



Full wwPDB EM Validation Report ⓘ

Dec 13, 2023 – 04:38 PM JST

PDB ID : 8HRI
EMDB ID : EMD-34974
Title : SARS-CoV-2 Delta variant spike protein
Authors : Xu, J.; Cheng, H.; Liu, N.; Wang, H.W.
Deposited on : 2022-12-15
Resolution : 2.90 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.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

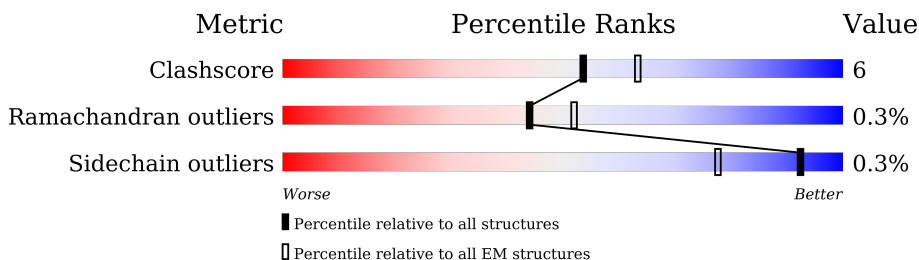
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1249	
1	B	1249	
1	C	1249	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24531 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
			Total	C	N	O	S		
1	A	1041	8170	5233	1360	1539	38	0	0
1	B	1044	8191	5245	1366	1542	38	0	0
1	C	1041	8170	5233	1360	1539	38	0	0

There are 303 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	MET	-	initiating methionine	UNP P0DTC2
A	-3	PRO	-	expression tag	UNP P0DTC2
A	-2	ARG	-	expression tag	UNP P0DTC2
A	-1	GLY	-	expression tag	UNP P0DTC2
A	0	PRO	-	expression tag	UNP P0DTC2
A	1	VAL	-	expression tag	UNP P0DTC2
A	2	ALA	-	expression tag	UNP P0DTC2
A	3	ALA	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	ILE	-	expression tag	UNP P0DTC2
A	9	LEU	-	expression tag	UNP P0DTC2
A	10	HIS	-	expression tag	UNP P0DTC2
A	11	GLY	-	expression tag	UNP P0DTC2
A	12	ALA	-	expression tag	UNP P0DTC2
A	13	TRP	-	expression tag	UNP P0DTC2
A	14	SER	-	expression tag	UNP P0DTC2
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	142	ASP	TYR	conflict	UNP P0DTC2
A	210A	ILE	LEU	conflict	UNP P0DTC2
A	210D	GLU	-	insertion	UNP P0DTC2
A	210E	PRO	-	insertion	UNP P0DTC2
A	210F	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1209	LEU	-	expression tag	UNP P0DTC2
A	1210	VAL	-	expression tag	UNP P0DTC2
A	1211	PRO	-	expression tag	UNP P0DTC2
A	1212	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	TYR	-	expression tag	UNP P0DTC2
A	1217	ILE	-	expression tag	UNP P0DTC2
A	1218	PRO	-	expression tag	UNP P0DTC2
A	1219	GLU	-	expression tag	UNP P0DTC2
A	1220	ALA	-	expression tag	UNP P0DTC2
A	1221	PRO	-	expression tag	UNP P0DTC2
A	1222	ARG	-	expression tag	UNP P0DTC2
A	1223	ASP	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	GLN	-	expression tag	UNP P0DTC2
A	1226	ALA	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	VAL	-	expression tag	UNP P0DTC2
A	1229	ARG	-	expression tag	UNP P0DTC2
A	1230	LYS	-	expression tag	UNP P0DTC2
A	1231	ASP	-	expression tag	UNP P0DTC2
A	1232	GLY	-	expression tag	UNP P0DTC2
A	1233	GLU	-	expression tag	UNP P0DTC2
A	1234	TRP	-	expression tag	UNP P0DTC2
A	1235	VAL	-	expression tag	UNP P0DTC2
A	1236	LEU	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	SER	-	expression tag	UNP P0DTC2
A	1239	THR	-	expression tag	UNP P0DTC2
A	1240	PHE	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	HIS	-	expression tag	UNP P0DTC2
A	1243	HIS	-	expression tag	UNP P0DTC2
A	1244	HIS	-	expression tag	UNP P0DTC2
A	1245	HIS	-	expression tag	UNP P0DTC2
A	1246	HIS	-	expression tag	UNP P0DTC2
A	1247	HIS	-	expression tag	UNP P0DTC2
B	-4	MET	-	initiating methionine	UNP P0DTC2
B	-3	PRO	-	expression tag	UNP P0DTC2
B	-2	ARG	-	expression tag	UNP P0DTC2
B	-1	GLY	-	expression tag	UNP P0DTC2
B	0	PRO	-	expression tag	UNP P0DTC2
B	1	VAL	-	expression tag	UNP P0DTC2
B	2	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	ILE	-	expression tag	UNP P0DTC2
B	9	LEU	-	expression tag	UNP P0DTC2
B	10	HIS	-	expression tag	UNP P0DTC2
B	11	GLY	-	expression tag	UNP P0DTC2
B	12	ALA	-	expression tag	UNP P0DTC2
B	13	TRP	-	expression tag	UNP P0DTC2
B	14	SER	-	expression tag	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	142	ASP	TYR	conflict	UNP P0DTC2
B	210A	ILE	LEU	conflict	UNP P0DTC2
B	210D	GLU	-	insertion	UNP P0DTC2
B	210E	PRO	-	insertion	UNP P0DTC2
B	210F	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	LEU	-	expression tag	UNP P0DTC2
B	1210	VAL	-	expression tag	UNP P0DTC2
B	1211	PRO	-	expression tag	UNP P0DTC2
B	1212	ARG	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2
B	1216	TYR	-	expression tag	UNP P0DTC2
B	1217	ILE	-	expression tag	UNP P0DTC2
B	1218	PRO	-	expression tag	UNP P0DTC2
B	1219	GLU	-	expression tag	UNP P0DTC2
B	1220	ALA	-	expression tag	UNP P0DTC2
B	1221	PRO	-	expression tag	UNP P0DTC2
B	1222	ARG	-	expression tag	UNP P0DTC2
B	1223	ASP	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	GLN	-	expression tag	UNP P0DTC2
B	1226	ALA	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	VAL	-	expression tag	UNP P0DTC2
B	1229	ARG	-	expression tag	UNP P0DTC2
B	1230	LYS	-	expression tag	UNP P0DTC2
B	1231	ASP	-	expression tag	UNP P0DTC2
B	1232	GLY	-	expression tag	UNP P0DTC2
B	1233	GLU	-	expression tag	UNP P0DTC2
B	1234	TRP	-	expression tag	UNP P0DTC2
B	1235	VAL	-	expression tag	UNP P0DTC2
B	1236	LEU	-	expression tag	UNP P0DTC2
B	1237	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1238	SER	-	expression tag	UNP P0DTC2
B	1239	THR	-	expression tag	UNP P0DTC2
B	1240	PHE	-	expression tag	UNP P0DTC2
B	1241	LEU	-	expression tag	UNP P0DTC2
B	1242	HIS	-	expression tag	UNP P0DTC2
B	1243	HIS	-	expression tag	UNP P0DTC2
B	1244	HIS	-	expression tag	UNP P0DTC2
B	1245	HIS	-	expression tag	UNP P0DTC2
B	1246	HIS	-	expression tag	UNP P0DTC2
B	1247	HIS	-	expression tag	UNP P0DTC2
C	-4	MET	-	initiating methionine	UNP P0DTC2
C	-3	PRO	-	expression tag	UNP P0DTC2
C	-2	ARG	-	expression tag	UNP P0DTC2
C	-1	GLY	-	expression tag	UNP P0DTC2
C	0	PRO	-	expression tag	UNP P0DTC2
C	1	VAL	-	expression tag	UNP P0DTC2
C	2	ALA	-	expression tag	UNP P0DTC2
C	3	ALA	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2
C	8	ILE	-	expression tag	UNP P0DTC2
C	9	LEU	-	expression tag	UNP P0DTC2
C	10	HIS	-	expression tag	UNP P0DTC2
C	11	GLY	-	expression tag	UNP P0DTC2
C	12	ALA	-	expression tag	UNP P0DTC2
C	13	TRP	-	expression tag	UNP P0DTC2
C	14	SER	-	expression tag	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	142	ASP	TYR	conflict	UNP P0DTC2
C	210A	ILE	LEU	conflict	UNP P0DTC2
C	210D	GLU	-	insertion	UNP P0DTC2
C	210E	PRO	-	insertion	UNP P0DTC2
C	210F	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1209	LEU	-	expression tag	UNP P0DTC2
C	1210	VAL	-	expression tag	UNP P0DTC2
C	1211	PRO	-	expression tag	UNP P0DTC2
C	1212	ARG	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	TYR	-	expression tag	UNP P0DTC2
C	1217	ILE	-	expression tag	UNP P0DTC2
C	1218	PRO	-	expression tag	UNP P0DTC2
C	1219	GLU	-	expression tag	UNP P0DTC2
C	1220	ALA	-	expression tag	UNP P0DTC2

