



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:33 PM UTC

PDB ID : 5W9L / pdb_00005w9l
EMDB ID : EMD-8787
Title : MERS S ectodomain trimer in complex with variable domain of neutralizing antibody G4
Authors : Pallesen, J.; Ward, A.B.
Deposited on : 2017-06-23
Resolution : 4.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

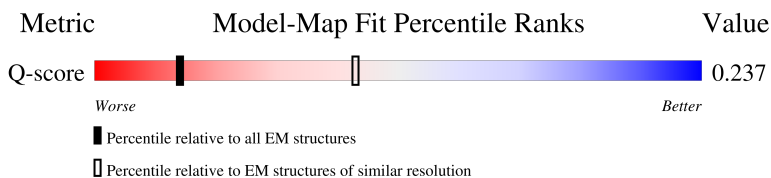
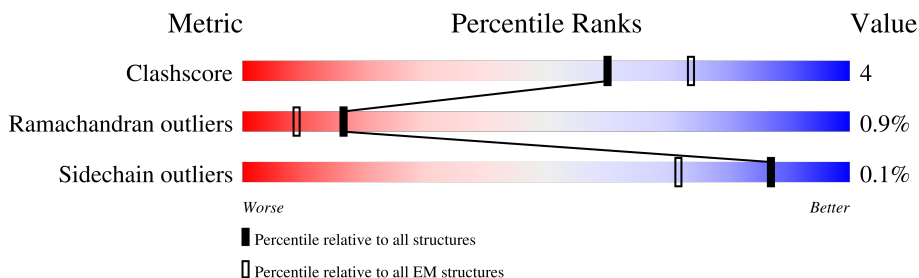
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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	1575 (4.30 - 5.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1329	
1	B	1329	
1	C	1329	
1	D	1329	

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Mol	Chain	Length	Quality of chain
1	G	1329	30% 65%
1	J	1329	14% 47% 7% 45%
2	E	233	47% 49%
2	H	233	48% 49%
3	F	218	6% 46% 5% 49%
3	I	218	6% 47% 49%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31118 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	456	Total	C	N	O	S	0	0
			3488	2210	588	673	17		
1	D	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	G	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	B	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	C	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	J	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		

There are 258 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	506	PHE	LEU	conflict	UNP W5ZZF5
A	748	ALA	ARG	conflict	UNP W5ZZF5
A	751	GLY	ARG	conflict	UNP W5ZZF5
A	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
A	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
A	1292	GLY	-	expression tag	UNP W5ZZF5
A	1293	SER	-	expression tag	UNP W5ZZF5
A	1294	GLY	-	expression tag	UNP W5ZZF5
A	1295	TYR	-	expression tag	UNP W5ZZF5
A	1296	ILE	-	expression tag	UNP W5ZZF5
A	1297	PRO	-	expression tag	UNP W5ZZF5
A	1298	GLU	-	expression tag	UNP W5ZZF5
A	1299	ALA	-	expression tag	UNP W5ZZF5
A	1300	PRO	-	expression tag	UNP W5ZZF5
A	1301	ARG	-	expression tag	UNP W5ZZF5
A	1302	ASP	-	expression tag	UNP W5ZZF5
A	1303	GLY	-	expression tag	UNP W5ZZF5
A	1304	GLN	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1305	ALA	-	expression tag	UNP W5ZZF5
A	1306	TYR	-	expression tag	UNP W5ZZF5
A	1307	VAL	-	expression tag	UNP W5ZZF5
A	1308	ARG	-	expression tag	UNP W5ZZF5
A	1309	LYS	-	expression tag	UNP W5ZZF5
A	1310	ASP	-	expression tag	UNP W5ZZF5
A	1311	GLY	-	expression tag	UNP W5ZZF5
A	1312	GLU	-	expression tag	UNP W5ZZF5
A	1313	TRP	-	expression tag	UNP W5ZZF5
A	1314	VAL	-	expression tag	UNP W5ZZF5
A	1315	LEU	-	expression tag	UNP W5ZZF5
A	1316	LEU	-	expression tag	UNP W5ZZF5
A	1317	SER	-	expression tag	UNP W5ZZF5
A	1318	THR	-	expression tag	UNP W5ZZF5
A	1319	PHE	-	expression tag	UNP W5ZZF5
A	1320	LEU	-	expression tag	UNP W5ZZF5
A	1321	GLY	-	expression tag	UNP W5ZZF5
A	1322	ARG	-	expression tag	UNP W5ZZF5
A	1323	SER	-	expression tag	UNP W5ZZF5
A	1324	LEU	-	expression tag	UNP W5ZZF5
A	1325	GLU	-	expression tag	UNP W5ZZF5
A	1326	VAL	-	expression tag	UNP W5ZZF5
A	1327	LEU	-	expression tag	UNP W5ZZF5
A	1328	PHE	-	expression tag	UNP W5ZZF5
A	1329	GLN	-	expression tag	UNP W5ZZF5
D	506	PHE	LEU	conflict	UNP W5ZZF5
D	748	ALA	ARG	conflict	UNP W5ZZF5
D	751	GLY	ARG	conflict	UNP W5ZZF5
D	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
D	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
D	1292	GLY	-	expression tag	UNP W5ZZF5
D	1293	SER	-	expression tag	UNP W5ZZF5
D	1294	GLY	-	expression tag	UNP W5ZZF5
D	1295	TYR	-	expression tag	UNP W5ZZF5
D	1296	ILE	-	expression tag	UNP W5ZZF5
D	1297	PRO	-	expression tag	UNP W5ZZF5
D	1298	GLU	-	expression tag	UNP W5ZZF5
D	1299	ALA	-	expression tag	UNP W5ZZF5
D	1300	PRO	-	expression tag	UNP W5ZZF5
D	1301	ARG	-	expression tag	UNP W5ZZF5
D	1302	ASP	-	expression tag	UNP W5ZZF5
D	1303	GLY	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1304	GLN	-	expression tag	UNP W5ZZF5
D	1305	ALA	-	expression tag	UNP W5ZZF5
D	1306	TYR	-	expression tag	UNP W5ZZF5
D	1307	VAL	-	expression tag	UNP W5ZZF5
D	1308	ARG	-	expression tag	UNP W5ZZF5
D	1309	LYS	-	expression tag	UNP W5ZZF5
D	1310	ASP	-	expression tag	UNP W5ZZF5
D	1311	GLY	-	expression tag	UNP W5ZZF5
D	1312	GLU	-	expression tag	UNP W5ZZF5
D	1313	TRP	-	expression tag	UNP W5ZZF5
D	1314	VAL	-	expression tag	UNP W5ZZF5
D	1315	LEU	-	expression tag	UNP W5ZZF5
D	1316	LEU	-	expression tag	UNP W5ZZF5
D	1317	SER	-	expression tag	UNP W5ZZF5
D	1318	THR	-	expression tag	UNP W5ZZF5
D	1319	PHE	-	expression tag	UNP W5ZZF5
D	1320	LEU	-	expression tag	UNP W5ZZF5
D	1321	GLY	-	expression tag	UNP W5ZZF5
D	1322	ARG	-	expression tag	UNP W5ZZF5
D	1323	SER	-	expression tag	UNP W5ZZF5
D	1324	LEU	-	expression tag	UNP W5ZZF5
D	1325	GLU	-	expression tag	UNP W5ZZF5
D	1326	VAL	-	expression tag	UNP W5ZZF5
D	1327	LEU	-	expression tag	UNP W5ZZF5
D	1328	PHE	-	expression tag	UNP W5ZZF5
D	1329	GLN	-	expression tag	UNP W5ZZF5
G	506	PHE	LEU	conflict	UNP W5ZZF5
G	748	ALA	ARG	conflict	UNP W5ZZF5
G	751	GLY	ARG	conflict	UNP W5ZZF5
G	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
G	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
G	1292	GLY	-	expression tag	UNP W5ZZF5
G	1293	SER	-	expression tag	UNP W5ZZF5
G	1294	GLY	-	expression tag	UNP W5ZZF5
G	1295	TYR	-	expression tag	UNP W5ZZF5
G	1296	ILE	-	expression tag	UNP W5ZZF5
G	1297	PRO	-	expression tag	UNP W5ZZF5
G	1298	GLU	-	expression tag	UNP W5ZZF5
G	1299	ALA	-	expression tag	UNP W5ZZF5
G	1300	PRO	-	expression tag	UNP W5ZZF5
G	1301	ARG	-	expression tag	UNP W5ZZF5
G	1302	ASP	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1303	GLY	-	expression tag	UNP W5ZZF5
G	1304	GLN	-	expression tag	UNP W5ZZF5
G	1305	ALA	-	expression tag	UNP W5ZZF5
G	1306	TYR	-	expression tag	UNP W5ZZF5
G	1307	VAL	-	expression tag	UNP W5ZZF5
G	1308	ARG	-	expression tag	UNP W5ZZF5
G	1309	LYS	-	expression tag	UNP W5ZZF5
G	1310	ASP	-	expression tag	UNP W5ZZF5
G	1311	GLY	-	expression tag	UNP W5ZZF5
G	1312	GLU	-	expression tag	UNP W5ZZF5
G	1313	TRP	-	expression tag	UNP W5ZZF5
G	1314	VAL	-	expression tag	UNP W5ZZF5
G	1315	LEU	-	expression tag	UNP W5ZZF5
G	1316	LEU	-	expression tag	UNP W5ZZF5
G	1317	SER	-	expression tag	UNP W5ZZF5
G	1318	THR	-	expression tag	UNP W5ZZF5
G	1319	PHE	-	expression tag	UNP W5ZZF5
G	1320	LEU	-	expression tag	UNP W5ZZF5
G	1321	GLY	-	expression tag	UNP W5ZZF5
G	1322	ARG	-	expression tag	UNP W5ZZF5
G	1323	SER	-	expression tag	UNP W5ZZF5
G	1324	LEU	-	expression tag	UNP W5ZZF5
G	1325	GLU	-	expression tag	UNP W5ZZF5
G	1326	VAL	-	expression tag	UNP W5ZZF5
G	1327	LEU	-	expression tag	UNP W5ZZF5
G	1328	PHE	-	expression tag	UNP W5ZZF5
G	1329	GLN	-	expression tag	UNP W5ZZF5
B	506	PHE	LEU	conflict	UNP W5ZZF5
B	748	ALA	ARG	conflict	UNP W5ZZF5
B	751	GLY	ARG	conflict	UNP W5ZZF5
B	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
B	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
B	1292	GLY	-	expression tag	UNP W5ZZF5
B	1293	SER	-	expression tag	UNP W5ZZF5
B	1294	GLY	-	expression tag	UNP W5ZZF5
B	1295	TYR	-	expression tag	UNP W5ZZF5
B	1296	ILE	-	expression tag	UNP W5ZZF5
B	1297	PRO	-	expression tag	UNP W5ZZF5
B	1298	GLU	-	expression tag	UNP W5ZZF5
B	1299	ALA	-	expression tag	UNP W5ZZF5
B	1300	PRO	-	expression tag	UNP W5ZZF5
B	1301	ARG	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1302	ASP	-	expression tag	UNP W5ZZF5
B	1303	GLY	-	expression tag	UNP W5ZZF5
B	1304	GLN	-	expression tag	UNP W5ZZF5
B	1305	ALA	-	expression tag	UNP W5ZZF5
B	1306	TYR	-	expression tag	UNP W5ZZF5
B	1307	VAL	-	expression tag	UNP W5ZZF5
B	1308	ARG	-	expression tag	UNP W5ZZF5
B	1309	LYS	-	expression tag	UNP W5ZZF5
B	1310	ASP	-	expression tag	UNP W5ZZF5
B	1311	GLY	-	expression tag	UNP W5ZZF5
B	1312	GLU	-	expression tag	UNP W5ZZF5
B	1313	TRP	-	expression tag	UNP W5ZZF5
B	1314	VAL	-	expression tag	UNP W5ZZF5
B	1315	LEU	-	expression tag	UNP W5ZZF5
B	1316	LEU	-	expression tag	UNP W5ZZF5
B	1317	SER	-	expression tag	UNP W5ZZF5
B	1318	THR	-	expression tag	UNP W5ZZF5
B	1319	PHE	-	expression tag	UNP W5ZZF5
B	1320	LEU	-	expression tag	UNP W5ZZF5
B	1321	GLY	-	expression tag	UNP W5ZZF5
B	1322	ARG	-	expression tag	UNP W5ZZF5
B	1323	SER	-	expression tag	UNP W5ZZF5
B	1324	LEU	-	expression tag	UNP W5ZZF5
B	1325	GLU	-	expression tag	UNP W5ZZF5
B	1326	VAL	-	expression tag	UNP W5ZZF5
B	1327	LEU	-	expression tag	UNP W5ZZF5
B	1328	PHE	-	expression tag	UNP W5ZZF5
B	1329	GLN	-	expression tag	UNP W5ZZF5
C	506	PHE	LEU	conflict	UNP W5ZZF5
C	748	ALA	ARG	conflict	UNP W5ZZF5
C	751	GLY	ARG	conflict	UNP W5ZZF5
C	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
C	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
C	1292	GLY	-	expression tag	UNP W5ZZF5
C	1293	SER	-	expression tag	UNP W5ZZF5
C	1294	GLY	-	expression tag	UNP W5ZZF5
C	1295	TYR	-	expression tag	UNP W5ZZF5
C	1296	ILE	-	expression tag	UNP W5ZZF5
C	1297	PRO	-	expression tag	UNP W5ZZF5
C	1298	GLU	-	expression tag	UNP W5ZZF5
C	1299	ALA	-	expression tag	UNP W5ZZF5
C	1300	PRO	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1301	ARG	-	expression tag	UNP W5ZZF5
C	1302	ASP	-	expression tag	UNP W5ZZF5
C	1303	GLY	-	expression tag	UNP W5ZZF5
C	1304	GLN	-	expression tag	UNP W5ZZF5
C	1305	ALA	-	expression tag	UNP W5ZZF5
C	1306	TYR	-	expression tag	UNP W5ZZF5
C	1307	VAL	-	expression tag	UNP W5ZZF5
C	1308	ARG	-	expression tag	UNP W5ZZF5
C	1309	LYS	-	expression tag	UNP W5ZZF5
C	1310	ASP	-	expression tag	UNP W5ZZF5
C	1311	GLY	-	expression tag	UNP W5ZZF5
C	1312	GLU	-	expression tag	UNP W5ZZF5
C	1313	TRP	-	expression tag	UNP W5ZZF5
C	1314	VAL	-	expression tag	UNP W5ZZF5
C	1315	LEU	-	expression tag	UNP W5ZZF5
C	1316	LEU	-	expression tag	UNP W5ZZF5
C	1317	SER	-	expression tag	UNP W5ZZF5
C	1318	THR	-	expression tag	UNP W5ZZF5
C	1319	PHE	-	expression tag	UNP W5ZZF5
C	1320	LEU	-	expression tag	UNP W5ZZF5
C	1321	GLY	-	expression tag	UNP W5ZZF5
C	1322	ARG	-	expression tag	UNP W5ZZF5
C	1323	SER	-	expression tag	UNP W5ZZF5
C	1324	LEU	-	expression tag	UNP W5ZZF5
C	1325	GLU	-	expression tag	UNP W5ZZF5
C	1326	VAL	-	expression tag	UNP W5ZZF5
C	1327	LEU	-	expression tag	UNP W5ZZF5
C	1328	PHE	-	expression tag	UNP W5ZZF5
C	1329	GLN	-	expression tag	UNP W5ZZF5
J	506	PHE	LEU	conflict	UNP W5ZZF5
J	748	ALA	ARG	conflict	UNP W5ZZF5
J	751	GLY	ARG	conflict	UNP W5ZZF5
J	1060	PRO	VAL	engineered mutation	UNP W5ZZF5
J	1061	PRO	LEU	engineered mutation	UNP W5ZZF5
J	1292	GLY	-	expression tag	UNP W5ZZF5
J	1293	SER	-	expression tag	UNP W5ZZF5
J	1294	GLY	-	expression tag	UNP W5ZZF5
J	1295	TYR	-	expression tag	UNP W5ZZF5
J	1296	ILE	-	expression tag	UNP W5ZZF5
J	1297	PRO	-	expression tag	UNP W5ZZF5
J	1298	GLU	-	expression tag	UNP W5ZZF5
J	1299	ALA	-	expression tag	UNP W5ZZF5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5
J	1302	ASP	-	expression tag	UNP W5ZZF5
J	1303	GLY	-	expression tag	UNP W5ZZF5
J	1304	GLN	-	expression tag	UNP W5ZZF5
J	1305	ALA	-	expression tag	UNP W5ZZF5
J	1306	TYR	-	expression tag	UNP W5ZZF5
J	1307	VAL	-	expression tag	UNP W5ZZF5
J	1308	ARG	-	expression tag	UNP W5ZZF5
J	1309	LYS	-	expression tag	UNP W5ZZF5
J	1310	ASP	-	expression tag	UNP W5ZZF5
J	1311	GLY	-	expression tag	UNP W5ZZF5
J	1312	GLU	-	expression tag	UNP W5ZZF5
J	1313	TRP	-	expression tag	UNP W5ZZF5
J	1314	VAL	-	expression tag	UNP W5ZZF5
J	1315	LEU	-	expression tag	UNP W5ZZF5
J	1316	LEU	-	expression tag	UNP W5ZZF5
J	1317	SER	-	expression tag	UNP W5ZZF5
J	1318	THR	-	expression tag	UNP W5ZZF5
J	1319	PHE	-	expression tag	UNP W5ZZF5
J	1320	LEU	-	expression tag	UNP W5ZZF5
J	1321	GLY	-	expression tag	UNP W5ZZF5
J	1322	ARG	-	expression tag	UNP W5ZZF5
J	1323	SER	-	expression tag	UNP W5ZZF5
J	1324	LEU	-	expression tag	UNP W5ZZF5
J	1325	GLU	-	expression tag	UNP W5ZZF5
J	1326	VAL	-	expression tag	UNP W5ZZF5
J	1327	LEU	-	expression tag	UNP W5ZZF5
J	1328	PHE	-	expression tag	UNP W5ZZF5
J	1329	GLN	-	expression tag	UNP W5ZZF5

