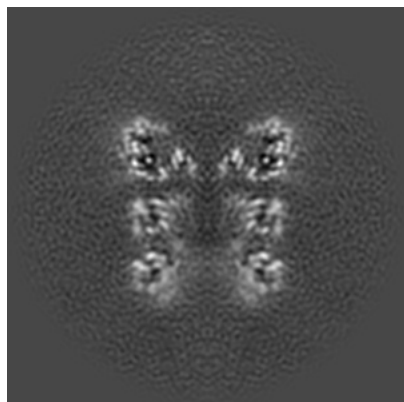


Z

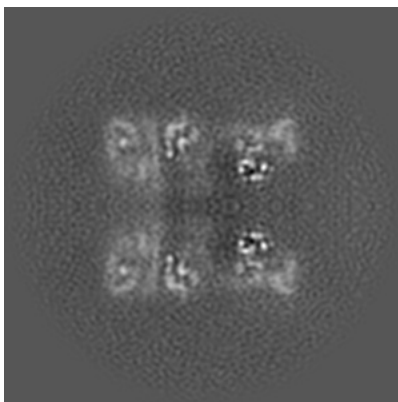
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

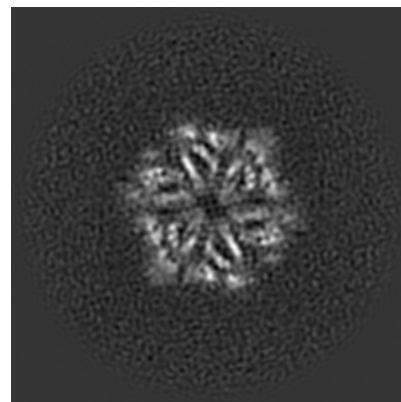
6.2.1 Primary map



X Index: 190

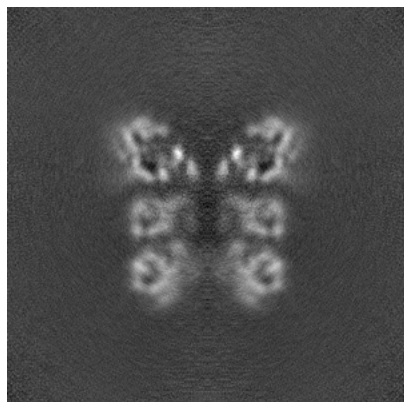


Y Index: 190

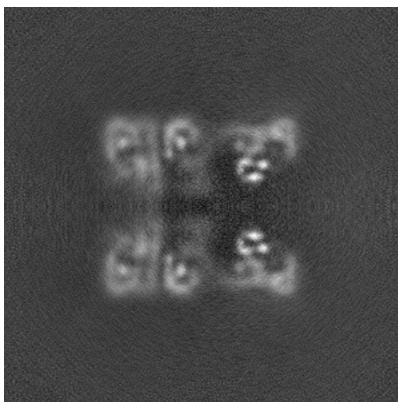


Z Index: 190

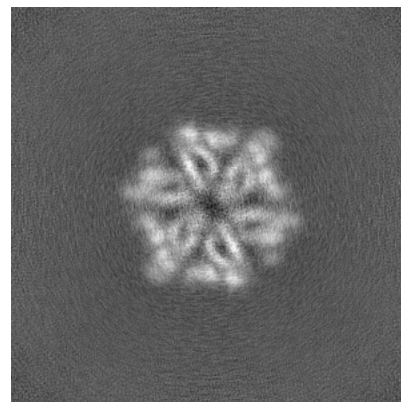
6.2.2 Raw map



X Index: 190



Y Index: 190

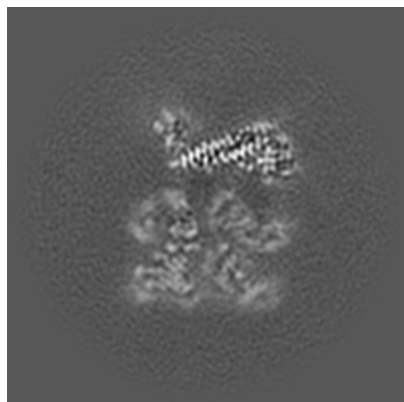


Z Index: 190

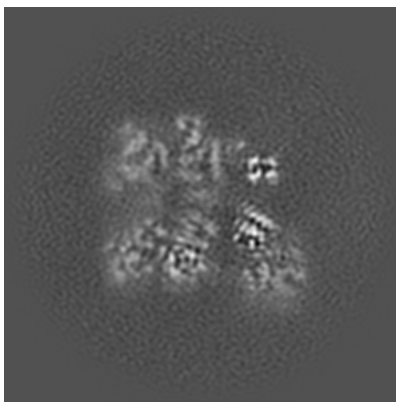
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

