



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:57 PM UTC

PDB ID : 5W9J / pdb_00005w9j
EMDB ID : EMD-8785
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:

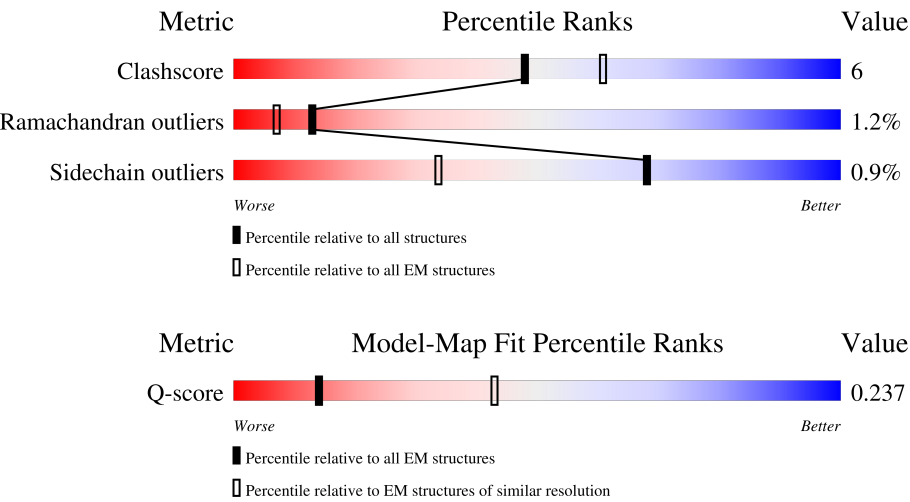
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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	D	1329	
1	G	1329	
1	J	1329	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	1329	
1	L	1329	
2	B	233	
2	E	233	
2	H	233	
3	C	218	
3	F	218	
3	I	218	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 32958 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	D	463	Total	C	N	O	S	0	0
			3545	2243	600	685	17		
1	A	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	J	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	K	726	Total	C	N	O	S	0	0
			5658	3601	926	1097	34		
1	L	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
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	conflict	UNP W5ZZF5
D	1061	PRO	LEU	conflict	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
D	1304	GLN	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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	conflict	UNP W5ZZF5
A	1061	PRO	LEU	conflict	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1304	GLN	-	expression tag	UNP W5ZZF5
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
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	conflict	UNP W5ZZF5
G	1061	PRO	LEU	conflict	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

Continued on next page...

Continued from previous page...

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
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	conflict	UNP W5ZZF5
J	1061	PRO	LEU	conflict	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
J	1300	PRO	-	expression tag	UNP W5ZZF5
J	1301	ARG	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
K	506	PHE	LEU	conflict	UNP W5ZZF5
K	748	ALA	ARG	conflict	UNP W5ZZF5
K	751	GLY	ARG	conflict	UNP W5ZZF5
K	1060	PRO	VAL	conflict	UNP W5ZZF5
K	1061	PRO	LEU	conflict	UNP W5ZZF5
K	1292	GLY	-	expression tag	UNP W5ZZF5
K	1293	SER	-	expression tag	UNP W5ZZF5
K	1294	GLY	-	expression tag	UNP W5ZZF5
K	1295	TYR	-	expression tag	UNP W5ZZF5
K	1296	ILE	-	expression tag	UNP W5ZZF5
K	1297	PRO	-	expression tag	UNP W5ZZF5
K	1298	GLU	-	expression tag	UNP W5ZZF5
K	1299	ALA	-	expression tag	UNP W5ZZF5
K	1300	PRO	-	expression tag	UNP W5ZZF5

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

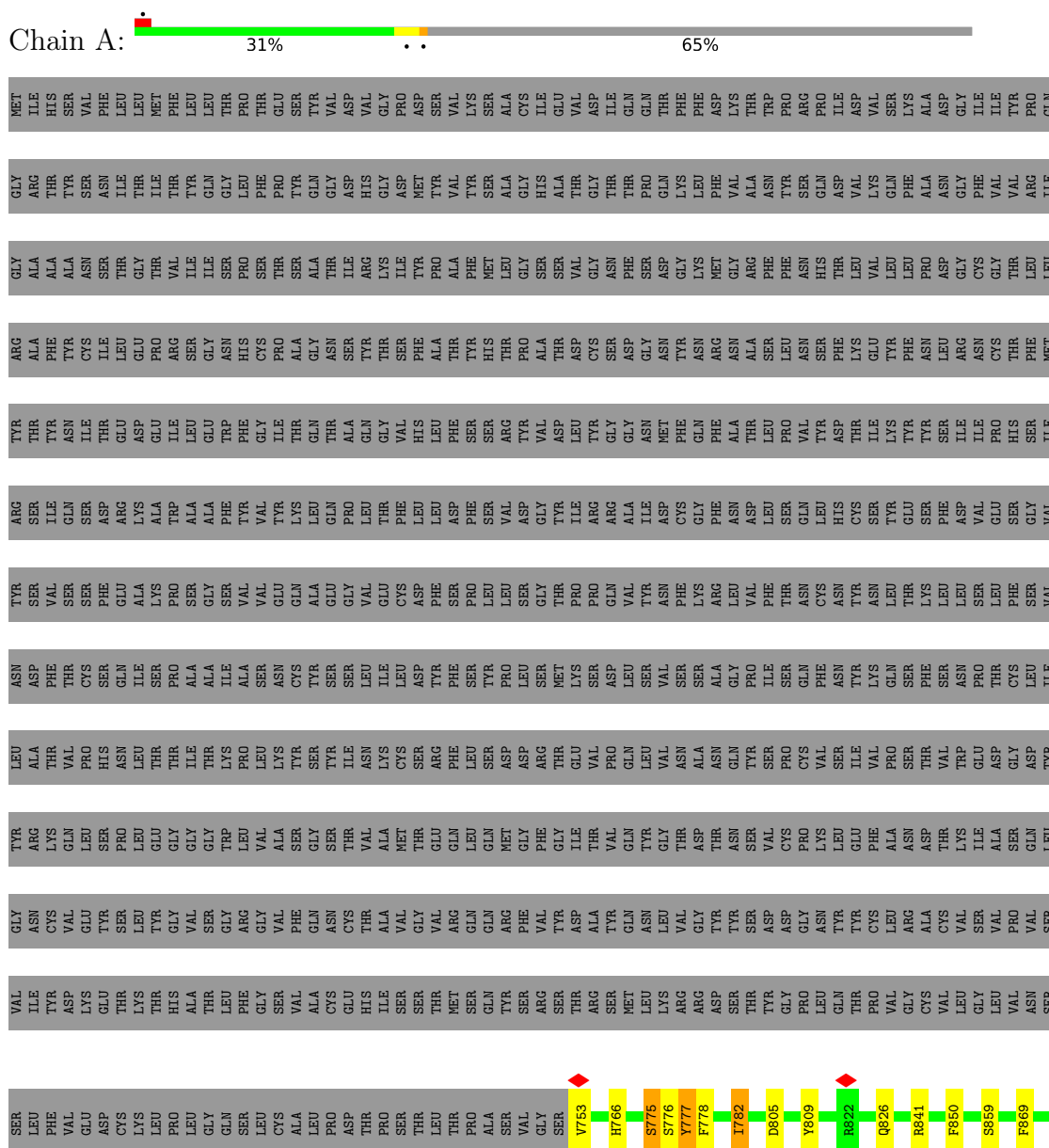
- Molecule 2 is a protein called G4 VH.

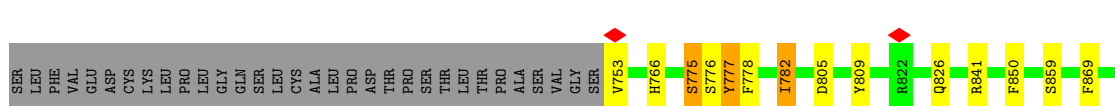
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	B	119	Total	C	N	O	S	0	0
			948	602	156	185	5		
2	H	119	Total	C	N	O	S	0	0
			948	602	156	185	5		

- Molecule 3 is a protein called G4 VL.

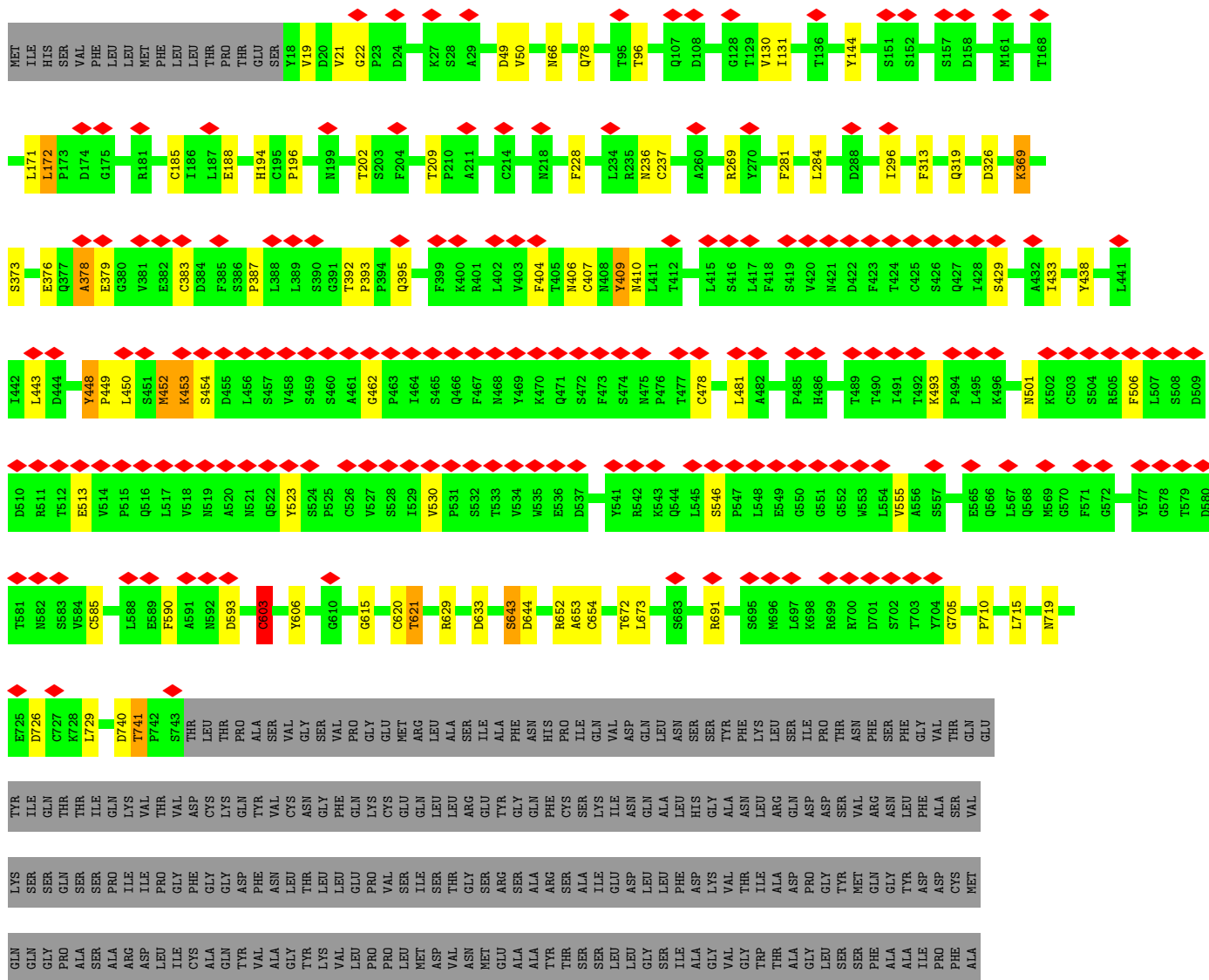
Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	C	111	Total 835	C 522	N 143	O 166	S 4	0	0
3	I	111	Total 835	C 522	N 143	O 166	S 4	0	0

