



Full wwPDB EM Validation Report ⓘ

Apr 9, 2026 – 09:44 PM UTC

PDB ID : 9I3O / pdb_00009i3o
EMDB ID : EMD-52602
Title : Csu pilus rod type 2 stack
Authors : Malmi, H.; Pakharukova, N.; Zavialov, A.V.
Deposited on : 2025-01-23
Resolution : 4.70 Å (reported)
Based on initial model : 7ZL4

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:

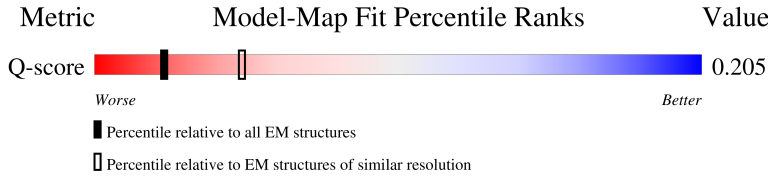
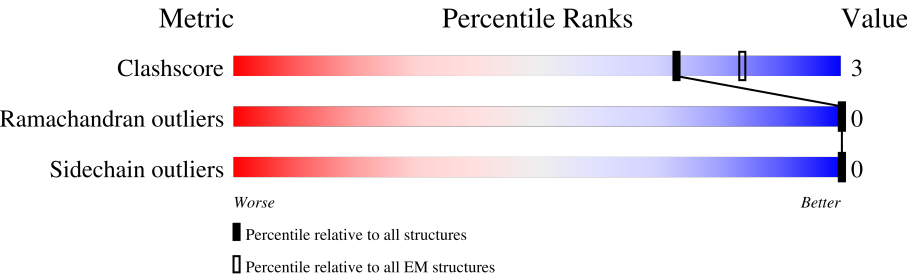
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 4.70 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.





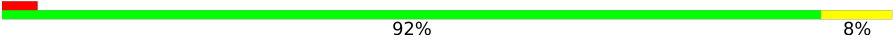
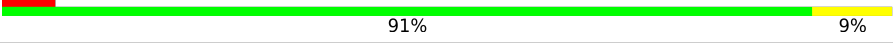
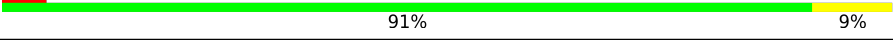
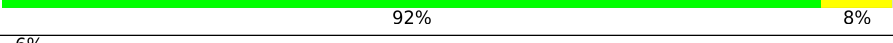
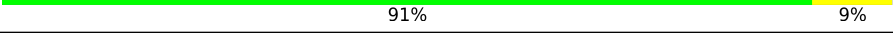
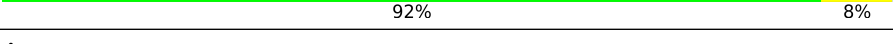
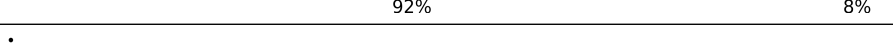
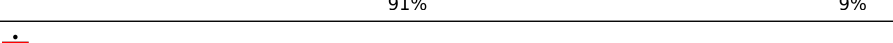
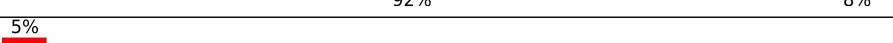








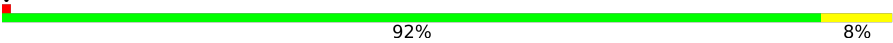
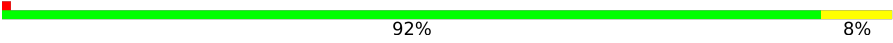
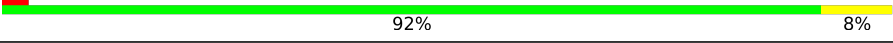
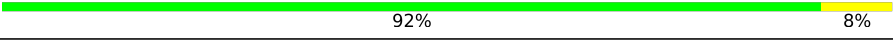


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	A1	155	
1	A2	155	
1	A3	155	
1	A4	155	

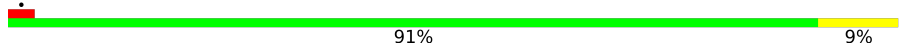
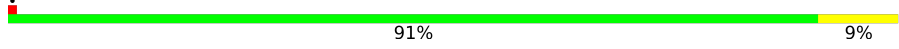
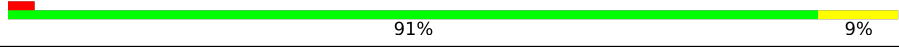
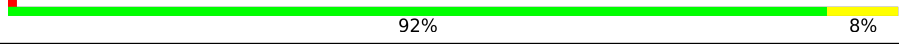
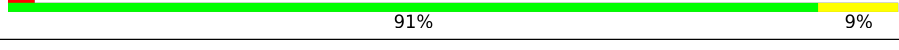
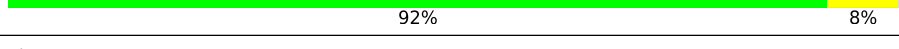
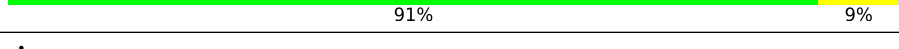
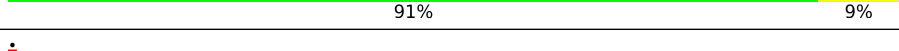
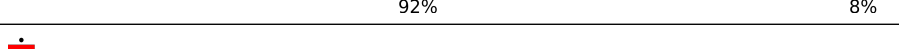
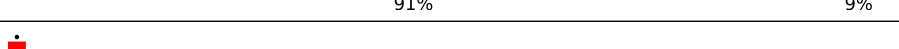
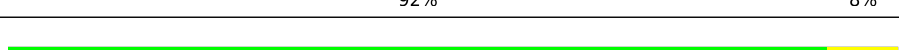
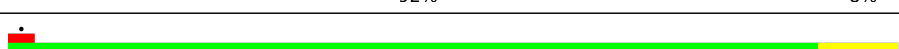
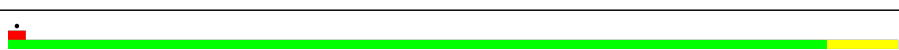
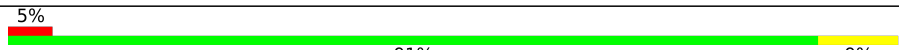
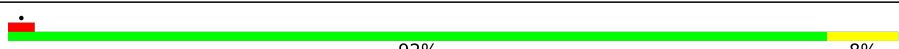


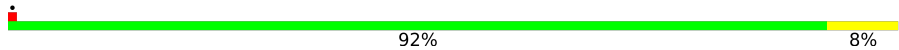
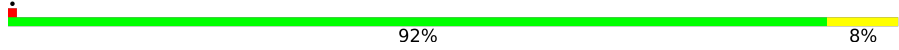
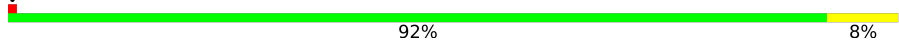
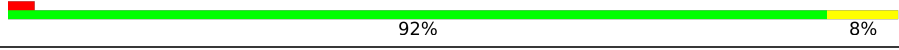
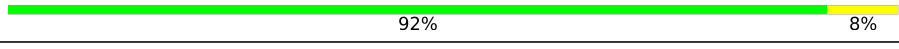
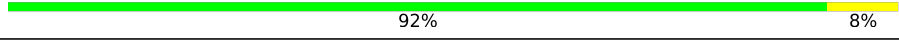
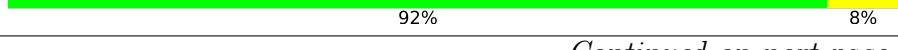

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	B1	155	 92% 8%
1	B2	155	 91% 9%
1	B3	155	 92% 8%
1	B4	155	 91% 9% 6%
1	C1	155	 91% 9% 5%
1	C2	155	 92% 8%
1	C3	155	 91% 9% 6%
1	C4	155	 92% 8%
1	D1	155	 92% 8%
1	D2	155	 91% 9%
1	D3	155	 92% 8%
1	D4	155	 91% 9% 5%
1	E1	155	 92% 8%
1	E2	155	 92% 8% 5%
1	E3	155	 92% 8%
1	E4	155	 92% 8%
1	F1	155	 92% 8%
1	F2	155	 92% 8%
1	F3	155	 92% 8%
1	F4	155	 92% 8%
1	G1	155	 92% 8%
1	G2	155	 92% 8%
1	G3	155	 92% 8%
1	G4	155	 92% 8%
1	H1	155	 91% 9%

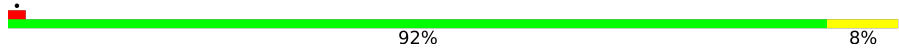
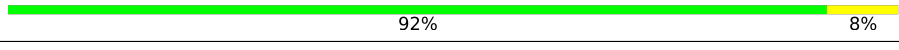
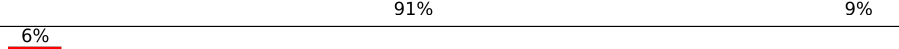
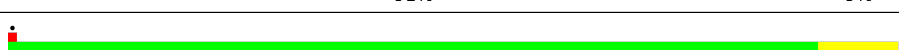
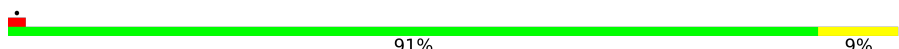
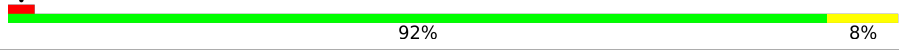
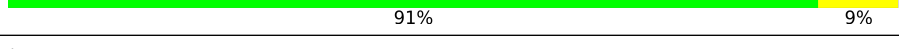
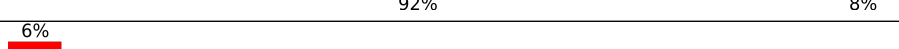

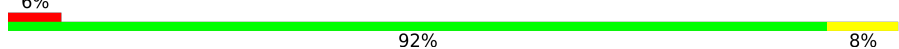
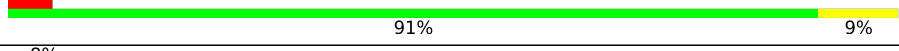
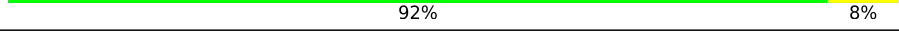






Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H2	155	 91%9%
1	H3	155	 91%9%
1	H4	155	 91%9%
1	I1	155	 92%8%
1	I2	155	 91%9%
1	I3	155	 92%8%
1	I4	155	 91%9%
1	J1	155	 91%9%
1	J2	155	 92%8%
1	J3	155	 91%9%
1	J4	155	 92%8%
1	K1	155	 92%8%
1	K2	155	 91%9%
1	K3	155	 92%8%
1	K4	155	 5%91%9%
1	L1	155	 92%8%
1	L2	155	 92%8%
1	L3	155	 92%8%
1	L4	155	 92%8%
1	M1	155	 92%8%
1	M2	155	 92%8%
1	M3	155	 92%8%
1	M4	155	 92%8%
1	N1	155	 92%8%
1	N2	155	 92%8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	N3	155	 92%8%
1	N4	155	 92%8%
1	O1	155	 91%9%
1	O2	155	 6%91%9%
1	O3	155	 91%9%
1	O4	155	 91%9%
1	P1	155	 92%8%
1	P2	155	 91%9%
1	P3	155	 92%8%
1	P4	155	 6%91%9%
1	Q1	155	 91%9%
1	Q2	155	 6%92%8%
1	Q3	155	 5%91%9%
1	Q4	155	 8%92%8%
1	R1	155	 6%91%
1	R2	155	 6%91%
1	R3	155	 6%91%
1	R4	155	 6%91%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 151368 atoms, of which 74596 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 CsuA/B.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	141	Total	C	H	N	O	S	0	0
			2017	634	988	177	215	3		
1	B1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	C1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	D1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	E1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	F1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	G1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	H1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	I1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	J1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	K1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	L1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	M1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	N1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	O1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	P1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		
1	Q1	155	Total	C	H	N	O	S	0	0
			2226	696	1097	194	236	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R1	14	Total	C	H	N	O	0	0
			209	62	109	17	21		
1	A2	141	Total	C	H	N	O	S	0
			2017	634	988	177	215	3	0
1	B2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	C2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	D2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	E2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	F2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	G2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	H2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	I2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	J2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	K2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	L2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	M2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	N2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	O2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	P2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	Q2	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0
1	R2	14	Total	C	H	N	O	0	0
			209	62	109	17	21		
1	A3	141	Total	C	H	N	O	S	0
			2017	634	988	177	215	3	0
1	B3	155	Total	C	H	N	O	S	0
			2226	696	1097	194	236	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	D3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	E3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	F3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	G3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	H3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	I3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	J3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	K3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	L3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	M3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	N3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	O3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	P3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	Q3	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	R3	14	Total 209	C 62	H 109	N 17	O 21		0	0
1	A4	141	Total 2017	C 634	H 988	N 177	O 215	S 3	0	0
1	B4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	C4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	D4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	E4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0

Continued on next page...

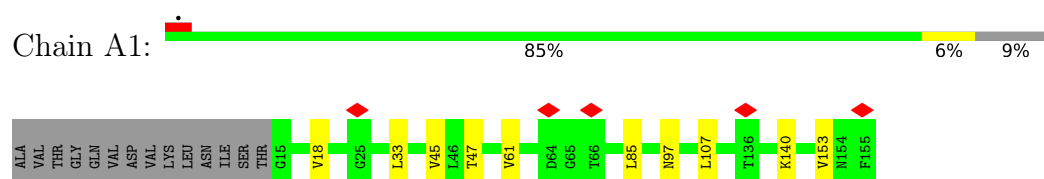
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
1	F4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	G4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	H4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	I4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	J4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	K4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	L4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	M4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	N4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	O4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	P4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	Q4	155	Total 2226	C 696	H 1097	N 194	O 236	S 3	0	0
1	R4	14	Total 209	C 62	H 109	N 17	O 21		0	0

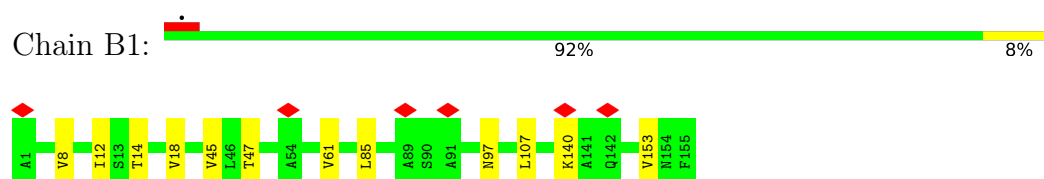
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

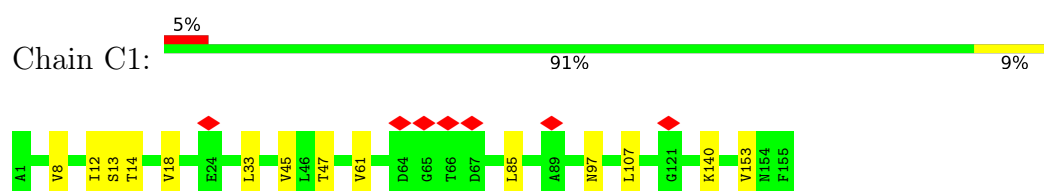
- Molecule 1: CsuA/B



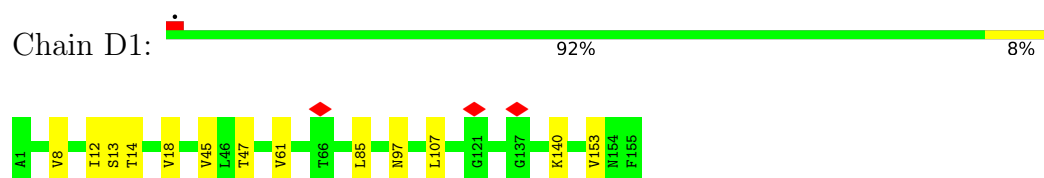
- Molecule 1: CsuA/B



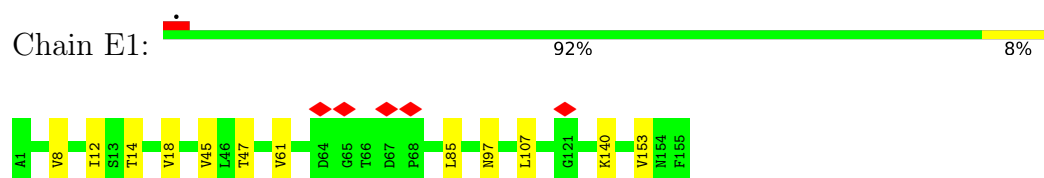
- Molecule 1: CsuA/B



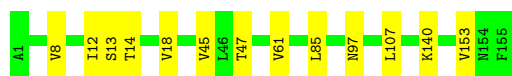
- Molecule 1: CsuA/B



- Molecule 1: CsuA/B



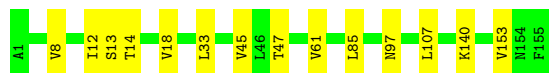
● Molecule 1: CsuA/B

Chain F1:  92% 8%

● Molecule 1: CsuA/B

Chain G1:  92% 8%

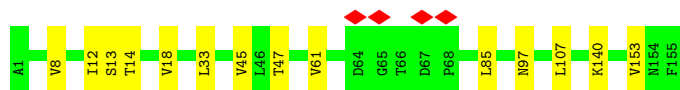
● Molecule 1: CsuA/B

Chain H1:  91% 9%

● Molecule 1: CsuA/B

Chain I1:  92% 8%

● Molecule 1: CsuA/B

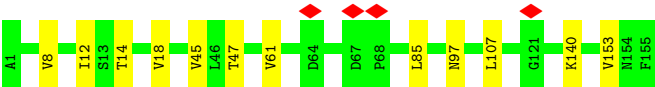
Chain J1:  91% 9%

● Molecule 1: CsuA/B

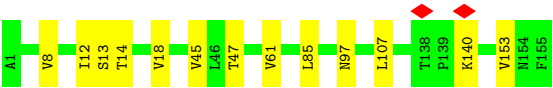
Chain K1:  92% 8%

● Molecule 1: CsuA/B

Chain L1:  92% 8%



• Molecule 1: CsuA/B



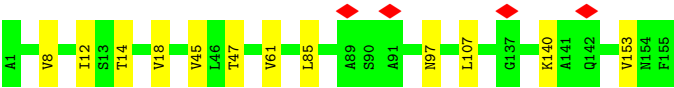
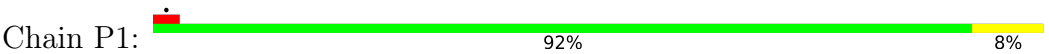
• Molecule 1: CsuA/B



