



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:31 PM UTC

PDB ID : 6QXM / pdb_00006qxm
EMDB ID : EMD-4669
Title : Cryo-EM structure of T7 bacteriophage portal protein, 12mer, open valve
Authors : Fabrega-Ferrer, M.; Cuervo, A.; Machon, C.; Fernandez, F.J.; Perez-Luque, R.; Pous, J.; Vega, M.C.; Carrascosa, J.L.; Coll, M.
Deposited on : 2019-03-07
Resolution : 4.10 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:

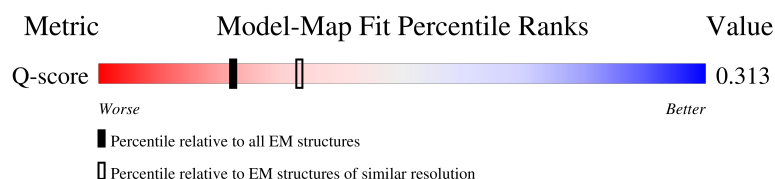
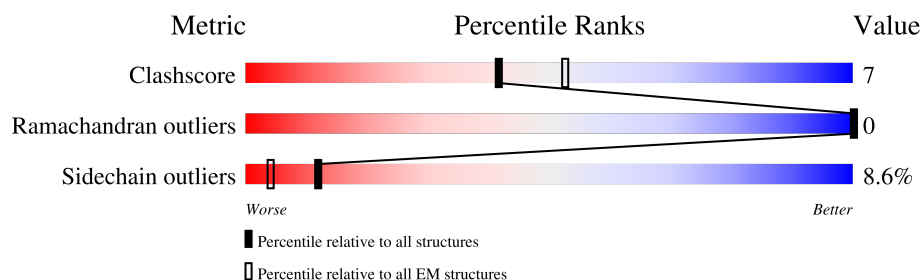
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.10 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	6458 (3.60 - 4.60)

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	547	<div> <div>24%</div> <div>55%</div> <div>16%</div> <div>28%</div> </div>
1	B	547	<div> <div>24%</div> <div>54%</div> <div>17%</div> <div>28%</div> </div>
1	C	547	<div> <div>26%</div> <div>54%</div> <div>16%</div> <div>28%</div> </div>
1	D	547	<div> <div>24%</div> <div>54%</div> <div>16%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
1	E	547	
1	F	547	
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 37164 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	B	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	C	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	D	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	E	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	F	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	G	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	H	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	I	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	J	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	K	392	Total 3097	C 1961	N 522	O 600	S 14	0	0
1	L	392	Total 3097	C 1961	N 522	O 600	S 14	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	ALA	-	expression tag	UNP P03728
A	538	ALA	-	expression tag	UNP P03728
A	539	ALA	-	expression tag	UNP P03728
A	540	LEU	-	expression tag	UNP P03728
A	541	GLU	-	expression tag	UNP P03728
A	542	HIS	-	expression tag	UNP P03728

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Chain	Residue	Modelled	Actual	Comment	Reference
A	543	HIS	-	expression tag	UNP P03728
A	544	HIS	-	expression tag	UNP P03728
A	545	HIS	-	expression tag	UNP P03728
A	546	HIS	-	expression tag	UNP P03728
A	547	HIS	-	expression tag	UNP P03728
B	537	ALA	-	expression tag	UNP P03728
B	538	ALA	-	expression tag	UNP P03728
B	539	ALA	-	expression tag	UNP P03728
B	540	LEU	-	expression tag	UNP P03728
B	541	GLU	-	expression tag	UNP P03728
B	542	HIS	-	expression tag	UNP P03728
B	543	HIS	-	expression tag	UNP P03728
B	544	HIS	-	expression tag	UNP P03728
B	545	HIS	-	expression tag	UNP P03728
B	546	HIS	-	expression tag	UNP P03728
B	547	HIS	-	expression tag	UNP P03728
C	537	ALA	-	expression tag	UNP P03728
C	538	ALA	-	expression tag	UNP P03728
C	539	ALA	-	expression tag	UNP P03728
C	540	LEU	-	expression tag	UNP P03728
C	541	GLU	-	expression tag	UNP P03728
C	542	HIS	-	expression tag	UNP P03728
C	543	HIS	-	expression tag	UNP P03728
C	544	HIS	-	expression tag	UNP P03728
C	545	HIS	-	expression tag	UNP P03728
C	546	HIS	-	expression tag	UNP P03728
C	547	HIS	-	expression tag	UNP P03728
D	537	ALA	-	expression tag	UNP P03728
D	538	ALA	-	expression tag	UNP P03728
D	539	ALA	-	expression tag	UNP P03728
D	540	LEU	-	expression tag	UNP P03728
D	541	GLU	-	expression tag	UNP P03728
D	542	HIS	-	expression tag	UNP P03728
D	543	HIS	-	expression tag	UNP P03728
D	544	HIS	-	expression tag	UNP P03728
D	545	HIS	-	expression tag	UNP P03728
D	546	HIS	-	expression tag	UNP P03728
D	547	HIS	-	expression tag	UNP P03728
E	537	ALA	-	expression tag	UNP P03728
E	538	ALA	-	expression tag	UNP P03728
E	539	ALA	-	expression tag	UNP P03728
E	540	LEU	-	expression tag	UNP P03728

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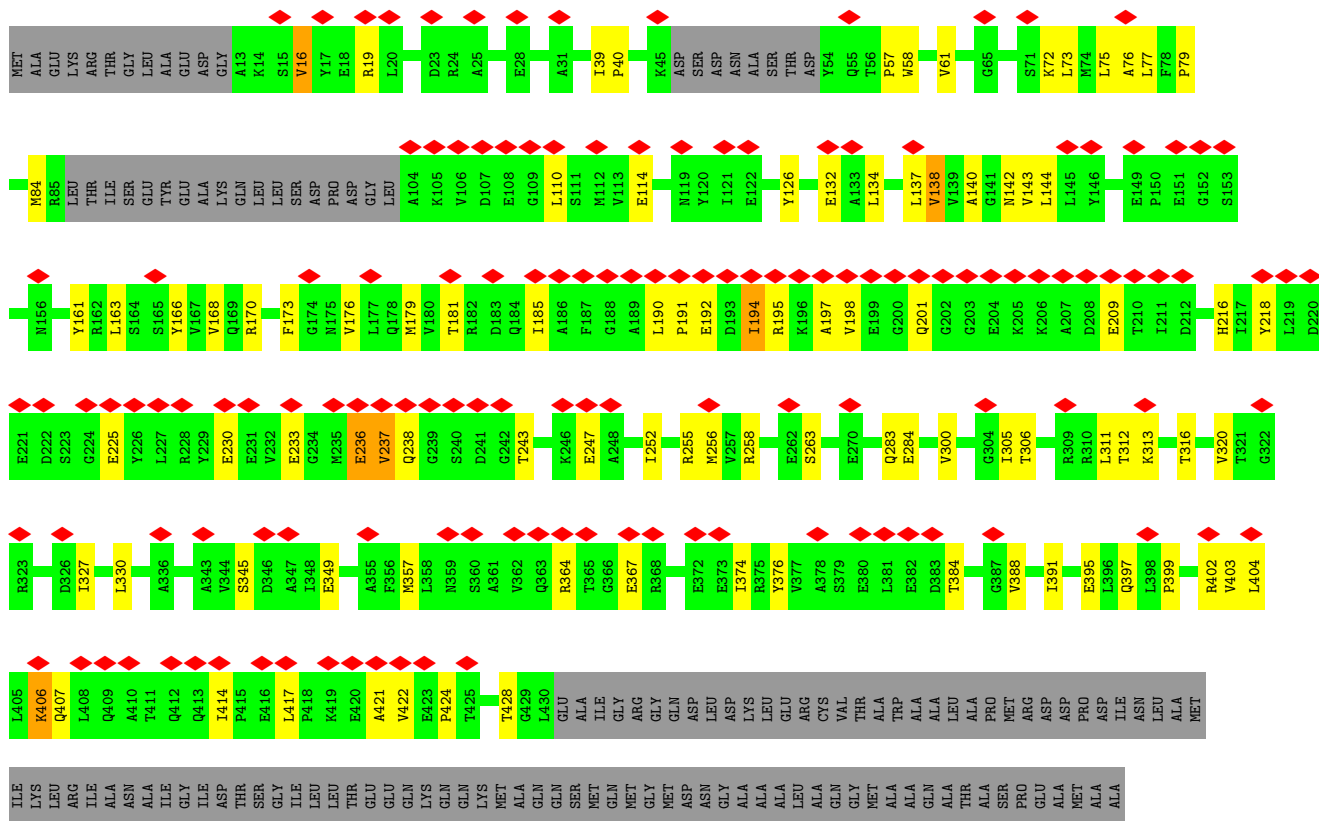
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Chain	Residue	Modelled	Actual	Comment	Reference
E	541	GLU	-	expression tag	UNP P03728
E	542	HIS	-	expression tag	UNP P03728
E	543	HIS	-	expression tag	UNP P03728
E	544	HIS	-	expression tag	UNP P03728
E	545	HIS	-	expression tag	UNP P03728
E	546	HIS	-	expression tag	UNP P03728
E	547	HIS	-	expression tag	UNP P03728
F	537	ALA	-	expression tag	UNP P03728
F	538	ALA	-	expression tag	UNP P03728
F	539	ALA	-	expression tag	UNP P03728
F	540	LEU	-	expression tag	UNP P03728
F	541	GLU	-	expression tag	UNP P03728
F	542	HIS	-	expression tag	UNP P03728
F	543	HIS	-	expression tag	UNP P03728
F	544	HIS	-	expression tag	UNP P03728
F	545	HIS	-	expression tag	UNP P03728
F	546	HIS	-	expression tag	UNP P03728
F	547	HIS	-	expression tag	UNP P03728
G	537	ALA	-	expression tag	UNP P03728
G	538	ALA	-	expression tag	UNP P03728
G	539	ALA	-	expression tag	UNP P03728
G	540	LEU	-	expression tag	UNP P03728
G	541	GLU	-	expression tag	UNP P03728
G	542	HIS	-	expression tag	UNP P03728
G	543	HIS	-	expression tag	UNP P03728
G	544	HIS	-	expression tag	UNP P03728
G	545	HIS	-	expression tag	UNP P03728
G	546	HIS	-	expression tag	UNP P03728
G	547	HIS	-	expression tag	UNP P03728
H	537	ALA	-	expression tag	UNP P03728
H	538	ALA	-	expression tag	UNP P03728
H	539	ALA	-	expression tag	UNP P03728
H	540	LEU	-	expression tag	UNP P03728
H	541	GLU	-	expression tag	UNP P03728
H	542	HIS	-	expression tag	UNP P03728
H	543	HIS	-	expression tag	UNP P03728
H	544	HIS	-	expression tag	UNP P03728
H	545	HIS	-	expression tag	UNP P03728
H	546	HIS	-	expression tag	UNP P03728
H	547	HIS	-	expression tag	UNP P03728
I	537	ALA	-	expression tag	UNP P03728
I	538	ALA	-	expression tag	UNP P03728

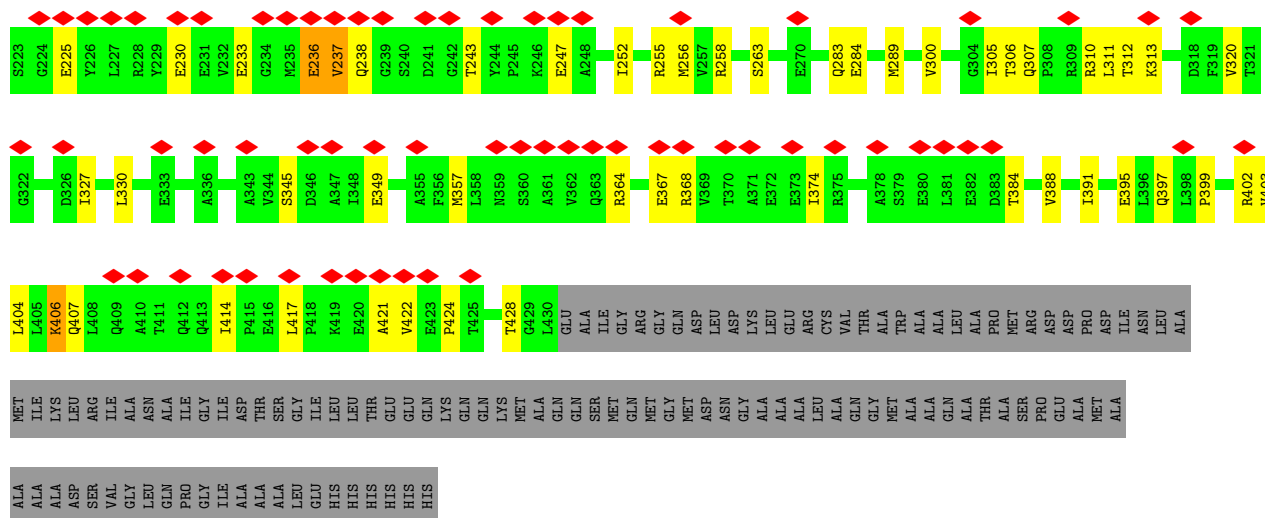
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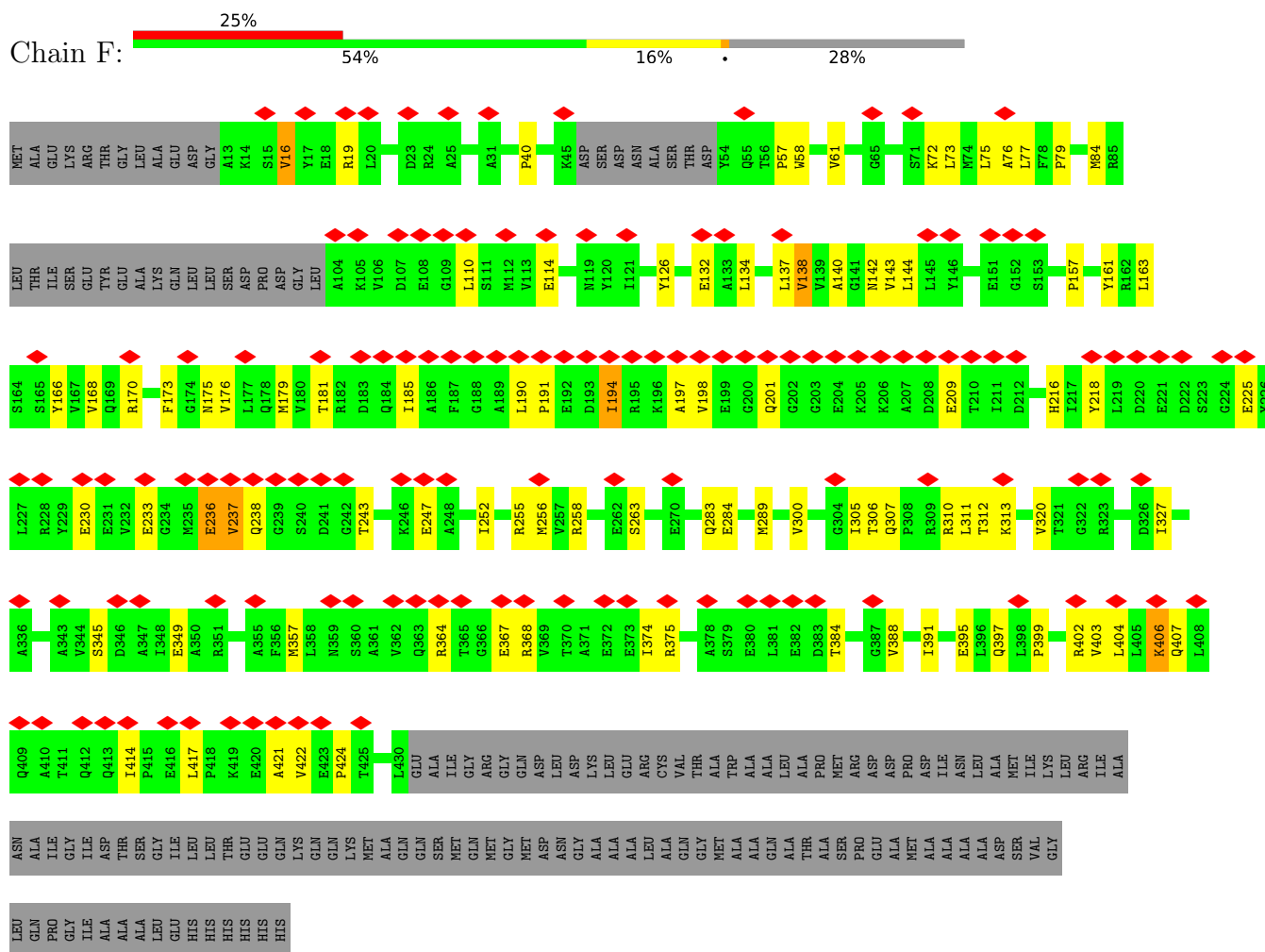
Chain	Residue	Modelled	Actual	Comment	Reference
I	539	ALA	-	expression tag	UNP P03728
I	540	LEU	-	expression tag	UNP P03728
I	541	GLU	-	expression tag	UNP P03728
I	542	HIS	-	expression tag	UNP P03728
I	543	HIS	-	expression tag	UNP P03728
I	544	HIS	-	expression tag	UNP P03728
I	545	HIS	-	expression tag	UNP P03728
I	546	HIS	-	expression tag	UNP P03728
I	547	HIS	-	expression tag	UNP P03728
J	537	ALA	-	expression tag	UNP P03728
J	538	ALA	-	expression tag	UNP P03728
J	539	ALA	-	expression tag	UNP P03728
J	540	LEU	-	expression tag	UNP P03728
J	541	GLU	-	expression tag	UNP P03728
J	542	HIS	-	expression tag	UNP P03728
J	543	HIS	-	expression tag	UNP P03728
J	544	HIS	-	expression tag	UNP P03728
J	545	HIS	-	expression tag	UNP P03728
J	546	HIS	-	expression tag	UNP P03728
J	547	HIS	-	expression tag	UNP P03728
K	537	ALA	-	expression tag	UNP P03728
K	538	ALA	-	expression tag	UNP P03728
K	539	ALA	-	expression tag	UNP P03728
K	540	LEU	-	expression tag	UNP P03728
K	541	GLU	-	expression tag	UNP P03728
K	542	HIS	-	expression tag	UNP P03728
K	543	HIS	-	expression tag	UNP P03728
K	544	HIS	-	expression tag	UNP P03728
K	545	HIS	-	expression tag	UNP P03728
K	546	HIS	-	expression tag	UNP P03728
K	547	HIS	-	expression tag	UNP P03728
L	537	ALA	-	expression tag	UNP P03728
L	538	ALA	-	expression tag	UNP P03728
L	539	ALA	-	expression tag	UNP P03728
L	540	LEU	-	expression tag	UNP P03728
L	541	GLU	-	expression tag	UNP P03728
L	542	HIS	-	expression tag	UNP P03728
L	543	HIS	-	expression tag	UNP P03728
L	544	HIS	-	expression tag	UNP P03728
L	545	HIS	-	expression tag	UNP P03728
L	546	HIS	-	expression tag	UNP P03728
L	547	HIS	-	expression tag	UNP P03728