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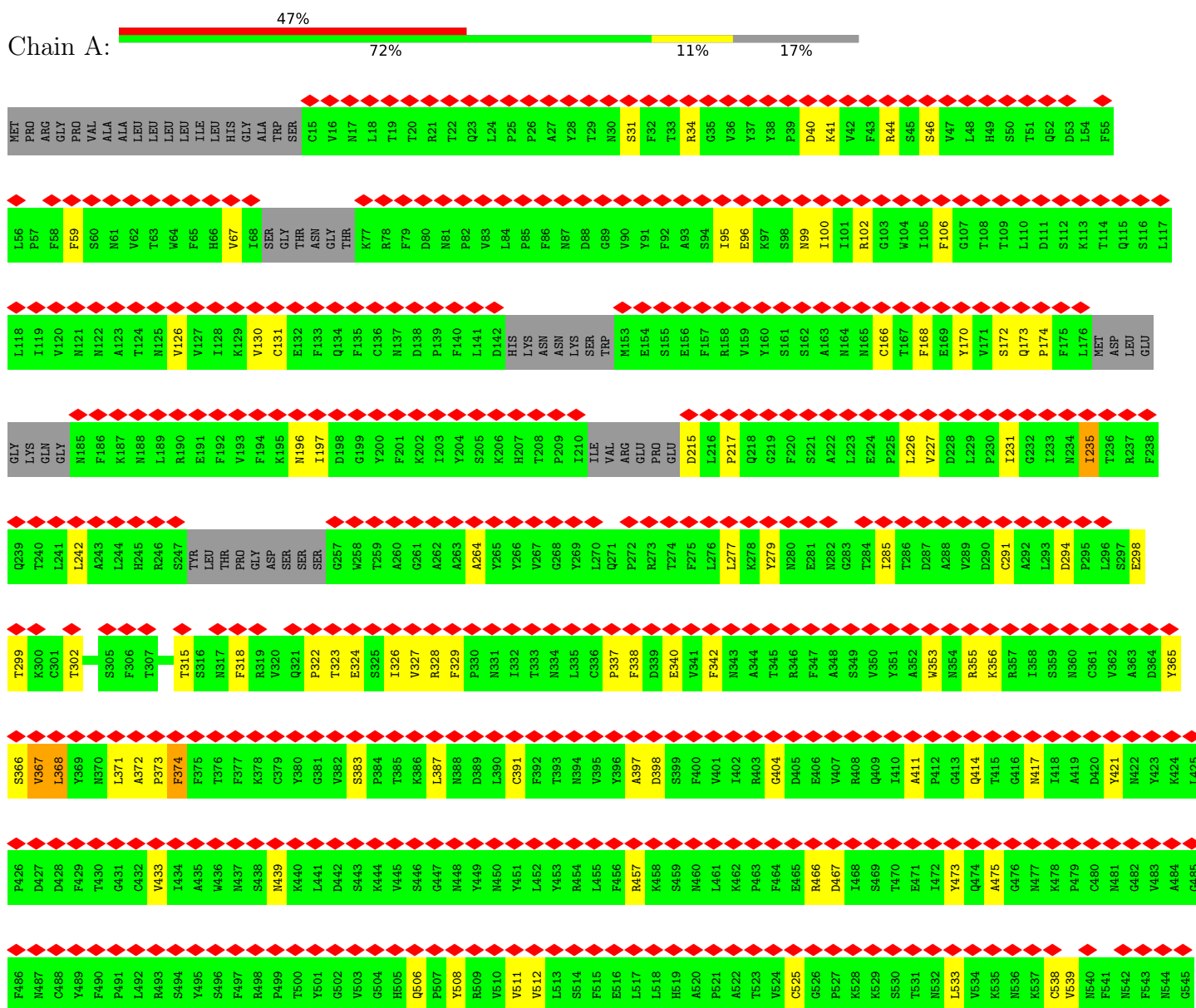
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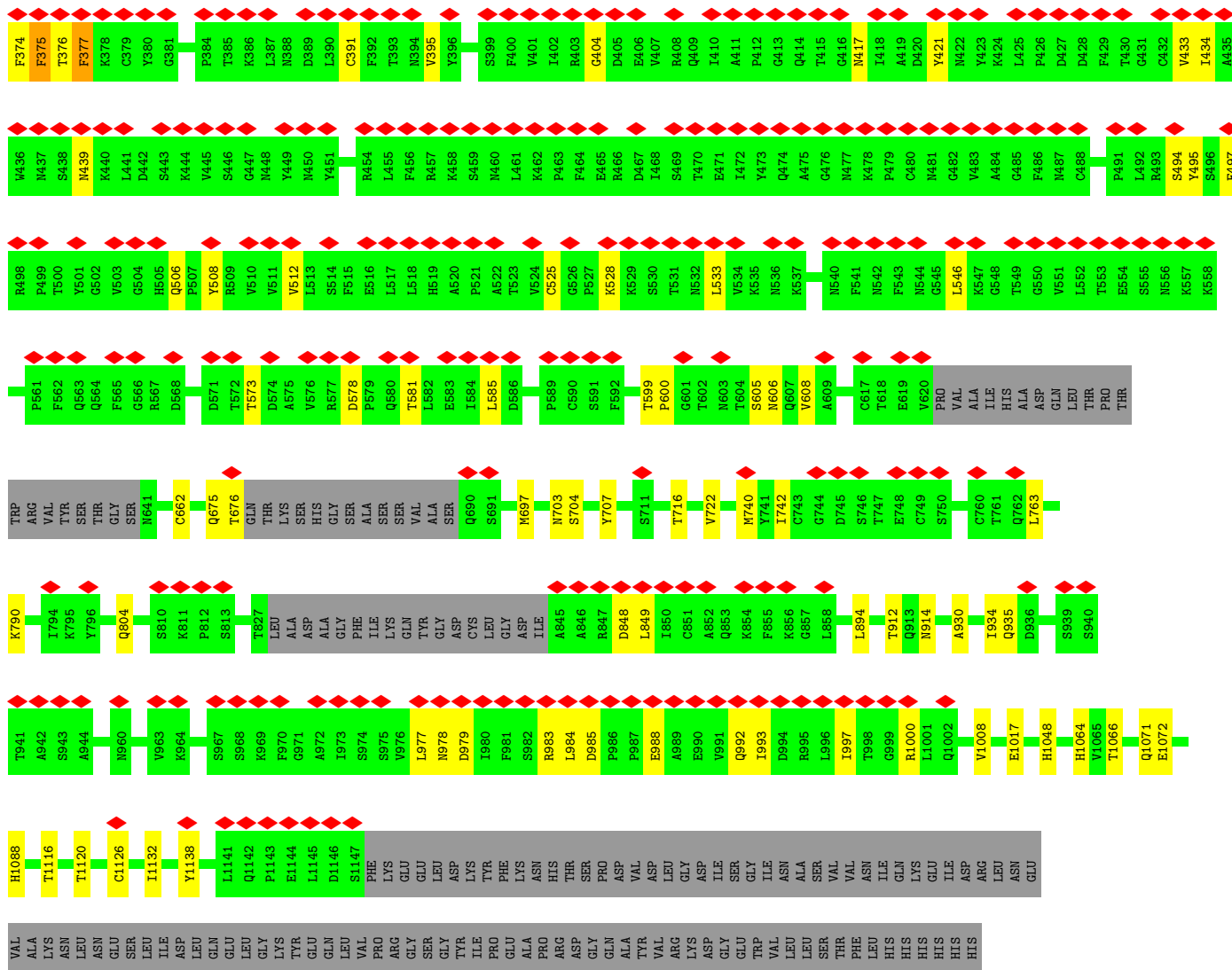
Chain	Residue	Modelled	Actual	Comment	Reference
C	1221	PRO	-	expression tag	UNP P0DTC2
C	1222	ARG	-	expression tag	UNP P0DTC2
C	1223	ASP	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	GLN	-	expression tag	UNP P0DTC2
C	1226	ALA	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	VAL	-	expression tag	UNP P0DTC2
C	1229	ARG	-	expression tag	UNP P0DTC2
C	1230	LYS	-	expression tag	UNP P0DTC2
C	1231	ASP	-	expression tag	UNP P0DTC2
C	1232	GLY	-	expression tag	UNP P0DTC2
C	1233	GLU	-	expression tag	UNP P0DTC2
C	1234	TRP	-	expression tag	UNP P0DTC2
C	1235	VAL	-	expression tag	UNP P0DTC2
C	1236	LEU	-	expression tag	UNP P0DTC2
C	1237	LEU	-	expression tag	UNP P0DTC2
C	1238	SER	-	expression tag	UNP P0DTC2
C	1239	THR	-	expression tag	UNP P0DTC2
C	1240	PHE	-	expression tag	UNP P0DTC2
C	1241	LEU	-	expression tag	UNP P0DTC2
C	1242	HIS	-	expression tag	UNP P0DTC2
C	1243	HIS	-	expression tag	UNP P0DTC2
C	1244	HIS	-	expression tag	UNP P0DTC2
C	1245	HIS	-	expression tag	UNP P0DTC2
C	1246	HIS	-	expression tag	UNP P0DTC2
C	1247	HIS	-	expression tag	UNP P0DTC2

3 Residue-property plots

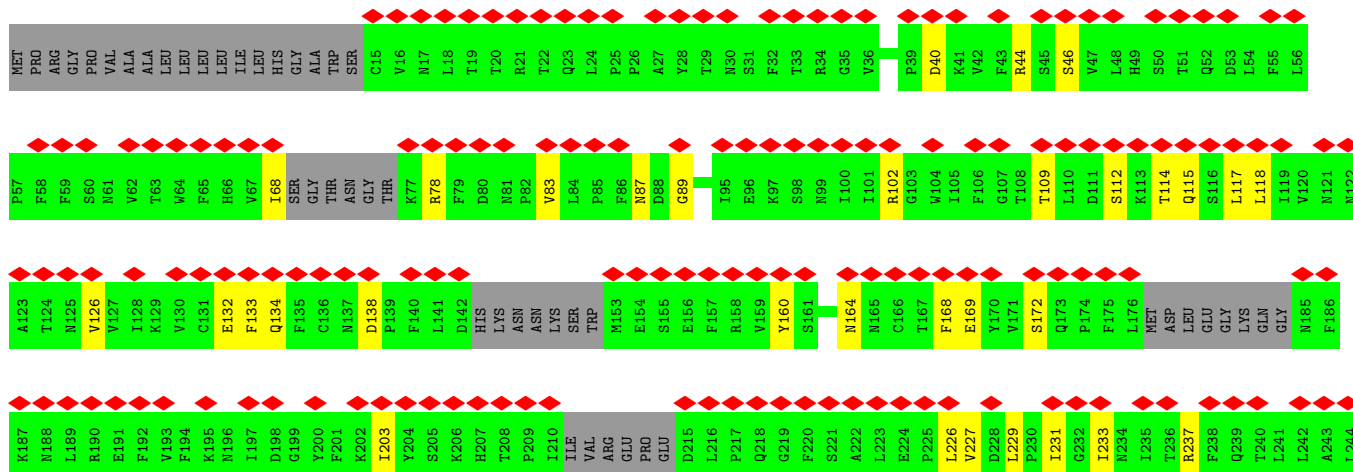
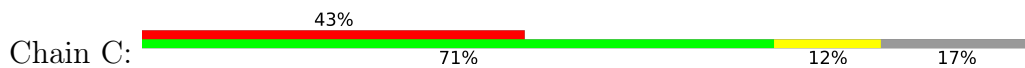
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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