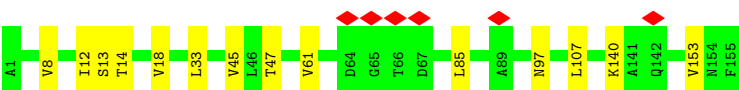
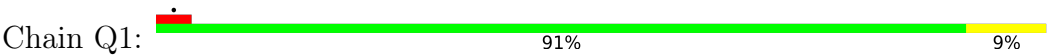
• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



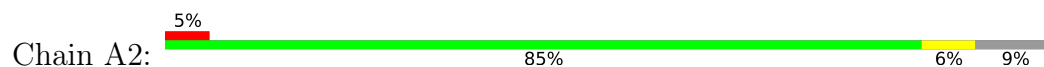
• Molecule 1: CsuA/B



A1	V8	I12	S13	T14	GLY	CYS	THR	THR	VAL	GLY	GLY	ARG	THR	ASP	ARG	THR	GLU	GLY	ASN	LYS	ASN	THR	ALA	LYS	PHE	GLY	ALA	THR	ASP	VAL	VAL	VAL	ALA	PHE	GLY	ASN	LYS	THR	VAL	TYR	ALA	THR	VAL	THR	ARG	GLY	ASP	ALA	ALA	ASN	THR	VAL	ASN	LEU	THR	TYR	VAL	GLN	PRO	ALA	ALA	THR	PHE	GLY	THR	THR	ASN	ILE	VAL	THR	GLY	VAL	GLN	ALA	THR	GLY	ASP	CYS	THR	ALA	VAL	THR	VAL	PRO
----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ILE PHE GLY ALA ILE ALA PRO ASN THR GLY THR PRO LYS ALA GLN GLY ASP TYR LYS ASP THR LEU VAL THR VAL ASN PHE

• Molecule 1: CsuA/B



ALA VAL THR GLN VAL ASP VAL LYS ASN LEU ILE SER THR G15 V18 V45 L46 T47 V61 D64 G65 T66 L85 A89 S90 A91 N97 L107 G121 T136 G137 T138 P139 K140 V153 N154 F155

• Molecule 1: CsuA/B



A1 V8 I12 S13 T14 V18 L33 V45 L46 T47 A54 T55 V61 G65 T66 D67 L85 N97 L107 G121 K140 V153 N154 F155

• Molecule 1: CsuA/B



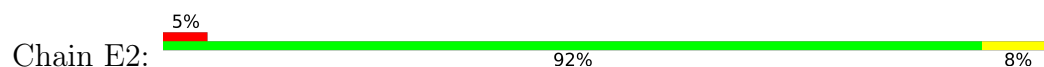
A1 V8 I12 S13 T14 V18 L33 V45 L46 T47 V61 L85 N97 L107 K140 V153 N154 F155

• Molecule 1: CsuA/B



A1 V8 I12 S13 T14 V18 L33 V45 L46 T47 V61 L85 A89 N97 L107 G137 K140 A141 Q142 V153 N154 F155

• Molecule 1: CsuA/B



A1 V8 I12 S13 T14 V18 V45 L46 T47 V61 D64 G65 T66 D67 P68 V69 D70 L85 A89 N97 L107 K140 V153 N154 F155

• Molecule 1: CsuA/B

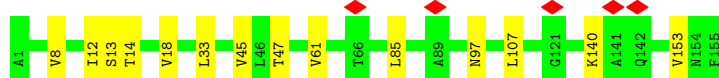


A1 V8 I12 S13 T14 V18 V45 L46 T47 V61 G65 T66 L85 N97 L107 K140 V153 N154 F155

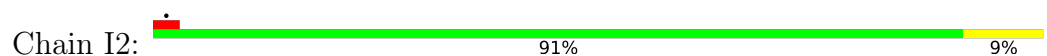
• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



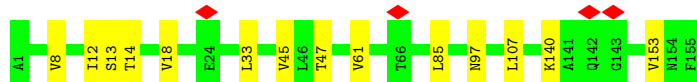
• Molecule 1: CsuA/B



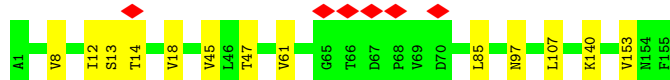
• Molecule 1: CsuA/B



• Molecule 1: CsuA/B

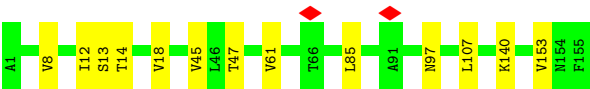


• Molecule 1: CsuA/B

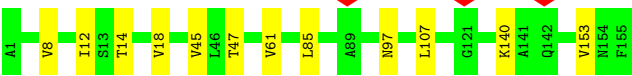


• Molecule 1: CsuA/B

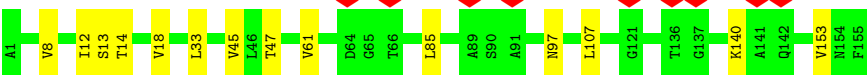
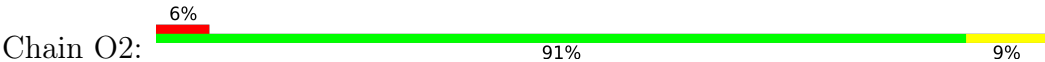




• Molecule 1: CsuA/B



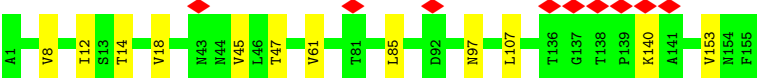
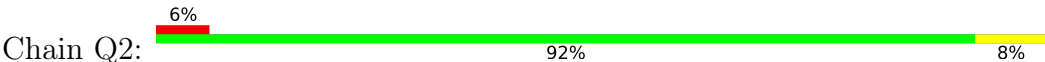
• Molecule 1: CsuA/B



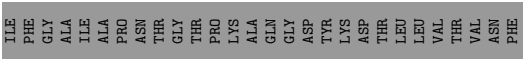
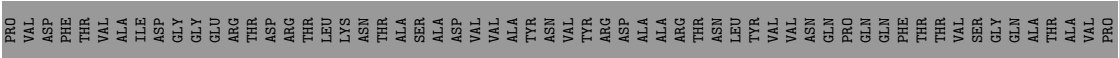
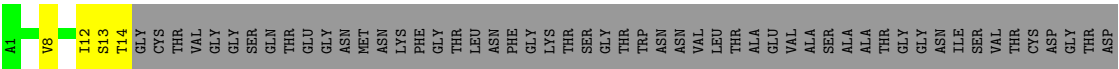
• Molecule 1: CsuA/B



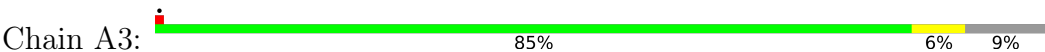
• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



• Molecule 1: CsuA/B

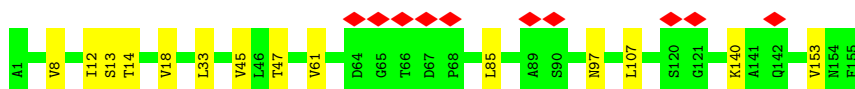
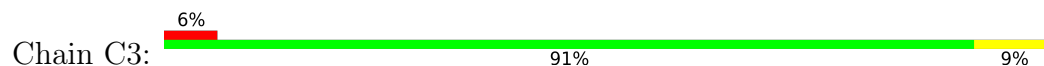




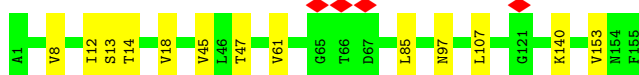
- Molecule 1: CsuA/B



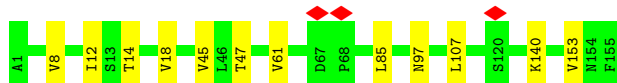
- Molecule 1: CsuA/B



- Molecule 1: CsuA/B



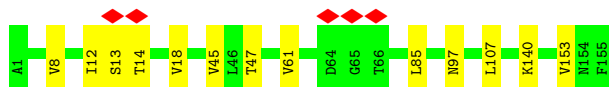
- Molecule 1: CsuA/B



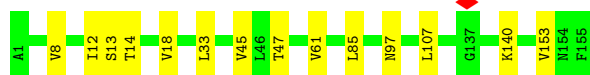
- Molecule 1: CsuA/B



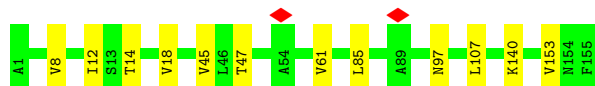
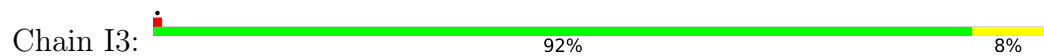
- Molecule 1: CsuA/B



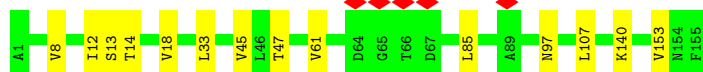
- Molecule 1: CsuA/B



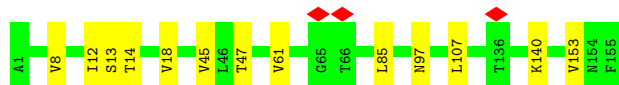
• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



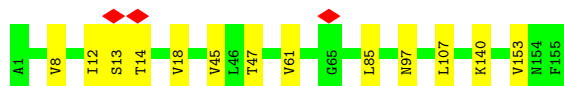
• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



A horizontal bar chart showing the distribution of 15 items. The items are labeled A1, V8, T12, S13, T14, V18, L33, V45, L46, T47, V61, L85, N97, L107, G137, K140, V153, N154, and F155. The bars are colored green or yellow. A red diamond is placed above the bar for G137.

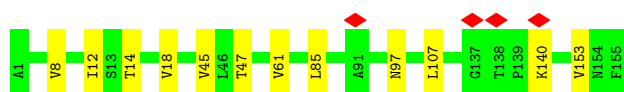
Category	Count
A1	1
V8	1
T12	1
S13	1
T14	1
V18	1
V45	1
L46	1
T47	1
A54	1
V61	1
L85	1
A89	1
N97	1
L107	1
K140	1
V153	1
N154	1
F155	1

[illegible]

Residue	Position	Frequency	Conservation	Phylogenetic	Structural	Functional	Evolutionary	Biophysical	Genetic	Protein	Cellular	Organismal	Environmental	Systemic	Global	Planetary	Universal
ALA	1	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
VAL	2	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
THR	3	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
GLY	4	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
GLN	5	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
VAL	6	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
ASP	7	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
VAL	8	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
LYS	9	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
LEU	10	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
ASN	11	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
ILE	12	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
SER	13	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
THR	14	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
G15	15	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
V18	18	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
V45	45	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
L46	46	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
T47	47	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
V61	61	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
G65	65	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
T66	66	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
D67	67	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
P68	68	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
L85	85	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
A89	89	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2	1.3	1.4	1.5
N97	97	0.05	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0					

