



Full wwPDB EM Validation Report ⓘ

Jan 13, 2025 – 12:40 PM JST

PDB ID : 8YZC
EMDB ID : EMD-39689
Title : Structure of BA.2.86 spike protein in complex with ACE2.
Authors : Wang, Y.J.; Zang, X.; Sun, L.
Deposited on : 2024-04-06
Resolution : 2.70 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:

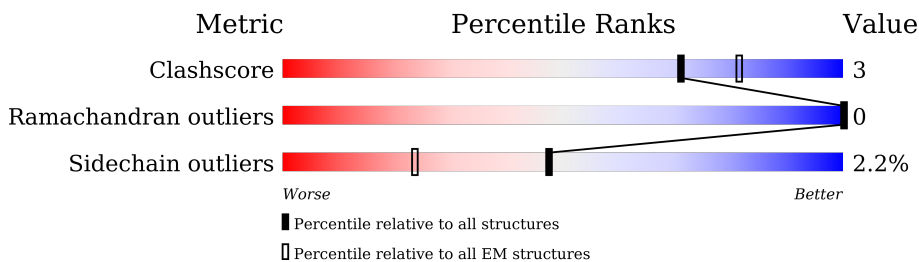
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1291	70% 10% 20%
1	B	1291	71% 9% 20%
1	C	1291	71% 9% 20%
2	G	742	11% 72% 8% 20%
2	H	742	11% 72% 8% 20%
2	I	742	12% 72% 9% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38973 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,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1033	8121	5204	1344	1537	36	0	0
1	B	1033	8121	5204	1344	1537	36	0	0
1	C	1033	8121	5204	1344	1537	36	0	0

There are 285 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP P0DTC2
A	-2	PRO	-	expression tag	UNP P0DTC2
A	-1	MET	-	expression tag	UNP P0DTC2
A	0	GLY	-	expression tag	UNP P0DTC2
A	1	SER	-	expression tag	UNP P0DTC2
A	2	LEU	-	expression tag	UNP P0DTC2
A	3	GLN	-	expression tag	UNP P0DTC2
A	4	PRO	-	expression tag	UNP P0DTC2
A	5	LEU	-	expression tag	UNP P0DTC2
A	6	ALA	-	expression tag	UNP P0DTC2
A	7	THR	-	expression tag	UNP P0DTC2
A	8	LEU	-	expression tag	UNP P0DTC2
A	9	TYR	-	expression tag	UNP P0DTC2
A	10	LEU	-	expression tag	UNP P0DTC2
A	11	LEU	-	expression tag	UNP P0DTC2
A	12	GLY	-	expression tag	UNP P0DTC2
A	13	MET	-	expression tag	UNP P0DTC2
A	14	LEU	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	ALA	-	expression tag	UNP P0DTC2
A	17	SER	-	expression tag	UNP P0DTC2
A	18	VAL	-	expression tag	UNP P0DTC2
A	19	LEU	-	expression tag	UNP P0DTC2
A	20	ALA	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ILE	THR	variant	UNP P0DTC2
A	28	THR	ARG	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	31	SER	ALA	variant	UNP P0DTC2
A	54	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	128	PHE	VAL	conflict	UNP P0DTC2
A	144	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	158	SER	PHE	conflict	UNP P0DTC2
A	159	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	conflict	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	variant	UNP P0DTC2
A	245	ASN	HIS	variant	UNP P0DTC2
A	264	ASP	ALA	variant	UNP P0DTC2
A	332	VAL	ILE	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	HIS	VAL	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	450	ASP	ASN	variant	UNP P0DTC2
A	452	TRP	LEU	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	PRO	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	670	VAL	ILE	conflict	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	ARG	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	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
B	-3	MET	-	initiating methionine	UNP P0DTC2
B	-2	PRO	-	expression tag	UNP P0DTC2
B	-1	MET	-	expression tag	UNP P0DTC2
B	0	GLY	-	expression tag	UNP P0DTC2
B	1	SER	-	expression tag	UNP P0DTC2
B	2	LEU	-	expression tag	UNP P0DTC2
B	3	GLN	-	expression tag	UNP P0DTC2
B	4	PRO	-	expression tag	UNP P0DTC2
B	5	LEU	-	expression tag	UNP P0DTC2
B	6	ALA	-	expression tag	UNP P0DTC2
B	7	THR	-	expression tag	UNP P0DTC2
B	8	LEU	-	expression tag	UNP P0DTC2
B	9	TYR	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	LEU	-	expression tag	UNP P0DTC2
B	11	LEU	-	expression tag	UNP P0DTC2
B	12	GLY	-	expression tag	UNP P0DTC2
B	13	MET	-	expression tag	UNP P0DTC2
B	14	LEU	-	expression tag	UNP P0DTC2
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	ALA	-	expression tag	UNP P0DTC2
B	17	SER	-	expression tag	UNP P0DTC2
B	18	VAL	-	expression tag	UNP P0DTC2
B	19	LEU	-	expression tag	UNP P0DTC2
B	20	ALA	-	expression tag	UNP P0DTC2
B	26	ILE	THR	variant	UNP P0DTC2
B	28	THR	ARG	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	31	SER	ALA	variant	UNP P0DTC2
B	54	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	128	PHE	VAL	conflict	UNP P0DTC2
B	144	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	158	SER	PHE	conflict	UNP P0DTC2
B	159	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	conflict	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	variant	UNP P0DTC2
B	264	ASP	ALA	variant	UNP P0DTC2
B	332	VAL	ILE	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	variant	UNP P0DTC2
B	452	TRP	LEU	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	670	VAL	ILE	conflict	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	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	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
C	-3	MET	-	initiating methionine	UNP P0DTC2
C	-2	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	expression tag	UNP P0DTC2
C	0	GLY	-	expression tag	UNP P0DTC2
C	1	SER	-	expression tag	UNP P0DTC2
C	2	LEU	-	expression tag	UNP P0DTC2
C	3	GLN	-	expression tag	UNP P0DTC2
C	4	PRO	-	expression tag	UNP P0DTC2
C	5	LEU	-	expression tag	UNP P0DTC2
C	6	ALA	-	expression tag	UNP P0DTC2
C	7	THR	-	expression tag	UNP P0DTC2
C	8	LEU	-	expression tag	UNP P0DTC2
C	9	TYR	-	expression tag	UNP P0DTC2
C	10	LEU	-	expression tag	UNP P0DTC2
C	11	LEU	-	expression tag	UNP P0DTC2
C	12	GLY	-	expression tag	UNP P0DTC2
C	13	MET	-	expression tag	UNP P0DTC2
C	14	LEU	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	ALA	-	expression tag	UNP P0DTC2
C	17	SER	-	expression tag	UNP P0DTC2
C	18	VAL	-	expression tag	UNP P0DTC2
C	19	LEU	-	expression tag	UNP P0DTC2
C	20	ALA	-	expression tag	UNP P0DTC2
C	26	ILE	THR	variant	UNP P0DTC2
C	28	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	31	SER	ALA	variant	UNP P0DTC2
C	54	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	128	PHE	VAL	conflict	UNP P0DTC2
C	144	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	158	SER	PHE	conflict	UNP P0DTC2
C	159	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	conflict	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2
C	245	ASN	HIS	variant	UNP P0DTC2
C	264	ASP	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	332	VAL	ILE	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	variant	UNP P0DTC2
C	452	TRP	LEU	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	670	VAL	ILE	conflict	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	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	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	H	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	I	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	733	SER	-	expression tag	UNP Q9BYF1
G	734	GLY	-	expression tag	UNP Q9BYF1
G	735	HIS	-	expression tag	UNP Q9BYF1
G	736	HIS	-	expression tag	UNP Q9BYF1
G	737	HIS	-	expression tag	UNP Q9BYF1
G	738	HIS	-	expression tag	UNP Q9BYF1
G	739	HIS	-	expression tag	UNP Q9BYF1
G	740	HIS	-	expression tag	UNP Q9BYF1
G	741	HIS	-	expression tag	UNP Q9BYF1
G	742	HIS	-	expression tag	UNP Q9BYF1
H	733	SER	-	expression tag	UNP Q9BYF1
H	734	GLY	-	expression tag	UNP Q9BYF1
H	735	HIS	-	expression tag	UNP Q9BYF1
H	736	HIS	-	expression tag	UNP Q9BYF1
H	737	HIS	-	expression tag	UNP Q9BYF1
H	738	HIS	-	expression tag	UNP Q9BYF1
H	739	HIS	-	expression tag	UNP Q9BYF1
H	740	HIS	-	expression tag	UNP Q9BYF1
H	741	HIS	-	expression tag	UNP Q9BYF1

