



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 12:50 AM UTC

PDB ID : 6VAL / pdb_00006val
EMDB ID : EMD-21142
Title : Cryo-EM structure of an undecameric chicken CALHM1 and human CALHM2 chimera
Authors : Syrjanen, J.L.; Chou, T.H.; Furukawa, H.
Deposited on : 2019-12-17
Resolution : 3.87 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:

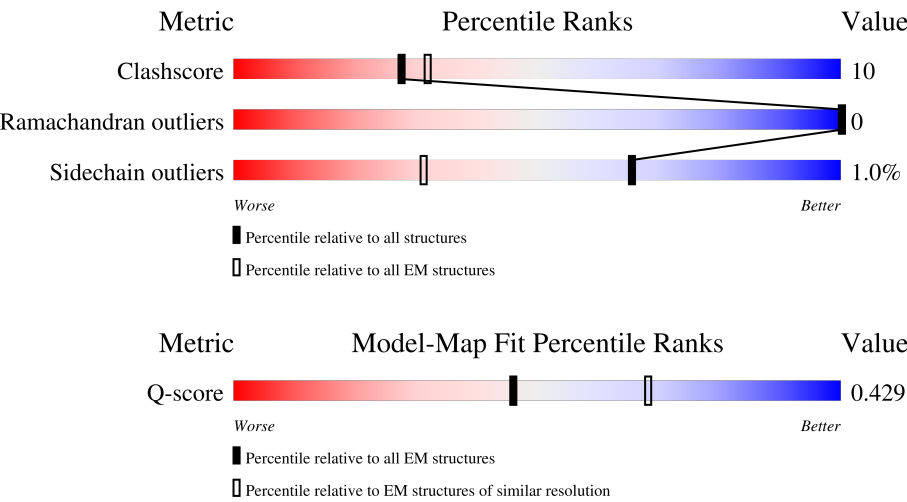
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.87 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.



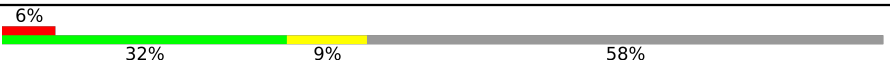
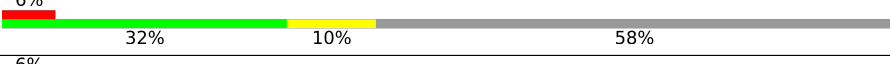
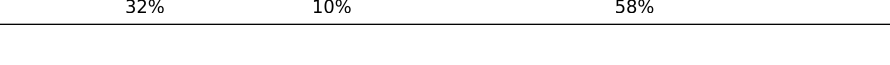
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8831 (3.37 - 4.37)

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	615	
1	B	615	
1	C	615	
1	D	615	

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Mol	Chain	Length	Quality of chain
1	E	615	
1	F	615	
1	G	615	
1	H	615	
1	I	615	
1	J	615	
1	K	615	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 21615 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 Green fluorescent protein, CALHM1,CALMH2 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	B	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	C	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	D	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	E	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	F	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	G	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	H	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	I	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	J	257	Total 1965	C 1277	N 333	O 340	S 15	0	0
1	K	257	Total 1965	C 1277	N 333	O 340	S 15	0	0