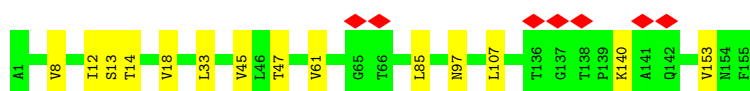
• Molecule 1: CsuA/B

Chain C4:  92% 8%



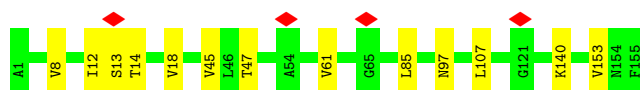
• Molecule 1: CsuA/B

Chain D4:  91% 9%



• Molecule 1: CsuA/B

Chain E4:  92% 8%



• Molecule 1: CsuA/B

Chain F4:  92% 8%



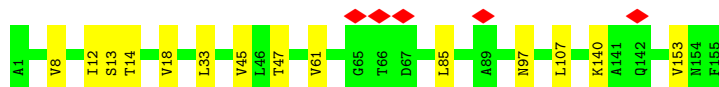
• Molecule 1: CsuA/B

Chain G4:  92% 8%




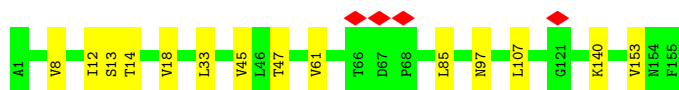
• Molecule 1: CsuA/B

Chain H4:  91% 9%



• Molecule 1: CsuA/B

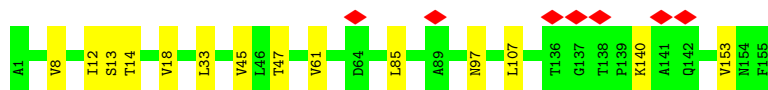
Chain I4:  91% 9%



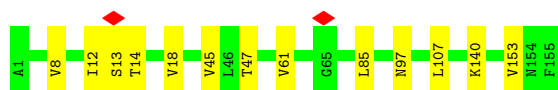
- Molecule 1: CsuA/B



- Molecule 1: CsuA/B



- Molecule 1: CsuA/B



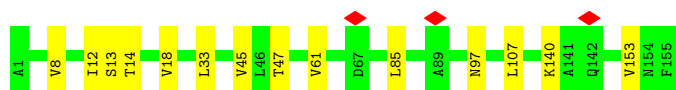
- Molecule 1: CsuA/B



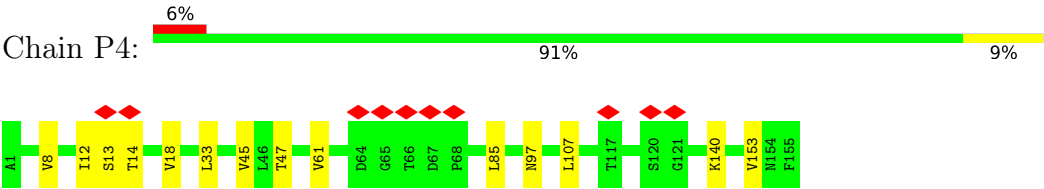
- Molecule 1: CsuA/B



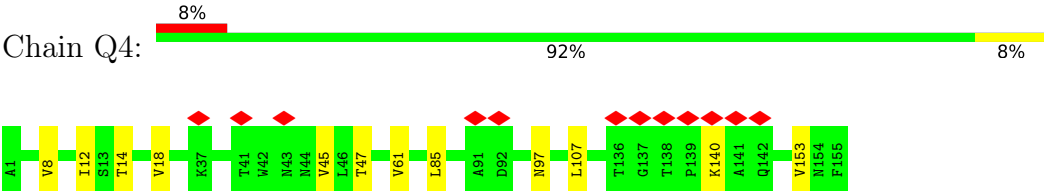
- Molecule 1: CsuA/B



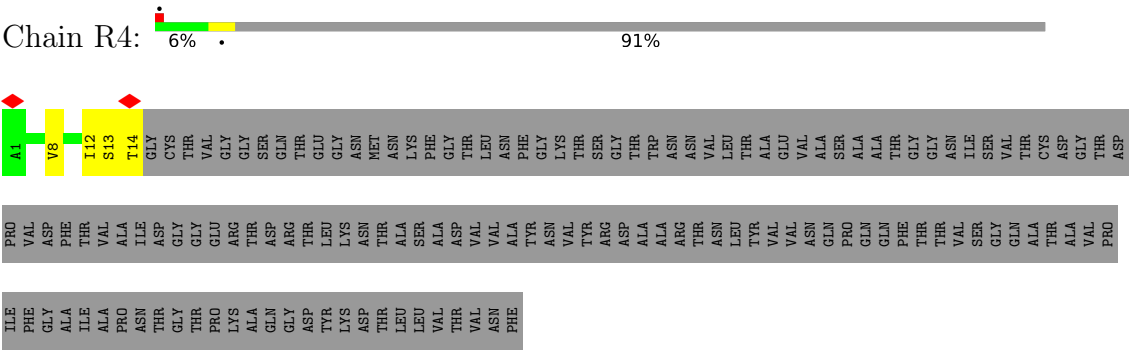
- Molecule 1: CsuA/B



• Molecule 1: CsuA/B



• Molecule 1: CsuA/B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	687088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	59.848	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.247	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	179.74538, 122.02897, 484.81778	wwPDB
Map dimensions	588, 148, 218	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82452005, 0.82452005, 0.82452005	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A1	0.51	0/1045	0.87	0/1427
1	A2	0.50	0/1045	0.87	0/1427
1	A3	0.51	0/1045	0.87	0/1427
1	A4	0.50	0/1045	0.87	0/1427
1	B1	0.52	0/1145	0.89	0/1564
1	B2	0.51	0/1145	0.87	0/1564
1	B3	0.52	0/1145	0.89	0/1564
1	B4	0.52	0/1145	0.87	0/1564
1	C1	0.51	0/1145	0.87	0/1564
1	C2	0.52	0/1145	0.89	0/1564
1	C3	0.52	0/1145	0.87	0/1564
1	C4	0.52	0/1145	0.89	0/1564
1	D1	0.52	0/1145	0.87	0/1564
1	D2	0.52	0/1145	0.87	0/1564
1	D3	0.52	0/1145	0.87	0/1564
1	D4	0.51	0/1145	0.87	0/1564
1	E1	0.52	0/1145	0.89	0/1564
1	E2	0.52	0/1145	0.87	0/1564
1	E3	0.52	0/1145	0.89	0/1564
1	E4	0.52	0/1145	0.87	0/1564
1	F1	0.51	0/1145	0.87	0/1564
1	F2	0.52	0/1145	0.87	0/1564
1	F3	0.52	0/1145	0.87	0/1564
1	F4	0.51	0/1145	0.87	0/1564
1	G1	0.52	0/1145	0.87	0/1564
1	G2	0.52	0/1145	0.89	0/1564
1	G3	0.52	0/1145	0.87	0/1564
1	G4	0.51	0/1145	0.89	0/1564
1	H1	0.52	0/1145	0.87	0/1564
1	H2	0.51	0/1145	0.87	0/1564
1	H3	0.52	0/1145	0.87	0/1564
1	H4	0.52	0/1145	0.87	0/1564
1	I1	0.52	0/1145	0.89	0/1564
1	I2	0.51	0/1145	0.87	0/1564

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I3	0.52	0/1145	0.89	0/1564
1	I4	0.51	0/1145	0.87	0/1564
1	J1	0.52	0/1145	0.87	0/1564
1	J2	0.52	0/1145	0.89	0/1564
1	J3	0.51	0/1145	0.87	0/1564
1	J4	0.52	0/1145	0.89	0/1564
1	K1	0.51	0/1145	0.87	0/1564
1	K2	0.52	0/1145	0.87	0/1564
1	K3	0.51	0/1145	0.87	0/1564
1	K4	0.51	0/1145	0.87	0/1564
1	L1	0.52	0/1145	0.89	0/1564
1	L2	0.51	0/1145	0.87	0/1564
1	L3	0.52	0/1145	0.89	0/1564
1	L4	0.51	0/1145	0.87	0/1564
1	M1	0.51	0/1145	0.87	0/1564
1	M2	0.51	0/1145	0.87	0/1564
1	M3	0.51	0/1145	0.87	0/1564
1	M4	0.51	0/1145	0.87	0/1564
1	N1	0.52	0/1145	0.87	0/1564
1	N2	0.52	0/1145	0.89	0/1564
1	N3	0.52	0/1145	0.87	0/1564
1	N4	0.52	0/1145	0.89	0/1564
1	O1	0.52	0/1145	0.87	0/1564
1	O2	0.51	0/1145	0.87	0/1564
1	O3	0.51	0/1145	0.87	0/1564
1	O4	0.52	0/1145	0.87	0/1564
1	P1	0.52	0/1145	0.89	0/1564
1	P2	0.52	0/1145	0.87	0/1564
1	P3	0.52	0/1145	0.89	0/1564
1	P4	0.52	0/1145	0.87	0/1564
1	Q1	0.52	0/1145	0.87	0/1564
1	Q2	0.52	0/1145	0.89	0/1564
1	Q3	0.52	0/1145	0.87	0/1564
1	Q4	0.52	0/1145	0.89	0/1564
1	R1	0.59	0/99	0.82	0/134
1	R2	0.58	0/99	0.83	0/134
1	R3	0.58	0/99	0.83	0/134
1	R4	0.58	0/99	0.83	0/134
All	All	0.52	0/77856	0.88	0/106340

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

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	A1	1029	988	987	7	0
1	A2	1029	988	987	6	0
1	A3	1029	988	987	7	0
1	A4	1029	988	987	6	0
1	B1	1129	1097	1097	9	0
1	B2	1129	1097	1097	10	0
1	B3	1129	1097	1097	9	0
1	B4	1129	1097	1097	10	0
1	C1	1129	1097	1097	10	0
1	C2	1129	1097	1097	9	0
1	C3	1129	1097	1097	10	0
1	C4	1129	1097	1097	9	0
1	D1	1129	1097	1097	9	0
1	D2	1129	1097	1097	10	0
1	D3	1129	1097	1097	9	0
1	D4	1129	1097	1097	10	0
1	E1	1129	1097	1097	9	0
1	E2	1129	1097	1097	9	0
1	E3	1129	1097	1097	9	0
1	E4	1129	1097	1097	9	0
1	F1	1129	1097	1097	9	0
1	F2	1129	1097	1097	9	0
1	F3	1129	1097	1097	9	0
1	F4	1129	1097	1097	9	0
1	G1	1129	1097	1097	9	0
1	G2	1129	1097	1097	9	0
1	G3	1129	1097	1097	9	0
1	G4	1129	1097	1097	9	0
1	H1	1129	1097	1097	10	0
1	H2	1129	1097	1097	10	0
1	H3	1129	1097	1097	10	0
1	H4	1129	1097	1097	10	0
1	I1	1129	1097	1097	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I2	1129	1097	1097	10	0
1	I3	1129	1097	1097	9	0
1	I4	1129	1097	1097	10	0
1	J1	1129	1097	1097	10	0
1	J2	1129	1097	1097	9	0
1	J3	1129	1097	1097	10	0
1	J4	1129	1097	1097	9	0
1	K1	1129	1097	1097	9	0
1	K2	1129	1097	1097	10	0
1	K3	1129	1097	1097	9	0
1	K4	1129	1097	1097	10	0
1	L1	1129	1097	1097	9	0
1	L2	1129	1097	1097	9	0
1	L3	1129	1097	1097	9	0
1	L4	1129	1097	1097	9	0
1	M1	1129	1097	1097	9	0
1	M2	1129	1097	1097	9	0
1	M3	1129	1097	1097	9	0
1	M4	1129	1097	1097	9	0
1	N1	1129	1097	1097	9	0
1	N2	1129	1097	1097	9	0
1	N3	1129	1097	1097	9	0
1	N4	1129	1097	1097	9	0
1	O1	1129	1097	1097	10	0
1	O2	1129	1097	1097	10	0
1	O3	1129	1097	1097	10	0
1	O4	1129	1097	1097	10	0
1	P1	1129	1097	1097	9	0
1	P2	1129	1097	1097	10	0
1	P3	1129	1097	1097	9	0
1	P4	1129	1097	1097	10	0
1	Q1	1129	1097	1097	10	0
1	Q2	1129	1097	1097	9	0
1	Q3	1129	1097	1097	10	0
1	Q4	1129	1097	1097	9	0
1	R1	100	109	109	3	0
1	R2	100	109	109	3	0
1	R3	100	109	109	3	0
1	R4	100	109	109	3	0
All	All	76772	74596	74592	502	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 3.