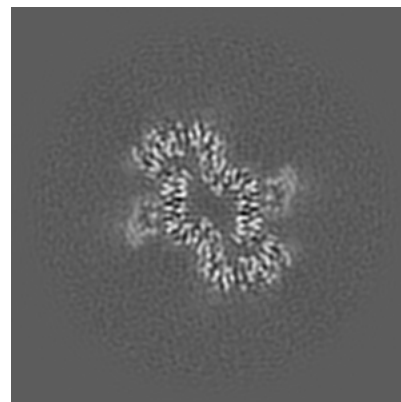
6.3.1 Primary map



X Index: 150

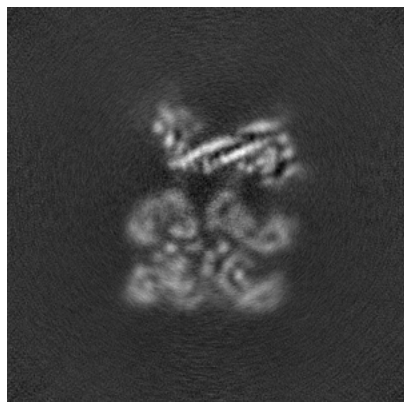


Y Index: 171

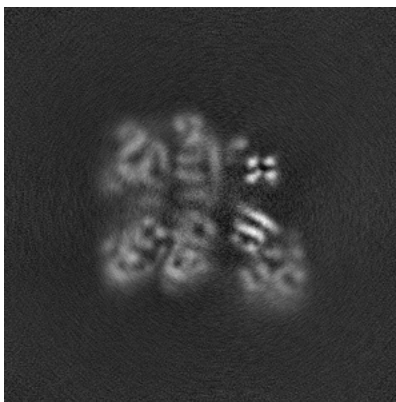


Z Index: 235

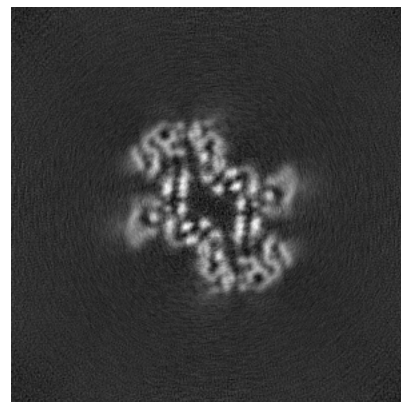
6.3.2 Raw map



X Index: 150



Y Index: 171

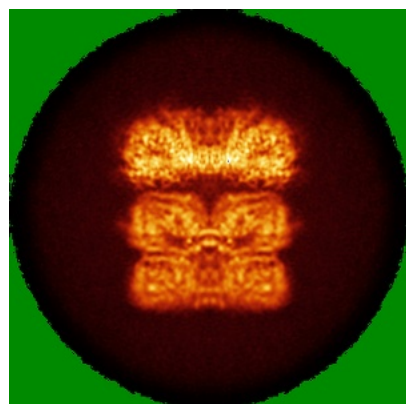


Z Index: 235

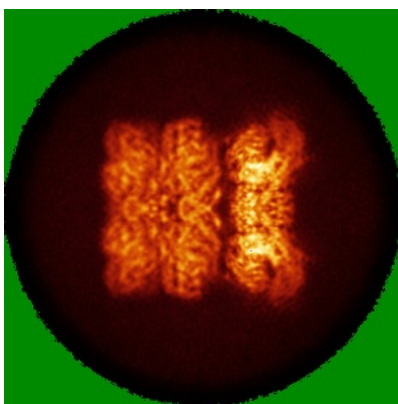
The images above show the largest variance slices of the map in three orthogonal directions.