● Molecule 1: Spike glycoprotein



H245	R246	S247	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	G257	W258	T259	A260	G261	A262	A263	A264	Y265	Y266	Y267	G268	Y269	L270	Q271	P272	R273	T274	F275	L276	L277	K278	Y279	N280	E281	N282	I285	T286	D287	A288	V289	D290	C291	A292	L293	D294	P295	L296	S297	E298	T299	K300	L303	K304	S305	F306		
T307	T315	S316	N317	F318	R319	V320	Q321	P322	T323	E324	S325	V327	R328	F329	P330	N331	I332	N334	L335	C336	P337	F338	D339	E340	V341	F342	N343	R346	F347	A348	S349	V350	Y351	A352	W353	N354	R355	K356	R357	I358	S359	N360	C361	V362	Y423	K424	L425	P426	D427	D428	F429	T430	G431	C432	V433	F373	F374	
F375	T376	F377	K378	C379	G381	V382	S383	F384	T385	K386	L387	N388	D389	L390	C391	F392	T393	N394	V395	Y396	D398	S399	F400	I401	I402	R403	G404	D405	E406	R408	Q409	I410	A411	P412	G413	Q414	T415	G416	M417	I418	A419	D420	Y421	M422	Y423	K424	L425	P426	D427	D428	F429	T430	G431	C432	V433	I434		
A435	W436	M437	S438	M439	K440	L441	D442	S443	K444	Y445	S446	C447	M448	Y449	M450	Y451	L452	Y453	R454	L455	F456	R457	S459	M460	L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	M477	K478	F479	C480	M481	G482	V483	A484	G485	F486	M487	C488	Y489	F490	P491	L492	R493	S494
Y495	S496	F497	R498	P499	T500	Y501	G502	V503	G504	H505	Q506	P507	Y508	R509	V510	V511	L513	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	N540	F541	N542	F543	N544	G545	L546	K547	G548	T549	G550	V551	L552	T553	E554
S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565	G566	R567	D568	L569	A570	D571	T572	L573	D574	V576	R577	F579	Q580	T581	L582	E583	L584	L585	D586	L587	C590	S591	F592	G593	G601	T602	N603	T604	Q607	V608	A609	L610	L611	N615	N616	C617	V620	PRO	VAL	ALA	ILE	HIS						
ALA	ASP	GLN	THR	PRO	THR	TRP	ARG	VAL	TYR	THR	GLY	SER	N641	R646	A647	G648	L650	A653	E654	D663	V674	Q675	T676	GLN	THR	LYS	SER	HIS	ALA	SER	SER	VAL	VAL	SER	D690	S691	L699	N710	A713	V722	M740	Y741	I742	D745														
S746	T747	E748	C749	S750	N751	L752	L753	L754	W755	G757	S758	F759	C760	L763	P792	T796	Q804	S810	K811	P812	F823	N824	K825	N826	R827	LEU	ALA	ASP	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	S691	L699	N710	A713	V722	M740	Y741	I742	D745	D848	L849	R850	C851	A852	K853	R854						
F855	K856	L894	R902	V915	L916	N919	I931	I934	Q935	L938	S939	S940	T941	A942	S943	A944	L945	D950	H954	L959	R964	Q965	A972	I973	L977	R978	D979	I980	F981	S982	R983	L984	D985	F986	P987	E988	A989	Y991	Q992	I993	N994	L996	I997															
R1000	L1001	Q1002	V1008	R1019	K1028	F1042	H1048	P1057	V1065	T1066	E1072	K1086	E1092	S1097	H1101	W1102	T1116	V1122	N1135	Y1138	L1141	Q1142	P1143	E1144	L1145	D1146	S1147	PHE	GLU	GLY	SER	GLY	LEU	ASP	LYS	TYR	GLY	GLN	VAL	PRO	ARG	GLY	SER	GLY	TYR	ILE	PRO	GLY	ALA	ASN	HIS	THR	SER	PRO				
ASP	VAL	ASP	LEU	TYR	VAL	ARG	LYS	ASP	GLY	ILE	ASN	ALA	TRP	VAL	LEU	VAL	VAL	VAL	ASN	THR	PHE	GLN	LEU	HIS	HIS	HIS	HIS	HIS	ASP	VAL	PRO	ARG	GLY	SER	GLY	LEU	ASP	LYS	TYR	GLY	GLN	VAL	PRO	ARG	GLY	SER	GLY	TYR	ILE	PRO	GLY	ALA	ASN	HIS	THR	SER	PRO	
ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	ILE	ASN	ALA	TRP	VAL	LEU	VAL	VAL	VAL	ASN	THR	PHE	GLN	LEU	HIS	HIS	HIS	HIS	ASP	VAL	PRO	ARG	GLY	SER	GLY	LEU	ASP	LYS	TYR	GLY	GLN	VAL	PRO	ARG	GLY	SER	GLY	TYR	ILE	PRO	GLY	ALA	ASN	HIS	THR	SER	PRO		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	167167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	8.683	Depositor
Minimum map value	-4.943	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.115	Depositor
Recommended contour level	0.7	Depositor
Map size (\AA)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/8359	0.50	0/11367
1	B	0.27	0/8380	0.50	0/11395
1	C	0.27	0/8359	0.49	0/11367
All	All	0.27	0/25098	0.50	0/34129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8170	0	8006	94	0
1	B	8191	0	8029	88	0
1	C	8170	0	8006	102	0
All	All	24531	0	24041	268	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 (268) 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:C:391:CYS:HA	1:C:525:CYS:HB3	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:PHE:HE1	1:B:434:ILE:HG23	1.27	0.97
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.48	0.91
1:A:372:ALA:HB1	1:A:373:PRO:HD2	1.66	0.78
1:B:176:LEU:HG	1:B:190:ARG:HE	1.48	0.78
1:C:132:GLU:HB3	1:C:164:ASN:HB3	1.64	0.78
1:A:391:CYS:HB2	1:A:525:CYS:HA	1.65	0.76
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.69	0.75
1:A:46:SER:HA	1:A:279:TYR:O	1.89	0.72
1:B:96:GLU:O	1:B:188:ASN:HB2	1.89	0.72
1:A:365:TYR:HA	1:A:368:LEU:HD23	1.72	0.71
1:B:375:PHE:CE1	1:B:434:ILE:HG23	2.19	0.70
1:B:83:VAL:HG11	1:B:237:ARG:HH11	1.56	0.70
1:B:81:ASN:HD21	1:B:242:LEU:HD23	1.57	0.69
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.26	0.69
1:C:422:ASN:HD21	1:C:454:ARG:H	1.41	0.68
1:A:983:ARG:HG2	1:C:390:LEU:HD21	1.75	0.68
1:C:112:SER:HB3	1:C:134:GLN:NE2	2.08	0.68
1:B:113:LYS:HG3	1:B:114:THR:HG23	1.76	0.67
1:A:40:ASP:OD2	1:A:44:ARG:NH1	2.26	0.66
1:C:203:ILE:HB	1:C:227:VAL:HB	1.75	0.66
1:C:676:THR:HB	1:C:691:SER:H	1.61	0.65
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.78	0.65
1:C:391:CYS:HA	1:C:525:CYS:CB	2.26	0.65
1:C:902:MET:HB3	1:C:916:LEU:HD11	1.79	0.65
1:C:115:GLN:HG2	1:C:233:ILE:HG21	1.79	0.64
1:B:439:ASN:ND2	1:B:506:GLN:OE1	2.30	0.64
1:B:848:ASP:OD1	1:B:849:LEU:N	2.30	0.64
1:B:370:ASN:O	1:B:371:LEU:C	2.36	0.64
1:C:329:PHE:O	1:C:580:GLN:NE2	2.30	0.63
1:B:126:VAL:HB	1:B:174:PRO:HA	1.81	0.62
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.81	0.62
1:C:40:ASP:OD2	1:C:44:ARG:NH2	2.31	0.62
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	1.81	0.62
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.81	0.62
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.82	0.61
1:A:96:GLU:OE2	1:A:100:ILE:N	2.32	0.61
1:C:540:ASN:HB3	1:C:549:THR:HG22	1.81	0.61
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.65	0.61
1:C:367:VAL:HG23	1:C:368:LEU:HD12	1.83	0.61
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.83	0.61
1:A:318:PHE:O	1:A:592:PHE:HA	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.34	0.61
1:A:659:SER:HB3	1:A:698:SER:HB2	1.83	0.60
1:B:173:GLN:OE1	1:B:174:PRO:HD2	2.01	0.60
1:B:172:SER:OG	1:B:173:GLN:N	2.34	0.60
1:A:433:VAL:HG22	1:A:512:VAL:HG22	1.83	0.59
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.83	0.59
1:C:126:VAL:HB	1:C:172:SER:HB2	1.84	0.59
1:A:353:TRP:O	1:A:466:ARG:NH2	2.31	0.59
1:A:1142:GLN:HG3	1:A:1143:PRO:HD3	1.83	0.59
1:C:117:LEU:HD11	1:C:231:ILE:HG21	1.85	0.58
1:B:358:ILE:HB	1:B:395:VAL:HB	1.85	0.58
1:C:89:GLY:HA3	1:C:270:LEU:HD12	1.85	0.58
1:C:991:VAL:HG23	1:C:992:GLN:HE21	1.68	0.58
1:B:1072:GLU:HG2	1:C:894:LEU:HD21	1.85	0.57
1:A:404:GLY:HA2	1:A:508:TYR:HD2	1.68	0.57
1:A:329:PHE:O	1:A:580:GLN:NE2	2.38	0.57
1:B:139:PRO:HA	1:B:158:ARG:O	2.05	0.57
1:A:869:MET:HG2	1:C:699:LEU:HD21	1.86	0.57
1:B:375:PHE:HE1	1:B:434:ILE:CG2	2.11	0.57
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.86	0.56
1:B:599:THR:HB	1:B:608:VAL:HG12	1.87	0.56
1:B:95:ILE:HG13	1:B:186:PHE:HB2	1.88	0.56
1:C:763:LEU:HG	1:C:1008:VAL:HG21	1.87	0.56
1:A:326:ILE:HG22	1:A:328:ARG:HG2	1.86	0.56
1:A:763:LEU:HG	1:A:1008:VAL:HG21	1.86	0.56
1:B:100:ILE:HG22	1:B:242:LEU:HD12	1.88	0.56
1:B:376:THR:O	1:B:377:PHE:HB2	2.05	0.55
1:B:978:ASN:OD1	1:B:979:ASP:N	2.40	0.55
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.88	0.55
1:A:291:CYS:HB2	1:A:298:GLU:HA	1.89	0.55
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.24	0.55
1:C:433:VAL:HG22	1:C:512:VAL:HG22	1.89	0.55
1:A:931:ILE:O	1:A:934:ILE:HG22	2.06	0.55
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.89	0.55
1:A:31:SER:O	1:A:59:PHE:HA	2.07	0.54
1:A:99:ASN:O	1:A:102:ARG:NH1	2.40	0.54
1:B:707:TYR:HB3	1:C:792:PRO:HG3	1.88	0.54
1:B:99:ASN:O	1:B:102:ARG:NH1	2.38	0.54
1:A:337:PRO:HB2	1:A:340:GLU:OE1	2.07	0.54
1:B:675:GLN:O	1:B:676:THR:C	2.45	0.54
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:CYS:HB2	1:B:133:PHE:CD1	2.43	0.54
1:B:125:ASN:HA	1:B:174:PRO:HD3	1.89	0.53
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.74	0.53
1:C:756:TYR:HE2	1:C:997:ILE:HG21	1.73	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.89	0.53
1:B:68:ILE:HG22	1:B:78:ARG:HB2	1.90	0.53
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.90	0.53
1:C:112:SER:HB3	1:C:134:GLN:HE21	1.73	0.53
1:C:328:ARG:NH2	1:C:578:ASP:OD2	2.29	0.53