All (502) 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:J2:45:VAL:HG12	1:J2:47:THR:HG23	1.87	0.57
1:Q4:45:VAL:HG12	1:Q4:47:THR:HG23	1.87	0.57
1:M1:45:VAL:HG12	1:M1:47:THR:HG23	1.87	0.57
1:C2:45:VAL:HG12	1:C2:47:THR:HG23	1.87	0.57
1:F3:45:VAL:HG12	1:F3:47:THR:HG23	1.87	0.57
1:C4:45:VAL:HG12	1:C4:47:THR:HG23	1.87	0.57
1:H4:45:VAL:HG12	1:H4:47:THR:HG23	1.87	0.57
1:O4:45:VAL:HG12	1:O4:47:THR:HG23	1.87	0.57
1:H2:45:VAL:HG12	1:H2:47:THR:HG23	1.87	0.57
1:O2:45:VAL:HG12	1:O2:47:THR:HG23	1.87	0.57
1:Q2:45:VAL:HG12	1:Q2:47:THR:HG23	1.87	0.57
1:A4:45:VAL:HG12	1:A4:47:THR:HG23	1.87	0.57
1:J4:45:VAL:HG12	1:J4:47:THR:HG23	1.87	0.57
1:F1:45:VAL:HG12	1:F1:47:THR:HG23	1.87	0.57
1:A2:45:VAL:HG12	1:A2:47:THR:HG23	1.87	0.57
1:M3:45:VAL:HG12	1:M3:47:THR:HG23	1.87	0.57
1:P2:18:VAL:HG21	1:P2:153:VAL:HG21	1.87	0.57
1:P4:18:VAL:HG21	1:P4:153:VAL:HG21	1.87	0.57
1:H1:45:VAL:HG12	1:H1:47:THR:HG23	1.87	0.57
1:I2:18:VAL:HG21	1:I2:153:VAL:HG21	1.87	0.57
1:A3:45:VAL:HG12	1:A3:47:THR:HG23	1.87	0.57
1:I4:18:VAL:HG21	1:I4:153:VAL:HG21	1.87	0.57
1:A1:45:VAL:HG12	1:A1:47:THR:HG23	1.87	0.56
1:D1:45:VAL:HG12	1:D1:47:THR:HG23	1.87	0.56
1:B2:18:VAL:HG21	1:B2:153:VAL:HG21	1.87	0.56
1:D3:45:VAL:HG12	1:D3:47:THR:HG23	1.87	0.56
1:H3:45:VAL:HG12	1:H3:47:THR:HG23	1.87	0.56
1:O3:45:VAL:HG12	1:O3:47:THR:HG23	1.87	0.56
1:C1:45:VAL:HG12	1:C1:47:THR:HG23	1.87	0.56
1:J1:45:VAL:HG12	1:J1:47:THR:HG23	1.87	0.56
1:K1:45:VAL:HG12	1:K1:47:THR:HG23	1.87	0.56
1:O1:45:VAL:HG12	1:O1:47:THR:HG23	1.87	0.56
1:K3:45:VAL:HG12	1:K3:47:THR:HG23	1.87	0.56
1:B4:18:VAL:HG21	1:B4:153:VAL:HG21	1.87	0.56
1:Q1:45:VAL:HG12	1:Q1:47:THR:HG23	1.87	0.56
1:D2:18:VAL:HG21	1:D2:153:VAL:HG21	1.87	0.56
1:G2:18:VAL:HG21	1:G2:153:VAL:HG21	1.87	0.56
1:K2:18:VAL:HG21	1:K2:153:VAL:HG21	1.87	0.56
1:M2:45:VAL:HG12	1:M2:47:THR:HG23	1.87	0.56
1:N2:18:VAL:HG21	1:N2:153:VAL:HG21	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C3:45:VAL:HG12	1:C3:47:THR:HG23	1.87	0.56
1:J3:45:VAL:HG12	1:J3:47:THR:HG23	1.87	0.56
1:Q3:45:VAL:HG12	1:Q3:47:THR:HG23	1.87	0.56
1:D4:18:VAL:HG21	1:D4:153:VAL:HG21	1.87	0.56
1:F4:45:VAL:HG12	1:F4:47:THR:HG23	1.87	0.56
1:K4:18:VAL:HG21	1:K4:153:VAL:HG21	1.87	0.56
1:M4:45:VAL:HG12	1:M4:47:THR:HG23	1.87	0.56
1:N4:18:VAL:HG21	1:N4:153:VAL:HG21	1.87	0.56
1:B2:45:VAL:HG12	1:B2:47:THR:HG23	1.87	0.56
1:E2:45:VAL:HG12	1:E2:47:THR:HG23	1.87	0.56
1:F2:45:VAL:HG12	1:F2:47:THR:HG23	1.87	0.56
1:I2:45:VAL:HG12	1:I2:47:THR:HG23	1.87	0.56
1:B4:45:VAL:HG12	1:B4:47:THR:HG23	1.87	0.56
1:G4:18:VAL:HG21	1:G4:153:VAL:HG21	1.87	0.56
1:P4:45:VAL:HG12	1:P4:47:THR:HG23	1.87	0.56
1:N1:18:VAL:HG21	1:N1:153:VAL:HG21	1.87	0.56
1:L2:45:VAL:HG12	1:L2:47:THR:HG23	1.87	0.56
1:P2:45:VAL:HG12	1:P2:47:THR:HG23	1.87	0.56
1:N3:18:VAL:HG21	1:N3:153:VAL:HG21	1.87	0.56
1:P3:18:VAL:HG21	1:P3:153:VAL:HG21	1.87	0.56
1:E4:45:VAL:HG12	1:E4:47:THR:HG23	1.87	0.56
1:I4:45:VAL:HG12	1:I4:47:THR:HG23	1.87	0.56
1:L4:45:VAL:HG12	1:L4:47:THR:HG23	1.87	0.56
1:B1:18:VAL:HG21	1:B1:153:VAL:HG21	1.87	0.56
1:I1:18:VAL:HG21	1:I1:153:VAL:HG21	1.87	0.56
1:P1:18:VAL:HG21	1:P1:153:VAL:HG21	1.87	0.56
1:B3:18:VAL:HG21	1:B3:153:VAL:HG21	1.87	0.56
1:I3:18:VAL:HG21	1:I3:153:VAL:HG21	1.87	0.56
1:G1:18:VAL:HG21	1:G1:153:VAL:HG21	1.87	0.56
1:N1:45:VAL:HG12	1:N1:47:THR:HG23	1.87	0.56
1:G3:18:VAL:HG21	1:G3:153:VAL:HG21	1.87	0.56
1:G3:45:VAL:HG12	1:G3:47:THR:HG23	1.87	0.56
1:N3:45:VAL:HG12	1:N3:47:THR:HG23	1.87	0.56
1:G1:45:VAL:HG12	1:G1:47:THR:HG23	1.87	0.56
1:C2:18:VAL:HG21	1:C2:153:VAL:HG21	1.87	0.56
1:J4:18:VAL:HG21	1:J4:153:VAL:HG21	1.87	0.56
1:H1:18:VAL:HG21	1:H1:153:VAL:HG21	1.87	0.56
1:L1:45:VAL:HG12	1:L1:47:THR:HG23	1.87	0.56
1:O1:18:VAL:HG21	1:O1:153:VAL:HG21	1.87	0.56
1:J2:18:VAL:HG21	1:J2:153:VAL:HG21	1.87	0.56
1:L3:45:VAL:HG12	1:L3:47:THR:HG23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O3:18:VAL:HG21	1:O3:153:VAL:HG21	1.87	0.56
1:Q4:18:VAL:HG21	1:Q4:153:VAL:HG21	1.87	0.56
1:A1:18:VAL:HG21	1:A1:153:VAL:HG21	1.87	0.56
1:E1:45:VAL:HG12	1:E1:47:THR:HG23	1.87	0.56
1:M1:18:VAL:HG21	1:M1:153:VAL:HG21	1.87	0.56
1:O2:18:VAL:HG21	1:O2:153:VAL:HG21	1.87	0.56
1:Q2:18:VAL:HG21	1:Q2:153:VAL:HG21	1.87	0.56
1:A3:18:VAL:HG21	1:A3:153:VAL:HG21	1.87	0.56
1:E3:45:VAL:HG12	1:E3:47:THR:HG23	1.87	0.56
1:H3:18:VAL:HG21	1:H3:153:VAL:HG21	1.87	0.56
1:A4:18:VAL:HG21	1:A4:153:VAL:HG21	1.87	0.56
1:C4:18:VAL:HG21	1:C4:153:VAL:HG21	1.87	0.56
1:A2:18:VAL:HG21	1:A2:153:VAL:HG21	1.87	0.55
1:G2:45:VAL:HG12	1:G2:47:THR:HG23	1.87	0.55
1:H2:18:VAL:HG21	1:H2:153:VAL:HG21	1.87	0.55
1:N2:45:VAL:HG12	1:N2:47:THR:HG23	1.87	0.55
1:H4:18:VAL:HG21	1:H4:153:VAL:HG21	1.87	0.55
1:E1:18:VAL:HG21	1:E1:153:VAL:HG21	1.87	0.55
1:L1:18:VAL:HG21	1:L1:153:VAL:HG21	1.87	0.55
1:D2:45:VAL:HG12	1:D2:47:THR:HG23	1.87	0.55
1:K2:45:VAL:HG12	1:K2:47:THR:HG23	1.87	0.55
1:F3:18:VAL:HG21	1:F3:153:VAL:HG21	1.87	0.55
1:I3:45:VAL:HG12	1:I3:47:THR:HG23	1.87	0.55
1:M3:18:VAL:HG21	1:M3:153:VAL:HG21	1.87	0.55
1:D4:45:VAL:HG12	1:D4:47:THR:HG23	1.87	0.55
1:G4:45:VAL:HG12	1:G4:47:THR:HG23	1.87	0.55
1:K4:45:VAL:HG12	1:K4:47:THR:HG23	1.87	0.55
1:N4:45:VAL:HG12	1:N4:47:THR:HG23	1.87	0.55
1:O4:18:VAL:HG21	1:O4:153:VAL:HG21	1.87	0.55
1:F1:18:VAL:HG21	1:F1:153:VAL:HG21	1.87	0.55
1:I1:45:VAL:HG12	1:I1:47:THR:HG23	1.87	0.55
1:P1:45:VAL:HG12	1:P1:47:THR:HG23	1.87	0.55
1:E2:18:VAL:HG21	1:E2:153:VAL:HG21	1.87	0.55
1:L2:18:VAL:HG21	1:L2:153:VAL:HG21	1.87	0.55
1:B3:45:VAL:HG12	1:B3:47:THR:HG23	1.87	0.55
1:E3:18:VAL:HG21	1:E3:153:VAL:HG21	1.87	0.55
1:L3:18:VAL:HG21	1:L3:153:VAL:HG21	1.87	0.55
1:P3:45:VAL:HG12	1:P3:47:THR:HG23	1.87	0.55
1:L4:18:VAL:HG21	1:L4:153:VAL:HG21	1.87	0.55
1:B1:45:VAL:HG12	1:B1:47:THR:HG23	1.87	0.55
1:F2:18:VAL:HG21	1:F2:153:VAL:HG21	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M2:18:VAL:HG21	1:M2:153:VAL:HG21	1.87	0.55
1:E4:18:VAL:HG21	1:E4:153:VAL:HG21	1.87	0.55
1:F4:18:VAL:HG21	1:F4:153:VAL:HG21	1.87	0.55
1:M4:18:VAL:HG21	1:M4:153:VAL:HG21	1.87	0.55
1:D1:18:VAL:HG21	1:D1:153:VAL:HG21	1.87	0.55
1:K3:18:VAL:HG21	1:K3:153:VAL:HG21	1.87	0.55
1:D3:18:VAL:HG21	1:D3:153:VAL:HG21	1.87	0.55
1:K1:18:VAL:HG21	1:K1:153:VAL:HG21	1.87	0.55
1:Q3:18:VAL:HG21	1:Q3:153:VAL:HG21	1.87	0.55
1:C1:18:VAL:HG21	1:C1:153:VAL:HG21	1.87	0.55
1:J3:18:VAL:HG21	1:J3:153:VAL:HG21	1.87	0.55
1:Q1:18:VAL:HG21	1:Q1:153:VAL:HG21	1.87	0.54
1:A2:18:VAL:HG13	1:A2:61:VAL:HG22	1.90	0.54
1:H2:18:VAL:HG13	1:H2:61:VAL:HG22	1.90	0.54
1:I2:18:VAL:HG13	1:I2:61:VAL:HG22	1.90	0.54
1:O2:18:VAL:HG13	1:O2:61:VAL:HG22	1.90	0.54
1:P2:18:VAL:HG13	1:P2:61:VAL:HG22	1.90	0.54
1:C3:18:VAL:HG21	1:C3:153:VAL:HG21	1.87	0.54
1:A4:18:VAL:HG13	1:A4:61:VAL:HG22	1.90	0.54
1:B4:18:VAL:HG13	1:B4:61:VAL:HG22	1.90	0.54
1:H4:18:VAL:HG13	1:H4:61:VAL:HG22	1.90	0.54
1:I4:18:VAL:HG13	1:I4:61:VAL:HG22	1.90	0.54
1:O4:18:VAL:HG13	1:O4:61:VAL:HG22	1.90	0.54
1:J1:18:VAL:HG21	1:J1:153:VAL:HG21	1.87	0.54
1:B2:18:VAL:HG13	1:B2:61:VAL:HG22	1.90	0.54
1:K2:18:VAL:HG13	1:K2:61:VAL:HG22	1.90	0.54
1:P4:18:VAL:HG13	1:P4:61:VAL:HG22	1.90	0.54
1:M2:18:VAL:HG13	1:M2:61:VAL:HG22	1.90	0.54
1:F4:18:VAL:HG13	1:F4:61:VAL:HG22	1.90	0.54
1:K4:18:VAL:HG13	1:K4:61:VAL:HG22	1.90	0.54
1:M4:18:VAL:HG13	1:M4:61:VAL:HG22	1.90	0.54
1:M1:18:VAL:HG13	1:M1:61:VAL:HG22	1.90	0.54
1:D2:18:VAL:HG13	1:D2:61:VAL:HG22	1.90	0.54
1:F2:18:VAL:HG13	1:F2:61:VAL:HG22	1.90	0.54
1:J2:18:VAL:HG13	1:J2:61:VAL:HG22	1.89	0.54
1:D4:18:VAL:HG13	1:D4:61:VAL:HG22	1.90	0.54
1:G2:18:VAL:HG13	1:G2:61:VAL:HG22	1.90	0.54
1:N2:18:VAL:HG13	1:N2:61:VAL:HG22	1.90	0.54
1:F3:18:VAL:HG13	1:F3:61:VAL:HG22	1.90	0.54
1:G4:18:VAL:HG13	1:G4:61:VAL:HG22	1.90	0.54
1:F1:18:VAL:HG13	1:F1:61:VAL:HG22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q2:18:VAL:HG13	1:Q2:61:VAL:HG22	1.90	0.54
1:M3:18:VAL:HG13	1:M3:61:VAL:HG22	1.90	0.54
1:C4:18:VAL:HG13	1:C4:61:VAL:HG22	1.90	0.54
1:N4:18:VAL:HG13	1:N4:61:VAL:HG22	1.90	0.54
1:Q4:18:VAL:HG13	1:Q4:61:VAL:HG22	1.90	0.54
1:C2:18:VAL:HG13	1:C2:61:VAL:HG22	1.90	0.54
1:D3:18:VAL:HG13	1:D3:61:VAL:HG22	1.90	0.54
1:J4:18:VAL:HG13	1:J4:61:VAL:HG22	1.90	0.54
1:A1:18:VAL:HG13	1:A1:61:VAL:HG22	1.90	0.54
1:D1:18:VAL:HG13	1:D1:61:VAL:HG22	1.90	0.54
1:K1:18:VAL:HG13	1:K1:61:VAL:HG22	1.90	0.54
1:H3:18:VAL:HG13	1:H3:61:VAL:HG22	1.90	0.54
1:H1:18:VAL:HG13	1:H1:61:VAL:HG22	1.90	0.54
1:O1:18:VAL:HG13	1:O1:61:VAL:HG22	1.90	0.54
1:E2:18:VAL:HG13	1:E2:61:VAL:HG22	1.90	0.54
1:L2:18:VAL:HG13	1:L2:61:VAL:HG22	1.90	0.54
1:A3:18:VAL:HG13	1:A3:61:VAL:HG22	1.90	0.54
1:K3:18:VAL:HG13	1:K3:61:VAL:HG22	1.90	0.54
1:E4:18:VAL:HG13	1:E4:61:VAL:HG22	1.90	0.54
1:N3:18:VAL:HG13	1:N3:61:VAL:HG22	1.90	0.54
1:O3:18:VAL:HG13	1:O3:61:VAL:HG22	1.90	0.54
1:L4:18:VAL:HG13	1:L4:61:VAL:HG22	1.90	0.54
1:B1:18:VAL:HG13	1:B1:61:VAL:HG22	1.90	0.53
1:I1:18:VAL:HG13	1:I1:61:VAL:HG22	1.90	0.53
1:P1:18:VAL:HG13	1:P1:61:VAL:HG22	1.90	0.53
1:G3:18:VAL:HG13	1:G3:61:VAL:HG22	1.90	0.53
1:P3:18:VAL:HG13	1:P3:61:VAL:HG22	1.90	0.53
1:G1:18:VAL:HG13	1:G1:61:VAL:HG22	1.90	0.53
1:N1:18:VAL:HG13	1:N1:61:VAL:HG22	1.90	0.53
1:B3:18:VAL:HG13	1:B3:61:VAL:HG22	1.90	0.53
1:I3:18:VAL:HG13	1:I3:61:VAL:HG22	1.90	0.53
1:L3:18:VAL:HG13	1:L3:61:VAL:HG22	1.90	0.53
1:J1:18:VAL:HG13	1:J1:61:VAL:HG22	1.90	0.53
1:L1:18:VAL:HG13	1:L1:61:VAL:HG22	1.90	0.53
1:J3:18:VAL:HG13	1:J3:61:VAL:HG22	1.90	0.53
1:Q1:18:VAL:HG13	1:Q1:61:VAL:HG22	1.90	0.53
1:C3:18:VAL:HG13	1:C3:61:VAL:HG22	1.90	0.53
1:Q3:18:VAL:HG13	1:Q3:61:VAL:HG22	1.90	0.53
1:C1:18:VAL:HG13	1:C1:61:VAL:HG22	1.90	0.53
1:E1:18:VAL:HG13	1:E1:61:VAL:HG22	1.90	0.53
1:E3:18:VAL:HG13	1:E3:61:VAL:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q4:14:THR:HG22	1:Q4:14:THR:O	2.12	0.50
1:J2:14:THR:O	1:J2:14:THR:HG22	2.12	0.50
1:Q2:14:THR:O	1:Q2:14:THR:HG22	2.12	0.50
1:J4:14:THR:HG22	1:J4:14:THR:O	2.12	0.50
1:C2:14:THR:HG22	1:C2:14:THR:O	2.12	0.50
1:C4:14:THR:HG22	1:C4:14:THR:O	2.12	0.50
1:B3:14:THR:O	1:B3:14:THR:HG22	2.12	0.50
1:I3:14:THR:O	1:I3:14:THR:HG22	2.12	0.50
1:P3:14:THR:HG22	1:P3:14:THR:O	2.12	0.50
1:B1:14:THR:HG22	1:B1:14:THR:O	2.12	0.50
1:P1:14:THR:HG22	1:P1:14:THR:O	2.12	0.50
1:I1:14:THR:HG22	1:I1:14:THR:O	2.12	0.50
1:N2:14:THR:HG22	1:N2:14:THR:O	2.12	0.49
1:G4:14:THR:HG22	1:G4:14:THR:O	2.12	0.49
1:N4:14:THR:O	1:N4:14:THR:HG22	2.12	0.49
1:G2:14:THR:HG22	1:G2:14:THR:O	2.12	0.49
1:L1:14:THR:HG22	1:L1:14:THR:O	2.12	0.48
1:E1:14:THR:HG22	1:E1:14:THR:O	2.12	0.48
1:E3:14:THR:HG22	1:E3:14:THR:O	2.12	0.48
1:L3:14:THR:O	1:L3:14:THR:HG22	2.12	0.48
1:Q1:97:ASN:ND2	1:Q1:107:LEU:HD11	2.30	0.47
1:F2:97:ASN:ND2	1:F2:107:LEU:HD11	2.30	0.47
1:A1:97:ASN:ND2	1:A1:107:LEU:HD11	2.30	0.47
1:C1:97:ASN:ND2	1:C1:107:LEU:HD11	2.30	0.47
1:H1:97:ASN:ND2	1:H1:107:LEU:HD11	2.30	0.47
1:K2:97:ASN:ND2	1:K2:107:LEU:HD11	2.30	0.47
1:A3:97:ASN:ND2	1:A3:107:LEU:HD11	2.30	0.47
1:C3:97:ASN:ND2	1:C3:107:LEU:HD11	2.30	0.47
1:H3:97:ASN:ND2	1:H3:107:LEU:HD11	2.30	0.47
1:O3:97:ASN:ND2	1:O3:107:LEU:HD11	2.30	0.47
1:D4:97:ASN:ND2	1:D4:107:LEU:HD11	2.30	0.47
1:F4:97:ASN:ND2	1:F4:107:LEU:HD11	2.30	0.47
1:K4:97:ASN:ND2	1:K4:107:LEU:HD11	2.30	0.47
1:J1:97:ASN:ND2	1:J1:107:LEU:HD11	2.30	0.47
1:O1:97:ASN:ND2	1:O1:107:LEU:HD11	2.30	0.47
1:C2:97:ASN:ND2	1:C2:107:LEU:HD11	2.30	0.47
1:D2:97:ASN:ND2	1:D2:107:LEU:HD11	2.30	0.47
1:J2:97:ASN:ND2	1:J2:107:LEU:HD11	2.30	0.47
1:M2:97:ASN:ND2	1:M2:107:LEU:HD11	2.30	0.47
1:Q2:97:ASN:ND2	1:Q2:107:LEU:HD11	2.30	0.47
1:J3:97:ASN:ND2	1:J3:107:LEU:HD11	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q3:97:ASN:ND2	1:Q3:107:LEU:HD11	2.30	0.47
1:J4:97:ASN:ND2	1:J4:107:LEU:HD11	2.30	0.47
1:M4:97:ASN:ND2	1:M4:107:LEU:HD11	2.30	0.47
1:Q4:97:ASN:ND2	1:Q4:107:LEU:HD11	2.30	0.47
1:B1:97:ASN:ND2	1:B1:107:LEU:HD11	2.30	0.47
1:I3:97:ASN:ND2	1:I3:107:LEU:HD11	2.30	0.47
1:C4:97:ASN:ND2	1:C4:107:LEU:HD11	2.30	0.47
1:I1:97:ASN:ND2	1:I1:107:LEU:HD11	2.30	0.47
1:P1:97:ASN:ND2	1:P1:107:LEU:HD11	2.30	0.47
1:B3:97:ASN:ND2	1:B3:107:LEU:HD11	2.30	0.47
1:P3:97:ASN:ND2	1:P3:107:LEU:HD11	2.30	0.47
1:D3:97:ASN:ND2	1:D3:107:LEU:HD11	2.30	0.47
1:I4:97:ASN:ND2	1:I4:107:LEU:HD11	2.30	0.47
1:H2:97:ASN:ND2	1:H2:107:LEU:HD11	2.30	0.46
1:I2:97:ASN:ND2	1:I2:107:LEU:HD11	2.30	0.46
1:P2:97:ASN:ND2	1:P2:107:LEU:HD11	2.30	0.46
1:G3:97:ASN:ND2	1:G3:107:LEU:HD11	2.30	0.46
1:K3:97:ASN:ND2	1:K3:107:LEU:HD11	2.30	0.46
1:N3:97:ASN:ND2	1:N3:107:LEU:HD11	2.30	0.46
1:B4:97:ASN:ND2	1:B4:107:LEU:HD11	2.30	0.46
1:D1:97:ASN:ND2	1:D1:107:LEU:HD11	2.30	0.46
1:G1:97:ASN:ND2	1:G1:107:LEU:HD11	2.30	0.46
1:K1:97:ASN:ND2	1:K1:107:LEU:HD11	2.30	0.46
1:B2:97:ASN:ND2	1:B2:107:LEU:HD11	2.30	0.46
1:L2:97:ASN:ND2	1:L2:107:LEU:HD11	2.30	0.46
1:O2:97:ASN:ND2	1:O2:107:LEU:HD11	2.30	0.46
1:A4:97:ASN:ND2	1:A4:107:LEU:HD11	2.30	0.46
1:O4:97:ASN:ND2	1:O4:107:LEU:HD11	2.30	0.46
1:P4:97:ASN:ND2	1:P4:107:LEU:HD11	2.30	0.46
1:L1:97:ASN:ND2	1:L1:107:LEU:HD11	2.30	0.46
1:N1:97:ASN:ND2	1:N1:107:LEU:HD11	2.30	0.46
1:A2:97:ASN:ND2	1:A2:107:LEU:HD11	2.30	0.46
1:E2:97:ASN:ND2	1:E2:107:LEU:HD11	2.30	0.46
1:L3:97:ASN:ND2	1:L3:107:LEU:HD11	2.30	0.46
1:E4:97:ASN:ND2	1:E4:107:LEU:HD11	2.30	0.46
1:H4:97:ASN:ND2	1:H4:107:LEU:HD11	2.30	0.46
1:L4:97:ASN:ND2	1:L4:107:LEU:HD11	2.30	0.46
1:E1:97:ASN:ND2	1:E1:107:LEU:HD11	2.30	0.46
1:E3:97:ASN:ND2	1:E3:107:LEU:HD11	2.30	0.46
1:G2:97:ASN:ND2	1:G2:107:LEU:HD11	2.30	0.46
1:G4:97:ASN:ND2	1:G4:107:LEU:HD11	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N4:97:ASN:ND2	1:N4:107:LEU:HD11	2.30	0.46
1:N2:97:ASN:ND2	1:N2:107:LEU:HD11	2.30	0.46
1:F1:97:ASN:ND2	1:F1:107:LEU:HD11	2.30	0.46
1:M1:97:ASN:ND2	1:M1:107:LEU:HD11	2.30	0.46
1:F3:97:ASN:ND2	1:F3:107:LEU:HD11	2.30	0.46
1:M3:97:ASN:ND2	1:M3:107:LEU:HD11	2.30	0.46
1:H4:33:LEU:HD12	1:H4:33:LEU:HA	1.85	0.45
1:O4:33:LEU:HD12	1:O4:33:LEU:HA	1.85	0.45
1:H2:33:LEU:HD12	1:H2:33:LEU:HA	1.86	0.45
1:O2:33:LEU:HD12	1:O2:33:LEU:HA	1.85	0.45
1:D1:140:LYS:HB2	1:E1:12:ILE:HD13	2.00	0.44
1:K1:140:LYS:HB2	1:L1:12:ILE:HD13	2.00	0.44
1:J4:140:LYS:HB2	1:K4:12:ILE:HD13	2.00	0.44
1:Q4:140:LYS:HB2	1:R4:12:ILE:HD13	2.00	0.44
1:M1:140:LYS:HB2	1:N1:12:ILE:HD13	2.00	0.43
1:A2:140:LYS:HB2	1:B2:12:ILE:HD13	2.00	0.43
1:C2:140:LYS:HB2	1:D2:12:ILE:HD13	2.00	0.43
1:H2:140:LYS:HB2	1:I2:12:ILE:HD13	2.00	0.43
1:D3:140:LYS:HB2	1:E3:12:ILE:HD13	2.00	0.43
1:F3:140:LYS:HB2	1:G3:12:ILE:HD13	2.00	0.43
1:K3:140:LYS:HB2	1:L3:12:ILE:HD13	2.00	0.43
1:A4:140:LYS:HB2	1:B4:12:ILE:HD13	2.00	0.43
1:C4:140:LYS:HB2	1:D4:12:ILE:HD13	2.00	0.43
1:H4:140:LYS:HB2	1:I4:12:ILE:HD13	2.00	0.43
1:F1:140:LYS:HB2	1:G1:12:ILE:HD13	2.00	0.43
1:J2:140:LYS:HB2	1:K2:12:ILE:HD13	2.01	0.43
1:O2:140:LYS:HB2	1:P2:12:ILE:HD13	2.00	0.43
1:Q2:140:LYS:HB2	1:R2:12:ILE:HD13	2.01	0.43
1:M3:140:LYS:HB2	1:N3:12:ILE:HD13	2.00	0.43
1:O4:140:LYS:HB2	1:P4:12:ILE:HD13	2.00	0.43
1:O1:140:LYS:HB2	1:P1:12:ILE:HD13	2.00	0.43
1:F2:140:LYS:HB2	1:G2:12:ILE:HD13	2.00	0.43
1:A3:140:LYS:HB2	1:B3:12:ILE:HD13	2.00	0.43
1:O3:140:LYS:HB2	1:P3:12:ILE:HD13	2.00	0.43
1:H1:140:LYS:HB2	1:I1:12:ILE:HD13	2.00	0.43
1:Q1:140:LYS:HB2	1:R1:12:ILE:HD13	2.00	0.43
1:D2:140:LYS:HB2	1:E2:12:ILE:HD13	2.00	0.43
1:K2:140:LYS:HB2	1:L2:12:ILE:HD13	2.00	0.43
1:M2:140:LYS:HB2	1:N2:12:ILE:HD13	2.00	0.43
1:H3:140:LYS:HB2	1:I3:12:ILE:HD13	2.00	0.43
1:D4:140:LYS:HB2	1:E4:12:ILE:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F4:140:LYS:HB2	1:G4:12:ILE:HD13	2.00	0.43
1:K4:140:LYS:HB2	1:L4:12:ILE:HD13	2.00	0.43
1:M4:140:LYS:HB2	1:N4:12:ILE:HD13	2.00	0.43
1:A1:140:LYS:HB2	1:B1:12:ILE:HD13	2.00	0.43
1:C1:140:LYS:HB2	1:D1:12:ILE:HD13	2.00	0.43
1:E2:140:LYS:HB2	1:F2:12:ILE:HD13	2.00	0.43
1:B3:140:LYS:HB2	1:C3:12:ILE:HD13	2.00	0.43
1:Q3:140:LYS:HB2	1:R3:12:ILE:HD13	2.00	0.43
1:E4:140:LYS:HB2	1:F4:12:ILE:HD13	2.00	0.43
1:L4:140:LYS:HB2	1:M4:12:ILE:HD13	2.00	0.43
1:B1:140:LYS:HB2	1:C1:12:ILE:HD13	2.00	0.43
1:I1:140:LYS:HB2	1:J1:12:ILE:HD13	2.00	0.43
1:J1:140:LYS:HB2	1:K1:12:ILE:HD13	2.00	0.43
1:P1:140:LYS:HB2	1:Q1:12:ILE:HD13	2.00	0.43
1:L2:140:LYS:HB2	1:M2:12:ILE:HD13	2.01	0.43
1:C3:140:LYS:HB2	1:D3:12:ILE:HD13	2.00	0.43
1:J3:140:LYS:HB2	1:K3:12:ILE:HD13	2.00	0.43
1:I3:140:LYS:HB2	1:J3:12:ILE:HD13	2.00	0.43
1:P3:140:LYS:HB2	1:Q3:12:ILE:HD13	2.00	0.43
1:E1:85:LEU:HD21	1:F1:8:VAL:HG12	2.01	0.43
1:L1:85:LEU:HD21	1:M1:8:VAL:HG12	2.01	0.43
1:E3:85:LEU:HD21	1:F3:8:VAL:HG12	2.01	0.43
1:L3:85:LEU:HD21	1:M3:8:VAL:HG12	2.01	0.43
1:G1:85:LEU:HD21	1:H1:8:VAL:HG12	2.01	0.43
1:G3:85:LEU:HD21	1:H3:8:VAL:HG12	2.01	0.43
1:N3:85:LEU:HD21	1:O3:8:VAL:HG12	2.01	0.43
1:C1:85:LEU:HD21	1:D1:8:VAL:HG12	2.01	0.42
1:E1:140:LYS:HB2	1:F1:12:ILE:HD13	2.00	0.42
1:J1:85:LEU:HD21	1:K1:8:VAL:HG12	2.01	0.42
1:L1:140:LYS:HB2	1:M1:12:ILE:HD13	2.00	0.42
1:N1:85:LEU:HD21	1:O1:8:VAL:HG12	2.01	0.42
1:Q1:85:LEU:HD21	1:R1:8:VAL:HG12	2.01	0.42
1:P2:140:LYS:HB2	1:Q2:12:ILE:HD13	2.00	0.42
1:C3:85:LEU:HD21	1:D3:8:VAL:HG12	2.01	0.42
1:E3:140:LYS:HB2	1:F3:12:ILE:HD13	2.00	0.42
1:Q3:85:LEU:HD21	1:R3:8:VAL:HG12	2.01	0.42
1:P4:140:LYS:HB2	1:Q4:12:ILE:HD13	2.00	0.42
1:B2:140:LYS:HB2	1:C2:12:ILE:HD13	2.00	0.42
1:J3:85:LEU:HD21	1:K3:8:VAL:HG12	2.01	0.42
1:L3:140:LYS:HB2	1:M3:12:ILE:HD13	2.01	0.42
1:B4:140:LYS:HB2	1:C4:12:ILE:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I2:140:LYS:HB2	1:J2:12:ILE:HD13	2.01	0.42
1:I4:140:LYS:HB2	1:J4:12:ILE:HD13	2.00	0.42
1:D1:85:LEU:HD21	1:E1:8:VAL:HG12	2.01	0.42
1:G1:140:LYS:HB2	1:H1:12:ILE:HD13	2.00	0.42
1:N1:140:LYS:HB2	1:O1:12:ILE:HD13	2.00	0.42
1:G3:140:LYS:HB2	1:H3:12:ILE:HD13	2.00	0.42
1:N3:140:LYS:HB2	1:O3:12:ILE:HD13	2.00	0.42
1:O3:33:LEU:HD12	1:O3:33:LEU:HA	1.85	0.42
1:H1:33:LEU:HD12	1:H1:33:LEU:HA	1.85	0.42
1:M1:85:LEU:HD21	1:N1:8:VAL:HG12	2.01	0.42
1:A3:33:LEU:HD12	1:A3:33:LEU:HA	1.85	0.42
1:A1:33:LEU:HD12	1:A1:33:LEU:HA	1.85	0.42
1:F1:85:LEU:HD21	1:G1:8:VAL:HG12	2.01	0.42
1:N2:140:LYS:HB2	1:O2:12:ILE:HD13	2.00	0.42
1:D3:85:LEU:HD21	1:E3:8:VAL:HG12	2.01	0.42
1:F3:85:LEU:HD21	1:G3:8:VAL:HG12	2.01	0.42
1:H3:33:LEU:HD12	1:H3:33:LEU:HA	1.85	0.42
1:G4:140:LYS:HB2	1:H4:12:ILE:HD13	2.00	0.42
1:K1:85:LEU:HD21	1:L1:8:VAL:HG12	2.01	0.42
1:O1:33:LEU:HD12	1:O1:33:LEU:HA	1.85	0.42
1:F2:85:LEU:HD21	1:G2:8:VAL:HG12	2.01	0.42
1:G2:140:LYS:HB2	1:H2:12:ILE:HD13	2.00	0.42
1:H2:85:LEU:HD21	1:I2:8:VAL:HG12	2.01	0.42
1:K3:85:LEU:HD21	1:L3:8:VAL:HG12	2.01	0.42
1:F4:85:LEU:HD21	1:G4:8:VAL:HG12	2.01	0.42
1:H4:85:LEU:HD21	1:I4:8:VAL:HG12	2.01	0.42
1:B1:85:LEU:HD21	1:C1:8:VAL:HG12	2.01	0.42
1:O1:85:LEU:HD21	1:P1:8:VAL:HG12	2.01	0.42
1:A2:85:LEU:HD21	1:B2:8:VAL:HG12	2.01	0.42
1:H3:85:LEU:HD21	1:I3:8:VAL:HG12	2.01	0.42
1:M3:85:LEU:HD21	1:N3:8:VAL:HG12	2.01	0.42
1:A4:85:LEU:HD21	1:B4:8:VAL:HG12	2.01	0.42
1:N4:140:LYS:HB2	1:O4:12:ILE:HD13	2.01	0.42
1:A1:85:LEU:HD21	1:B1:8:VAL:HG12	2.01	0.42
1:M2:85:LEU:HD21	1:N2:8:VAL:HG12	2.01	0.42
1:O2:85:LEU:HD21	1:P2:8:VAL:HG12	2.01	0.42
1:A3:85:LEU:HD21	1:B3:8:VAL:HG12	2.01	0.42
1:B3:85:LEU:HD21	1:C3:8:VAL:HG12	2.01	0.42
1:O3:85:LEU:HD21	1:P3:8:VAL:HG12	2.01	0.42
1:O4:85:LEU:HD21	1:P4:8:VAL:HG12	2.01	0.42
1:I1:85:LEU:HD21	1:J1:8:VAL:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L2:85:LEU:HD21	1:M2:8:VAL:HG12	2.01	0.42
1:P3:85:LEU:HD21	1:Q3:8:VAL:HG12	2.01	0.42
1:L4:85:LEU:HD21	1:M4:8:VAL:HG12	2.01	0.42
1:M4:85:LEU:HD21	1:N4:8:VAL:HG12	2.01	0.42
1:C1:33:LEU:HD12	1:C1:33:LEU:HA	1.85	0.41
1:H1:85:LEU:HD21	1:I1:8:VAL:HG12	2.01	0.41
1:K1:13:SER:O	1:K1:14:THR:HG23	2.20	0.41
1:P1:85:LEU:HD21	1:Q1:8:VAL:HG12	2.01	0.41
1:E2:85:LEU:HD21	1:F2:8:VAL:HG12	2.01	0.41
1:G2:85:LEU:HD21	1:H2:8:VAL:HG12	2.01	0.41
1:K2:13:SER:O	1:K2:14:THR:HG23	2.20	0.41
1:N2:85:LEU:HD21	1:O2:8:VAL:HG12	2.01	0.41
1:R2:13:SER:O	1:R2:14:THR:HG23	2.20	0.41
1:C3:33:LEU:HD12	1:C3:33:LEU:HA	1.85	0.41
1:I3:85:LEU:HD21	1:J3:8:VAL:HG12	2.01	0.41
1:E4:85:LEU:HD21	1:F4:8:VAL:HG12	2.01	0.41
1:N4:85:LEU:HD21	1:O4:8:VAL:HG12	2.01	0.41
1:J1:33:LEU:HD12	1:J1:33:LEU:HA	1.85	0.41
1:R1:13:SER:O	1:R1:14:THR:HG23	2.20	0.41
1:B2:85:LEU:HD21	1:C2:8:VAL:HG12	2.01	0.41
1:J3:33:LEU:HD12	1:J3:33:LEU:HA	1.85	0.41
1:R3:13:SER:O	1:R3:14:THR:HG23	2.20	0.41
1:B4:85:LEU:HD21	1:C4:8:VAL:HG12	2.01	0.41
1:G4:85:LEU:HD21	1:H4:8:VAL:HG12	2.01	0.41
1:I4:85:LEU:HD21	1:J4:8:VAL:HG12	2.01	0.41
1:D1:13:SER:O	1:D1:14:THR:HG23	2.20	0.41
1:D2:13:SER:O	1:D2:14:THR:HG23	2.20	0.41
1:I2:85:LEU:HD21	1:J2:8:VAL:HG12	2.01	0.41
1:P2:85:LEU:HD21	1:Q2:8:VAL:HG12	2.01	0.41
1:D3:13:SER:O	1:D3:14:THR:HG23	2.20	0.41
1:K3:13:SER:O	1:K3:14:THR:HG23	2.20	0.41
1:D4:13:SER:O	1:D4:14:THR:HG23	2.20	0.41
1:K4:13:SER:O	1:K4:14:THR:HG23	2.20	0.41
1:P4:85:LEU:HD21	1:Q4:8:VAL:HG12	2.01	0.41
1:R4:13:SER:O	1:R4:14:THR:HG23	2.20	0.41
1:C1:13:SER:O	1:C1:14:THR:HG23	2.20	0.41
1:M1:13:SER:O	1:M1:14:THR:HG23	2.20	0.41
1:Q1:33:LEU:HD12	1:Q1:33:LEU:HA	1.85	0.41
1:B2:13:SER:O	1:B2:14:THR:HG23	2.20	0.41
1:Q3:33:LEU:HD12	1:Q3:33:LEU:HA	1.85	0.41
1:B4:13:SER:O	1:B4:14:THR:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D4:85:LEU:HD21	1:E4:8:VAL:HG12	2.01	0.41
1:K4:85:LEU:HD21	1:L4:8:VAL:HG12	2.01	0.41
1:J1:13:SER:O	1:J1:14:THR:HG23	2.20	0.41
1:I2:13:SER:O	1:I2:14:THR:HG23	2.20	0.41
1:K2:85:LEU:HD21	1:L2:8:VAL:HG12	2.01	0.41
1:P2:13:SER:O	1:P2:14:THR:HG23	2.20	0.41
1:C3:13:SER:O	1:C3:14:THR:HG23	2.20	0.41
1:F3:13:SER:O	1:F3:14:THR:HG23	2.20	0.41
1:Q3:13:SER:O	1:Q3:14:THR:HG23	2.20	0.41
1:I4:13:SER:O	1:I4:14:THR:HG23	2.20	0.41
1:L4:13:SER:O	1:L4:14:THR:HG23	2.20	0.41
1:P4:13:SER:O	1:P4:14:THR:HG23	2.20	0.41
1:Q4:85:LEU:HD21	1:R4:8:VAL:HG12	2.01	0.41
1:F1:13:SER:O	1:F1:14:THR:HG23	2.20	0.41
1:O1:13:SER:O	1:O1:14:THR:HG23	2.20	0.41
1:Q1:13:SER:O	1:Q1:14:THR:HG23	2.20	0.41
1:C2:85:LEU:HD21	1:D2:8:VAL:HG12	2.01	0.41
1:D2:85:LEU:HD21	1:E2:8:VAL:HG12	2.01	0.41
1:E2:13:SER:O	1:E2:14:THR:HG23	2.20	0.41
1:L2:13:SER:O	1:L2:14:THR:HG23	2.20	0.41
1:H3:13:SER:O	1:H3:14:THR:HG23	2.20	0.41
1:J3:13:SER:O	1:J3:14:THR:HG23	2.20	0.41
1:M3:13:SER:O	1:M3:14:THR:HG23	2.20	0.41
1:O3:13:SER:O	1:O3:14:THR:HG23	2.20	0.41
1:C4:85:LEU:HD21	1:D4:8:VAL:HG12	2.01	0.41
1:D4:33:LEU:HD12	1:D4:33:LEU:HA	1.85	0.41
1:H1:13:SER:O	1:H1:14:THR:HG23	2.20	0.41
1:N1:13:SER:O	1:N1:14:THR:HG23	2.20	0.41
1:B2:33:LEU:HD12	1:B2:33:LEU:HA	1.85	0.41
1:I2:33:LEU:HD12	1:I2:33:LEU:HA	1.85	0.41
1:J2:85:LEU:HD21	1:K2:8:VAL:HG12	2.01	0.41
1:K2:33:LEU:HD12	1:K2:33:LEU:HA	1.85	0.41
1:Q2:85:LEU:HD21	1:R2:8:VAL:HG12	2.01	0.41
1:E4:13:SER:O	1:E4:14:THR:HG23	2.20	0.41
1:J4:85:LEU:HD21	1:K4:8:VAL:HG12	2.01	0.41
1:G1:13:SER:O	1:G1:14:THR:HG23	2.20	0.41
1:D2:33:LEU:HD12	1:D2:33:LEU:HA	1.85	0.41
1:O2:13:SER:O	1:O2:14:THR:HG23	2.20	0.41
1:N3:13:SER:O	1:N3:14:THR:HG23	2.20	0.41
1:B4:33:LEU:HD12	1:B4:33:LEU:HA	1.85	0.41
1:I4:33:LEU:HD12	1:I4:33:LEU:HA	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K4:33:LEU:HD12	1:K4:33:LEU:HA	1.85	0.41
1:H2:13:SER:O	1:H2:14:THR:HG23	2.20	0.41
1:P2:33:LEU:HD12	1:P2:33:LEU:HA	1.85	0.41
1:G3:13:SER:O	1:G3:14:THR:HG23	2.20	0.41
1:H4:13:SER:O	1:H4:14:THR:HG23	2.20	0.41
1:P4:33:LEU:HD12	1:P4:33:LEU:HA	1.86	0.41
1:O4:13:SER:O	1:O4:14:THR:HG23	2.20	0.41
1:F4:13:SER:O	1:F4:14:THR:HG23	2.20	0.40
1:F2:13:SER:O	1:F2:14:THR:HG23	2.20	0.40
1:M2:13:SER:O	1:M2:14:THR:HG23	2.20	0.40
1:M4:13:SER:O	1:M4:14:THR:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	139/155 (90%)	138 (99%)	1 (1%)	0	100	100
1	A2	139/155 (90%)	138 (99%)	1 (1%)	0	100	100
1	A3	139/155 (90%)	138 (99%)	1 (1%)	0	100	100
1	A4	139/155 (90%)	138 (99%)	1 (1%)	0	100	100
1	B1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	B2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	B3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	B4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	C1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	C2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	C3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	D1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	D2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	D3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	D4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	E1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	E2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	E3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	E4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	F1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	F2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	F3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	F4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	G1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	G2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	G3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	G4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	H1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	H2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	H3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	H4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	I1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	I2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	I3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	I4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	J1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	J2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	J3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	J4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	K1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	K2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	K4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	L1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	L2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	L3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	L4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	M1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	M2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	M3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	M4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	N1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	N2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	N3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	N4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	O1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	O2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	O3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	O4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	P1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	P2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	P3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	P4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	Q1	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	Q2	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	Q3	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	Q4	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
1	R1	12/155 (8%)	11 (92%)	1 (8%)	0	100	100
1	R2	12/155 (8%)	11 (92%)	1 (8%)	0	100	100
1	R3	12/155 (8%)	11 (92%)	1 (8%)	0	100	100
1	R4	12/155 (8%)	11 (92%)	1 (8%)	0	100	100
All	All	10396/11160 (93%)	10196 (98%)	200 (2%)	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	A1	110/122 (90%)	110 (100%)	0	100	100
1	A2	110/122 (90%)	110 (100%)	0	100	100
1	A3	110/122 (90%)	110 (100%)	0	100	100
1	A4	110/122 (90%)	110 (100%)	0	100	100
1	B1	122/122 (100%)	122 (100%)	0	100	100
1	B2	122/122 (100%)	122 (100%)	0	100	100
1	B3	122/122 (100%)	122 (100%)	0	100	100
1	B4	122/122 (100%)	122 (100%)	0	100	100
1	C1	122/122 (100%)	122 (100%)	0	100	100
1	C2	122/122 (100%)	122 (100%)	0	100	100
1	C3	122/122 (100%)	122 (100%)	0	100	100
1	C4	122/122 (100%)	122 (100%)	0	100	100
1	D1	122/122 (100%)	122 (100%)	0	100	100
1	D2	122/122 (100%)	122 (100%)	0	100	100
1	D3	122/122 (100%)	122 (100%)	0	100	100
1	D4	122/122 (100%)	122 (100%)	0	100	100
1	E1	122/122 (100%)	122 (100%)	0	100	100
1	E2	122/122 (100%)	122 (100%)	0	100	100
1	E3	122/122 (100%)	122 (100%)	0	100	100
1	E4	122/122 (100%)	122 (100%)	0	100	100
1	F1	122/122 (100%)	122 (100%)	0	100	100
1	F2	122/122 (100%)	122 (100%)	0	100	100
1	F3	122/122 (100%)	122 (100%)	0	100	100
1	F4	122/122 (100%)	122 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G1	122/122 (100%)	122 (100%)	0	100	100
1	G2	122/122 (100%)	122 (100%)	0	100	100
1	G3	122/122 (100%)	122 (100%)	0	100	100
1	G4	122/122 (100%)	122 (100%)	0	100	100
1	H1	122/122 (100%)	122 (100%)	0	100	100
1	H2	122/122 (100%)	122 (100%)	0	100	100
1	H3	122/122 (100%)	122 (100%)	0	100	100
1	H4	122/122 (100%)	122 (100%)	0	100	100
1	I1	122/122 (100%)	122 (100%)	0	100	100
1	I2	122/122 (100%)	122 (100%)	0	100	100
1	I3	122/122 (100%)	122 (100%)	0	100	100
1	I4	122/122 (100%)	122 (100%)	0	100	100
1	J1	122/122 (100%)	122 (100%)	0	100	100
1	J2	122/122 (100%)	122 (100%)	0	100	100
1	J3	122/122 (100%)	122 (100%)	0	100	100
1	J4	122/122 (100%)	122 (100%)	0	100	100
1	K1	122/122 (100%)	122 (100%)	0	100	100
1	K2	122/122 (100%)	122 (100%)	0	100	100
1	K3	122/122 (100%)	122 (100%)	0	100	100
1	K4	122/122 (100%)	122 (100%)	0	100	100
1	L1	122/122 (100%)	122 (100%)	0	100	100
1	L2	122/122 (100%)	122 (100%)	0	100	100
1	L3	122/122 (100%)	122 (100%)	0	100	100
1	L4	122/122 (100%)	122 (100%)	0	100	100
1	M1	122/122 (100%)	122 (100%)	0	100	100
1	M2	122/122 (100%)	122 (100%)	0	100	100
1	M3	122/122 (100%)	122 (100%)	0	100	100
1	M4	122/122 (100%)	122 (100%)	0	100	100
1	N1	122/122 (100%)	122 (100%)	0	100	100
1	N2	122/122 (100%)	122 (100%)	0	100	100
1	N3	122/122 (100%)	122 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N4	122/122 (100%)	122 (100%)	0	100	100
1	O1	122/122 (100%)	122 (100%)	0	100	100
1	O2	122/122 (100%)	122 (100%)	0	100	100
1	O3	122/122 (100%)	122 (100%)	0	100	100
1	O4	122/122 (100%)	122 (100%)	0	100	100
1	P1	122/122 (100%)	122 (100%)	0	100	100
1	P2	122/122 (100%)	122 (100%)	0	100	100
1	P3	122/122 (100%)	122 (100%)	0	100	100
1	P4	122/122 (100%)	122 (100%)	0	100	100
1	Q1	122/122 (100%)	122 (100%)	0	100	100
1	Q2	122/122 (100%)	122 (100%)	0	100	100
1	Q3	122/122 (100%)	122 (100%)	0	100	100
1	Q4	122/122 (100%)	122 (100%)	0	100	100
1	R1	12/122 (10%)	12 (100%)	0	100	100
1	R2	12/122 (10%)	12 (100%)	0	100	100
1	R3	12/122 (10%)	12 (100%)	0	100	100
1	R4	12/122 (10%)	12 (100%)	0	100	100
All	All	8296/8784 (94%)	8296 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	26	ASN
1	B1	26	ASN
1	C1	26	ASN
1	D1	26	ASN
1	E1	26	ASN
1	F1	26	ASN
1	G1	26	ASN
1	H1	26	ASN
1	I1	26	ASN
1	J1	26	ASN
1	K1	26	ASN
1	L1	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M1	26	ASN
1	N1	26	ASN
1	O1	26	ASN
1	P1	26	ASN
1	Q1	26	ASN
1	A2	26	ASN
1	B2	26	ASN
1	C2	26	ASN
1	D2	26	ASN
1	E2	26	ASN
1	F2	26	ASN
1	G2	26	ASN
1	H2	26	ASN
1	I2	26	ASN
1	J2	26	ASN
1	K2	26	ASN
1	L2	26	ASN
1	M2	26	ASN
1	N2	26	ASN
1	O2	26	ASN
1	P2	26	ASN
1	Q2	26	ASN
1	A3	26	ASN
1	B3	26	ASN
1	C3	26	ASN
1	D3	26	ASN
1	E3	26	ASN
1	F3	26	ASN
1	G3	26	ASN
1	H3	26	ASN
1	I3	26	ASN
1	J3	26	ASN
1	K3	26	ASN
1	L3	26	ASN
1	M3	26	ASN
1	N3	26	ASN
1	O3	26	ASN
1	P3	26	ASN
1	Q3	26	ASN
1	A4	26	ASN
1	B4	26	ASN
1	C4	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D4	26	ASN
1	E4	26	ASN
1	F4	26	ASN
1	G4	26	ASN
1	H4	26	ASN
1	I4	26	ASN
1	J4	26	ASN
1	K4	26	ASN
1	L4	26	ASN
1	M4	26	ASN
1	N4	26	ASN
1	O4	26	ASN
1	P4	26	ASN
1	Q4	26	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