- Molecule 1: Spike glycoprotein



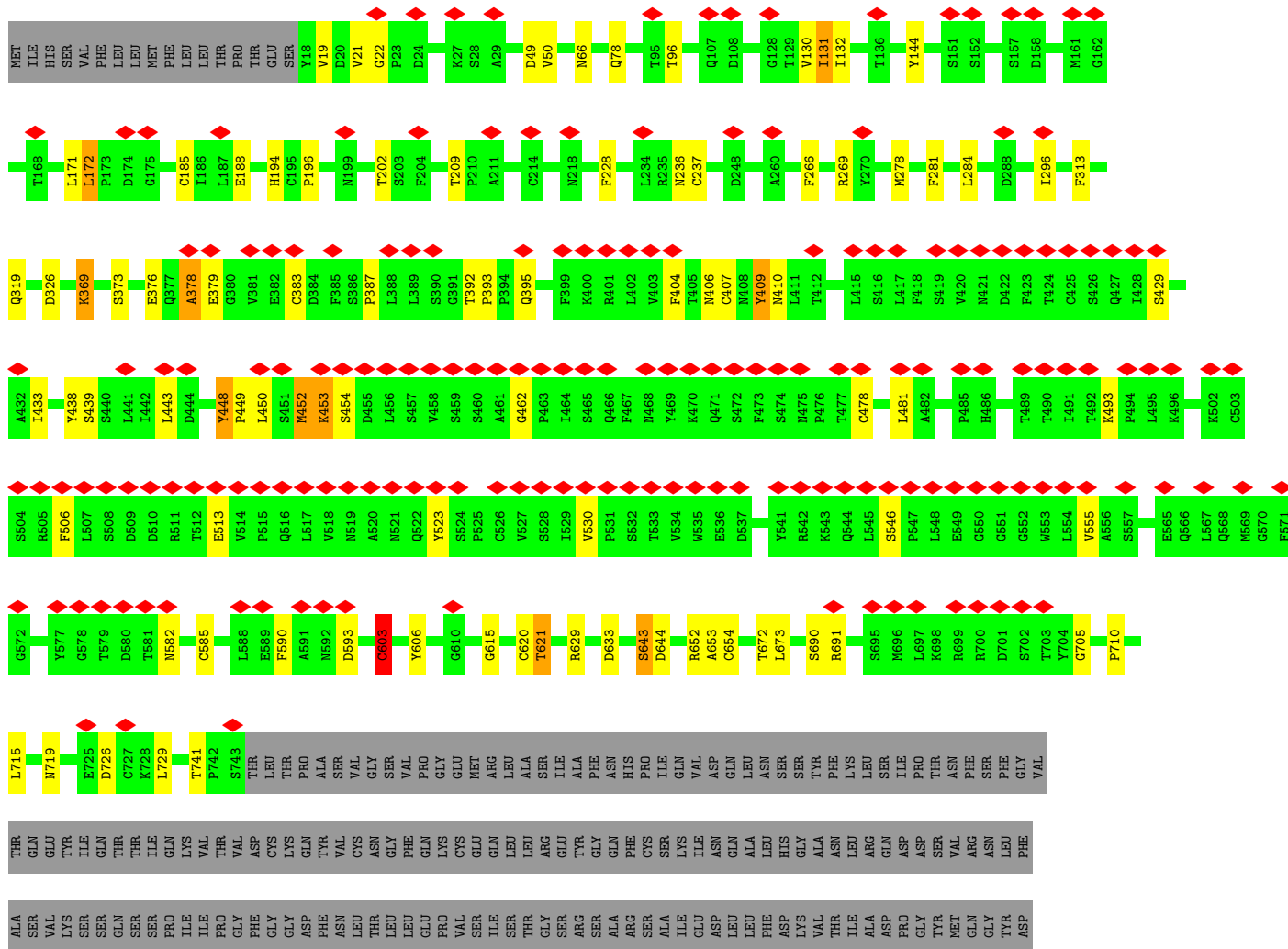


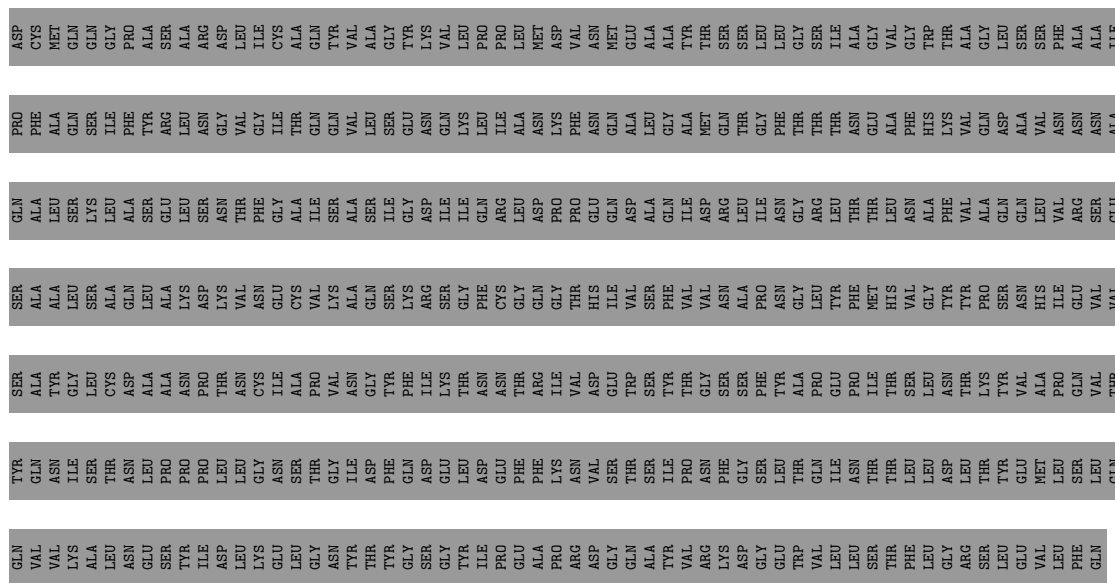
- Molecule 1: Spike glycoprotein



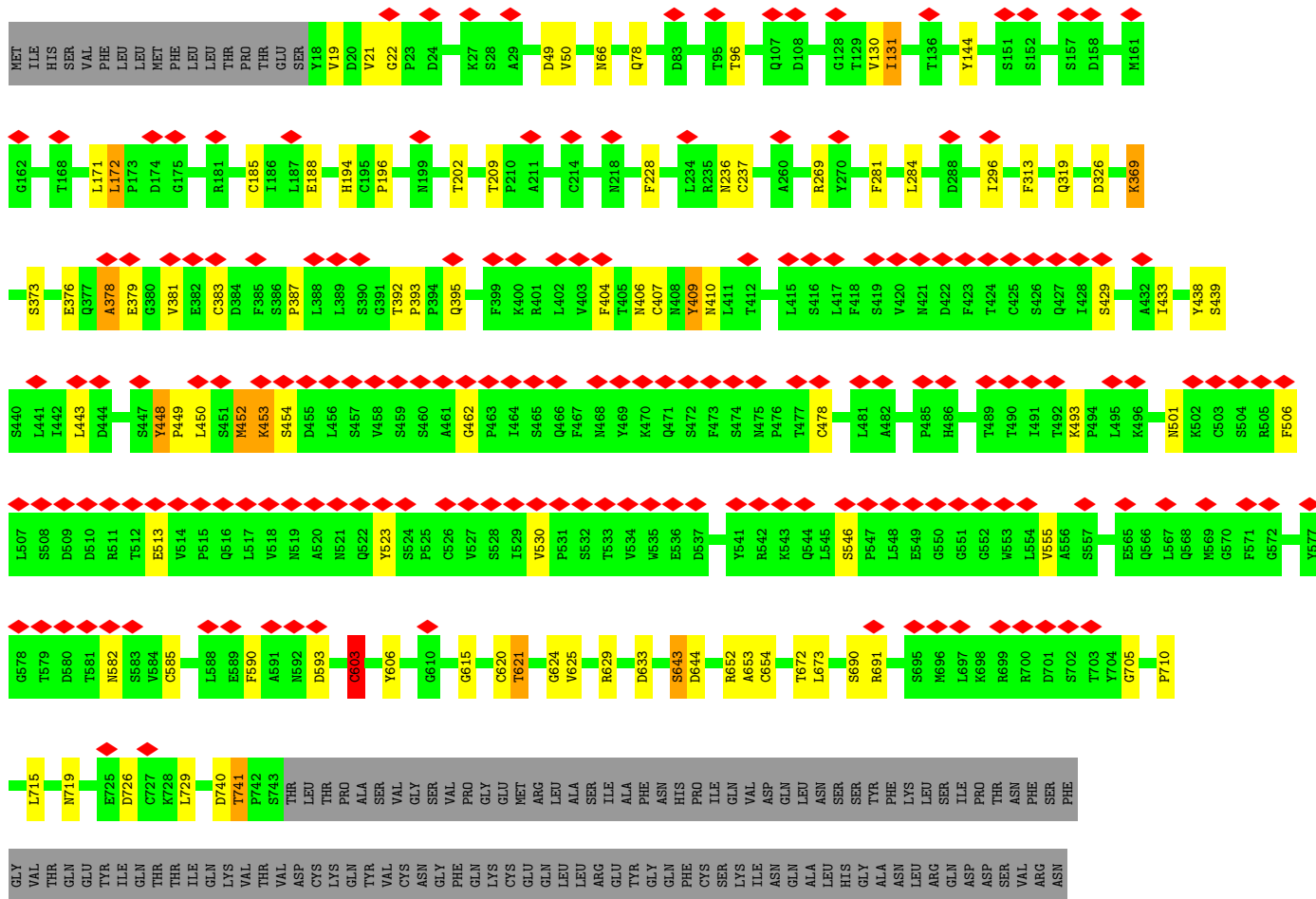
[illegible]

- Molecule 1: Spike glycoprotein



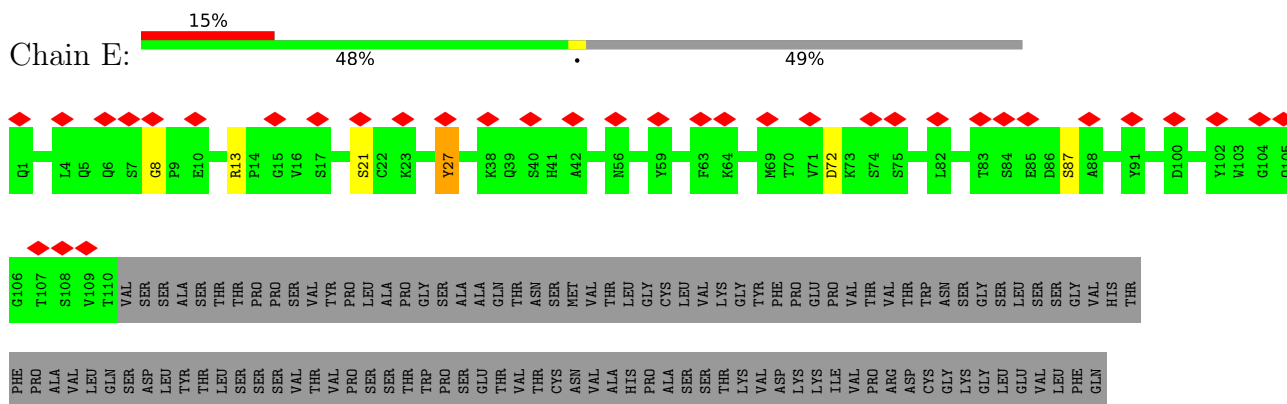


- Molecule 1: Spike glycoprotein

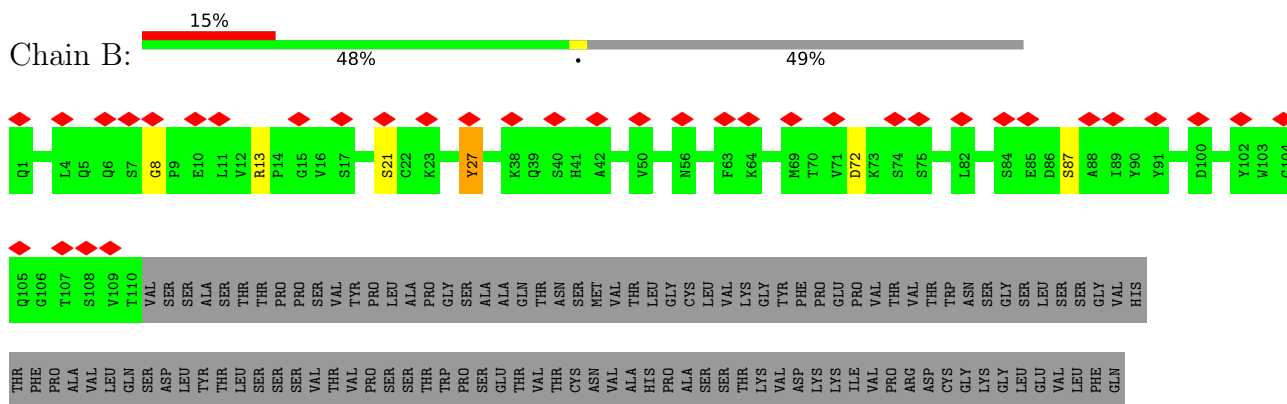


LEU	GLN	THR	VAL	VAL	VAL	SER	ASN	ALA	THR	THR	LEU
GLN	THR	VAL	THR	VAL	GLU	GLU	ALA	ILE	ASP	ASP	PHE
GLN	GLN	SER	GLN	SER	GLN	SER	GLN	PRO	ASP	ASP	ALA
VAL	GLN	ASN	ASN	ALA	ALA	ALA	LEU	ALA	CYS	MET	SER
LYS	ILE	SER	ILE	GLY	LEU	LEU	SER	GLN	GLN	GLN	LYS
ALA	THR	SER	LEU	LEU	ALA	ALA	LYS	SER	GLY	SER	SER
LEU	THR	ASN	ASN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

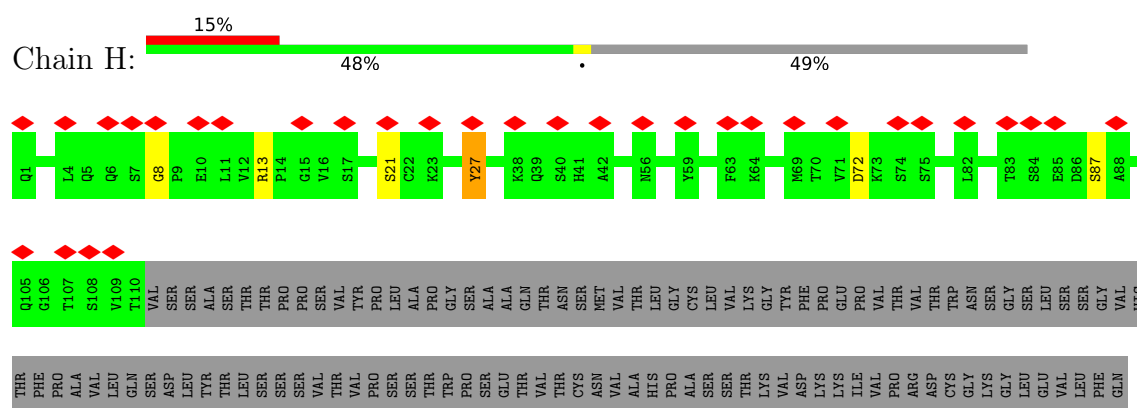
- Molecule 2: G4 VH



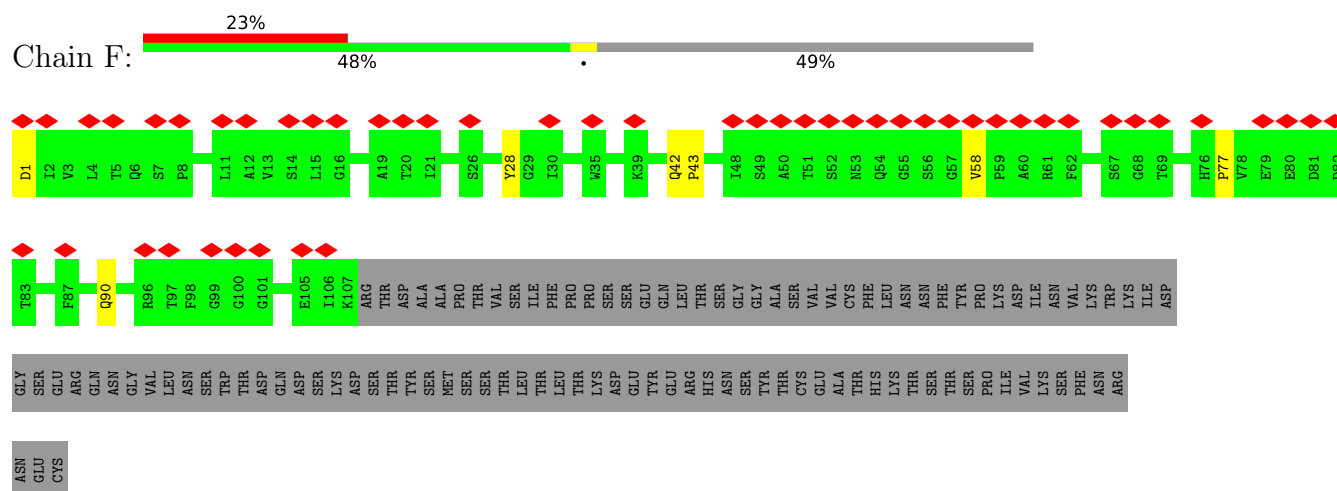
- Molecule 2: G4 VH



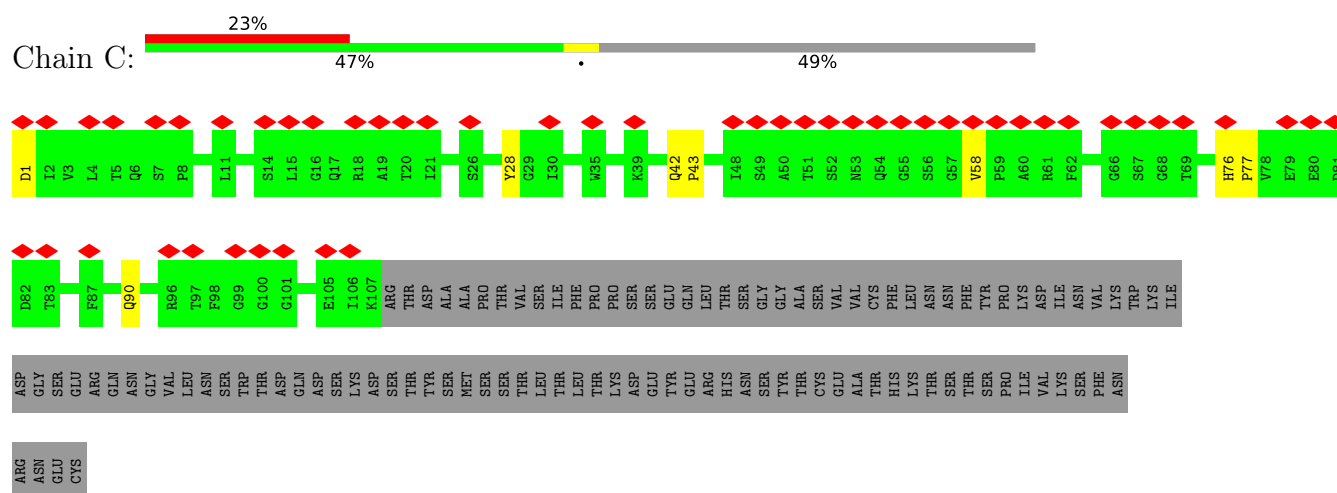
- Molecule 2: G4 VH



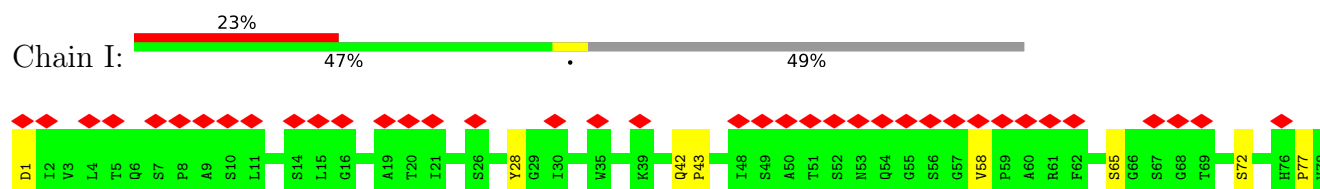
• Molecule 3: G4 VL

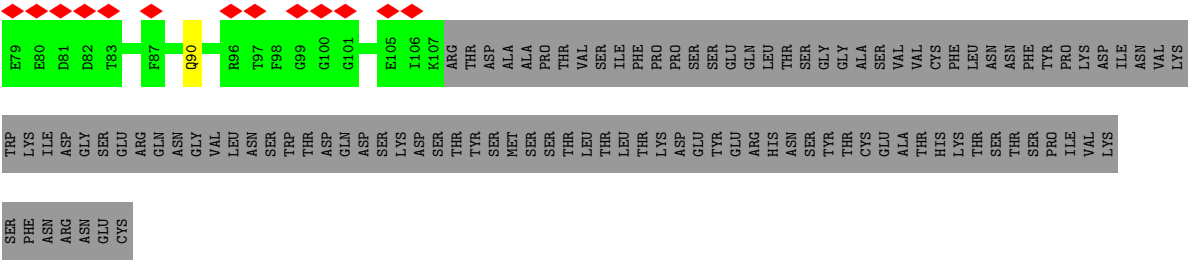


• Molecule 3: G4 VL



• Molecule 3: G4 VL





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	1988	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	0.047	Depositor
Minimum map value	-0.022	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	0/3618	1.11	27/4921 (0.5%)
1	D	0.92	0/3618	1.11	27/4921 (0.5%)
1	G	0.92	0/3618	1.11	27/4921 (0.5%)
1	J	0.86	6/5803 (0.1%)	1.17	53/7901 (0.7%)
1	K	0.86	6/5803 (0.1%)	1.17	53/7901 (0.7%)
1	L	0.86	6/5803 (0.1%)	1.18	53/7901 (0.7%)
2	B	0.78	0/972	1.09	5/1317 (0.4%)
2	E	0.78	0/972	1.09	5/1317 (0.4%)
2	H	0.78	0/972	1.10	5/1317 (0.4%)
3	C	0.79	0/852	1.20	6/1153 (0.5%)
3	F	0.80	0/852	1.20	6/1153 (0.5%)
3	I	0.79	0/852	1.20	6/1153 (0.5%)
All	All	0.87	18/33735 (0.1%)	1.15	273/45876 (0.6%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	236	ASN	CA-C	-7.48	1.45	1.53
1	L	236	ASN	CA-C	-7.45	1.45	1.53
1	J	236	ASN	CA-C	-7.39	1.45	1.53
1	K	383	CYS	C-O	-6.31	1.16	1.23
1	L	383	CYS	C-O	-6.25	1.16	1.23
1	J	438	TYR	N-CA	6.20	1.54	1.45
1	J	383	CYS	C-O	-6.19	1.16	1.23
1	L	438	TYR	N-CA	6.15	1.54	1.45
1	K	438	TYR	N-CA	6.12	1.53	1.45
1	J	383	CYS	N-CA	-5.80	1.39	1.46
1	L	383	CYS	N-CA	-5.79	1.39	1.46
1	K	383	CYS	N-CA	-5.76	1.39	1.46
1	J	585	CYS	N-CA	5.67	1.54	1.46
1	J	654	CYS	CA-C	-5.64	1.45	1.52
1	L	585	CYS	N-CA	5.64	1.54	1.46
1	L	654	CYS	CA-C	-5.64	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	654	CYS	CA-C	-5.62	1.45	1.52
1	K	585	CYS	N-CA	5.60	1.54	1.46