Protein	Residue	Score	Category	
MET	Y161	0.85	High	
	L162	0.85	High	
	L163	0.85	High	
	S164	0.85	High	
	S165	0.85	High	
	Y166	0.85	High	
	Y167	0.85	High	
	Y168	0.85	High	
	Q169	0.85	High	
	R170	0.85	High	
ALA	F173	0.85	High	
	G174	0.85	High	
	N175	0.85	High	
	Y176	0.85	High	
	L177	0.85	High	
	Q178	0.85	High	
	M179	0.85	High	
	H180	0.85	High	
	T181	0.85	High	
	D182	0.85	High	
LYS	Q184	0.85	High	
	I185	0.85	High	
	A186	0.85	High	
	F187	0.85	High	
	G188	0.85	High	
	L189	0.85	High	
	L190	0.85	High	
	P191	0.85	High	
	E192	0.85	High	
	D193	0.85	High	
GLU	I194	0.85	High	
	R195	0.85	High	
	K196	0.85	High	
	A197	0.85	High	
	E198	0.85	High	
	E199	0.85	High	
	G200	0.85	High	
	Q201	0.85	High	
	G202	0.85	High	
	E203	0.85	High	
THR	E204	0.85	High	
	K205	0.85	High	
	K206	0.85	High	
	A207	0.85	High	
	D208	0.85	High	
	E209	0.85	High	
	T210	0.85	High	
	I211	0.85	High	
	D212	0.85	High	
	GLY	H216	0.85	High
L217		0.85	High	
Y218		0.85	High	
L219		0.85	High	
D220		0.85	High	
E221		0.85	High	
D222		0.85	High	
ASP		Y216	0.85	High
		P217	0.85	High
		SER	H24	0.85
	R85		0.85	High
	LEU		0.85	High
	THR		0.85	High
	TLE		0.85	High
	SER		0.85	High
	GLU		0.85	High
	TYR		0.85	High
GLU	0.85		High	
ALA	0.85		High	
THR	LVS	0.85	High	
	GLN	0.85	High	
	LEU	0.85	High	
	LEU	0.85	High	
	SER	0.85	High	
	ASP	0.85	High	
	PRO	0.85	High	
	ASP	0.85	High	
	GLY	0.85	High	
	LEU	0.85	High	
ASP	A104	0.85	High	
	K105	0.85	High	
	V106	0.85	High	
	D107	0.85	High	
	E108	0.85	High	
	G109	0.85	High	
	L110	0.85	High	
	S111	0.85	High	
	M112	0.85	High	
	V113	0.85	High	
SER	E114	0.85	High	
	R115	0.85	High	
	N119	0.85	High	
	Y126	0.85	High	
	E132	0.85	High	
	A133	0.85	High	
	L134	0.85	High	
	L137	0.85	High	
	V138	0.85	High	
	A140	0.85	High	
THR	G141	0.85	High	
	N142	0.85	High	
	V143	0.85	High	
	L144	0.85	High	
	L145	0.85	High	
	Y146	0.85	High	
	E149	0.85	High	
	P150	0.85	High	
	E151	0.85	High	
	G152	0.85	High	
ASP	Y155	0.85	High	
	P157	0.85	High	
	SER	K45	0.85	High
		ASP	0.85	High
		ASP	0.85	High
		ASN	0.85	High
		ALA	0.85	High
		SER	0.85	High
		THR	0.85	High
		ASP	0.85	High
Y54		0.85	High	
GLY		P57	0.85	High
	W58	0.85	High	
	V61	0.85	High	
	G65	0.85	High	
	S71	0.85	High	
	K72	0.85	High	
	L73	0.85	High	
	W74	0.85	High	
	L75	0.85	High	
	A76	0.85	High	
ASP	L77	0.85	High	
	F76	0.85	High	
	P79	0.85	High	
	GLY	A13	0.85	High
		K14	0.85	High
		S15	0.85	High
		V16	0.85	High
		Y17	0.85	High
		E18	0.85	High
		R19	0.85	High
L20		0.85	High	