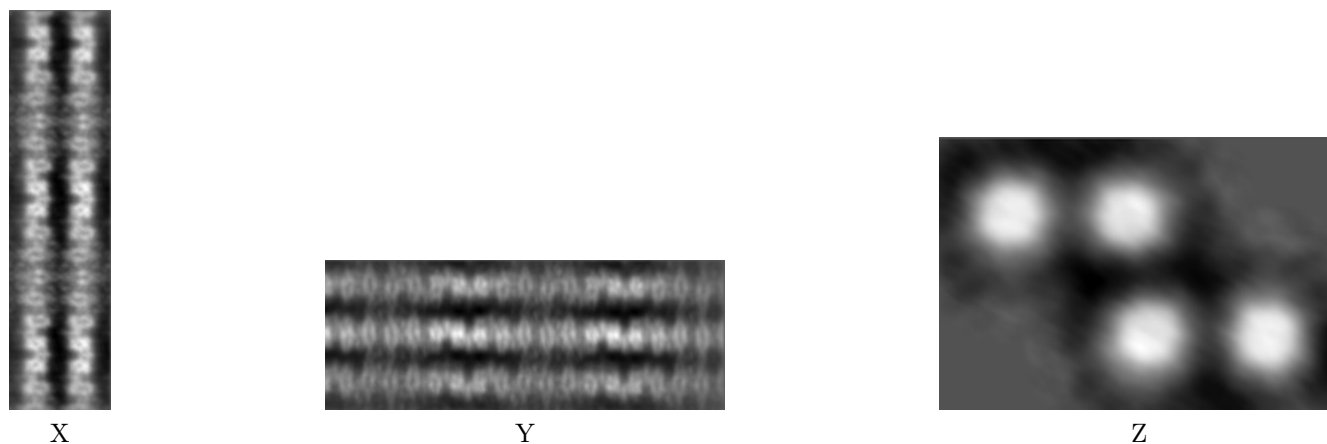
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52602. These allow visual inspection of the internal detail of the map and identification of artifacts.