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

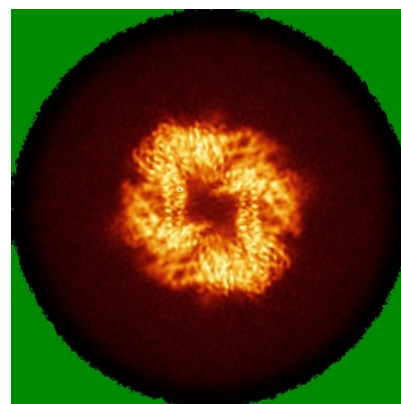
6.4.1 Primary map



X

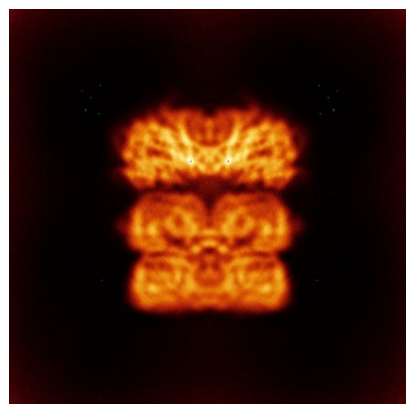


Y

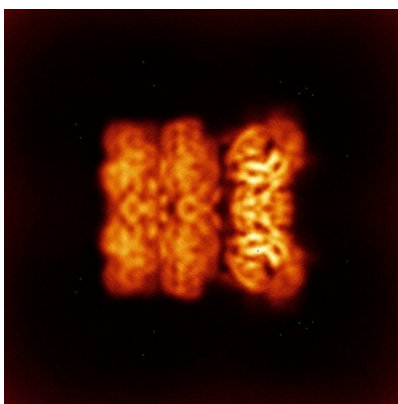


Z

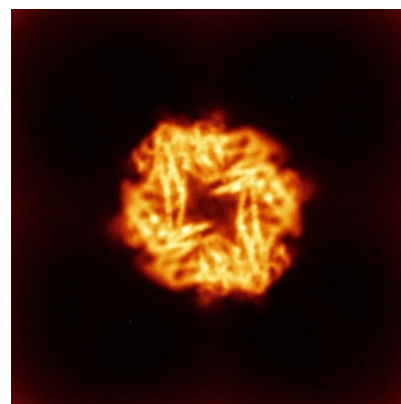
6.4.2 Raw map



X



Y

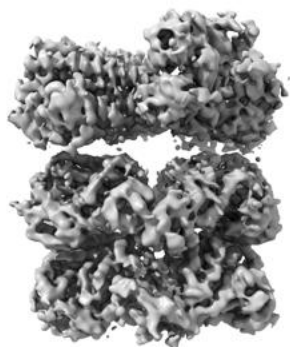


Z

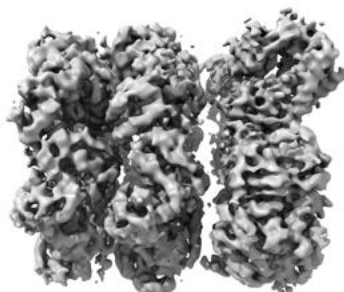
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

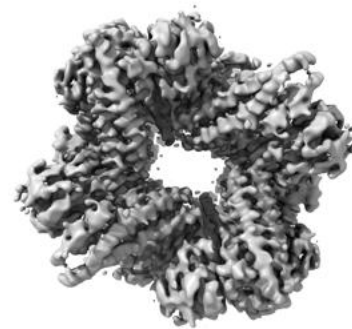
6.5.1 Primary map



X



Y



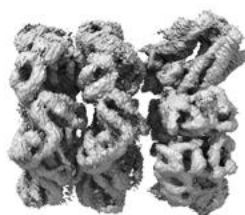
Z

The images above show the 3D surface view of the map at the recommended contour level 0.131. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

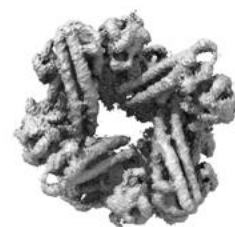
6.5.2 Raw map



X



Y



Z

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

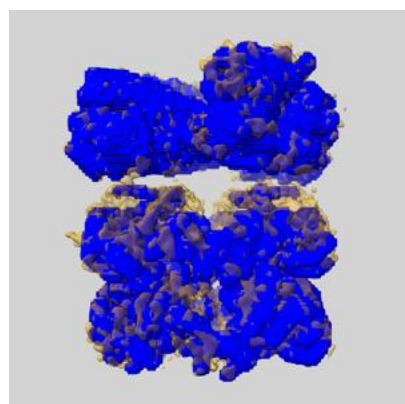
6.6 Mask visualisation [i](#)

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

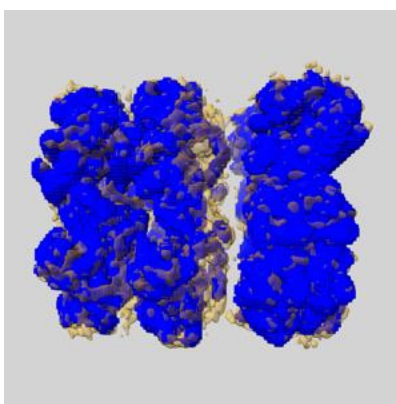
A mask typically either:

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

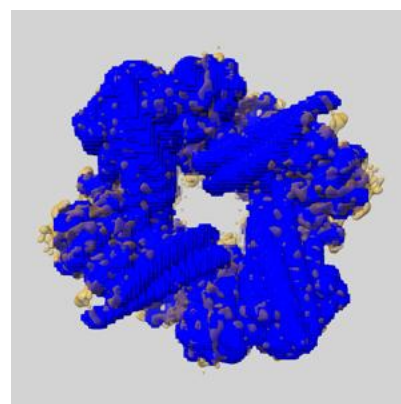
6.6.1 emd_19177_msk_1.map [i](#)