1:C:357:ARG:NH2	1:C:396:TYR:OH	2.41	0.52
1:C:988:GLU:O	1:C:992:GLN:HG2	2.09	0.52
1:A:383:SER:HB2	1:C:456:PHE:HE1	1.74	0.52
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.46	0.51
1:B:319:ARG:HH22	1:C:740:MET:HG2	1.74	0.51
1:C:226:LEU:HD23	1:C:227:VAL:HG23	1.91	0.51
1:A:170:TYR:HE1	1:A:172:SER:HB2	1.75	0.51
1:A:196:ASN:HD22	1:A:235:ILE:HG21	1.76	0.51
1:C:68:ILE:HD12	1:C:78:ARG:HG3	1.93	0.51
1:C:409:GLN:OE1	1:C:416:GLY:HA3	2.11	0.51
1:C:823:PHE:CD1	1:C:1057:PRO:HD3	2.46	0.51
1:B:433:VAL:HG22	1:B:512:VAL:HG22	1.93	0.51
1:C:823:PHE:HD1	1:C:1057:PRO:HD3	1.76	0.51
1:A:748:GLU:O	1:A:752:LEU:HG	2.11	0.50
1:C:915:VAL:O	1:C:919:ASN:ND2	2.43	0.50
1:C:950:ASP:O	1:C:954:HIS:ND1	2.44	0.50
1:B:231:ILE:HG22	1:B:233:ILE:HG23	1.93	0.50
1:B:993:ILE:O	1:B:997:ILE:HG12	2.10	0.50
1:C:979:ASP:O	1:C:983:ARG:HB2	2.11	0.50
1:A:592:PHE:CE1	1:B:740:MET:HE1	2.47	0.50
1:B:404:GLY:HA2	1:B:508:TYR:CD2	2.47	0.50
1:B:763:LEU:HG	1:B:1008:VAL:HG21	1.92	0.50
1:A:961:THR:O	1:A:965:GLN:HG2	2.12	0.50
1:B:139:PRO:HB3	1:B:159:VAL:HA	1.94	0.50
1:B:495:TYR:HB3	1:B:497:PHE:CE1	2.46	0.50
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.93	0.50
1:C:133:PHE:CE1	1:C:160:TYR:HB3	2.47	0.50
1:C:490:PHE:CE2	1:C:492:LEU:HB2	2.46	0.50
1:A:702:GLU:OE2	1:B:790:LYS:NZ	2.34	0.49
1:C:338:PHE:HD2	1:C:368:LEU:HD11	1.76	0.49
1:C:519:HIS:HB3	1:C:565:PHE:HE1	1.78	0.49
1:A:173:GLN:HG3	1:A:174:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASN:O	1:A:421:TYR:HB2	2.12	0.49
1:A:342:PHE:CZ	1:A:511:VAL:HG21	2.47	0.49
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.45	0.49
1:A:371:LEU:O	1:A:372:ALA:HB2	2.13	0.49
1:B:131:CYS:HB2	1:B:133:PHE:CE1	2.47	0.49
1:B:716:THR:OG1	1:B:1071:GLN:O	2.20	0.49
1:B:81:ASN:ND2	1:B:242:LEU:HD23	2.24	0.49
1:C:336:CYS:HB2	1:C:337:PRO:HD2	1.94	0.49
1:B:118:LEU:HD21	1:B:120:VAL:HG23	1.95	0.49
1:B:988:GLU:O	1:B:992:GLN:HG2	2.12	0.49
1:C:676:THR:HB	1:C:691:SER:N	2.28	0.48
1:C:931:ILE:O	1:C:934:ILE:HG22	2.14	0.48
1:C:985:ASP:HB3	1:C:987:PRO:HD2	1.95	0.48
1:B:294:ASP:N	1:B:294:ASP:OD1	2.46	0.48
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.96	0.48
1:C:358:ILE:HB	1:C:395:VAL:HB	1.96	0.48
1:C:988:GLU:OE1	1:C:988:GLU:N	2.45	0.48
1:A:323:THR:O	1:A:539:VAL:HG12	2.14	0.48
1:C:497:PHE:CE2	1:C:507:PRO:HB3	2.48	0.48
1:A:41:LYS:HG2	1:C:562:PHE:HD2	1.78	0.48
1:A:338:PHE:HE2	1:A:365:TYR:CE1	2.32	0.48
1:A:372:ALA:HB1	1:A:373:PRO:CD	2.42	0.48
1:C:409:GLN:NE2	1:C:418:ILE:HG12	2.28	0.47
1:C:445:VAL:O	1:C:498:ARG:NH1	2.47	0.47
1:A:373:PRO:O	1:A:373:PRO:HG2	2.13	0.47
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.95	0.47
1:A:884:SER:OG	1:A:887:THR:OG1	2.33	0.47
1:B:119:ILE:HG23	1:B:128:ILE:HG13	1.96	0.47
1:B:374:PHE:O	1:B:375:PHE:HB2	2.14	0.47
1:A:777:ASN:O	1:A:781:VAL:HG23	2.15	0.47
1:B:984:LEU:HD13	1:B:988:GLU:HB3	1.97	0.47
1:A:299:THR:HA	1:A:302:THR:HG22	1.96	0.47
1:A:41:LYS:HE2	1:C:562:PHE:HB2	1.96	0.47
1:A:605:SER:OG	1:A:606:ASN:N	2.48	0.47
1:A:294:ASP:OD1	1:A:294:ASP:N	2.46	0.46
1:A:130:VAL:HG12	1:A:168:PHE:HB3	1.97	0.46
1:A:858:LEU:HD13	1:A:959:LEU:HD22	1.97	0.46
1:B:130:VAL:HG12	1:B:168:PHE:HB3	1.96	0.46
1:C:350:VAL:HG12	1:C:422:ASN:HB3	1.97	0.46
1:C:533:LEU:HD23	1:C:533:LEU:H	1.80	0.46
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:GLN:HG2	1:A:963:VAL:HG21	1.96	0.46
1:B:662:CYS:HB2	1:B:697:MET:HG2	1.97	0.46
1:C:444:LYS:HG3	1:C:447:GLY:H	1.81	0.45
1:B:494:SER:OG	1:B:495:TYR:N	2.48	0.45
1:C:439:ASN:CG	1:C:506:GLN:HG2	2.36	0.45
1:A:356:LYS:HB2	1:A:397:ALA:HB3	1.99	0.45
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.99	0.45
1:A:328:ARG:NH2	1:A:580:GLN:HB2	2.32	0.45
1:A:398:ASP:O	1:A:511:VAL:HA	2.16	0.45
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.98	0.45
1:B:578:ASP:HB3	1:B:581:THR:O	2.17	0.45
1:B:1088:HIS:HB3	1:B:1120:THR:HG21	1.98	0.45
1:B:605:SER:OG	1:B:606:ASN:N	2.49	0.45
1:A:1002:GLN:HE22	1:C:1002:GLN:NE2	2.14	0.45
1:B:368:LEU:O	1:B:370:ASN:N	2.49	0.45
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.98	0.44
1:B:977:LEU:HD23	1:B:977:LEU:H	1.81	0.44
1:C:46:SER:HA	1:C:279:TYR:O	2.17	0.44
1:B:80:ASP:OD1	1:B:80:ASP:N	2.49	0.44
1:B:121:ASN:HD21	1:B:176:LEU:HB2	1.82	0.44
1:A:355:ARG:HG2	1:A:466:ARG:HH12	1.82	0.44
1:A:538:CYS:HB3	1:A:551:VAL:HG23	1.99	0.44
1:B:111:ASP:OD1	1:B:113:LYS:HG2	2.17	0.44
1:C:168:PHE:CE2	1:C:229:LEU:HD22	2.53	0.44
1:C:611:LEU:HD12	1:C:650:LEU:HD13	1.99	0.44
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.33	0.44
1:B:142:ASP:O	1:B:156:GLU:HB3	2.18	0.44
1:A:815:ARG:HD2	1:A:819:GLU:HB3	1.98	0.44
1:B:722:VAL:HA	1:B:1064:HIS:O	2.17	0.44
1:C:138:ASP:N	1:C:138:ASP:OD1	2.51	0.44
1:C:560:LEU:HB2	1:C:561:PRO:HD2	2.00	0.44
1:B:417:ASN:O	1:B:421:TYR:HB2	2.18	0.43
1:C:977:LEU:HD22	1:C:993:ILE:HD12	1.99	0.43
1:A:366:SER:C	1:A:368:LEU:H	2.22	0.43
1:A:298:GLU:HG2	1:A:315:THR:CG2	2.47	0.43
1:A:323:THR:HG23	1:A:324:GLU:OE1	2.18	0.43
1:A:533:LEU:H	1:A:533:LEU:HD23	1.84	0.43
1:A:46:SER:CA	1:A:279:TYR:O	2.61	0.43
1:B:703:ASN:OD1	1:B:704:SER:N	2.51	0.43
1:C:87:ASN:O	1:C:89:GLY:N	2.52	0.43
1:C:502:GLY:O	1:C:506:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:ASN:OD1	1:A:964:LYS:HE2	2.19	0.43
1:C:393:THR:O	1:C:523:THR:OG1	2.36	0.43
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.53	0.43
1:A:34:ARG:NH1	1:A:217:PRO:O	2.51	0.43
1:A:355:ARG:NH2	1:A:356:LYS:O	2.51	0.43
1:B:118:LEU:HD13	1:B:133:PHE:CE2	2.53	0.43
1:C:710:ASN:N	1:C:710:ASN:OD1	2.52	0.43
1:C:462:LYS:HD3	1:C:463:PRO:HD2	2.01	0.43
1:A:67:VAL:HG21	1:A:242:LEU:HD22	2.00	0.42
1:A:95:ILE:HG22	1:A:264:ALA:HB3	2.00	0.42
1:A:979:ASP:OD1	1:A:980:ILE:N	2.51	0.42
1:C:825:LYS:HB3	1:C:945:LEU:HD12	2.00	0.42
1:A:277:LEU:HD23	1:A:285:ILE:HD13	2.01	0.42
1:A:387:LEU:H	1:A:387:LEU:HD23	1.84	0.42
1:B:376:THR:HG22	1:B:377:PHE:H	1.83	0.42
1:B:912:THR:OG1	1:B:914:ASN:OD1	2.22	0.42
1:A:473:TYR:CE2	1:A:475:ALA:HB2	2.54	0.42
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.52	0.42
1:C:387:LEU:H	1:C:387:LEU:HD23	1.85	0.42
1:C:428:ASP:OD1	1:C:428:ASP:N	2.52	0.42
1:A:322:PRO:HB3	1:A:538:CYS:SG	2.60	0.42
1:B:366:SER:HA	1:B:369:TYR:CE2	2.54	0.42
1:C:825:LYS:HE2	1:C:825:LYS:HB2	1.84	0.42
1:A:106:PHE:HB3	1:A:235:ILE:CD1	2.50	0.42
1:A:215:ASP:N	1:A:215:ASP:OD1	2.53	0.42
1:C:102:ARG:HA	1:C:102:ARG:HD3	1.88	0.42
1:C:676:THR:HG22	1:C:690:GLN:HB3	2.01	0.42
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.44	0.42
1:C:118:LEU:HD21	1:C:133:PHE:CE2	2.55	0.42
1:C:169:GLU:OE1	1:C:169:GLU:N	2.52	0.42
1:B:339:ASP:OD1	1:B:340:GLU:N	2.53	0.41
1:B:984:LEU:HD12	1:B:985:ASP:O	2.20	0.41
1:C:40:ASP:N	1:C:40:ASP:OD1	2.52	0.41
1:A:722:VAL:HA	1:A:1064:HIS:O	2.20	0.41
1:A:758:SER:H	1:C:965:GLN:NE2	2.18	0.41
1:C:168:PHE:HE2	1:C:229:LEU:HD22	1.86	0.41
1:A:130:VAL:HG11	1:A:231:ILE:HD12	2.01	0.41
1:A:197:ILE:HD12	1:A:197:ILE:HA	1.98	0.41
1:A:373:PRO:O	1:A:373:PRO:CG	2.69	0.41
1:B:1072:GLU:HG2	1:C:894:LEU:CD2	2.48	0.41
1:C:854:LYS:HB2	1:C:854:LYS:HE2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.85	0.41
1:C:1072:GLU:OE1	1:C:1072:GLU:N	2.49	0.41
1:A:736:VAL:HG22	1:A:858:LEU:HD22	2.03	0.41
1:C:1086:LYS:HD2	1:C:1122:VAL:HG21	2.03	0.41
1:B:87:ASN:HD22	1:B:269:TYR:HE2	1.69	0.41
1:C:756:TYR:CE2	1:C:997:ILE:HG21	2.52	0.41
1:B:1017:GLU:OE1	1:C:1019:ARG:NH2	2.54	0.41
1:C:83:VAL:HG11	1:C:237:ARG:NH2	2.35	0.41
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.56	0.41
1:A:726:ILE:HD13	1:A:945:LEU:HD13	2.02	0.41
1:B:930:ALA:O	1:B:934:ILE:HG12	2.21	0.41
1:A:569:ILE:HD12	1:A:569:ILE:H	1.86	0.40
1:B:109:THR:HA	1:B:237:ARG:NH2	2.37	0.40
1:B:495:TYR:HB3	1:B:497:PHE:CD1	2.56	0.40
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.56	0.40
1:A:327:VAL:O	1:A:327:VAL:HG12	2.22	0.40
1:A:439:ASN:CG	1:A:506:GLN:HG2	2.42	0.40
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.03	0.40
1:B:78:ARG:NH2	1:B:80:ASP:OD2	2.55	0.40
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.03	0.40
1:C:109:THR:HG22	1:C:114:THR:HG22	2.04	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	1023/1249 (82%)	970 (95%)	50 (5%)	3 (0%)	41	71
1	B	1026/1249 (82%)	967 (94%)	53 (5%)	6 (1%)	25	58
1	C	1023/1249 (82%)	974 (95%)	49 (5%)	0	100	100
All	All	3072/3747 (82%)	2911 (95%)	152 (5%)	9 (0%)	44	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	LEU
1	B	377	PHE
1	A	235	ILE
1	A	374	PHE
1	B	368	LEU
1	B	373	PRO
1	B	375	PHE
1	B	528	LYS
1	A	367	VAL