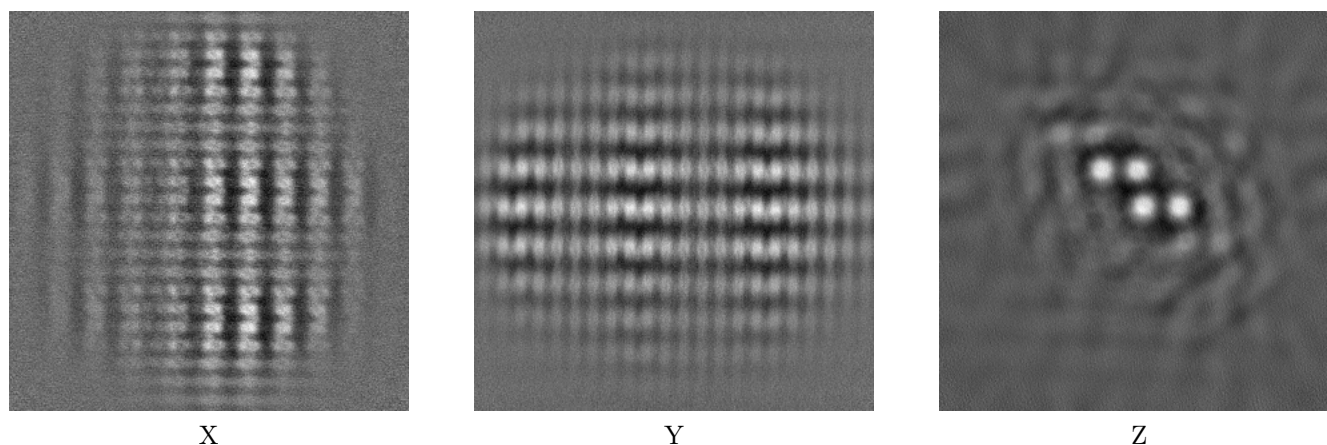
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



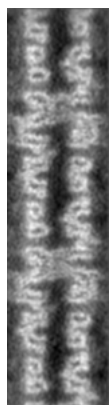
6.1.2 Raw map



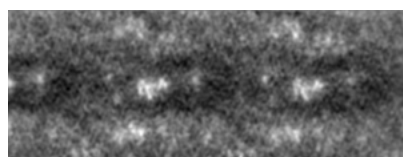
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

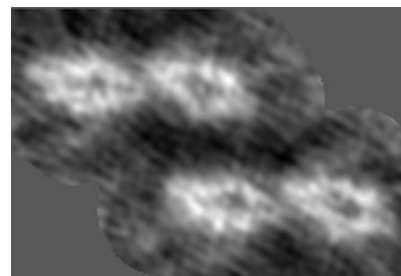
6.2.1 Primary map



X Index:
109

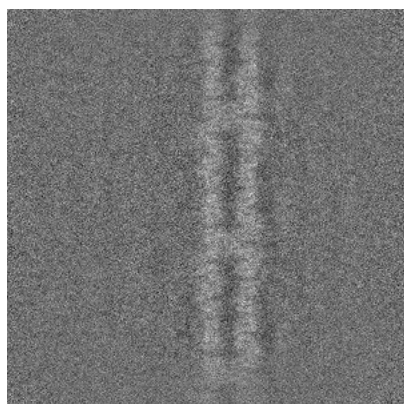


Y Index: 74

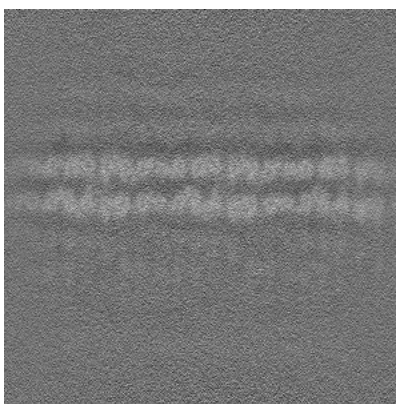


Z Index: 294

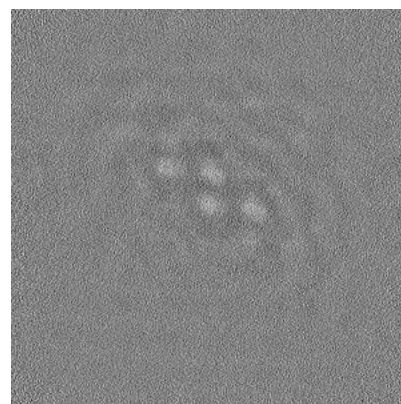
6.2.2 Raw map



X Index: 360



Y Index: 360

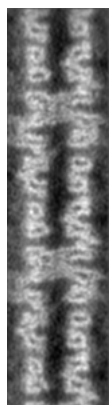


Z Index: 360

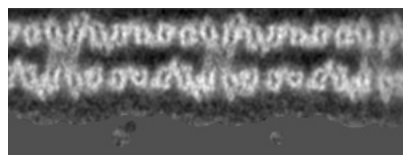
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