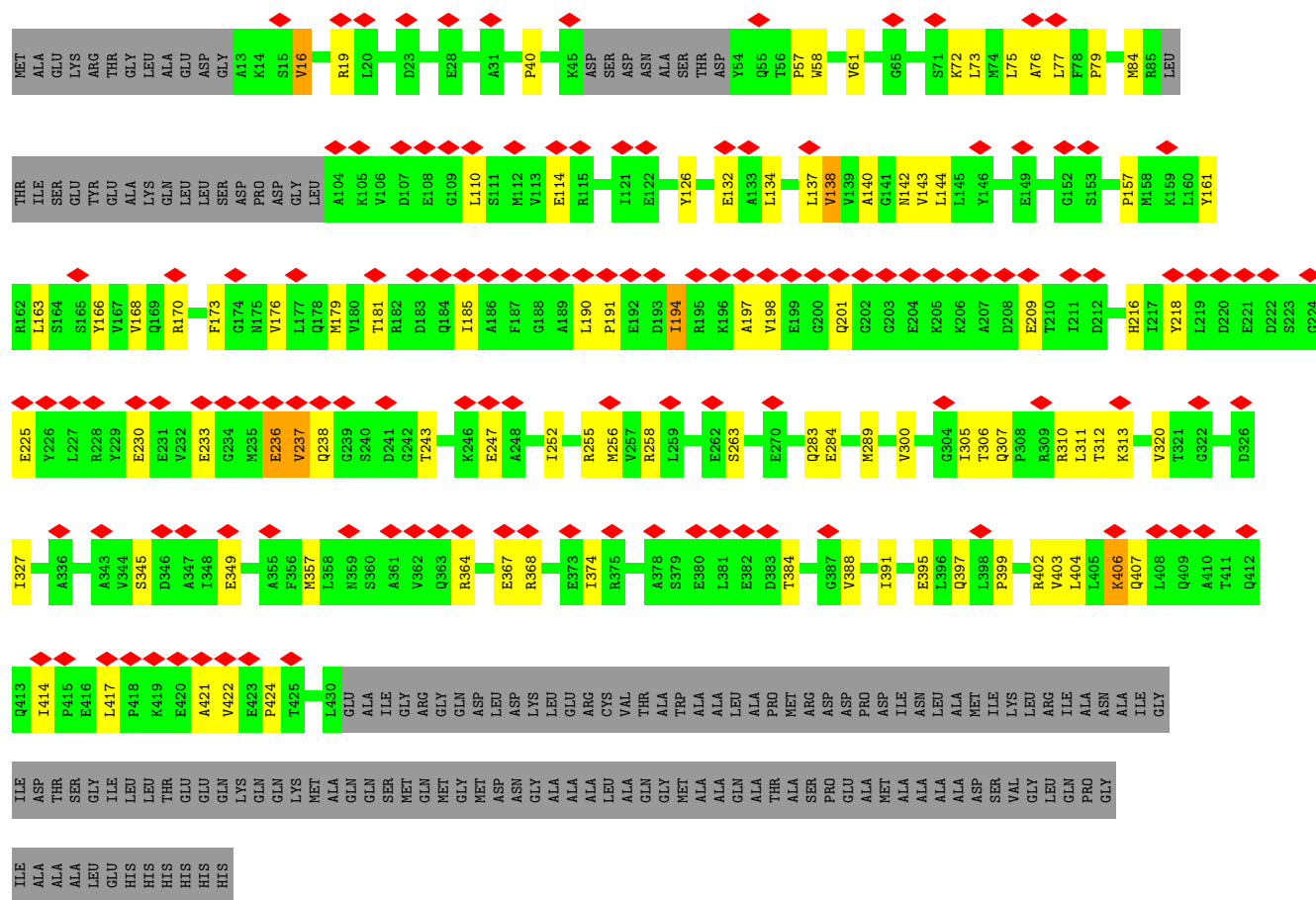


• Molecule 1: Portal protein

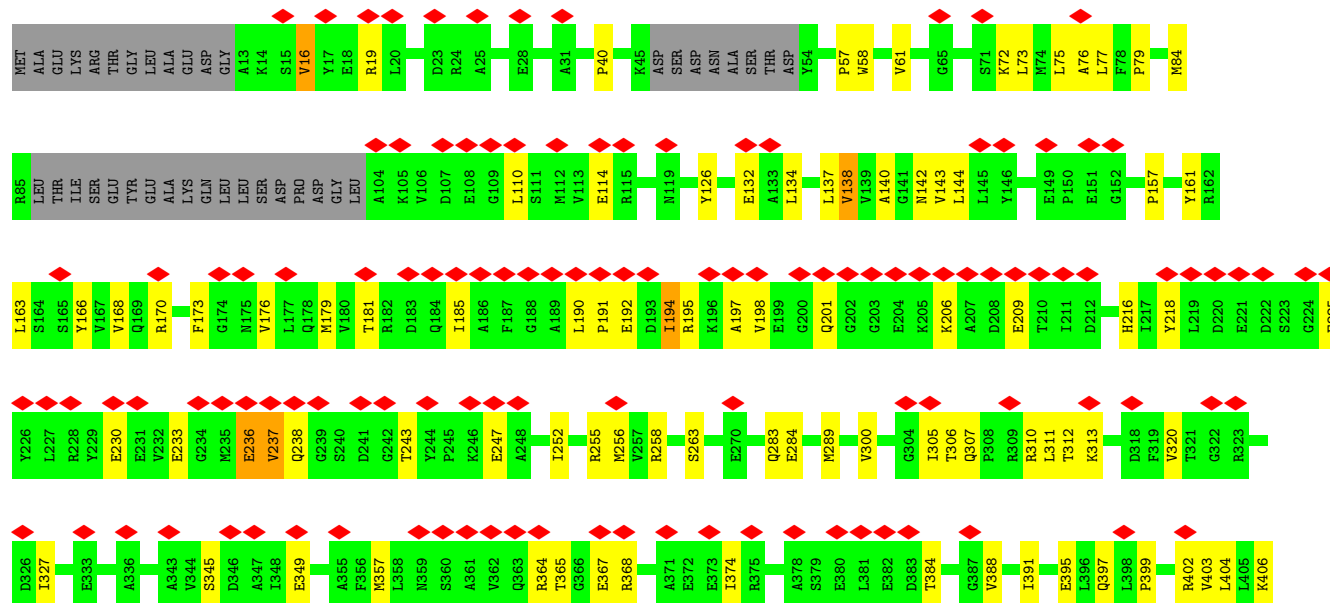


• Molecule 1: Portal protein

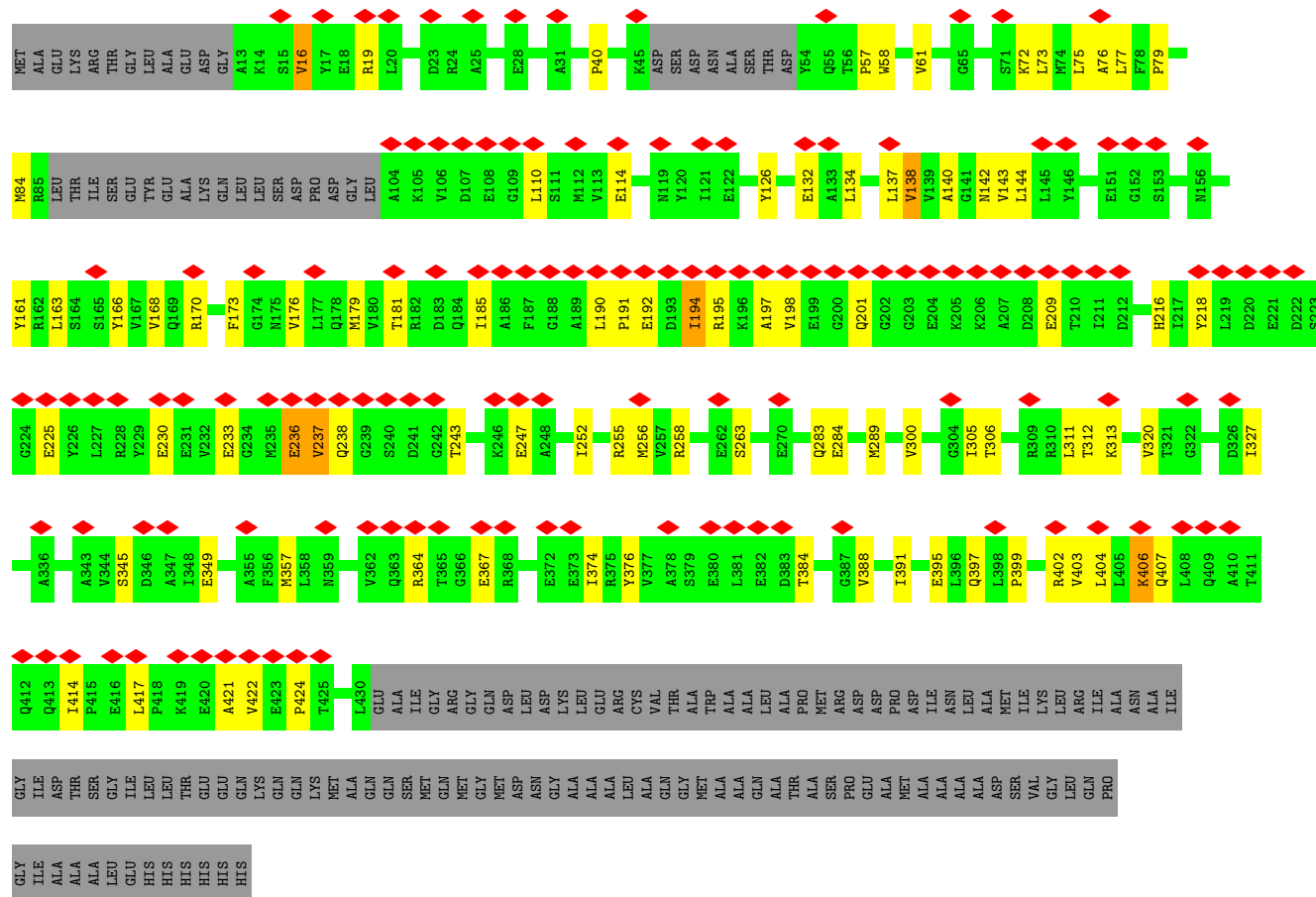




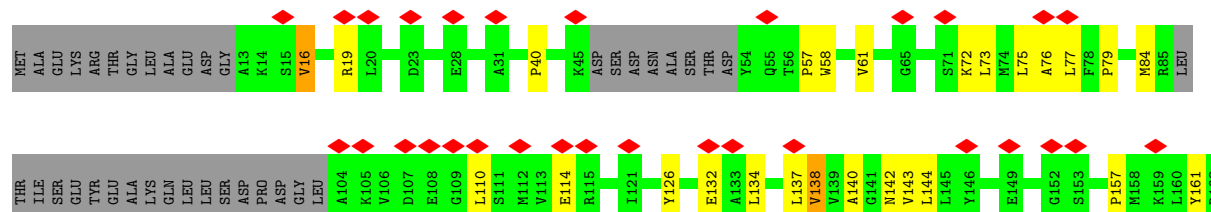
● Molecule 1: Portal protein

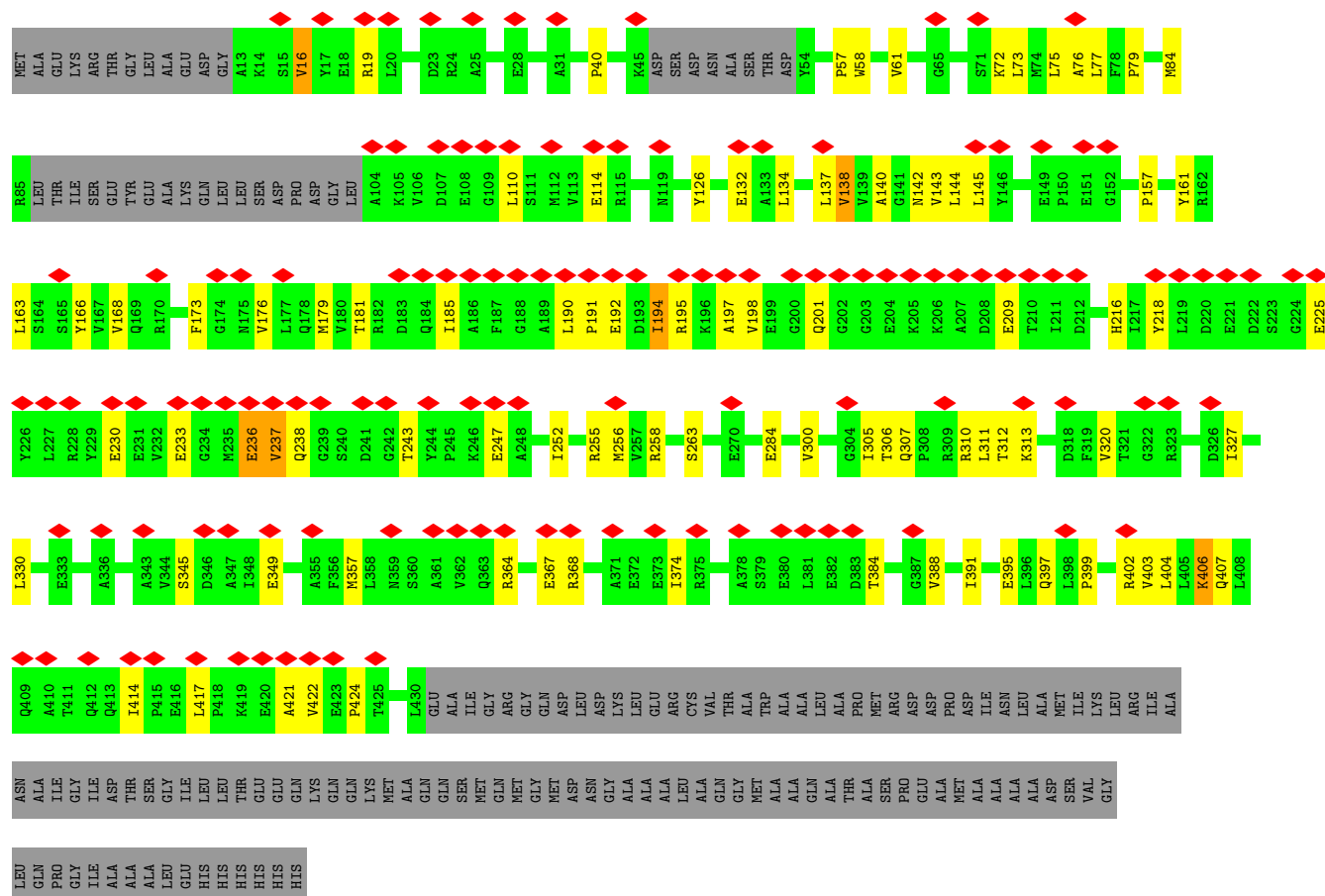


- Molecule 1: Portal protein

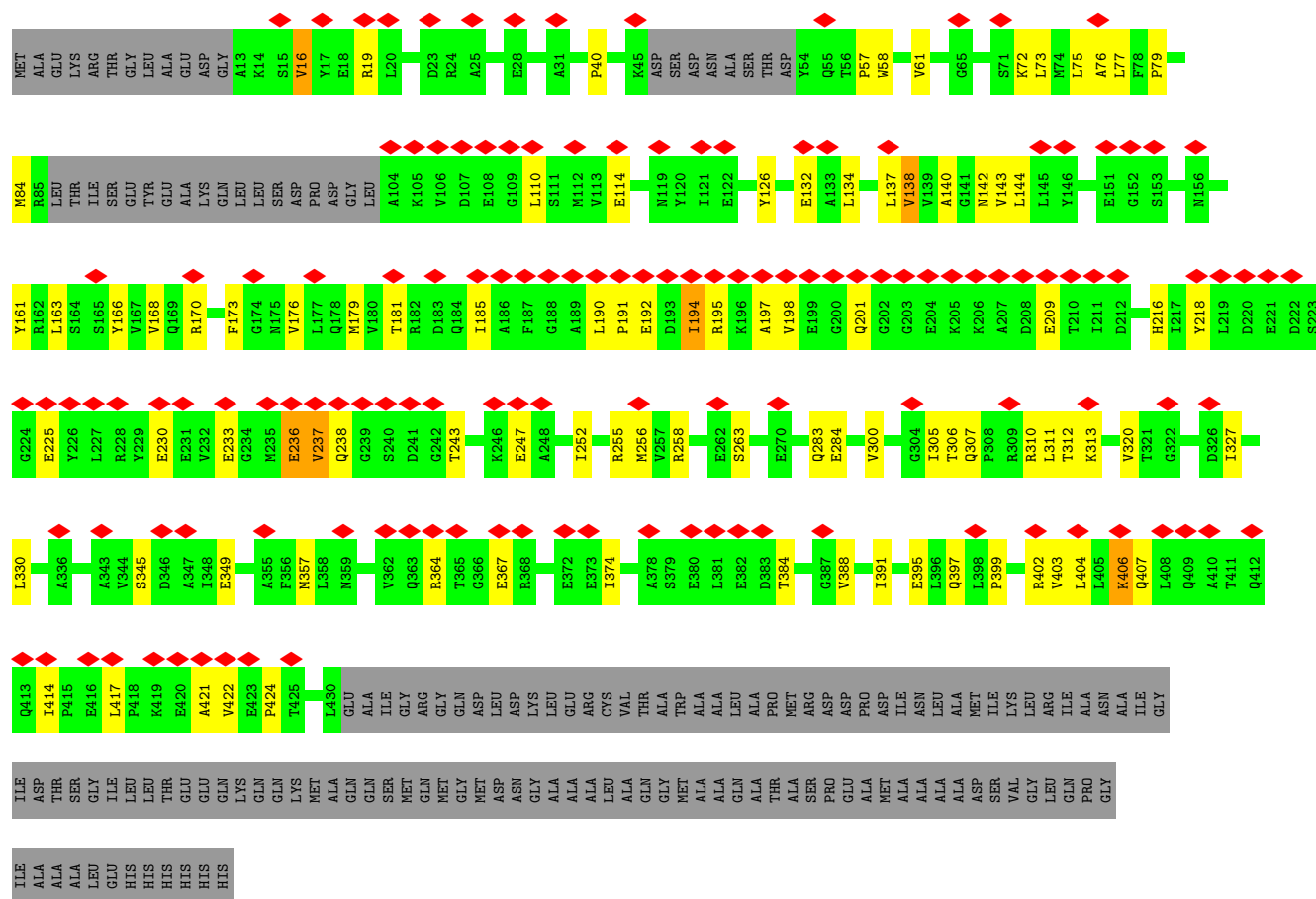


- Molecule 1: Portal protein





• Molecule 1: Portal protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C12	Depositor
Number of particles used	32688	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 ($e^-/\text{\AA}^2$)	39.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.487	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0577	Depositor
Map size (Å)	228.79999, 228.79999, 228.79999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/3149	0.76	2/4261 (0.0%)
1	B	0.37	0/3149	0.76	2/4261 (0.0%)
1	C	0.37	0/3149	0.76	2/4261 (0.0%)
1	D	0.37	0/3149	0.76	2/4261 (0.0%)
1	E	0.37	0/3149	0.76	2/4261 (0.0%)
1	F	0.37	0/3149	0.76	2/4261 (0.0%)
1	G	0.37	0/3149	0.76	2/4261 (0.0%)
1	H	0.37	0/3149	0.76	2/4261 (0.0%)
1	I	0.37	0/3149	0.76	2/4261 (0.0%)
1	J	0.37	0/3149	0.76	2/4261 (0.0%)
1	K	0.37	0/3149	0.76	2/4261 (0.0%)
1	L	0.37	0/3149	0.76	2/4261 (0.0%)
All	All	0.37	0/37788	0.76	24/51132 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	305	ILE	N-CA-C	-6.12	106.84	112.96
1	D	305	ILE	N-CA-C	-6.11	106.85	112.96
1	H	305	ILE	N-CA-C	-6.10	106.86	112.96
1	B	305	ILE	N-CA-C	-6.10	106.86	112.96
1	E	305	ILE	N-CA-C	-6.09	106.87	112.96
1	L	305	ILE	N-CA-C	-6.08	106.88	112.96
1	C	305	ILE	N-CA-C	-6.07	106.89	112.96
1	F	305	ILE	N-CA-C	-6.07	106.89	112.96
1	G	305	ILE	N-CA-C	-6.07	106.89	112.96
1	K	305	ILE	N-CA-C	-6.07	106.89	112.96
1	A	305	ILE	N-CA-C	-6.07	106.89	112.96
1	J	305	ILE	N-CA-C	-6.07	106.89	112.96
1	J	194	ILE	N-CA-C	-5.21	108.42	113.53
1	B	194	ILE	N-CA-C	-5.18	108.46	113.53
1	C	194	ILE	N-CA-C	-5.17	108.46	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	194	ILE	N-CA-C	-5.14	108.49	113.53
1	F	194	ILE	N-CA-C	-5.14	108.49	113.53
1	I	194	ILE	N-CA-C	-5.14	108.49	113.53
1	K	194	ILE	N-CA-C	-5.14	108.49	113.53
1	G	194	ILE	N-CA-C	-5.14	108.49	113.53
1	L	194	ILE	N-CA-C	-5.13	108.50	113.53
1	A	194	ILE	N-CA-C	-5.12	108.51	113.53
1	D	194	ILE	N-CA-C	-5.12	108.52	113.53
1	H	194	ILE	N-CA-C	-5.10	108.53	113.53

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	3097	0	3104	42	0
1	B	3097	0	3104	45	0
1	C	3097	0	3104	46	0
1	D	3097	0	3104	45	0
1	E	3097	0	3104	50	0
1	F	3097	0	3104	46	0
1	G	3097	0	3104	42	0
1	H	3097	0	3104	45	0
1	I	3097	0	3104	42	0
1	J	3097	0	3104	41	0
1	K	3097	0	3104	44	0
1	L	3097	0	3104	43	0
All	All	37164	0	37248	508	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 7.