5.3.2 Protein sidechains [i](#)

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	912/1086 (84%)	909 (100%)	3 (0%)	92	98
1	B	913/1086 (84%)	910 (100%)	3 (0%)	92	98
1	C	912/1086 (84%)	909 (100%)	3 (0%)	92	98
All	All	2737/3258 (84%)	2728 (100%)	9 (0%)	92	98

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	VAL
1	A	368	LEU
1	A	374	PHE
1	B	368	LEU
1	B	370	ASN
1	B	983	ARG
1	C	675	GLN
1	C	676	THR
1	C	690	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1002	GLN
1	B	81	ASN
1	B	439	ASN
1	B	804	GLN
1	C	165	ASN
1	C	804	GLN
1	C	935	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 monosaccharides 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.

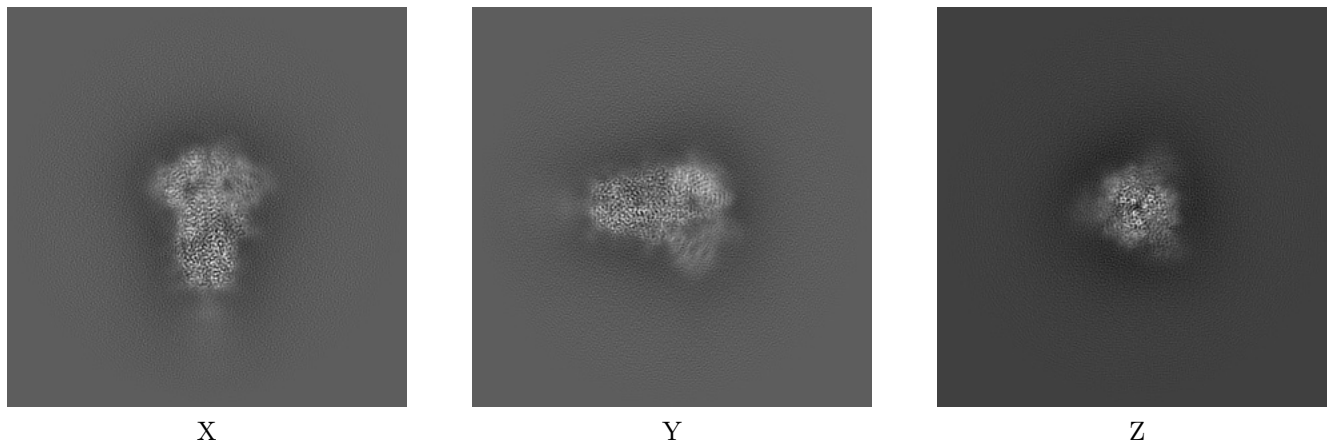
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34974. These allow visual inspection of the internal detail of the map and identification of artifacts.

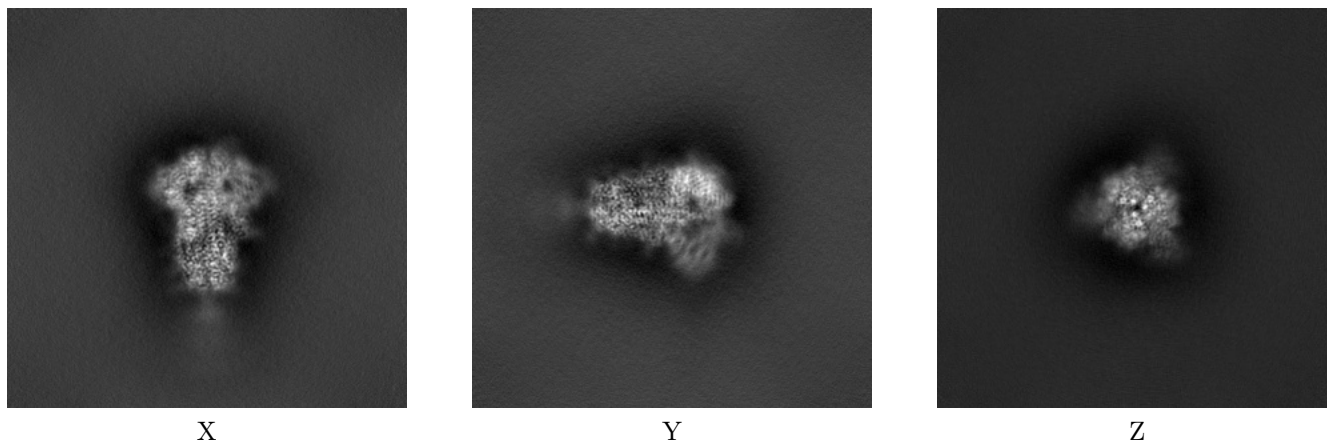
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



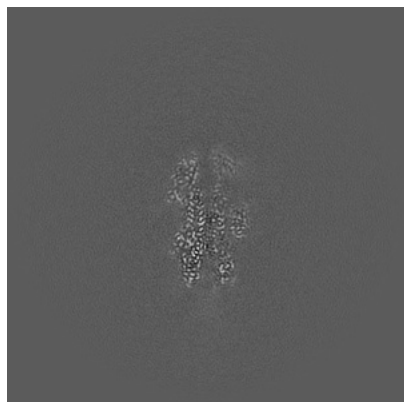
6.1.2 Raw map



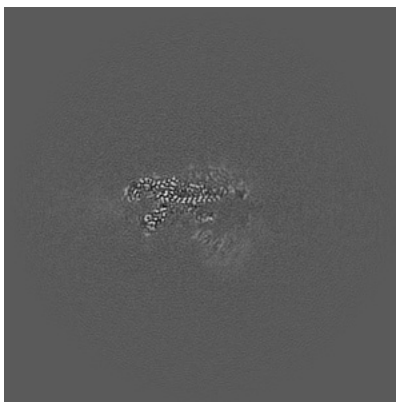
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

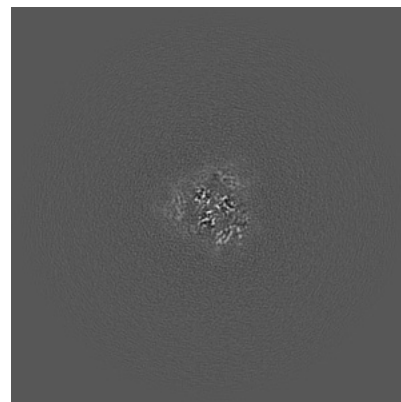
6.2.1 Primary map



X Index: 256

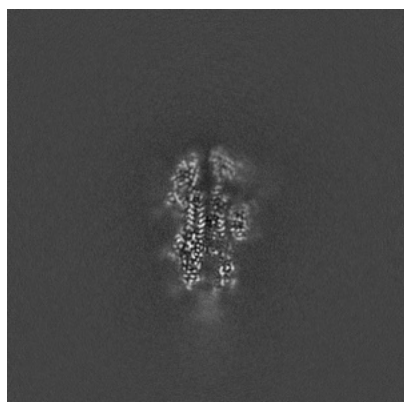


Y Index: 256

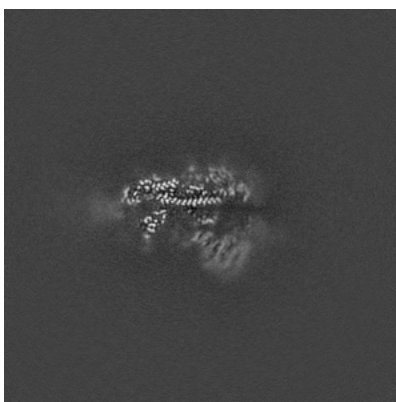


Z Index: 256

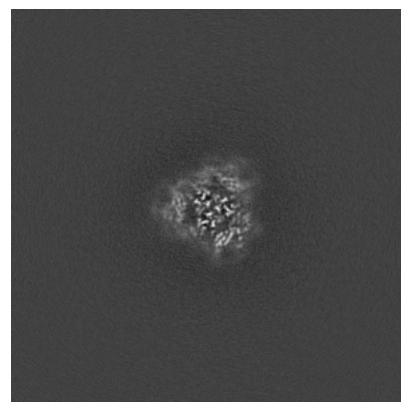
6.2.2 Raw map



X Index: 256



Y Index: 256

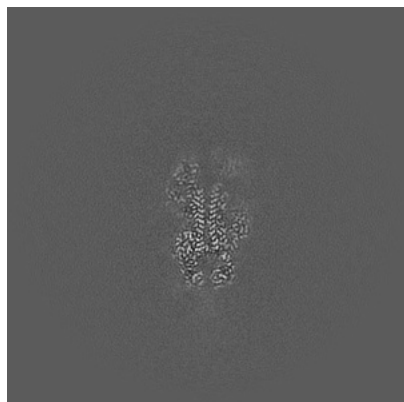


Z Index: 256

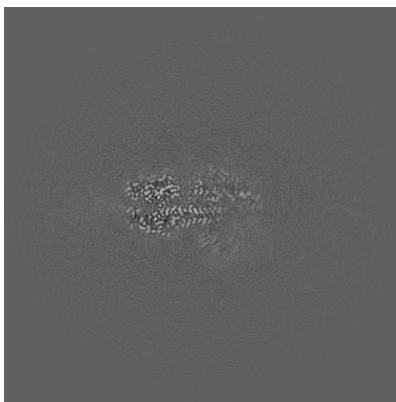
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