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	58	VAL	CA-C-N	10.16	129.96	120.21
3	C	58	VAL	C-N-CA	10.16	129.96	120.21
3	I	58	VAL	CA-C-N	10.11	129.92	120.21
3	I	58	VAL	C-N-CA	10.11	129.92	120.21
3	F	58	VAL	CA-C-N	10.11	129.92	120.21
3	F	58	VAL	C-N-CA	10.11	129.92	120.21
3	I	42	GLN	CA-C-N	9.94	126.82	119.66
3	I	42	GLN	C-N-CA	9.94	126.82	119.66
3	C	42	GLN	CA-C-N	9.92	126.80	119.66
3	C	42	GLN	C-N-CA	9.92	126.80	119.66
3	F	42	GLN	CA-C-N	9.86	126.76	119.66
3	F	42	GLN	C-N-CA	9.86	126.76	119.66
1	G	1160	ASN	CA-C-N	9.60	129.35	119.56
1	G	1160	ASN	C-N-CA	9.60	129.35	119.56
1	J	393	PRO	CA-C-N	9.58	129.51	120.03
1	J	393	PRO	C-N-CA	9.58	129.51	120.03
1	L	393	PRO	CA-C-N	9.58	129.51	120.03
1	L	393	PRO	C-N-CA	9.58	129.51	120.03
1	D	1160	ASN	CA-C-N	9.58	129.33	119.56
1	D	1160	ASN	C-N-CA	9.58	129.33	119.56
1	A	1160	ASN	CA-C-N	9.55	129.31	119.56
1	A	1160	ASN	C-N-CA	9.55	129.31	119.56
1	K	393	PRO	CA-C-N	9.53	129.46	120.03
1	K	393	PRO	C-N-CA	9.53	129.46	120.03
2	H	8	GLY	CA-C-N	8.98	128.92	119.85
2	H	8	GLY	C-N-CA	8.98	128.92	119.85
2	B	8	GLY	CA-C-N	8.95	128.89	119.85
2	B	8	GLY	C-N-CA	8.95	128.89	119.85
2	E	8	GLY	CA-C-N	8.92	128.86	119.85
2	E	8	GLY	C-N-CA	8.92	128.86	119.85
1	D	753	VAL	CA-C-N	8.60	128.54	120.03
1	D	753	VAL	C-N-CA	8.60	128.54	120.03
1	G	753	VAL	CA-C-N	8.55	128.49	120.03
1	G	753	VAL	C-N-CA	8.55	128.49	120.03
1	A	753	VAL	CA-C-N	8.52	128.47	120.03
1	A	753	VAL	C-N-CA	8.52	128.47	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	936	PRO	CA-C-N	8.50	128.44	119.85
1	G	936	PRO	C-N-CA	8.50	128.44	119.85
1	D	936	PRO	CA-C-N	8.48	128.41	119.85
1	D	936	PRO	C-N-CA	8.48	128.41	119.85
1	A	936	PRO	CA-C-N	8.47	128.41	119.85
1	A	936	PRO	C-N-CA	8.47	128.41	119.85
1	J	705	GLY	CA-C-N	8.19	128.12	119.85
1	J	705	GLY	C-N-CA	8.19	128.12	119.85
1	K	705	GLY	CA-C-N	8.16	128.10	119.85
1	K	705	GLY	C-N-CA	8.16	128.10	119.85
1	L	96	THR	CA-C-N	8.14	128.07	119.85
1	L	96	THR	C-N-CA	8.14	128.07	119.85
1	J	96	THR	CA-C-N	8.14	128.07	119.85
1	J	96	THR	C-N-CA	8.14	128.07	119.85
1	L	705	GLY	CA-C-N	8.14	128.07	119.85
1	L	705	GLY	C-N-CA	8.14	128.07	119.85
1	K	96	THR	CA-C-N	8.12	128.05	119.85
1	K	96	THR	C-N-CA	8.12	128.05	119.85
1	L	144	TYR	CA-C-N	7.73	127.66	119.85
1	L	144	TYR	C-N-CA	7.73	127.66	119.85
1	G	1219	PRO	CA-C-N	7.70	128.31	120.38
1	G	1219	PRO	C-N-CA	7.70	128.31	120.38
1	D	1219	PRO	CA-C-N	7.70	128.31	120.38
1	D	1219	PRO	C-N-CA	7.70	128.31	120.38
1	K	144	TYR	CA-C-N	7.70	127.62	119.85
1	K	144	TYR	C-N-CA	7.70	127.62	119.85
1	A	1219	PRO	CA-C-N	7.69	128.30	120.38
1	A	1219	PRO	C-N-CA	7.69	128.30	120.38
1	J	144	TYR	CA-C-N	7.65	127.61	120.03
1	J	144	TYR	C-N-CA	7.65	127.61	120.03
1	J	530	VAL	CA-C-N	7.64	127.65	119.78
1	J	530	VAL	C-N-CA	7.64	127.65	119.78
1	L	429	SER	CA-C-N	7.63	127.68	119.28
1	L	429	SER	C-N-CA	7.63	127.68	119.28
1	K	429	SER	CA-C-N	7.63	127.67	119.28
1	K	429	SER	C-N-CA	7.63	127.67	119.28
1	K	530	VAL	CA-C-N	7.62	127.62	119.78
1	K	530	VAL	C-N-CA	7.62	127.62	119.78
1	J	429	SER	CA-C-N	7.61	127.65	119.28
1	J	429	SER	C-N-CA	7.61	127.65	119.28
1	L	530	VAL	CA-C-N	7.60	127.61	119.78
1	L	530	VAL	C-N-CA	7.60	127.61	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	22	GLY	CA-C-N	7.44	127.44	119.78
1	J	22	GLY	C-N-CA	7.44	127.44	119.78
1	L	22	GLY	CA-C-N	7.43	127.43	119.78
1	L	22	GLY	C-N-CA	7.43	127.43	119.78
1	K	22	GLY	CA-C-N	7.41	127.41	119.78
1	K	22	GLY	C-N-CA	7.41	127.41	119.78
1	L	209	THR	CA-C-N	7.41	129.10	119.84
1	L	209	THR	C-N-CA	7.41	129.10	119.84
3	I	43	PRO	CA-C-N	7.39	127.31	119.85
3	I	43	PRO	C-N-CA	7.39	127.31	119.85
1	J	209	THR	CA-C-N	7.39	129.08	119.84
1	J	209	THR	C-N-CA	7.39	129.08	119.84
1	K	209	THR	CA-C-N	7.37	129.05	119.84
1	K	209	THR	C-N-CA	7.37	129.05	119.84
1	G	766	HIS	CA-C-N	7.36	127.29	119.85
1	G	766	HIS	C-N-CA	7.36	127.29	119.85
1	J	462	GLY	CA-C-N	7.36	128.00	119.47
1	J	462	GLY	C-N-CA	7.36	128.00	119.47
1	K	462	GLY	CA-C-N	7.35	127.99	119.47
1	K	462	GLY	C-N-CA	7.35	127.99	119.47
1	L	462	GLY	CA-C-N	7.34	127.99	119.47
1	L	462	GLY	C-N-CA	7.34	127.99	119.47
3	C	43	PRO	CA-C-N	7.34	127.26	119.85
3	C	43	PRO	C-N-CA	7.34	127.26	119.85
1	D	766	HIS	CA-C-N	7.33	127.26	119.85
1	D	766	HIS	C-N-CA	7.33	127.26	119.85
3	F	43	PRO	CA-C-N	7.32	127.25	119.85
3	F	43	PRO	C-N-CA	7.32	127.25	119.85
1	A	766	HIS	CA-C-N	7.32	127.24	119.85
1	A	766	HIS	C-N-CA	7.32	127.24	119.85
1	L	296	ILE	CA-C-N	7.25	127.01	119.76
1	L	296	ILE	C-N-CA	7.25	127.01	119.76
1	J	296	ILE	CA-C-N	7.24	127.00	119.76
1	J	296	ILE	C-N-CA	7.24	127.00	119.76
1	K	296	ILE	CA-C-N	7.20	126.96	119.76
1	K	296	ILE	C-N-CA	7.20	126.96	119.76
1	K	729	LEU	CA-C-N	7.02	126.99	119.76
1	K	729	LEU	C-N-CA	7.02	126.99	119.76
1	L	729	LEU	CA-C-N	7.02	126.99	119.76
1	L	729	LEU	C-N-CA	7.02	126.99	119.76
1	J	729	LEU	CA-C-N	7.01	126.98	119.76
1	J	729	LEU	C-N-CA	7.01	126.98	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	369	LYS	CA-C-N	6.99	126.97	119.78
1	J	369	LYS	C-N-CA	6.99	126.97	119.78
1	L	369	LYS	CA-C-N	6.98	126.97	119.78
1	L	369	LYS	C-N-CA	6.98	126.97	119.78
1	K	369	LYS	CA-C-N	6.93	126.92	119.78
1	K	369	LYS	C-N-CA	6.93	126.92	119.78
1	J	373	SER	N-CA-C	6.67	119.33	110.53
1	K	373	SER	N-CA-C	6.64	119.30	110.53
1	L	373	SER	N-CA-C	6.61	119.25	110.53
1	J	378	ALA	CA-C-N	6.58	133.54	121.70
1	J	378	ALA	C-N-CA	6.58	133.54	121.70
1	K	378	ALA	CA-C-N	6.56	133.51	121.70
1	K	378	ALA	C-N-CA	6.56	133.51	121.70
1	L	378	ALA	CA-C-N	6.55	133.50	121.70
1	L	378	ALA	C-N-CA	6.55	133.50	121.70
1	L	448	TYR	CA-C-N	6.45	127.90	119.84
1	L	448	TYR	C-N-CA	6.45	127.90	119.84
1	L	392	THR	CA-C-N	6.44	124.30	119.66
1	L	392	THR	C-N-CA	6.44	124.30	119.66
1	K	448	TYR	CA-C-N	6.43	127.87	119.84
1	K	448	TYR	C-N-CA	6.43	127.87	119.84
1	J	392	THR	CA-C-N	6.42	124.28	119.66
1	J	392	THR	C-N-CA	6.42	124.28	119.66
1	K	392	THR	CA-C-N	6.41	124.27	119.66
1	K	392	THR	C-N-CA	6.41	124.27	119.66
1	J	448	TYR	CA-C-N	6.40	127.84	119.84
1	J	448	TYR	C-N-CA	6.40	127.84	119.84
1	L	284	LEU	CA-C-N	6.40	128.63	120.89
1	L	284	LEU	C-N-CA	6.40	128.63	120.89
1	K	284	LEU	CA-C-N	6.37	128.60	120.89
1	K	284	LEU	C-N-CA	6.37	128.60	120.89
1	J	284	LEU	CA-C-N	6.37	128.59	120.89
1	J	284	LEU	C-N-CA	6.37	128.59	120.89
1	L	188	GLU	CA-C-N	6.35	126.32	119.78
1	L	188	GLU	C-N-CA	6.35	126.32	119.78
1	J	188	GLU	CA-C-N	6.32	126.29	119.78
1	J	188	GLU	C-N-CA	6.32	126.29	119.78
1	K	188	GLU	CA-C-N	6.32	126.29	119.78
1	K	188	GLU	C-N-CA	6.32	126.29	119.78
1	G	1206	ALA	CA-C-N	6.29	126.20	119.85
1	G	1206	ALA	C-N-CA	6.29	126.20	119.85
1	J	319	GLN	CA-C-N	6.26	127.67	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	319	GLN	C-N-CA	6.26	127.67	119.84
1	A	1206	ALA	CA-C-N	6.25	126.16	119.85
1	A	1206	ALA	C-N-CA	6.25	126.16	119.85
1	K	319	GLN	CA-C-N	6.24	127.64	119.84
1	K	319	GLN	C-N-CA	6.24	127.64	119.84
1	D	1206	ALA	CA-C-N	6.23	126.15	119.85
1	D	1206	ALA	C-N-CA	6.23	126.15	119.85
1	L	319	GLN	CA-C-N	6.22	127.62	119.84
1	L	319	GLN	C-N-CA	6.22	127.62	119.84
1	A	970	ILE	CA-C-N	6.13	127.50	119.84
1	A	970	ILE	C-N-CA	6.13	127.50	119.84
2	E	13	ARG	CA-C-N	6.13	126.04	119.85
2	E	13	ARG	C-N-CA	6.13	126.04	119.85
1	D	970	ILE	CA-C-N	6.12	127.49	119.84
1	D	970	ILE	C-N-CA	6.12	127.49	119.84
2	H	13	ARG	CA-C-N	6.09	126.00	119.85
2	H	13	ARG	C-N-CA	6.09	126.00	119.85
1	G	970	ILE	CA-C-N	6.09	127.45	119.84
1	G	970	ILE	C-N-CA	6.09	127.45	119.84
2	B	13	ARG	CA-C-N	6.07	125.98	119.85
2	B	13	ARG	C-N-CA	6.07	125.98	119.85
1	D	1142	TYR	CA-C-N	6.04	126.00	119.78
1	D	1142	TYR	C-N-CA	6.04	126.00	119.78
1	A	1142	TYR	CA-C-N	6.04	126.00	119.78
1	A	1142	TYR	C-N-CA	6.04	126.00	119.78
1	J	406	ASN	CA-C-N	-6.04	111.96	121.87
1	J	406	ASN	C-N-CA	-6.04	111.96	121.87
1	G	1142	TYR	CA-C-N	6.01	125.97	119.78
1	G	1142	TYR	C-N-CA	6.01	125.97	119.78
1	K	406	ASN	CA-C-N	-6.01	112.02	121.87
1	K	406	ASN	C-N-CA	-6.01	112.02	121.87
1	L	406	ASN	CA-C-N	-6.00	112.03	121.87
1	L	406	ASN	C-N-CA	-6.00	112.03	121.87
1	K	493	LYS	CA-C-N	5.99	125.95	119.78
1	K	493	LYS	C-N-CA	5.99	125.95	119.78
1	L	493	LYS	CA-C-N	5.98	125.94	119.78
1	L	493	LYS	C-N-CA	5.98	125.94	119.78
1	J	493	LYS	CA-C-N	5.98	125.94	119.78
1	J	493	LYS	C-N-CA	5.98	125.94	119.78
1	J	409	TYR	N-CA-C	5.97	118.04	109.14
1	L	409	TYR	N-CA-C	5.95	118.01	109.14
1	K	409	TYR	N-CA-C	5.94	118.00	109.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	850	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	850	PHE	CA-CB-CG	-5.86	107.94	113.80
1	G	850	PHE	CA-CB-CG	-5.85	107.95	113.80
1	D	935	LEU	CA-C-N	5.80	126.35	120.38
1	D	935	LEU	C-N-CA	5.80	126.35	120.38
1	A	935	LEU	CA-C-N	5.79	126.35	120.38
1	A	935	LEU	C-N-CA	5.79	126.35	120.38
1	G	935	LEU	CA-C-N	5.77	126.32	120.38
1	G	935	LEU	C-N-CA	5.77	126.32	120.38
1	L	643	SER	N-CA-C	5.59	117.91	110.53
1	J	643	SER	N-CA-C	5.58	117.90	110.53
1	K	643	SER	N-CA-C	5.58	117.90	110.53
1	G	1060	PRO	N-CA-C	5.48	117.39	110.70
1	A	859	SER	CA-C-N	5.47	125.37	119.85
1	A	859	SER	C-N-CA	5.47	125.37	119.85
1	A	1060	PRO	N-CA-C	5.46	117.37	110.70
1	G	859	SER	CA-C-N	5.46	125.37	119.85
1	G	859	SER	C-N-CA	5.46	125.37	119.85
1	D	1060	PRO	N-CA-C	5.46	117.36	110.70
1	J	603	CYS	CA-C-N	5.44	128.47	120.91
1	J	603	CYS	C-N-CA	5.44	128.47	120.91
1	K	603	CYS	CA-C-N	5.42	128.45	120.91
1	K	603	CYS	C-N-CA	5.42	128.45	120.91
1	G	1060	PRO	CA-C-N	5.42	125.06	119.05
1	G	1060	PRO	C-N-CA	5.42	125.06	119.05
1	L	603	CYS	CA-C-N	5.41	128.44	120.91
1	L	603	CYS	C-N-CA	5.41	128.44	120.91
1	A	1060	PRO	CA-C-N	5.41	125.06	119.05
1	A	1060	PRO	C-N-CA	5.41	125.06	119.05
1	L	172	LEU	CA-C-N	5.40	125.30	119.85
1	L	172	LEU	C-N-CA	5.40	125.30	119.85
1	D	859	SER	CA-C-N	5.39	125.30	119.85
1	D	859	SER	C-N-CA	5.39	125.30	119.85
1	D	1060	PRO	CA-C-N	5.38	125.03	119.05
1	D	1060	PRO	C-N-CA	5.38	125.03	119.05
1	J	172	LEU	CA-C-N	5.38	125.28	119.85
1	J	172	LEU	C-N-CA	5.38	125.28	119.85
1	K	172	LEU	CA-C-N	5.36	125.26	119.85
1	K	172	LEU	C-N-CA	5.36	125.26	119.85
1	J	546	SER	CA-C-N	5.32	125.14	119.28
1	J	546	SER	C-N-CA	5.32	125.14	119.28
1	D	869	PHE	CA-CB-CG	-5.31	108.49	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	546	SER	CA-C-N	5.29	125.10	119.28
1	L	546	SER	C-N-CA	5.29	125.10	119.28
1	A	869	PHE	CA-CB-CG	-5.28	108.52	113.80
1	G	869	PHE	CA-CB-CG	-5.26	108.54	113.80
1	K	546	SER	CA-C-N	5.26	125.07	119.28
1	K	546	SER	C-N-CA	5.26	125.07	119.28
1	K	653	ALA	CB-CA-C	-5.26	110.50	116.54
1	G	782	ILE	CA-C-N	5.24	125.00	119.76
1	G	782	ILE	C-N-CA	5.24	125.00	119.76
1	J	741	THR	CA-C-N	5.24	125.17	119.78
1	J	741	THR	C-N-CA	5.24	125.17	119.78
1	A	782	ILE	CA-C-N	5.24	125.00	119.76
1	A	782	ILE	C-N-CA	5.24	125.00	119.76
1	L	653	ALA	CB-CA-C	-5.23	110.52	116.54
1	J	653	ALA	CB-CA-C	-5.22	110.53	116.54
1	L	741	THR	CA-C-N	5.21	125.14	119.78
1	L	741	THR	C-N-CA	5.21	125.14	119.78
1	D	782	ILE	CA-C-N	5.20	124.96	119.76
1	D	782	ILE	C-N-CA	5.20	124.96	119.76
1	K	741	THR	CA-C-N	5.20	125.14	119.78
1	K	741	THR	C-N-CA	5.20	125.14	119.78
1	J	593	ASP	CA-CB-CG	5.19	117.79	112.60
1	K	593	ASP	CA-CB-CG	5.19	117.79	112.60
1	L	593	ASP	CA-CB-CG	5.15	117.75	112.60
2	E	21	SER	N-CA-C	5.07	116.89	109.24
2	H	21	SER	N-CA-C	5.06	116.88	109.24
2	B	21	SER	N-CA-C	5.05	116.86	109.24