All (508) 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:E:157:PRO:HG2	1:F:173:PHE:HB3	1.78	0.66
1:I:168:VAL:HG22	1:I:179:MET:HG2	1.84	0.60
1:E:168:VAL:HG22	1:E:179:MET:HG2	1.84	0.60
1:J:168:VAL:HG22	1:J:179:MET:HG2	1.83	0.60
1:D:168:VAL:HG22	1:D:179:MET:HG2	1.84	0.60
1:F:168:VAL:HG22	1:F:179:MET:HG2	1.83	0.60
1:H:168:VAL:HG22	1:H:179:MET:HG2	1.84	0.60
1:C:168:VAL:HG22	1:C:179:MET:HG2	1.84	0.59
1:K:168:VAL:HG22	1:K:179:MET:HG2	1.83	0.59
1:G:255:ARG:NH1	1:G:263:SER:O	2.35	0.59
1:B:168:VAL:HG22	1:B:179:MET:HG2	1.83	0.59
1:E:255:ARG:NH1	1:E:263:SER:O	2.35	0.59
1:F:255:ARG:NH1	1:F:263:SER:O	2.35	0.59
1:H:255:ARG:NH1	1:H:263:SER:O	2.35	0.59
1:H:368:ARG:HH12	1:I:374:ILE:HD11	1.68	0.59
1:D:255:ARG:NH1	1:D:263:SER:O	2.35	0.59
1:G:168:VAL:HG22	1:G:179:MET:HG2	1.83	0.59
1:A:168:VAL:HG22	1:A:179:MET:HG2	1.83	0.58
1:L:255:ARG:NH1	1:L:263:SER:O	2.35	0.58
1:C:255:ARG:NH1	1:C:263:SER:O	2.35	0.58
1:I:255:ARG:NH1	1:I:263:SER:O	2.35	0.58
1:B:255:ARG:NH1	1:B:263:SER:O	2.35	0.58
1:K:255:ARG:NH1	1:K:263:SER:O	2.35	0.58
1:L:168:VAL:HG22	1:L:179:MET:HG2	1.83	0.58
1:A:255:ARG:NH1	1:A:263:SER:O	2.35	0.58
1:J:255:ARG:NH1	1:J:263:SER:O	2.35	0.58
1:G:157:PRO:HG2	1:H:173:PHE:HB3	1.87	0.57
1:A:157:PRO:HG2	1:B:173:PHE:HB3	1.86	0.57
1:B:368:ARG:HH12	1:C:374:ILE:HD11	1.71	0.56
1:J:142:ASN:ND2	1:J:166:TYR:OH	2.39	0.55
1:L:142:ASN:ND2	1:L:166:TYR:OH	2.39	0.55
1:A:142:ASN:ND2	1:A:166:TYR:OH	2.39	0.55
1:E:142:ASN:ND2	1:E:166:TYR:OH	2.39	0.55
1:I:142:ASN:ND2	1:I:166:TYR:OH	2.39	0.55
1:B:142:ASN:ND2	1:B:166:TYR:OH	2.39	0.55
1:F:142:ASN:ND2	1:F:166:TYR:OH	2.39	0.55
1:K:142:ASN:ND2	1:K:166:TYR:OH	2.39	0.55
1:D:142:ASN:ND2	1:D:166:TYR:OH	2.39	0.55
1:G:142:ASN:ND2	1:G:166:TYR:OH	2.39	0.55
1:C:142:ASN:ND2	1:C:166:TYR:OH	2.39	0.55
1:H:142:ASN:ND2	1:H:166:TYR:OH	2.39	0.54
1:D:138:VAL:HG13	1:D:256:MET:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ARG:HH12	1:F:374:ILE:HD11	1.72	0.54
1:J:157:PRO:HG2	1:K:173:PHE:HB3	1.90	0.54
1:C:138:VAL:HG13	1:C:256:MET:HE1	1.90	0.53
1:E:138:VAL:HG13	1:E:256:MET:HE1	1.90	0.53
1:J:368:ARG:HH12	1:K:374:ILE:HD11	1.73	0.53
1:B:138:VAL:HG13	1:B:256:MET:HE1	1.90	0.53
1:F:138:VAL:HG13	1:F:256:MET:HE1	1.90	0.53
1:G:138:VAL:HG13	1:G:256:MET:HE1	1.90	0.53
1:I:138:VAL:HG13	1:I:256:MET:HE1	1.90	0.53
1:A:138:VAL:HG13	1:A:256:MET:HE1	1.90	0.52
1:J:138:VAL:HG13	1:J:256:MET:HE1	1.90	0.52
1:J:84:MET:HE2	1:J:114:GLU:HG2	1.92	0.52
1:L:138:VAL:HG13	1:L:256:MET:HE1	1.90	0.52
1:L:84:MET:HE2	1:L:114:GLU:HG2	1.92	0.52
1:A:84:MET:HE2	1:A:114:GLU:HG2	1.92	0.52
1:H:138:VAL:HG13	1:H:256:MET:HE1	1.90	0.52
1:C:84:MET:HE2	1:C:114:GLU:HG2	1.92	0.52
1:H:84:MET:HE2	1:H:114:GLU:HG2	1.92	0.52
1:K:138:VAL:HG13	1:K:256:MET:HE1	1.90	0.52
1:K:84:MET:HE2	1:K:114:GLU:HG2	1.92	0.51
1:H:157:PRO:HG2	1:I:173:PHE:HB3	1.93	0.51
1:I:84:MET:HE2	1:I:114:GLU:HG2	1.92	0.51
1:B:84:MET:HE2	1:B:114:GLU:HG2	1.92	0.51
1:B:157:PRO:HG2	1:C:173:PHE:HB3	1.92	0.51
1:K:368:ARG:HH12	1:L:374:ILE:HD11	1.75	0.51
1:B:77:LEU:O	1:B:397:GLN:NE2	2.44	0.51
1:F:77:LEU:O	1:F:397:GLN:NE2	2.44	0.51
1:A:77:LEU:O	1:A:397:GLN:NE2	2.44	0.51
1:G:84:MET:HE2	1:G:114:GLU:HG2	1.92	0.51
1:G:368:ARG:HH12	1:H:374:ILE:HD11	1.76	0.51
1:A:126:TYR:HE2	1:A:404:LEU:HD11	1.76	0.51
1:G:77:LEU:O	1:G:397:GLN:NE2	2.44	0.51
1:C:77:LEU:O	1:C:397:GLN:NE2	2.44	0.51
1:E:77:LEU:O	1:E:397:GLN:NE2	2.44	0.51
1:E:84:MET:HE2	1:E:114:GLU:HG2	1.92	0.51
1:F:84:MET:HE2	1:F:114:GLU:HG2	1.92	0.51
1:D:77:LEU:O	1:D:397:GLN:NE2	2.44	0.50
1:F:126:TYR:HE2	1:F:404:LEU:HD11	1.76	0.50
1:J:126:TYR:HE2	1:J:404:LEU:HD11	1.76	0.50
1:L:77:LEU:O	1:L:397:GLN:NE2	2.44	0.50
1:D:84:MET:HE2	1:D:114:GLU:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:TYR:HE2	1:B:404:LEU:HD11	1.76	0.50
1:G:126:TYR:HE2	1:G:404:LEU:HD11	1.76	0.50
1:I:126:TYR:HE2	1:I:404:LEU:HD11	1.76	0.50
1:E:126:TYR:HE2	1:E:404:LEU:HD11	1.76	0.50
1:H:77:LEU:O	1:H:397:GLN:NE2	2.44	0.50
1:K:77:LEU:O	1:K:397:GLN:NE2	2.44	0.50
1:L:126:TYR:HE2	1:L:404:LEU:HD11	1.76	0.50
1:A:345:SER:O	1:A:349:GLU:HB2	2.12	0.50
1:A:368:ARG:HH12	1:B:374:ILE:HD11	1.77	0.50
1:L:345:SER:O	1:L:349:GLU:HB2	2.12	0.49
1:B:345:SER:O	1:B:349:GLU:HB2	2.12	0.49
1:D:126:TYR:HE2	1:D:404:LEU:HD11	1.76	0.49
1:K:126:TYR:HE2	1:K:404:LEU:HD11	1.76	0.49
1:C:345:SER:O	1:C:349:GLU:HB2	2.12	0.49
1:J:77:LEU:O	1:J:397:GLN:NE2	2.44	0.49
1:K:345:SER:O	1:K:349:GLU:HB2	2.13	0.49
1:I:77:LEU:O	1:I:397:GLN:NE2	2.44	0.49
1:C:126:TYR:HE2	1:C:404:LEU:HD11	1.76	0.49
1:J:345:SER:O	1:J:349:GLU:HB2	2.12	0.49
1:E:142:ASN:HB3	1:E:163:LEU:HD21	1.95	0.49
1:J:142:ASN:HB3	1:J:163:LEU:HD21	1.95	0.49
1:A:142:ASN:HB3	1:A:163:LEU:HD21	1.95	0.49
1:D:142:ASN:HB3	1:D:163:LEU:HD21	1.95	0.49
1:I:142:ASN:HB3	1:I:163:LEU:HD21	1.95	0.49
1:I:345:SER:O	1:I:349:GLU:HB2	2.13	0.49
1:D:258:ARG:NH2	1:D:395:GLU:OE1	2.46	0.49
1:D:345:SER:O	1:D:349:GLU:HB2	2.13	0.49
1:H:345:SER:O	1:H:349:GLU:HB2	2.12	0.49
1:B:403:VAL:O	1:B:407:GLN:HB2	2.13	0.49
1:E:345:SER:O	1:E:349:GLU:HB2	2.12	0.49
1:F:142:ASN:HB3	1:F:163:LEU:HD21	1.95	0.49
1:F:258:ARG:NH2	1:F:395:GLU:OE1	2.46	0.49
1:H:126:TYR:HE2	1:H:404:LEU:HD11	1.76	0.49
1:H:142:ASN:HB3	1:H:163:LEU:HD21	1.95	0.49
1:H:258:ARG:NH2	1:H:395:GLU:OE1	2.46	0.49
1:K:142:ASN:HB3	1:K:163:LEU:HD21	1.95	0.49
1:L:142:ASN:HB3	1:L:163:LEU:HD21	1.95	0.49
1:L:258:ARG:NH2	1:L:395:GLU:OE1	2.46	0.49
1:L:403:VAL:O	1:L:407:GLN:HB2	2.13	0.49
1:A:403:VAL:O	1:A:407:GLN:HB2	2.13	0.49
1:B:142:ASN:HB3	1:B:163:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ASN:HB3	1:C:163:LEU:HD21	1.95	0.49
1:G:345:SER:O	1:G:349:GLU:HB2	2.12	0.49
1:I:236:GLU:OE2	1:I:237:VAL:N	2.46	0.49
1:C:190:LEU:HD12	1:C:191:PRO:HD2	1.95	0.48
1:F:345:SER:O	1:F:349:GLU:HB2	2.13	0.48
1:G:142:ASN:HB3	1:G:163:LEU:HD21	1.95	0.48
1:B:190:LEU:HD12	1:B:191:PRO:HD2	1.95	0.48
1:C:258:ARG:NH2	1:C:395:GLU:OE1	2.46	0.48
1:I:258:ARG:NH2	1:I:395:GLU:OE1	2.46	0.48
1:B:258:ARG:NH2	1:B:395:GLU:OE1	2.46	0.48
1:C:403:VAL:O	1:C:407:GLN:HB2	2.13	0.48
1:J:403:VAL:O	1:J:407:GLN:HB2	2.13	0.48
1:K:258:ARG:NH2	1:K:395:GLU:OE1	2.46	0.48
1:K:403:VAL:O	1:K:407:GLN:HB2	2.13	0.48
1:B:236:GLU:OE2	1:B:237:VAL:N	2.46	0.48
1:F:190:LEU:HD12	1:F:191:PRO:HD2	1.95	0.48
1:I:403:VAL:O	1:I:407:GLN:HB2	2.13	0.48
1:A:258:ARG:NH2	1:A:395:GLU:OE1	2.46	0.48
1:I:197:ALA:O	1:I:201:GLN:NE2	2.47	0.48
1:E:155:TYR:HD2	1:F:175:ASN:HD21	1.61	0.48
1:G:197:ALA:O	1:G:201:GLN:NE2	2.47	0.48
1:J:236:GLU:OE2	1:J:237:VAL:N	2.46	0.48
1:K:197:ALA:O	1:K:201:GLN:NE2	2.47	0.48
1:G:190:LEU:HD12	1:G:191:PRO:HD2	1.96	0.48
1:J:258:ARG:NH2	1:J:395:GLU:OE1	2.46	0.48
1:L:197:ALA:O	1:L:201:GLN:NE2	2.47	0.48
1:A:190:LEU:HD12	1:A:191:PRO:HD2	1.95	0.48
1:D:190:LEU:HD12	1:D:191:PRO:HD2	1.95	0.48
1:G:403:VAL:O	1:G:407:GLN:HB2	2.13	0.48
1:A:197:ALA:O	1:A:201:GLN:NE2	2.47	0.48
1:C:197:ALA:O	1:C:201:GLN:NE2	2.47	0.48
1:D:197:ALA:O	1:D:201:GLN:NE2	2.47	0.48
1:H:403:VAL:O	1:H:407:GLN:HB2	2.13	0.48
1:I:194:ILE:HD12	1:I:238:GLN:HB2	1.96	0.48
1:K:16:VAL:HG22	1:K:19:ARG:HH22	1.79	0.48
1:E:190:LEU:HD12	1:E:191:PRO:HD2	1.95	0.47
1:E:197:ALA:O	1:E:201:GLN:NE2	2.47	0.47
1:G:258:ARG:NH2	1:G:395:GLU:OE1	2.46	0.47
1:J:194:ILE:HD12	1:J:238:GLN:HB2	1.96	0.47
1:L:16:VAL:HG22	1:L:19:ARG:HH22	1.79	0.47
1:E:258:ARG:NH2	1:E:395:GLU:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:190:LEU:HD12	1:H:191:PRO:HD2	1.95	0.47
1:A:16:VAL:HG22	1:A:19:ARG:HH22	1.79	0.47
1:B:197:ALA:O	1:B:201:GLN:NE2	2.47	0.47
1:D:403:VAL:O	1:D:407:GLN:HB2	2.13	0.47
1:E:236:GLU:OE2	1:E:237:VAL:N	2.46	0.47
1:F:16:VAL:HG22	1:F:19:ARG:HH22	1.79	0.47
1:H:194:ILE:HD12	1:H:238:GLN:HB2	1.96	0.47
1:H:197:ALA:O	1:H:201:GLN:NE2	2.47	0.47
1:E:403:VAL:O	1:E:407:GLN:HB2	2.13	0.47
1:F:388:VAL:HA	1:F:391:ILE:HG22	1.97	0.47
1:K:194:ILE:HD12	1:K:238:GLN:HB2	1.96	0.47
1:I:190:LEU:HD12	1:I:191:PRO:HD2	1.95	0.47
1:J:16:VAL:HG22	1:J:19:ARG:HH22	1.79	0.47
1:E:16:VAL:HG22	1:E:19:ARG:HH22	1.79	0.47
1:E:368:ARG:HA	1:F:375:ARG:HG3	1.96	0.47
1:I:388:VAL:HA	1:I:391:ILE:HG22	1.97	0.47
1:J:197:ALA:O	1:J:201:GLN:NE2	2.47	0.47
1:J:388:VAL:HA	1:J:391:ILE:HG22	1.97	0.47
1:K:236:GLU:OE2	1:K:237:VAL:N	2.46	0.47
1:C:236:GLU:OE2	1:C:237:VAL:N	2.46	0.47
1:F:197:ALA:O	1:F:201:GLN:NE2	2.47	0.47
1:F:368:ARG:HH12	1:G:374:ILE:HD11	1.80	0.47
1:F:403:VAL:O	1:F:407:GLN:HB2	2.13	0.47
1:G:194:ILE:HD12	1:G:238:GLN:HB2	1.96	0.47
1:K:190:LEU:HD12	1:K:191:PRO:HD2	1.95	0.47
1:L:194:ILE:HD12	1:L:238:GLN:HB2	1.96	0.47
1:L:388:VAL:HA	1:L:391:ILE:HG22	1.97	0.47
1:H:16:VAL:HG22	1:H:19:ARG:HH22	1.79	0.47
1:I:16:VAL:HG22	1:I:19:ARG:HH22	1.79	0.47
1:J:190:LEU:HD12	1:J:191:PRO:HD2	1.95	0.47
1:L:190:LEU:HD12	1:L:191:PRO:HD2	1.95	0.47
1:A:388:VAL:HA	1:A:391:ILE:HG22	1.97	0.47
1:B:16:VAL:HG22	1:B:19:ARG:HH22	1.79	0.47
1:F:236:GLU:OE2	1:F:237:VAL:N	2.46	0.47
1:G:16:VAL:HG22	1:G:19:ARG:HH22	1.79	0.47
1:C:388:VAL:HA	1:C:391:ILE:HG22	1.97	0.47
1:G:388:VAL:HA	1:G:391:ILE:HG22	1.97	0.47
1:I:144:LEU:HB2	1:I:166:TYR:CZ	2.50	0.47
1:A:144:LEU:HB2	1:A:166:TYR:CZ	2.50	0.46
1:D:144:LEU:HB2	1:D:166:TYR:CZ	2.50	0.46
1:G:144:LEU:HB2	1:G:166:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ILE:HD12	1:C:238:GLN:HB2	1.96	0.46
1:D:194:ILE:HD12	1:D:238:GLN:HB2	1.96	0.46
1:D:388:VAL:HA	1:D:391:ILE:HG22	1.97	0.46
1:A:194:ILE:HD12	1:A:238:GLN:HB2	1.96	0.46
1:C:16:VAL:HG22	1:C:19:ARG:HH22	1.79	0.46
1:C:144:LEU:HB2	1:C:166:TYR:CZ	2.50	0.46
1:C:406:LYS:HA	1:C:406:LYS:HD3	1.63	0.46
1:E:388:VAL:HA	1:E:391:ILE:HG22	1.97	0.46
1:F:157:PRO:HG2	1:G:173:PHE:HB3	1.97	0.46
1:K:144:LEU:HB2	1:K:166:TYR:CZ	2.50	0.46
1:B:144:LEU:HB2	1:B:166:TYR:CZ	2.50	0.46
1:H:388:VAL:HA	1:H:391:ILE:HG22	1.97	0.46
1:F:144:LEU:HB2	1:F:166:TYR:CZ	2.50	0.46
1:F:194:ILE:HD12	1:F:238:GLN:HB2	1.96	0.46
1:B:194:ILE:HD12	1:B:238:GLN:HB2	1.96	0.46
1:D:16:VAL:HG22	1:D:19:ARG:HH22	1.79	0.46
1:E:194:ILE:HD12	1:E:238:GLN:HB2	1.96	0.46
1:L:144:LEU:HB2	1:L:166:TYR:CZ	2.50	0.46
1:H:144:LEU:HB2	1:H:166:TYR:CZ	2.50	0.46
1:J:40:PRO:HG3	1:J:57:PRO:HD3	1.98	0.46
1:J:144:LEU:HB2	1:J:166:TYR:CZ	2.50	0.46
1:K:388:VAL:HA	1:K:391:ILE:HG22	1.97	0.46
1:I:40:PRO:HG3	1:I:57:PRO:HD3	1.98	0.46
1:J:73:LEU:HD23	1:J:134:LEU:HD21	1.98	0.46
1:L:40:PRO:HG3	1:L:57:PRO:HD3	1.98	0.46
1:L:236:GLU:OE2	1:L:237:VAL:N	2.46	0.46
1:A:40:PRO:HG3	1:A:57:PRO:HD3	1.98	0.46
1:I:73:LEU:HD23	1:I:134:LEU:HD21	1.98	0.46
1:K:40:PRO:HG3	1:K:57:PRO:HD3	1.98	0.46
1:L:73:LEU:HD23	1:L:134:LEU:HD21	1.98	0.46
1:A:73:LEU:HD23	1:A:134:LEU:HD21	1.98	0.45
1:A:140:ALA:HB1	1:A:163:LEU:HD12	1.99	0.45
1:B:40:PRO:HG3	1:B:57:PRO:HD3	1.98	0.45
1:C:40:PRO:HG3	1:C:57:PRO:HD3	1.98	0.45
1:B:140:ALA:HB1	1:B:163:LEU:HD12	1.99	0.45
1:B:388:VAL:HA	1:B:391:ILE:HG22	1.97	0.45
1:D:40:PRO:HG3	1:D:57:PRO:HD3	1.98	0.45
1:E:140:ALA:HB1	1:E:163:LEU:HD12	1.99	0.45
1:E:144:LEU:HB2	1:E:166:TYR:CZ	2.50	0.45
1:F:140:ALA:HB1	1:F:163:LEU:HD12	1.99	0.45
1:L:140:ALA:HB1	1:L:163:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:PRO:HG3	1:E:57:PRO:HD3	1.98	0.45
1:D:140:ALA:HB1	1:D:163:LEU:HD12	1.99	0.45
1:G:236:GLU:OE2	1:G:237:VAL:N	2.46	0.45
1:G:421:ALA:HB1	1:G:424:PRO:HB3	1.98	0.45
1:H:40:PRO:HG3	1:H:57:PRO:HD3	1.98	0.45
1:K:140:ALA:HB1	1:K:163:LEU:HD12	1.99	0.45
1:A:236:GLU:OE2	1:A:237:VAL:N	2.46	0.45
1:C:140:ALA:HB1	1:C:163:LEU:HD12	1.99	0.45
1:F:40:PRO:HG3	1:F:57:PRO:HD3	1.98	0.45
1:G:140:ALA:HB1	1:G:163:LEU:HD12	1.99	0.45
1:H:421:ALA:HB1	1:H:424:PRO:HB3	1.98	0.45
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.81	0.45
1:C:58:TRP:CD2	1:C:284:GLU:HG3	2.52	0.45
1:F:144:LEU:HD23	1:F:161:TYR:HD2	1.82	0.45
1:G:58:TRP:CD2	1:G:284:GLU:HG3	2.52	0.45
1:H:58:TRP:CD2	1:H:284:GLU:HG3	2.52	0.45
1:G:40:PRO:HG3	1:G:57:PRO:HD3	1.98	0.45
1:B:306:THR:HG21	1:B:327:ILE:HD11	1.99	0.45
1:C:144:LEU:HD23	1:C:161:TYR:HD2	1.82	0.45
1:C:306:THR:HG21	1:C:327:ILE:HD11	1.99	0.45
1:C:330:LEU:HA	1:C:330:LEU:HD23	1.81	0.45
1:D:58:TRP:CD2	1:D:284:GLU:HG3	2.52	0.45
1:F:306:THR:HG21	1:F:327:ILE:HD11	1.99	0.45