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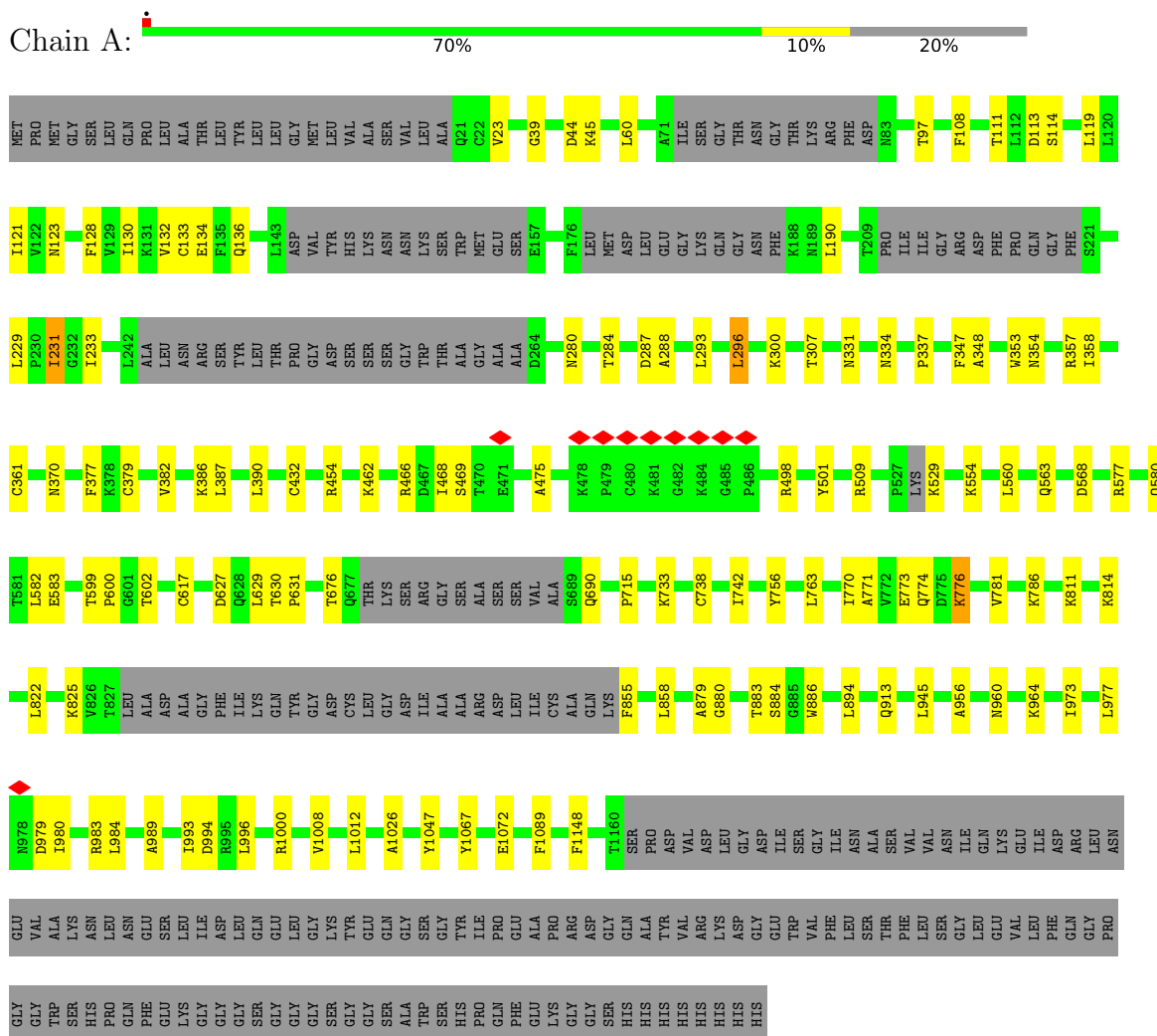
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Chain	Residue	Modelled	Actual	Comment	Reference
H	742	HIS	-	expression tag	UNP Q9BYF1
I	733	SER	-	expression tag	UNP Q9BYF1
I	734	GLY	-	expression tag	UNP Q9BYF1
I	735	HIS	-	expression tag	UNP Q9BYF1
I	736	HIS	-	expression tag	UNP Q9BYF1
I	737	HIS	-	expression tag	UNP Q9BYF1
I	738	HIS	-	expression tag	UNP Q9BYF1
I	739	HIS	-	expression tag	UNP Q9BYF1
I	740	HIS	-	expression tag	UNP Q9BYF1
I	741	HIS	-	expression tag	UNP Q9BYF1
I	742	HIS	-	expression tag	UNP Q9BYF1