- Molecule 2 is a protein called G4 VH.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	H	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

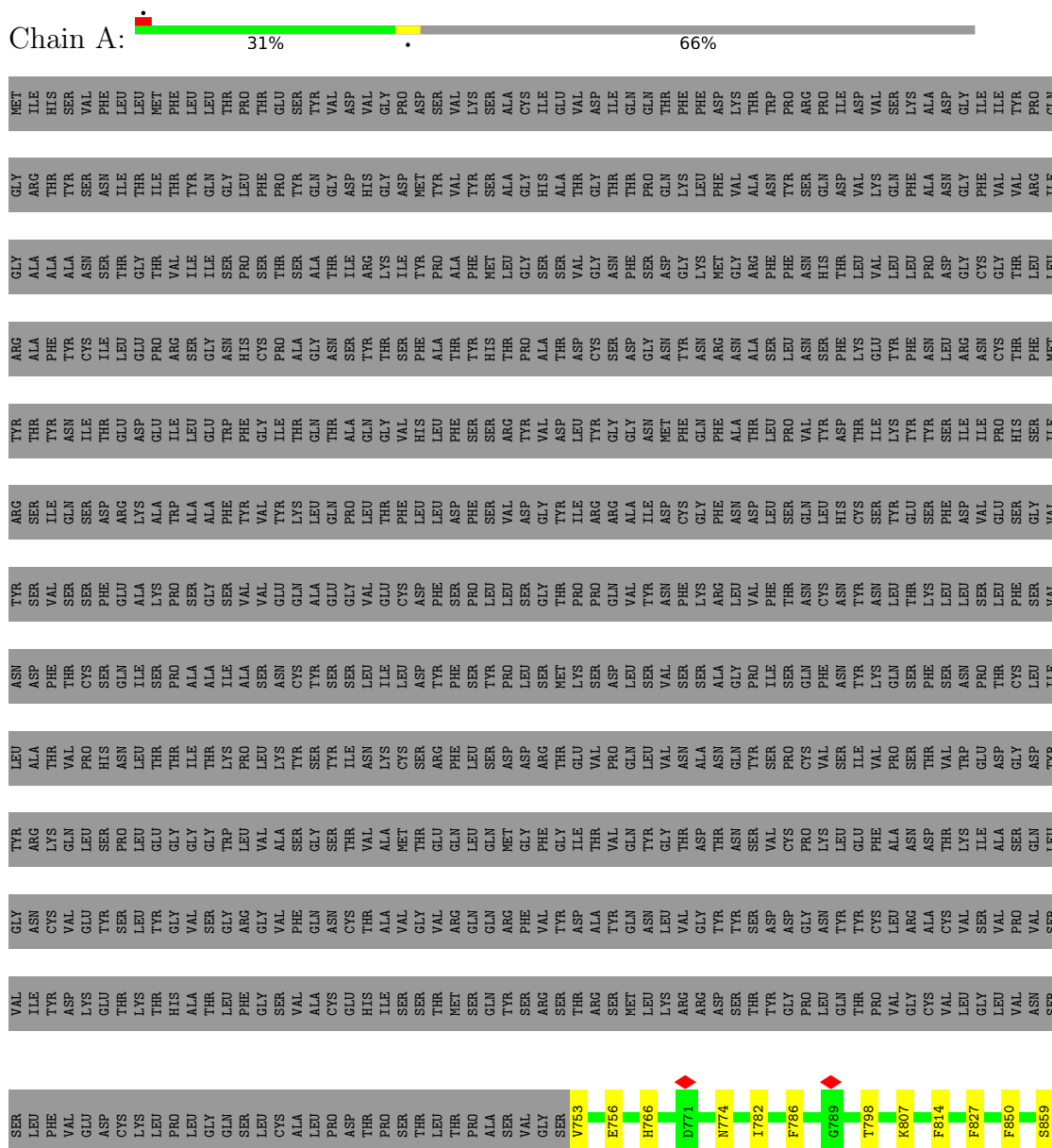
- Molecule 3 is a protein called G4 VL.

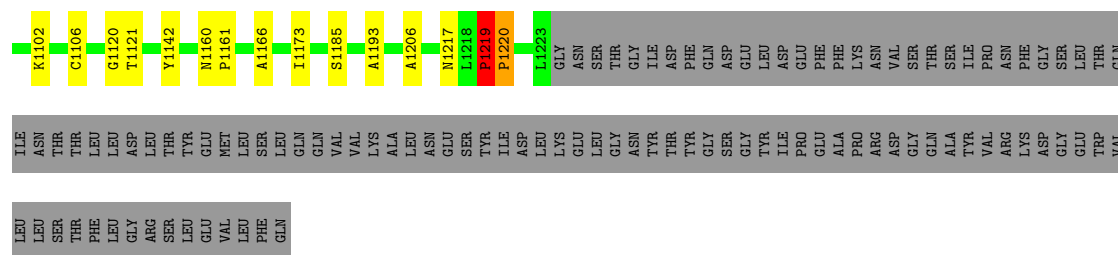
Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	I	111	Total 835	C 522	N 143	O 166	S 4	0	0