1:G:306:THR:HG21	1:G:327:ILE:HD11	1.99	0.45
1:K:58:TRP:CD2	1:K:284:GLU:HG3	2.52	0.45
1:B:58:TRP:CD2	1:B:284:GLU:HG3	2.52	0.45
1:D:306:THR:HG21	1:D:327:ILE:HD11	1.99	0.45
1:E:73:LEU:HD12	1:E:76:ALA:HB3	1.99	0.45
1:F:421:ALA:HB1	1:F:424:PRO:HB3	1.98	0.45
1:H:140:ALA:HB1	1:H:163:LEU:HD12	1.99	0.45
1:I:58:TRP:CD2	1:I:284:GLU:HG3	2.52	0.45
1:I:421:ALA:HB1	1:I:424:PRO:HB3	1.98	0.45
1:J:140:ALA:HB1	1:J:163:LEU:HD12	1.99	0.45
1:A:73:LEU:HD12	1:A:76:ALA:HB3	1.99	0.45
1:E:306:THR:HG21	1:E:327:ILE:HD11	1.99	0.45
1:F:58:TRP:CD2	1:F:284:GLU:HG3	2.52	0.45
1:I:140:ALA:HB1	1:I:163:LEU:HD12	1.99	0.45
1:A:58:TRP:CD2	1:A:284:GLU:HG3	2.52	0.44
1:A:306:THR:HG21	1:A:327:ILE:HD11	1.99	0.44
1:D:73:LEU:HD12	1:D:76:ALA:HB3	1.99	0.44
1:D:73:LEU:HD23	1:D:134:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HD23	1:D:161:TYR:HD2	1.82	0.44
1:D:236:GLU:OE2	1:D:237:VAL:N	2.46	0.44
1:F:73:LEU:HD12	1:F:76:ALA:HB3	1.99	0.44
1:H:306:THR:HG21	1:H:327:ILE:HD11	1.99	0.44
1:B:73:LEU:HD12	1:B:76:ALA:HB3	1.99	0.44
1:L:73:LEU:HD12	1:L:76:ALA:HB3	1.99	0.44
1:L:421:ALA:HB1	1:L:424:PRO:HB3	1.98	0.44
1:B:406:LYS:HA	1:B:406:LYS:HD3	1.63	0.44
1:E:73:LEU:HD23	1:E:134:LEU:HD21	1.98	0.44
1:G:72:LYS:HG3	1:G:357:MET:HE2	2.00	0.44
1:G:73:LEU:HD23	1:G:134:LEU:HD21	1.98	0.44
1:J:421:ALA:HB1	1:J:424:PRO:HB3	1.99	0.44
1:K:144:LEU:HD23	1:K:161:TYR:HD2	1.82	0.44
1:L:144:LEU:HD23	1:L:161:TYR:HD2	1.82	0.44
1:C:73:LEU:HD23	1:C:134:LEU:HD21	1.98	0.44
1:E:406:LYS:HA	1:E:406:LYS:HD3	1.63	0.44
1:H:72:LYS:HG3	1:H:357:MET:HE2	2.00	0.44
1:J:73:LEU:HD12	1:J:76:ALA:HB3	1.99	0.44
1:K:73:LEU:HD12	1:K:76:ALA:HB3	1.99	0.44
1:K:73:LEU:HD23	1:K:134:LEU:HD21	1.98	0.44
1:E:58:TRP:CD2	1:E:284:GLU:HG3	2.52	0.44
1:E:421:ALA:HB1	1:E:424:PRO:HB3	1.99	0.44
1:F:73:LEU:HD23	1:F:134:LEU:HD21	1.98	0.44
1:G:73:LEU:HD12	1:G:76:ALA:HB3	1.99	0.44
1:H:73:LEU:HD12	1:H:76:ALA:HB3	1.99	0.44
1:I:72:LYS:HG3	1:I:357:MET:HE2	2.00	0.44
1:I:306:THR:HG21	1:I:327:ILE:HD11	1.99	0.44
1:K:252:ILE:HD13	1:K:399:PRO:HB2	2.00	0.44
1:K:421:ALA:HB1	1:K:424:PRO:HB3	1.99	0.44
1:L:252:ILE:HD13	1:L:399:PRO:HB2	2.00	0.44
1:A:252:ILE:HD13	1:A:399:PRO:HB2	2.00	0.44
1:B:73:LEU:HD23	1:B:134:LEU:HD21	1.98	0.44
1:C:73:LEU:HD12	1:C:76:ALA:HB3	1.99	0.44
1:E:72:LYS:HG3	1:E:357:MET:HE2	2.00	0.44
1:E:144:LEU:HD23	1:E:161:TYR:HD2	1.82	0.44
1:F:72:LYS:HG3	1:F:357:MET:HE2	2.00	0.44
1:H:365:THR:HG22	1:I:376:TYR:CE1	2.53	0.44
1:I:73:LEU:HD12	1:I:76:ALA:HB3	1.99	0.44
1:I:406:LYS:HA	1:I:406:LYS:HD3	1.63	0.44
1:J:306:THR:HG21	1:J:327:ILE:HD11	1.99	0.44
1:A:144:LEU:HD23	1:A:161:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:GLU:O	1:C:402:ARG:NH1	2.51	0.44
1:D:247:GLU:O	1:D:402:ARG:NH1	2.51	0.44
1:H:73:LEU:HD23	1:H:134:LEU:HD21	1.98	0.44
1:J:58:TRP:CD2	1:J:284:GLU:HG3	2.52	0.44
1:J:247:GLU:O	1:J:402:ARG:NH1	2.51	0.44
1:K:306:THR:HG21	1:K:327:ILE:HD11	1.99	0.44
1:L:306:THR:HG21	1:L:327:ILE:HD11	1.99	0.44
1:A:39:ILE:HD12	1:A:39:ILE:HA	1.93	0.44
1:A:283:GLN:NE2	1:A:345:SER:OG	2.51	0.44
1:A:421:ALA:HB1	1:A:424:PRO:HB3	1.98	0.44
1:C:72:LYS:HG3	1:C:357:MET:HE2	2.00	0.44
1:I:247:GLU:O	1:I:402:ARG:NH1	2.51	0.44
1:I:252:ILE:HD13	1:I:399:PRO:HB2	2.00	0.44
1:J:144:LEU:HD23	1:J:161:TYR:HD2	1.82	0.44
1:J:252:ILE:HD13	1:J:399:PRO:HB2	2.00	0.44
1:D:72:LYS:HG3	1:D:357:MET:HE2	2.00	0.44
1:D:421:ALA:HB1	1:D:424:PRO:HB3	1.99	0.44
1:E:39:ILE:HD12	1:E:39:ILE:HA	1.93	0.44
1:F:406:LYS:HA	1:F:406:LYS:HD3	1.63	0.44
1:J:72:LYS:HG3	1:J:357:MET:HE2	2.00	0.44
1:K:247:GLU:O	1:K:402:ARG:NH1	2.51	0.44
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.86	0.43
1:B:247:GLU:O	1:B:402:ARG:NH1	2.51	0.43
1:E:247:GLU:O	1:E:402:ARG:NH1	2.51	0.43
1:F:247:GLU:O	1:F:402:ARG:NH1	2.51	0.43
1:G:144:LEU:HD23	1:G:161:TYR:HD2	1.82	0.43
1:B:230:GLU:OE2	1:B:230:GLU:N	2.51	0.43
1:B:252:ILE:HD13	1:B:399:PRO:HB2	2.00	0.43
1:C:230:GLU:N	1:C:230:GLU:OE2	2.51	0.43
1:I:144:LEU:HD23	1:I:161:TYR:HD2	1.82	0.43
1:B:72:LYS:HG3	1:B:357:MET:HE2	2.00	0.43
1:C:421:ALA:HB1	1:C:424:PRO:HB3	1.98	0.43
1:E:289:MET:HE2	1:E:289:MET:HB3	1.93	0.43
1:J:283:GLN:NE2	1:J:345:SER:OG	2.51	0.43
1:L:58:TRP:CD2	1:L:284:GLU:HG3	2.52	0.43
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.81	0.43
1:B:144:LEU:HD23	1:B:161:TYR:HD2	1.82	0.43
1:E:79:PRO:HG3	1:E:374:ILE:HG21	2.01	0.43
1:H:79:PRO:HG3	1:H:374:ILE:HG21	2.01	0.43
1:H:236:GLU:OE2	1:H:237:VAL:N	2.46	0.43
1:H:247:GLU:O	1:H:402:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:ILE:HD13	1:H:399:PRO:HB2	2.00	0.43
1:A:72:LYS:HG3	1:A:357:MET:HE2	2.00	0.43
1:A:230:GLU:N	1:A:230:GLU:OE2	2.51	0.43
1:D:252:ILE:HD13	1:D:399:PRO:HB2	2.00	0.43
1:F:79:PRO:HG3	1:F:374:ILE:HG21	2.01	0.43
1:G:79:PRO:HG3	1:G:374:ILE:HG21	2.01	0.43
1:G:230:GLU:OE2	1:G:230:GLU:N	2.51	0.43
1:K:72:LYS:HG3	1:K:357:MET:HE2	2.00	0.43
1:L:247:GLU:O	1:L:402:ARG:NH1	2.51	0.43
1:B:421:ALA:HB1	1:B:424:PRO:HB3	1.98	0.43
1:D:230:GLU:OE2	1:D:230:GLU:N	2.51	0.43
1:F:252:ILE:HD13	1:F:399:PRO:HB2	2.00	0.43
1:G:247:GLU:O	1:G:402:ARG:NH1	2.51	0.43
1:H:144:LEU:HD23	1:H:161:TYR:HD2	1.82	0.43
1:H:163:LEU:HD23	1:H:163:LEU:HA	1.86	0.43
1:L:307:GLN:OE1	1:L:310:ARG:NH2	2.49	0.43
1:F:230:GLU:OE2	1:F:230:GLU:N	2.51	0.43
1:I:79:PRO:HG3	1:I:374:ILE:HG21	2.01	0.43
1:L:230:GLU:OE2	1:L:230:GLU:N	2.51	0.43
1:L:330:LEU:HD23	1:L:330:LEU:HA	1.81	0.43
1:A:247:GLU:O	1:A:402:ARG:NH1	2.51	0.43
1:D:79:PRO:HG3	1:D:374:ILE:HG21	2.01	0.43
1:H:230:GLU:N	1:H:230:GLU:OE2	2.51	0.43
1:L:72:LYS:HG3	1:L:357:MET:HE2	2.00	0.43
1:D:39:ILE:HD12	1:D:39:ILE:HA	1.93	0.43
1:D:406:LYS:HA	1:D:406:LYS:HD3	1.63	0.43
1:G:252:ILE:HD13	1:G:399:PRO:HB2	2.00	0.43
1:H:283:GLN:NE2	1:H:345:SER:OG	2.51	0.43
1:K:230:GLU:OE2	1:K:230:GLU:N	2.51	0.43
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.93	0.43
1:C:252:ILE:HD13	1:C:399:PRO:HB2	2.00	0.43
1:D:283:GLN:NE2	1:D:345:SER:OG	2.51	0.43
1:I:230:GLU:OE2	1:I:230:GLU:N	2.51	0.43
1:J:79:PRO:HG3	1:J:374:ILE:HG21	2.01	0.43
1:D:289:MET:HE2	1:D:289:MET:HB3	1.93	0.42
1:E:230:GLU:N	1:E:230:GLU:OE2	2.51	0.42
1:G:283:GLN:NE2	1:G:345:SER:OG	2.51	0.42
1:J:230:GLU:N	1:J:230:GLU:OE2	2.51	0.42
1:C:283:GLN:NE2	1:C:345:SER:OG	2.51	0.42
1:F:72:LYS:HA	1:F:72:LYS:HD3	1.86	0.42
1:J:406:LYS:HA	1:J:406:LYS:HD3	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:LEU:HD23	1:D:330:LEU:HA	1.81	0.42
1:D:380:GLU:O	1:D:384:THR:OG1	2.33	0.42
1:H:289:MET:HE2	1:H:289:MET:HB3	1.93	0.42
1:I:289:MET:HE2	1:I:289:MET:HB3	1.93	0.42
1:J:192:GLU:OE2	1:J:195:ARG:NH1	2.53	0.42
1:L:283:GLN:NE2	1:L:345:SER:OG	2.51	0.42
1:B:79:PRO:HG3	1:B:374:ILE:HG21	2.01	0.42
1:C:39:ILE:HD12	1:C:39:ILE:HA	1.93	0.42
1:C:79:PRO:HG3	1:C:374:ILE:HG21	2.01	0.42
1:F:283:GLN:NE2	1:F:345:SER:OG	2.51	0.42
1:A:79:PRO:HG3	1:A:374:ILE:HG21	2.01	0.42
1:E:170:ARG:HD2	1:E:263:SER:HA	2.02	0.42
1:E:252:ILE:HD13	1:E:399:PRO:HB2	2.00	0.42
1:A:307:GLN:OE1	1:A:310:ARG:NH2	2.49	0.42
1:I:163:LEU:HD23	1:I:163:LEU:HA	1.86	0.42
1:K:79:PRO:HG3	1:K:374:ILE:HG21	2.01	0.42
1:K:192:GLU:OE2	1:K:195:ARG:NH1	2.53	0.42
1:D:157:PRO:HG2	1:E:173:PHE:HB3	2.01	0.42
1:F:289:MET:HE2	1:F:289:MET:HB3	1.93	0.42
1:A:406:LYS:HA	1:A:406:LYS:HD3	1.63	0.42
1:J:216:HIS:CE1	1:J:218:TYR:HB3	2.55	0.42
1:K:185:ILE:HG12	1:K:190:LEU:HB2	2.02	0.42
1:K:406:LYS:HA	1:K:406:LYS:HD3	1.63	0.42
1:L:79:PRO:HG3	1:L:374:ILE:HG21	2.01	0.42
1:A:185:ILE:HG12	1:A:190:LEU:HB2	2.02	0.42
1:B:185:ILE:HG12	1:B:190:LEU:HB2	2.02	0.42
1:B:365:THR:HG22	1:C:376:TYR:CE1	2.55	0.42
1:C:185:ILE:HG12	1:C:190:LEU:HB2	2.02	0.42
1:G:170:ARG:HD2	1:G:263:SER:HA	2.02	0.42
1:H:216:HIS:CE1	1:H:218:TYR:HB3	2.55	0.42
1:K:157:PRO:HG2	1:L:173:PHE:HB3	2.01	0.42
1:C:170:ARG:HD2	1:C:263:SER:HA	2.02	0.41
1:G:216:HIS:CE1	1:G:218:TYR:HB3	2.55	0.41
1:H:170:ARG:HD2	1:H:263:SER:HA	2.02	0.41
1:I:216:HIS:CE1	1:I:218:TYR:HB3	2.55	0.41
1:J:185:ILE:HG12	1:J:190:LEU:HB2	2.02	0.41
1:K:72:LYS:HA	1:K:72:LYS:HD3	1.86	0.41
1:K:307:GLN:OE1	1:K:310:ARG:NH2	2.49	0.41
1:L:185:ILE:HG12	1:L:190:LEU:HB2	2.02	0.41
1:L:406:LYS:HA	1:L:406:LYS:HD3	1.63	0.41
1:D:185:ILE:HG12	1:D:190:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:ILE:HG12	1:I:190:LEU:HB2	2.02	0.41
1:L:216:HIS:CE1	1:L:218:TYR:HB3	2.55	0.41
1:D:368:ARG:HH12	1:E:374:ILE:HD11	1.85	0.41
1:F:170:ARG:HD2	1:F:263:SER:HA	2.02	0.41
1:G:289:MET:HE2	1:G:289:MET:HB3	1.93	0.41
1:E:330:LEU:HD23	1:E:330:LEU:HA	1.81	0.41
1:D:192:GLU:OE2	1:D:195:ARG:NH1	2.53	0.41
1:I:192:GLU:OE2	1:I:195:ARG:NH1	2.53	0.41
1:K:163:LEU:HD23	1:K:163:LEU:HA	1.86	0.41
1:C:192:GLU:OE2	1:C:195:ARG:NH1	2.53	0.41
1:E:185:ILE:HG12	1:E:190:LEU:HB2	2.02	0.41
1:E:283:GLN:NE2	1:E:345:SER:OG	2.51	0.41
1:F:185:ILE:HG12	1:F:190:LEU:HB2	2.02	0.41
1:G:185:ILE:HG12	1:G:190:LEU:HB2	2.02	0.41
1:H:185:ILE:HG12	1:H:190:LEU:HB2	2.02	0.41
1:A:216:HIS:CE1	1:A:218:TYR:HB3	2.55	0.41
1:F:216:HIS:CE1	1:F:218:TYR:HB3	2.55	0.41
1:G:307:GLN:OE1	1:G:310:ARG:NH2	2.49	0.41
1:C:72:LYS:HD3	1:C:72:LYS:HA	1.86	0.41
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.86	0.41
1:D:216:HIS:CE1	1:D:218:TYR:HB3	2.55	0.41
1:E:192:GLU:OE2	1:E:195:ARG:NH1	2.53	0.41
1:F:163:LEU:HD23	1:F:163:LEU:HA	1.86	0.41
1:F:307:GLN:OE1	1:F:310:ARG:NH2	2.49	0.41
1:I:283:GLN:NE2	1:I:345:SER:OG	2.51	0.41
1:K:216:HIS:CE1	1:K:218:TYR:HB3	2.55	0.41
1:L:72:LYS:HD3	1:L:72:LYS:HA	1.86	0.41
1:A:170:ARG:HD2	1:A:263:SER:HA	2.02	0.41
1:C:316:THR:HG22	1:D:295:LYS:HB2	2.03	0.41
1:C:397:GLN:HB3	1:C:428:THR:HB	2.03	0.41
1:D:397:GLN:HB3	1:D:428:THR:HB	2.03	0.41
1:G:406:LYS:HA	1:G:406:LYS:HD3	1.63	0.41
1:B:192:GLU:OE2	1:B:195:ARG:NH1	2.53	0.40
1:B:216:HIS:CE1	1:B:218:TYR:HB3	2.55	0.40
1:B:283:GLN:NE2	1:B:345:SER:OG	2.51	0.40
1:D:170:ARG:HD2	1:D:263:SER:HA	2.02	0.40
1:E:216:HIS:CE1	1:E:218:TYR:HB3	2.55	0.40
1:H:206:LYS:HA	1:H:206:LYS:HD2	1.91	0.40
1:I:170:ARG:HD2	1:I:263:SER:HA	2.02	0.40
1:B:289:MET:HE2	1:B:289:MET:HB3	1.93	0.40
1:B:307:GLN:OE1	1:B:310:ARG:NH2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:HIS:CE1	1:C:218:TYR:HB3	2.55	0.40
1:H:192:GLU:OE2	1:H:195:ARG:NH1	2.53	0.40
1:H:307:GLN:OE1	1:H:310:ARG:NH2	2.49	0.40
1:J:289:MET:HE2	1:J:289:MET:HB3	1.93	0.40
1:L:170:ARG:HD2	1:L:263:SER:HA	2.02	0.40
1:E:108:GLU:O	1:E:112:MET:HG3	2.22	0.40
1:E:397:GLN:HB3	1:E:428:THR:HB	2.04	0.40
1:E:206:LYS:HA	1:E:206:LYS:HD2	1.91	0.40
1:E:307:GLN:OE1	1:E:310:ARG:NH2	2.49	0.40
1:J:170:ARG:HD2	1:J:263:SER:HA	2.02	0.40
1:K:145:LEU:HD23	1:K:145:LEU:HA	1.94	0.40
1:K:330:LEU:HD23	1:K:330:LEU:HA	1.81	0.40
1:L:163:LEU:HD23	1:L:163:LEU:HA	1.86	0.40
1:J:72:LYS:HA	1:J:72:LYS:HD3	1.86	0.40
1:L:192:GLU:OE2	1:L:195:ARG:NH1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
1	B	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
1	C	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
1	D	386/547 (71%)	351 (91%)	35 (9%)	0	100	100
1	E	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
1	F	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
1	G	386/547 (71%)	351 (91%)	35 (9%)	0	100	100
1	H	386/547 (71%)	349 (90%)	37 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
1	J	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
1	K	386/547 (71%)	351 (91%)	35 (9%)	0	100	100
1	L	386/547 (71%)	350 (91%)	36 (9%)	0	100	100
All	All	4632/6564 (71%)	4202 (91%)	430 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	B	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	C	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	D	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	E	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	F	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	G	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	H	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	I	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	J	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	K	336/450 (75%)	307 (91%)	29 (9%)	10	32
1	L	336/450 (75%)	307 (91%)	29 (9%)	10	32
All	All	4032/5400 (75%)	3684 (91%)	348 (9%)	12	32