3 Residue-property plots

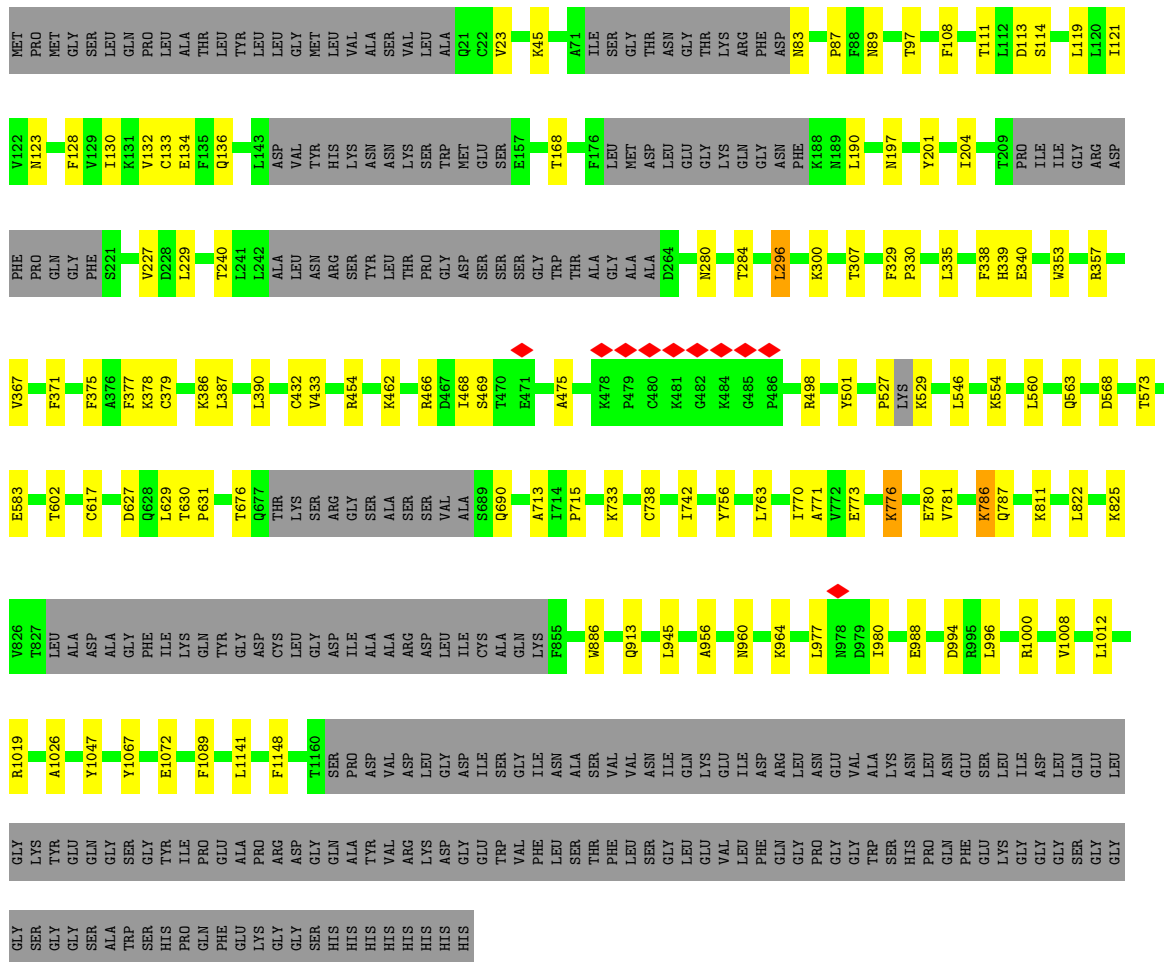
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