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	3545	0	3471	35	0
1	D	3545	0	3471	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3545	0	3471	34	0
1	J	5658	0	5425	79	0
1	K	5658	0	5425	85	0
1	L	5658	0	5425	85	0
2	B	948	0	904	4	0
2	E	948	0	904	4	0
2	H	948	0	904	4	0
3	C	835	0	816	5	0
3	F	835	0	816	4	0
3	I	835	0	816	5	0
All	All	32958	0	31848	374	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 6.

All (374) 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:K:506:PHE:CE2	1:K:555:VAL:HG21	1.01	1.54
1:L:506:PHE:CE2	1:L:555:VAL:HG21	1.01	1.52
1:L:506:PHE:CE2	1:L:555:VAL:CG2	1.93	1.51
1:J:506:PHE:CE2	1:J:555:VAL:CG2	1.88	1.50
1:K:506:PHE:CE2	1:K:555:VAL:CG2	1.93	1.49
1:J:506:PHE:CE2	1:J:555:VAL:HG21	0.96	1.48
1:L:506:PHE:HE2	1:L:555:VAL:CG2	1.31	1.37
1:J:506:PHE:CD2	1:J:555:VAL:HG21	1.63	1.33
1:K:506:PHE:HE2	1:K:555:VAL:CG2	1.31	1.32
1:K:506:PHE:CD2	1:K:555:VAL:HG21	1.63	1.31
1:L:506:PHE:CD2	1:L:555:VAL:HG21	1.63	1.31
1:J:506:PHE:HE2	1:J:555:VAL:CG2	1.25	1.29
1:K:506:PHE:CE1	1:K:513:GLU:OE1	1.88	1.25
1:L:506:PHE:CE1	1:L:513:GLU:OE1	1.88	1.25
1:J:506:PHE:CE1	1:J:513:GLU:OE1	1.88	1.24
1:J:506:PHE:CD2	1:J:555:VAL:CG2	2.23	1.20
1:K:506:PHE:CD2	1:K:555:VAL:CG2	2.24	1.15
1:L:506:PHE:CD2	1:L:555:VAL:CG2	2.24	1.15
1:A:909:TYR:HD1	1:A:909:TYR:O	1.37	1.05
1:G:909:TYR:HD1	1:G:909:TYR:O	1.37	1.04
1:D:909:TYR:O	1:D:909:TYR:HD1	1.37	1.03
1:L:185:CYS:HG	1:L:237:CYS:HG	1.00	0.96
1:D:986:THR:HG21	1:D:1195:GLU:OE2	1.66	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:986:THR:HG21	1:G:1195:GLU:OE2	1.66	0.96
1:A:986:THR:HG21	1:A:1195:GLU:OE2	1.66	0.96
1:L:603:CYS:SG	1:L:603:CYS:O	2.26	0.94
1:K:603:CYS:O	1:K:603:CYS:SG	2.26	0.93
1:D:914:GLN:O	1:D:914:GLN:HG3	1.68	0.93
1:J:603:CYS:SG	1:J:603:CYS:O	2.26	0.92
1:A:914:GLN:HG3	1:A:914:GLN:O	1.68	0.92
1:G:914:GLN:O	1:G:914:GLN:HG3	1.68	0.91
1:J:185:CYS:HG	1:J:237:CYS:HG	1.08	0.91
1:J:506:PHE:CD2	1:J:555:VAL:HG23	2.07	0.87
1:G:909:TYR:O	1:G:909:TYR:CD1	2.27	0.87
1:D:909:TYR:O	1:D:909:TYR:CD1	2.27	0.86
1:K:691:ARG:HA	1:K:691:ARG:NE	1.90	0.86
1:A:909:TYR:O	1:A:909:TYR:CD1	2.27	0.86
1:K:506:PHE:CD2	1:K:555:VAL:HG23	2.10	0.86
1:J:691:ARG:HA	1:J:691:ARG:NE	1.91	0.85
1:J:506:PHE:HE2	1:J:555:VAL:CB	1.89	0.85
1:L:691:ARG:HA	1:L:691:ARG:NE	1.90	0.85
1:L:506:PHE:CD2	1:L:555:VAL:HG23	2.10	0.84
1:L:506:PHE:HE2	1:L:555:VAL:CB	1.91	0.83
1:K:452:MET:C	1:K:454:SER:H	1.86	0.83
1:K:506:PHE:HE2	1:K:555:VAL:CB	1.92	0.83
1:L:452:MET:C	1:L:454:SER:H	1.86	0.82
1:K:185:CYS:HG	1:K:237:CYS:HG	1.27	0.81
1:J:452:MET:C	1:J:454:SER:H	1.86	0.81
1:J:506:PHE:CE2	1:J:555:VAL:CB	2.65	0.79
1:L:448:TYR:CE2	1:L:453:LYS:HA	2.19	0.78
1:K:450:LEU:C	1:K:453:LYS:HG2	2.09	0.78
1:J:450:LEU:C	1:J:453:LYS:HG2	2.09	0.78
1:L:450:LEU:C	1:L:453:LYS:HG2	2.09	0.78
1:L:506:PHE:HD2	1:L:555:VAL:HG23	1.49	0.78
1:K:448:TYR:CE2	1:K:453:LYS:HA	2.19	0.77
1:A:909:TYR:HD1	1:A:909:TYR:C	1.91	0.77
1:L:450:LEU:O	1:L:453:LYS:HG2	1.84	0.77
1:J:448:TYR:CE2	1:J:453:LYS:HA	2.19	0.77
1:L:506:PHE:HD2	1:L:555:VAL:CG2	1.97	0.77
1:G:909:TYR:HD1	1:G:909:TYR:C	1.91	0.76
1:K:450:LEU:O	1:K:453:LYS:HG2	1.84	0.76
1:K:506:PHE:HD2	1:K:555:VAL:HG23	1.49	0.76
1:J:450:LEU:O	1:J:453:LYS:HG2	1.84	0.76
1:D:909:TYR:HD1	1:D:909:TYR:C	1.91	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:78:GLN:C	1:L:78:GLN:OE1	2.29	0.76
1:L:652:ARG:NE	1:L:652:ARG:HA	2.00	0.76
1:K:78:GLN:C	1:K:78:GLN:OE1	2.29	0.76
1:K:652:ARG:HA	1:K:652:ARG:NE	2.00	0.76
1:A:909:TYR:CD1	1:A:909:TYR:C	2.64	0.75
1:J:78:GLN:OE1	1:J:78:GLN:C	2.29	0.75
1:J:652:ARG:NE	1:J:652:ARG:HA	2.00	0.75
1:G:909:TYR:CD1	1:G:909:TYR:C	2.64	0.74
1:J:452:MET:O	1:J:454:SER:N	2.21	0.74
1:L:452:MET:O	1:L:454:SER:N	2.21	0.74
1:J:506:PHE:HD2	1:J:555:VAL:CG2	1.98	0.73
1:J:506:PHE:HD2	1:J:555:VAL:HG23	1.49	0.73
1:L:78:GLN:OE1	1:L:78:GLN:O	2.07	0.73
1:G:1059:ASP:OD1	1:G:1059:ASP:O	2.06	0.73
1:K:452:MET:O	1:K:454:SER:N	2.21	0.73
1:K:78:GLN:OE1	1:K:78:GLN:O	2.07	0.73
1:J:78:GLN:OE1	1:J:78:GLN:O	2.07	0.72
1:A:1059:ASP:OD1	1:A:1059:ASP:O	2.06	0.72
1:J:506:PHE:CD1	1:J:513:GLU:OE1	2.43	0.72
1:D:1059:ASP:OD1	1:D:1059:ASP:O	2.06	0.72
1:D:1059:ASP:OD1	1:D:1059:ASP:C	2.33	0.71
1:K:506:PHE:CE2	1:K:555:VAL:CB	2.68	0.71
1:L:506:PHE:CE2	1:L:555:VAL:CB	2.68	0.71
1:L:506:PHE:CD1	1:L:513:GLU:OE1	2.44	0.71
1:G:1059:ASP:OD1	1:G:1059:ASP:C	2.33	0.70
1:J:452:MET:C	1:J:454:SER:N	2.49	0.70
1:A:1059:ASP:OD1	1:A:1059:ASP:C	2.33	0.70
1:J:172:LEU:HD12	1:J:172:LEU:O	1.92	0.70
1:L:172:LEU:HD12	1:L:172:LEU:O	1.92	0.70
1:K:172:LEU:O	1:K:172:LEU:HD12	1.92	0.69
1:D:909:TYR:CD1	1:D:909:TYR:C	2.64	0.69
1:K:506:PHE:CD1	1:K:513:GLU:OE1	2.44	0.69
1:D:1141:TYR:CD1	1:D:1141:TYR:C	2.71	0.69
1:G:1141:TYR:C	1:G:1141:TYR:CD1	2.71	0.69
1:L:452:MET:C	1:L:454:SER:N	2.49	0.69
1:A:1141:TYR:CD1	1:A:1141:TYR:C	2.71	0.69
1:D:914:GLN:O	1:D:914:GLN:CG	2.43	0.67
1:D:1122:HIS:HE2	1:D:1125:SER:HG	1.41	0.66
3:C:90:GLN:OE1	3:C:90:GLN:HA	1.95	0.66
1:L:652:ARG:HA	1:L:652:ARG:HE	1.58	0.66
3:F:90:GLN:HA	3:F:90:GLN:OE1	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:452:MET:C	1:K:454:SER:N	2.49	0.66
1:A:914:GLN:O	1:A:914:GLN:CG	2.43	0.66
3:I:90:GLN:HA	3:I:90:GLN:OE1	1.95	0.66
1:K:652:ARG:HA	1:K:652:ARG:HE	1.58	0.66
1:D:1141:TYR:HD1	1:D:1141:TYR:O	1.79	0.65
1:A:1122:HIS:HE2	1:A:1125:SER:HG	1.43	0.65
1:J:652:ARG:HA	1:J:652:ARG:HE	1.58	0.65
1:A:1141:TYR:HD1	1:A:1141:TYR:O	1.79	0.65
1:G:1141:TYR:HD1	1:G:1141:TYR:O	1.79	0.64
1:G:777:TYR:CD1	1:G:777:TYR:C	2.75	0.64
1:L:21:VAL:HG11	1:L:237:CYS:SG	2.39	0.62
1:A:777:TYR:C	1:A:777:TYR:CD1	2.75	0.62
1:L:369:LYS:O	1:L:369:LYS:HG2	2.00	0.62
1:A:776:SER:OG	3:C:28:TYR:OH	2.18	0.62
1:K:21:VAL:HG11	1:K:237:CYS:SG	2.39	0.62
1:D:776:SER:OG	3:F:28:TYR:OH	2.18	0.61
1:G:776:SER:OG	3:I:28:TYR:OH	2.18	0.61
1:J:369:LYS:O	1:J:369:LYS:HG2	2.00	0.61
1:J:21:VAL:HG11	1:J:237:CYS:SG	2.39	0.61
1:D:777:TYR:CD1	1:D:777:TYR:C	2.75	0.61
1:J:130:VAL:HG12	1:J:130:VAL:O	2.00	0.61
1:K:369:LYS:O	1:K:369:LYS:HG2	2.00	0.61
1:L:130:VAL:HG12	1:L:130:VAL:O	2.00	0.60
1:K:620:CYS:O	1:K:620:CYS:SG	2.59	0.60
1:K:130:VAL:HG12	1:K:130:VAL:O	2.00	0.60
2:B:72:ASP:C	2:B:72:ASP:OD1	2.45	0.59
1:J:620:CYS:SG	1:J:620:CYS:O	2.59	0.59
1:L:448:TYR:HE2	1:L:453:LYS:HA	1.68	0.59
2:E:72:ASP:C	2:E:72:ASP:OD1	2.45	0.59
1:L:620:CYS:SG	1:L:620:CYS:O	2.59	0.59
1:K:506:PHE:HD2	1:K:555:VAL:CG2	1.97	0.58
2:H:72:ASP:OD1	2:H:72:ASP:C	2.45	0.58
1:K:448:TYR:HE2	1:K:453:LYS:HA	1.68	0.58
1:J:448:TYR:HE2	1:J:453:LYS:HA	1.68	0.57
1:A:1141:TYR:C	1:A:1141:TYR:HD1	2.13	0.56
1:A:970:ILE:O	1:A:970:ILE:HD12	2.06	0.56
1:L:409:TYR:CD1	1:L:409:TYR:C	2.84	0.56
1:K:171:LEU:HD23	1:K:171:LEU:C	2.31	0.56
1:D:809:TYR:O	1:D:809:TYR:CD1	2.59	0.56
1:J:130:VAL:O	1:J:130:VAL:CG1	2.54	0.56
1:L:171:LEU:C	1:L:171:LEU:HD23	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:409:TYR:CD1	1:K:409:TYR:C	2.84	0.55
1:D:970:ILE:HD12	1:D:970:ILE:O	2.06	0.55
1:A:809:TYR:CD1	1:A:809:TYR:O	2.60	0.55
1:J:409:TYR:CD1	1:J:409:TYR:C	2.84	0.55
1:K:281:PHE:CD1	1:K:281:PHE:O	2.60	0.55
1:G:809:TYR:O	1:G:809:TYR:CD1	2.60	0.55
1:J:171:LEU:C	1:J:171:LEU:HD23	2.31	0.55
1:J:281:PHE:O	1:J:281:PHE:CD1	2.60	0.55
1:L:130:VAL:O	1:L:130:VAL:CG1	2.55	0.55
1:L:281:PHE:O	1:L:281:PHE:CD1	2.60	0.55
2:B:27:TYR:N	2:B:27:TYR:HD1	2.05	0.55
1:G:1141:TYR:C	1:G:1141:TYR:HD1	2.13	0.55
3:I:65:SER:HG	3:I:72:SER:HG	1.54	0.55
3:I:90:GLN:OE1	3:I:90:GLN:CA	2.54	0.55
2:H:27:TYR:HD1	2:H:27:TYR:N	2.05	0.54
2:E:27:TYR:CD1	2:E:27:TYR:N	2.76	0.54
3:F:90:GLN:OE1	3:F:90:GLN:CA	2.54	0.54
1:G:970:ILE:HD12	1:G:970:ILE:O	2.06	0.54
1:D:1141:TYR:C	1:D:1141:TYR:HD1	2.13	0.54
1:K:130:VAL:O	1:K:130:VAL:CG1	2.55	0.54
1:G:914:GLN:O	1:G:914:GLN:CG	2.43	0.54
1:G:903:PRO:HB2	1:G:905:TYR:CE2	2.43	0.54
1:L:378:ALA:HB1	1:L:379:GLU:HA	1.90	0.54
1:D:903:PRO:HB2	1:D:905:TYR:CE2	2.43	0.54
2:E:27:TYR:N	2:E:27:TYR:HD1	2.05	0.54
2:B:27:TYR:N	2:B:27:TYR:CD1	2.76	0.53
1:K:378:ALA:HB1	1:K:379:GLU:HA	1.90	0.53
1:A:903:PRO:HB2	1:A:905:TYR:CE2	2.43	0.53
1:K:506:PHE:HE1	1:K:513:GLU:OE1	1.81	0.53
1:J:194:HIS:O	1:J:194:HIS:ND1	2.42	0.53
1:L:194:HIS:ND1	1:L:194:HIS:O	2.42	0.53
1:L:376:GLU:O	1:L:376:GLU:HG3	2.09	0.53
1:J:378:ALA:HB1	1:J:379:GLU:HA	1.90	0.53
1:K:376:GLU:O	1:K:376:GLU:HG3	2.09	0.53
1:J:673:LEU:C	1:J:673:LEU:HD23	2.33	0.53
1:J:376:GLU:HG3	1:J:376:GLU:O	2.09	0.53
3:C:90:GLN:OE1	3:C:90:GLN:CA	2.54	0.53
1:G:809:TYR:CD1	1:G:809:TYR:C	2.87	0.52
1:J:633:ASP:C	1:J:633:ASP:OD1	2.53	0.52
1:K:194:HIS:O	1:K:194:HIS:ND1	2.42	0.52
1:J:450:LEU:HA	1:J:453:LYS:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:673:LEU:HD23	1:L:673:LEU:C	2.34	0.52
2:H:27:TYR:N	2:H:27:TYR:CD1	2.76	0.52