3 Residue-property plots

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

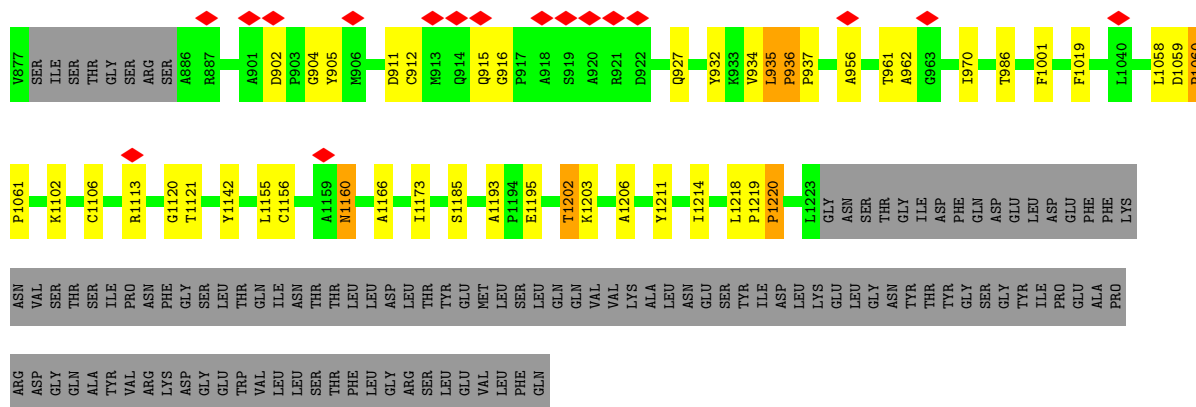
• Molecule 1: Spike glycoprotein



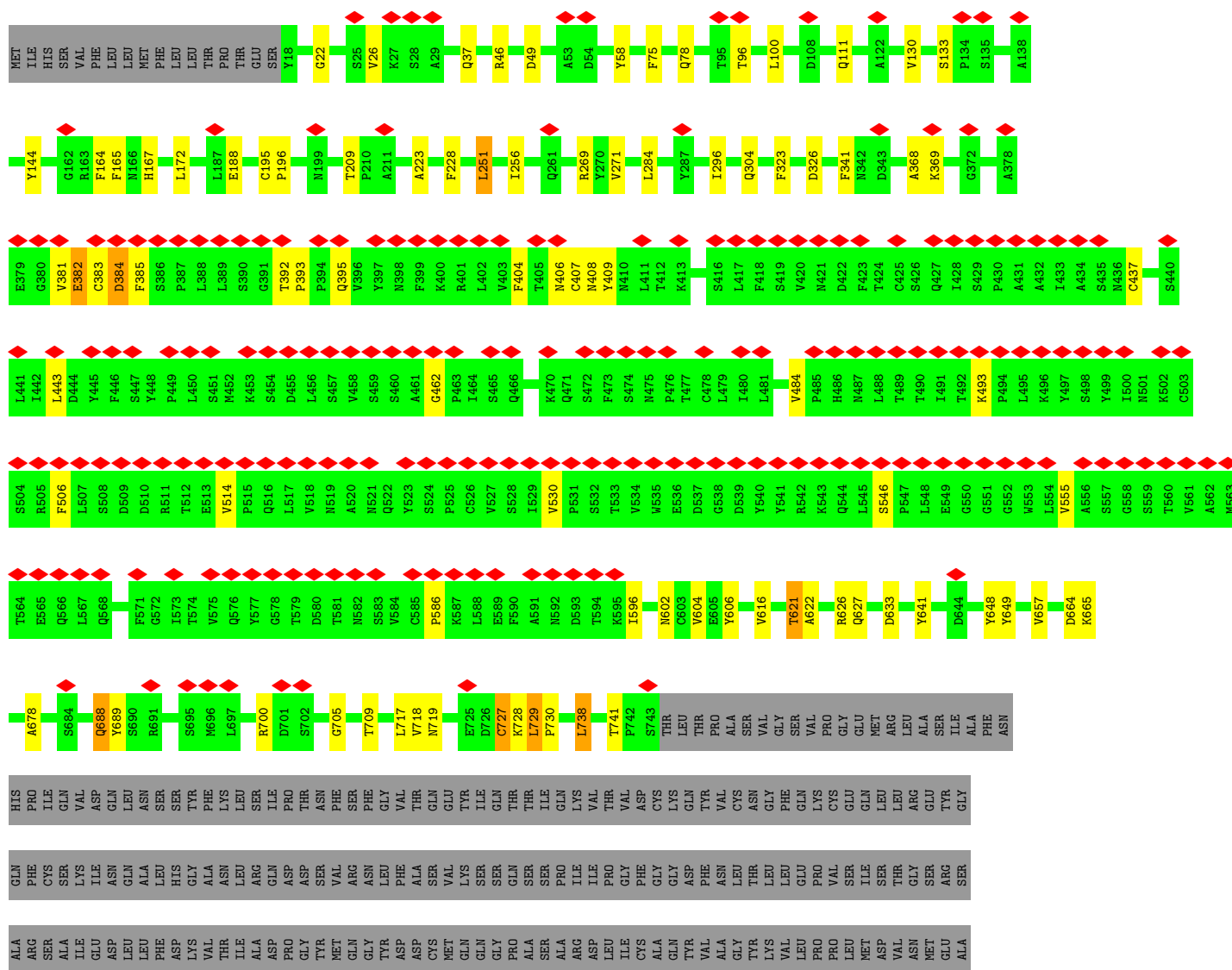


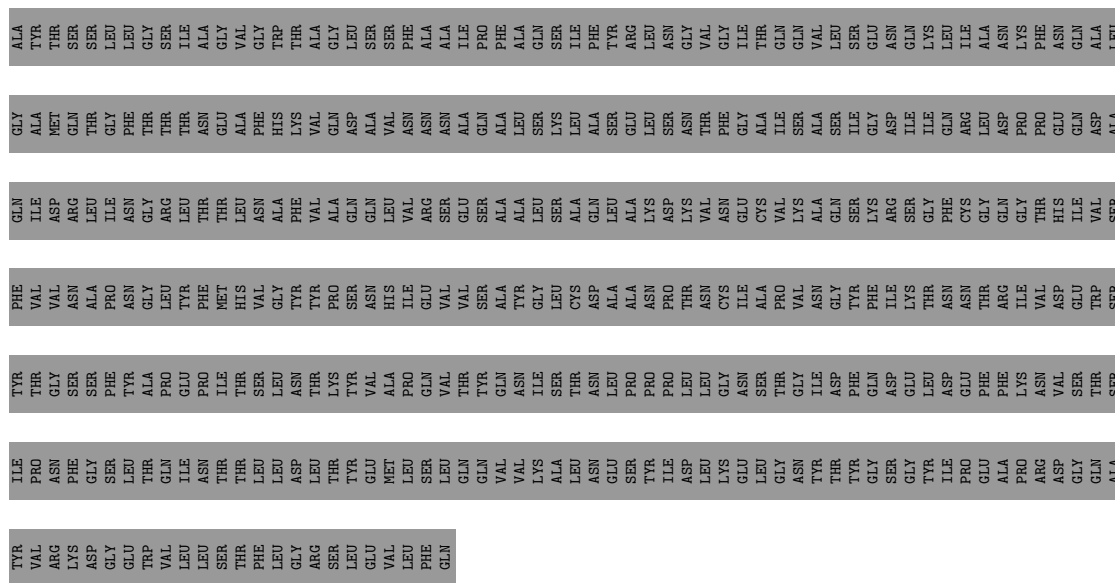
Chain G: 30% 65%



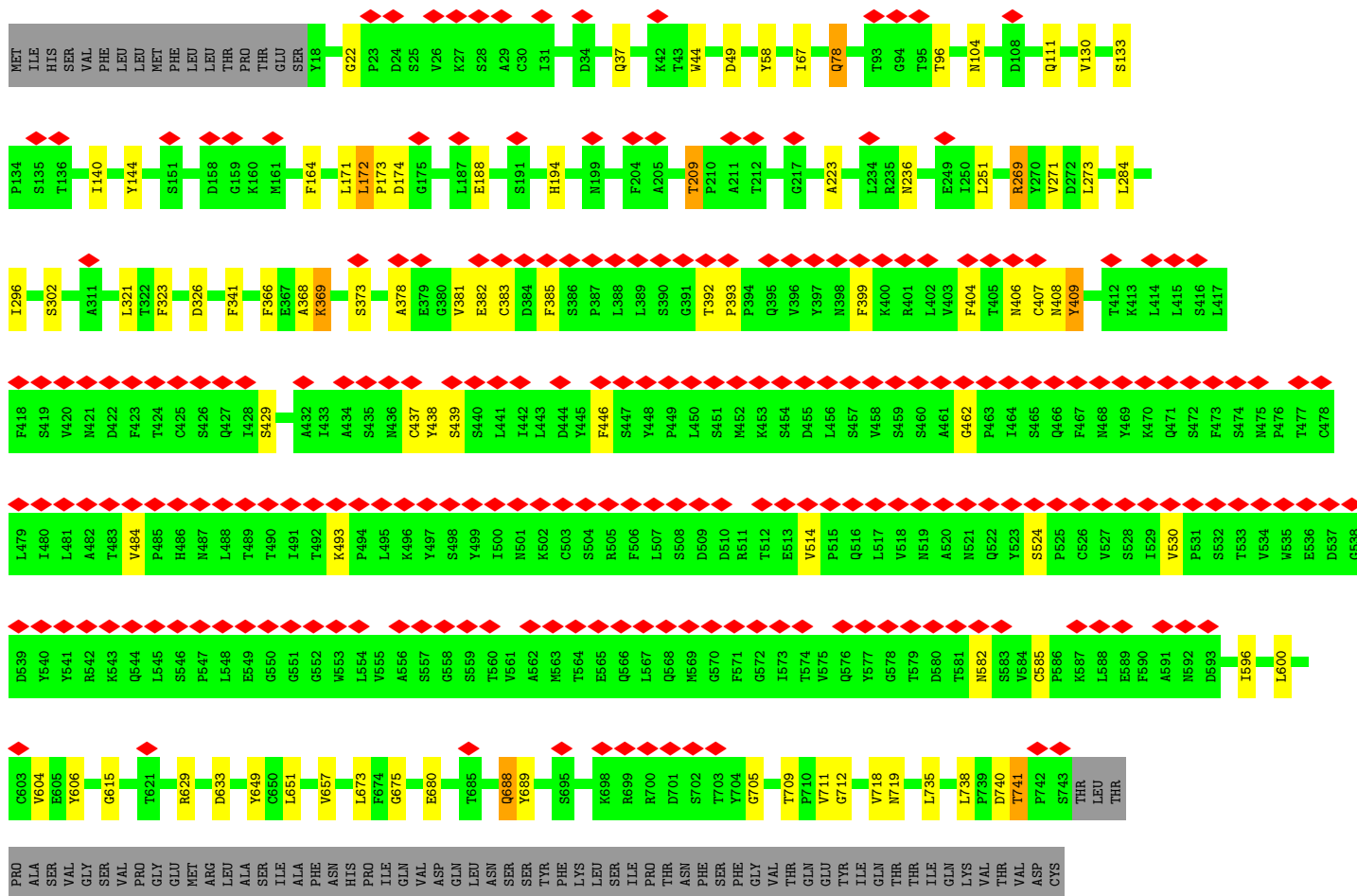


• Molecule 1: Spike glycoprotein



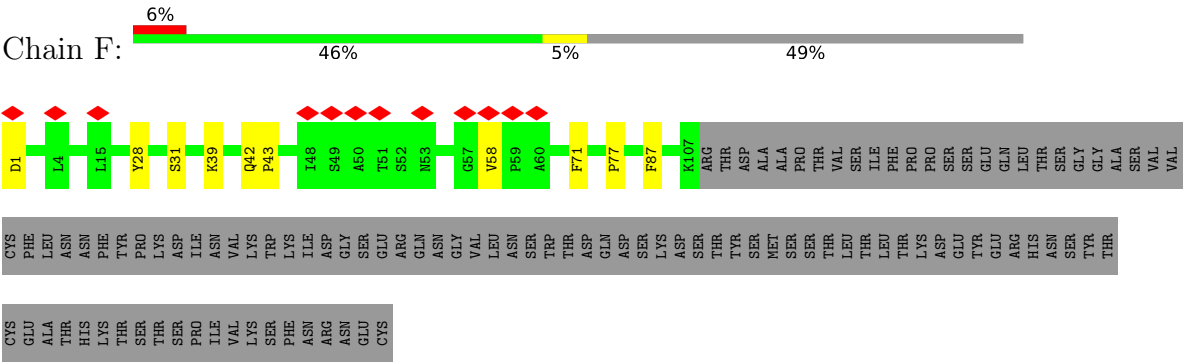


- Molecule 1: Spike glycoprotein

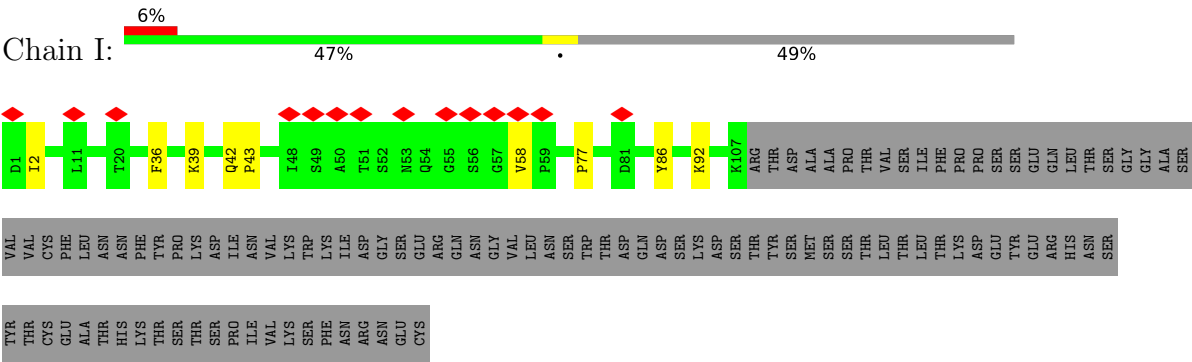




● Molecule 3: G4 VL



● Molecule 3: G4 VL



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	8496	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.89	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	310.08, 310.08, 310.08	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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	A	0.92	0/3560	1.18	40/4840 (0.8%)
1	B	0.84	2/5803 (0.0%)	1.34	79/7901 (1.0%)
1	C	0.85	2/5803 (0.0%)	1.38	84/7901 (1.1%)
1	D	0.91	0/3618	1.20	35/4921 (0.7%)
1	G	0.91	0/3618	1.23	46/4921 (0.9%)
1	J	0.86	3/5803 (0.1%)	1.41	89/7901 (1.1%)
2	E	0.83	0/972	1.09	6/1317 (0.5%)
2	H	0.79	0/972	1.12	4/1317 (0.3%)
3	F	0.85	0/852	1.32	11/1153 (1.0%)
3	I	0.84	0/852	1.28	10/1153 (0.9%)
All	All	0.87	7/31853 (0.0%)	1.30	404/43325 (0.9%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	585	CYS	N-CA	-9.62	1.37	1.46
1	J	584	VAL	CA-C	-8.07	1.42	1.52
1	B	437	CYS	CA-C	7.42	1.62	1.52
1	J	437	CYS	C-O	6.71	1.31	1.23
1	C	437	CYS	C-N	5.66	1.40	1.33
1	B	437	CYS	C-N	-5.66	1.26	1.33
1	C	369	LYS	N-CA	5.29	1.50	1.46