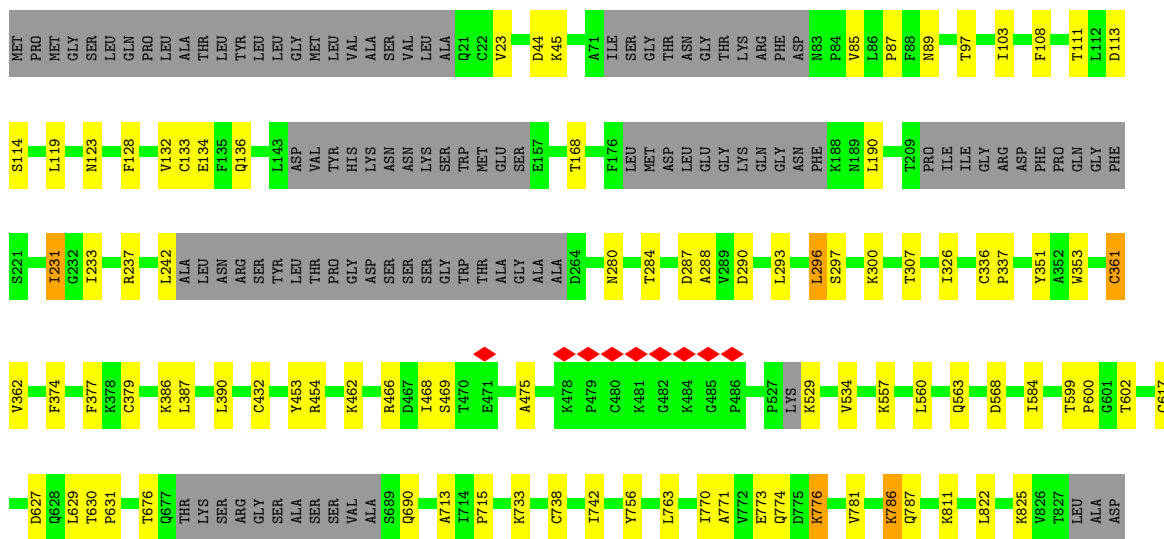


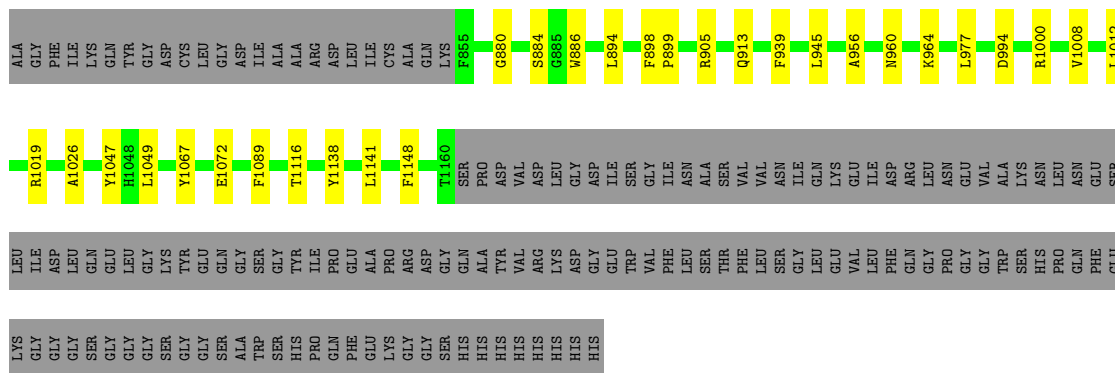
- Molecule 1: Spike glycoprotein,Fibrin,Expression Tag