1:K:673:LEU:C	1:K:673:LEU:HD23	2.34	0.52
1:D:809:TYR:CD1	1:D:809:TYR:C	2.87	0.52
1:A:809:TYR:CD1	1:A:809:TYR:C	2.87	0.52
1:K:506:PHE:CZ	1:K:513:GLU:OE1	2.57	0.52
1:L:450:LEU:HA	1:L:453:LYS:HB3	1.91	0.51
1:K:450:LEU:HA	1:K:453:LYS:HB3	1.92	0.51
2:H:27:TYR:HD1	2:H:27:TYR:H	1.57	0.51
1:K:269:ARG:HD3	1:K:269:ARG:C	2.36	0.51
1:K:590:PHE:O	1:K:590:PHE:CD1	2.64	0.51
1:K:633:ASP:OD1	1:K:633:ASP:C	2.53	0.51
1:L:606:TYR:CD1	1:L:606:TYR:C	2.88	0.51
1:J:433:ILE:HD13	1:J:478:CYS:HB2	1.93	0.51
1:J:606:TYR:CD1	1:J:606:TYR:C	2.88	0.51
1:J:691:ARG:HA	1:J:691:ARG:HE	1.75	0.51
1:D:777:TYR:CD1	1:D:777:TYR:O	2.64	0.50
2:E:27:TYR:HD1	2:E:27:TYR:H	1.57	0.50
1:J:443:LEU:C	1:J:443:LEU:HD23	2.36	0.50
1:K:606:TYR:CD1	1:K:606:TYR:C	2.88	0.50
1:L:590:PHE:CD1	1:L:590:PHE:O	2.64	0.50
1:J:269:ARG:C	1:J:269:ARG:HD3	2.36	0.50
1:J:590:PHE:O	1:J:590:PHE:CD1	2.64	0.50
1:K:433:ILE:HD13	1:K:478:CYS:HB2	1.93	0.50
1:K:443:LEU:C	1:K:443:LEU:HD23	2.36	0.50
1:A:777:TYR:CD1	1:A:777:TYR:O	2.64	0.50
1:L:633:ASP:C	1:L:633:ASP:OD1	2.52	0.50
1:G:1122:HIS:NE2	1:G:1125:SER:OG	2.35	0.50
1:L:443:LEU:HD23	1:L:443:LEU:C	2.36	0.50
1:K:410:ASN:C	1:K:410:ASN:OD1	2.55	0.49
1:L:269:ARG:HD3	1:L:269:ARG:C	2.36	0.49
2:B:27:TYR:HD1	2:B:27:TYR:H	1.57	0.49
1:G:777:TYR:CD1	1:G:777:TYR:O	2.64	0.49
1:L:433:ILE:HD13	1:L:478:CYS:HB2	1.93	0.49
1:L:506:PHE:CZ	1:L:513:GLU:OE1	2.58	0.49
1:D:986:THR:CG2	1:D:1195:GLU:OE2	2.52	0.49
1:K:719:ASN:OD1	1:K:719:ASN:C	2.55	0.49
1:A:974:GLN:O	1:A:974:GLN:CD	2.56	0.49
1:J:719:ASN:C	1:J:719:ASN:OD1	2.55	0.49
1:L:410:ASN:OD1	1:L:410:ASN:C	2.55	0.49
1:G:970:ILE:HD12	1:G:970:ILE:C	2.38	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:841:ARG:HA	1:G:841:ARG:NE	2.28	0.49
1:D:841:ARG:NE	1:D:841:ARG:HA	2.28	0.49
1:D:974:GLN:O	1:D:974:GLN:CD	2.56	0.49
1:G:974:GLN:CD	1:G:974:GLN:O	2.56	0.49
1:D:970:ILE:HD12	1:D:970:ILE:C	2.38	0.48
1:A:841:ARG:HA	1:A:841:ARG:NE	2.28	0.48
1:J:410:ASN:OD1	1:J:410:ASN:C	2.55	0.48
1:A:970:ILE:HD12	1:A:970:ILE:C	2.38	0.48
1:L:719:ASN:OD1	1:L:719:ASN:C	2.55	0.47
1:A:1141:TYR:CD1	1:A:1141:TYR:O	2.63	0.47
1:G:1141:TYR:CD1	1:G:1141:TYR:O	2.63	0.47
1:J:506:PHE:HE2	1:J:555:VAL:CG1	2.26	0.47
1:L:449:PRO:O	1:L:453:LYS:HB3	2.15	0.47
1:L:691:ARG:HA	1:L:691:ARG:HE	1.75	0.47
1:G:986:THR:CG2	1:G:1195:GLU:OE2	2.52	0.47
1:J:449:PRO:O	1:J:453:LYS:HB3	2.15	0.47
1:K:66:ASN:CG	1:K:66:ASN:O	2.58	0.47
1:J:506:PHE:HE1	1:J:513:GLU:OE1	1.79	0.47
1:J:66:ASN:O	1:J:66:ASN:OD1	2.33	0.47
1:K:621:THR:O	1:K:621:THR:HG22	2.15	0.47
1:K:449:PRO:O	1:K:453:LYS:HB3	2.15	0.46
1:L:313:PHE:CD1	1:L:313:PHE:C	2.94	0.46
1:A:986:THR:CG2	1:A:1195:GLU:OE2	2.52	0.46
1:G:826:GLN:H	1:G:826:GLN:CD	2.21	0.46
1:J:621:THR:HG22	1:J:621:THR:O	2.15	0.46
1:L:21:VAL:CG1	1:L:237:CYS:SG	3.03	0.46
1:K:506:PHE:HE2	1:K:555:VAL:CG1	2.27	0.46
1:D:826:GLN:H	1:D:826:GLN:CD	2.21	0.46
1:L:66:ASN:OD1	1:L:66:ASN:O	2.33	0.46
1:A:775:SER:OG	1:A:776:SER:N	2.48	0.46
1:K:21:VAL:CG1	1:K:237:CYS:SG	3.03	0.46
1:K:66:ASN:O	1:K:66:ASN:OD1	2.33	0.46
1:L:506:PHE:HE2	1:L:555:VAL:CG1	2.27	0.46
1:L:621:THR:O	1:L:621:THR:HG22	2.15	0.46
1:D:775:SER:OG	1:D:776:SER:N	2.48	0.45
1:A:974:GLN:C	1:A:974:GLN:OE1	2.60	0.45
1:L:194:HIS:NE2	1:L:202:THR:OG1	2.40	0.45
1:J:66:ASN:O	1:J:66:ASN:CG	2.58	0.45
1:G:974:GLN:OE1	1:G:974:GLN:C	2.60	0.45
1:D:974:GLN:C	1:D:974:GLN:OE1	2.60	0.45
1:K:281:PHE:CD1	1:K:281:PHE:C	2.93	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:590:PHE:O	1:L:590:PHE:CG	2.69	0.45
1:J:21:VAL:CG1	1:J:237:CYS:SG	3.03	0.45
3:C:1:ASP:OD1	3:C:1:ASP:C	2.60	0.45
1:J:590:PHE:O	1:J:590:PHE:CG	2.69	0.45
1:G:775:SER:OG	1:G:776:SER:N	2.48	0.45
1:D:1141:TYR:CD1	1:D:1141:TYR:O	2.63	0.45
1:K:590:PHE:O	1:K:590:PHE:CG	2.69	0.45
1:L:395:GLN:HA	1:L:395:GLN:OE1	2.17	0.45
1:A:909:TYR:HA	1:A:912:CYS:SG	2.57	0.45
1:D:909:TYR:HA	1:D:912:CYS:SG	2.57	0.44
3:I:1:ASP:OD1	3:I:1:ASP:C	2.60	0.44
3:F:1:ASP:OD1	3:F:1:ASP:C	2.60	0.44
1:K:19:VAL:HB	1:K:237:CYS:HB3	2.00	0.44
1:G:909:TYR:HA	1:G:912:CYS:SG	2.57	0.44
1:K:194:HIS:NE2	1:K:202:THR:OG1	2.40	0.44
1:K:395:GLN:OE1	1:K:395:GLN:HA	2.17	0.44
1:J:19:VAL:HB	1:J:237:CYS:HB3	2.00	0.44
1:J:523:TYR:CD1	1:J:523:TYR:N	2.86	0.44
1:J:395:GLN:OE1	1:J:395:GLN:HA	2.17	0.44
1:K:313:PHE:CD1	1:K:313:PHE:C	2.94	0.44
1:A:1122:HIS:NE2	1:A:1125:SER:OG	2.35	0.44
1:G:1001:PHE:CD1	1:G:1001:PHE:C	2.96	0.44
1:K:691:ARG:HA	1:K:691:ARG:HE	1.75	0.44
1:L:19:VAL:HB	1:L:237:CYS:HB3	2.00	0.44
1:L:448:TYR:OH	1:L:452:MET:O	2.34	0.43
1:D:778:PHE:CD1	1:D:778:PHE:N	2.87	0.43
1:K:523:TYR:CD1	1:K:523:TYR:N	2.86	0.43
1:K:172:LEU:HD12	1:K:172:LEU:C	2.43	0.43
1:D:1001:PHE:CD1	1:D:1001:PHE:C	2.96	0.43
1:L:66:ASN:OD1	1:L:66:ASN:C	2.61	0.43
1:L:281:PHE:CD1	1:L:281:PHE:C	2.93	0.43
1:L:523:TYR:CD1	1:L:523:TYR:N	2.86	0.43
1:A:826:GLN:H	1:A:826:GLN:CD	2.21	0.43
1:A:1001:PHE:CD1	1:A:1001:PHE:C	2.96	0.43
1:K:326:ASP:OD1	1:K:326:ASP:C	2.61	0.43
1:J:228:PHE:CD1	1:J:228:PHE:C	2.96	0.43
1:J:313:PHE:CD1	1:J:313:PHE:C	2.94	0.43
1:G:778:PHE:CD1	1:G:778:PHE:N	2.87	0.43
1:K:228:PHE:CD1	1:K:228:PHE:C	2.96	0.43
1:G:805:ASP:C	1:G:805:ASP:OD1	2.62	0.43
1:J:281:PHE:CD1	1:J:281:PHE:C	2.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:691:ARG:NE	1:K:691:ARG:CA	2.70	0.43
1:L:66:ASN:O	1:L:66:ASN:CG	2.58	0.43
1:L:624:GLY:HA2	1:L:625:VAL:HA	1.83	0.43
1:J:726:ASP:OD1	1:J:726:ASP:C	2.61	0.42
1:K:66:ASN:OD1	1:K:66:ASN:C	2.61	0.42
1:L:404:PHE:HB3	1:L:407:CYS:SG	2.60	0.42
1:J:66:ASN:OD1	1:J:66:ASN:C	2.61	0.42
1:L:643:SER:OG	1:L:644:ASP:N	2.52	0.42
1:J:404:PHE:HB3	1:J:407:CYS:SG	2.60	0.42
1:L:228:PHE:CD1	1:L:228:PHE:C	2.96	0.42
1:L:603:CYS:HB2	1:L:615:GLY:HA2	2.01	0.42
1:A:1211:TYR:N	1:A:1211:TYR:CD1	2.88	0.42
1:L:172:LEU:HD12	1:L:172:LEU:C	2.43	0.42
1:A:778:PHE:CD1	1:A:778:PHE:N	2.87	0.42
1:G:1211:TYR:N	1:G:1211:TYR:CD1	2.88	0.42
1:J:50:VAL:HB	1:J:78:GLN:HG2	2.01	0.42
1:J:172:LEU:HD12	1:J:172:LEU:C	2.43	0.42
1:K:450:LEU:HA	1:K:453:LYS:CG	2.50	0.42
1:A:805:ASP:OD1	1:A:805:ASP:C	2.62	0.42
1:J:326:ASP:OD1	1:J:326:ASP:C	2.61	0.42
1:J:450:LEU:HA	1:J:453:LYS:CG	2.50	0.42
1:J:643:SER:OG	1:J:644:ASP:N	2.52	0.42
1:K:726:ASP:C	1:K:726:ASP:OD1	2.61	0.42
1:L:501:ASN:OD1	1:L:501:ASN:C	2.63	0.42
1:D:805:ASP:OD1	1:D:805:ASP:C	2.62	0.42
1:L:450:LEU:HA	1:L:453:LYS:CG	2.50	0.42
1:J:501:ASN:OD1	1:J:501:ASN:C	2.63	0.42
1:K:49:ASP:C	1:K:49:ASP:OD1	2.62	0.42
1:K:643:SER:OG	1:K:644:ASP:N	2.52	0.42
1:L:326:ASP:OD1	1:L:326:ASP:C	2.61	0.41
1:L:726:ASP:OD1	1:L:726:ASP:C	2.61	0.41
1:J:450:LEU:CA	1:J:453:LYS:HG2	2.50	0.41
1:K:404:PHE:HB3	1:K:407:CYS:SG	2.60	0.41
1:K:506:PHE:HE2	1:K:555:VAL:HG21	0.61	0.41
1:K:672:THR:HG22	1:K:715:LEU:HB2	2.02	0.41
1:K:603:CYS:HB2	1:K:615:GLY:HA2	2.01	0.41
1:D:1211:TYR:N	1:D:1211:TYR:CD1	2.88	0.41
1:J:603:CYS:HB2	1:J:615:GLY:HA2	2.01	0.41
1:K:50:VAL:HB	1:K:78:GLN:HG2	2.01	0.41
1:L:50:VAL:HB	1:L:78:GLN:HG2	2.01	0.41
1:L:672:THR:HG22	1:L:715:LEU:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:672:THR:HG22	1:J:715:LEU:HB2	2.02	0.41
1:L:130:VAL:O	1:L:131:ILE:HB	2.21	0.41
1:L:450:LEU:CA	1:L:453:LYS:HG2	2.50	0.41
1:K:439:SER:HA	1:K:582:ASN:HA	2.03	0.41
1:K:450:LEU:CA	1:K:453:LYS:HG2	2.50	0.41
1:J:49:ASP:OD1	1:J:49:ASP:C	2.63	0.41
1:K:132:ILE:HD12	1:K:132:ILE:HA	1.92	0.41
1:A:782:ILE:O	1:A:782:ILE:HG23	2.21	0.40
1:G:782:ILE:O	1:G:782:ILE:HG23	2.21	0.40
1:J:194:HIS:NE2	1:J:202:THR:OG1	2.40	0.40
1:L:381:VAL:O	1:L:407:CYS:HA	2.21	0.40
1:L:690:SER:OG	1:L:691:ARG:N	2.54	0.40
3:C:76:HIS:N	3:C:76:HIS:CD2	2.89	0.40
1:K:130:VAL:O	1:K:131:ILE:HB	2.21	0.40
1:K:266:PHE:HB3	1:K:278:MET:HB3	2.03	0.40
1:K:453:LYS:HB2	1:K:481:LEU:HD13	2.03	0.40
1:J:453:LYS:HB2	1:J:481:LEU:HD13	2.03	0.40
1:L:49:ASP:C	1:L:49:ASP:OD1	2.63	0.40
1:L:439:SER:HA	1:L:582:ASN:HA	2.03	0.40
1:L:740:ASP:O	1:L:741:THR:C	2.65	0.40
1:J:740:ASP:O	1:J:741:THR:C	2.65	0.40
1:K:690:SER:OG	1:K:691:ARG:N	2.54	0.40
1:L:691:ARG:NE	1:L:691:ARG:CA	2.70	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	A	459/1329 (34%)	434 (95%)	14 (3%)	11 (2%)	4	27
1	D	459/1329 (34%)	434 (95%)	14 (3%)	11 (2%)	4	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	459/1329 (34%)	434 (95%)	14 (3%)	11 (2%)	4	27
1	J	724/1329 (54%)	686 (95%)	34 (5%)	4 (1%)	21	58
1	K	724/1329 (54%)	686 (95%)	34 (5%)	4 (1%)	21	58
1	L	724/1329 (54%)	686 (95%)	34 (5%)	4 (1%)	21	58
2	B	117/233 (50%)	115 (98%)	1 (1%)	1 (1%)	14	49
2	E	117/233 (50%)	115 (98%)	1 (1%)	1 (1%)	14	49
2	H	117/233 (50%)	115 (98%)	1 (1%)	1 (1%)	14	49
3	C	109/218 (50%)	101 (93%)	7 (6%)	1 (1%)	14	49
3	F	109/218 (50%)	101 (93%)	7 (6%)	1 (1%)	14	49
3	I	109/218 (50%)	101 (93%)	7 (6%)	1 (1%)	14	49
All	All	4227/9327 (45%)	4008 (95%)	168 (4%)	51 (1%)	13	42