There are 682 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-293	MET	-	expression tag	UNP P42212
A	-292	TRP	-	expression tag	UNP P42212
A	-291	SER	-	expression tag	UNP P42212
A	-290	HIS	-	expression tag	UNP P42212
A	-289	PRO	-	expression tag	UNP P42212
A	-288	GLN	-	expression tag	UNP P42212
A	-287	PHE	-	expression tag	UNP P42212
A	-286	GLU	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-285	LYS	-	expression tag	UNP P42212
A	-284	GLY	-	expression tag	UNP P42212
A	-283	GLY	-	expression tag	UNP P42212
A	-282	GLY	-	expression tag	UNP P42212
A	-281	SER	-	expression tag	UNP P42212
A	-280	GLY	-	expression tag	UNP P42212
A	-279	GLY	-	expression tag	UNP P42212
A	-278	GLY	-	expression tag	UNP P42212
A	-277	SER	-	expression tag	UNP P42212
A	-276	GLY	-	expression tag	UNP P42212
A	-275	GLY	-	expression tag	UNP P42212
A	-274	SER	-	expression tag	UNP P42212
A	-273	ALA	-	expression tag	UNP P42212
A	-272	TRP	-	expression tag	UNP P42212
A	-271	SER	-	expression tag	UNP P42212
A	-270	HIS	-	expression tag	UNP P42212
A	-269	PRO	-	expression tag	UNP P42212
A	-268	GLN	-	expression tag	UNP P42212
A	-267	PHE	-	expression tag	UNP P42212
A	-266	GLU	-	expression tag	UNP P42212
A	-265	LYS	-	expression tag	UNP P42212
A	-264	GLY	-	expression tag	UNP P42212
A	-263	ALA	-	expression tag	UNP P42212
A	-262	HIS	-	expression tag	UNP P42212
A	-261	HIS	-	expression tag	UNP P42212
A	-260	HIS	-	expression tag	UNP P42212
A	-259	HIS	-	expression tag	UNP P42212
A	-258	HIS	-	expression tag	UNP P42212
A	-257	HIS	-	expression tag	UNP P42212
A	-256	HIS	-	expression tag	UNP P42212
A	-255	HIS	-	expression tag	UNP P42212
A	-254	ALA	-	expression tag	UNP P42212
A	-253	ALA	-	expression tag	UNP P42212
A	-252	ALA	-	expression tag	UNP P42212
A	-250	VAL	-	insertion	UNP P42212
A	-187	LEU	PHE	conflict	UNP P42212
A	-186	THR	SER	conflict	UNP P42212
A	-45	LYS	ALA	conflict	UNP P42212
A	-20	LEU	HIS	conflict	UNP P42212
A	-12	SER	-	linker	UNP P42212
A	-11	GLY	-	linker	UNP P42212
A	-10	LEU	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ARG	-	linker	UNP P42212
A	-8	SER	-	linker	UNP P42212
A	-7	GLY	-	linker	UNP P42212
A	-6	LEU	-	linker	UNP P42212
A	-5	VAL	-	linker	UNP P42212
A	-4	PRO	-	linker	UNP P42212
A	-3	ARG	-	linker	UNP P42212
A	-2	GLY	-	linker	UNP P42212
A	-1	SER	-	linker	UNP P42212
A	0	GLU	-	linker	UNP P42212
A	1	PHE	-	linker	UNP P42212
A	204	LYS	ARG	conflict	UNP A0A1D5NWS1
B	-293	MET	-	expression tag	UNP P42212
B	-292	TRP	-	expression tag	UNP P42212
B	-291	SER	-	expression tag	UNP P42212
B	-290	HIS	-	expression tag	UNP P42212
B	-289	PRO	-	expression tag	UNP P42212
B	-288	GLN	-	expression tag	UNP P42212
B	-287	PHE	-	expression tag	UNP P42212
B	-286	GLU	-	expression tag	UNP P42212
B	-285	LYS	-	expression tag	UNP P42212
B	-284	GLY	-	expression tag	UNP P42212
B	-283	GLY	-	expression tag	UNP P42212
B	-282	GLY	-	expression tag	UNP P42212
B	-281	SER	-	expression tag	UNP P42212
B	-280	GLY	-	expression tag	UNP P42212
B	-279	GLY	-	expression tag	UNP P42212
B	-278	GLY	-	expression tag	UNP P42212
B	-277	SER	-	expression tag	UNP P42212
B	-276	GLY	-	expression tag	UNP P42212
B	-275	GLY	-	expression tag	UNP P42212
B	-274	SER	-	expression tag	UNP P42212
B	-273	ALA	-	expression tag	UNP P42212
B	-272	TRP	-	expression tag	UNP P42212
B	-271	SER	-	expression tag	UNP P42212
B	-270	HIS	-	expression tag	UNP P42212
B	-269	PRO	-	expression tag	UNP P42212
B	-268	GLN	-	expression tag	UNP P42212
B	-267	PHE	-	expression tag	UNP P42212
B	-266	GLU	-	expression tag	UNP P42212
B	-265	LYS	-	expression tag	UNP P42212
B	-264	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-263	ALA	-	expression tag	UNP P42212
B	-262	HIS	-	expression tag	UNP P42212
B	-261	HIS	-	expression tag	UNP P42212
B	-260	HIS	-	expression tag	UNP P42212
B	-259	HIS	-	expression tag	UNP P42212
B	-258	HIS	-	expression tag	UNP P42212
B	-257	HIS	-	expression tag	UNP P42212
B	-256	HIS	-	expression tag	UNP P42212
B	-255	HIS	-	expression tag	UNP P42212
B	-254	ALA	-	expression tag	UNP P42212
B	-253	ALA	-	expression tag	UNP P42212
B	-252	ALA	-	expression tag	UNP P42212
B	-250	VAL	-	insertion	UNP P42212
B	-187	LEU	PHE	conflict	UNP P42212
B	-186	THR	SER	conflict	UNP P42212
B	-45	LYS	ALA	conflict	UNP P42212
B	-20	LEU	HIS	conflict	UNP P42212
B	-12	SER	-	linker	UNP P42212
B	-11	GLY	-	linker	UNP P42212
B	-10	LEU	-	linker	UNP P42212
B	-9	ARG	-	linker	UNP P42212
B	-8	SER	-	linker	UNP P42212
B	-7	GLY	-	linker	UNP P42212
B	-6	LEU	-	linker	UNP P42212
B	-5	VAL	-	linker	UNP P42212
B	-4	PRO	-	linker	UNP P42212
B	-3	ARG	-	linker	UNP P42212
B	-2	GLY	-	linker	UNP P42212
B	-1	SER	-	linker	UNP P42212
B	0	GLU	-	linker	UNP P42212
B	1	PHE	-	linker	UNP P42212
B	204	LYS	ARG	conflict	UNP A0A1D5NWS1
C	-293	MET	-	expression tag	UNP P42212
C	-292	TRP	-	expression tag	UNP P42212
C	-291	SER	-	expression tag	UNP P42212
C	-290	HIS	-	expression tag	UNP P42212
C	-289	PRO	-	expression tag	UNP P42212
C	-288	GLN	-	expression tag	UNP P42212
C	-287	PHE	-	expression tag	UNP P42212
C	-286	GLU	-	expression tag	UNP P42212
C	-285	LYS	-	expression tag	UNP P42212
C	-284	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-283	GLY	-	expression tag	UNP P42212
C	-282	GLY	-	expression tag	UNP P42212
C	-281	SER	-	expression tag	UNP P42212
C	-280	GLY	-	expression tag	UNP P42212
C	-279	GLY	-	expression tag	UNP P42212
C	-278	GLY	-	expression tag	UNP P42212
C	-277	SER	-	expression tag	UNP P42212
C	-276	GLY	-	expression tag	UNP P42212
C	-275	GLY	-	expression tag	UNP P42212
C	-274	SER	-	expression tag	UNP P42212
C	-273	ALA	-	expression tag	UNP P42212
C	-272	TRP	-	expression tag	UNP P42212
C	-271	SER	-	expression tag	UNP P42212
C	-270	HIS	-	expression tag	UNP P42212
C	-269	PRO	-	expression tag	UNP P42212
C	-268	GLN	-	expression tag	UNP P42212
C	-267	PHE	-	expression tag	UNP P42212
C	-266	GLU	-	expression tag	UNP P42212
C	-265	LYS	-	expression tag	UNP P42212
C	-264	GLY	-	expression tag	UNP P42212
C	-263	ALA	-	expression tag	UNP P42212
C	-262	HIS	-	expression tag	UNP P42212
C	-261	HIS	-	expression tag	UNP P42212
C	-260	HIS	-	expression tag	UNP P42212
C	-259	HIS	-	expression tag	UNP P42212
C	-258	HIS	-	expression tag	UNP P42212
C	-257	HIS	-	expression tag	UNP P42212
C	-256	HIS	-	expression tag	UNP P42212
C	-255	HIS	-	expression tag	UNP P42212
C	-254	ALA	-	expression tag	UNP P42212
C	-253	ALA	-	expression tag	UNP P42212
C	-252	ALA	-	expression tag	UNP P42212
C	-250	VAL	-	insertion	UNP P42212
C	-187	LEU	PHE	conflict	UNP P42212
C	-186	THR	SER	conflict	UNP P42212
C	-45	LYS	ALA	conflict	UNP P42212
C	-20	LEU	HIS	conflict	UNP P42212
C	-12	SER	-	linker	UNP P42212
C	-11	GLY	-	linker	UNP P42212
C	-10	LEU	-	linker	UNP P42212
C	-9	ARG	-	linker	UNP P42212
C	-8	SER	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	linker	UNP P42212
C	-6	LEU	-	linker	UNP P42212
C	-5	VAL	-	linker	UNP P42212
C	-4	PRO	-	linker	UNP P42212
C	-3	ARG	-	linker	UNP P42212
C	-2	GLY	-	linker	UNP P42212
C	-1	SER	-	linker	UNP P42212
C	0	GLU	-	linker	UNP P42212
C	1	PHE	-	linker	UNP P42212
C	204	LYS	ARG	conflict	UNP A0A1D5NWS1
D	-293	MET	-	expression tag	UNP P42212
D	-292	TRP	-	expression tag	UNP P42212
D	-291	SER	-	expression tag	UNP P42212
D	-290	HIS	-	expression tag	UNP P42212
D	-289	PRO	-	expression tag	UNP P42212
D	-288	GLN	-	expression tag	UNP P42212
D	-287	PHE	-	expression tag	UNP P42212
D	-286	GLU	-	expression tag	UNP P42212
D	-285	LYS	-	expression tag	UNP P42212
D	-284	GLY	-	expression tag	UNP P42212
D	-283	GLY	-	expression tag	UNP P42212
D	-282	GLY	-	expression tag	UNP P42212
D	-281	SER	-	expression tag	UNP P42212
D	-280	GLY	-	expression tag	UNP P42212
D	-279	GLY	-	expression tag	UNP P42212
D	-278	GLY	-	expression tag	UNP P42212
D	-277	SER	-	expression tag	UNP P42212
D	-276	GLY	-	expression tag	UNP P42212
D	-275	GLY	-	expression tag	UNP P42212
D	-274	SER	-	expression tag	UNP P42212
D	-273	ALA	-	expression tag	UNP P42212
D	-272	TRP	-	expression tag	UNP P42212
D	-271	SER	-	expression tag	UNP P42212
D	-270	HIS	-	expression tag	UNP P42212
D	-269	PRO	-	expression tag	UNP P42212
D	-268	GLN	-	expression tag	UNP P42212
D	-267	PHE	-	expression tag	UNP P42212
D	-266	GLU	-	expression tag	UNP P42212
D	-265	LYS	-	expression tag	UNP P42212
D	-264	GLY	-	expression tag	UNP P42212
D	-263	ALA	-	expression tag	UNP P42212
D	-262	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-261	HIS	-	expression tag	UNP P42212
D	-260	HIS	-	expression tag	UNP P42212
D	-259	HIS	-	expression tag	UNP P42212
D	-258	HIS	-	expression tag	UNP P42212
D	-257	HIS	-	expression tag	UNP P42212
D	-256	HIS	-	expression tag	UNP P42212
D	-255	HIS	-	expression tag	UNP P42212
D	-254	ALA	-	expression tag	UNP P42212
D	-253	ALA	-	expression tag	UNP P42212
D	-252	ALA	-	expression tag	UNP P42212
D	-250	VAL	-	insertion	UNP P42212
D	-187	LEU	PHE	conflict	UNP P42212
D	-186	THR	SER	conflict	UNP P42212
D	-45	LYS	ALA	conflict	UNP P42212
D	-20	LEU	HIS	conflict	UNP P42212
D	-12	SER	-	linker	UNP P42212
D	-11	GLY	-	linker	UNP P42212
D	-10	LEU	-	linker	UNP P42212
D	-9	ARG	-	linker	UNP P42212
D	-8	SER	-	linker	UNP P42212
D	-7	GLY	-	linker	UNP P42212
D	-6	LEU	-	linker	UNP P42212
D	-5	VAL	-	linker	UNP P42212
D	-4	PRO	-	linker	UNP P42212
D	-3	ARG	-	linker	UNP P42212
D	-2	GLY	-	linker	UNP P42212
D	-1	SER	-	linker	UNP P42212
D	0	GLU	-	linker	UNP P42212
D	1	PHE	-	linker	UNP P42212
D	204	LYS	ARG	conflict	UNP A0A1D5NWS1
E	-293	MET	-	expression tag	UNP P42212
E	-292	TRP	-	expression tag	UNP P42212
E	-291	SER	-	expression tag	UNP P42212
E	-290	HIS	-	expression tag	UNP P42212
E	-289	PRO	-	expression tag	UNP P42212
E	-288	GLN	-	expression tag	UNP P42212
E	-287	PHE	-	expression tag	UNP P42212
E	-286	GLU	-	expression tag	UNP P42212
E	-285	LYS	-	expression tag	UNP P42212
E	-284	GLY	-	expression tag	UNP P42212
E	-283	GLY	-	expression tag	UNP P42212
E	-282	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-281	SER	-	expression tag	UNP P42212
E	-280	GLY	-	expression tag	UNP P42212
E	-279	GLY	-	expression tag	UNP P42212
E	-278	GLY	-	expression tag	UNP P42212
E	-277	SER	-	expression tag	UNP P42212
E	-276	GLY	-	expression tag	UNP P42212
E	-275	GLY	-	expression tag	UNP P42212
E	-274	SER	-	expression tag	UNP P42212
E	-273	ALA	-	expression tag	UNP P42212
E	-272	TRP	-	expression tag	UNP P42212
E	-271	SER	-	expression tag	UNP P42212
E	-270	HIS	-	expression tag	UNP P42212
E	-269	PRO	-	expression tag	UNP P42212
E	-268	GLN	-	expression tag	UNP P42212
E	-267	PHE	-	expression tag	UNP P42212
E	-266	GLU	-	expression tag	UNP P42212
E	-265	LYS	-	expression tag	UNP P42212
E	-264	GLY	-	expression tag	UNP P42212
E	-263	ALA	-	expression tag	UNP P42212
E	-262	HIS	-	expression tag	UNP P42212
E	-261	HIS	-	expression tag	UNP P42212
E	-260	HIS	-	expression tag	UNP P42212
E	-259	HIS	-	expression tag	UNP P42212
E	-258	HIS	-	expression tag	UNP P42212
E	-257	HIS	-	expression tag	UNP P42212
E	-256	HIS	-	expression tag	UNP P42212
E	-255	HIS	-	expression tag	UNP P42212
E	-254	ALA	-	expression tag	UNP P42212
E	-253	ALA	-	expression tag	UNP P42212
E	-252	ALA	-	expression tag	UNP P42212
E	-250	VAL	-	insertion	UNP P42212
E	-187	LEU	PHE	conflict	UNP P42212
E	-186	THR	SER	conflict	UNP P42212
E	-45	LYS	ALA	conflict	UNP P42212
E	-20	LEU	HIS	conflict	UNP P42212
E	-12	SER	-	linker	UNP P42212
E	-11	GLY	-	linker	UNP P42212
E	-10	LEU	-	linker	UNP P42212
E	-9	ARG	-	linker	UNP P42212
E	-8	SER	-	linker	UNP P42212
E	-7	GLY	-	linker	UNP P42212
E	-6	LEU	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	VAL	-	linker	UNP P42212
E	-4	PRO	-	linker	UNP P42212
E	-3	ARG	-	linker	UNP P42212
E	-2	GLY	-	linker	UNP P42212
E	-1	SER	-	linker	UNP P42212
E	0	GLU	-	linker	UNP P42212
E	1	PHE	-	linker	UNP P42212
E	204	LYS	ARG	conflict	UNP A0A1D5NWS1
F	-293	MET	-	expression tag	UNP P42212
F	-292	TRP	-	expression tag	UNP P42212
F	-291	SER	-	expression tag	UNP P42212
F	-290	HIS	-	expression tag	UNP P42212
F	-289	PRO	-	expression tag	UNP P42212
F	-288	GLN	-	expression tag	UNP P42212
F	-287	PHE	-	expression tag	UNP P42212
F	-286	GLU	-	expression tag	UNP P42212
F	-285	LYS	-	expression tag	UNP P42212
F	-284	GLY	-	expression tag	UNP P42212
F	-283	GLY	-	expression tag	UNP P42212
F	-282	GLY	-	expression tag	UNP P42212
F	-281	SER	-	expression tag	UNP P42212
F	-280	GLY	-	expression tag	UNP P42212
F	-279	GLY	-	expression tag	UNP P42212
F	-278	GLY	-	expression tag	UNP P42212
F	-277	SER	-	expression tag	UNP P42212
F	-276	GLY	-	expression tag	UNP P42212
F	-275	GLY	-	expression tag	UNP P42212
F	-274	SER	-	expression tag	UNP P42212
F	-273	ALA	-	expression tag	UNP P42212
F	-272	TRP	-	expression tag	UNP P42212
F	-271	SER	-	expression tag	UNP P42212
F	-270	HIS	-	expression tag	UNP P42212
F	-269	PRO	-	expression tag	UNP P42212
F	-268	GLN	-	expression tag	UNP P42212
F	-267	PHE	-	expression tag	UNP P42212
F	-266	GLU	-	expression tag	UNP P42212
F	-265	LYS	-	expression tag	UNP P42212
F	-264	GLY	-	expression tag	UNP P42212
F	-263	ALA	-	expression tag	UNP P42212
F	-262	HIS	-	expression tag	UNP P42212
F	-261	HIS	-	expression tag	UNP P42212
F	-260	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-259	HIS	-	expression tag	UNP P42212
F	-258	HIS	-	expression tag	UNP P42212
F	-257	HIS	-	expression tag	UNP P42212
F	-256	HIS	-	expression tag	UNP P42212
F	-255	HIS	-	expression tag	UNP P42212
F	-254	ALA	-	expression tag	UNP P42212
F	-253	ALA	-	expression tag	UNP P42212
F	-252	ALA	-	expression tag	UNP P42212
F	-250	VAL	-	insertion	UNP P42212
F	-187	LEU	PHE	conflict	UNP P42212
F	-186	THR	SER	conflict	UNP P42212
F	-45	LYS	ALA	conflict	UNP P42212
F	-20	LEU	HIS	conflict	UNP P42212
F	-12	SER	-	linker	UNP P42212
F	-11	GLY	-	linker	UNP P42212
F	-10	LEU	-	linker	UNP P42212
F	-9	ARG	-	linker	UNP P42212
F	-8	SER	-	linker	UNP P42212
F	-7	GLY	-	linker	UNP P42212
F	-6	LEU	-	linker	UNP P42212
F	-5	VAL	-	linker	UNP P42212
F	-4	PRO	-	linker	UNP P42212
F	-3	ARG	-	linker	UNP P42212
F	-2	GLY	-	linker	UNP P42212
F	-1	SER	-	linker	UNP P42212
F	0	GLU	-	linker	UNP P42212
F	1	PHE	-	linker	UNP P42212
F	204	LYS	ARG	conflict	UNP A0A1D5NWS1
G	-293	MET	-	expression tag	UNP P42212
G	-292	TRP	-	expression tag	UNP P42212
G	-291	SER	-	expression tag	UNP P42212
G	-290	HIS	-	expression tag	UNP P42212
G	-289	PRO	-	expression tag	UNP P42212
G	-288	GLN	-	expression tag	UNP P42212
G	-287	PHE	-	expression tag	UNP P42212
G	-286	GLU	-	expression tag	UNP P42212
G	-285	LYS	-	expression tag	UNP P42212
G	-284	GLY	-	expression tag	UNP P42212
G	-283	GLY	-	expression tag	UNP P42212
G	-282	GLY	-	expression tag	UNP P42212
G	-281	SER	-	expression tag	UNP P42212
G	-280	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-279	GLY	-	expression tag	UNP P42212
G	-278	GLY	-	expression tag	UNP P42212
G	-277	SER	-	expression tag	UNP P42212
G	-276	GLY	-	expression tag	UNP P42212
G	-275	GLY	-	expression tag	UNP P42212
G	-274	SER	-	expression tag	UNP P42212
G	-273	ALA	-	expression tag	UNP P42212
G	-272	TRP	-	expression tag	UNP P42212
G	-271	SER	-	expression tag	UNP P42212
G	-270	HIS	-	expression tag	UNP P42212
G	-269	PRO	-	expression tag	UNP P42212
G	-268	GLN	-	expression tag	UNP P42212
G	-267	PHE	-	expression tag	UNP P42212
G	-266	GLU	-	expression tag	UNP P42212
G	-265	LYS	-	expression tag	UNP P42212
G	-264	GLY	-	expression tag	UNP P42212
G	-263	ALA	-	expression tag	UNP P42212
G	-262	HIS	-	expression tag	UNP P42212
G	-261	HIS	-	expression tag	UNP P42212
G	-260	HIS	-	expression tag	UNP P42212
G	-259	HIS	-	expression tag	UNP P42212
G	-258	HIS	-	expression tag	UNP P42212
G	-257	HIS	-	expression tag	UNP P42212
G	-256	HIS	-	expression tag	UNP P42212
G	-255	HIS	-	expression tag	UNP P42212
G	-254	ALA	-	expression tag	UNP P42212
G	-253	ALA	-	expression tag	UNP P42212
G	-252	ALA	-	expression tag	UNP P42212
G	-250	VAL	-	insertion	UNP P42212
G	-187	LEU	PHE	conflict	UNP P42212
G	-186	THR	SER	conflict	UNP P42212
G	-45	LYS	ALA	conflict	UNP P42212
G	-20	LEU	HIS	conflict	UNP P42212
G	-12	SER	-	linker	UNP P42212
G	-11	GLY	-	linker	UNP P42212
G	-10	LEU	-	linker	UNP P42212
G	-9	ARG	-	linker	UNP P42212
G	-8	SER	-	linker	UNP P42212
G	-7	GLY	-	linker	UNP P42212
G	-6	LEU	-	linker	UNP P42212
G	-5	VAL	-	linker	UNP P42212
G	-4	PRO	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	ARG	-	linker	UNP P42212
G	-2	GLY	-	linker	UNP P42212
G	-1	SER	-	linker	UNP P42212
G	0	GLU	-	linker	UNP P42212
G	1	PHE	-	linker	UNP P42212
G	204	LYS	ARG	conflict	UNP A0A1D5NWS1
H	-293	MET	-	expression tag	UNP P42212
H	-292	TRP	-	expression tag	UNP P42212
H	-291	SER	-	expression tag	UNP P42212
H	-290	HIS	-	expression tag	UNP P42212
H	-289	PRO	-	expression tag	UNP P42212
H	-288	GLN	-	expression tag	UNP P42212
H	-287	PHE	-	expression tag	UNP P42212
H	-286	GLU	-	expression tag	UNP P42212
H	-285	LYS	-	expression tag	UNP P42212
H	-284	GLY	-	expression tag	UNP P42212
H	-283	GLY	-	expression tag	UNP P42212
H	-282	GLY	-	expression tag	UNP P42212
H	-281	SER	-	expression tag	UNP P42212
H	-280	GLY	-	expression tag	UNP P42212
H	-279	GLY	-	expression tag	UNP P42212
H	-278	GLY	-	expression tag	UNP P42212
H	-277	SER	-	expression tag	UNP P42212
H	-276	GLY	-	expression tag	UNP P42212
H	-275	GLY	-	expression tag	UNP P42212
H	-274	SER	-	expression tag	UNP P42212
H	-273	ALA	-	expression tag	UNP P42212
H	-272	TRP	-	expression tag	UNP P42212
H	-271	SER	-	expression tag	UNP P42212
H	-270	HIS	-	expression tag	UNP P42212
H	-269	PRO	-	expression tag	UNP P42212
H	-268	GLN	-	expression tag	UNP P42212
H	-267	PHE	-	expression tag	UNP P42212
H	-266	GLU	-	expression tag	UNP P42212
H	-265	LYS	-	expression tag	UNP P42212
H	-264	GLY	-	expression tag	UNP P42212
H	-263	ALA	-	expression tag	UNP P42212
H	-262	HIS	-	expression tag	UNP P42212
H	-261	HIS	-	expression tag	UNP P42212
H	-260	HIS	-	expression tag	UNP P42212
H	-259	HIS	-	expression tag	UNP P42212
H	-258	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-257	HIS	-	expression tag	UNP P42212
H	-256	HIS	-	expression tag	UNP P42212
H	-255	HIS	-	expression tag	UNP P42212
H	-254	ALA	-	expression tag	UNP P42212
H	-253	ALA	-	expression tag	UNP P42212
H	-252	ALA	-	expression tag	UNP P42212
H	-250	VAL	-	insertion	UNP P42212
H	-187	LEU	PHE	conflict	UNP P42212
H	-186	THR	SER	conflict	UNP P42212
H	-45	LYS	ALA	conflict	UNP P42212
H	-20	LEU	HIS	conflict	UNP P42212
H	-12	SER	-	linker	UNP P42212
H	-11	GLY	-	linker	UNP P42212
H	-10	LEU	-	linker	UNP P42212
H	-9	ARG	-	linker	UNP P42212
H	-8	SER	-	linker	UNP P42212
H	-7	GLY	-	linker	UNP P42212
H	-6	LEU	-	linker	UNP P42212
H	-5	VAL	-	linker	UNP P42212
H	-4	PRO	-	linker	UNP P42212
H	-3	ARG	-	linker	UNP P42212
H	-2	GLY	-	linker	UNP P42212
H	-1	SER	-	linker	UNP P42212
H	0	GLU	-	linker	UNP P42212
H	1	PHE	-	linker	UNP P42212
H	204	LYS	ARG	conflict	UNP A0A1D5NWS1
I	-293	MET	-	expression tag	UNP P42212
I	-292	TRP	-	expression tag	UNP P42212
I	-291	SER	-	expression tag	UNP P42212
I	-290	HIS	-	expression tag	UNP P42212
I	-289	PRO	-	expression tag	UNP P42212
I	-288	GLN	-	expression tag	UNP P42212
I	-287	PHE	-	expression tag	UNP P42212
I	-286	GLU	-	expression tag	UNP P42212
I	-285	LYS	-	expression tag	UNP P42212
I	-284	GLY	-	expression tag	UNP P42212
I	-283	GLY	-	expression tag	UNP P42212
I	-282	GLY	-	expression tag	UNP P42212
I	-281	SER	-	expression tag	UNP P42212
I	-280	GLY	-	expression tag	UNP P42212
I	-279	GLY	-	expression tag	UNP P42212
I	-278	GLY	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-277	SER	-	expression tag	UNP P42212
I	-276	GLY	-	expression tag	UNP P42212
I	-275	GLY	-	expression tag	UNP P42212
I	-274	SER	-	expression tag	UNP P42212
I	-273	ALA	-	expression tag	UNP P42212
I	-272	TRP	-	expression tag	UNP P42212
I	-271	SER	-	expression tag	UNP P42212
I	-270	HIS	-	expression tag	UNP P42212
I	-269	PRO	-	expression tag	UNP P42212
I	-268	GLN	-	expression tag	UNP P42212
I	-267	PHE	-	expression tag	UNP P42212
I	-266	GLU	-	expression tag	UNP P42212
I	-265	LYS	-	expression tag	UNP P42212
I	-264	GLY	-	expression tag	UNP P42212
I	-263	ALA	-	expression tag	UNP P42212
I	-262	HIS	-	expression tag	UNP P42212
I	-261	HIS	-	expression tag	UNP P42212
I	-260	HIS	-	expression tag	UNP P42212
I	-259	HIS	-	expression tag	UNP P42212
I	-258	HIS	-	expression tag	UNP P42212
I	-257	HIS	-	expression tag	UNP P42212
I	-256	HIS	-	expression tag	UNP P42212
I	-255	HIS	-	expression tag	UNP P42212
I	-254	ALA	-	expression tag	UNP P42212
I	-253	ALA	-	expression tag	UNP P42212
I	-252	ALA	-	expression tag	UNP P42212
I	-250	VAL	-	insertion	UNP P42212
I	-187	LEU	PHE	conflict	UNP P42212
I	-186	THR	SER	conflict	UNP P42212
I	-45	LYS	ALA	conflict	UNP P42212
I	-20	LEU	HIS	conflict	UNP P42212
I	-12	SER	-	linker	UNP P42212
I	-11	GLY	-	linker	UNP P42212
I	-10	LEU	-	linker	UNP P42212
I	-9	ARG	-	linker	UNP P42212
I	-8	SER	-	linker	UNP P42212
I	-7	GLY	-	linker	UNP P42212
I	-6	LEU	-	linker	UNP P42212
I	-5	VAL	-	linker	UNP P42212
I	-4	PRO	-	linker	UNP P42212
I	-3	ARG	-	linker	UNP P42212
I	-2	GLY	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	SER	-	linker	UNP P42212
I	0	GLU	-	linker	UNP P42212
I	1	PHE	-	linker	UNP P42212
I	204	LYS	ARG	conflict	UNP A0A1D5NWS1
J	-293	MET	-	expression tag	UNP P42212
J	-292	TRP	-	expression tag	UNP P42212
J	-291	SER	-	expression tag	UNP P42212
J	-290	HIS	-	expression tag	UNP P42212
J	-289	PRO	-	expression tag	UNP P42212
J	-288	GLN	-	expression tag	UNP P42212
J	-287	PHE	-	expression tag	UNP P42212
J	-286	GLU	-	expression tag	UNP P42212
J	-285	LYS	-	expression tag	UNP P42212
J	-284	GLY	-	expression tag	UNP P42212
J	-283	GLY	-	expression tag	UNP P42212
J	-282	GLY	-	expression tag	UNP P42212
J	-281	SER	-	expression tag	UNP P42212
J	-280	GLY	-	expression tag	UNP P42212
J	-279	GLY	-	expression tag	UNP P42212
J	-278	GLY	-	expression tag	UNP P42212
J	-277	SER	-	expression tag	UNP P42212
J	-276	GLY	-	expression tag	UNP P42212
J	-275	GLY	-	expression tag	UNP P42212
J	-274	SER	-	expression tag	UNP P42212
J	-273	ALA	-	expression tag	UNP P42212
J	-272	TRP	-	expression tag	UNP P42212
J	-271	SER	-	expression tag	UNP P42212
J	-270	HIS	-	expression tag	UNP P42212
J	-269	PRO	-	expression tag	UNP P42212
J	-268	GLN	-	expression tag	UNP P42212
J	-267	PHE	-	expression tag	UNP P42212
J	-266	GLU	-	expression tag	UNP P42212
J	-265	LYS	-	expression tag	UNP P42212
J	-264	GLY	-	expression tag	UNP P42212
J	-263	ALA	-	expression tag	UNP P42212
J	-262	HIS	-	expression tag	UNP P42212
J	-261	HIS	-	expression tag	UNP P42212
J	-260	HIS	-	expression tag	UNP P42212
J	-259	HIS	-	expression tag	UNP P42212
J	-258	HIS	-	expression tag	UNP P42212
J	-257	HIS	-	expression tag	UNP P42212
J	-256	HIS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-255	HIS	-	expression tag	UNP P42212
J	-254	ALA	-	expression tag	UNP P42212
J	-253	ALA	-	expression tag	UNP P42212
J	-252	ALA	-	expression tag	UNP P42212
J	-250	VAL	-	insertion	UNP P42212
J	-187	LEU	PHE	conflict	UNP P42212
J	-186	THR	SER	conflict	UNP P42212
J	-45	LYS	ALA	conflict	UNP P42212
J	-20	LEU	HIS	conflict	UNP P42212
J	-12	SER	-	linker	UNP P42212
J	-11	GLY	-	linker	UNP P42212
J	-10	LEU	-	linker	UNP P42212
J	-9	ARG	-	linker	UNP P42212
J	-8	SER	-	linker	UNP P42212
J	-7	GLY	-	linker	UNP P42212
J	-6	LEU	-	linker	UNP P42212
J	-5	VAL	-	linker	UNP P42212
J	-4	PRO	-	linker	UNP P42212
J	-3	ARG	-	linker	UNP P42212
J	-2	GLY	-	linker	UNP P42212
J	-1	SER	-	linker	UNP P42212
J	0	GLU	-	linker	UNP P42212
J	1	PHE	-	linker	UNP P42212
J	204	LYS	ARG	conflict	UNP A0A1D5NWS1
K	-293	MET	-	expression tag	UNP P42212
K	-292	TRP	-	expression tag	UNP P42212
K	-291	SER	-	expression tag	UNP P42212
K	-290	HIS	-	expression tag	UNP P42212
K	-289	PRO	-	expression tag	UNP P42212
K	-288	GLN	-	expression tag	UNP P42212
K	-287	PHE	-	expression tag	UNP P42212
K	-286	GLU	-	expression tag	UNP P42212
K	-285	LYS	-	expression tag	UNP P42212
K	-284	GLY	-	expression tag	UNP P42212
K	-283	GLY	-	expression tag	UNP P42212
K	-282	GLY	-	expression tag	UNP P42212
K	-281	SER	-	expression tag	UNP P42212
K	-280	GLY	-	expression tag	UNP P42212
K	-279	GLY	-	expression tag	UNP P42212
K	-278	GLY	-	expression tag	UNP P42212
K	-277	SER	-	expression tag	UNP P42212
K	-276	GLY	-	expression tag	UNP P42212