All (404) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	935	LEU	CA-C-N	10.83	127.46	119.66
1	D	935	LEU	C-N-CA	10.83	127.46	119.66
3	F	42	GLN	CA-C-N	10.46	127.19	119.66
3	F	42	GLN	C-N-CA	10.46	127.19	119.66
1	A	935	LEU	CA-C-N	10.39	127.14	119.66
1	A	935	LEU	C-N-CA	10.39	127.14	119.66
2	E	8	GLY	CA-C-N	10.01	129.96	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	8	GLY	C-N-CA	10.01	129.96	119.85
1	J	437	CYS	O-C-N	-9.88	111.63	123.19
2	H	8	GLY	CA-C-N	9.79	129.73	119.85
2	H	8	GLY	C-N-CA	9.79	129.73	119.85
1	B	144	TYR	CA-C-N	9.64	129.59	119.85
1	B	144	TYR	C-N-CA	9.64	129.59	119.85
1	C	284	LEU	CA-C-N	9.51	129.16	119.56
1	C	284	LEU	C-N-CA	9.51	129.16	119.56
1	D	902	ASP	CA-C-N	9.25	129.19	120.03
1	D	902	ASP	C-N-CA	9.25	129.19	120.03
1	J	741	THR	CA-C-N	9.14	129.08	120.03
1	J	741	THR	C-N-CA	9.14	129.08	120.03
1	J	144	TYR	CA-C-N	9.13	129.08	119.85
1	J	144	TYR	C-N-CA	9.13	129.08	119.85
1	B	738	LEU	CA-C-N	9.12	129.06	120.03
1	B	738	LEU	C-N-CA	9.12	129.06	120.03
1	C	373	SER	N-CA-C	9.12	122.75	110.35
1	G	935	LEU	CA-C-N	9.02	126.16	119.66
1	G	935	LEU	C-N-CA	9.02	126.16	119.66
1	J	530	VAL	CA-C-N	9.02	129.07	119.78
1	J	530	VAL	C-N-CA	9.02	129.07	119.78
1	J	392	THR	CA-C-N	8.97	126.21	119.66
1	J	392	THR	C-N-CA	8.97	126.21	119.66
1	C	393	PRO	CA-C-N	8.93	128.87	120.03
1	C	393	PRO	C-N-CA	8.93	128.87	120.03
1	B	462	GLY	CA-C-N	8.93	128.67	119.56
1	B	462	GLY	C-N-CA	8.93	128.67	119.56
1	J	284	LEU	CA-C-N	8.86	129.08	119.87
1	J	284	LEU	C-N-CA	8.86	129.08	119.87
1	C	144	TYR	CA-C-N	8.75	128.69	119.85
1	C	144	TYR	C-N-CA	8.75	128.69	119.85
3	I	58	VAL	N-CA-C	8.74	118.94	108.45
1	J	393	PRO	CA-C-N	8.71	128.65	119.85
1	J	393	PRO	C-N-CA	8.71	128.65	119.85
1	B	209	THR	CA-C-N	8.71	128.44	119.56
1	B	209	THR	C-N-CA	8.71	128.44	119.56
1	J	738	LEU	CA-C-N	8.69	128.83	120.31
1	J	738	LEU	C-N-CA	8.69	128.83	120.31
1	B	393	PRO	CA-C-N	8.67	128.61	119.85
1	B	393	PRO	C-N-CA	8.67	128.61	119.85
1	C	741	THR	CA-C-N	8.66	128.70	119.78
1	C	741	THR	C-N-CA	8.66	128.70	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	902	ASP	CA-C-N	8.63	128.57	120.03
1	G	902	ASP	C-N-CA	8.63	128.57	120.03
1	G	1193	ALA	CA-C-N	8.61	128.65	119.78
1	G	1193	ALA	C-N-CA	8.61	128.65	119.78
1	G	1218	LEU	CA-C-N	8.57	129.20	120.38
1	G	1218	LEU	C-N-CA	8.57	129.20	120.38
3	I	58	VAL	CA-C-N	8.56	128.70	120.31
3	I	58	VAL	C-N-CA	8.56	128.70	120.31
1	J	209	THR	CA-C-N	8.47	128.20	119.56
1	J	209	THR	C-N-CA	8.47	128.20	119.56
1	J	493	LYS	CA-C-N	8.43	128.36	119.85
1	J	493	LYS	C-N-CA	8.43	128.36	119.85
1	C	96	THR	CA-C-N	8.42	128.45	119.78
1	C	96	THR	C-N-CA	8.42	128.45	119.78
1	A	766	HIS	CA-C-N	8.38	128.33	120.03
1	A	766	HIS	C-N-CA	8.38	128.33	120.03
1	G	1160	ASN	CA-C-N	8.38	130.31	119.84
1	G	1160	ASN	C-N-CA	8.38	130.31	119.84
1	A	1160	ASN	CA-C-N	8.36	130.29	119.84
1	A	1160	ASN	C-N-CA	8.36	130.29	119.84
3	F	58	VAL	CA-C-N	8.36	128.80	120.52
3	F	58	VAL	C-N-CA	8.36	128.80	120.52
1	B	741	THR	CA-C-N	8.36	128.39	119.78
1	B	741	THR	C-N-CA	8.36	128.39	119.78
1	J	484	VAL	CA-C-N	8.35	128.38	119.78
1	J	484	VAL	C-N-CA	8.35	128.38	119.78
1	C	209	THR	CA-C-N	8.32	128.04	119.56
1	C	209	THR	C-N-CA	8.32	128.04	119.56
1	D	766	HIS	CA-C-N	8.24	128.26	119.78
1	D	766	HIS	C-N-CA	8.24	128.26	119.78
1	J	22	GLY	CA-C-N	8.20	128.22	119.78
1	J	22	GLY	C-N-CA	8.20	128.22	119.78
1	D	1160	ASN	CA-C-N	8.14	130.01	119.84
1	D	1160	ASN	C-N-CA	8.14	130.01	119.84
1	G	1142	TYR	CA-C-N	8.14	128.16	119.78
1	G	1142	TYR	C-N-CA	8.14	128.16	119.78
1	B	530	VAL	CA-C-N	8.12	128.61	119.92
1	B	530	VAL	C-N-CA	8.12	128.61	119.92
1	C	530	VAL	CA-C-N	8.06	128.09	119.78
1	C	530	VAL	C-N-CA	8.06	128.09	119.78
1	D	1142	TYR	CA-C-N	8.03	128.03	119.76
1	D	1142	TYR	C-N-CA	8.03	128.03	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	LEU	CA-C-N	8.02	127.66	119.56
1	B	284	LEU	C-N-CA	8.02	127.66	119.56
1	C	649	TYR	CA-C-N	-8.01	109.55	122.36
1	C	649	TYR	C-N-CA	-8.01	109.55	122.36
1	C	493	LYS	CA-C-N	7.96	127.89	119.85
1	C	493	LYS	C-N-CA	7.96	127.89	119.85
1	G	1059	ASP	CA-C-N	7.95	128.57	120.38
1	G	1059	ASP	C-N-CA	7.95	128.57	120.38
1	D	1193	ALA	CA-C-N	7.94	127.96	119.78
1	D	1193	ALA	C-N-CA	7.94	127.96	119.78
1	B	22	GLY	CA-C-N	7.93	127.95	119.78
1	B	22	GLY	C-N-CA	7.93	127.95	119.78
1	J	399	PHE	N-CA-C	7.91	121.39	110.24
1	C	462	GLY	CA-C-N	7.90	127.61	119.56
1	C	462	GLY	C-N-CA	7.90	127.61	119.56
1	G	766	HIS	CA-C-N	7.88	127.81	119.85
1	G	766	HIS	C-N-CA	7.88	127.81	119.85
1	C	705	GLY	CA-C-N	7.86	127.87	119.78
1	C	705	GLY	C-N-CA	7.86	127.87	119.78
1	A	1059	ASP	CA-C-N	7.85	128.47	120.38
1	A	1059	ASP	C-N-CA	7.85	128.47	120.38
1	J	462	GLY	CA-C-N	7.78	127.50	119.56
1	J	462	GLY	C-N-CA	7.78	127.50	119.56
1	J	96	THR	CA-C-N	7.77	127.78	119.78
1	J	96	THR	C-N-CA	7.77	127.78	119.78
1	G	1219	PRO	N-CA-C	7.75	120.15	110.70
1	A	1142	TYR	CA-C-N	7.73	127.65	119.85
1	A	1142	TYR	C-N-CA	7.73	127.65	119.85
1	B	493	LYS	CA-C-N	7.71	127.64	119.85
1	B	493	LYS	C-N-CA	7.71	127.64	119.85
1	A	902	ASP	CA-C-N	7.71	127.63	119.85
1	A	902	ASP	C-N-CA	7.71	127.63	119.85
1	G	1219	PRO	CA-C-N	7.67	128.28	120.38
1	G	1219	PRO	C-N-CA	7.67	128.28	120.38
1	J	688	GLN	N-CA-C	7.65	119.41	111.14
1	B	223	ALA	N-CA-C	7.64	119.24	111.07
1	J	657	VAL	CA-C-N	7.64	127.62	119.76
1	J	657	VAL	C-N-CA	7.64	127.62	119.76
1	D	929	VAL	N-CA-C	-7.61	105.74	111.90
1	C	269	ARG	N-CA-C	7.61	119.57	111.28
1	C	133	SER	CA-C-N	7.53	127.24	119.56
1	C	133	SER	C-N-CA	7.53	127.24	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	705	GLY	CA-C-N	7.53	127.53	119.78
1	B	705	GLY	C-N-CA	7.53	127.53	119.78
3	I	42	GLN	CA-C-N	7.47	128.08	120.38
3	I	42	GLN	C-N-CA	7.47	128.08	120.38
3	F	43	PRO	CA-C-N	7.45	127.40	120.03
3	F	43	PRO	C-N-CA	7.45	127.40	120.03
3	F	58	VAL	N-CA-C	7.44	117.38	108.45
1	C	392	THR	CA-C-N	7.43	125.01	119.66
1	C	392	THR	C-N-CA	7.43	125.01	119.66
1	J	705	GLY	CA-C-N	7.38	127.38	119.78
1	J	705	GLY	C-N-CA	7.38	127.38	119.78
1	B	369	LYS	CA-C-N	7.37	127.30	119.85
1	B	369	LYS	C-N-CA	7.37	127.30	119.85
1	J	709	THR	CA-C-N	7.37	127.72	119.32
1	J	709	THR	C-N-CA	7.37	127.72	119.32
1	D	936	PRO	CA-C-N	7.35	127.28	119.85
1	D	936	PRO	C-N-CA	7.35	127.28	119.85
1	G	970	ILE	CA-C-N	7.29	127.29	119.78
1	G	970	ILE	C-N-CA	7.29	127.29	119.78
1	D	1206	ALA	CA-C-N	7.26	127.26	119.78
1	D	1206	ALA	C-N-CA	7.26	127.26	119.78
1	D	753	VAL	CA-C-N	7.24	127.24	119.78
1	D	753	VAL	C-N-CA	7.24	127.24	119.78
1	C	709	THR	CA-C-N	7.23	126.94	119.56
1	C	709	THR	C-N-CA	7.23	126.94	119.56
3	I	43	PRO	CA-C-N	7.23	127.22	119.78
3	I	43	PRO	C-N-CA	7.23	127.22	119.78
1	J	649	TYR	CA-C-N	-7.23	110.80	122.36
1	J	649	TYR	C-N-CA	-7.23	110.80	122.36
1	J	406	ASN	CA-C-N	-7.21	110.04	121.87
1	J	406	ASN	C-N-CA	-7.21	110.04	121.87
1	G	753	VAL	CA-C-N	7.20	127.20	119.78
1	G	753	VAL	C-N-CA	7.20	127.20	119.78
1	D	1059	ASP	CA-C-N	7.14	127.73	120.38
1	D	1059	ASP	C-N-CA	7.14	127.73	120.38
1	A	1193	ALA	CA-C-N	7.14	127.18	119.90
1	A	1193	ALA	C-N-CA	7.14	127.18	119.90
1	C	406	ASN	CA-C-N	-7.13	110.18	121.87
1	C	406	ASN	C-N-CA	-7.13	110.18	121.87
1	A	1206	ALA	CA-C-N	7.09	127.08	119.78
1	A	1206	ALA	C-N-CA	7.09	127.08	119.78
1	J	584	VAL	CB-CA-C	-7.07	102.40	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	753	VAL	CA-C-N	7.04	127.03	119.78
1	A	753	VAL	C-N-CA	7.04	127.03	119.78
1	B	96	THR	CA-C-N	7.02	127.01	119.78
1	B	96	THR	C-N-CA	7.02	127.01	119.78
1	J	584	VAL	O-C-N	-7.02	114.38	122.94
1	B	709	THR	CA-C-N	7.01	126.83	119.05
1	B	709	THR	C-N-CA	7.01	126.83	119.05
1	G	1206	ALA	CA-C-N	7.00	126.98	119.78
1	G	1206	ALA	C-N-CA	7.00	126.98	119.78
1	C	514	VAL	CA-C-N	7.00	126.98	119.78
1	C	514	VAL	C-N-CA	7.00	126.98	119.78
1	B	269	ARG	N-CA-C	6.98	118.89	111.28
1	B	133	SER	CA-C-N	6.93	126.63	119.56
1	B	133	SER	C-N-CA	6.93	126.63	119.56
1	C	378	ALA	CA-C-N	6.93	134.18	121.70
1	C	378	ALA	C-N-CA	6.93	134.18	121.70
1	J	37	GLN	N-CA-C	6.92	120.60	111.75
1	C	585	CYS	CA-C-N	6.91	126.89	119.78
1	C	585	CYS	C-N-CA	6.91	126.89	119.78
1	B	657	VAL	CA-C-N	6.90	126.87	119.76
1	B	657	VAL	C-N-CA	6.90	126.87	119.76
1	C	657	VAL	CA-C-N	6.90	126.87	119.76
1	C	657	VAL	C-N-CA	6.90	126.87	119.76
1	D	782	ILE	CA-C-N	6.88	126.64	119.76
1	D	782	ILE	C-N-CA	6.88	126.64	119.76
1	J	446	PHE	N-CA-C	6.88	119.32	108.79
1	G	936	PRO	CA-C-N	6.85	126.82	119.76
1	G	936	PRO	C-N-CA	6.85	126.82	119.76
1	J	167	HIS	CA-CB-CG	6.83	120.63	113.80
1	B	484	VAL	CA-C-N	6.82	126.81	119.78
1	B	484	VAL	C-N-CA	6.82	126.81	119.78
1	C	399	PHE	N-CA-C	6.79	119.81	110.24
1	G	875	GLU	CA-C-N	6.78	128.31	119.84
1	G	875	GLU	C-N-CA	6.78	128.31	119.84
1	A	936	PRO	CA-C-N	6.76	126.73	119.76
1	A	936	PRO	C-N-CA	6.76	126.73	119.76
1	C	22	GLY	CA-C-N	6.76	126.75	119.78
1	C	22	GLY	C-N-CA	6.76	126.75	119.78
1	J	369	LYS	CA-C-N	6.74	126.72	119.78
1	J	369	LYS	C-N-CA	6.74	126.72	119.78
1	J	269	ARG	N-CA-C	6.74	118.62	111.28
1	C	484	VAL	CA-C-N	6.67	126.65	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	484	VAL	C-N-CA	6.67	126.65	119.78
1	J	484	VAL	N-CA-C	6.63	114.33	108.63
1	D	970	ILE	CA-C-N	6.62	126.58	119.76
1	D	970	ILE	C-N-CA	6.62	126.58	119.76
1	J	373	SER	N-CA-C	6.62	119.83	110.50
1	J	688	GLN	CA-C-N	6.60	133.58	121.70
1	J	688	GLN	C-N-CA	6.60	133.58	121.70
1	C	236	ASN	CA-C-N	-6.59	112.07	121.50
1	C	236	ASN	C-N-CA	-6.59	112.07	121.50
1	G	782	ILE	CA-C-N	6.59	126.35	119.76
1	G	782	ILE	C-N-CA	6.59	126.35	119.76
1	J	271	VAL	N-CA-C	6.58	117.23	111.90
1	G	1220	PRO	N-CA-C	6.57	118.72	110.70
1	B	688	GLN	CA-C-N	6.54	133.46	121.70
1	B	688	GLN	C-N-CA	6.54	133.46	121.70
1	B	717	LEU	N-CA-C	6.46	120.37	112.23
1	C	302	SER	CA-C-N	6.43	129.12	120.50
1	C	302	SER	C-N-CA	6.43	129.12	120.50
1	C	738	LEU	CA-C-N	6.41	126.78	119.92
1	C	738	LEU	C-N-CA	6.41	126.78	119.92
1	B	546	SER	CA-C-N	6.40	126.32	119.28
1	B	546	SER	C-N-CA	6.40	126.32	119.28
1	B	100	LEU	N-CA-C	6.39	119.50	110.23
1	C	368	ALA	N-CA-C	6.39	120.38	112.58
1	C	711	VAL	N-CA-C	-6.36	106.34	111.81
1	J	368	ALA	N-CA-C	6.33	120.30	112.58
1	A	782	ILE	CA-C-N	6.32	126.08	119.76
1	A	782	ILE	C-N-CA	6.32	126.08	119.76
1	J	78	GLN	N-CA-C	6.32	118.17	111.28
1	C	409	TYR	N-CA-C	6.31	118.77	109.24
1	B	37	GLN	N-CA-C	6.30	119.82	111.75
1	C	366	PHE	CA-CB-CG	6.29	120.09	113.80
1	B	271	VAL	N-CA-C	6.24	116.93	111.56
1	B	26	VAL	N-CA-C	6.24	117.02	110.72
1	C	323	PHE	N-CA-C	6.23	119.29	108.76
3	I	39	LYS	CA-C-N	6.21	126.57	119.93
3	I	39	LYS	C-N-CA	6.21	126.57	119.93
1	J	188	GLU	CA-C-N	6.19	126.16	119.78
1	J	188	GLU	C-N-CA	6.19	126.16	119.78
1	C	223	ALA	N-CA-C	6.15	117.65	111.07
1	J	162	GLY	N-CA-C	6.11	123.80	115.30
1	G	1019	PHE	CA-CB-CG	6.11	119.91	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1219	PRO	CA-C-N	6.10	126.67	120.38
1	D	1219	PRO	C-N-CA	6.10	126.67	120.38
1	D	916	GLY	CA-C-N	6.08	127.45	119.84
1	D	916	GLY	C-N-CA	6.08	127.45	119.84
1	B	164	PHE	CA-CB-CG	6.08	119.88	113.80
1	G	916	GLY	CA-C-N	6.08	126.28	119.90
1	G	916	GLY	C-N-CA	6.08	126.28	119.90
1	A	916	GLY	CA-C-N	6.07	125.83	119.76
1	A	916	GLY	C-N-CA	6.07	125.83	119.76
3	I	58	VAL	CB-CA-C	-6.06	102.36	110.97
1	A	1166	ALA	CA-C-N	6.04	125.95	119.85
1	A	1166	ALA	C-N-CA	6.04	125.95	119.85
1	J	223	ALA	N-CA-C	6.02	117.85	111.28
1	B	75	PHE	CA-C-N	6.01	125.92	119.85
1	B	75	PHE	C-N-CA	6.01	125.92	119.85
1	A	807	LYS	N-CA-C	-6.00	105.04	112.72
2	E	13	ARG	CA-C-N	6.00	125.96	119.78
2	E	13	ARG	C-N-CA	6.00	125.96	119.78
1	G	912	CYS	N-CA-C	-6.00	103.50	111.24
1	J	302	SER	CA-C-N	5.98	128.51	120.50
1	J	302	SER	C-N-CA	5.98	128.51	120.50
1	C	321	LEU	N-CA-C	5.97	118.92	110.50
1	B	649	TYR	CA-C-N	-5.95	113.29	122.87
1	B	649	TYR	C-N-CA	-5.95	113.29	122.87
1	G	807	LYS	N-CA-C	-5.92	105.06	112.93
1	A	1219	PRO	CA-C-N	5.90	126.45	120.38
1	A	1219	PRO	C-N-CA	5.90	126.45	120.38
1	B	188	GLU	CA-C-N	5.89	125.85	119.78
1	B	188	GLU	C-N-CA	5.89	125.85	119.78
1	C	437	CYS	O-C-N	-5.89	116.33	123.10
1	D	807	LYS	N-CA-C	-5.87	105.20	112.72
1	G	1166	ALA	CA-C-N	5.87	125.77	119.85
1	G	1166	ALA	C-N-CA	5.87	125.77	119.85
1	B	484	VAL	N-CA-C	5.86	113.67	108.63
1	C	188	GLU	CA-C-N	5.86	125.81	119.78
1	C	188	GLU	C-N-CA	5.86	125.81	119.78
1	C	438	TYR	N-CA-C	5.85	117.96	109.07
2	H	13	ARG	CA-C-N	5.82	125.77	119.78
2	H	13	ARG	C-N-CA	5.82	125.77	119.78
1	C	296	ILE	CA-C-N	5.79	125.70	119.85
1	C	296	ILE	C-N-CA	5.79	125.70	119.85
1	C	484	VAL	N-CA-C	5.79	113.61	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	399	PHE	CA-CB-CG	-5.78	108.02	113.80
1	D	862	ILE	CA-C-N	5.76	125.69	119.76
1	D	862	ILE	C-N-CA	5.76	125.69	119.76
1	C	172	LEU	CA-C-N	5.75	125.66	119.85
1	C	172	LEU	C-N-CA	5.75	125.66	119.85
1	J	514	VAL	CA-C-N	5.74	125.69	119.78
1	J	514	VAL	C-N-CA	5.74	125.69	119.78
1	B	392	THR	CA-C-N	5.72	123.78	119.66
1	B	392	THR	C-N-CA	5.72	123.78	119.66
1	J	438	TYR	N-CA-C	5.72	117.87	109.24
1	C	37	GLN	N-CA-C	5.70	119.04	111.75
1	J	546	SER	CA-C-N	5.69	125.54	119.28
1	J	546	SER	C-N-CA	5.69	125.54	119.28
1	J	585	CYS	CA-C-N	5.68	125.64	119.78
1	J	585	CYS	C-N-CA	5.68	125.64	119.78
3	F	71	PHE	CA-CB-CG	-5.65	108.15	113.80
1	C	271	VAL	N-CA-C	5.63	116.85	112.12
1	J	296	ILE	CA-C-N	5.63	125.54	119.85
1	J	296	ILE	C-N-CA	5.63	125.54	119.85
1	C	341	PHE	N-CA-C	5.62	117.48	111.36
1	A	850	PHE	CA-CB-CG	-5.61	108.19	113.80
3	F	39	LYS	CA-C-N	5.60	125.87	119.83
3	F	39	LYS	C-N-CA	5.60	125.87	119.83
1	J	304	GLN	N-CA-C	5.59	118.09	111.33
1	B	196	PRO	N-CA-C	5.57	121.27	113.53
1	A	970	ILE	CA-C-N	5.56	125.49	119.76
1	A	970	ILE	C-N-CA	5.56	125.49	119.76
1	A	859	SER	CA-C-N	5.56	125.50	119.78
1	A	859	SER	C-N-CA	5.56	125.50	119.78
1	G	859	SER	CA-C-N	5.55	125.50	119.78
1	G	859	SER	C-N-CA	5.55	125.50	119.78
1	B	341	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	1060	PRO	CA-C-N	5.54	125.89	119.47
1	A	1060	PRO	C-N-CA	5.54	125.89	119.47
1	A	814	PHE	CA-CB-CG	-5.53	108.27	113.80
1	A	1044	PHE	CA-CB-CG	-5.53	108.27	113.80
1	D	850	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	296	ILE	CA-C-N	5.50	125.40	119.85
1	B	296	ILE	C-N-CA	5.50	125.40	119.85
1	B	172	LEU	CA-C-N	5.49	125.39	119.85
1	B	172	LEU	C-N-CA	5.49	125.39	119.85
1	G	1060	PRO	CA-C-N	5.46	125.81	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1060	PRO	C-N-CA	5.46	125.81	119.47
1	J	429	SER	CA-C-N	5.46	124.98	119.19
1	J	429	SER	C-N-CA	5.46	124.98	119.19
1	B	406	ASN	CA-C-N	-5.44	112.95	121.87
1	B	406	ASN	C-N-CA	-5.44	112.95	121.87
1	J	323	PHE	N-CA-C	5.43	117.94	108.76
1	B	271	VAL	CB-CA-C	-5.42	106.29	111.44
1	B	195	CYS	CA-C-N	5.41	125.06	119.05
1	B	195	CYS	C-N-CA	5.41	125.06	119.05
1	J	409	TYR	N-CA-C	5.41	117.41	109.24
1	B	167	HIS	CA-CB-CG	5.41	119.20	113.80
1	G	1202	THR	N-CA-C	5.40	116.19	108.74
1	B	323	PHE	N-CA-C	5.39	117.58	109.23
1	J	366	PHE	CA-CB-CG	5.38	119.18	113.80
1	B	165	PHE	CA-CB-CG	-5.37	108.43	113.80
1	J	19	VAL	N-CA-C	5.37	116.50	109.58
1	J	321	LEU	N-CA-C	5.37	118.06	110.50
1	J	236	ASN	CA-C-N	-5.34	113.28	120.87
1	J	236	ASN	C-N-CA	-5.34	113.28	120.87
1	C	369	LYS	CB-CA-C	-5.33	107.42	111.20
1	C	429	SER	CA-C-N	5.33	125.14	119.28
1	C	429	SER	C-N-CA	5.33	125.14	119.28
1	C	164	PHE	CA-CB-CG	5.31	119.11	113.80
1	C	273	LEU	N-CA-C	5.30	117.06	111.28
1	B	641	TYR	N-CA-C	5.29	118.01	108.48
1	B	606	TYR	N-CA-C	5.27	117.08	109.07
1	J	732	GLY	N-CA-C	-5.27	106.38	112.29
1	J	378	ALA	CA-C-N	5.27	131.18	121.70
1	J	378	ALA	C-N-CA	5.27	131.18	121.70
1	B	58	TYR	CA-C-N	5.25	125.18	119.78
1	B	58	TYR	C-N-CA	5.25	125.18	119.78
1	A	798	THR	N-CA-C	5.23	117.02	109.07
1	D	1166	ALA	CA-C-N	5.22	125.12	119.85
1	D	1166	ALA	C-N-CA	5.22	125.12	119.85
1	J	738	LEU	N-CA-C	5.21	116.39	109.93
1	J	172	LEU	CA-C-N	5.20	125.10	119.85
1	J	172	LEU	C-N-CA	5.20	125.10	119.85
1	C	524	SER	CA-C-N	5.18	124.98	119.28
1	C	524	SER	C-N-CA	5.18	124.98	119.28
1	C	688	GLN	CA-C-N	5.18	131.03	121.70
1	C	688	GLN	C-N-CA	5.18	131.03	121.70
1	B	514	VAL	CA-C-N	5.18	125.11	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	VAL	C-N-CA	5.18	125.11	119.78
1	B	46	ARG	CA-C-N	5.17	125.10	119.78
1	B	46	ARG	C-N-CA	5.17	125.10	119.78
1	C	78	GLN	N-CA-C	5.16	116.91	111.28
1	C	341	PHE	CA-CB-CG	-5.16	108.64	113.80
1	G	1058	LEU	N-CA-C	5.15	117.97	109.72
1	B	323	PHE	CA-CB-CG	5.14	118.94	113.80
1	J	367	GLU	N-CA-C	5.14	119.18	113.01
1	J	58	TYR	CA-C-N	5.14	125.07	119.78
1	J	58	TYR	C-N-CA	5.14	125.07	119.78
3	F	87	PHE	N-CA-C	5.12	116.75	108.34
1	C	58	TYR	CA-C-N	5.11	125.04	119.78
1	C	58	TYR	C-N-CA	5.11	125.04	119.78
1	A	1045	GLY	N-CA-C	-5.11	108.28	115.32
2	E	57	THR	N-CA-C	5.09	116.81	109.07
1	C	173	PRO	N-CA-C	-5.08	103.30	111.38
2	E	91	TYR	N-CA-C	5.07	116.65	108.34
1	G	911	ASP	N-CA-C	-5.04	107.13	113.28
1	B	304	GLN	N-CA-C	5.02	117.41	111.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3488	0	3413	22	0
1	B	5658	0	5424	76	0
1	C	5658	0	5423	47	0
1	D	3545	0	3471	30	0
1	G	3545	0	3471	30	0
1	J	5658	0	5423	48	0
2	E	948	0	904	4	0
2	H	948	0	904	10	0
3	F	835	0	816	2	0
3	I	835	0	816	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31118	0	30065	274	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 4.