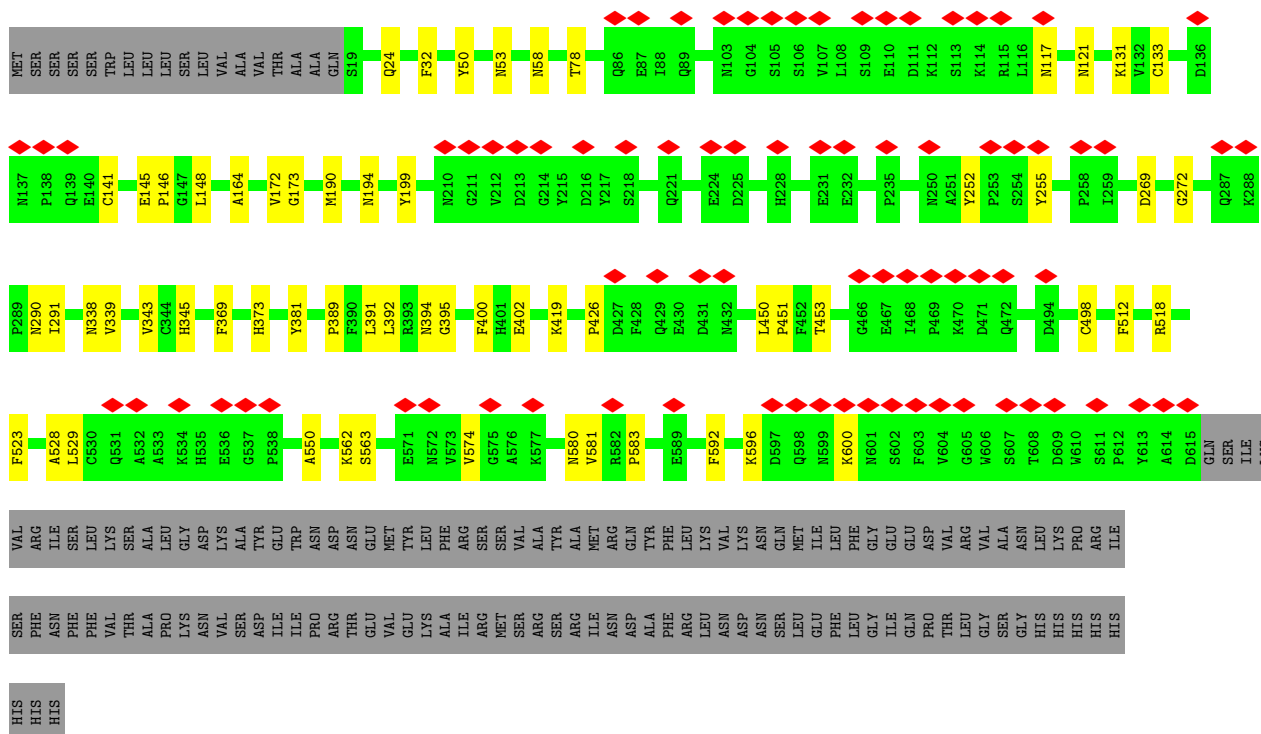


● Molecule 1: Spike glycoprotein,Fibrin,Expression Tag

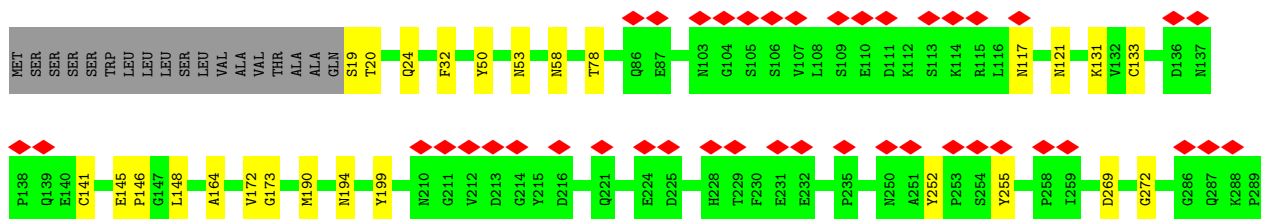


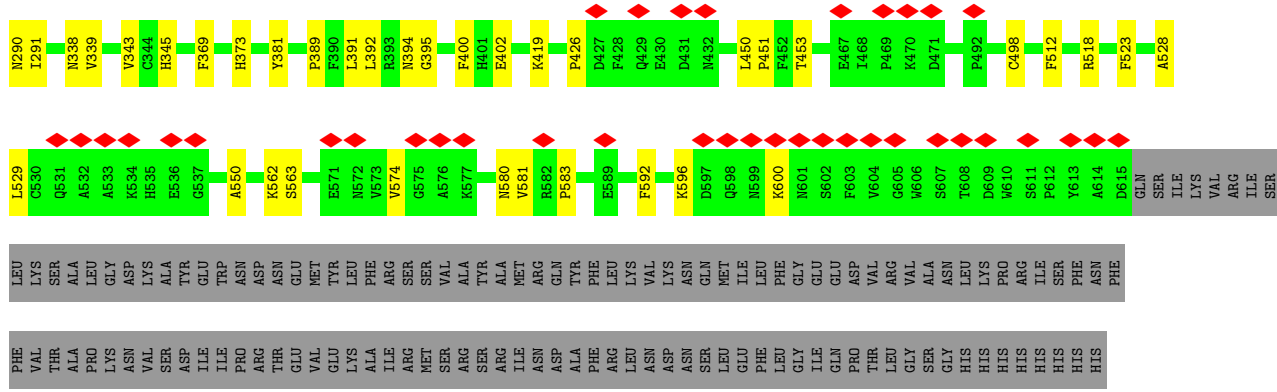


• Molecule 2: Angiotensin-converting enzyme 2

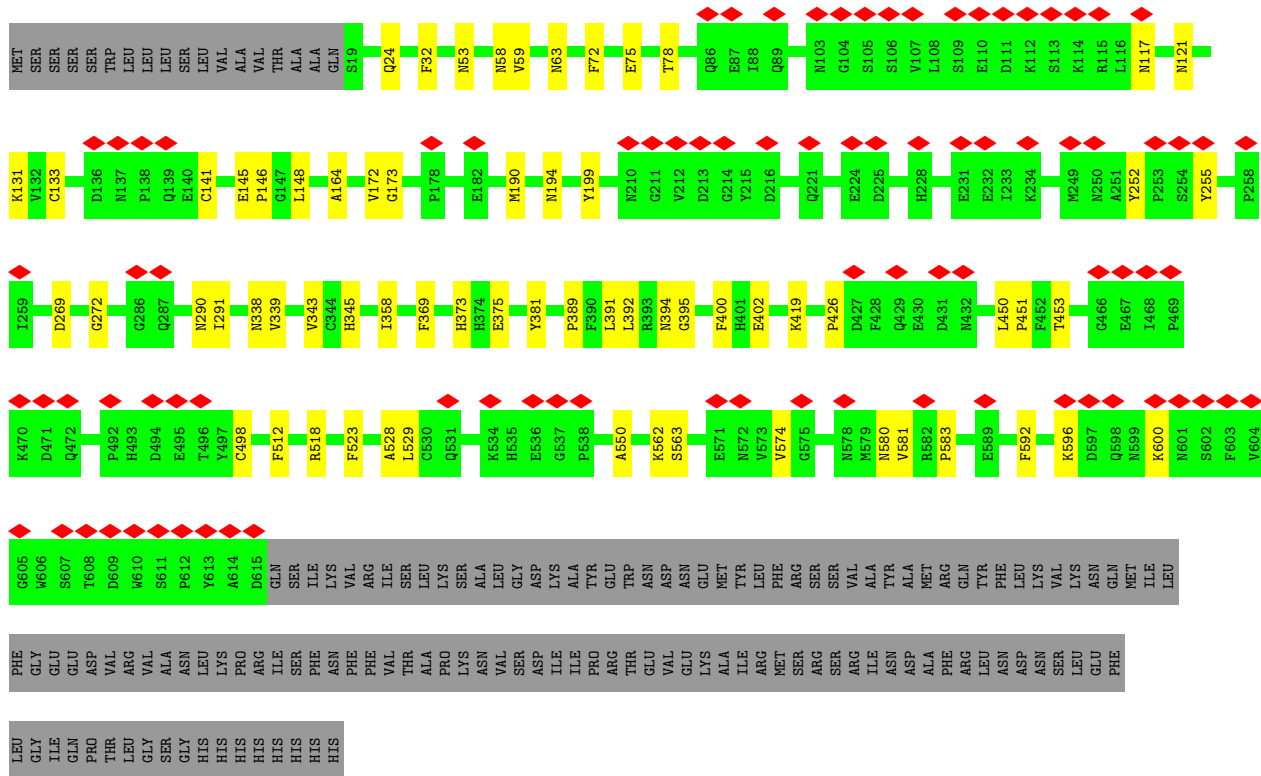


• Molecule 2: Angiotensin-converting enzyme 2





• Molecule 2: Angiotensin-converting enzyme 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	446892	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.865	Depositor
Minimum map value	-0.615	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	380.80002, 380.80002, 380.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.19, 1.19, 1.19	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/8316	0.41	0/11316
1	B	0.24	0/8316	0.42	0/11316
1	C	0.24	0/8316	0.42	0/11316
2	G	0.23	0/5007	0.36	0/6803
2	H	0.23	0/5007	0.36	0/6803
2	I	0.23	0/5007	0.36	0/6803
All	All	0.24	0/39969	0.40	0/54357