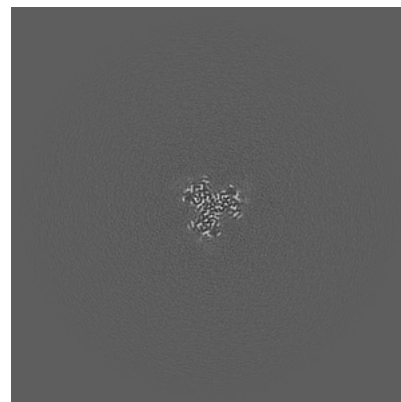
6.3.1 Primary map



X Index: 252

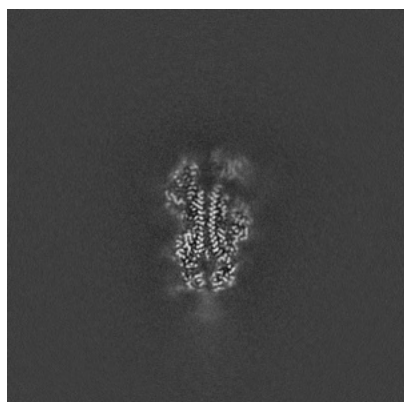


Y Index: 264

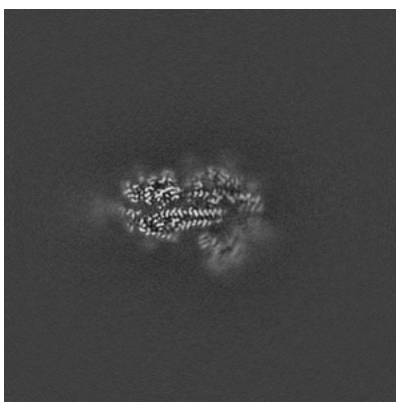


Z Index: 203

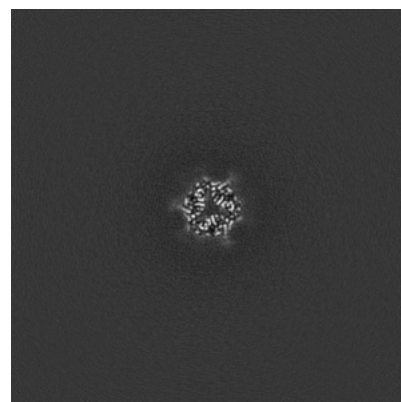
6.3.2 Raw map



X Index: 251



Y Index: 264

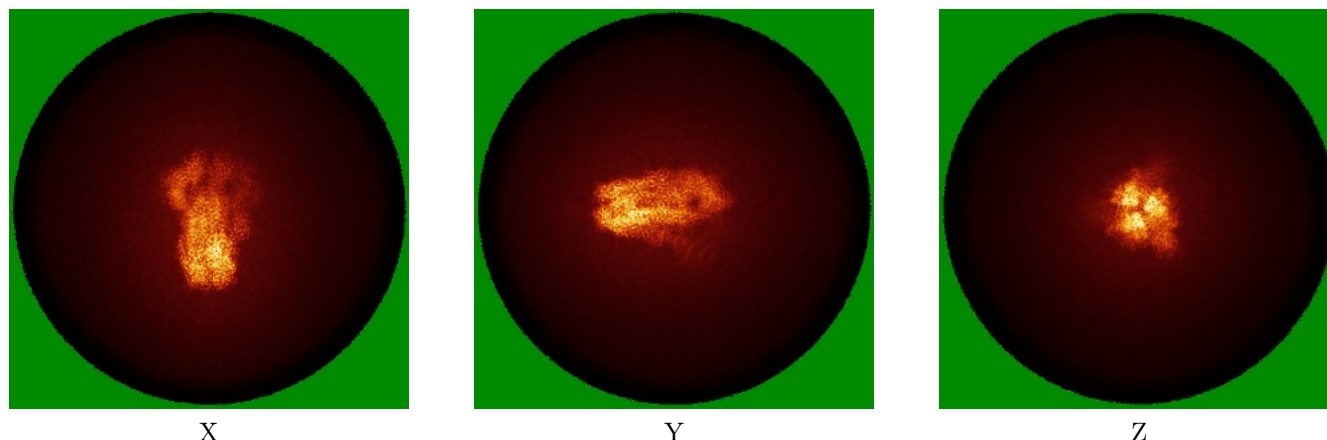


Z Index: 183

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

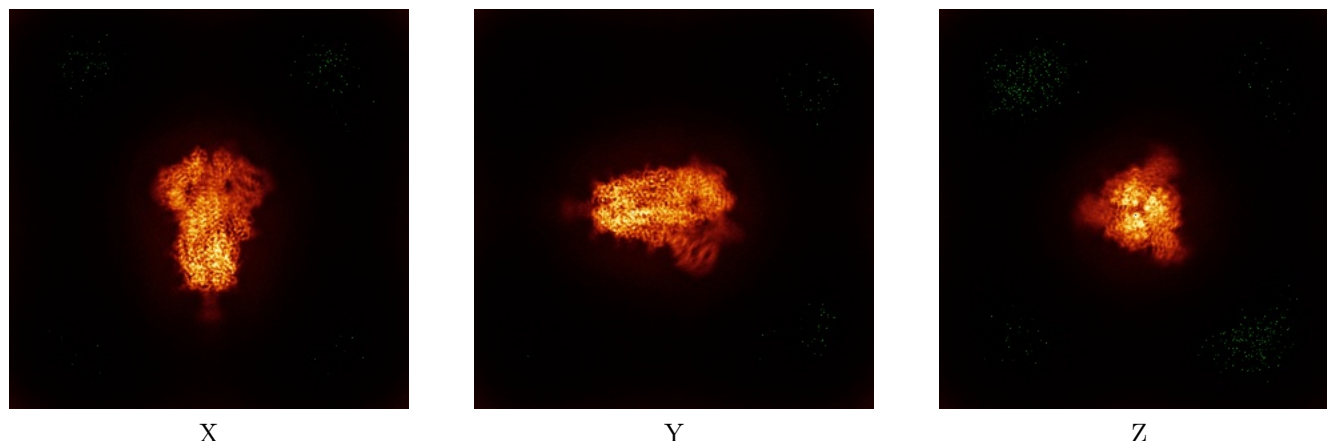


X

Y

Z

6.4.2 Raw map



X

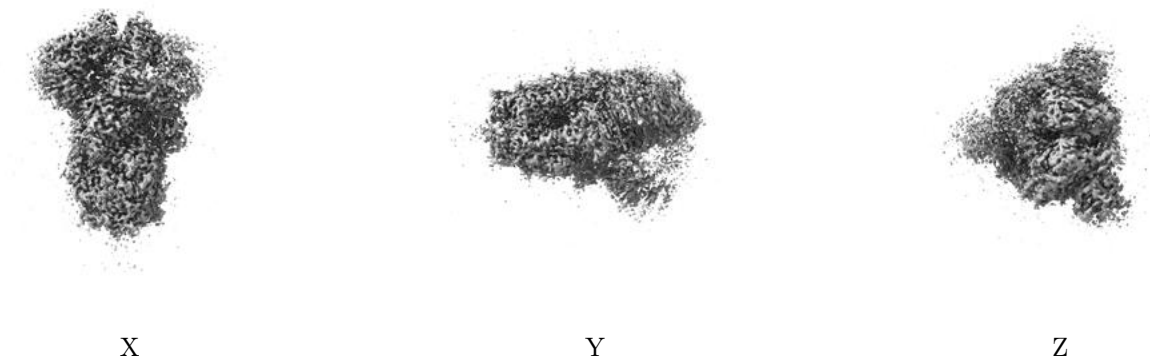
Y

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 0.7. 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.

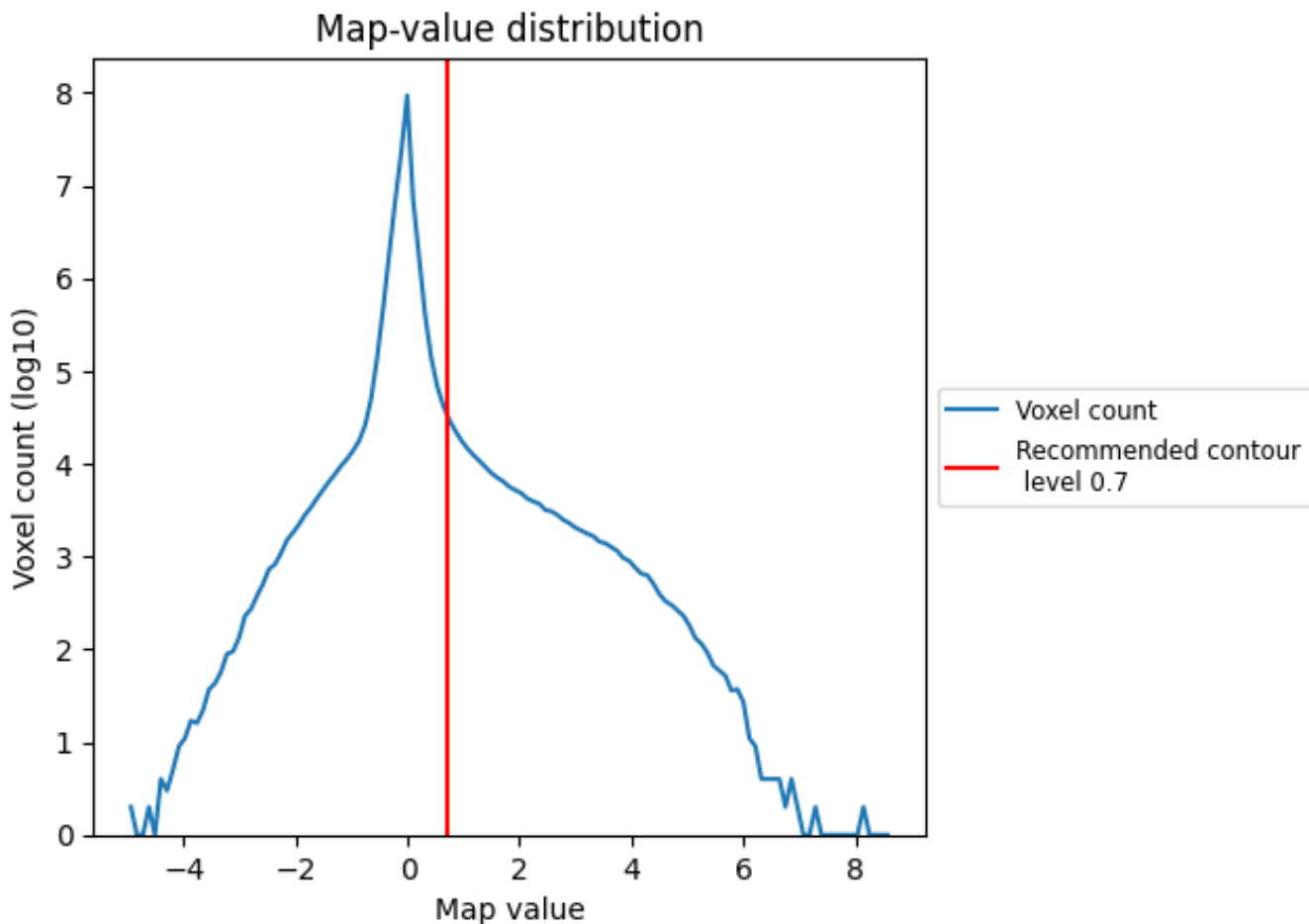
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