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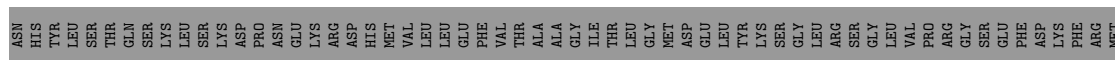
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Chain	Residue	Modelled	Actual	Comment	Reference
K	-275	GLY	-	expression tag	UNP P42212
K	-274	SER	-	expression tag	UNP P42212
K	-273	ALA	-	expression tag	UNP P42212
K	-272	TRP	-	expression tag	UNP P42212
K	-271	SER	-	expression tag	UNP P42212
K	-270	HIS	-	expression tag	UNP P42212
K	-269	PRO	-	expression tag	UNP P42212
K	-268	GLN	-	expression tag	UNP P42212
K	-267	PHE	-	expression tag	UNP P42212
K	-266	GLU	-	expression tag	UNP P42212
K	-265	LYS	-	expression tag	UNP P42212
K	-264	GLY	-	expression tag	UNP P42212
K	-263	ALA	-	expression tag	UNP P42212
K	-262	HIS	-	expression tag	UNP P42212
K	-261	HIS	-	expression tag	UNP P42212
K	-260	HIS	-	expression tag	UNP P42212
K	-259	HIS	-	expression tag	UNP P42212
K	-258	HIS	-	expression tag	UNP P42212
K	-257	HIS	-	expression tag	UNP P42212
K	-256	HIS	-	expression tag	UNP P42212
K	-255	HIS	-	expression tag	UNP P42212
K	-254	ALA	-	expression tag	UNP P42212
K	-253	ALA	-	expression tag	UNP P42212
K	-252	ALA	-	expression tag	UNP P42212
K	-250	VAL	-	insertion	UNP P42212
K	-187	LEU	PHE	conflict	UNP P42212
K	-186	THR	SER	conflict	UNP P42212
K	-45	LYS	ALA	conflict	UNP P42212
K	-20	LEU	HIS	conflict	UNP P42212
K	-12	SER	-	linker	UNP P42212
K	-11	GLY	-	linker	UNP P42212
K	-10	LEU	-	linker	UNP P42212
K	-9	ARG	-	linker	UNP P42212
K	-8	SER	-	linker	UNP P42212
K	-7	GLY	-	linker	UNP P42212
K	-6	LEU	-	linker	UNP P42212
K	-5	VAL	-	linker	UNP P42212
K	-4	PRO	-	linker	UNP P42212
K	-3	ARG	-	linker	UNP P42212
K	-2	GLY	-	linker	UNP P42212
K	-1	SER	-	linker	UNP P42212
K	0	GLU	-	linker	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	PHE	-	linker	UNP P42212
K	204	LYS	ARG	conflict	UNP A0A1D5NWS1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123664	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 ($e^-/\text{\AA}^2$)	57.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	11.974	Depositor
Minimum map value	-7.288	Depositor
Average map value	0.072	Depositor
Map value standard deviation	0.561	Depositor
Recommended contour level	2.82	Depositor
Map size ($\text{\AA}$)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	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	0.24	0/2013	0.44	0/2751
1	B	0.24	0/2013	0.44	0/2751
1	C	0.24	0/2013	0.44	0/2751
1	D	0.24	0/2013	0.44	0/2751
1	E	0.24	0/2013	0.44	0/2751
1	F	0.24	0/2013	0.44	0/2751
1	G	0.24	0/2013	0.44	0/2751
1	H	0.24	0/2013	0.44	0/2751
1	I	0.24	0/2013	0.44	0/2751
1	J	0.24	0/2013	0.44	0/2751
1	K	0.24	0/2013	0.44	0/2751
All	All	0.24	0/22143	0.44	0/30261