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1117	CYS
3	F	77	PRO
1	A	1117	CYS
3	C	77	PRO
1	G	1117	CYS
3	I	77	PRO
1	D	965	SER
1	D	1116	PHE
1	A	965	SER
1	A	1116	PHE
1	G	965	SER
1	G	1116	PHE
1	J	453	LYS
1	J	621	THR
1	K	453	LYS
1	K	621	THR
1	L	453	LYS
1	L	621	THR
1	D	775	SER
1	D	1219	PRO
1	A	775	SER
1	A	1219	PRO
1	G	775	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1219	PRO
1	J	131	ILE
1	J	629	ARG
1	K	131	ILE
1	K	629	ARG
1	L	131	ILE
1	L	629	ARG
1	D	917	PRO
1	D	1123	ILE
1	D	1220	PRO
2	E	87	SER
1	A	917	PRO
1	A	1123	ILE
1	A	1220	PRO
2	B	87	SER
1	G	917	PRO
1	G	1123	ILE
1	G	1220	PRO
2	H	87	SER
1	D	905	TYR
1	A	905	TYR
1	G	905	TYR
1	D	961	THR
1	A	961	THR
1	G	961	THR
1	D	908	GLY
1	G	908	GLY
1	A	908	GLY

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	388/1148 (34%)	383 (99%)	5 (1%)	61	72
1	D	388/1148 (34%)	383 (99%)	5 (1%)	61	72
1	G	388/1148 (34%)	383 (99%)	5 (1%)	61	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	635/1148 (55%)	630 (99%)	5 (1%)	73	78
1	K	635/1148 (55%)	630 (99%)	5 (1%)	73	78
1	L	635/1148 (55%)	630 (99%)	5 (1%)	73	78
2	B	102/202 (50%)	101 (99%)	1 (1%)	68	76
2	E	102/202 (50%)	101 (99%)	1 (1%)	68	76
2	H	102/202 (50%)	101 (99%)	1 (1%)	68	76
3	C	93/192 (48%)	93 (100%)	0	100	100
3	F	93/192 (48%)	93 (100%)	0	100	100
3	I	93/192 (48%)	93 (100%)	0	100	100
All	All	3654/8070 (45%)	3621 (99%)	33 (1%)	68	77

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	777	TYR
1	D	909	TYR
1	D	925	CYS
1	D	938	LEU
1	D	1141	TYR
2	E	27	TYR
1	A	777	TYR
1	A	909	TYR
1	A	925	CYS
1	A	938	LEU
1	A	1141	TYR
2	B	27	TYR
1	G	777	TYR
1	G	909	TYR
1	G	925	CYS
1	G	938	LEU
1	G	1141	TYR
2	H	27	TYR
1	J	196	PRO
1	J	387	PRO
1	J	452	MET
1	J	603	CYS
1	J	710	PRO
1	K	196	PRO
1	K	387	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	452	MET
1	K	603	CYS
1	K	710	PRO
1	L	196	PRO
1	L	387	PRO
1	L	452	MET
1	L	603	CYS
1	L	710	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	792	GLN
1	D	981	ASN
1	D	1002	ASN
1	D	1009	GLN
1	D	1023	GLN
1	D	1031	GLN
1	A	792	GLN
1	A	981	ASN
1	A	1002	ASN
1	A	1009	GLN
1	A	1023	GLN
1	A	1031	GLN
1	G	792	GLN
1	G	981	ASN
1	G	1002	ASN
1	G	1023	GLN
1	G	1031	GLN
1	J	60	GLN
1	J	264	HIS
1	J	280	GLN
1	J	346	GLN
1	J	427	GLN
1	J	566	GLN
1	K	60	GLN
1	K	199	ASN
1	K	264	HIS
1	K	280	GLN
1	K	346	GLN
1	K	427	GLN
1	K	566	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	681	HIS
1	L	60	GLN
1	L	264	HIS
1	L	280	GLN
1	L	346	GLN
1	L	427	GLN
1	L	566	GLN
1	L	628	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.

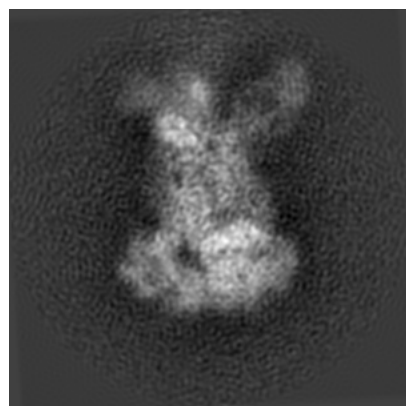
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8785. These allow visual inspection of the internal detail of the map and identification of artifacts.

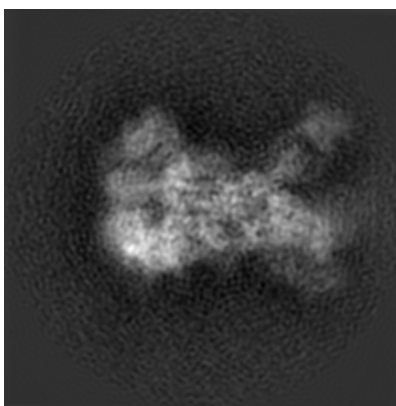
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

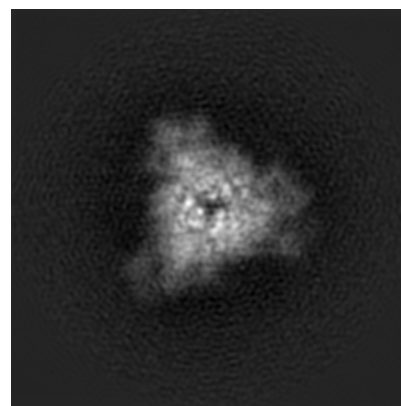
6.1.1 Primary map



X

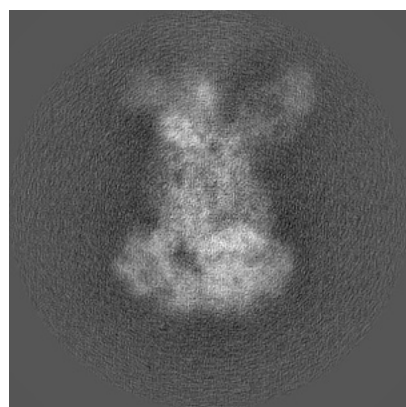


Y

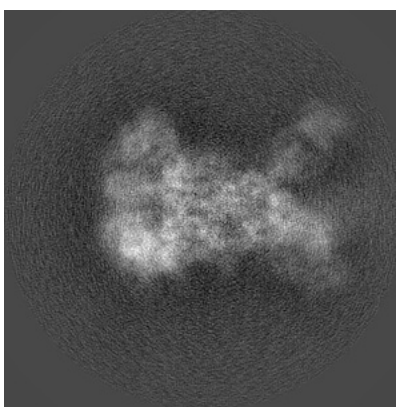


Z

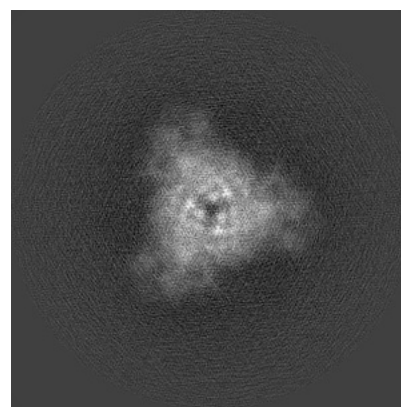
6.1.2 Raw map



X



Y

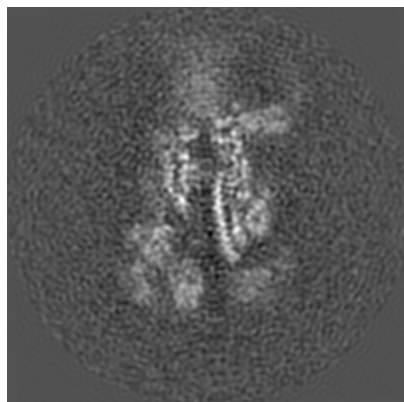


Z

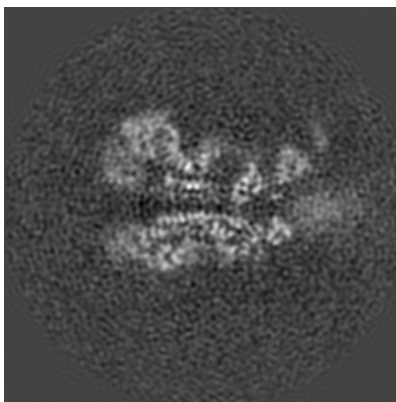
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

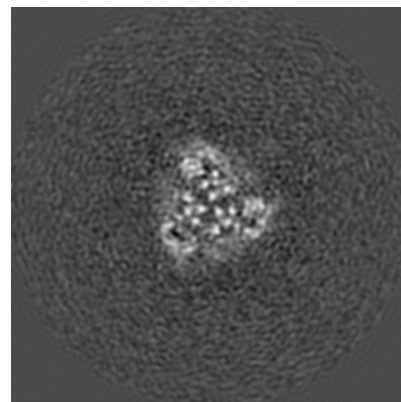
6.2.1 Primary map



X Index: 152

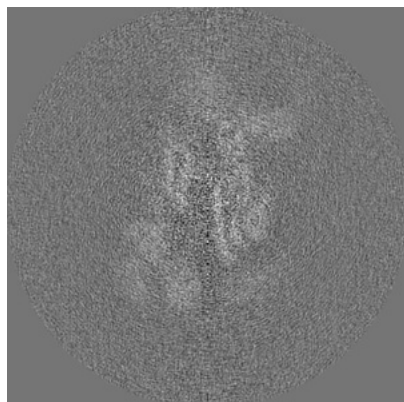


Y Index: 152

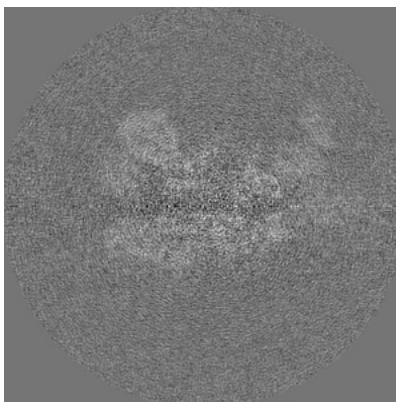


Z Index: 152

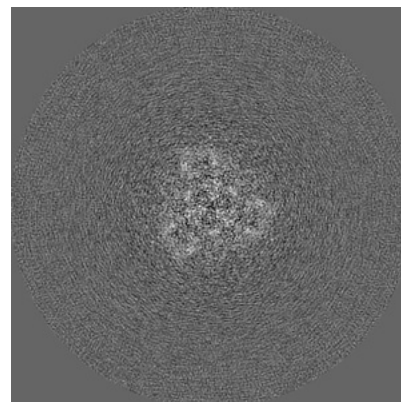
6.2.2 Raw map



X Index: 152



Y Index: 152

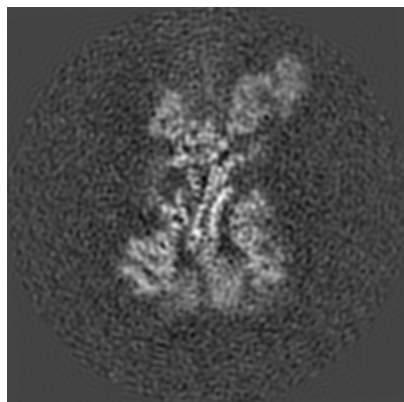


Z Index: 152

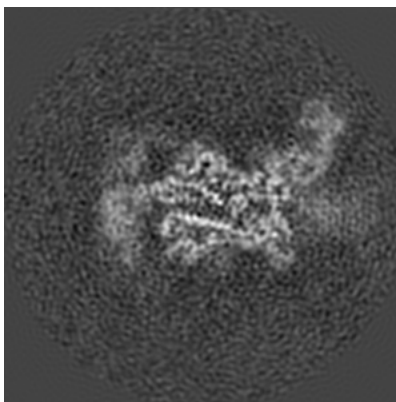
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