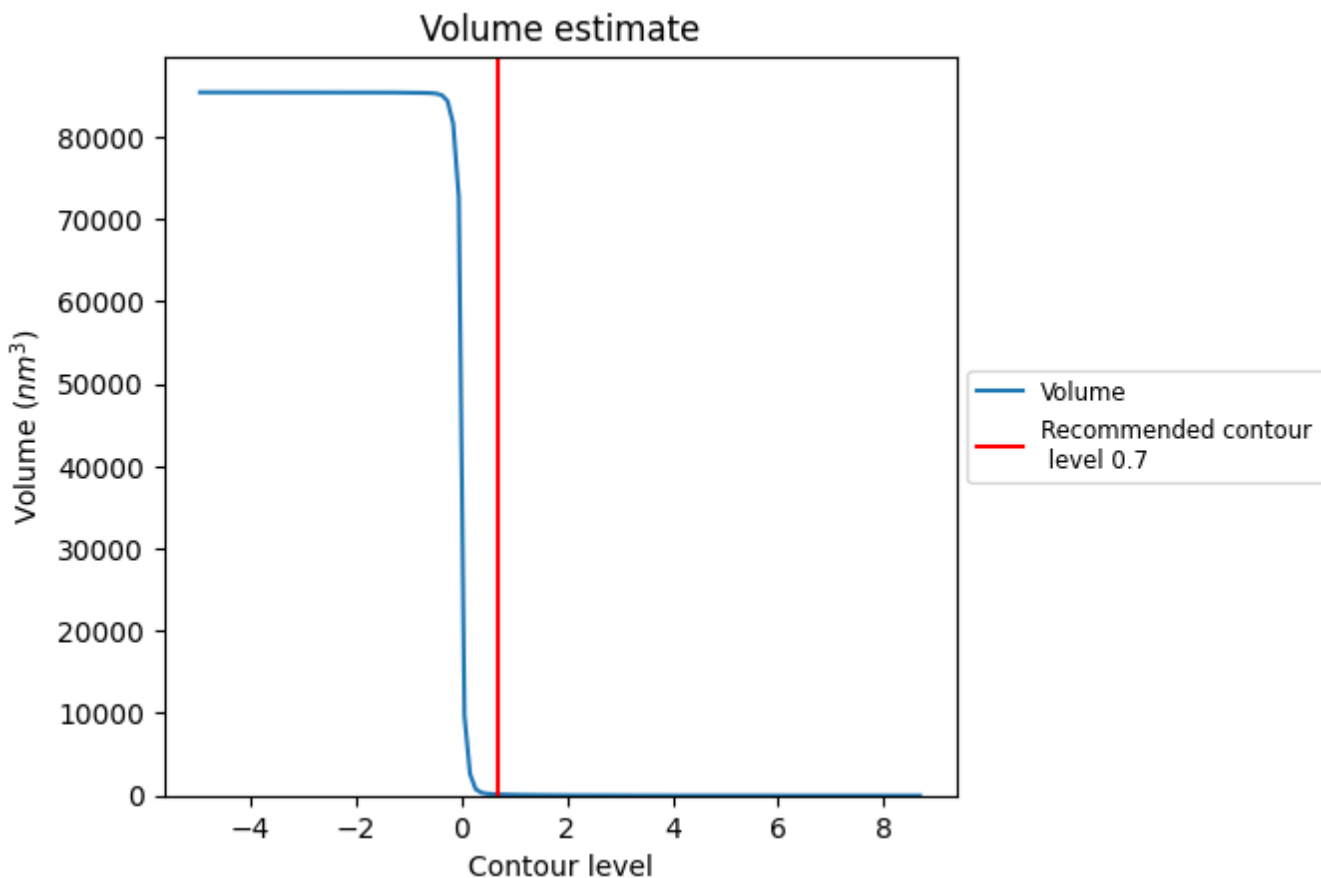
This section contains the results of statistical analysis of the map.

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.

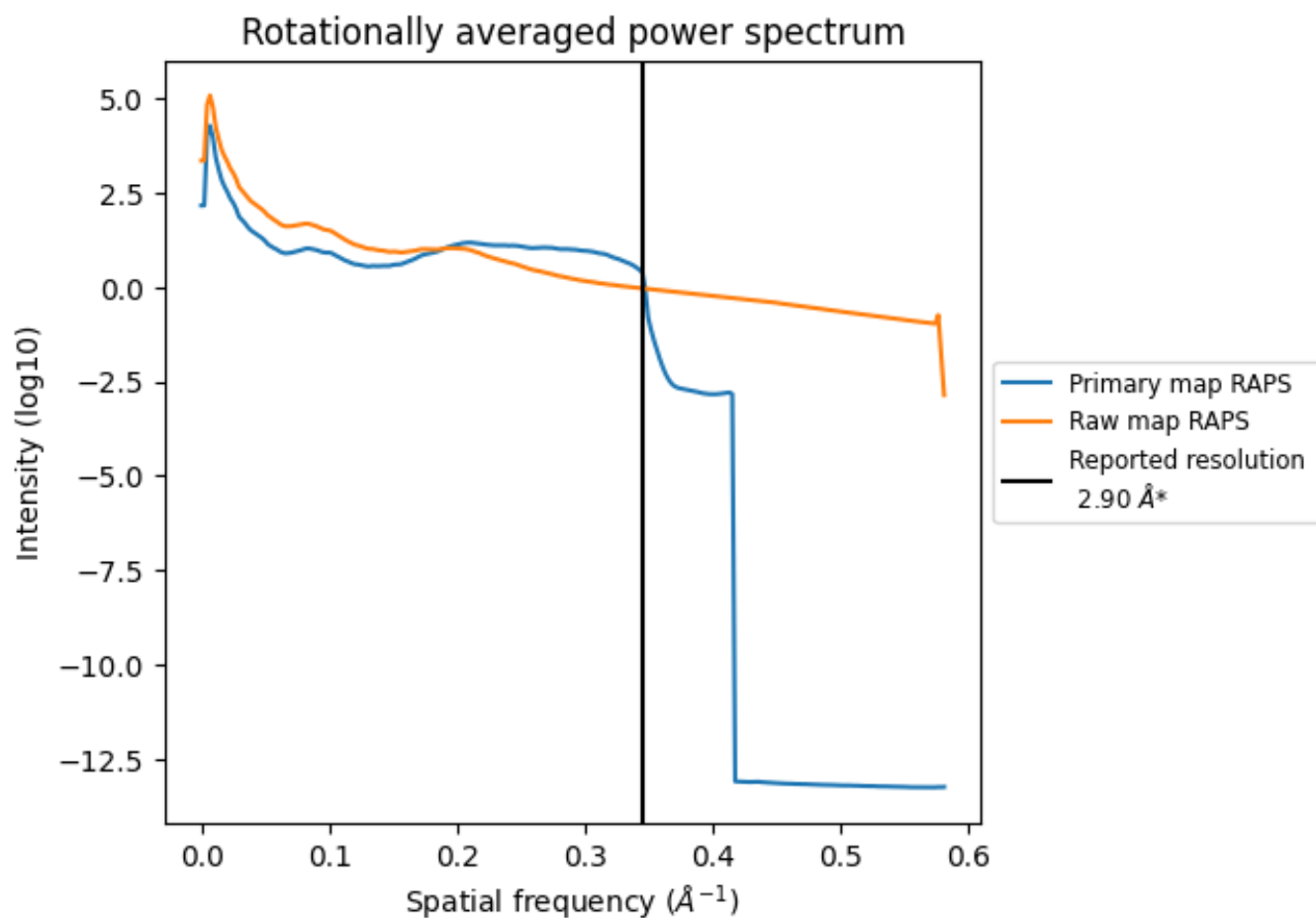
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 137 nm³; this corresponds to an approximate mass of 124 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