X



Y

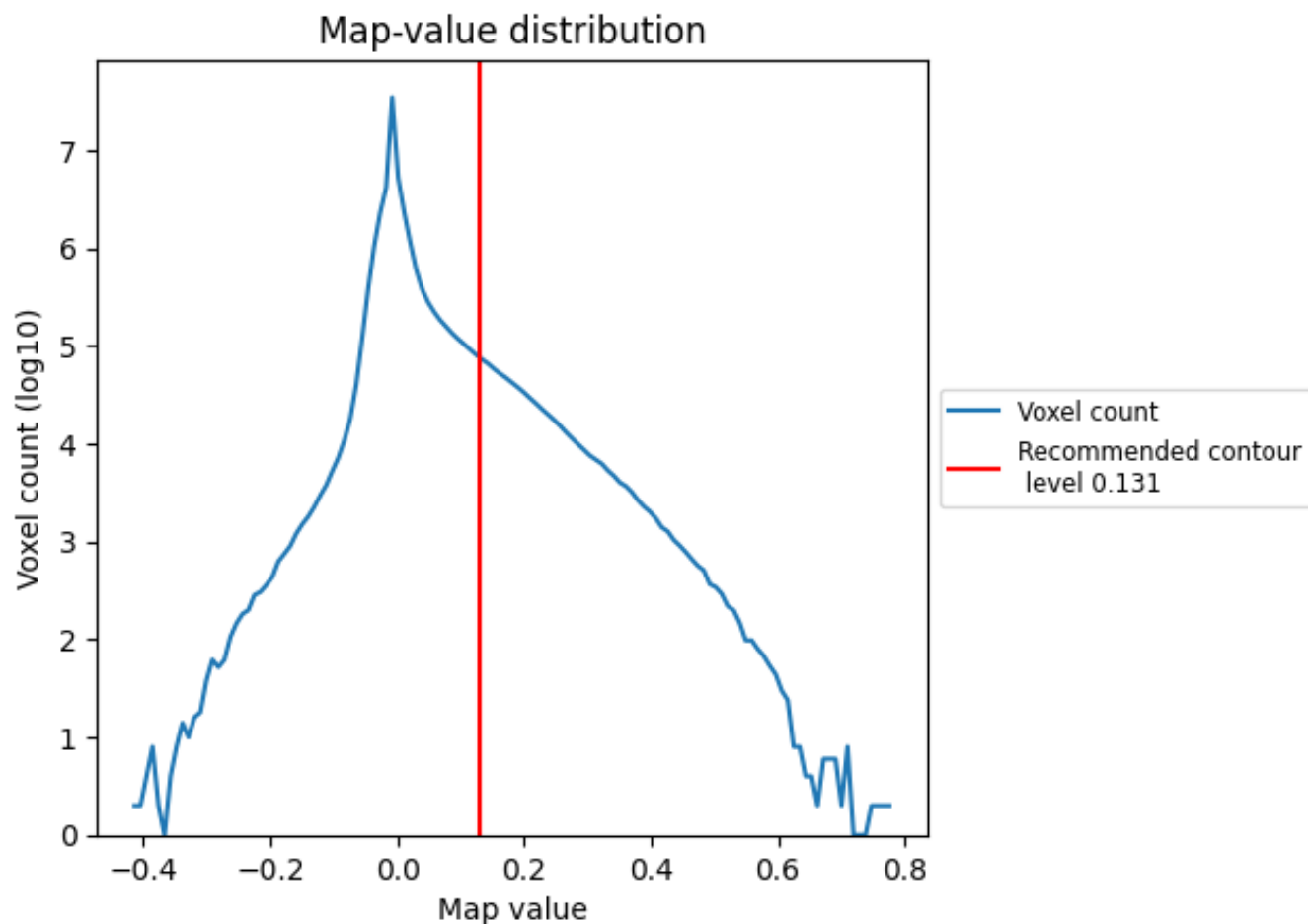


Z

7 Map analysis [i](#)

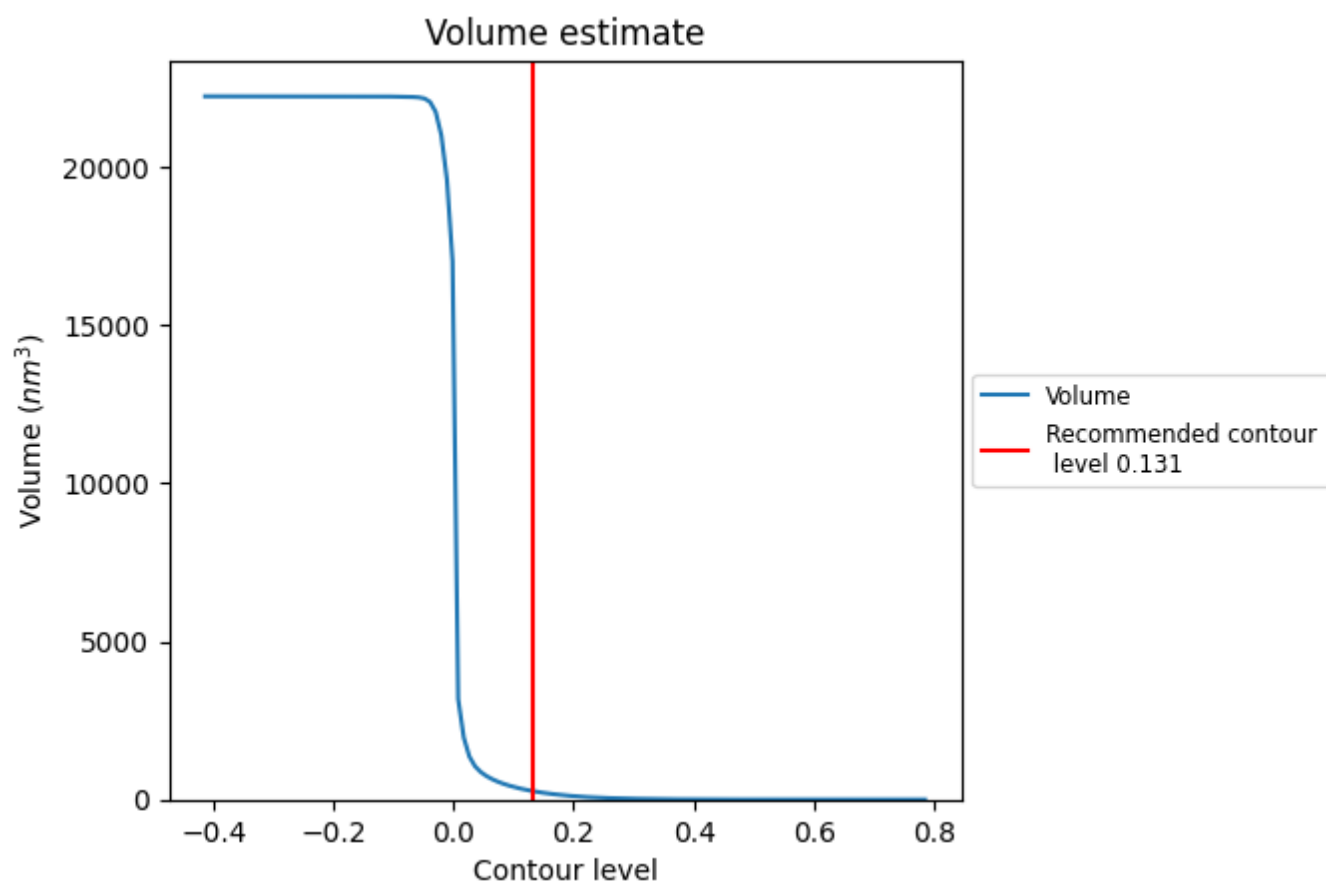
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