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	8121	0	7934	59	0
1	B	8121	0	7934	54	0
1	C	8121	0	7934	58	0
2	G	4870	0	4643	29	0
2	H	4870	0	4643	30	0
2	I	4870	0	4643	31	0
All	All	38973	0	37731	251	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (251) 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:B:629:LEU:HG	1:B:631:PRO:HD2	1.70	0.73
1:C:977:LEU:HB3	1:C:1000:ARG:HH22	1.55	0.71
1:C:629:LEU:HG	1:C:631:PRO:HD2	1.72	0.71
1:A:629:LEU:HG	1:A:631:PRO:HD2	1.72	0.71
1:A:763:LEU:HG	1:A:1008:VAL:HG21	1.75	0.69
1:C:763:LEU:HG	1:C:1008:VAL:HG21	1.74	0.67
1:B:197:ASN:ND2	1:B:201:TYR:O	2.30	0.65
1:B:763:LEU:HG	1:B:1008:VAL:HG21	1.78	0.64
2:I:453:THR:HG23	2:I:512:PHE:HB3	1.80	0.64
2:H:453:THR:HG23	2:H:512:PHE:HB3	1.79	0.64
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.31	0.64
2:G:453:THR:HG23	2:G:512:PHE:HB3	1.80	0.63
1:C:742:ILE:O	1:C:1000:ARG:NH1	2.31	0.63
1:A:331:ASN:HA	1:A:580:GLN:HG2	1.79	0.63
1:B:108:PHE:HB2	1:B:119:LEU:HB3	1.81	0.63
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.17	0.62
1:C:956:ALA:O	1:C:960:ASN:ND2	2.29	0.62
1:A:466:ARG:HE	1:A:468:ILE:HD11	1.63	0.62
1:C:466:ARG:HE	1:C:468:ILE:HD11	1.64	0.62
1:B:466:ARG:HE	1:B:468:ILE:HD11	1.65	0.62
1:C:353:TRP:O	1:C:466:ARG:NH2	2.33	0.61
2:H:117:ASN:O	2:H:121:ASN:ND2	2.32	0.61
1:C:361:CYS:SG	1:C:362:VAL:N	2.74	0.61
1:C:108:PHE:HB2	1:C:119:LEU:HB3	1.83	0.60
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.20	0.60
1:B:977:LEU:HB3	1:B:1000:ARG:HH22	1.66	0.60
1:A:111:THR:OG1	1:A:113:ASP:OD2	2.20	0.60
1:A:353:TRP:O	1:A:466:ARG:NH2	2.35	0.59
1:A:977:LEU:HB3	1:A:1000:ARG:HH22	1.66	0.59
2:I:117:ASN:O	2:I:121:ASN:ND2	2.32	0.59
1:A:956:ALA:O	1:A:960:ASN:ND2	2.32	0.59
2:G:117:ASN:O	2:G:121:ASN:ND2	2.32	0.59
1:A:108:PHE:HB2	1:A:119:LEU:HB3	1.84	0.58
1:B:111:THR:OG1	1:B:113:ASP:OD2	2.20	0.58
1:B:956:ALA:O	1:B:960:ASN:ND2	2.29	0.58
1:C:296:LEU:HD22	1:C:300:LYS:HE3	1.86	0.57
1:A:577:ARG:HH21	1:A:582:LEU:HB3	1.69	0.57
1:C:351:TYR:HB3	1:C:453:TYR:HA	1.85	0.57
1:A:554:LYS:NZ	1:A:583:GLU:OE2	2.37	0.57
1:A:379:CYS:HA	1:A:432:CYS:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.21	0.56
1:B:554:LYS:NZ	1:B:583:GLU:OE2	2.38	0.56
1:C:326:ILE:HD11	1:C:534:VAL:HG12	1.87	0.56
1:B:546:LEU:HD21	1:B:573:THR:HG21	1.87	0.55
1:B:133:CYS:SG	1:B:134:GLU:N	2.79	0.55
1:C:111:THR:OG1	1:C:113:ASP:OD2	2.19	0.55
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.39	0.55
1:C:231:ILE:HD12	1:C:233:ILE:HG23	1.89	0.55
2:G:53:ASN:O	2:G:58:ASN:ND2	2.39	0.55
1:B:353:TRP:O	1:B:466:ARG:NH2	2.35	0.55
2:H:419:LYS:HE3	2:H:426:PRO:HA	1.89	0.55
1:B:379:CYS:HA	1:B:432:CYS:HA	1.89	0.55
1:A:296:LEU:HD22	1:A:300:LYS:HE3	1.88	0.55
1:B:1089:PHE:HB3	1:C:913:GLN:HE21	1.72	0.55
1:B:114:SER:OG	1:B:136:GLN:NE2	2.39	0.54
1:A:913:GLN:HE21	1:C:1089:PHE:HB3	1.71	0.54
1:B:83:ASN:ND2	1:B:240:THR:O	2.40	0.54
1:C:379:CYS:HA	1:C:432:CYS:HA	1.89	0.54
2:G:419:LYS:HE3	2:G:426:PRO:HA	1.89	0.54
2:I:529:LEU:HD22	2:I:550:ALA:HB1	1.90	0.54
1:C:114:SER:OG	1:C:136:GLN:NE2	2.41	0.54
1:A:1089:PHE:HB3	1:B:913:GLN:HE21	1.73	0.54
1:A:114:SER:OG	1:A:136:GLN:NE2	2.40	0.54
2:I:419:LYS:HE3	2:I:426:PRO:HA	1.89	0.53
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.42	0.53
1:B:296:LEU:HD22	1:B:300:LYS:HE3	1.90	0.53
2:I:53:ASN:O	2:I:58:ASN:ND2	2.41	0.53
1:C:336:CYS:HB2	1:C:362:VAL:H	1.74	0.53
1:A:337:PRO:HD2	1:A:358:ILE:HG23	1.90	0.53
2:H:133:CYS:HA	2:H:141:CYS:HA	1.91	0.53