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL

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Mol	Chain	Res	Type
1	A	61	VAL
1	A	75	LEU
1	A	110	LEU
1	A	132	GLU
1	A	137	LEU
1	A	138	VAL
1	A	143	VAL
1	A	176	VAL
1	A	181	THR
1	A	198	VAL
1	A	209	GLU
1	A	225	GLU
1	A	233	GLU
1	A	236	GLU
1	A	237	VAL
1	A	243	THR
1	A	300	VAL
1	A	311	LEU
1	A	312	THR
1	A	313	LYS
1	A	320	VAL
1	A	364	ARG
1	A	367	GLU
1	A	384	THR
1	A	406	LYS
1	A	414	ILE
1	A	417	LEU
1	A	422	VAL
1	B	16	VAL
1	B	61	VAL
1	B	75	LEU
1	B	110	LEU
1	B	132	GLU
1	B	137	LEU
1	B	138	VAL
1	B	143	VAL
1	B	176	VAL
1	B	181	THR
1	B	198	VAL
1	B	209	GLU
1	B	225	GLU
1	B	233	GLU

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Mol	Chain	Res	Type
1	B	236	GLU
1	B	237	VAL
1	B	243	THR
1	B	300	VAL
1	B	311	LEU
1	B	312	THR
1	B	313	LYS
1	B	320	VAL
1	B	364	ARG
1	B	367	GLU
1	B	384	THR
1	B	406	LYS
1	B	414	ILE
1	B	417	LEU
1	B	422	VAL
1	C	16	VAL
1	C	61	VAL
1	C	75	LEU
1	C	110	LEU
1	C	132	GLU
1	C	137	LEU
1	C	138	VAL
1	C	143	VAL
1	C	176	VAL
1	C	181	THR
1	C	198	VAL
1	C	209	GLU
1	C	225	GLU
1	C	233	GLU
1	C	236	GLU
1	C	237	VAL
1	C	243	THR
1	C	300	VAL
1	C	311	LEU
1	C	312	THR
1	C	313	LYS
1	C	320	VAL
1	C	364	ARG
1	C	367	GLU
1	C	384	THR
1	C	406	LYS
1	C	414	ILE

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Mol	Chain	Res	Type
1	C	417	LEU
1	C	422	VAL
1	D	16	VAL
1	D	61	VAL
1	D	75	LEU
1	D	110	LEU
1	D	132	GLU
1	D	137	LEU
1	D	138	VAL
1	D	143	VAL
1	D	176	VAL
1	D	181	THR
1	D	198	VAL
1	D	209	GLU
1	D	225	GLU
1	D	233	GLU
1	D	236	GLU
1	D	237	VAL
1	D	243	THR
1	D	300	VAL
1	D	311	LEU
1	D	312	THR
1	D	313	LYS
1	D	320	VAL
1	D	364	ARG
1	D	367	GLU
1	D	384	THR
1	D	406	LYS
1	D	414	ILE
1	D	417	LEU
1	D	422	VAL
1	E	16	VAL
1	E	61	VAL
1	E	75	LEU
1	E	110	LEU
1	E	132	GLU
1	E	137	LEU
1	E	138	VAL
1	E	143	VAL
1	E	176	VAL
1	E	181	THR
1	E	198	VAL

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Mol	Chain	Res	Type
1	E	209	GLU
1	E	225	GLU
1	E	233	GLU
1	E	236	GLU
1	E	237	VAL
1	E	243	THR
1	E	300	VAL
1	E	311	LEU
1	E	312	THR
1	E	313	LYS
1	E	320	VAL
1	E	364	ARG
1	E	367	GLU
1	E	384	THR
1	E	406	LYS
1	E	414	ILE
1	E	417	LEU
1	E	422	VAL
1	F	16	VAL
1	F	61	VAL
1	F	75	LEU
1	F	110	LEU
1	F	132	GLU
1	F	137	LEU
1	F	138	VAL
1	F	143	VAL
1	F	176	VAL
1	F	181	THR
1	F	198	VAL
1	F	209	GLU
1	F	225	GLU
1	F	233	GLU
1	F	236	GLU
1	F	237	VAL
1	F	243	THR
1	F	300	VAL
1	F	311	LEU
1	F	312	THR
1	F	313	LYS
1	F	320	VAL
1	F	364	ARG
1	F	367	GLU

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Mol	Chain	Res	Type
1	F	384	THR
1	F	406	LYS
1	F	414	ILE
1	F	417	LEU
1	F	422	VAL
1	G	16	VAL
1	G	61	VAL
1	G	75	LEU
1	G	110	LEU
1	G	132	GLU
1	G	137	LEU
1	G	138	VAL
1	G	143	VAL
1	G	176	VAL
1	G	181	THR
1	G	198	VAL
1	G	209	GLU
1	G	225	GLU
1	G	233	GLU
1	G	236	GLU
1	G	237	VAL
1	G	243	THR
1	G	300	VAL
1	G	311	LEU
1	G	312	THR
1	G	313	LYS
1	G	320	VAL
1	G	364	ARG
1	G	367	GLU
1	G	384	THR
1	G	406	LYS
1	G	414	ILE
1	G	417	LEU
1	G	422	VAL
1	H	16	VAL
1	H	61	VAL
1	H	75	LEU
1	H	110	LEU
1	H	132	GLU
1	H	137	LEU
1	H	138	VAL
1	H	143	VAL

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Mol	Chain	Res	Type
1	H	176	VAL
1	H	181	THR
1	H	198	VAL
1	H	209	GLU
1	H	225	GLU
1	H	233	GLU
1	H	236	GLU
1	H	237	VAL
1	H	243	THR
1	H	300	VAL
1	H	311	LEU
1	H	312	THR
1	H	313	LYS
1	H	320	VAL
1	H	364	ARG
1	H	367	GLU
1	H	384	THR
1	H	406	LYS
1	H	414	ILE
1	H	417	LEU
1	H	422	VAL
1	I	16	VAL
1	I	61	VAL
1	I	75	LEU
1	I	110	LEU
1	I	132	GLU
1	I	137	LEU
1	I	138	VAL
1	I	143	VAL
1	I	176	VAL
1	I	181	THR
1	I	198	VAL
1	I	209	GLU
1	I	225	GLU
1	I	233	GLU
1	I	236	GLU
1	I	237	VAL
1	I	243	THR
1	I	300	VAL
1	I	311	LEU
1	I	312	THR
1	I	313	LYS

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Mol	Chain	Res	Type
1	I	320	VAL
1	I	364	ARG
1	I	367	GLU
1	I	384	THR
1	I	406	LYS
1	I	414	ILE
1	I	417	LEU
1	I	422	VAL
1	J	16	VAL
1	J	61	VAL
1	J	75	LEU
1	J	110	LEU
1	J	132	GLU
1	J	137	LEU
1	J	138	VAL
1	J	143	VAL
1	J	176	VAL
1	J	181	THR
1	J	198	VAL
1	J	209	GLU
1	J	225	GLU
1	J	233	GLU
1	J	236	GLU
1	J	237	VAL
1	J	243	THR
1	J	300	VAL
1	J	311	LEU
1	J	312	THR
1	J	313	LYS
1	J	320	VAL
1	J	364	ARG
1	J	367	GLU
1	J	384	THR
1	J	406	LYS
1	J	414	ILE
1	J	417	LEU
1	J	422	VAL
1	K	16	VAL
1	K	61	VAL
1	K	75	LEU
1	K	110	LEU
1	K	132	GLU

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Mol	Chain	Res	Type
1	K	137	LEU
1	K	138	VAL
1	K	143	VAL
1	K	176	VAL
1	K	181	THR
1	K	198	VAL
1	K	209	GLU
1	K	225	GLU
1	K	233	GLU
1	K	236	GLU
1	K	237	VAL
1	K	243	THR
1	K	300	VAL
1	K	311	LEU
1	K	312	THR
1	K	313	LYS
1	K	320	VAL
1	K	364	ARG
1	K	367	GLU
1	K	384	THR
1	K	406	LYS
1	K	414	ILE
1	K	417	LEU
1	K	422	VAL
1	L	16	VAL
1	L	61	VAL
1	L	75	LEU
1	L	110	LEU
1	L	132	GLU
1	L	137	LEU
1	L	138	VAL
1	L	143	VAL
1	L	176	VAL
1	L	181	THR
1	L	198	VAL
1	L	209	GLU
1	L	225	GLU
1	L	233	GLU
1	L	236	GLU
1	L	237	VAL
1	L	243	THR
1	L	300	VAL