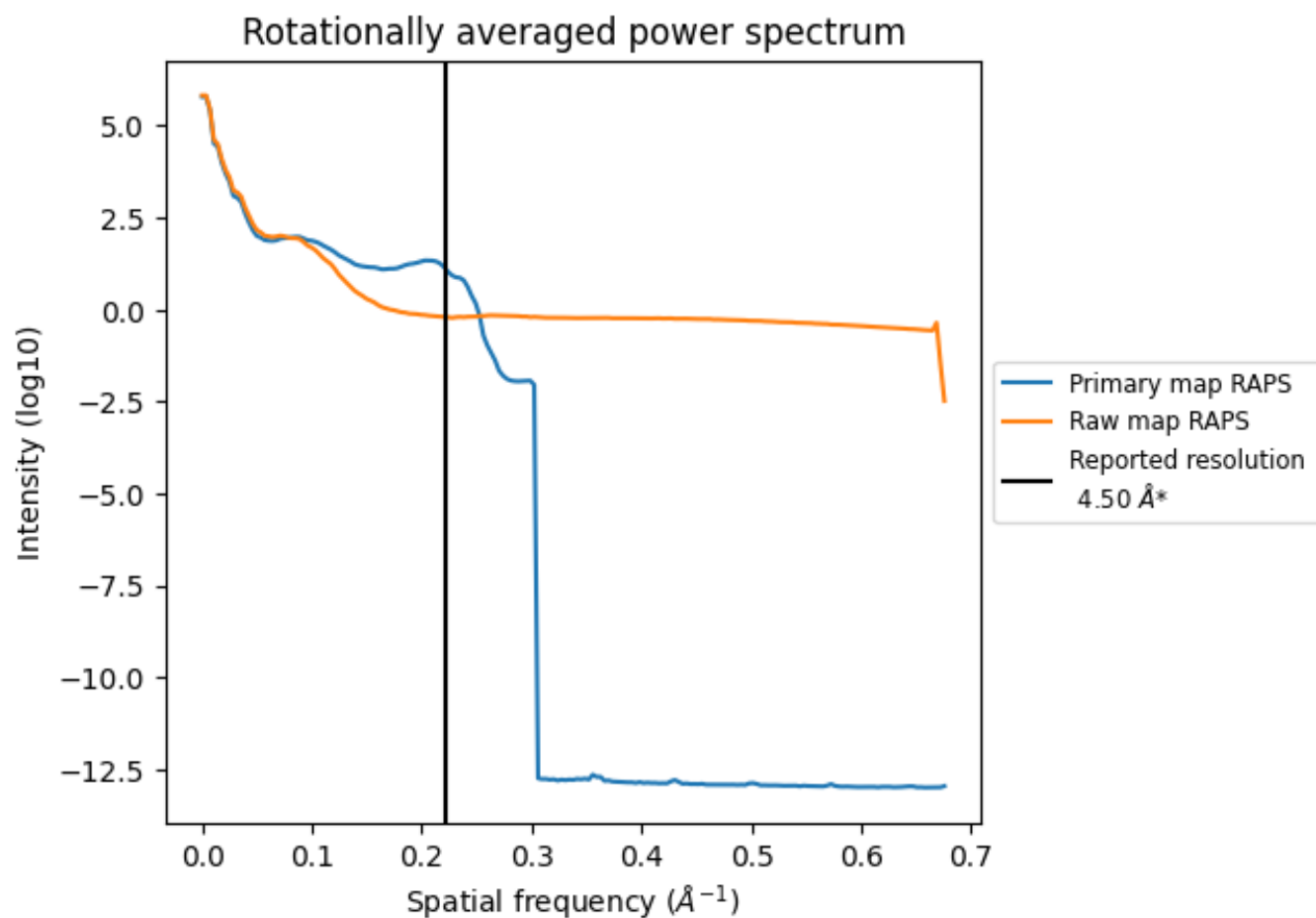
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 271 nm³; this corresponds to an approximate mass of 245 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 ⓘ