1:C:280:ASN:ND2	1:C:284:THR:O	2.42	0.53
2:G:529:LEU:HD22	2:G:550:ALA:HB1	1.90	0.53
2:G:269:ASP:OD1	2:G:272:GLY:N	2.40	0.52
2:H:529:LEU:HD22	2:H:550:ALA:HB1	1.90	0.52
2:H:53:ASN:O	2:H:58:ASN:ND2	2.41	0.51
1:A:287:ASP:OD1	1:A:288:ALA:N	2.43	0.51
1:A:773:GLU:HA	1:A:776:LYS:HG2	1.92	0.51
1:A:979:ASP:O	1:A:983:ARG:NE	2.37	0.51
2:I:133:CYS:HA	2:I:141:CYS:HA	1.91	0.51
2:I:269:ASP:OD1	2:I:272:GLY:N	2.40	0.51
2:G:133:CYS:HA	2:G:141:CYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:269:ASP:OD1	2:H:272:GLY:N	2.40	0.51
1:C:133:CYS:SG	1:C:134:GLU:N	2.85	0.50
1:A:280:ASN:ND2	1:A:284:THR:O	2.44	0.50
1:A:973:ILE:HD11	1:A:984:LEU:HD21	1.93	0.50
2:I:173:GLY:O	2:I:498:CYS:N	2.45	0.50
2:G:173:GLY:O	2:G:498:CYS:N	2.45	0.50
1:B:387:LEU:HD12	1:B:390:LEU:HD12	1.93	0.50
1:C:387:LEU:HD12	1:C:390:LEU:HD12	1.93	0.50
2:I:394:ASN:HB3	2:I:562:LYS:HD2	1.94	0.50
2:H:173:GLY:O	2:H:498:CYS:N	2.44	0.49
1:A:387:LEU:HD12	1:A:390:LEU:HD12	1.95	0.49
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.38	0.49
1:B:130:ILE:HD13	1:B:229:LEU:HD11	1.93	0.49
2:I:290:ASN:OD1	2:I:291:ILE:N	2.46	0.49
2:G:290:ASN:OD1	2:G:291:ILE:N	2.45	0.49
2:I:402:GLU:HB2	2:I:518:ARG:HG3	1.94	0.49
2:H:290:ASN:OD1	2:H:291:ILE:N	2.46	0.49
1:C:123:ASN:HD22	1:C:128:PHE:HD1	1.61	0.49
2:H:389:PRO:HD2	2:H:392:LEU:HD12	1.95	0.49
1:A:133:CYS:SG	1:A:134:GLU:N	2.85	0.48
2:G:145:GLU:HB3	2:G:146:PRO:HD3	1.96	0.48
2:G:389:PRO:HD2	2:G:392:LEU:HD12	1.96	0.48
2:H:145:GLU:HB3	2:H:146:PRO:HD3	1.96	0.48
1:A:334:ASN:HD21	1:A:361:CYS:HA	1.77	0.48
2:I:145:GLU:HB3	2:I:146:PRO:HD3	1.96	0.48
2:I:389:PRO:HD2	2:I:392:LEU:HD12	1.96	0.48
1:B:280:ASN:ND2	1:B:284:THR:OG1	2.41	0.48
1:A:348:ALA:HB1	1:A:354:ASN:H	1.79	0.48
2:H:528:ALA:HB2	2:H:574:VAL:HG12	1.96	0.48
1:A:676:THR:HA	1:A:690:GLN:HG2	1.96	0.48
1:A:822:LEU:HD22	1:A:945:LEU:HD21	1.96	0.48
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.96	0.48
1:C:627:ASP:OD1	1:C:627:ASP:N	2.47	0.48
2:H:190:MET:O	2:H:194:ASN:ND2	2.35	0.48
2:H:394:ASN:HB3	2:H:562:LYS:HD2	1.96	0.48
1:A:231:ILE:HD12	1:A:233:ILE:HG23	1.94	0.47
2:H:392:LEU:HD13	2:H:563:SER:HB3	1.96	0.47
2:H:402:GLU:HB2	2:H:518:ARG:HG3	1.94	0.47
1:C:287:ASP:OD1	1:C:288:ALA:N	2.43	0.47
2:G:402:GLU:HB2	2:G:518:ARG:HG3	1.94	0.47
2:I:528:ALA:HB2	2:I:574:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:GLY:O	1:A:884:SER:OG	2.27	0.47
1:B:204:ILE:HB	1:B:227:VAL:HG12	1.95	0.47
1:B:498:ARG:NH1	1:B:501:TYR:OH	2.45	0.47
1:C:454:ARG:NH2	1:C:469:SER:O	2.45	0.47
1:C:85:VAL:HG11	1:C:237:ARG:HE	1.80	0.47
1:A:454:ARG:NH2	1:A:469:SER:O	2.46	0.47
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.97	0.47
1:C:880:GLY:O	1:C:884:SER:OG	2.26	0.47
2:G:392:LEU:HD13	2:G:563:SER:HB3	1.97	0.47
2:G:580:ASN:OD1	2:G:581:VAL:N	2.48	0.47
2:H:343:VAL:HG12	2:H:345:HIS:H	1.80	0.47
2:I:369:PHE:O	2:I:373:HIS:ND1	2.47	0.47
1:C:560:LEU:HB2	1:C:563:GLN:HG2	1.96	0.47
2:G:394:ASN:HB3	2:G:562:LYS:HD2	1.96	0.47
2:H:580:ASN:OD1	2:H:581:VAL:N	2.48	0.47
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.96	0.46
1:C:676:THR:HA	1:C:690:GLN:HG2	1.97	0.46
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.96	0.46
2:I:392:LEU:HD13	2:I:563:SER:HB3	1.96	0.46
2:G:528:ALA:HB2	2:G:574:VAL:HG12	1.96	0.46
2:I:394:ASN:OD1	2:I:395:GLY:N	2.48	0.46
2:I:580:ASN:OD1	2:I:581:VAL:N	2.48	0.46
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.97	0.46
2:G:343:VAL:HG12	2:G:345:HIS:H	1.80	0.46
1:A:307:THR:HA	1:A:602:THR:HG21	1.97	0.46