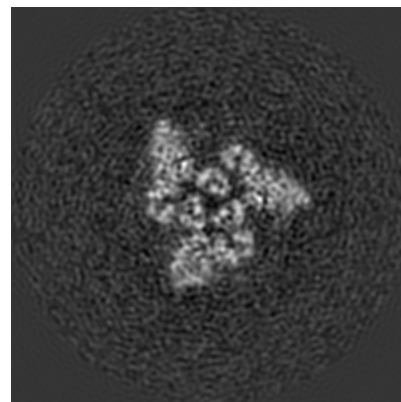
6.3.1 Primary map



X Index: 134

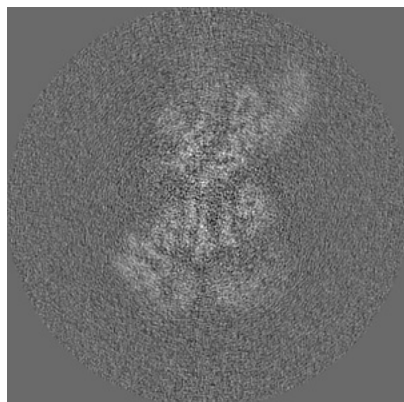


Y Index: 140

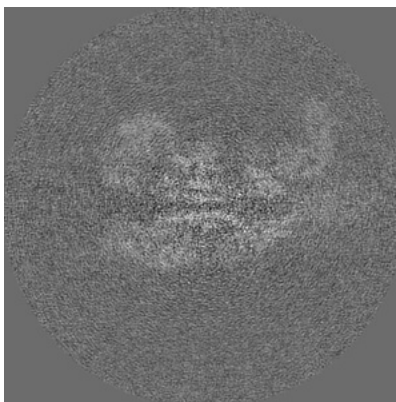


Z Index: 125

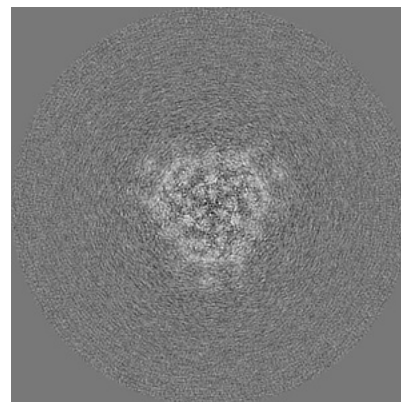
6.3.2 Raw map



X Index: 142



Y Index: 149

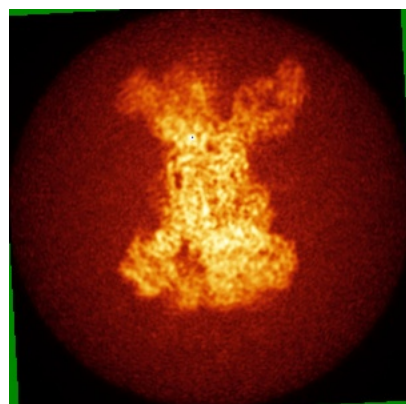


Z Index: 132

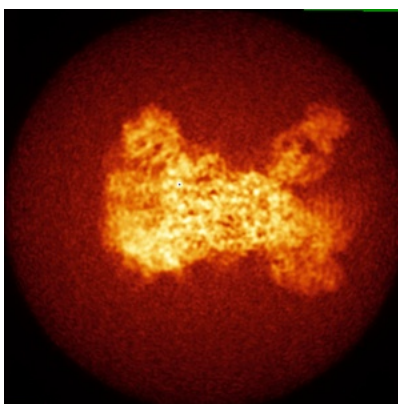
The images above show the largest variance slices of the map in three orthogonal directions.

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

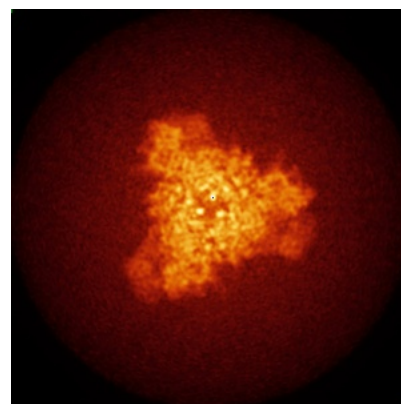
6.4.1 Primary map



X

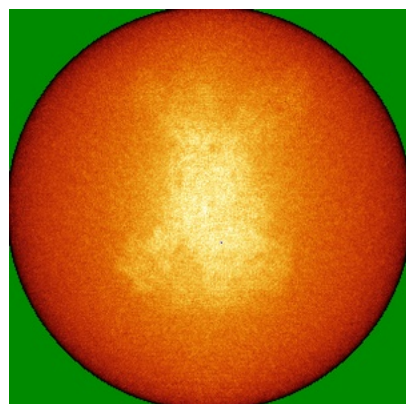


Y

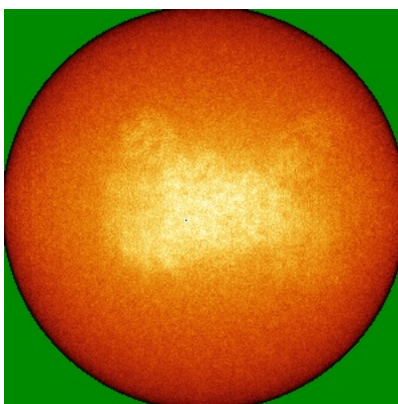


Z

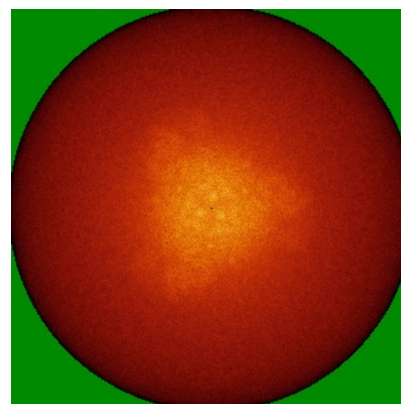
6.4.2 Raw map



X



Y

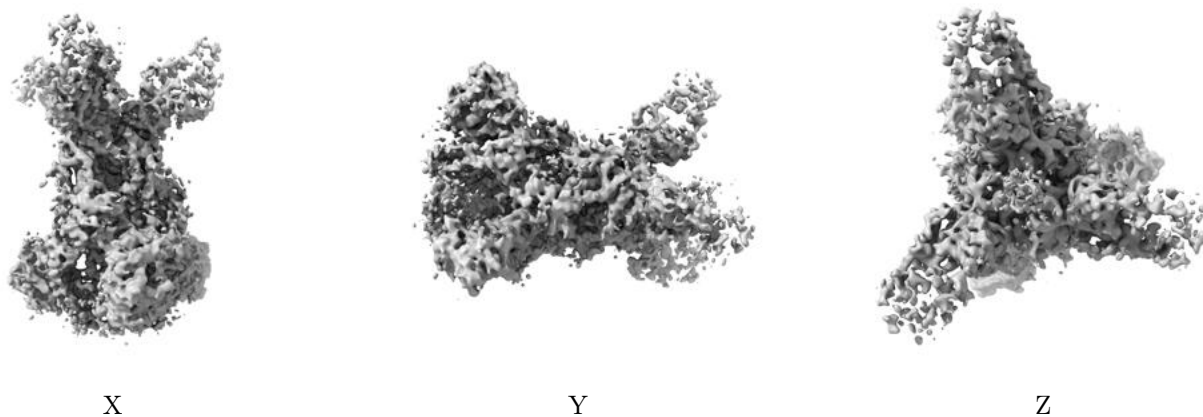


Z

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.

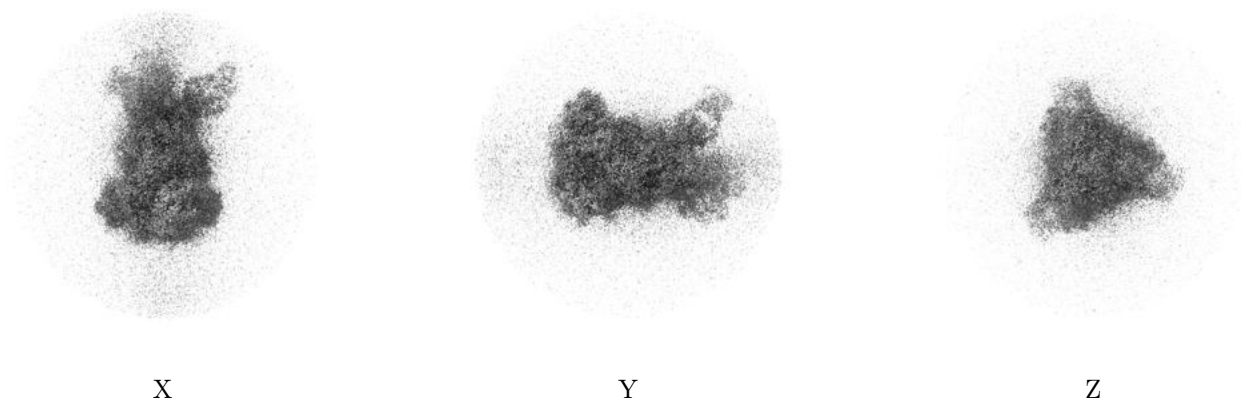
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

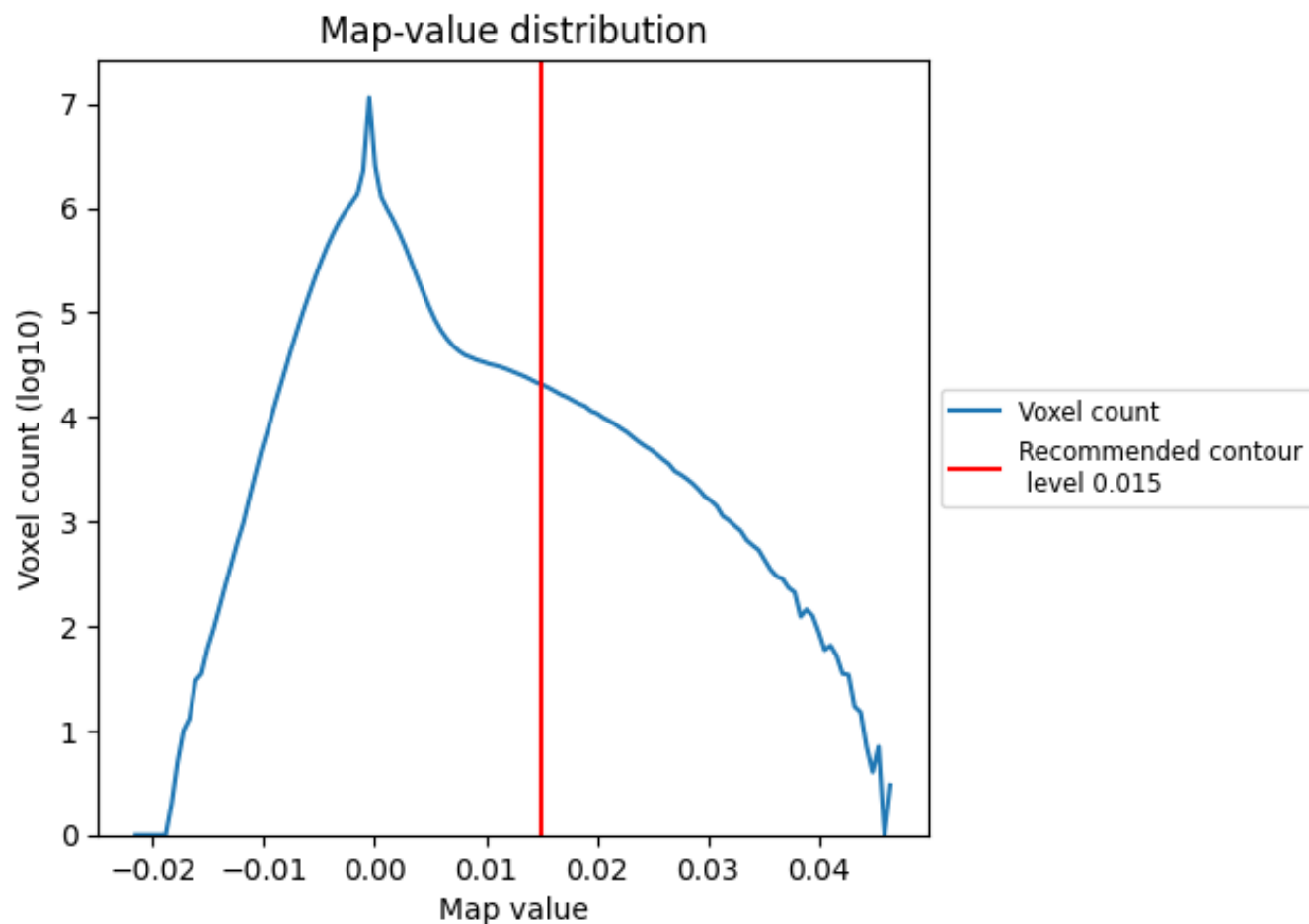
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

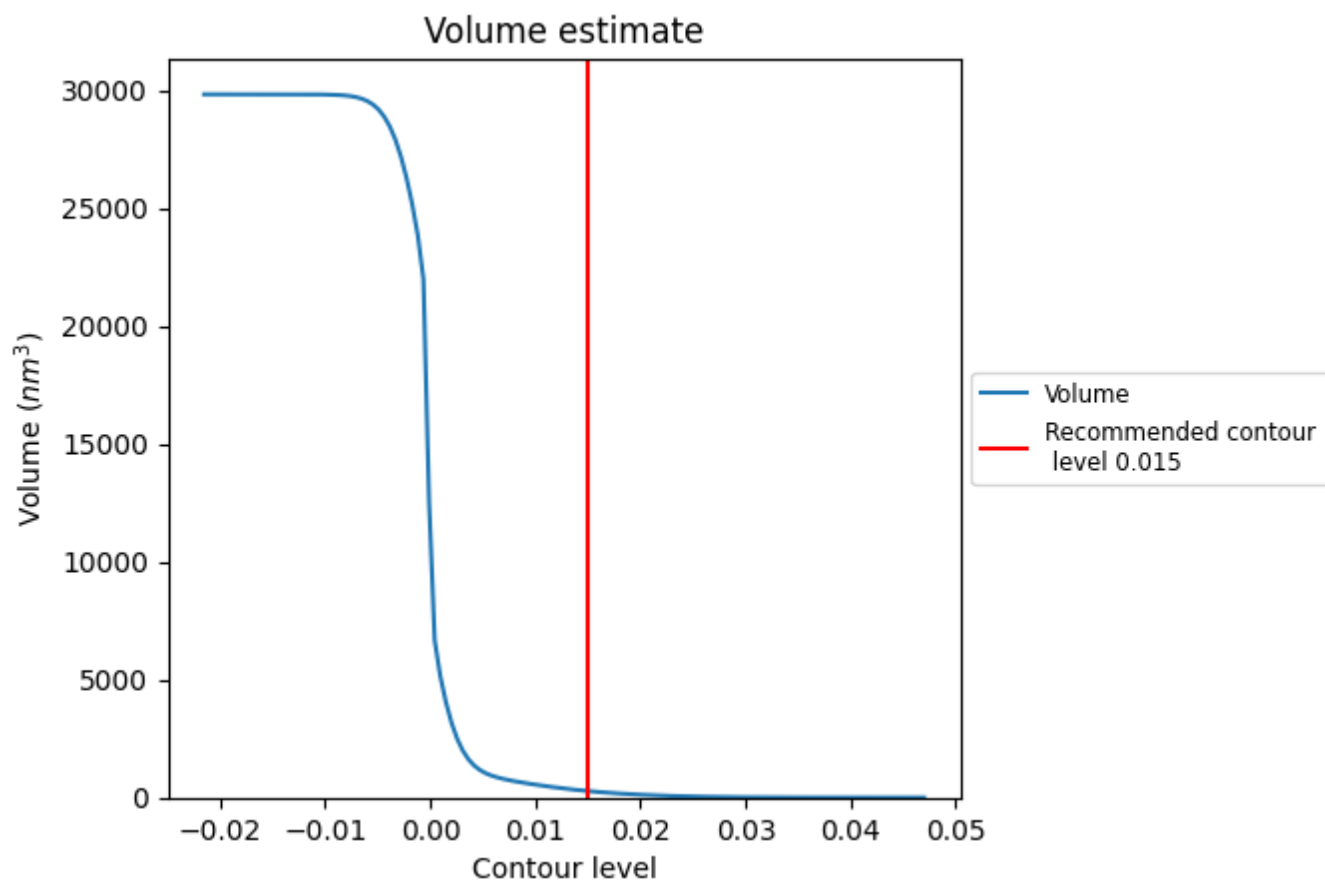
This section contains the results of statistical analysis of the map.

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.