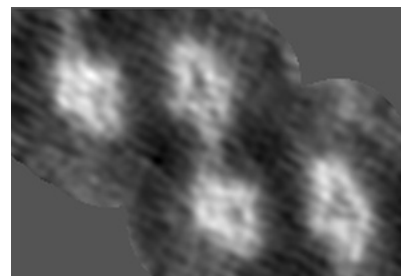
6.3.1 Primary map



X Index:
107

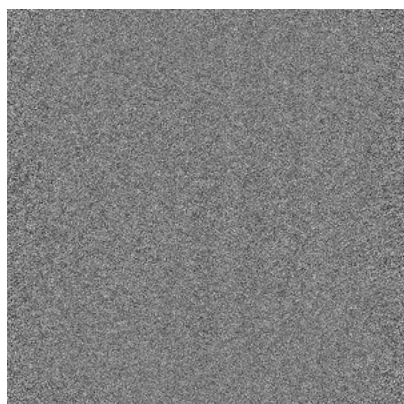


Y Index: 37

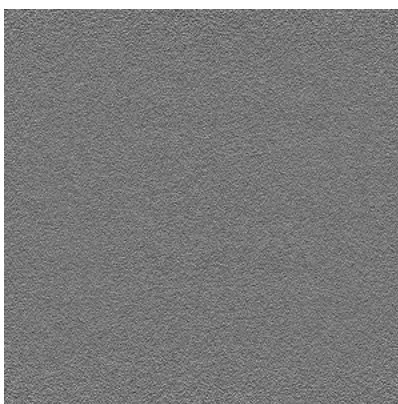


Z Index: 232

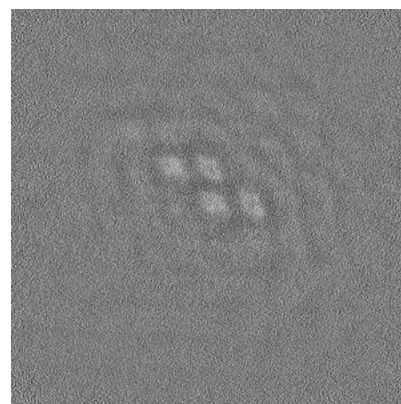
6.3.2 Raw map



X Index: 0



Y Index: 0

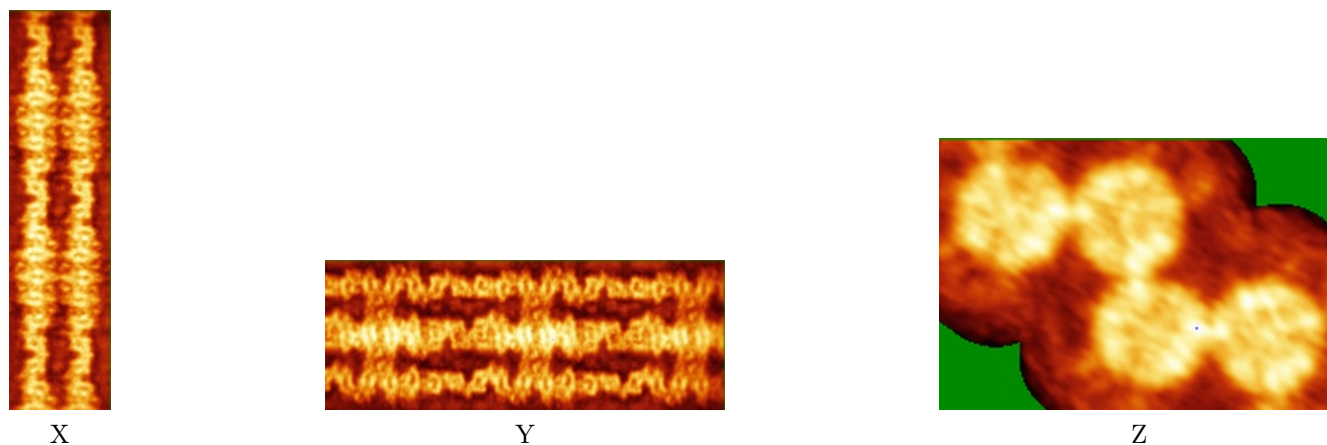


Z Index: 350

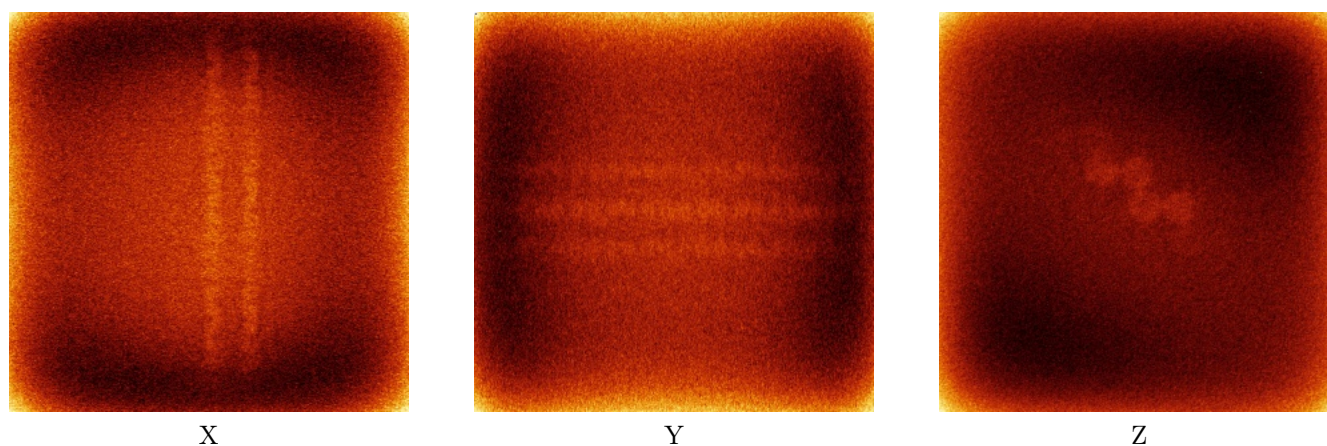
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



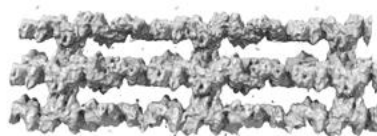
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



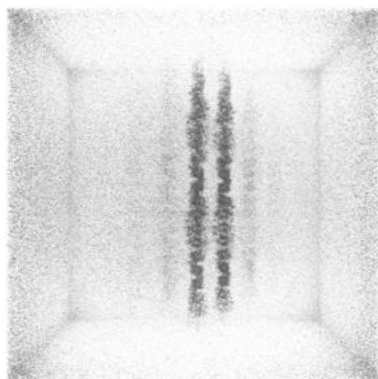
Y



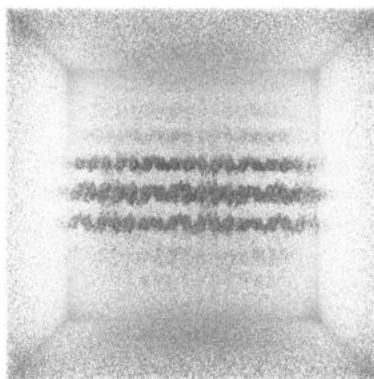
Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

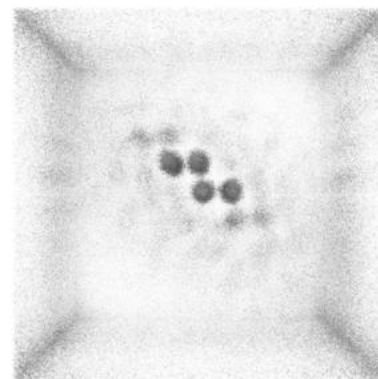
6.5.2 Raw map



X



Y



Z

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

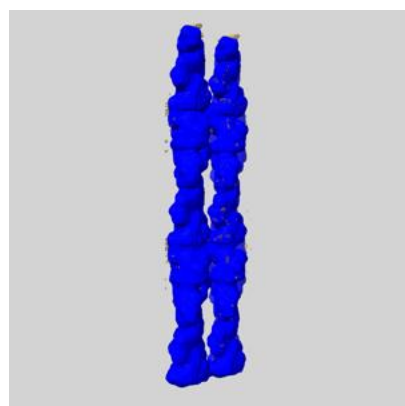
6.6 Mask visualisation [i](#)

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

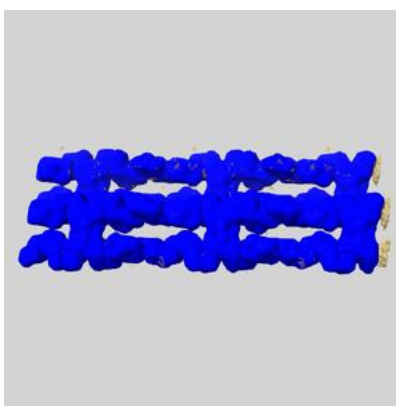
A mask typically either:

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

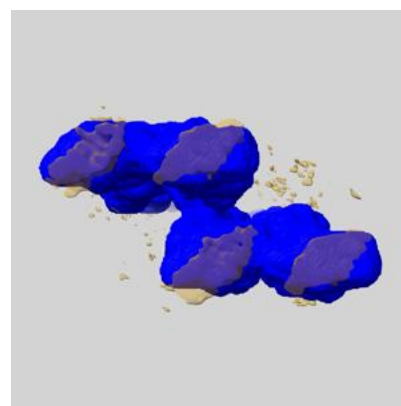
6.6.1 emd_52602_msk_1.map [i](#)



X



Y

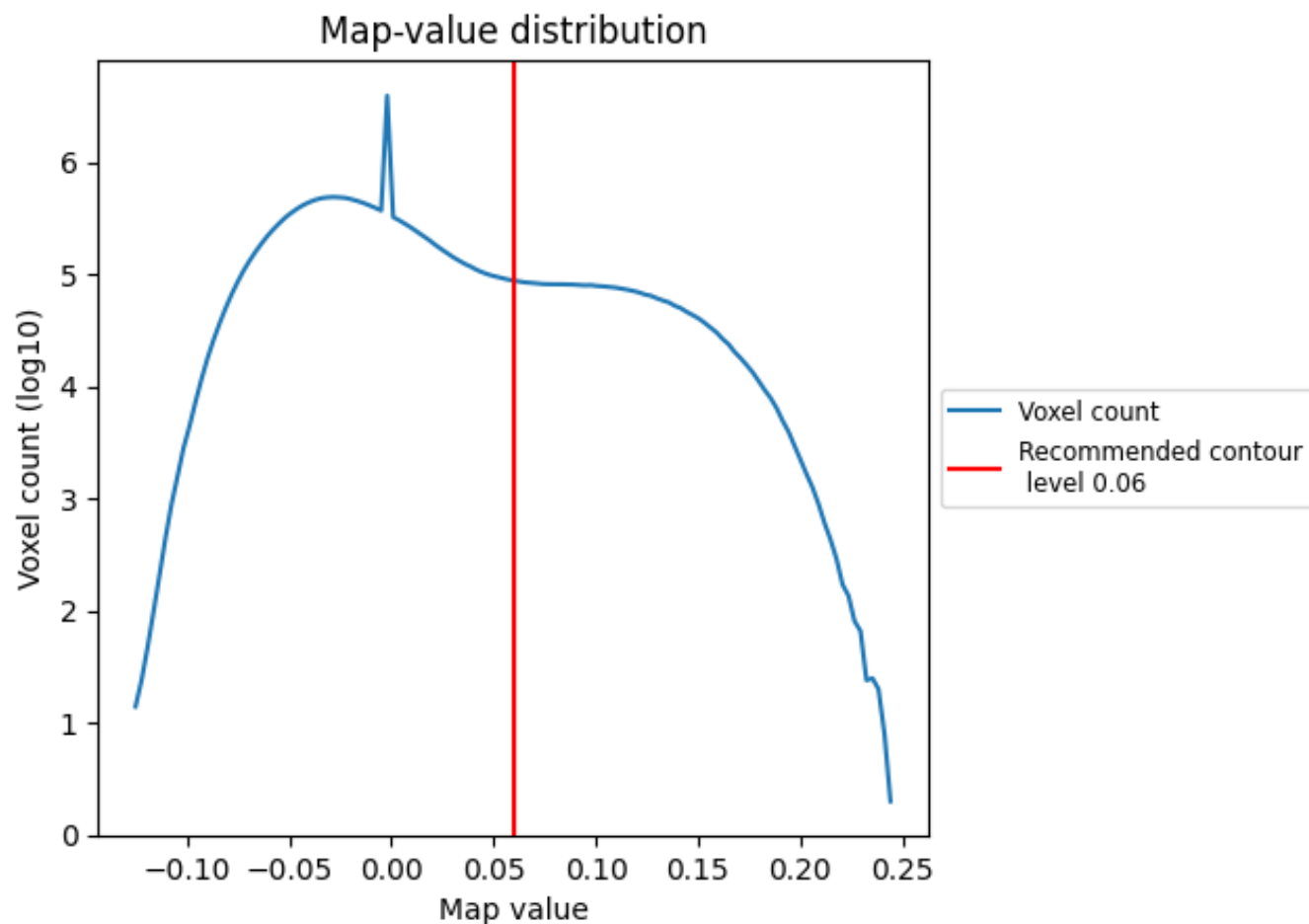


Z

7 Map analysis [i](#)

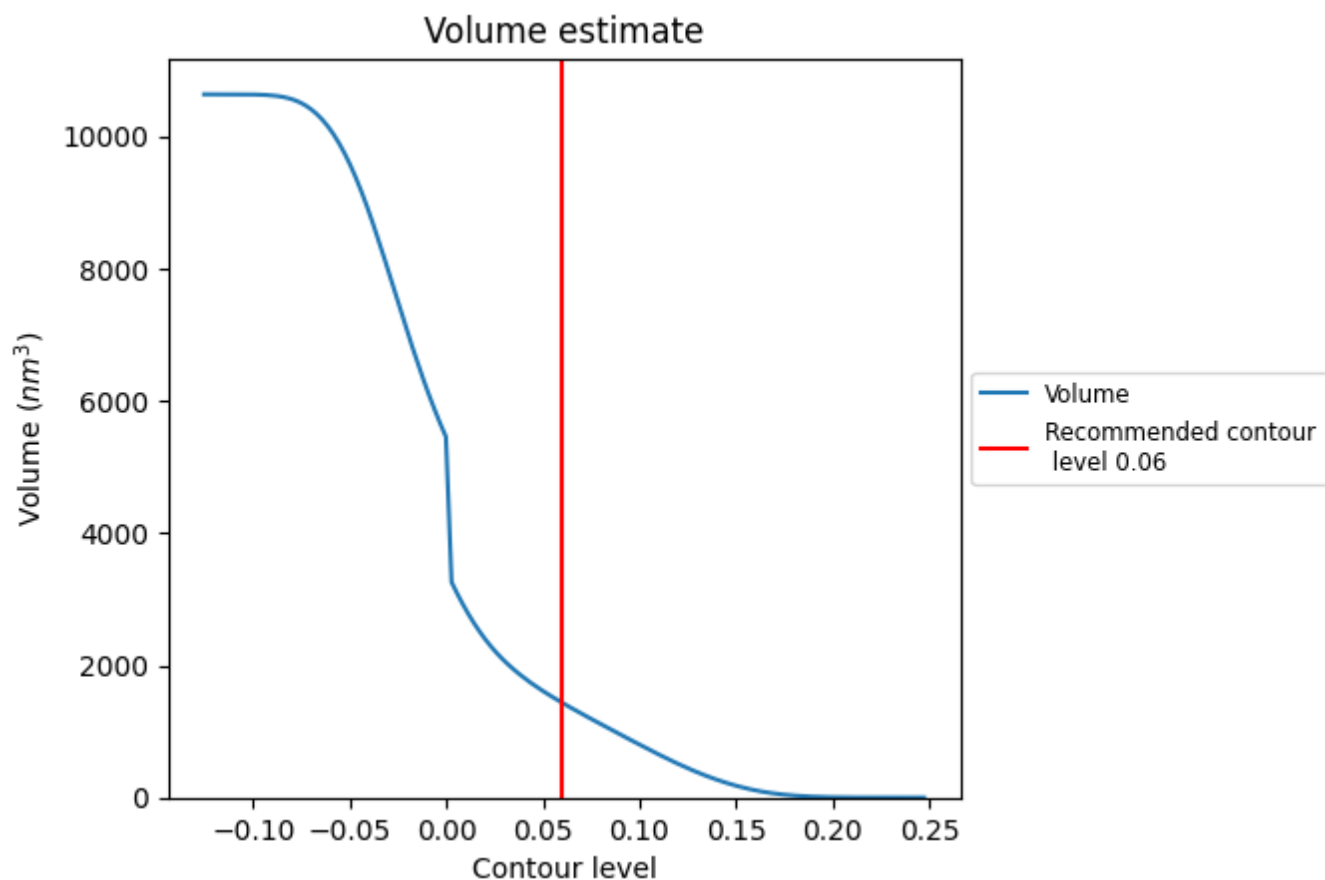
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1434 nm³; this corresponds to an approximate mass of 1295 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