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Mol	Chain	Res	Type
1	L	311	LEU
1	L	312	THR
1	L	313	LYS
1	L	320	VAL
1	L	364	ARG
1	L	367	GLU
1	L	384	THR
1	L	406	LYS
1	L	414	ILE
1	L	417	LEU
1	L	422	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	119	ASN
1	A	142	ASN
1	A	201	GLN
1	A	216	HIS
1	A	335	GLN
1	A	409	GLN
1	B	22	ASN
1	B	119	ASN
1	B	142	ASN
1	B	175	ASN
1	B	201	GLN
1	B	216	HIS
1	B	335	GLN
1	B	409	GLN
1	C	22	ASN
1	C	119	ASN
1	C	142	ASN
1	C	175	ASN
1	C	201	GLN
1	C	216	HIS
1	C	335	GLN
1	C	409	GLN
1	D	22	ASN
1	D	119	ASN
1	D	142	ASN
1	D	201	GLN

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Mol	Chain	Res	Type
1	D	216	HIS
1	D	335	GLN
1	D	409	GLN
1	E	22	ASN
1	E	119	ASN
1	E	142	ASN
1	E	175	ASN
1	E	201	GLN
1	E	216	HIS
1	E	409	GLN
1	F	22	ASN
1	F	119	ASN
1	F	142	ASN
1	F	175	ASN
1	F	201	GLN
1	F	216	HIS
1	F	335	GLN
1	F	409	GLN
1	G	22	ASN
1	G	119	ASN
1	G	142	ASN
1	G	175	ASN
1	G	201	GLN
1	G	216	HIS
1	G	335	GLN
1	G	409	GLN
1	H	22	ASN
1	H	119	ASN
1	H	142	ASN
1	H	175	ASN
1	H	201	GLN
1	H	216	HIS
1	H	409	GLN
1	I	22	ASN
1	I	119	ASN
1	I	142	ASN
1	I	175	ASN
1	I	201	GLN
1	I	216	HIS
1	I	335	GLN
1	I	409	GLN
1	J	22	ASN

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Mol	Chain	Res	Type
1	J	119	ASN
1	J	142	ASN
1	J	201	GLN
1	J	216	HIS
1	J	335	GLN
1	J	409	GLN
1	K	22	ASN
1	K	119	ASN
1	K	142	ASN
1	K	175	ASN
1	K	201	GLN
1	K	216	HIS
1	K	335	GLN
1	K	409	GLN
1	L	22	ASN
1	L	119	ASN
1	L	142	ASN
1	L	175	ASN
1	L	201	GLN
1	L	335	GLN
1	L	409	GLN

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](#)

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.

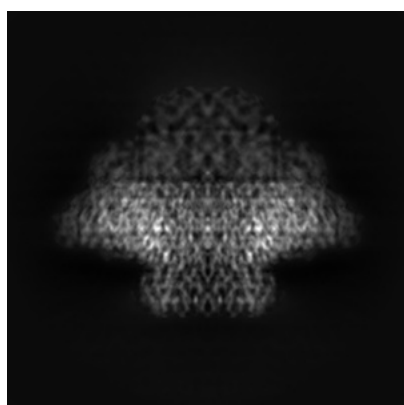
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4669. These allow visual inspection of the internal detail of the map and identification of artifacts.

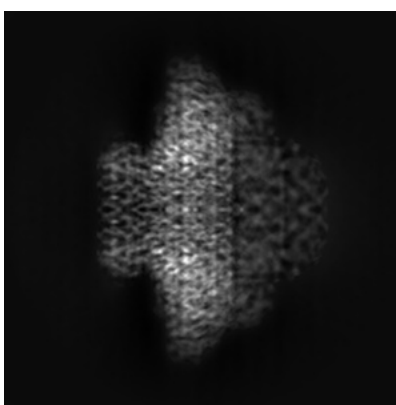
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

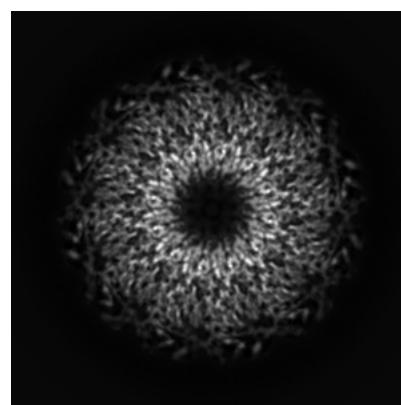
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 110



Y Index: 110



Z Index: 110

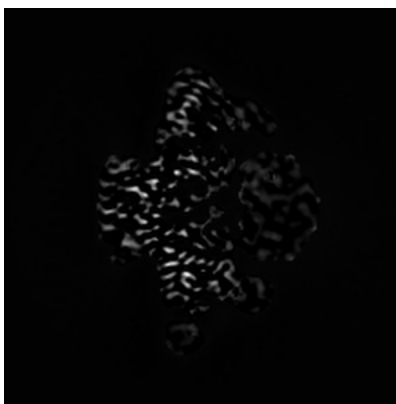
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 82



Y Index: 82

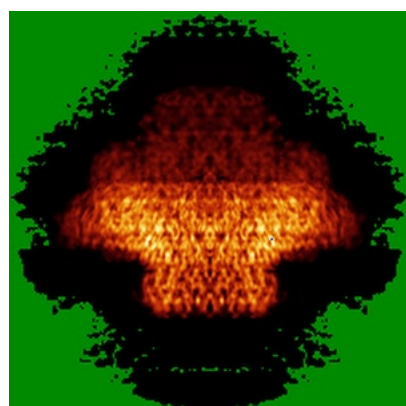


Z Index: 100

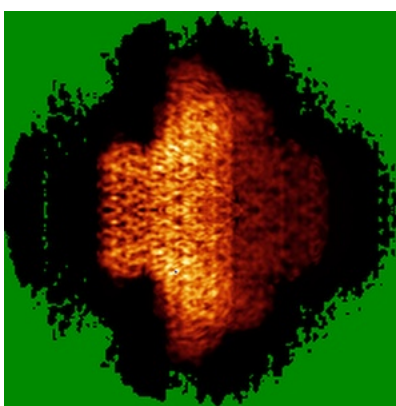
The images above show the largest variance slices of the map in three orthogonal directions.

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

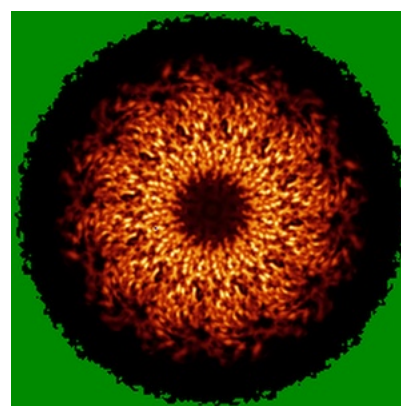
6.4.1 Primary map



X



Y

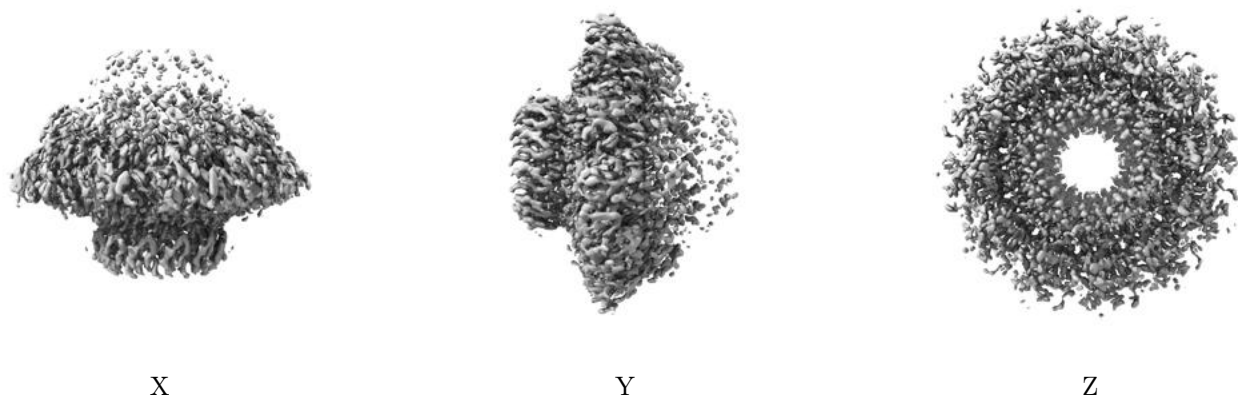


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0577. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

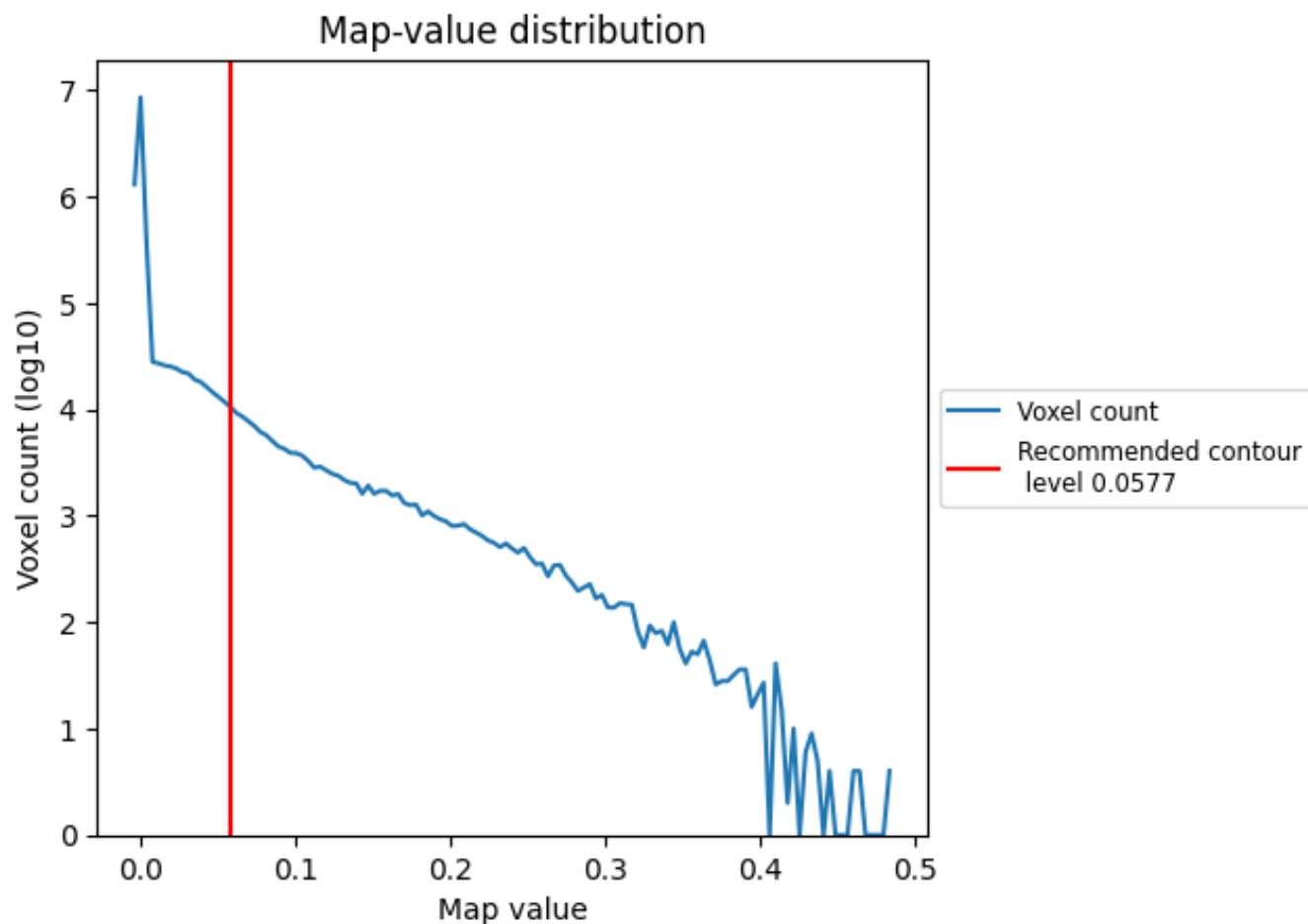
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

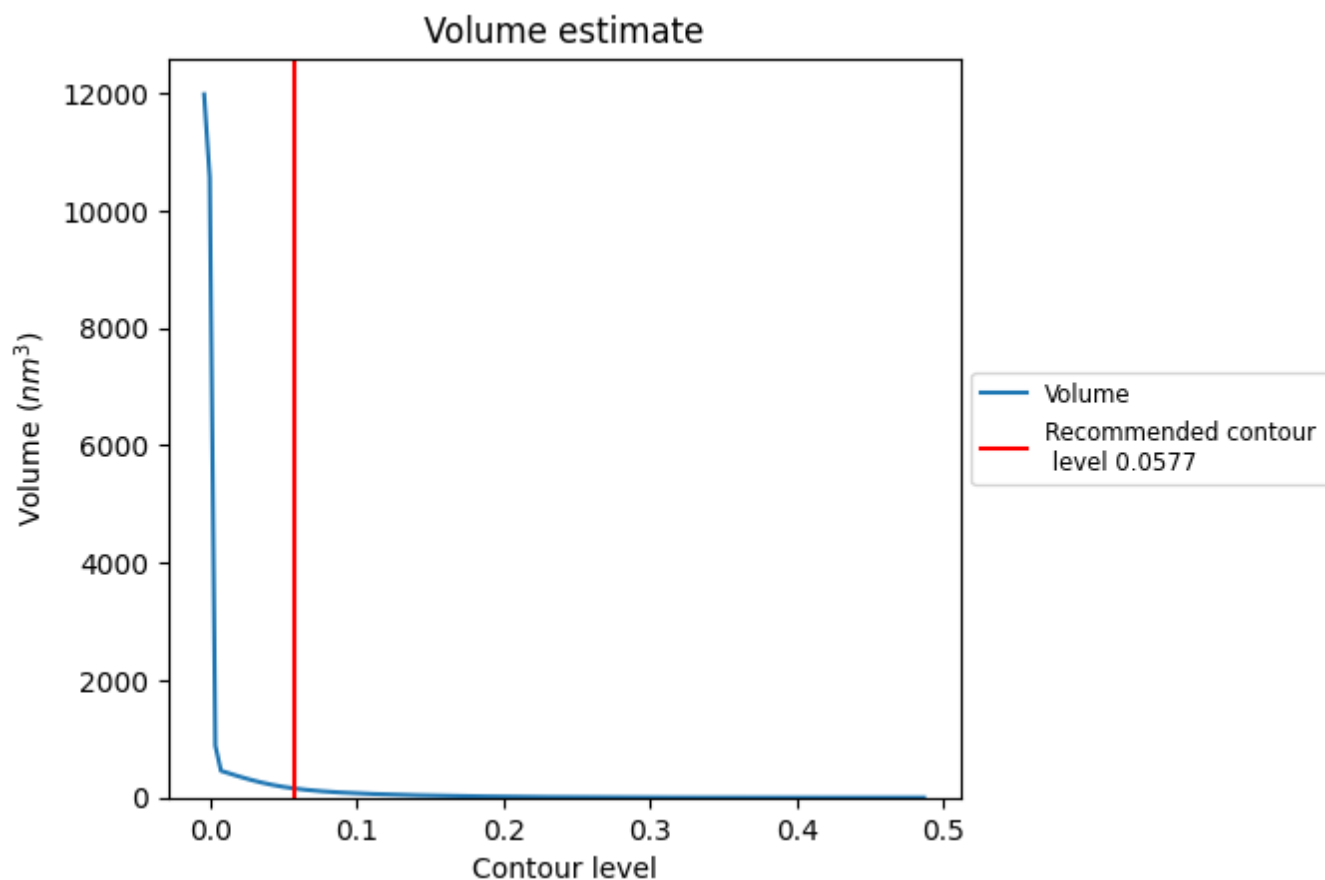
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