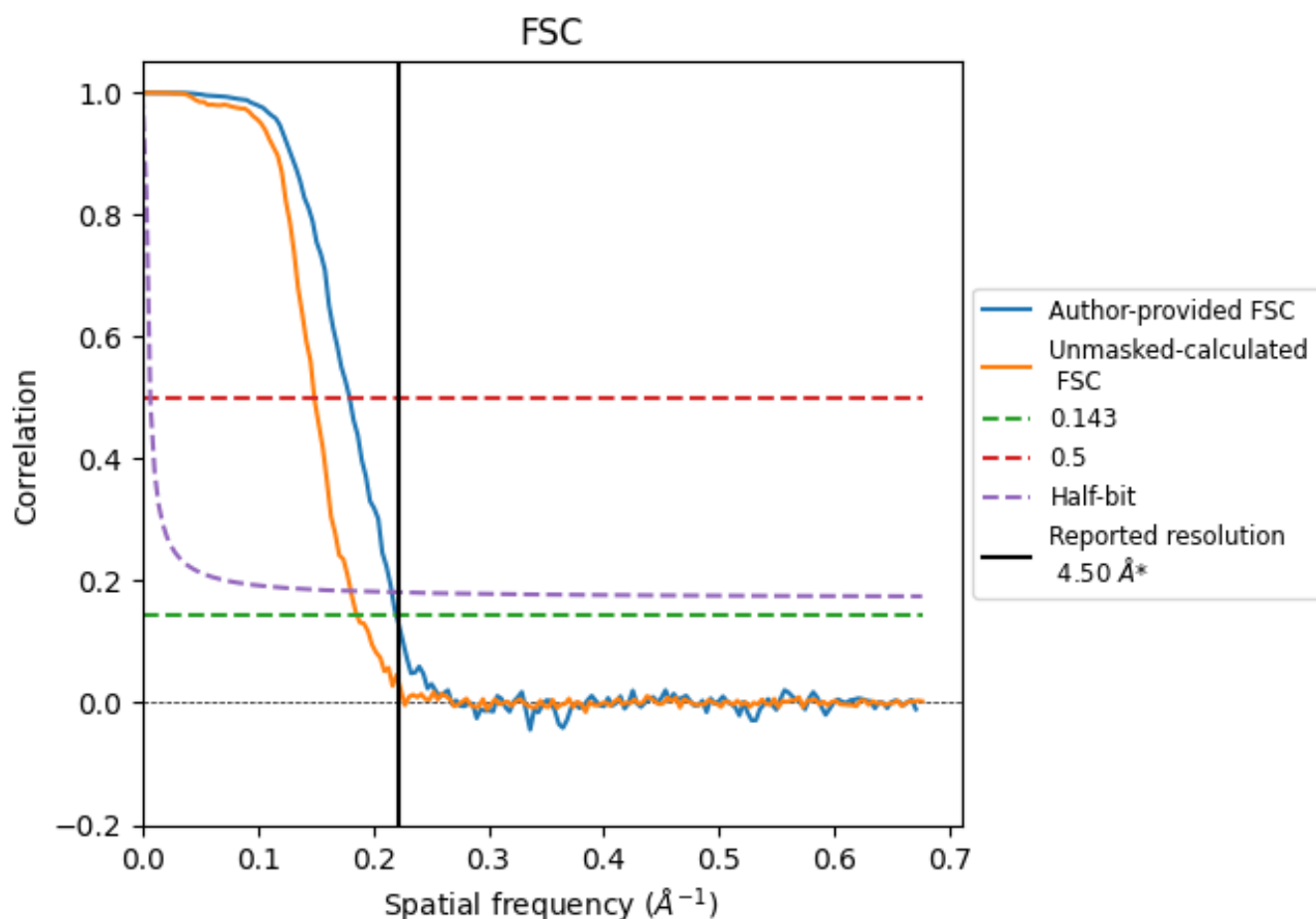


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

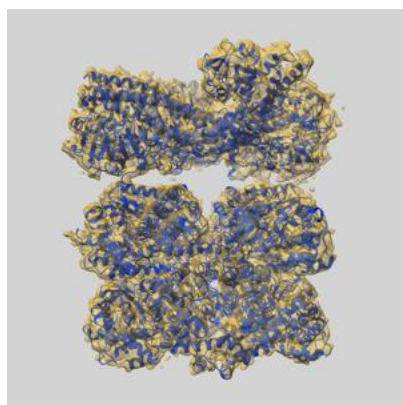
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.54	5.56	4.62
Unmasked-calculated*	5.37	6.71	5.53