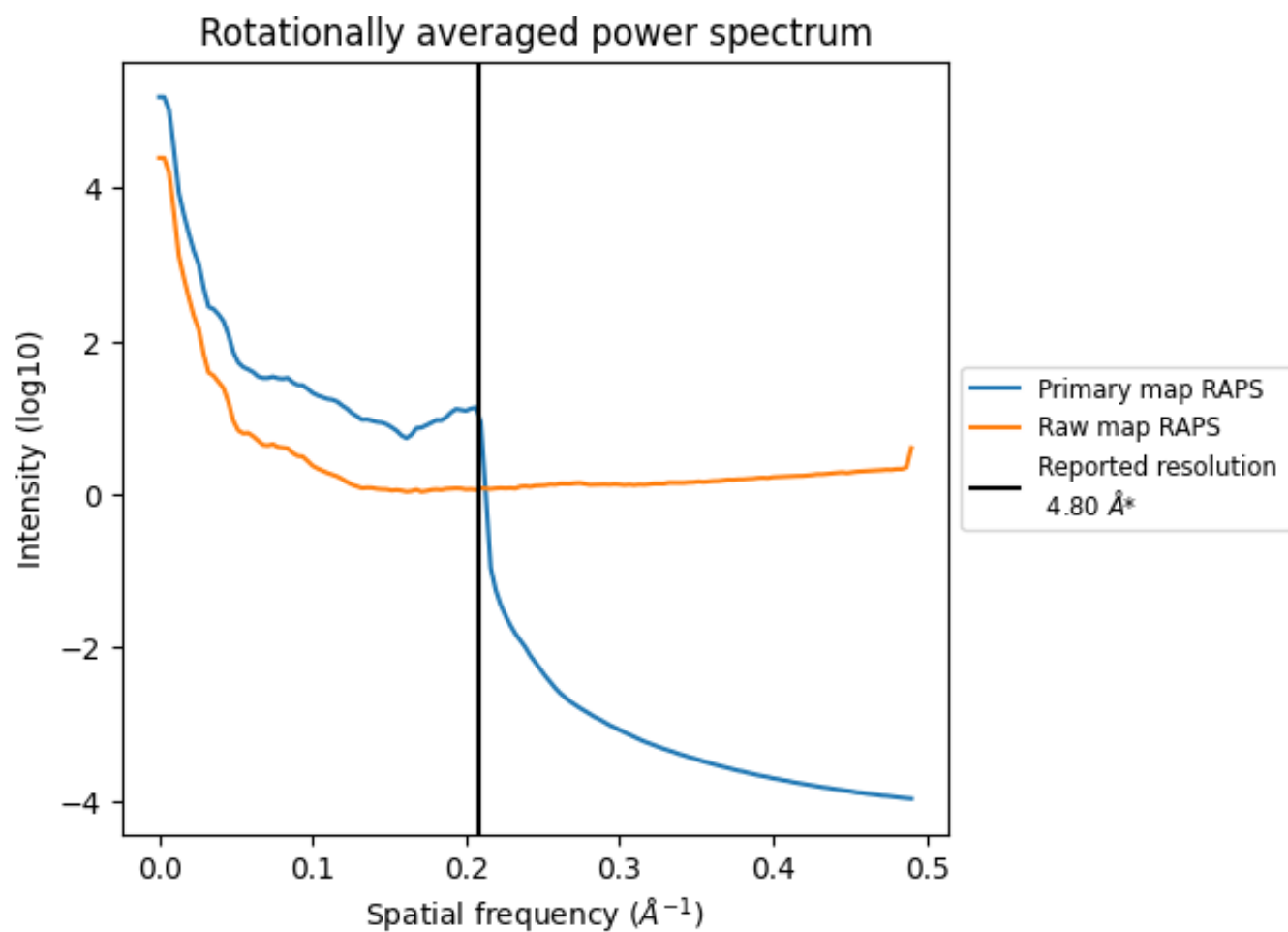
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 276 nm³; this corresponds to an approximate mass of 249 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 ⓘ

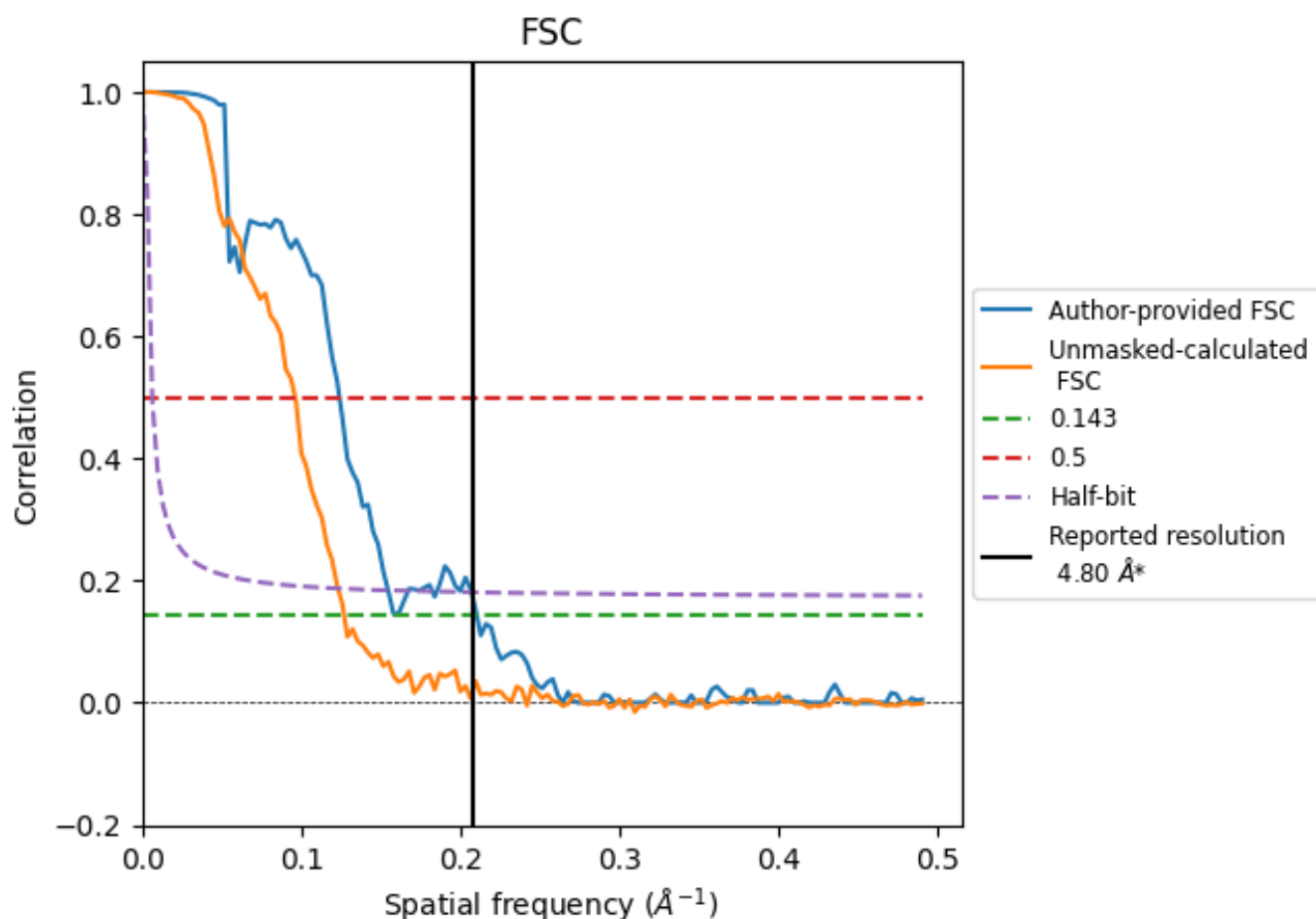


*Reported resolution corresponds to spatial frequency of 0.208 $\text{\AA}^{-1}$

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](#)

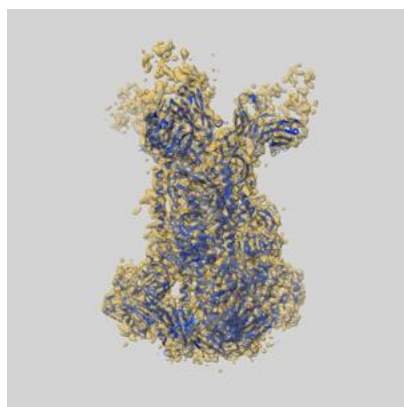
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.76	8.06	6.47
Unmasked-calculated*	7.88	10.40	8.12

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

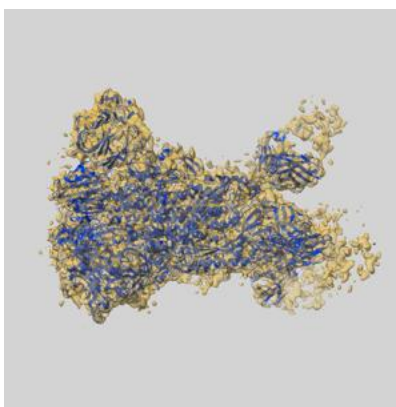
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8785 and PDB model 5W9J. Per-residue inclusion information can be found in section 3 on page 12.

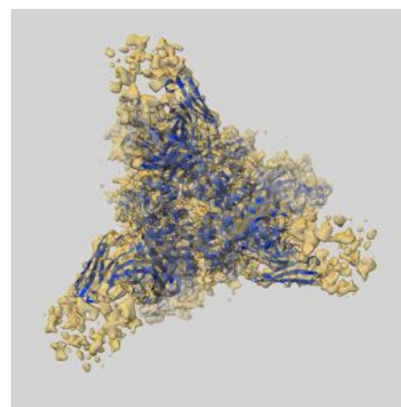
9.1 Map-model overlay [i](#)



X



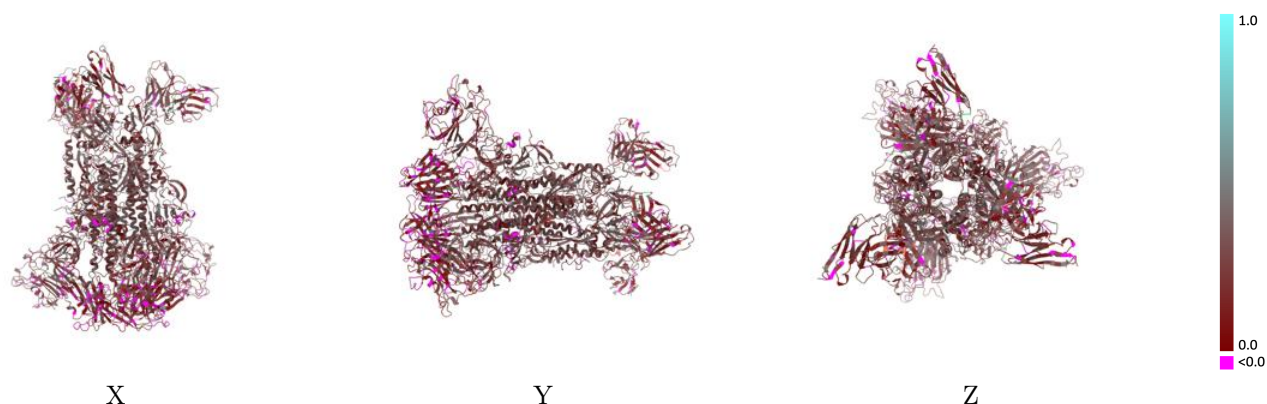
Y



Z

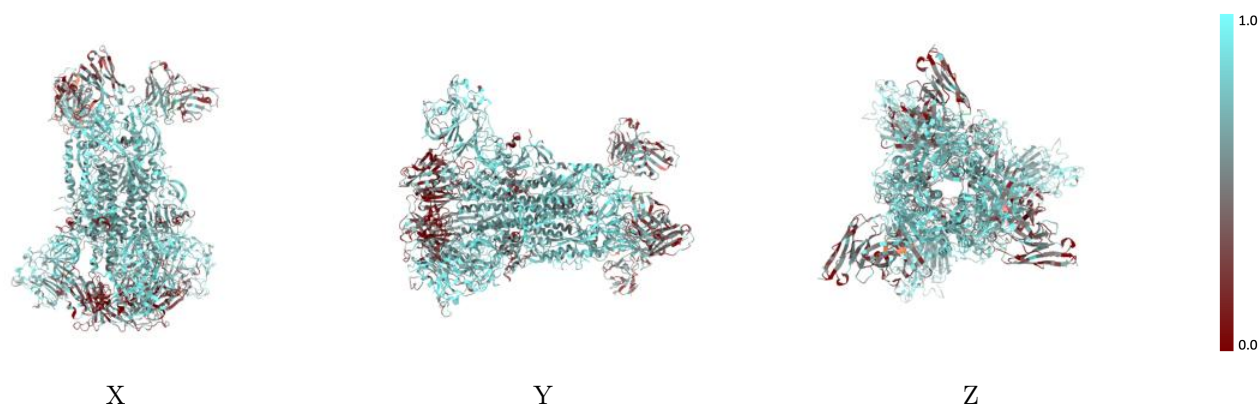
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



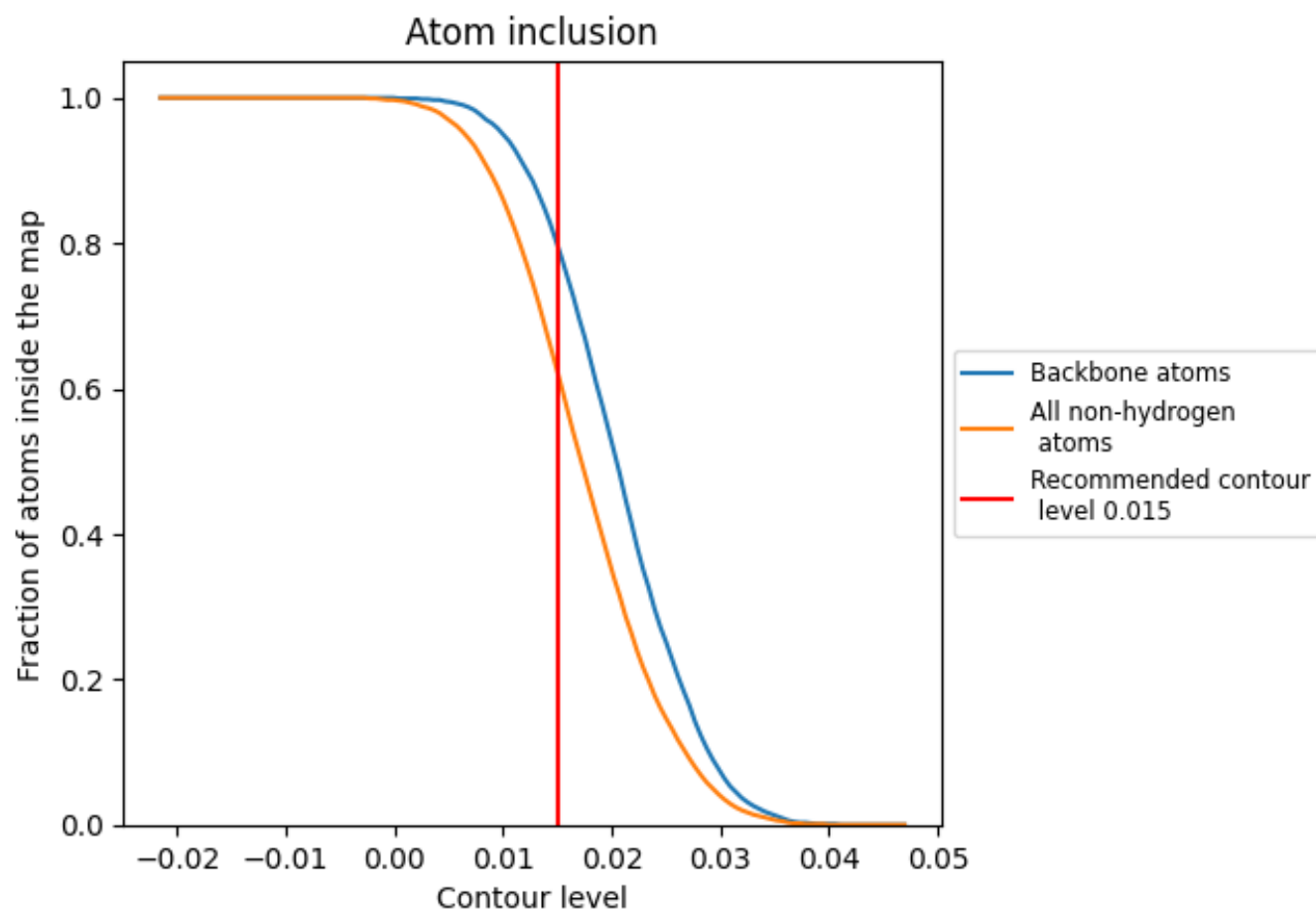
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 80% of all backbone atoms, 62% 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	0.6250	0.2370
A	0.7110	0.2840
B	0.5220	0.2340
C	0.4100	0.1910
D	0.7140	0.2840
E	0.5170	0.2360
F	0.4150	0.1930
G	0.7120	0.2840
H	0.5230	0.2350
I	0.4050	0.1920
J	0.6190	0.2130
K	0.6200	0.2140
L	0.6180	0.2130

1.0

0.0

<0.0