All (274) 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:J:506:PHE:CE2	1:J:555:VAL:HG21	1.15	1.61
1:B:506:PHE:CE2	1:B:555:VAL:HG21	1.03	1.54
1:B:506:PHE:CE2	1:B:555:VAL:CG2	1.97	1.48
1:J:506:PHE:CE2	1:J:555:VAL:CG2	2.03	1.40
1:B:506:PHE:HE2	1:B:555:VAL:CG2	1.30	1.36
1:B:384:ASP:O	1:B:404:PHE:CZ	1.81	1.32
1:B:381:VAL:CG1	1:B:408:ASN:N	1.99	1.25
1:D:905:TYR:CE1	1:D:936:PRO:HB3	1.75	1.20
1:B:381:VAL:HG12	1:B:408:ASN:N	1.55	1.17
1:B:381:VAL:HB	1:B:408:ASN:CB	1.64	1.10
1:B:506:PHE:CD2	1:B:555:VAL:HG21	1.88	1.08
1:B:381:VAL:HG12	1:B:408:ASN:H	0.93	1.08
1:J:506:PHE:CD2	1:J:555:VAL:HG21	1.88	1.08
1:B:381:VAL:CG1	1:B:407:CYS:HA	1.88	1.03
1:B:381:VAL:CG1	1:B:408:ASN:H	1.65	1.03
1:B:381:VAL:HB	1:B:408:ASN:HB2	1.39	1.03
1:B:506:PHE:CD2	1:B:555:VAL:CG2	2.43	1.02
1:J:506:PHE:HE2	1:J:555:VAL:CG2	1.49	1.02
1:B:384:ASP:O	1:B:404:PHE:HZ	1.22	1.00
1:D:905:TYR:OH	1:D:936:PRO:HA	1.63	0.99
1:B:381:VAL:HG11	1:B:407:CYS:C	1.89	0.96
1:B:381:VAL:HG11	1:B:408:ASN:N	1.81	0.95
1:G:905:TYR:OH	1:G:935:LEU:C	2.09	0.95
1:D:905:TYR:CE1	1:D:936:PRO:CB	2.50	0.95
1:B:728:LYS:C	1:B:730:PRO:HD3	1.90	0.95
1:J:506:PHE:CD2	1:J:555:VAL:CG2	2.46	0.93
1:B:728:LYS:O	1:B:730:PRO:CD	2.18	0.92
1:A:905:TYR:CE1	1:A:936:PRO:HB3	2.04	0.92
1:B:381:VAL:CG1	1:B:407:CYS:C	2.43	0.91
1:D:905:TYR:OH	1:D:936:PRO:CA	2.19	0.91
1:B:381:VAL:CG1	1:B:407:CYS:CA	2.49	0.90
1:B:384:ASP:O	1:B:404:PHE:CE2	2.28	0.87
1:D:905:TYR:HE1	1:D:936:PRO:CB	1.88	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:CYS:HB2	1:C:385:PHE:CE1	2.09	0.86
1:D:905:TYR:HE1	1:D:936:PRO:HB3	1.39	0.85
1:B:728:LYS:O	1:B:730:PRO:HD2	1.78	0.83
1:C:381:VAL:O	1:C:407:CYS:HB2	1.80	0.80
1:B:381:VAL:HG13	1:B:407:CYS:HA	1.64	0.79
1:B:728:LYS:O	1:B:730:PRO:HD3	1.80	0.79
1:J:691:ARG:HA	1:J:691:ARG:NE	2.00	0.77
1:B:506:PHE:CD2	1:B:555:VAL:HG23	2.19	0.77
1:C:680:GLU:OE1	1:C:680:GLU:N	2.17	0.77
1:B:728:LYS:C	1:B:730:PRO:CD	2.57	0.77
1:B:381:VAL:CB	1:B:408:ASN:CB	2.57	0.75
1:J:506:PHE:HE2	1:J:555:VAL:HG22	1.53	0.73
1:B:621:THR:HG22	1:B:622:ALA:H	1.53	0.72
1:B:382:GLU:H	1:B:408:ASN:HB2	1.54	0.72
1:D:905:TYR:OH	1:D:936:PRO:N	2.23	0.72
1:B:621:THR:HG22	1:B:622:ALA:N	2.04	0.72
1:B:384:ASP:CB	1:B:404:PHE:HE2	2.04	0.71
1:C:369:LYS:HG2	1:C:369:LYS:O	1.89	0.70
1:G:905:TYR:HH	1:G:935:LEU:C	1.97	0.70
1:C:385:PHE:CE2	1:C:404:PHE:CE1	2.80	0.69
1:D:871:LEU:O	1:D:871:LEU:HG	1.91	0.68
1:G:905:TYR:OH	1:G:936:PRO:N	2.28	0.67
1:C:381:VAL:O	1:C:407:CYS:CB	2.44	0.66
2:H:5:GLN:CD	2:H:5:GLN:O	2.39	0.65
1:J:506:PHE:CD2	1:J:555:VAL:HG23	2.30	0.65
1:J:506:PHE:HE2	1:J:555:VAL:HG21	0.91	0.64
1:D:905:TYR:OH	1:D:935:LEU:C	2.42	0.63
1:C:381:VAL:O	1:C:407:CYS:CA	2.46	0.63
1:J:381:VAL:O	1:J:407:CYS:HB2	1.98	0.63
1:B:382:GLU:O	1:B:407:CYS:HB2	1.98	0.63
1:B:688:GLN:HB2	1:B:689:TYR:HA	1.81	0.62
1:C:381:VAL:O	1:C:407:CYS:HA	1.98	0.62
1:G:915:GLN:O	1:G:915:GLN:HG2	1.99	0.62
1:C:596:ILE:C	1:C:596:ILE:HD12	2.26	0.61
2:H:110:THR:HG22	2:H:110:THR:O	2.00	0.61
2:H:5:GLN:O	2:H:5:GLN:OE1	2.19	0.61
1:B:256:ILE:HG23	1:B:256:ILE:O	2.01	0.60
1:C:194:HIS:O	1:C:194:HIS:ND1	2.35	0.60
1:D:905:TYR:CZ	1:D:936:PRO:HA	2.36	0.59
1:B:381:VAL:HG11	1:B:407:CYS:CA	2.24	0.59
1:D:905:TYR:HE1	1:D:936:PRO:CD	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:905:TYR:HE1	1:D:936:PRO:CG	2.15	0.59
1:D:905:TYR:CZ	1:D:936:PRO:CA	2.86	0.58
2:H:85:GLU:OE1	2:H:85:GLU:N	2.34	0.58
1:B:621:THR:O	1:B:648:TYR:HD2	1.87	0.57
2:H:11:LEU:HD23	2:H:11:LEU:C	2.29	0.57
2:H:11:LEU:HD23	2:H:11:LEU:O	2.05	0.57
1:C:385:PHE:HE2	1:C:404:PHE:CE1	2.22	0.57
1:G:905:TYR:HE1	1:G:936:PRO:HD3	1.70	0.56
1:B:700:ARG:HA	1:B:700:ARG:NE	2.21	0.56
1:D:1173:ILE:HG13	1:D:1185:SER:OG	2.06	0.56
1:D:897:LYS:HE2	1:D:897:LYS:HA	1.88	0.56
1:B:616:VAL:O	1:B:616:VAL:HG13	2.06	0.56
1:J:620:CYS:O	1:J:621:THR:C	2.49	0.55
1:B:382:GLU:N	1:B:408:ASN:HB2	2.21	0.55
2:E:20:ILE:C	2:E:20:ILE:HD12	2.32	0.55
1:B:382:GLU:C	1:B:408:ASN:O	2.50	0.55
1:J:399:PHE:CD1	1:J:399:PHE:N	2.73	0.55
1:A:756:GLU:OE1	1:A:756:GLU:N	2.36	0.54
1:B:381:VAL:HG12	1:B:407:CYS:C	2.19	0.54
1:B:727:CYS:HB3	1:B:738:LEU:HD23	1.89	0.54
1:B:385:PHE:CE2	1:B:404:PHE:CE1	2.97	0.53
1:B:381:VAL:HG12	1:B:407:CYS:CA	2.30	0.53
1:J:691:ARG:HA	1:J:691:ARG:HE	1.71	0.53
1:G:986:THR:HG21	1:G:1195:GLU:OE2	2.07	0.53
1:B:251:LEU:C	1:B:251:LEU:HD23	2.33	0.53
1:D:905:TYR:CE1	1:D:936:PRO:CA	2.91	0.53
1:J:67:ILE:HG13	1:J:67:ILE:O	2.09	0.53
1:C:385:PHE:CD2	1:C:404:PHE:CZ	2.97	0.52
1:B:604:VAL:HG23	1:B:604:VAL:O	2.09	0.52
1:J:395:GLN:HA	1:J:395:GLN:OE1	2.10	0.52
1:B:382:GLU:HG3	1:B:383:CYS:N	2.24	0.52
1:B:621:THR:CG2	1:B:622:ALA:H	2.21	0.52
1:B:621:THR:CG2	1:B:622:ALA:N	2.73	0.52
1:J:724:VAL:HG11	1:J:727:CYS:SG	2.50	0.52
1:B:506:PHE:HD2	1:B:555:VAL:HG23	1.70	0.52
1:J:409:TYR:CD1	1:J:409:TYR:C	2.89	0.51
1:G:1160:ASN:C	1:G:1160:ASN:OD1	2.53	0.51
1:B:382:GLU:HG3	1:B:383:CYS:H	1.75	0.51
3:I:92:LYS:O	3:I:92:LYS:HD3	2.10	0.51
1:J:369:LYS:O	1:J:369:LYS:HG2	2.10	0.51
1:C:67:ILE:HG23	1:C:67:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:SER:HA	1:C:582:ASN:HA	1.94	0.50
1:J:172:LEU:HD23	1:J:172:LEU:N	2.27	0.50
1:G:873:LEU:C	1:G:873:LEU:HD12	2.37	0.50
1:B:381:VAL:H	1:B:408:ASN:HD22	1.60	0.50
1:C:735:LEU:HD12	1:C:735:LEU:N	2.27	0.50
1:D:875:GLU:HB3	1:D:886:ALA:HB3	1.94	0.50
1:C:383:CYS:CB	1:C:385:PHE:CE1	2.89	0.50
1:G:756:GLU:CD	1:G:756:GLU:H	2.17	0.50
1:B:382:GLU:CA	1:B:408:ASN:O	2.60	0.50
1:G:905:TYR:CE1	1:G:936:PRO:HB3	2.47	0.50
3:F:1:ASP:C	3:F:1:ASP:OD1	2.55	0.49
1:J:240:MET:SD	1:J:240:MET:C	2.96	0.49
1:D:1219:PRO:HG2	1:D:1220:PRO:HD3	1.93	0.49
1:J:648:TYR:C	1:J:648:TYR:CD2	2.90	0.49
3:I:2:ILE:HD12	3:I:2:ILE:H	1.77	0.49
1:D:875:GLU:H	1:D:875:GLU:CD	2.19	0.49
1:J:439:SER:HA	1:J:582:ASN:HA	1.93	0.49
1:B:228:PHE:C	1:B:228:PHE:CD2	2.90	0.49
1:C:251:LEU:C	1:C:251:LEU:HD23	2.37	0.49
1:J:172:LEU:O	1:J:172:LEU:HG	2.12	0.49
2:E:72:ASP:C	2:E:72:ASP:OD1	2.54	0.49
2:H:11:LEU:O	2:H:11:LEU:CD2	2.61	0.48
1:B:395:GLN:HA	1:B:395:GLN:OE1	2.13	0.48
1:A:905:TYR:CE1	1:A:936:PRO:CB	2.89	0.48
1:A:905:TYR:HE1	1:A:936:PRO:HB3	1.72	0.48
1:A:1060:PRO:HA	1:A:1063:GLN:HB3	1.96	0.48
1:G:1120:GLY:O	1:G:1121:THR:OG1	2.22	0.48
1:B:111:GLN:OE1	1:B:111:GLN:N	2.39	0.48
1:D:1120:GLY:O	1:D:1121:THR:OG1	2.28	0.47
1:D:1005:LEU:C	1:D:1005:LEU:HD23	2.39	0.47
1:B:443:LEU:HD23	1:B:443:LEU:C	2.39	0.47
1:J:383:CYS:HB2	1:J:385:PHE:CZ	2.50	0.47
1:B:78:GLN:C	1:B:78:GLN:CD	2.82	0.47
1:G:905:TYR:CE1	1:G:936:PRO:HD3	2.49	0.47
1:G:1001:PHE:CD2	1:G:1001:PHE:C	2.93	0.47
1:C:606:TYR:CD1	1:C:606:TYR:C	2.92	0.47
1:G:1156:CYS:SG	1:G:1211:TYR:HB2	2.54	0.47
1:B:382:GLU:HA	1:B:408:ASN:O	2.15	0.47
1:B:49:ASP:OD1	1:B:49:ASP:C	2.56	0.47
3:I:92:LYS:HD3	3:I:92:LYS:C	2.40	0.47
1:C:78:GLN:C	1:C:78:GLN:CD	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:LEU:HD23	1:J:172:LEU:H	1.78	0.47
1:A:944:GLU:HA	1:A:944:GLU:OE1	2.13	0.46
1:J:49:ASP:C	1:J:49:ASP:OD1	2.57	0.46
1:A:956:ALA:N	1:A:957:GLY:CA	2.79	0.46
1:C:78:GLN:NE2	1:C:78:GLN:O	2.48	0.46
1:B:384:ASP:CA	1:B:404:PHE:HE2	2.29	0.46
1:G:927:GLN:HB2	1:G:932:TYR:HB2	1.98	0.46
1:J:111:GLN:OE1	1:J:111:GLN:N	2.44	0.46
1:J:425:CYS:HA	1:J:478:CYS:HA	1.97	0.46
1:B:602:ASN:O	1:B:616:VAL:HB	2.16	0.46
1:B:664:ASP:OD1	1:B:664:ASP:C	2.57	0.46
1:A:1160:ASN:OD1	1:A:1160:ASN:C	2.56	0.46
2:H:72:ASP:OD1	2:H:72:ASP:C	2.59	0.46
1:G:1102:LYS:O	1:G:1106:CYS:N	2.49	0.46
1:C:326:ASP:OD1	1:C:326:ASP:C	2.59	0.46
1:C:604:VAL:O	1:C:604:VAL:HG13	2.16	0.46
1:J:130:VAL:O	1:J:130:VAL:HG12	2.16	0.46
1:D:964:LEU:O	1:D:965:SER:CB	2.65	0.46
2:H:5:GLN:CD	2:H:5:GLN:C	2.83	0.45
1:A:1124:VAL:O	1:A:1124:VAL:HG13	2.16	0.45
1:C:385:PHE:CE2	1:C:404:PHE:CZ	3.04	0.45
3:F:28:TYR:CD1	3:F:28:TYR:N	2.84	0.45
1:A:1017:GLU:H	1:A:1017:GLU:CD	2.21	0.45
1:B:256:ILE:O	1:B:256:ILE:CG2	2.65	0.45
1:B:719:ASN:OD1	1:B:719:ASN:C	2.60	0.45
1:G:936:PRO:HA	1:G:937:PRO:HD3	1.83	0.45
1:J:593:ASP:N	1:J:594:THR:HA	2.31	0.45
1:A:935:LEU:HD12	1:A:935:LEU:N	2.31	0.45
1:C:633:ASP:OD1	1:C:633:ASP:C	2.60	0.45
1:G:986:THR:HG21	1:G:1195:GLU:CD	2.41	0.45
1:C:673:LEU:C	1:C:673:LEU:HD23	2.41	0.44
1:B:384:ASP:HB3	1:B:404:PHE:HE2	1.76	0.44
1:A:1219:PRO:HG2	1:A:1220:PRO:HD3	2.00	0.44
1:B:130:VAL:O	1:B:130:VAL:HG12	2.18	0.44
1:B:326:ASP:C	1:B:326:ASP:OD1	2.58	0.44
1:C:172:LEU:HD23	1:C:172:LEU:N	2.33	0.44
1:C:446:PHE:N	1:C:446:PHE:CD2	2.85	0.44
1:G:1113:ARG:HA	1:G:1113:ARG:NE	2.32	0.44
1:J:606:TYR:CD1	1:J:606:TYR:C	2.96	0.44
1:J:689:TYR:CD1	1:J:689:TYR:C	2.95	0.44
1:A:977:PHE:N	1:A:977:PHE:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:383:CYS:O	1:J:385:PHE:CD1	2.71	0.44
1:J:709:THR:HB	1:J:710:PRO:HD2	1.99	0.44
1:D:756:GLU:H	1:D:756:GLU:CD	2.26	0.43
1:C:409:TYR:CD1	1:C:409:TYR:C	2.95	0.43
1:G:1173:ILE:HG13	1:G:1185:SER:OG	2.18	0.43
1:C:600:LEU:H	1:C:600:LEU:HD12	1.83	0.43
1:A:1001:PHE:C	1:A:1001:PHE:CD2	2.97	0.43
1:J:396:VAL:HA	1:J:399:PHE:CE1	2.54	0.43
1:B:384:ASP:HB3	1:B:404:PHE:CE2	2.53	0.43
1:C:600:LEU:HD12	1:C:600:LEU:N	2.32	0.43
2:E:41:HIS:HB3	2:E:44:SER:HB3	2.00	0.43
1:G:1155:LEU:HD22	1:G:1214:ILE:HD11	2.01	0.43
1:B:409:TYR:O	1:B:586:PRO:HA	2.18	0.43
1:J:381:VAL:O	1:J:407:CYS:HA	2.19	0.43
1:J:633:ASP:C	1:J:633:ASP:OD1	2.60	0.43
1:C:130:VAL:O	1:C:130:VAL:HG12	2.18	0.43
1:C:172:LEU:O	1:C:172:LEU:HG	2.19	0.43
1:J:728:LYS:O	1:J:729:LEU:HG	2.19	0.43
1:C:171:LEU:C	1:C:171:LEU:HD23	2.44	0.43
3:I:2:ILE:HD12	3:I:2:ILE:N	2.33	0.42
1:B:665:LYS:HB3	1:B:665:LYS:HE3	1.84	0.42
1:D:775:SER:OG	1:D:776:SER:N	2.45	0.42
1:D:1217:ASN:C	1:D:1217:ASN:OD1	2.62	0.42
1:G:1060:PRO:HB2	1:G:1061:PRO:HD3	2.00	0.42
1:G:1202:THR:OG1	1:G:1203:LYS:N	2.52	0.42
1:J:330:ASP:OD1	1:J:330:ASP:C	2.62	0.42
2:H:110:THR:O	2:H:110:THR:CG2	2.66	0.42
1:B:626:ARG:O	1:B:627:GLN:HB2	2.19	0.42
1:J:378:ALA:HB1	1:J:379:GLU:HA	2.02	0.42
1:D:806:CYS:O	1:D:806:CYS:SG	2.77	0.42
1:D:905:TYR:OH	1:D:935:LEU:O	2.37	0.42
1:J:381:VAL:O	1:J:407:CYS:CB	2.65	0.42
1:A:786:PHE:CD1	1:A:786:PHE:C	2.96	0.42
1:C:740:ASP:O	1:C:741:THR:C	2.62	0.42
1:A:827:PHE:N	1:A:827:PHE:CD1	2.87	0.42
1:J:228:PHE:CD2	1:J:228:PHE:C	2.96	0.42
1:A:875:GLU:OE1	1:A:875:GLU:N	2.39	0.41
3:I:36:PHE:O	3:I:86:TYR:HA	2.20	0.41
1:B:633:ASP:C	1:B:633:ASP:OD1	2.62	0.41
1:J:240:MET:SD	1:J:240:MET:O	2.78	0.41
1:A:977:PHE:N	1:A:977:PHE:HD1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:826:GLN:H	1:G:826:GLN:CD	2.24	0.41
1:C:209:THR:O	1:C:209:THR:HG22	2.19	0.41
1:C:382:GLU:HA	1:C:408:ASN:O	2.19	0.41
1:A:871:LEU:N	1:A:871:LEU:HD12	2.36	0.41
1:A:1008:MET:O	1:A:1008:MET:HG3	2.19	0.41
1:C:104:ASN:OD1	1:C:104:ASN:C	2.63	0.41
1:C:675:GLY:HA2	1:C:712:GLY:HA3	2.03	0.41
1:C:688:GLN:HB2	1:C:689:TYR:HA	2.02	0.41
1:J:410:ASN:C	1:J:410:ASN:OD1	2.63	0.41
2:E:13:ARG:HA	2:E:14:PRO:HD3	1.95	0.41
1:G:961:THR:O	1:G:961:THR:HG22	2.20	0.41
1:C:719:ASN:C	1:C:719:ASN:OD1	2.61	0.41
1:D:905:TYR:CE1	1:D:936:PRO:CD	3.00	0.41
1:G:806:CYS:O	1:G:806:CYS:SG	2.78	0.41
1:C:172:LEU:HD23	1:C:172:LEU:H	1.85	0.41
1:D:1102:LYS:O	1:D:1106:CYS:N	2.53	0.41
1:G:777:TYR:CD2	1:G:777:TYR:N	2.89	0.41
1:A:774:ASN:OD1	1:A:774:ASN:C	2.64	0.41
1:C:49:ASP:OD1	1:C:49:ASP:C	2.63	0.41
1:C:111:GLN:OE1	1:C:111:GLN:N	2.45	0.41
1:C:174:ASP:C	1:C:174:ASP:OD1	2.61	0.41
1:J:689:TYR:CD2	1:J:689:TYR:N	2.88	0.41
1:G:764:PHE:CD2	1:G:764:PHE:C	2.99	0.40
1:C:140:ILE:HD13	1:C:140:ILE:HG21	1.80	0.40
1:A:1183:GLU:N	1:A:1183:GLU:OE1	2.55	0.40
1:D:756:GLU:OE1	1:D:756:GLU:N	2.42	0.40
1:G:904:GLY:O	1:G:905:TYR:HB2	2.20	0.40
1:G:905:TYR:OH	1:G:934:VAL:O	2.38	0.40
1:B:688:GLN:CB	1:B:689:TYR:HA	2.49	0.40
1:B:381:VAL:CB	1:B:408:ASN:HB2	2.29	0.40
1:C:269:ARG:O	1:C:269:ARG:HD2	2.20	0.40
1:B:727:CYS:O	1:B:729:LEU:N	2.45	0.40
1:C:615:GLY:HA3	1:C:651:LEU:HD11	2.03	0.40
1:J:615:GLY:HA2	1:J:654:CYS:SG	2.61	0.40
1:J:132:ILE:HD12	1:J:132:ILE:HA	1.89	0.40
1:J:719:ASN:C	1:J:719:ASN:OD1	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	450/1329 (34%)	422 (94%)	25 (6%)	3 (1%)	18	55
1	B	724/1329 (54%)	688 (95%)	28 (4%)	8 (1%)	11	45
1	C	724/1329 (54%)	686 (95%)	35 (5%)	3 (0%)	30	67
1	D	459/1329 (34%)	433 (94%)	19 (4%)	7 (2%)	8	38
1	G	459/1329 (34%)	431 (94%)	25 (5%)	3 (1%)	18	55
1	J	724/1329 (54%)	691 (95%)	27 (4%)	6 (1%)	16	52
2	E	117/233 (50%)	113 (97%)	3 (3%)	1 (1%)	14	49
2	H	117/233 (50%)	111 (95%)	6 (5%)	0	100	100
3	F	109/218 (50%)	102 (94%)	5 (5%)	2 (2%)	6	33
3	I	109/218 (50%)	102 (94%)	6 (6%)	1 (1%)	14	49
All	All	3992/8876 (45%)	3779 (95%)	179 (4%)	34 (1%)	16	49