*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 5.37 differs from the reported value 4.5 by more than 10 %

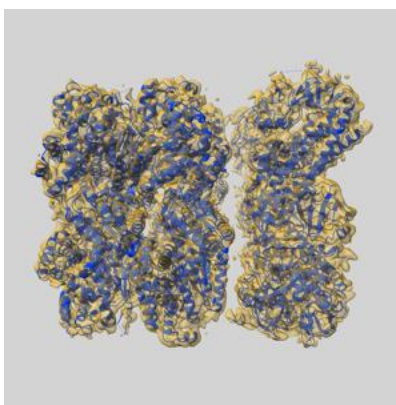
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19177 and PDB model 8RHN. Per-residue inclusion information can be found in section [3](#) on page [18](#).

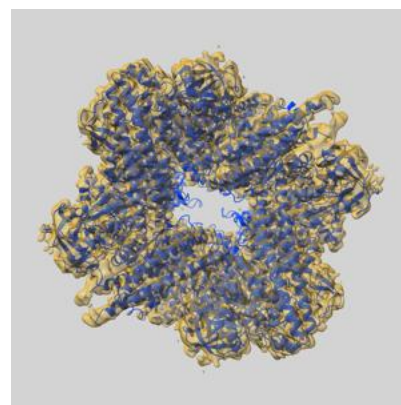
9.1 Map-model overlay [i](#)



X



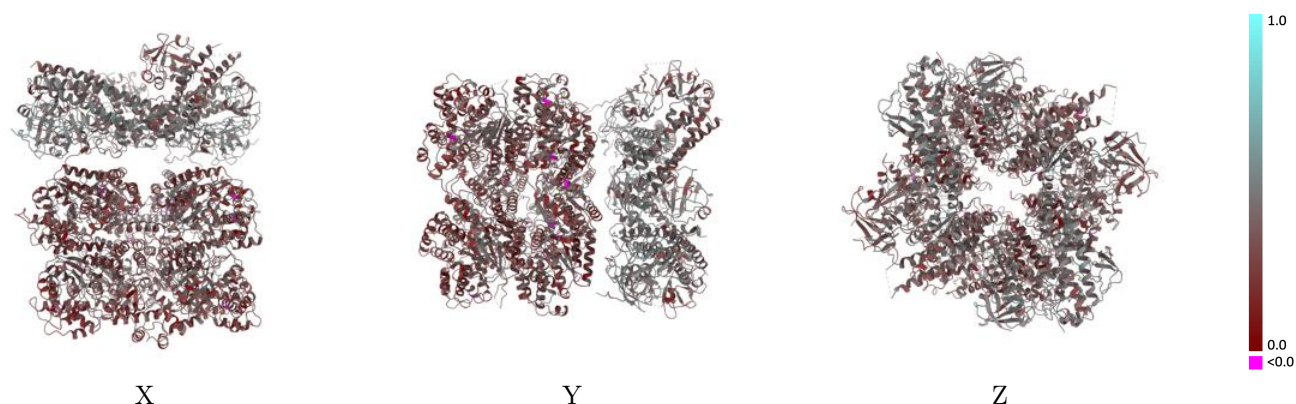
Y



Z

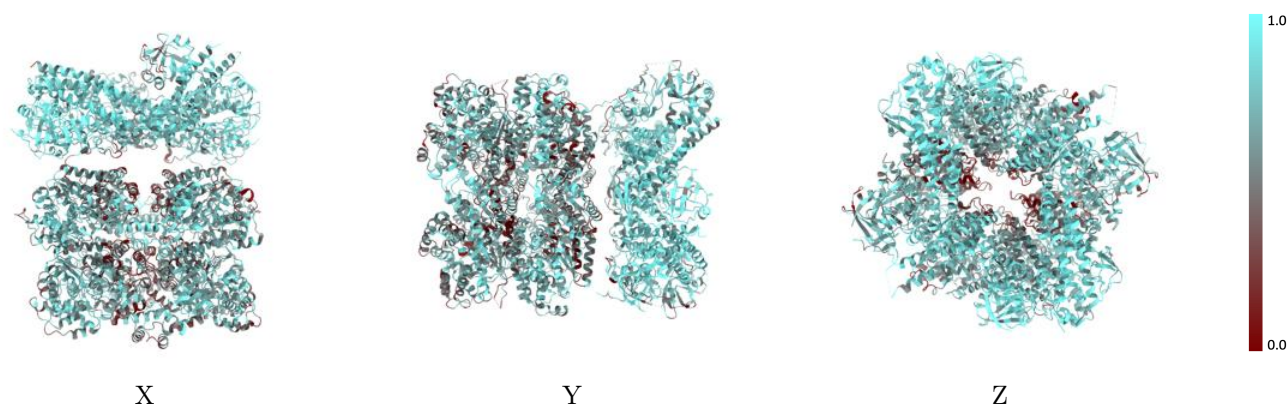
The images above show the 3D surface view of the map at the recommended contour level 0.131 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