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1965	0	1888	51	0
1	B	1965	0	1888	45	0
1	C	1965	0	1888	44	0
1	D	1965	0	1888	48	0
1	E	1965	0	1888	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1965	0	1888	46	0
1	G	1965	0	1888	47	0
1	H	1965	0	1888	46	0
1	I	1965	0	1888	47	0
1	J	1965	0	1888	43	0
1	K	1965	0	1888	46	0
All	All	21615	0	20768	413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (413) 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:A:214:GLN:HG3	1:K:276:TRP:CD1	2.15	0.82
1:F:276:TRP:CD1	1:G:214:GLN:HG3	2.18	0.79
1:C:276:TRP:CD1	1:D:214:GLN:HG3	2.19	0.78
1:H:276:TRP:CD1	1:I:214:GLN:HG3	2.19	0.78
1:D:276:TRP:CD1	1:E:214:GLN:HG3	2.18	0.78
1:A:214:GLN:HG3	1:K:276:TRP:NE1	2.00	0.77
1:I:276:TRP:CD1	1:J:214:GLN:HG3	2.20	0.76
1:A:276:TRP:CD1	1:B:214:GLN:HG3	2.21	0.76
1:G:276:TRP:CD1	1:H:214:GLN:HG3	2.21	0.76
1:J:276:TRP:CD1	1:K:214:GLN:HG3	2.21	0.76
1:B:276:TRP:CD1	1:C:214:GLN:HG3	2.20	0.75
1:H:97:TYR:OH	1:H:215:GLU:OE2	2.05	0.75
1:F:97:TYR:OH	1:F:215:GLU:OE2	2.05	0.74
1:J:97:TYR:OH	1:J:215:GLU:OE2	2.05	0.74
1:C:97:TYR:OH	1:C:215:GLU:OE2	2.05	0.73
1:D:97:TYR:OH	1:D:215:GLU:OE2	2.05	0.73
1:I:97:TYR:OH	1:I:215:GLU:OE2	2.05	0.73
1:B:97:TYR:OH	1:B:215:GLU:OE2	2.05	0.73
1:G:97:TYR:OH	1:G:215:GLU:OE2	2.05	0.73
1:K:97:TYR:OH	1:K:215:GLU:OE2	2.05	0.72
1:E:97:TYR:OH	1:E:215:GLU:OE2	2.05	0.72
1:A:97:TYR:OH	1:A:215:GLU:OE2	2.05	0.72
1:A:298:HIS:CD2	1:K:244:ASN:HD21	2.08	0.72
1:E:276:TRP:CD1	1:F:214:GLN:HG3	2.25	0.72
1:G:244:ASN:HD21	1:H:298:HIS:CD2	2.12	0.68
1:J:244:ASN:HD21	1:K:298:HIS:CD2	2.11	0.68
1:B:244:ASN:HD21	1:C:298:HIS:CD2	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ASN:HD21	1:B:298:HIS:CD2	2.13	0.67
1:I:244:ASN:HD21	1:J:298:HIS:CD2	2.13	0.66
1:H:244:ASN:HD21	1:I:298:HIS:CD2	2.14	0.65
1:C:244:ASN:HD21	1:D:298:HIS:CD2	2.14	0.65
1:B:276:TRP:NE1	1:C:214:GLN:HG3	2.12	0.64
1:F:244:ASN:HD21	1:G:298:HIS:CD2	2.15	0.64
1:F:276:TRP:NE1	1:G:214:GLN:HG3	2.12	0.64
1:H:276:TRP:NE1	1:I:214:GLN:HG3	2.11	0.64
1:C:276:TRP:NE1	1:D:214:GLN:HG3	2.12	0.64
1:H:137:LEU:HD23	1:H:173:VAL:HG22	1.80	0.64
1:I:137:LEU:HD23	1:I:173:VAL:HG22	1.80	0.64
1:K:94:VAL:HG21	1:K:284:LEU:HA	1.79	0.64
1:K:137:LEU:HD23	1:K:173:VAL:HG22	1.80	0.64
1:D:244:ASN:HD21	1:E:298:HIS:CD2	2.15	0.64
1:G:236:HIS:HE2	1:G:270:THR:HG1	1.46	0.64
1:D:276:TRP:NE1	1:E:214:GLN:HG3	2.12	0.64
1:G:137:LEU:HD23	1:G:173:VAL:HG22	1.80	0.64
1:H:94:VAL:HG21	1:H:284:LEU:HA	1.79	0.64
1:J:137:LEU:HD23	1:J:173:VAL:HG22	1.80	0.64
1:A:94:VAL:HG21	1:A:284:LEU:HA	1.80	0.64
1:G:94:VAL:HG21	1:G:284:LEU:HA	1.80	0.64
1:I:276:TRP:NE1	1:J:214:GLN:HG3	2.12	0.64
1:J:276:TRP:NE1	1:K:214:GLN:HG3	2.13	0.64
1:A:137:LEU:HD23	1:A:173:VAL:HG22	1.80	0.63
1:J:94:VAL:HG21	1:J:284:LEU:HA	1.79	0.63
1:F:94:VAL:HG21	1:F:284:LEU:HA	1.79	0.63
1:B:94:VAL:HG21	1:B:284:LEU:HA	1.79	0.63
1:I:94:VAL:HG21	1:I:284:LEU:HA	1.79	0.63
1:A:276:TRP:NE1	1:B:214:GLN:HG3	2.14	0.63
1:F:137:LEU:HD23	1:F:173:VAL:HG22	1.80	0.63
1:G:276:TRP:NE1	1:H:214:GLN:HG3	2.13	0.63
1:E:137:LEU:HD23	1:E:173:VAL:HG22	1.80	0.63
1:B:137:LEU:HD23	1:B:173:VAL:HG22	1.80	0.62
1:C:94:VAL:HG21	1:C:284:LEU:HA	1.79	0.62
1:D:94:VAL:HG21	1:D:284:LEU:HA	1.79	0.62
1:E:94:VAL:HG21	1:E:284:LEU:HA	1.79	0.62
1:D:137:LEU:HD23	1:D:173:VAL:HG22	1.80	0.62
1:C:137:LEU:HD23	1:C:173:VAL:HG22	1.80	0.62
1:E:62:ILE:HD11	1:F:191:LEU:HA	1.82	0.61
1:C:236:HIS:HE2	1:C:270:THR:HG1	1.49	0.61
1:E:244:ASN:HD21	1:F:298:HIS:CD2	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HA	1:K:62:ILE:HD11	1.85	0.59
1:E:236:HIS:HE2	1:E:270:THR:HG1	1.51	0.59
1:A:236:HIS:HE2	1:A:270:THR:HG1	1.51	0.58
1:I:236:HIS:HE2	1:I:270:THR:HG1	1.50	0.58
1:J:62:ILE:HD11	1:K:191:LEU:HA	1.86	0.58
1:B:62:ILE:HD11	1:C:191:LEU:HA	1.86	0.57
1:C:62:ILE:HD11	1:D:191:LEU:HA	1.86	0.57
1:I:62:ILE:HD11	1:J:191:LEU:HA	1.86	0.57
1:A:62:ILE:HD11	1:B:191:LEU:HA	1.87	0.57
1:G:62:ILE:HD11	1:H:191:LEU:HA	1.86	0.57
1:K:236:HIS:HE2	1:K:270:THR:HG1	1.51	0.57
1:J:236:HIS:HE2	1:J:270:THR:HG1	1.48	0.56
1:H:62:ILE:HD11	1:I:191:LEU:HA	1.87	0.56
1:F:62:ILE:HD11	1:G:191:LEU:HA	1.88	0.56
1:K:275:GLN:OE1	1:K:300:TRP:NE1	2.22	0.55
1:E:276:TRP:NE1	1:F:214:GLN:HG3	2.21	0.55
1:I:275:GLN:OE1	1:I:300:TRP:NE1	2.22	0.55
1:H:275:GLN:OE1	1:H:300:TRP:NE1	2.22	0.55
1:J:275:GLN:OE1	1:J:300:TRP:NE1	2.22	0.55
1:A:275:GLN:OE1	1:A:300:TRP:NE1	2.22	0.54
1:G:275:GLN:OE1	1:G:300:TRP:NE1	2.22	0.54
1:E:40:ASN:CG	1:F:179:ARG:HH21	2.16	0.53
1:F:275:GLN:OE1	1:F:300:TRP:NE1	2.22	0.53
1:E:239:VAL:HG22	1:E:262:ILE:HD13	1.91	0.52
1:F:239:VAL:HG22	1:F:262:ILE:HD13	1.91	0.52
1:G:163:TYR:OH	1:G:169:ILE:O	2.21	0.52
1:C:239:VAL:HG22	1:C:262:ILE:HD13	1.91	0.52
1:D:239:VAL:HG22	1:D:262:ILE:HD13	1.91	0.52
1:K:239:VAL:HG22	1:K:262:ILE:HD13	1.91	0.52
1:G:239:VAL:HG22	1:G:262:ILE:HD13	1.91	0.52
1:D:236:HIS:HE2	1:D:270:THR:HG1	1.48	0.52
1:J:239:VAL:HG22	1:J:262:ILE:HD13	1.91	0.52
1:B:239:VAL:HG22	1:B:262:ILE:HD13	1.91	0.51
1:H:239:VAL:HG22	1:H:262:ILE:HD13	1.91	0.51
1:I:239:VAL:HG22	1:I:262:ILE:HD13	1.91	0.51
1:B:275:GLN:OE1	1:B:300:TRP:NE1	2.22	0.51
1:C:257:ASP:OD1	1:C:258:ASP:N	2.44	0.51
1:B:204:LYS:HA	1:B:207:CYS:SG	2.51	0.51
1:E:204:LYS:HA	1:E:207:CYS:SG	2.51	0.51
1:G:204:LYS:HA	1:G:207:CYS:SG	2.51	0.51
1:B:257:ASP:OD1	1:B:258:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:ASP:OD1	1:G:258:ASP:N	2.44	0.51
1:H:257:ASP:OD1	1:H:258:ASP:N	2.44	0.51
1:J:204:LYS:HA	1:J:207:CYS:SG	2.51	0.51
1:F:257:ASP:OD1	1:F:258:ASP:N	2.44	0.51
1:I:204:LYS:HA	1:I:207:CYS:SG	2.51	0.51
1:I:257:ASP:OD1	1:I:258:ASP:N	2.44	0.51
1:J:257:ASP:OD1	1:J:258:ASP:N	2.44	0.51
1:K:257:ASP:OD1	1:K:258:ASP:N	2.44	0.51
1:A:204:LYS:HA	1:A:207:CYS:SG	2.51	0.51
1:D:204:LYS:HA	1:D:207:CYS:SG	2.51	0.51
1:H:204:LYS:HA	1:H:207:CYS:SG	2.51	0.51
1:K:204:LYS:HA	1:K:207:CYS:SG	2.51	0.51
1:A:239:VAL:HG22	1:A:262:ILE:HD13	1.91	0.50
1:A:257:ASP:OD1	1:A:258:ASP:N	2.44	0.50
1:E:275:GLN:OE1	1:E:300:TRP:NE1	2.22	0.50
1:D:257:ASP:OD1	1:D:258:ASP:N	2.44	0.50
1:F:204:LYS:HA	1:F:207:CYS:SG	2.51	0.50
1:E:257:ASP:OD1	1:E:258:ASP:N	2.44	0.50
1:D:62:ILE:HD11	1:E:191:LEU:HA	1.93	0.50
1:C:204:LYS:HA	1:C:207:CYS:SG	2.51	0.50
1:E:203:LEU:HD13	1:E:206:TYR:HD2	1.77	0.50
1:F:203:LEU:HD13	1:F:206:TYR:HD2	1.77	0.49
1:D:203:LEU:HD13	1:D:206:TYR:HD2	1.77	0.49
1:K:203:LEU:HD13	1:K:206:TYR:HD2	1.77	0.49
1:G:203:LEU:HD13	1:G:206:TYR:HD2	1.77	0.49
1:A:203:LEU:HD13	1:A:206:TYR:HD2	1.77	0.49
1:B:203:LEU:HD13	1:B:206:TYR:HD2	1.77	0.49
1:C:203:LEU:HD13	1:C:206:TYR:HD2	1.77	0.49
1:J:203:LEU:HD13	1:J:206:TYR:HD2	1.77	0.49
1:D:210:LEU:HD22	1:D:214:GLN:OE1	2.13	0.49
1:G:210:LEU:HD22	1:G:214:GLN:OE1	2.13	0.49
1:H:210:LEU:HD22	1:H:214:GLN:OE1	2.13	0.49
1:J:210:LEU:HD22	1:J:214:GLN:OE1	2.13	0.49
1:C:210:LEU:HD22	1:C:214:GLN:OE1	2.13	0.49
1:K:210:LEU:HD22	1:K:214:GLN:OE1	2.13	0.49
1:I:203:LEU:HD13	1:I:206:TYR:HD2	1.77	0.48
1:E:210:LEU:HD22	1:E:214:GLN:OE1	2.13	0.48
1:H:146:PRO:O	1:H:150:VAL:HG23	2.14	0.48
1:I:146:PRO:O	1:I:150:VAL:HG23	2.14	0.48
1:I:210:LEU:HD22	1:I:214:GLN:OE1	2.13	0.48
1:G:146:PRO:O	1:G:150:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:203:LEU:HD13	1:H:206:TYR:HD2	1.77	0.48
1:C:275:GLN:OE1	1:C:300:TRP:NE1	2.22	0.48
1:F:146:PRO:O	1:F:150:VAL:HG23	2.14	0.48
1:J:146:PRO:O	1:J:150:VAL:HG23	2.14	0.48
1:J:170:ALA:HB3	1:J:173:VAL:HG12	1.95	0.48
1:B:210:LEU:HD22	1:B:214:GLN:OE1	2.13	0.48
1:C:146:PRO:O	1:C:150:VAL:HG23	2.14	0.48
1:E:170:ALA:HB3	1:E:173:VAL:HG12	1.95	0.48
1:B:236:HIS:HE2	1:B:270:THR:HG1	1.48	0.48
1:K:170:ALA:HB3	1:K:173:VAL:HG12	1.95	0.48
1:A:210:LEU:HD22	1:A:214:GLN:OE1	2.13	0.47
1:I:170:ALA:HB3	1:I:173:VAL:HG12	1.95	0.47
1:D:146:PRO:O	1:D:150:VAL:HG23	2.14	0.47
1:B:146:PRO:O	1:B:150:VAL:HG23	2.14	0.47
1:D:275:GLN:OE1	1:D:300:TRP:NE1	2.22	0.47
1:H:170:ALA:HB3	1:H:173:VAL:HG12	1.95	0.47
1:A:170:ALA:HB3	1:A:173:VAL:HG12	1.95	0.47
1:C:170:ALA:HB3	1:C:173:VAL:HG12	1.95	0.47
1:F:210:LEU:HD22	1:F:214:GLN:OE1	2.13	0.47
1:A:146:PRO:O	1:A:150:VAL:HG23	2.14	0.47
1:G:170:ALA:HB3	1:G:173:VAL:HG12	1.95	0.47
1:A:238:ARG:HB2	1:B:224:ASN:ND2	2.29	0.47
1:D:248:PHE:CE1	1:E:271:GLN:HG2	2.50	0.47
1:E:146:PRO:O	1:E:150:VAL:HG23	2.14	0.47
1:F:163:TYR:OH	1:F:169:ILE:O	2.21	0.47
1:I:40:ASN:CG	1:J:179:ARG:HH21	2.23	0.47
1:I:121:GLY:HA2	1:I:182:SER:OG	2.15	0.47
1:K:146:PRO:O	1:K:150:VAL:HG23	2.14	0.47
1:F:170:ALA:HB3	1:F:173:VAL:HG12	1.95	0.47
1:J:40:ASN:CG	1:K:179:ARG:HH21	2.22	0.47
1:K:121:GLY:HA2	1:K:182:SER:OG	2.15	0.47
1:A:163:TYR:OH	1:A:169:ILE:O	2.21	0.47
1:A:121:GLY:HA2	1:A:182:SER:OG	2.15	0.47
1:B:121:GLY:HA2	1:B:182:SER:OG	2.15	0.47
1:C:121:GLY:HA2	1:C:182:SER:OG	2.15	0.47
1:B:170:ALA:HB3	1:B:173:VAL:HG12	1.95	0.46
1:F:121:GLY:HA2	1:F:182:SER:OG	2.15	0.46
1:H:121:GLY:HA2	1:H:182:SER:OG	2.15	0.46
1:A:211:SER:OG	1:K:280:THR:HG21	2.15	0.46
1:A:217:TYR:CE1	1:K:237:SER:HB2	2.51	0.46
1:D:170:ALA:HB3	1:D:173:VAL:HG12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:SER:OG	1:B:221:TYR:HA	2.16	0.46
1:B:210:LEU:HD13	1:B:214:GLN:HB3	1.98	0.46
1:F:254:LEU:HD23	1:F:258:ASP:HB3	1.98	0.46
1:J:121:GLY:HA2	1:J:182:SER:OG	2.15	0.46
1:C:210:LEU:HD13	1:C:214:GLN:HB3	1.98	0.46
1:D:247:ARG:HH21	1:E:301:ALA:HB1	1.79	0.46
1:G:40:ASN:CG	1:H:179:ARG:HH21	2.23	0.46
1:G:254:LEU:HD23	1:G:258:ASP:HB3	1.98	0.46
1:B:40:ASN:CG	1:C:179:ARG:HH21	2.23	0.46
1:E:254:LEU:HD23	1:E:258:ASP:HB3	1.98	0.46
1:G:121:GLY:HA2	1:G:182:SER:OG	2.15	0.46
1:A:210:LEU:HD13	1:A:214:GLN:HB3	1.98	0.46
1:D:121:GLY:HA2	1:D:182:SER:OG	2.15	0.46
1:H:254:LEU:HD23	1:H:258:ASP:HB3	1.98	0.46
1:D:210:LEU:HD13	1:D:214:GLN:HB3	1.98	0.46
1:E:121:GLY:HA2	1:E:182:SER:OG	2.15	0.46
1:I:254:LEU:HD23	1:I:258:ASP:HB3	1.98	0.46
1:J:210:LEU:HD13	1:J:214:GLN:HB3	1.98	0.46
1:E:210:LEU:HD13	1:E:214:GLN:HB3	1.98	0.45
1:K:210:LEU:HD13	1:K:214:GLN:HB3	1.98	0.45
1:D:254:LEU:HD23	1:D:258:ASP:HB3	1.98	0.45
1:F:210:LEU:HD13	1:F:214:GLN:HB3	1.98	0.45
1:C:40:ASN:CG	1:D:179:ARG:HH21	2.24	0.45
1:J:254:LEU:HD23	1:J:258:ASP:HB3	1.98	0.45
1:B:65:LEU:HD23	1:B:65:LEU:HA	1.84	0.45