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	961	THR
1	G	962	ALA
1	B	729	LEU
1	J	378	ALA
1	A	940	ASP
1	D	961	THR
1	D	965	SER
1	B	718	VAL
1	C	718	VAL
1	J	602	ASN
1	J	718	VAL
1	D	1220	PRO
2	E	28	THR
3	F	31	SER

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Mol	Chain	Res	Type
3	F	77	PRO
3	I	77	PRO
1	B	384	ASP
1	A	1220	PRO
1	D	956	ALA
1	D	1219	PRO
1	B	368	ALA
1	B	621	THR
1	C	629	ARG
1	J	596	ILE
1	J	598	SER
1	J	629	ARG
1	D	905	TYR
1	G	956	ALA
1	B	382	GLU
1	G	1220	PRO
1	B	678	ALA
1	B	596	ILE
1	C	44	TRP
1	D	1161	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/1148 (33%)	381 (100%)	0	100	100
1	B	635/1148 (55%)	633 (100%)	2 (0%)	86	84
1	C	635/1148 (55%)	635 (100%)	0	100	100
1	D	388/1148 (34%)	388 (100%)	0	100	100
1	G	388/1148 (34%)	388 (100%)	0	100	100
1	J	635/1148 (55%)	635 (100%)	0	100	100
2	E	102/202 (50%)	102 (100%)	0	100	100
2	H	102/202 (50%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	93/192 (48%)	93 (100%)	0	100	100
3	I	93/192 (48%)	93 (100%)	0	100	100
All	All	3452/7676 (45%)	3450 (100%)	2 (0%)	87	88

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	251	LEU
1	B	727	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	769	GLN
1	A	772	GLN
1	A	1146	HIS
1	A	1208	GLN
1	D	766	HIS
1	D	769	GLN
1	D	1146	HIS
3	F	74	ASN
1	G	766	HIS
1	G	772	GLN
1	G	815	GLN
1	G	981	ASN
1	G	987	GLN
3	I	74	ASN
1	B	36	GLN
1	B	618	GLN
1	C	36	GLN
1	C	78	GLN
1	C	91	HIS
1	C	167	HIS
1	C	319	GLN
1	C	628	GLN
1	J	36	GLN
1	J	194	HIS
1	J	471	GLN
1	J	688	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

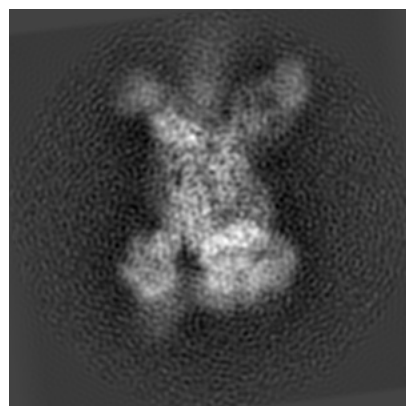
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8787. These allow visual inspection of the internal detail of the map and identification of artifacts.

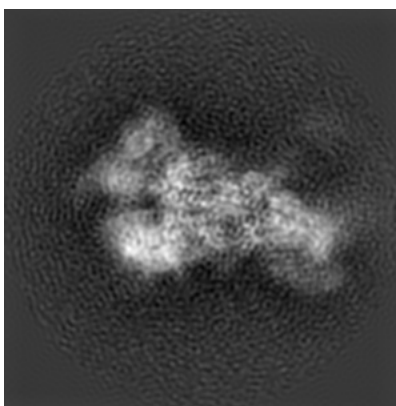
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

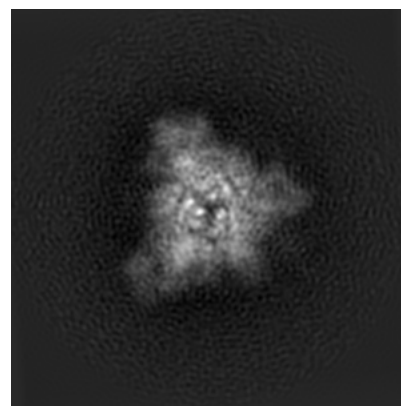
6.1.1 Primary map



X

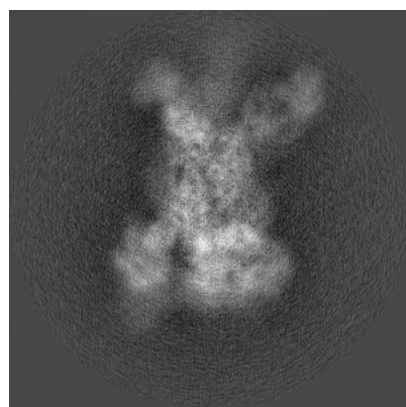


Y

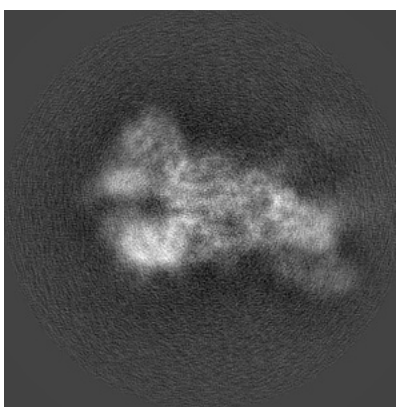


Z

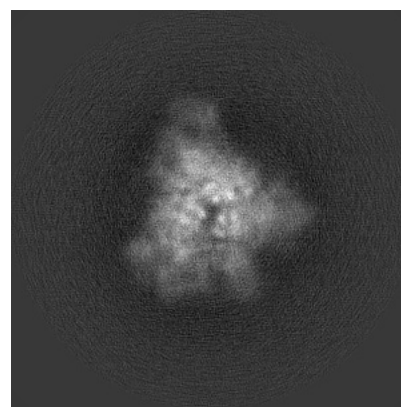
6.1.2 Raw map



X



Y

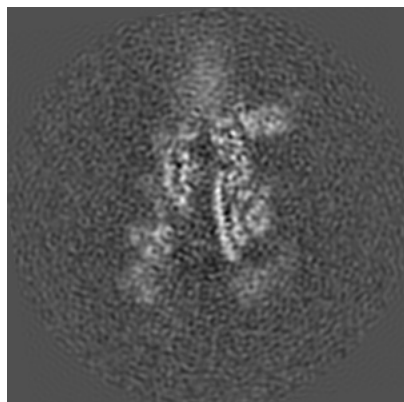


Z

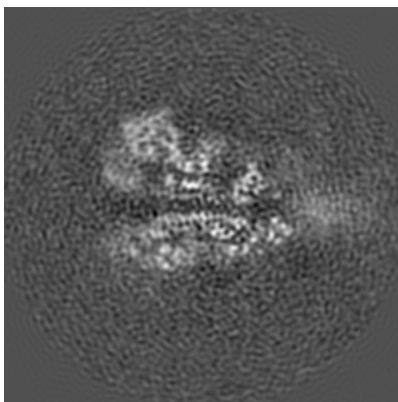
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