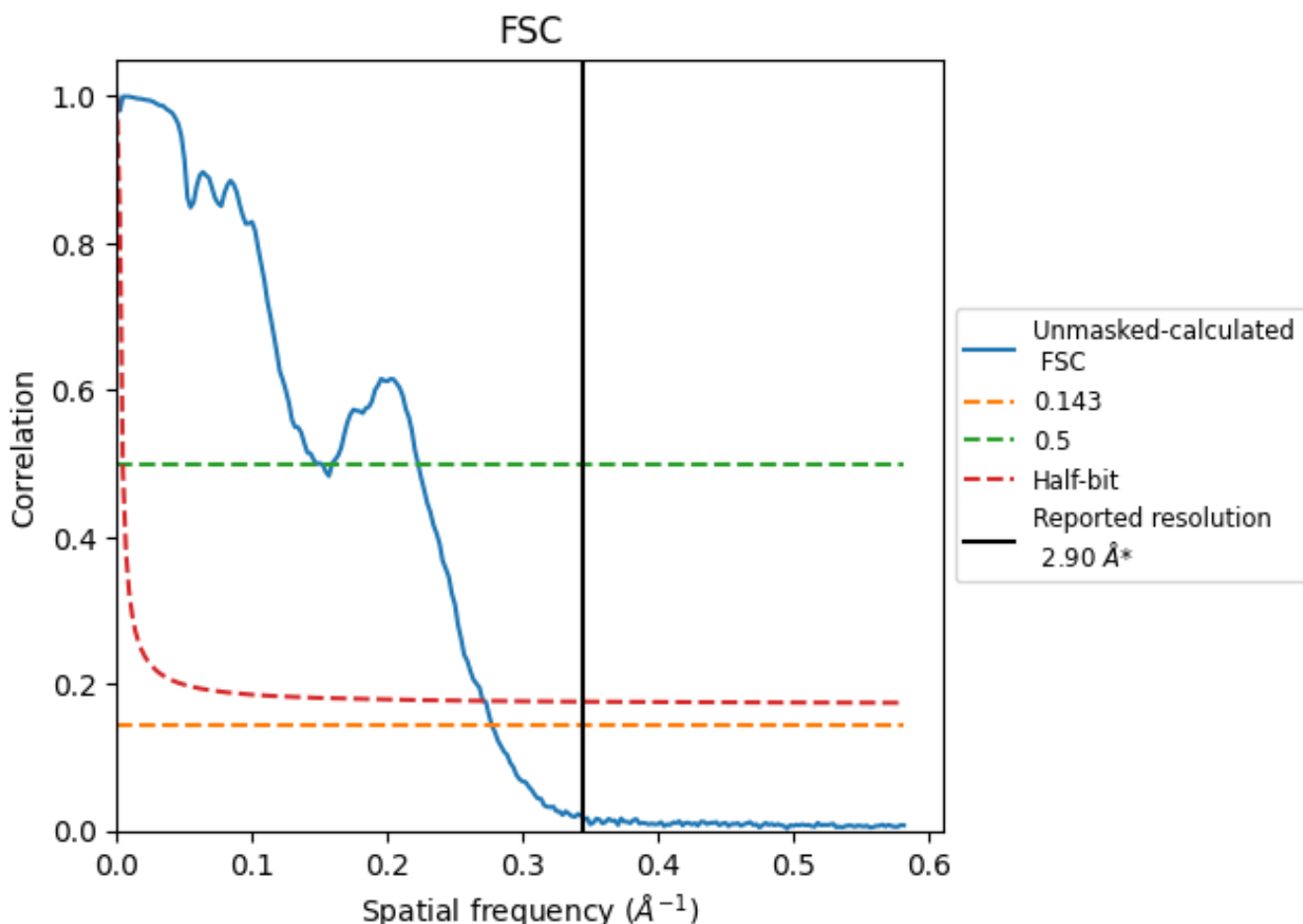


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345\AA^{-1}

8.2 Resolution estimates [i](#)

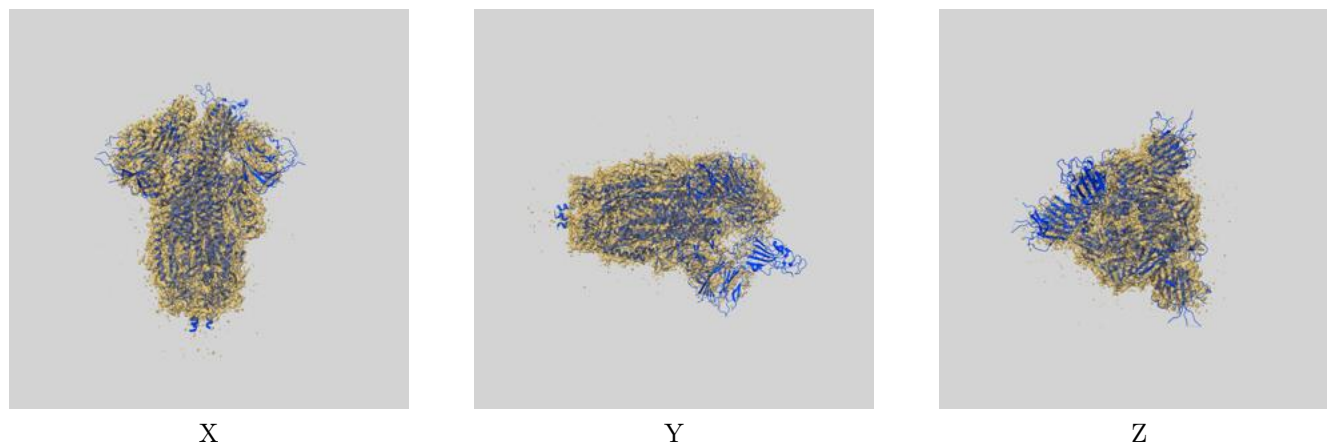
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.61	6.79	3.70

*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 3.61 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

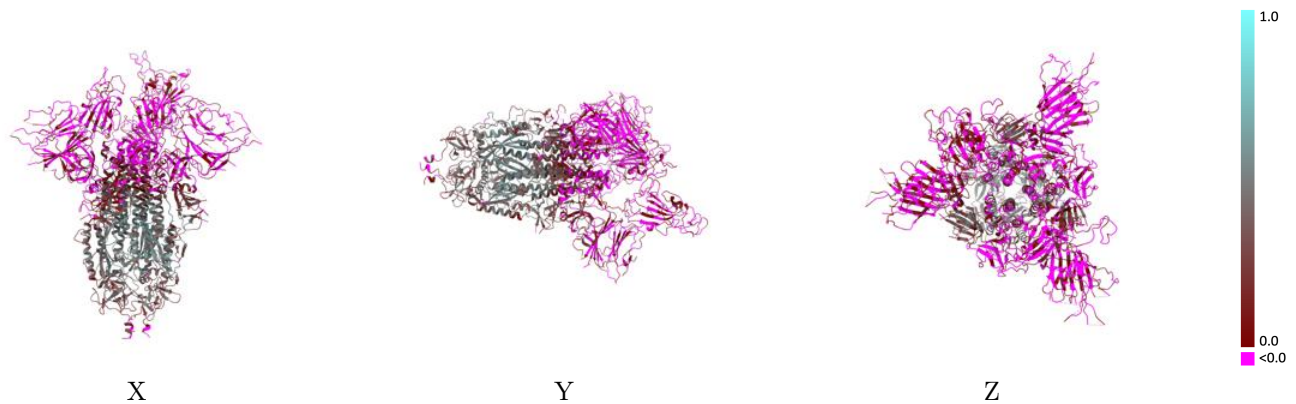
This section contains information regarding the fit between EMDB map EMD-34974 and PDB model 8HRI. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



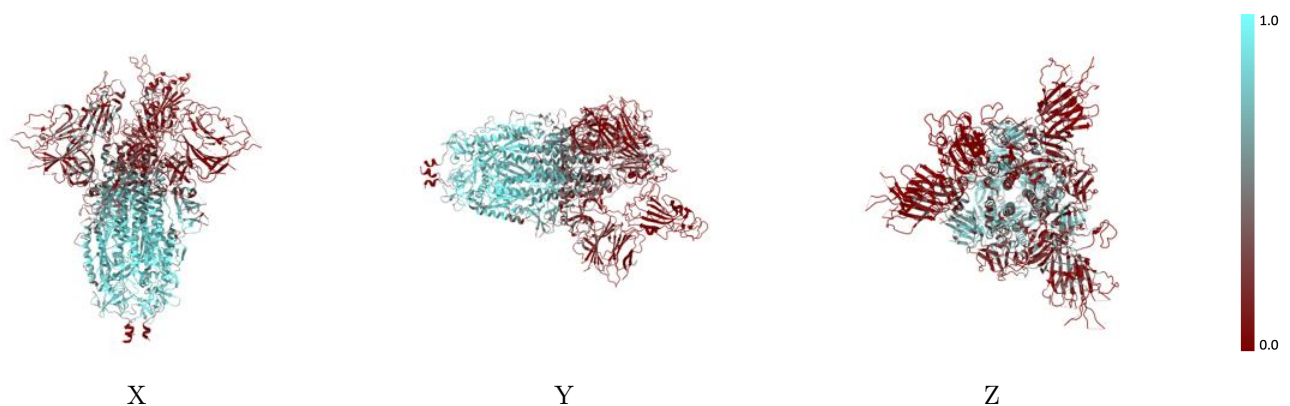
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



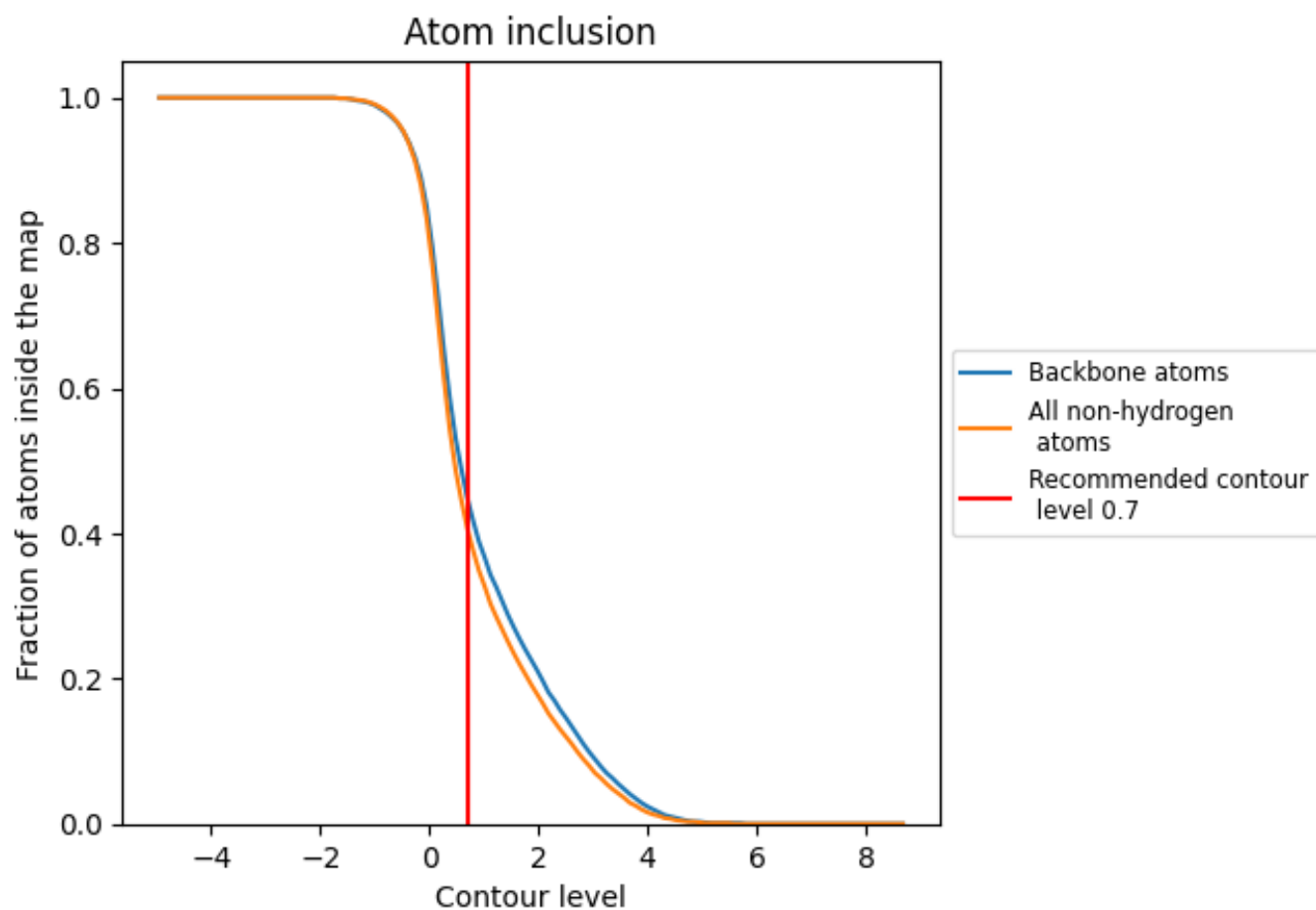
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).









9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 41% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4070	 0.1540
A	 0.3790	 0.1660
B	 0.4230	 0.1560
C	 0.4200	 0.1410