1:H:40:ASN:CG	1:I:179:ARG:HH21	2.25	0.45
1:I:210:LEU:HD13	1:I:214:GLN:HB3	1.98	0.45
1:C:254:LEU:HD23	1:C:258:ASP:HB3	1.98	0.45
1:D:65:LEU:HD23	1:D:65:LEU:HA	1.85	0.45
1:G:210:LEU:HD13	1:G:214:GLN:HB3	1.98	0.45
1:K:254:LEU:HD23	1:K:258:ASP:HB3	1.98	0.44
1:A:43:CYS:C	1:A:44:LEU:HD22	2.43	0.44
1:F:43:CYS:C	1:F:44:LEU:HD22	2.43	0.44
1:H:210:LEU:HD13	1:H:214:GLN:HB3	1.98	0.44
1:C:129:CYS:SG	1:C:158:PRO:HD3	2.58	0.44
1:E:129:CYS:SG	1:E:158:PRO:HD3	2.58	0.44
1:F:40:ASN:HD22	1:G:176:ARG:HH12	1.65	0.44
1:F:247:ARG:HH21	1:G:301:ALA:HB1	1.82	0.44
1:G:43:CYS:C	1:G:44:LEU:HD22	2.43	0.44
1:H:129:CYS:SG	1:H:158:PRO:HD3	2.58	0.44
1:A:254:LEU:HD23	1:A:258:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:CYS:C	1:D:44:LEU:HD22	2.43	0.44
1:F:40:ASN:CG	1:G:179:ARG:HH21	2.25	0.44
1:F:129:CYS:SG	1:F:158:PRO:HD3	2.58	0.44
1:G:65:LEU:HD23	1:G:65:LEU:HA	1.85	0.44
1:B:254:LEU:HD23	1:B:258:ASP:HB3	1.98	0.44
1:C:43:CYS:C	1:C:44:LEU:HD22	2.43	0.44
1:I:43:CYS:C	1:I:44:LEU:HD22	2.43	0.44
1:K:129:CYS:SG	1:K:158:PRO:HD3	2.58	0.44
1:A:129:CYS:SG	1:A:158:PRO:HD3	2.58	0.44
1:B:43:CYS:C	1:B:44:LEU:HD22	2.43	0.44
1:B:129:CYS:SG	1:B:158:PRO:HD3	2.58	0.44
1:J:43:CYS:C	1:J:44:LEU:HD22	2.43	0.44
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.83	0.44
1:D:129:CYS:SG	1:D:158:PRO:HD3	2.58	0.44
1:F:236:HIS:NE2	1:F:270:THR:OG1	2.40	0.44
1:J:129:CYS:SG	1:J:158:PRO:HD3	2.58	0.44
1:A:247:ARG:HH21	1:B:301:ALA:HB1	1.83	0.43
1:H:247:ARG:HH21	1:I:301:ALA:HB1	1.83	0.43
1:K:43:CYS:C	1:K:44:LEU:HD22	2.43	0.43
1:G:129:CYS:SG	1:G:158:PRO:HD3	2.58	0.43
1:I:129:CYS:SG	1:I:158:PRO:HD3	2.58	0.43
1:D:40:ASN:CG	1:E:179:ARG:HH21	2.27	0.43
1:E:43:CYS:C	1:E:44:LEU:HD22	2.43	0.43
1:A:221:TYR:HA	1:K:237:SER:OG	2.18	0.43
1:I:119:LEU:HD23	1:I:119:LEU:HA	1.83	0.43
1:H:43:CYS:C	1:H:44:LEU:HD22	2.43	0.43
1:E:273:ARG:N	1:E:274:PRO:HD2	2.34	0.43
1:A:301:ALA:HB1	1:K:247:ARG:HH21	1.84	0.43
1:B:273:ARG:N	1:B:274:PRO:HD2	2.34	0.43
1:I:102:MET:N	1:I:102:MET:HE2	2.34	0.43
1:J:102:MET:HE2	1:J:102:MET:N	2.34	0.43
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.83	0.43
1:C:273:ARG:N	1:C:274:PRO:HD2	2.34	0.42
1:D:102:MET:N	1:D:102:MET:HE2	2.34	0.42
1:D:237:SER:OG	1:E:221:TYR:HA	2.19	0.42
1:H:155:ALA:O	1:H:158:PRO:HD2	2.19	0.42
1:E:155:ALA:O	1:E:158:PRO:HD2	2.20	0.42
1:H:102:MET:HE2	1:H:102:MET:N	2.34	0.42
1:J:155:ALA:O	1:J:158:PRO:HD2	2.20	0.42
1:K:102:MET:N	1:K:102:MET:HE2	2.34	0.42
1:K:155:ALA:O	1:K:158:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:LEU:O	1:K:206:TYR:HB2	2.20	0.42
1:A:155:ALA:O	1:A:158:PRO:HD2	2.20	0.42
1:A:224:ASN:ND2	1:K:238:ARG:HB2	2.35	0.42
1:A:271:GLN:HG2	1:K:248:PHE:CE1	2.54	0.42
1:F:155:ALA:O	1:F:158:PRO:HD2	2.20	0.42
1:F:273:ARG:N	1:F:274:PRO:HD2	2.34	0.42
1:I:273:ARG:N	1:I:274:PRO:HD2	2.34	0.42
1:D:155:ALA:O	1:D:158:PRO:HD2	2.20	0.42
1:D:203:LEU:O	1:D:206:TYR:HB2	2.20	0.42
1:F:102:MET:HE2	1:F:102:MET:N	2.34	0.42
1:G:273:ARG:N	1:G:274:PRO:HD2	2.34	0.42
1:H:40:ASN:HD22	1:I:176:ARG:HH12	1.68	0.42
1:I:155:ALA:O	1:I:158:PRO:HD2	2.20	0.42
1:J:203:LEU:O	1:J:206:TYR:HB2	2.20	0.42
1:A:203:LEU:O	1:A:206:TYR:HB2	2.20	0.42
1:B:155:ALA:O	1:B:158:PRO:HD2	2.20	0.42
1:C:40:ASN:HD22	1:D:176:ARG:HH12	1.67	0.42
1:C:155:ALA:O	1:C:158:PRO:HD2	2.20	0.42
1:C:238:ARG:HB2	1:D:224:ASN:ND2	2.35	0.42
1:C:247:ARG:HH21	1:D:301:ALA:HB1	1.84	0.42
1:D:273:ARG:N	1:D:274:PRO:HD2	2.34	0.42
1:F:238:ARG:HB2	1:G:224:ASN:ND2	2.34	0.42
1:G:203:LEU:O	1:G:206:TYR:HB2	2.20	0.42
1:K:273:ARG:N	1:K:274:PRO:HD2	2.34	0.42
1:A:102:MET:HE2	1:A:102:MET:N	2.34	0.42
1:A:179:ARG:HH21	1:K:40:ASN:CG	2.27	0.42
1:A:273:ARG:N	1:A:274:PRO:HD2	2.34	0.42
1:C:203:LEU:O	1:C:206:TYR:HB2	2.19	0.42
1:E:102:MET:HE2	1:E:102:MET:N	2.34	0.42
1:G:102:MET:N	1:G:102:MET:HE2	2.34	0.42
1:A:40:ASN:HD22	1:B:176:ARG:HH12	1.68	0.42
1:A:43:CYS:HB3	1:A:156:ARG:HA	2.02	0.42
1:C:102:MET:HE2	1:C:102:MET:N	2.34	0.42
1:F:81:TRP:HE1	1:F:95:LEU:HD21	1.85	0.42
1:F:237:SER:OG	1:G:221:TYR:HA	2.19	0.42
1:G:155:ALA:O	1:G:158:PRO:HD2	2.20	0.42
1:H:81:TRP:HE1	1:H:95:LEU:HD21	1.85	0.42
1:H:119:LEU:HD23	1:H:119:LEU:HA	1.83	0.42
1:H:203:LEU:O	1:H:206:TYR:HB2	2.19	0.42
1:J:273:ARG:N	1:J:274:PRO:HD2	2.34	0.42
1:A:40:ASN:HD22	1:B:176:ARG:NH1	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:CYS:HB3	1:B:156:ARG:HA	2.02	0.42
1:D:43:CYS:HB3	1:D:156:ARG:HA	2.02	0.42
1:G:122:LYS:H	1:G:122:LYS:HG3	1.69	0.42
1:A:40:ASN:CG	1:B:179:ARG:HH21	2.27	0.42
1:C:280:THR:HG21	1:D:211:SER:OG	2.20	0.42
1:F:280:THR:HG21	1:G:211:SER:OG	2.20	0.42
1:H:273:ARG:N	1:H:274:PRO:HD2	2.34	0.42
1:J:43:CYS:HB3	1:J:156:ARG:HA	2.02	0.42
1:B:102:MET:N	1:B:102:MET:HE2	2.34	0.42
1:C:43:CYS:HB3	1:C:156:ARG:HA	2.02	0.42
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.88	0.42
1:E:62:ILE:CD1	1:F:191:LEU:HA	2.49	0.42
1:I:43:CYS:HB3	1:I:156:ARG:HA	2.02	0.42
1:I:247:ARG:HH21	1:J:301:ALA:HB1	1.85	0.42
1:K:43:CYS:HB3	1:K:156:ARG:HA	2.02	0.42
1:E:203:LEU:O	1:E:206:TYR:HB2	2.20	0.41
1:I:81:TRP:HE1	1:I:95:LEU:HD21	1.85	0.41
1:I:285:TYR:CE2	1:I:287:GLU:HB2	2.56	0.41
1:C:237:SER:OG	1:D:221:TYR:HA	2.20	0.41
1:H:261:LEU:HD23	1:H:261:LEU:HA	1.88	0.41
1:J:119:LEU:HD23	1:J:119:LEU:HA	1.83	0.41
1:C:285:TYR:CE2	1:C:287:GLU:HB2	2.56	0.41
1:D:81:TRP:HE1	1:D:95:LEU:HD21	1.85	0.41
1:F:203:LEU:O	1:F:206:TYR:HB2	2.20	0.41
1:G:40:ASN:HD22	1:H:176:ARG:HH12	1.69	0.41
1:I:40:ASN:HD22	1:J:176:ARG:HH12	1.68	0.41
1:I:203:LEU:O	1:I:206:TYR:HB2	2.20	0.41
1:B:203:LEU:O	1:B:206:TYR:HB2	2.20	0.41
1:E:43:CYS:HB3	1:E:156:ARG:HA	2.02	0.41
1:E:285:TYR:CE2	1:E:287:GLU:HB2	2.56	0.41
1:F:43:CYS:HB3	1:F:156:ARG:HA	2.02	0.41
1:G:285:TYR:CE2	1:G:287:GLU:HB2	2.56	0.41
1:H:43:CYS:HB3	1:H:156:ARG:HA	2.02	0.41
1:K:81:TRP:HE1	1:K:95:LEU:HD21	1.85	0.41
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.83	0.41
1:E:81:TRP:HE1	1:E:95:LEU:HD21	1.85	0.41
1:A:62:ILE:CD1	1:B:191:LEU:HA	2.51	0.41
1:B:285:TYR:CE2	1:B:287:GLU:HB2	2.56	0.41
1:K:285:TYR:CE2	1:K:287:GLU:HB2	2.56	0.41
1:J:81:TRP:HE1	1:J:95:LEU:HD21	1.85	0.41
1:C:81:TRP:HE1	1:C:95:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:LEU:HB2	1:F:123:CYS:SG	2.61	0.41
1:G:43:CYS:HB3	1:G:156:ARG:HA	2.02	0.41
1:H:237:SER:OG	1:I:221:TYR:HA	2.20	0.41
1:H:238:ARG:HB2	1:I:224:ASN:ND2	2.36	0.41
1:K:56:LEU:HB2	1:K:123:CYS:SG	2.61	0.41
1:B:81:TRP:HE1	1:B:95:LEU:HD21	1.85	0.41
1:K:73:ASN:OD1	1:K:76:MET:HG3	2.22	0.41
1:K:119:LEU:HD23	1:K:119:LEU:HA	1.83	0.41
1:B:253:ALA:C	1:B:254:LEU:HD12	2.47	0.40
1:C:56:LEU:HB2	1:C:123:CYS:SG	2.61	0.40
1:D:73:ASN:OD1	1:D:76:MET:HG3	2.22	0.40
1:E:253:ALA:C	1:E:254:LEU:HD12	2.47	0.40
1:E:261:LEU:HD23	1:E:261:LEU:HA	1.88	0.40
1:F:65:LEU:HA	1:F:65:LEU:HD23	1.85	0.40
1:G:56:LEU:HB2	1:G:123:CYS:SG	2.61	0.40
1:G:81:TRP:HE1	1:G:95:LEU:HD21	1.85	0.40
1:I:238:ARG:HB2	1:J:224:ASN:ND2	2.37	0.40
1:A:73:ASN:OD1	1:A:76:MET:HG3	2.22	0.40
1:A:150:VAL:O	1:A:154:LEU:HG	2.21	0.40
1:A:298:HIS:CG	1:K:244:ASN:HD21	2.38	0.40
1:B:56:LEU:HB2	1:B:123:CYS:SG	2.61	0.40
1:B:73:ASN:OD1	1:B:76:MET:HG3	2.22	0.40
1:C:73:ASN:OD1	1:C:76:MET:HG3	2.22	0.40
1:E:56:LEU:HB2	1:E:123:CYS:SG	2.61	0.40
1:E:73:ASN:OD1	1:E:76:MET:HG3	2.22	0.40
1:E:150:VAL:O	1:E:154:LEU:HG	2.22	0.40
1:G:150:VAL:O	1:G:154:LEU:HG	2.22	0.40
1:H:210:LEU:HD21	1:H:285:TYR:CD2	2.57	0.40
1:H:280:THR:HG21	1:I:211:SER:OG	2.21	0.40
1:I:280:THR:HG21	1:J:211:SER:OG	2.22	0.40
1:J:73:ASN:OD1	1:J:76:MET:HG3	2.22	0.40
1:J:210:LEU:HD21	1:J:285:TYR:CD2	2.57	0.40
1:A:81:TRP:HE1	1:A:95:LEU:HD21	1.85	0.40
1:A:285:TYR:CE2	1:A:287:GLU:HB2	2.56	0.40
1:F:285:TYR:CE2	1:F:287:GLU:HB2	2.56	0.40
1:G:237:SER:HB2	1:H:217:TYR:CE1	2.56	0.40
1:H:253:ALA:C	1:H:254:LEU:HD12	2.47	0.40
1:H:285:TYR:CE2	1:H:287:GLU:HB2	2.56	0.40
1:I:56:LEU:HB2	1:I:123:CYS:SG	2.61	0.40
1:I:73:ASN:OD1	1:I:76:MET:HG3	2.21	0.40
1:C:290:GLY:O	1:C:291:LEU:HD12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:LEU:HB2	1:D:123:CYS:SG	2.61	0.40
1:D:61:LEU:HD12	1:D:61:LEU:HA	1.95	0.40
1:D:285:TYR:CE2	1:D:287:GLU:HB2	2.56	0.40
1:E:210:LEU:HD21	1:E:285:TYR:CD2	2.57	0.40
1:F:73:ASN:OD1	1:F:76:MET:HG3	2.21	0.40
1:F:150:VAL:O	1:F:154:LEU:HG	2.22	0.40
1:F:210:LEU:HD21	1:F:285:TYR:CD2	2.57	0.40
1:H:61:LEU:HD12	1:H:61:LEU:HA	1.95	0.40
1:C:253:ALA:C	1:C:254:LEU:HD12	2.47	0.40
1:D:290:GLY:O	1:D:291:LEU:HD12	2.22	0.40
1:G:261:LEU:HD23	1:G:261:LEU:HA	1.88	0.40
1:H:169:ILE:HG22	1:H:170:ALA:O	2.22	0.40
1:I:169:ILE:HG22	1:I:170:ALA:O	2.22	0.40
1:J:237:SER:HB2	1:K:217:TYR:CE1	2.56	0.40
1:J:253:ALA:C	1:J:254:LEU:HD12	2.46	0.40
1:J:285:TYR:CE2	1:J:287:GLU:HB2	2.56	0.40
1:K:210:LEU:HD21	1:K:285:TYR:CD2	2.57	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	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	B	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	C	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	D	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	E	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	F	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	G	251/615 (41%)	236 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	I	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	J	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
1	K	251/615 (41%)	236 (94%)	15 (6%)	0	100	100
All	All	2761/6765 (41%)	2596 (94%)	165 (6%)	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	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	B	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	C	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	D	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	E	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	F	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	G	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	H	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	I	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	J	196/517 (38%)	194 (99%)	2 (1%)	68	75
1	K	196/517 (38%)	194 (99%)	2 (1%)	68	75
All	All	2156/5687 (38%)	2134 (99%)	22 (1%)	65	75