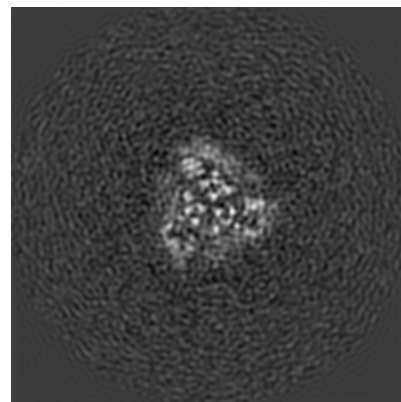
6.2.1 Primary map



X Index: 152

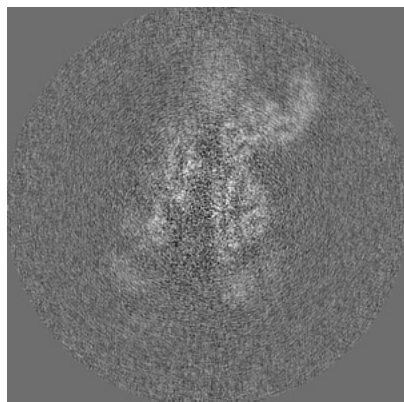


Y Index: 152

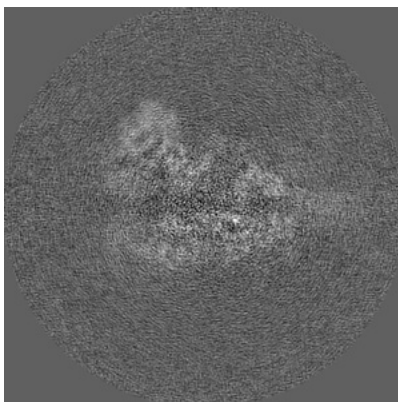


Z Index: 152

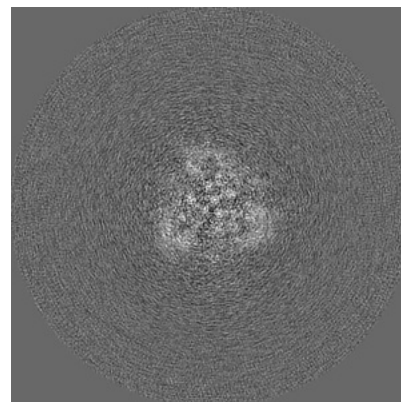
6.2.2 Raw map



X Index: 152



Y Index: 152

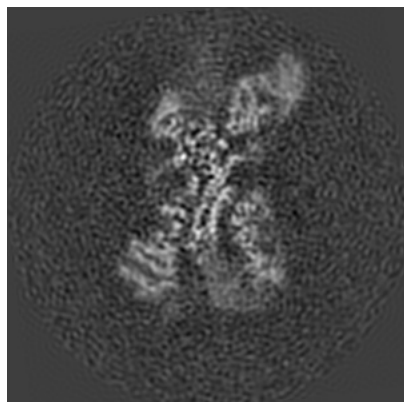


Z Index: 152

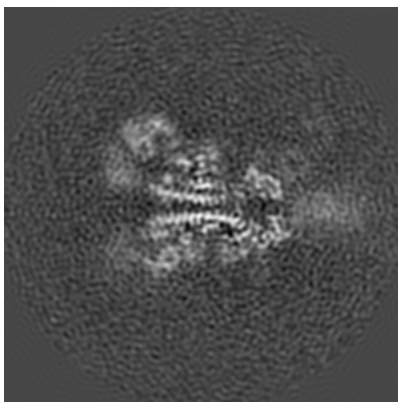
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

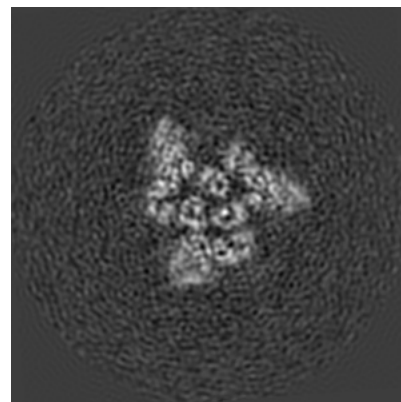
6.3.1 Primary map



X Index: 135

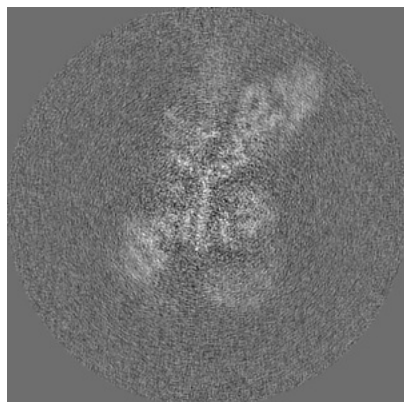


Y Index: 149

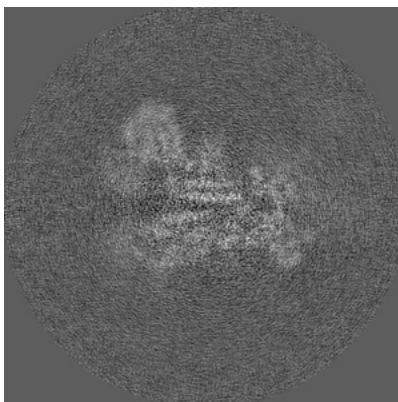


Z Index: 124

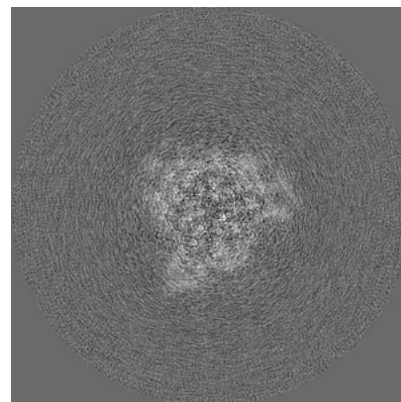
6.3.2 Raw map



X Index: 144



Y Index: 146

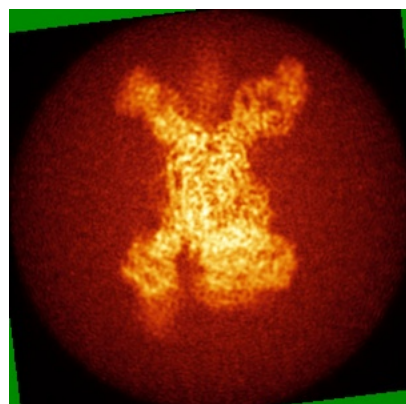


Z Index: 132

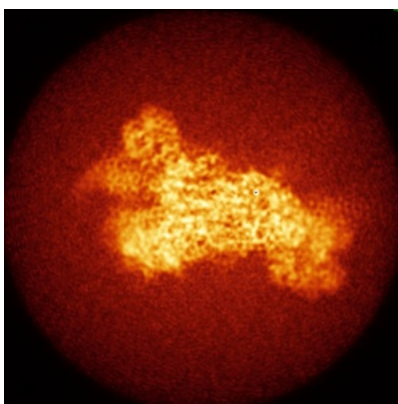
The images above show the largest variance slices of the map in three orthogonal directions.

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

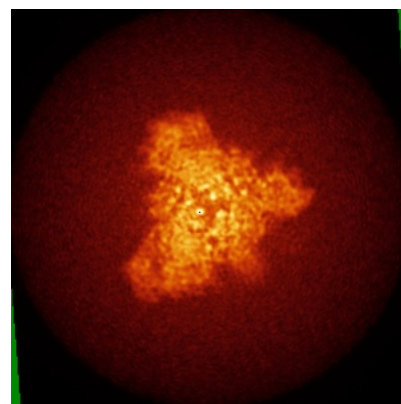
6.4.1 Primary map



X

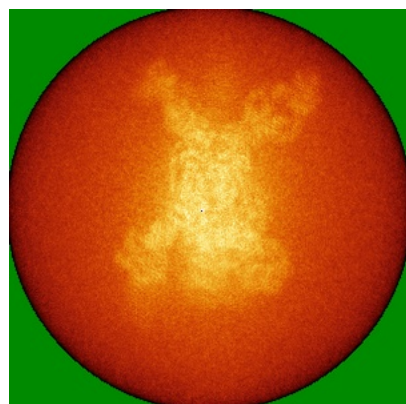


Y

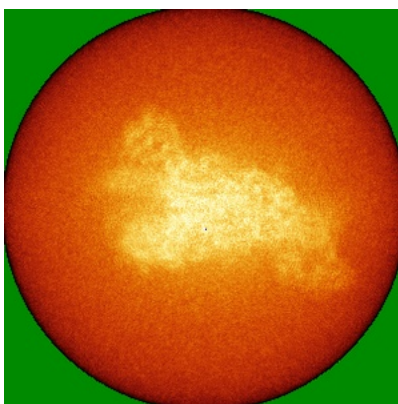


Z

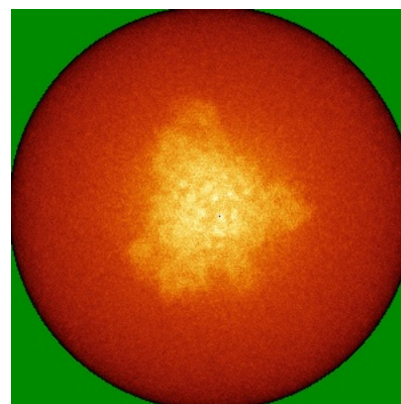
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



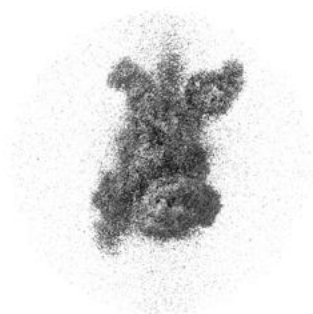
Y



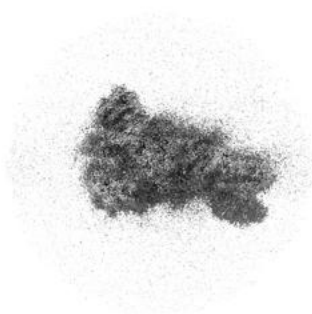
Z

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

6.5.2 Raw map



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.

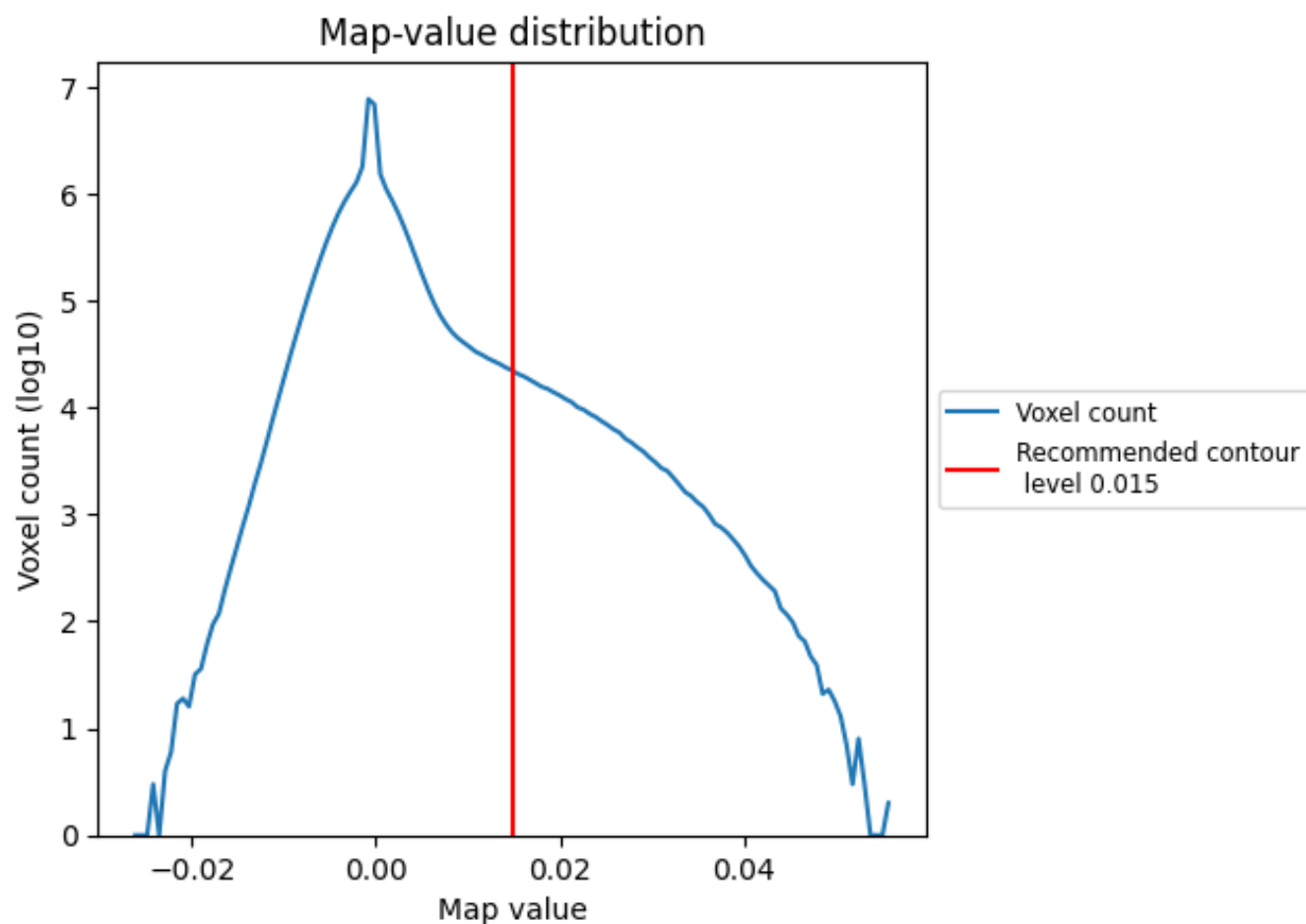
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

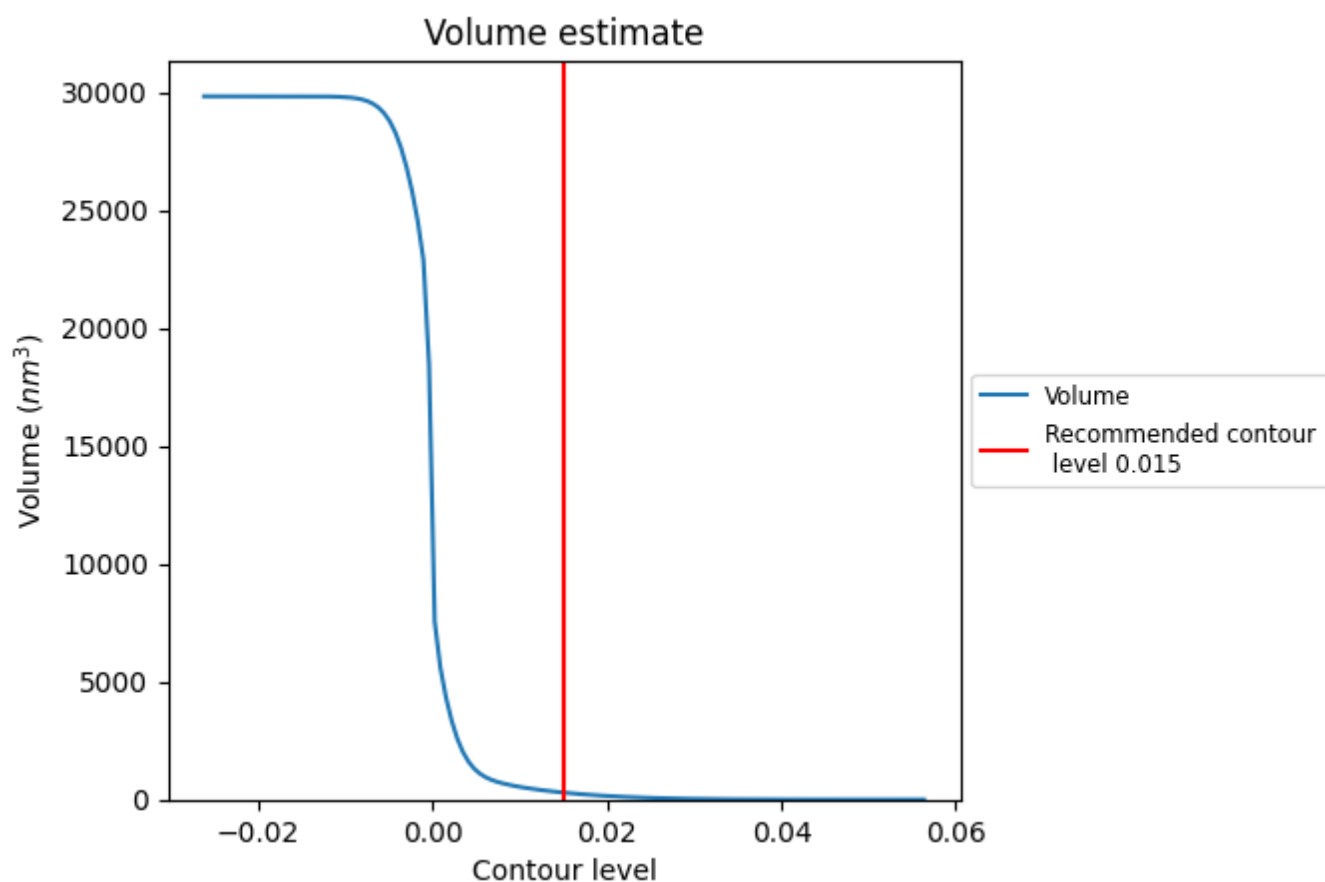
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