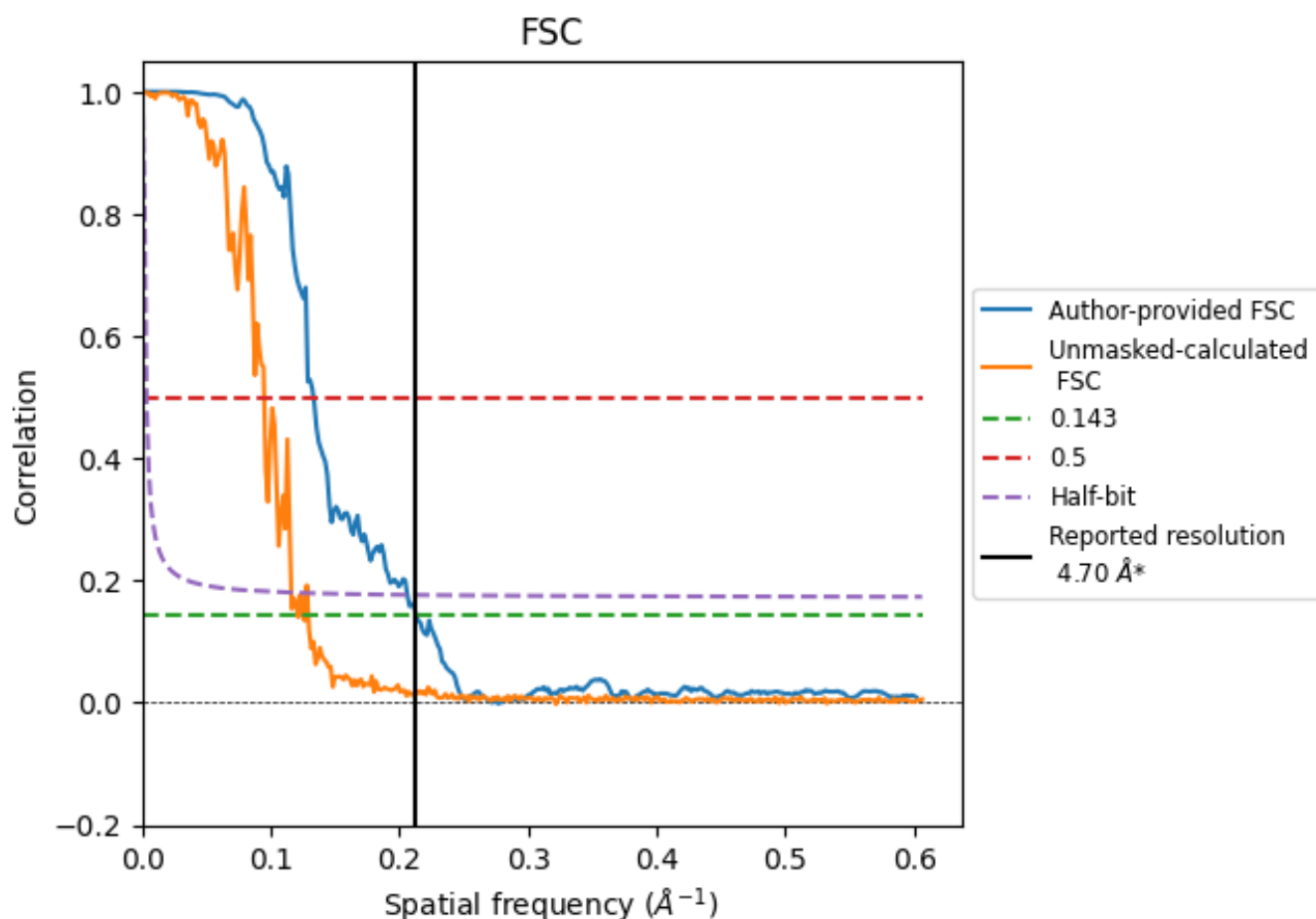
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.213 \AA^{-1}

8.2 Resolution estimates [i](#)

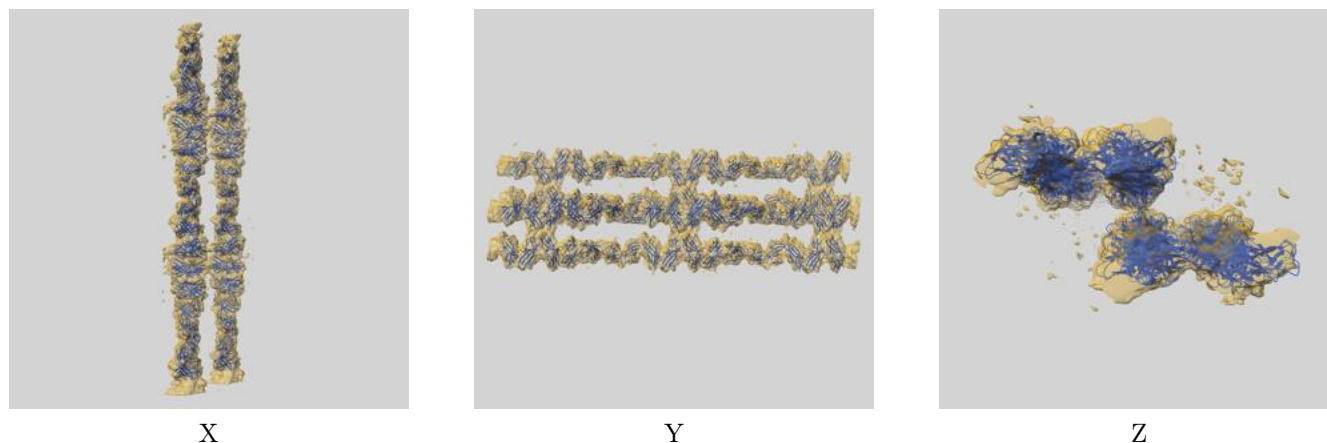
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.70	7.51	4.85
Unmasked-calculated*	8.26	10.55	8.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.26 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

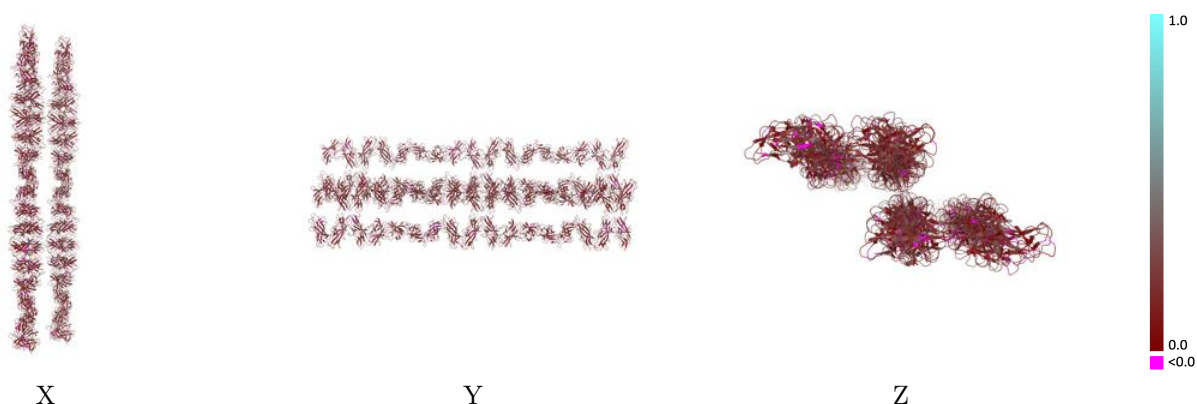
This section contains information regarding the fit between EMDB map EMD-52602 and PDB model 9I3O. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



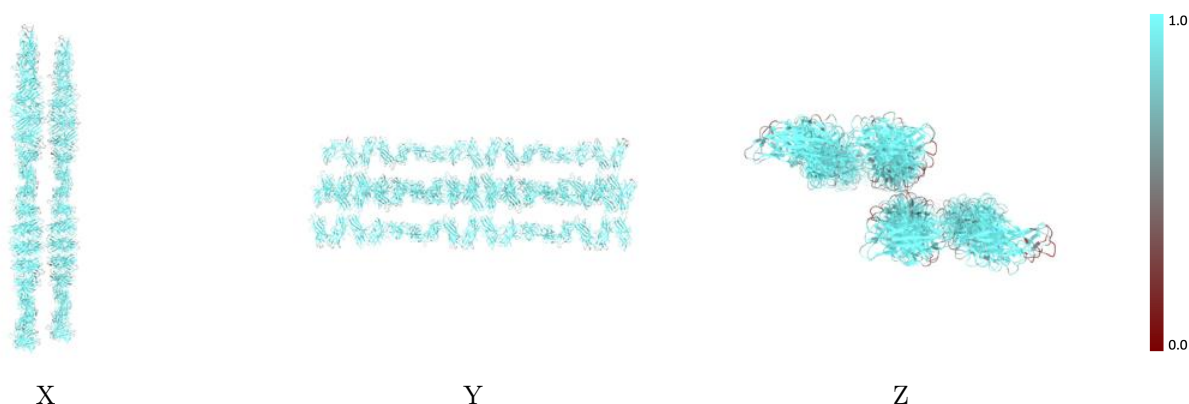
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



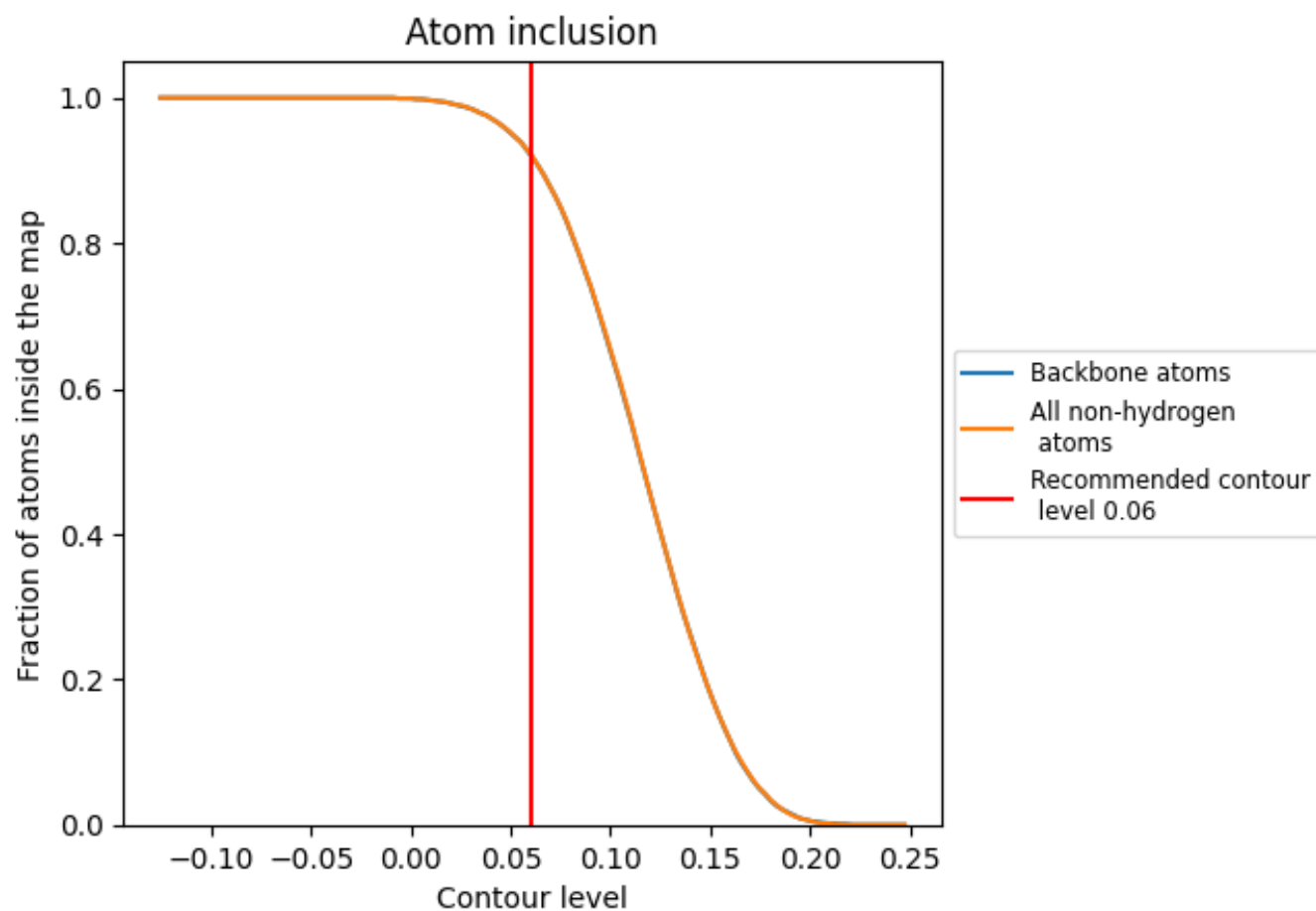
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9220	 0.2050
A1	 0.9130	 0.1860
A2	 0.8890	 0.1920
A3	 0.9300	 0.2020
A4	 0.9180	 0.1850
B1	 0.9050	 0.1820
B2	 0.9170	 0.2050
B3	 0.9040	 0.1890
B4	 0.8910	 0.1780
C1	 0.9000	 0.1980
C2	 0.9420	 0.2250
C3	 0.9110	 0.2150
C4	 0.9140	 0.2000
D1	 0.9250	 0.1920
D2	 0.9180	 0.2110
D3	 0.9140	 0.2220
D4	 0.9170	 0.1970
E1	 0.9210	 0.1910
E2	 0.8990	 0.2220
E3	 0.9170	 0.2150
E4	 0.9310	 0.1990
F1	 0.9300	 0.1990
F2	 0.9260	 0.2360
F3	 0.9030	 0.2180
F4	 0.9620	 0.1910
G1	 0.9410	 0.1990
G2	 0.9230	 0.2360
G3	 0.9250	 0.2120
G4	 0.9690	 0.2090
H1	 0.9590	 0.2150
H2	 0.9190	 0.2190
H3	 0.9540	 0.2210
H4	 0.9270	 0.1780
I1	 0.9330	 0.2090
I2	 0.9240	 0.2320



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
I3	 0.9370	 0.2160
I4	 0.9210	 0.2100
J1	 0.9300	 0.2070
J2	 0.9430	 0.2330
J3	 0.9140	 0.2280
J4	 0.9250	 0.2110
K1	 0.9450	 0.1970
K2	 0.9170	 0.2210
K3	 0.9250	 0.2250
K4	 0.9180	 0.1970
L1	 0.9240	 0.2000
L2	 0.8980	 0.2160
L3	 0.9350	 0.2280
L4	 0.9380	 0.1920
M1	 0.9300	 0.2060
M2	 0.9200	 0.2270
M3	 0.9110	 0.2140
M4	 0.9600	 0.1970
N1	 0.9390	 0.2000
N2	 0.9220	 0.2220
N3	 0.9270	 0.2070
N4	 0.9660	 0.1970
O1	 0.9580	 0.2060
O2	 0.9020	 0.1960
O3	 0.9430	 0.2080
O4	 0.9240	 0.1770
P1	 0.9370	 0.1960
P2	 0.9110	 0.1980
P3	 0.9250	 0.2070
P4	 0.8820	 0.1640
Q1	 0.8910	 0.1830
Q2	 0.8730	 0.1840
Q3	 0.9040	 0.2070
Q4	 0.8490	 0.1730
R1	 0.9600	 0.1590
R2	 0.9300	 0.1460
R3	 0.9600	 0.1440
R4	 0.8200	 0.1260