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	VAL
1	A	159	CYS

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Mol	Chain	Res	Type
1	B	116	VAL
1	B	159	CYS
1	C	116	VAL
1	C	159	CYS
1	D	116	VAL
1	D	159	CYS
1	E	116	VAL
1	E	159	CYS
1	F	116	VAL
1	F	159	CYS
1	G	116	VAL
1	G	159	CYS
1	H	116	VAL
1	H	159	CYS
1	I	116	VAL
1	I	159	CYS
1	J	116	VAL
1	J	159	CYS
1	K	116	VAL
1	K	159	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	230	GLN
1	A	244	ASN
1	A	298	HIS
1	B	227	GLN
1	B	230	GLN
1	C	227	GLN
1	C	230	GLN
1	C	298	HIS
1	D	227	GLN
1	D	230	GLN
1	D	244	ASN
1	D	298	HIS
1	E	227	GLN
1	E	230	GLN
1	F	227	GLN
1	F	230	GLN
1	F	244	ASN

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Mol	Chain	Res	Type
1	F	298	HIS
1	G	227	GLN
1	G	230	GLN
1	G	244	ASN
1	H	227	GLN
1	H	230	GLN
1	H	244	ASN
1	I	227	GLN
1	I	230	GLN
1	J	227	GLN
1	J	230	GLN
1	J	298	HIS
1	K	227	GLN
1	K	230	GLN
1	K	244	ASN
1	K	298	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

There are no chain breaks in this entry.

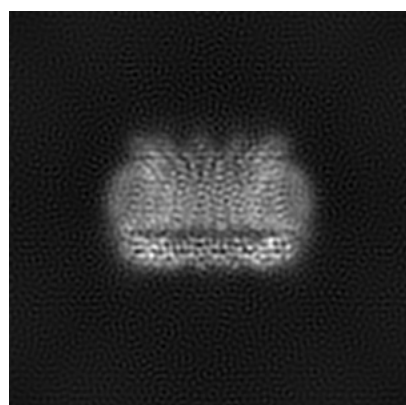
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21142. These allow visual inspection of the internal detail of the map and identification of artifacts.

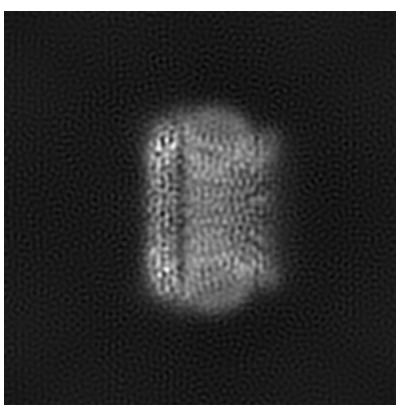
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

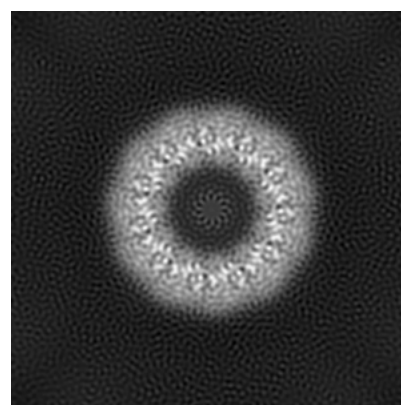
6.1.1 Primary map



X



Y

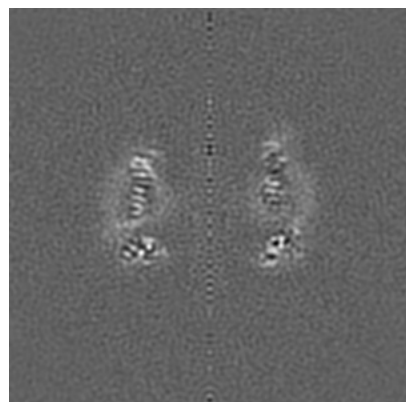


Z

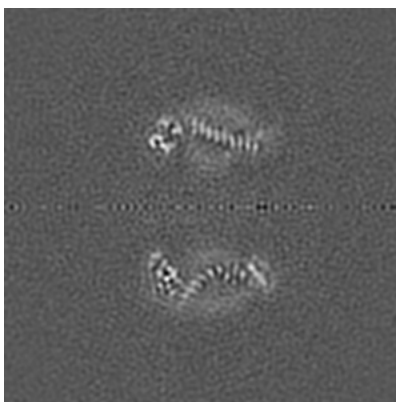
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