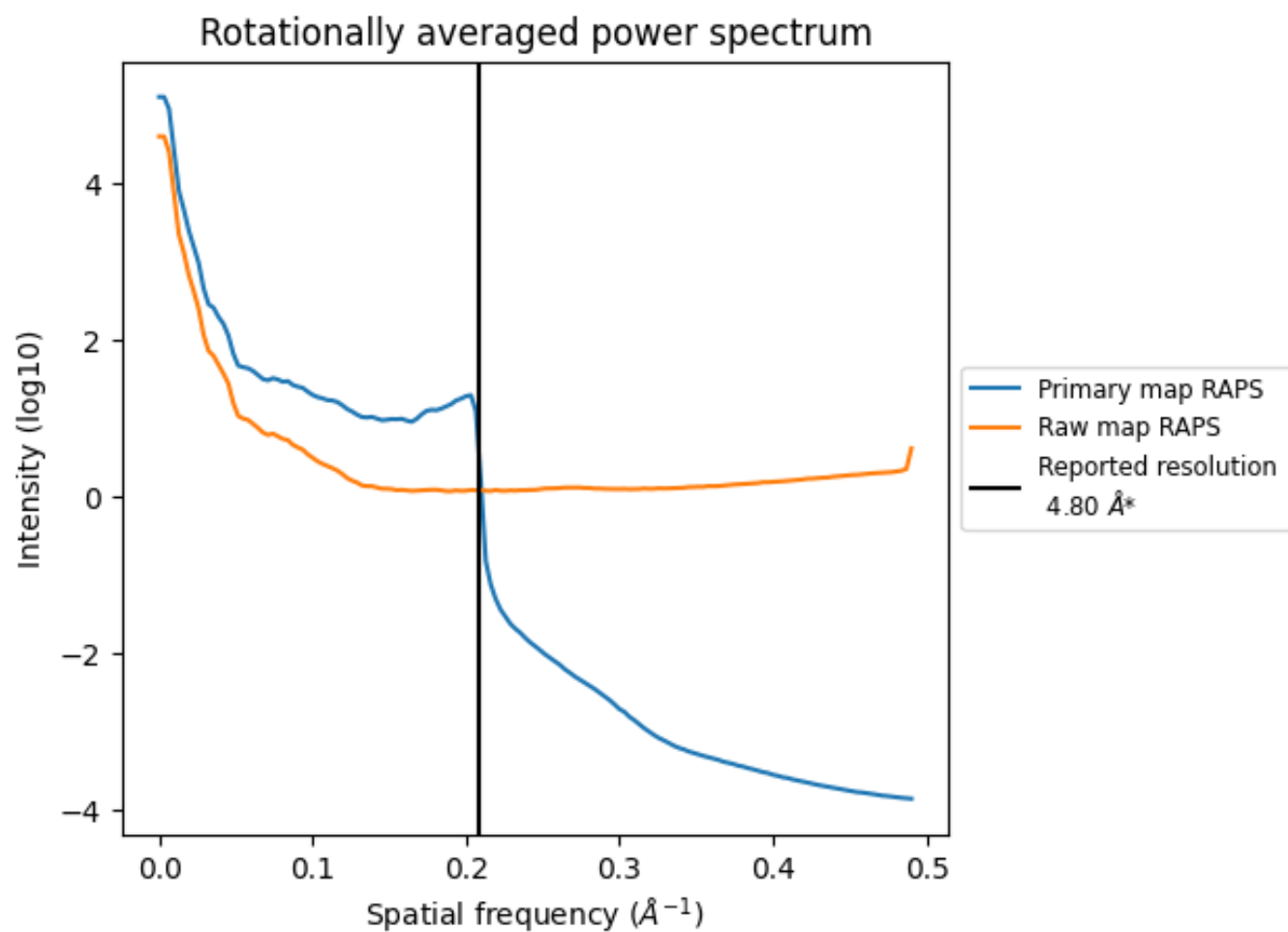
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm³; this corresponds to an approximate mass of 269 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

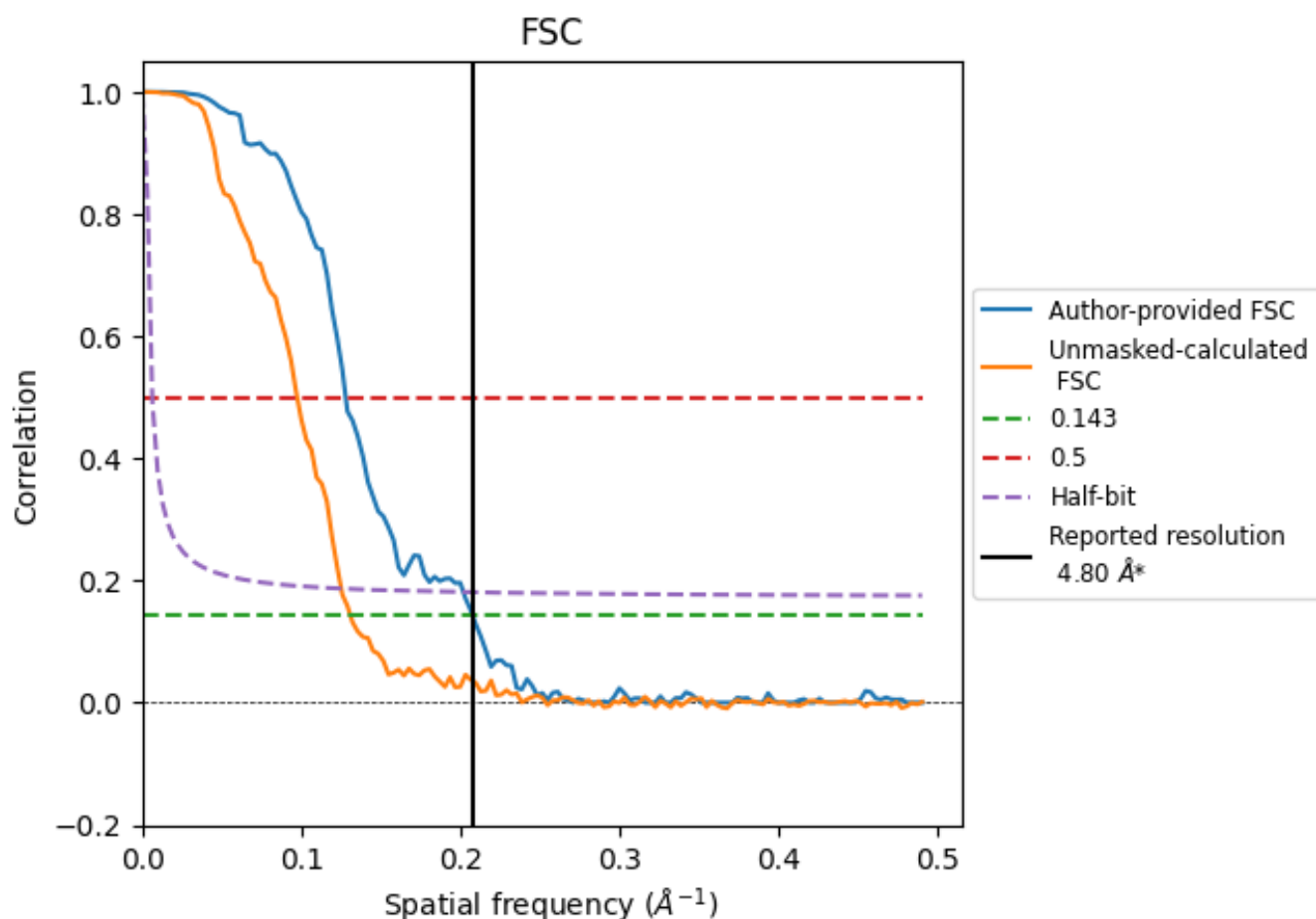


*Reported resolution corresponds to spatial frequency of $0.208 \text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.208 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

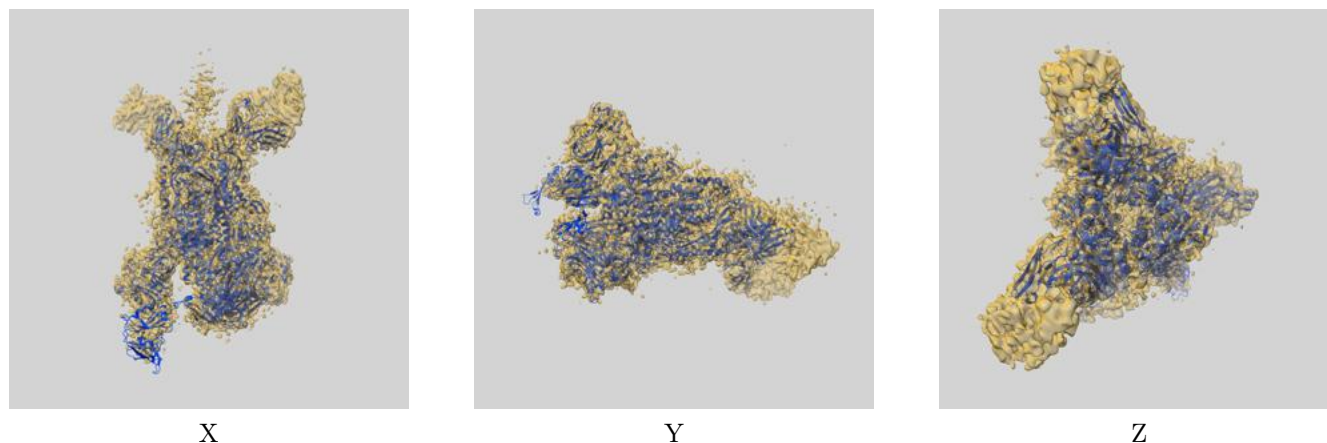
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.82	7.82	4.95
Unmasked-calculated*	7.65	10.27	7.99

*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 7.65 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

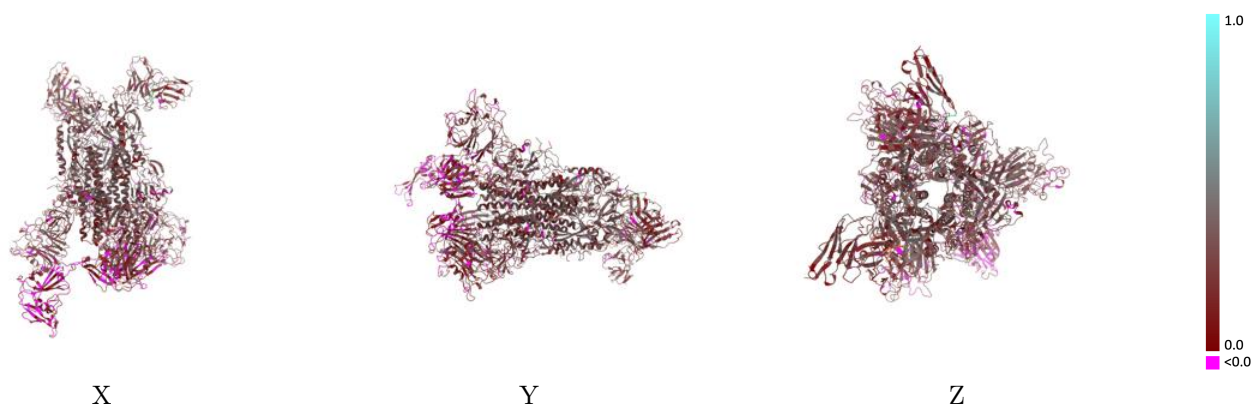
This section contains information regarding the fit between EMDB map EMD-8787 and PDB model 5W9L. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



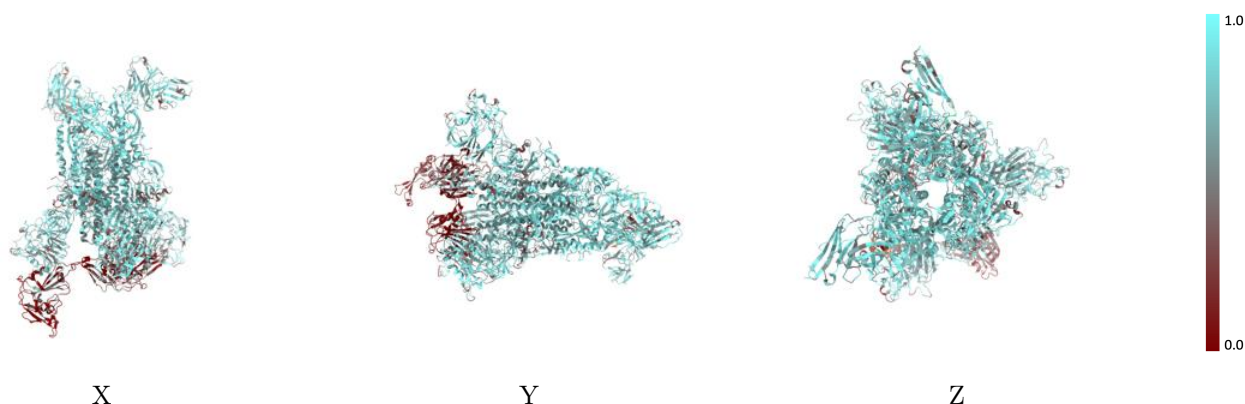
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



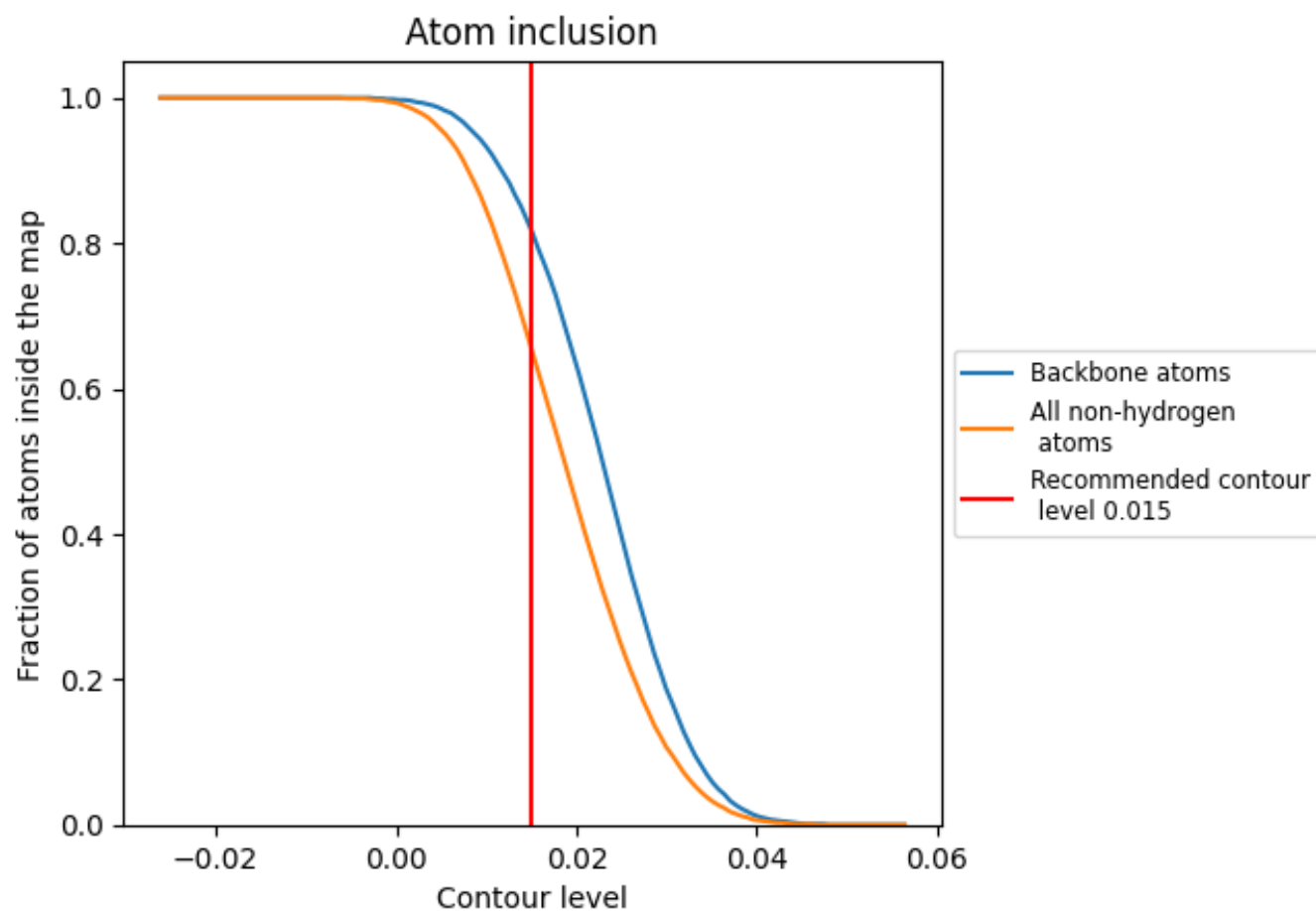
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6550	0.2370
A	0.7630	0.2970
B	0.5790	0.1900
C	0.5630	0.1960
D	0.7350	0.2910
E	0.7380	0.2580
F	0.6990	0.2260
G	0.7480	0.2990
H	0.7340	0.2410
I	0.6660	0.2420
J	0.6120	0.2140

1.0

0.0

<0.0