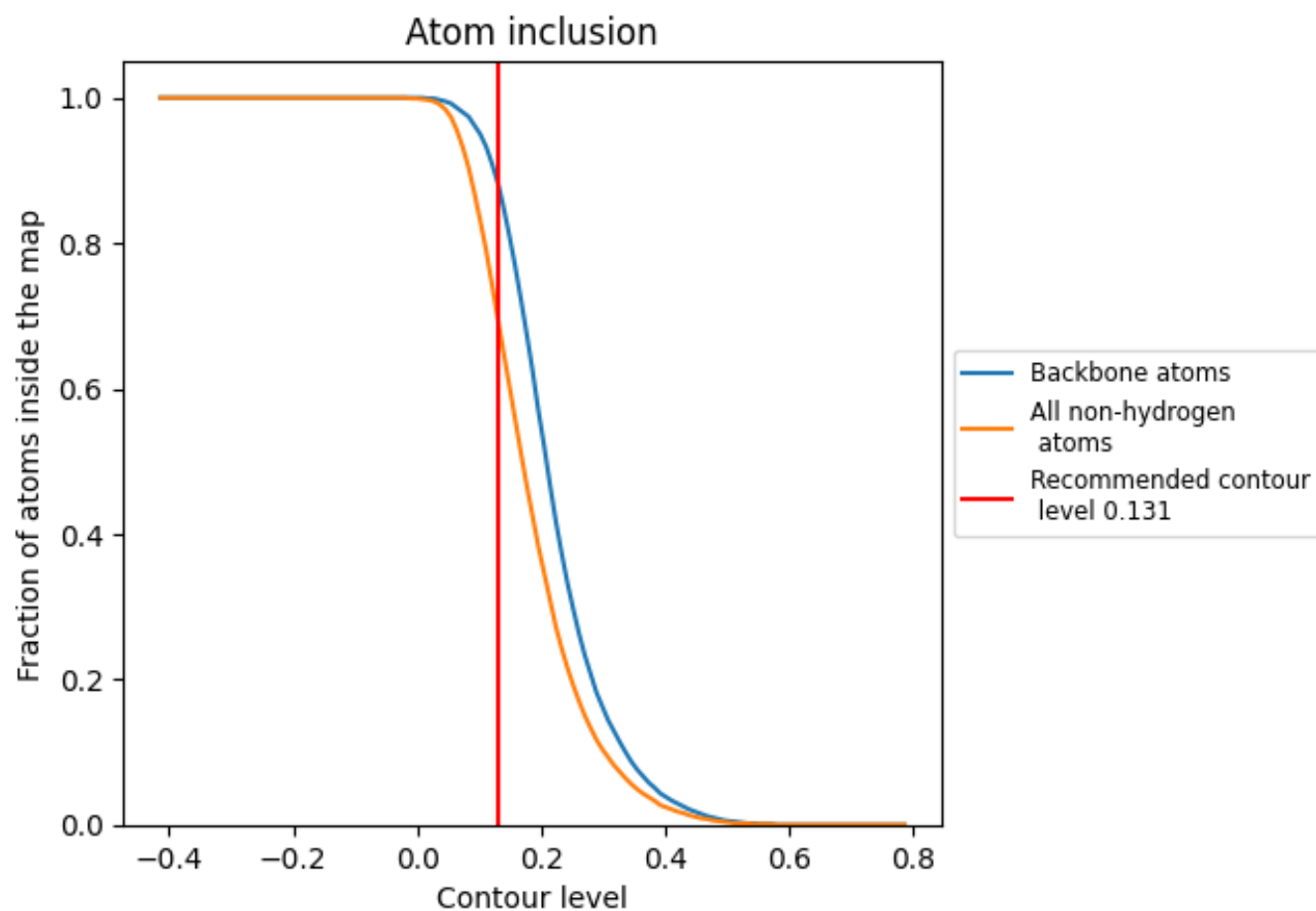
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.131).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 69% 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 (0.131) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.3610
A	 0.8740	 0.4530
B	 0.8790	 0.4550
C	 0.8280	 0.4120
D	 0.8240	 0.4130
E	 0.8400	 0.4510
F	 0.6760	 0.3780
G	 0.8380	 0.4420
H	 0.6890	 0.3920
I	 0.8310	 0.4560
J	 0.8380	 0.4600
K	 0.6510	 0.3190
L	 0.6550	 0.3330
M	 0.6520	 0.3210
N	 0.6580	 0.3360
O	 0.5620	 0.3070
P	 0.5560	 0.3060