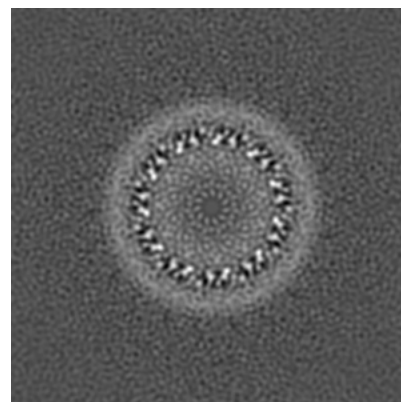
6.2.1 Primary map



X Index: 128



Y Index: 128

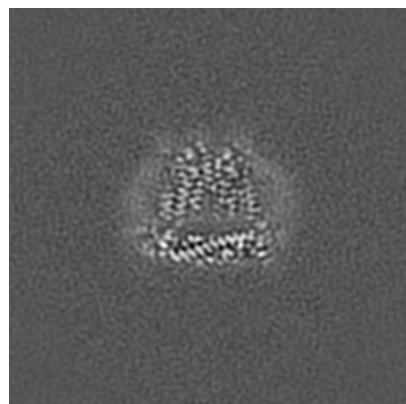


Z Index: 128

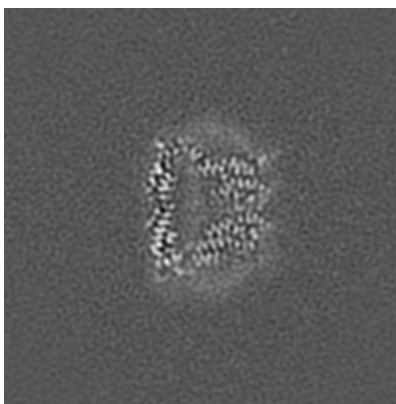
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

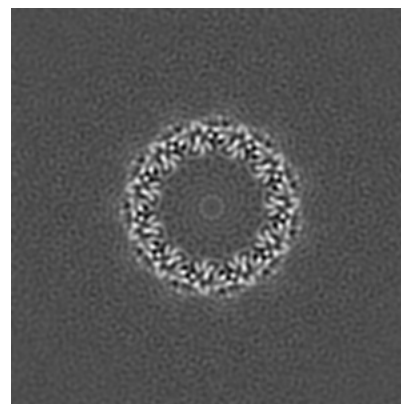
6.3.1 Primary map



X Index: 169



Y Index: 91

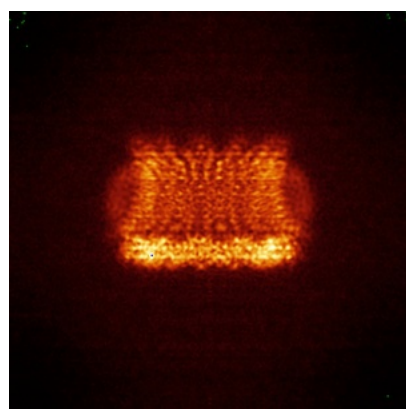


Z Index: 104

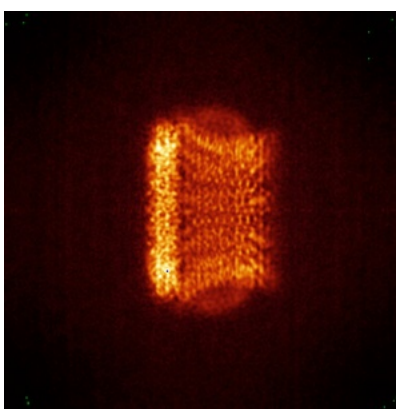
The images above show the largest variance slices of the map in three orthogonal directions.

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

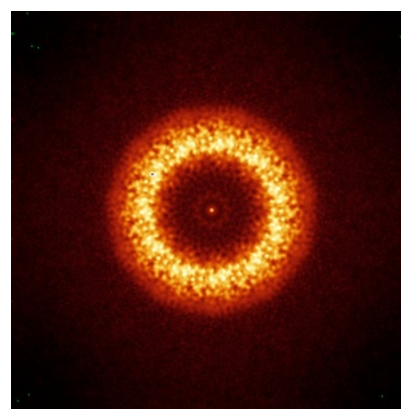
6.4.1 Primary map



X



Y

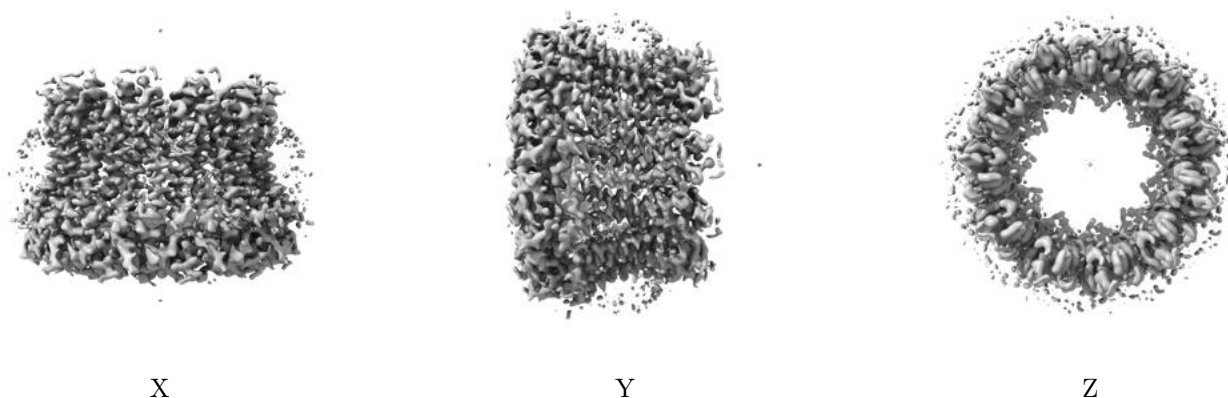


Z

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

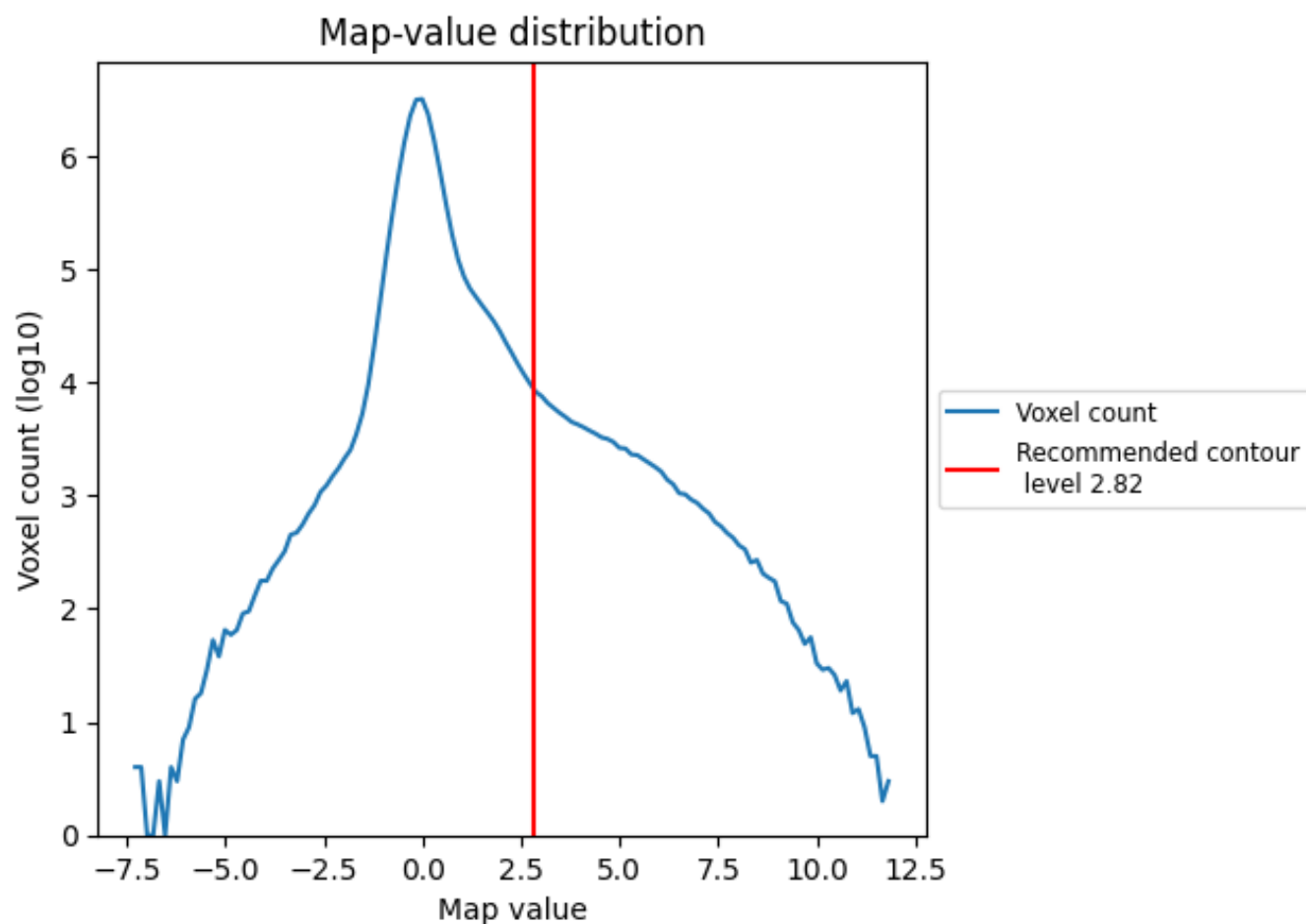
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

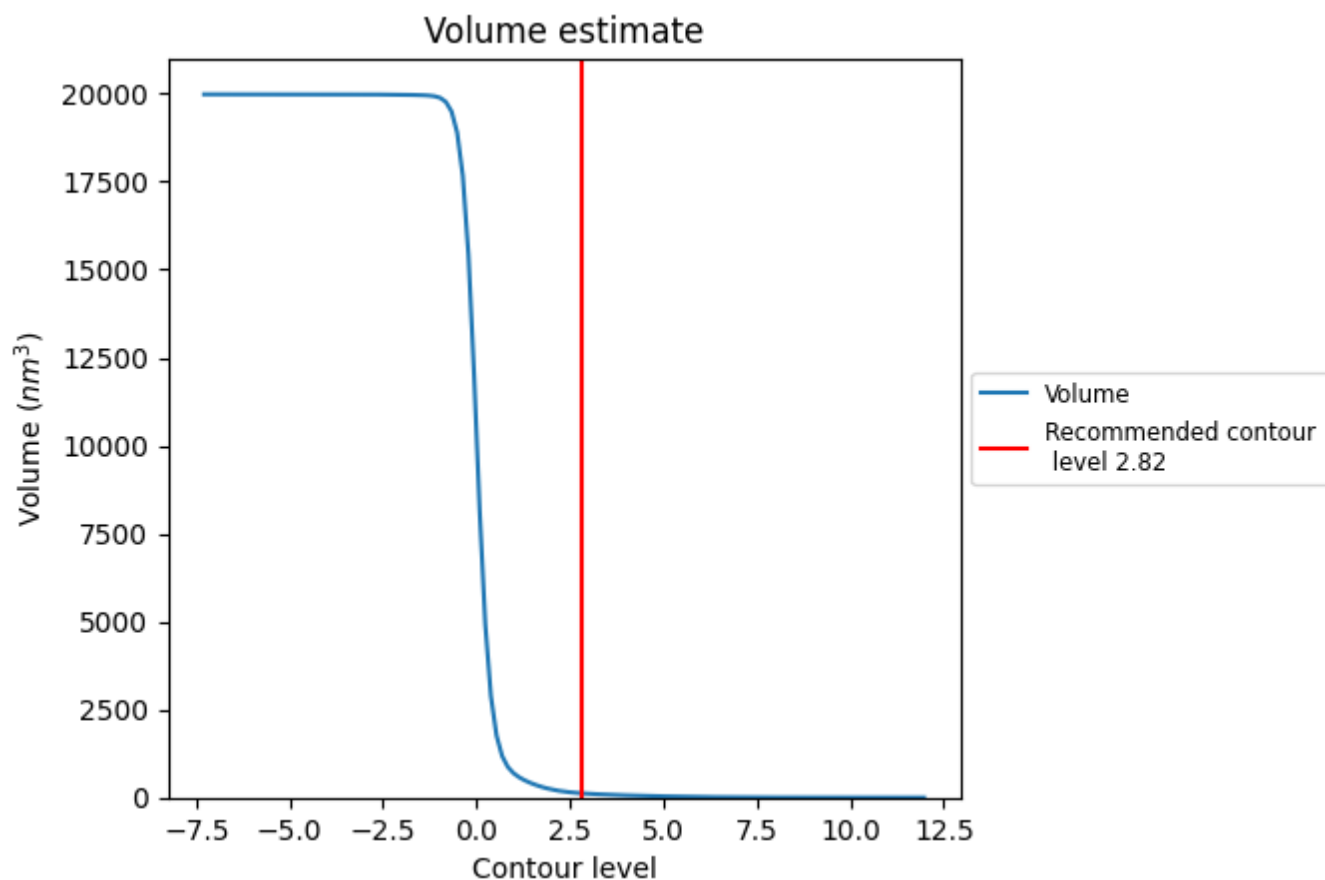
This section contains the results of statistical analysis of the map.