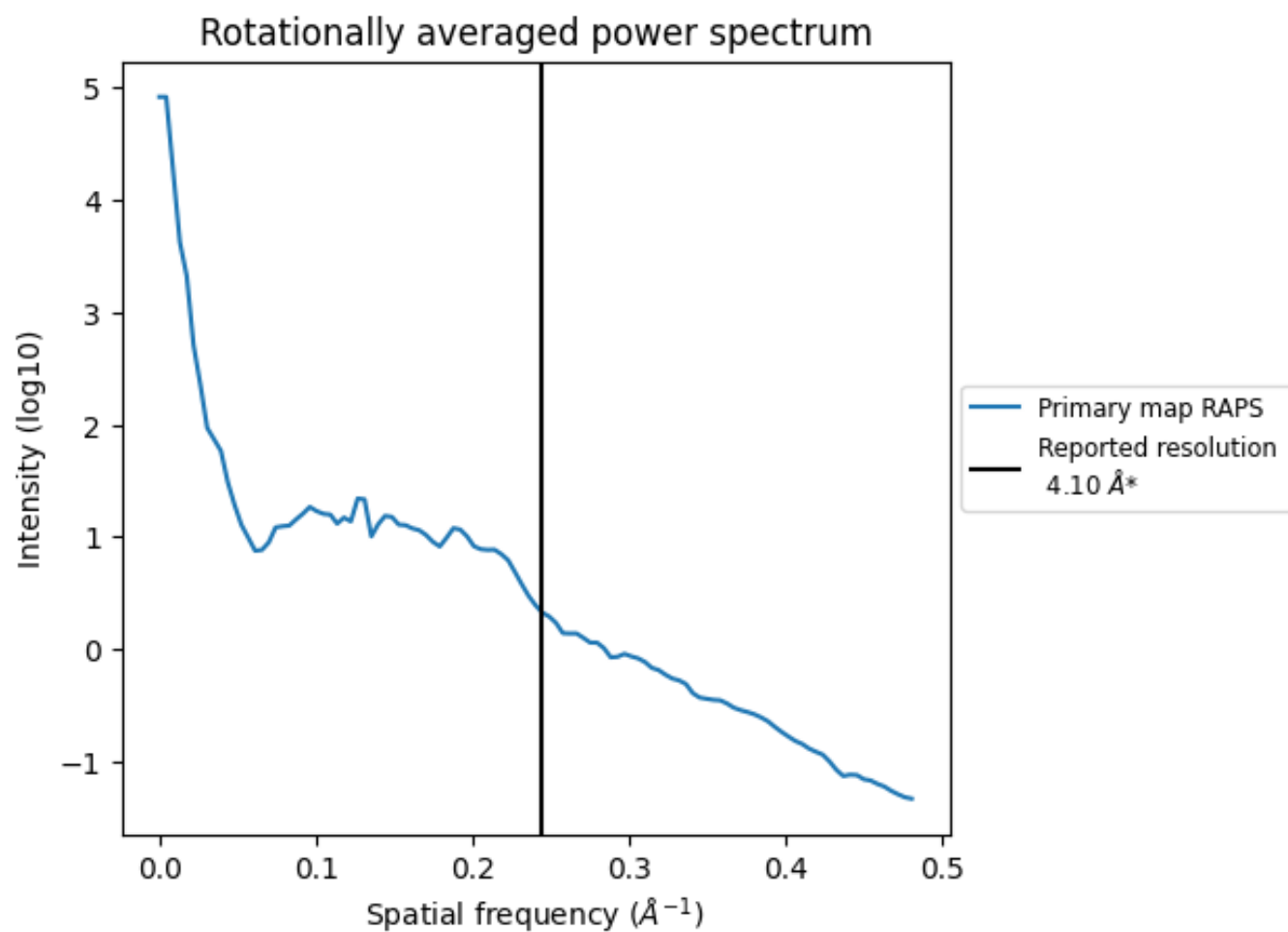
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

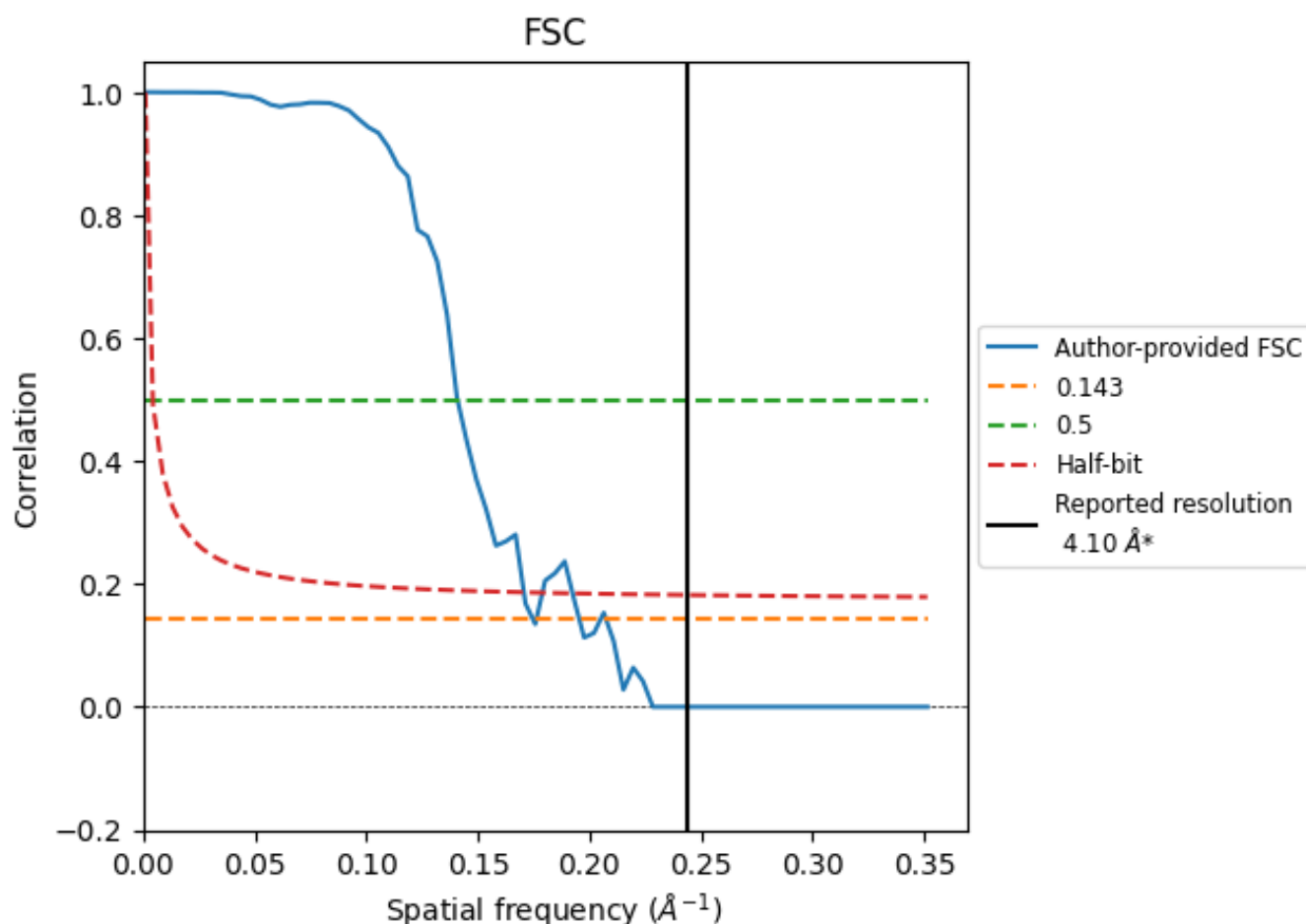


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

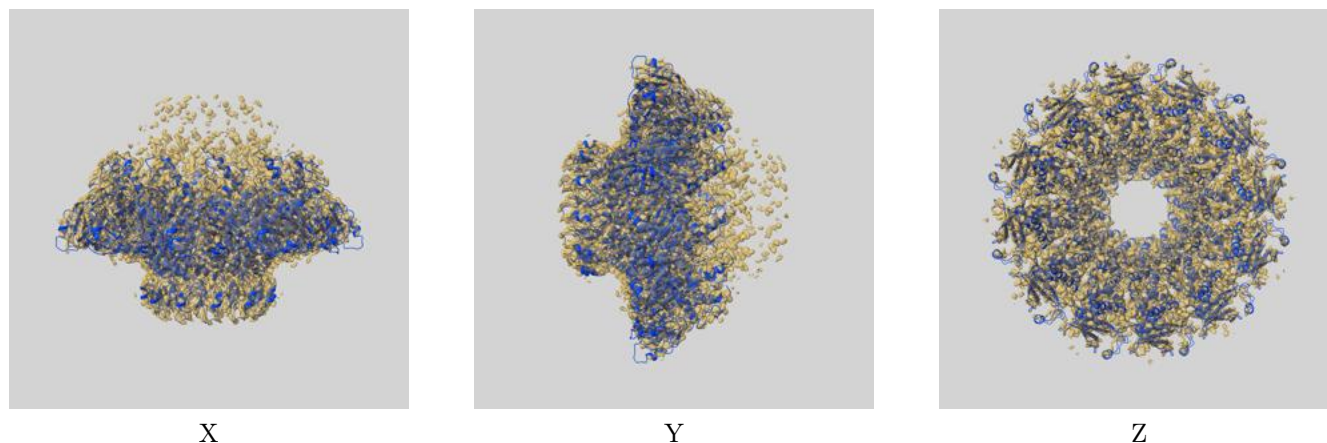
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	5.73	7.10	5.86
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 5.73 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4669 and PDB model 6QXM. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



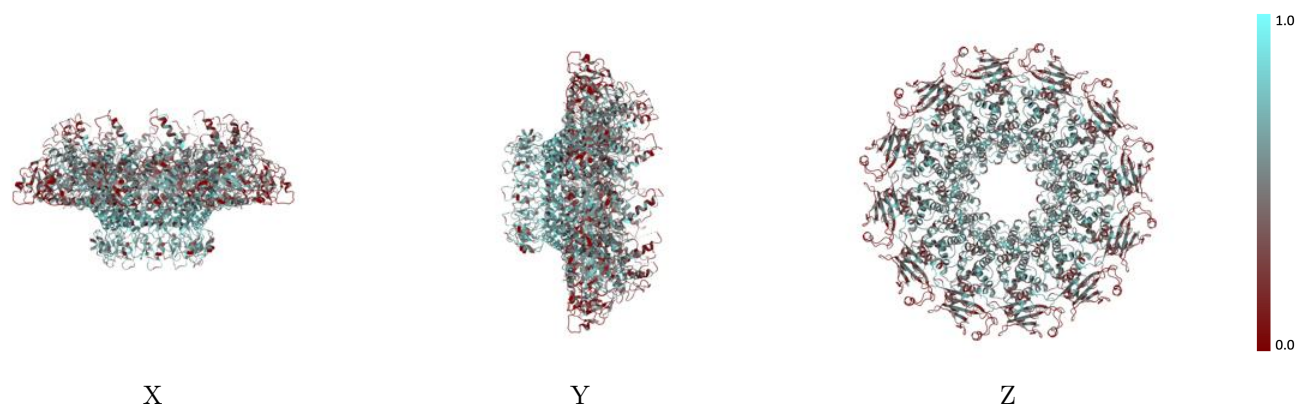
The images above show the 3D surface view of the map at the recommended contour level 0.0577 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



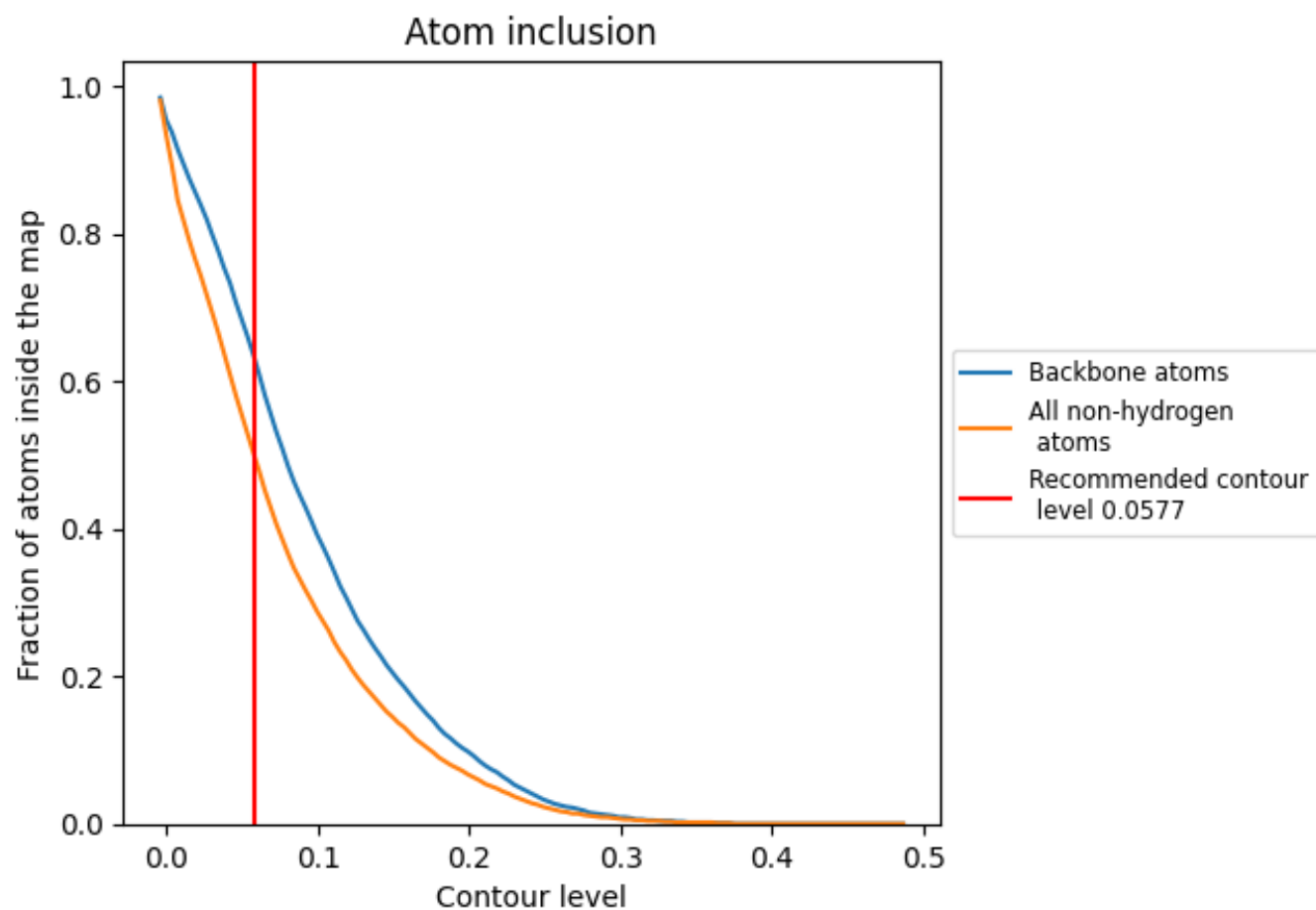
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0577).

9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 50% 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 (0.0577) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.5000</div>	<div><div></div>0.3130</div>
A	<div><div></div>0.4990</div>	<div><div></div>0.3170</div>
B	<div><div></div>0.5080</div>	<div><div></div>0.3110</div>
C	<div><div></div>0.4930</div>	<div><div></div>0.3130</div>
D	<div><div></div>0.5000</div>	<div><div></div>0.3190</div>
E	<div><div></div>0.5080</div>	<div><div></div>0.3100</div>
F	<div><div></div>0.4930</div>	<div><div></div>0.3140</div>
G	<div><div></div>0.5010</div>	<div><div></div>0.3170</div>
H	<div><div></div>0.5070</div>	<div><div></div>0.3110</div>
I	<div><div></div>0.4940</div>	<div><div></div>0.3120</div>
J	<div><div></div>0.5000</div>	<div><div></div>0.3170</div>
K	<div><div></div>0.5070</div>	<div><div></div>0.3100</div>
L	<div><div></div>0.4930</div>	<div><div></div>0.3110</div>

1.0

0.0

<0.0