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.

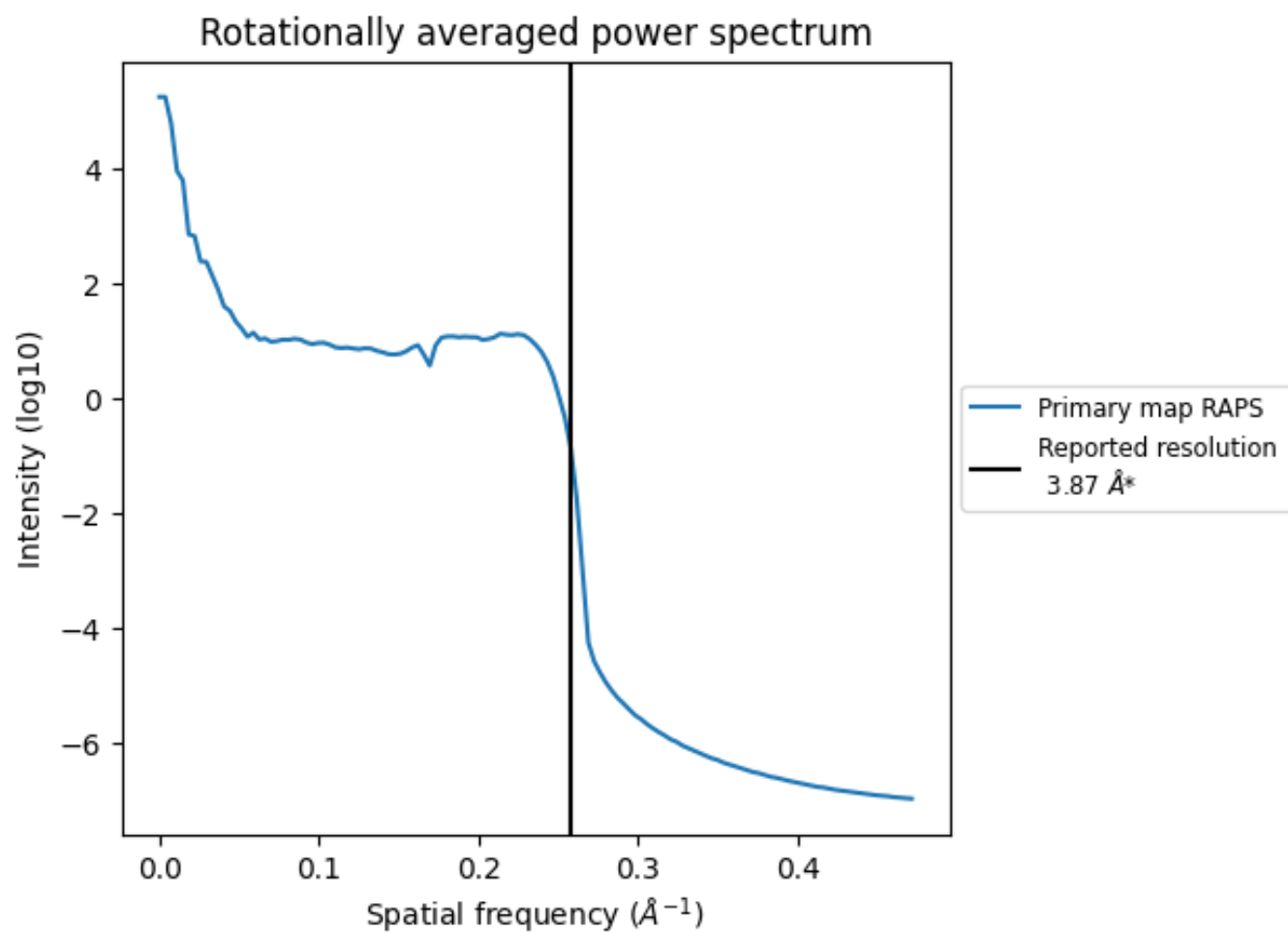
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 121 nm³; this corresponds to an approximate mass of 109 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 0.258 Å⁻¹

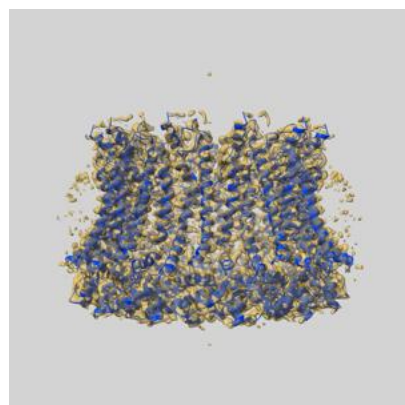
8 Fourier-Shell correlation

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

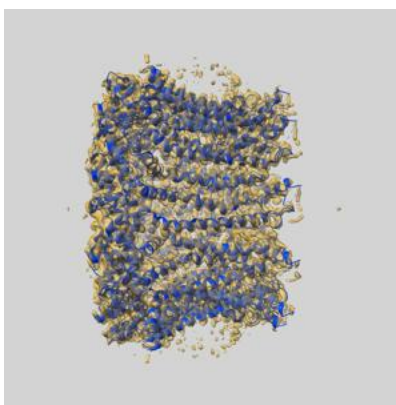
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21142 and PDB model 6VAL. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

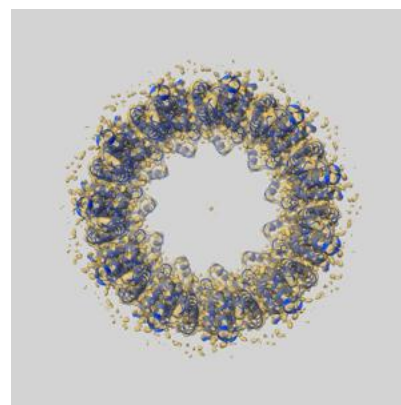
9.1 Map-model overlay [i](#)



X



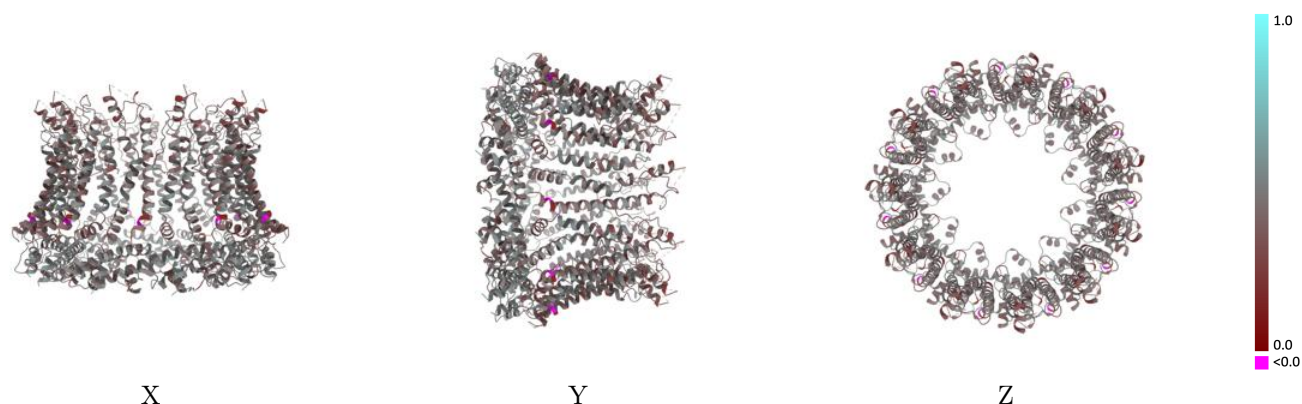
Y



Z

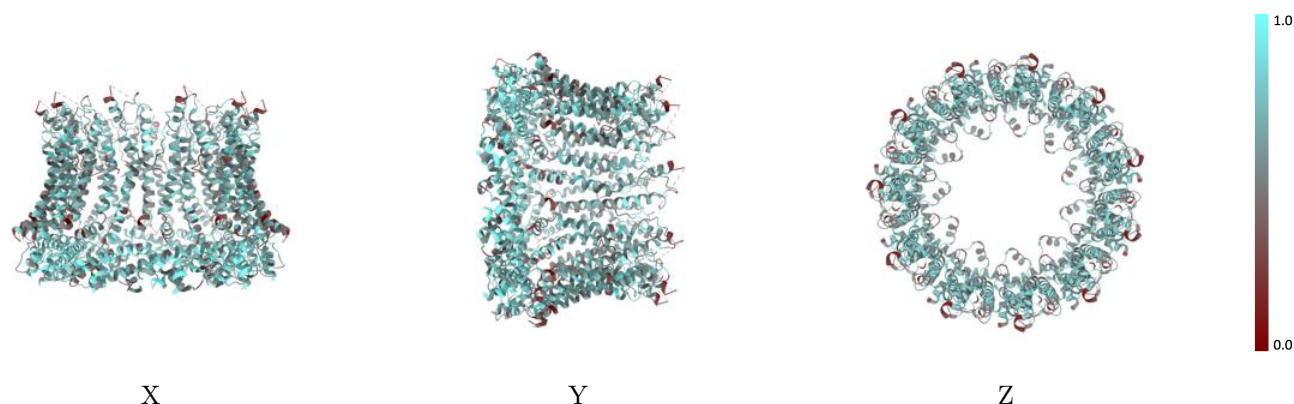
The images above show the 3D surface view of the map at the recommended contour level 2.82 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



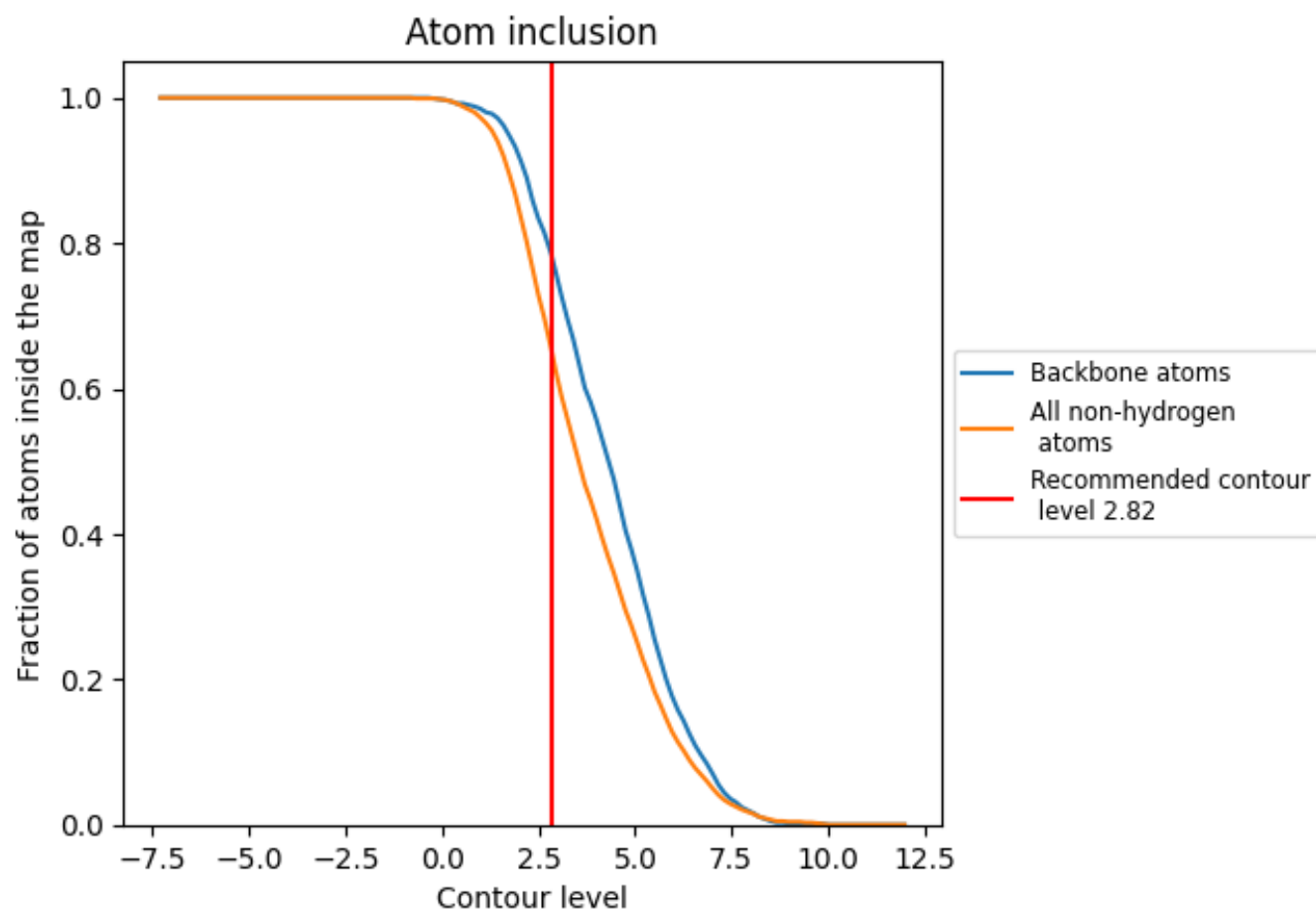
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.82).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 66% 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 (2.82) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.4290
A	0.6470	0.4300
B	0.6600	0.4290
C	0.6550	0.4290
D	0.6570	0.4300
E	0.6600	0.4280
F	0.6580	0.4290
G	0.6570	0.4300
H	0.6590	0.4290
I	0.6510	0.4280
J	0.6560	0.4300
K	0.6610	0.4290

1.0

0.0

<0.0