1:A:39:GLY:HA3	1:A:60:LEU:HB3	1.96	0.46
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.97	0.46
1:A:97:THR:HB	1:A:190:LEU:HD13	1.98	0.46
1:B:676:THR:HA	1:B:690:GLN:HG2	1.97	0.46
1:B:980:ILE:HD11	1:B:996:LEU:HD11	1.97	0.46
2:G:394:ASN:OD1	2:G:395:GLY:N	2.49	0.46
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.45
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.99	0.45
1:B:560:LEU:HB2	1:B:563:GLN:HG2	1.97	0.45
2:I:148:LEU:HD22	2:I:164:ALA:HB1	1.99	0.45
1:A:560:LEU:HB2	1:A:563:GLN:HG2	1.97	0.45
1:B:121:ILE:HG22	1:B:130:ILE:HG12	1.98	0.45
1:C:307:THR:HA	1:C:602:THR:HG21	1.99	0.45
2:H:394:ASN:OD1	2:H:395:GLY:N	2.50	0.45
2:G:450:LEU:HB2	2:G:451:PRO:HD3	1.99	0.45
1:C:786:LYS:HG2	1:C:787:GLN:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:LYS:HE3	1:A:771:ALA:HB1	1.99	0.45
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.99	0.45
1:B:454:ARG:NH2	1:B:469:SER:O	2.45	0.45
1:B:123:ASN:HD22	1:B:128:PHE:HD1	1.64	0.45
2:H:369:PHE:O	2:H:373:HIS:ND1	2.47	0.44
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.99	0.44
2:I:343:VAL:HG12	2:I:345:HIS:H	1.81	0.44
2:G:32:PHE:HE2	2:G:391:LEU:HD21	1.83	0.44
2:G:148:LEU:HD22	2:G:164:ALA:HB1	1.99	0.44
2:G:190:MET:O	2:G:194:ASN:ND2	2.34	0.44
1:B:97:THR:HB	1:B:190:LEU:HD13	1.99	0.44
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.99	0.44
1:B:781:VAL:HG22	1:B:1026:ALA:HB2	2.00	0.44
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.99	0.44
2:G:369:PHE:O	2:G:373:HIS:ND1	2.48	0.44
1:C:786:LYS:H	1:C:786:LYS:HD3	1.83	0.44
1:A:123:ASN:HD22	1:A:128:PHE:HD1	1.65	0.43
1:B:307:THR:HA	1:B:602:THR:HG21	2.01	0.43
1:B:527:PRO:O	1:B:529:LYS:NZ	2.50	0.43
1:A:357:ARG:NH2	1:B:168:THR:O	2.52	0.43
2:I:59:VAL:O	2:I:63:ASN:ND2	2.35	0.43
2:I:252:TYR:HB3	2:I:255:TYR:HD2	1.83	0.43
1:B:357:ARG:NH2	1:C:168:THR:O	2.52	0.43
2:H:252:TYR:HB3	2:H:255:TYR:HD2	1.83	0.43
1:B:475:ALA:O	2:H:24:GLN:NE2	2.51	0.43
1:C:1116:THR:HG22	1:C:1138:TYR:HB3	2.00	0.43
2:G:252:TYR:HB3	2:G:255:TYR:HD2	1.82	0.43
2:I:450:LEU:HB2	2:I:451:PRO:HD3	1.99	0.43
2:H:32:PHE:HE2	2:H:391:LEU:HD21	1.83	0.43
2:G:596:LYS:O	2:G:600:LYS:HG3	2.19	0.43
2:H:148:LEU:HD22	2:H:164:ALA:HB1	1.99	0.43
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.01	0.43
1:C:475:ALA:O	2:I:24:GLN:NE2	2.51	0.43
1:A:475:ALA:O	2:G:24:GLN:NE2	2.52	0.43
1:A:630:THR:HB	1:A:631:PRO:HD3	2.01	0.43
2:H:450:LEU:HB2	2:H:451:PRO:HD3	1.99	0.43
2:H:523:PHE:HB3	2:H:583:PRO:HB2	2.01	0.43
2:I:32:PHE:HE2	2:I:391:LEU:HD21	1.84	0.43
2:I:596:LYS:O	2:I:600:LYS:HG3	2.19	0.43
2:H:596:LYS:O	2:H:600:LYS:HG3	2.19	0.42
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:THR:HB	1:C:631:PRO:HD3	2.01	0.42
1:C:773:GLU:HA	1:C:776:LYS:HG2	2.01	0.42
2:I:523:PHE:HB3	2:I:583:PRO:HB2	2.00	0.42
1:B:378:LYS:HB2	1:B:433:VAL:HB	2.01	0.42
1:B:630:THR:HB	1:B:631:PRO:HD3	2.01	0.42
2:G:50:TYR:HA	2:G:58:ASN:HB3	2.01	0.42
1:A:627:ASP:OD1	1:A:627:ASP:N	2.47	0.42
2:I:338:ASN:ND2	2:I:339:VAL:H	2.18	0.42
2:H:50:TYR:HA	2:H:58:ASN:HB3	2.02	0.42
2:H:338:ASN:ND2	2:H:339:VAL:H	2.18	0.42
1:A:855:PHE:HD2	1:A:858:LEU:HD12	1.83	0.41
2:I:190:MET:O	2:I:194:ASN:ND2	2.35	0.41
1:A:989:ALA:O	1:A:993:ILE:HG12	2.21	0.41
1:B:776:LYS:NZ	1:B:780:GLU:OE2	2.51	0.41
1:B:786:LYS:HG2	1:B:787:GLN:HG3	2.02	0.41
1:C:557:LYS:HB2	1:C:584:ILE:HG21	2.02	0.41
1:C:599:THR:HA	1:C:600:PRO:HD3	1.92	0.41
1:B:87:PRO:HB2	1:B:89:ASN:HD21	1.85	0.41
1:A:599:THR:HA	1:A:600:PRO:HD3	1.92	0.41
1:B:339:HIS:ND1	1:B:340:GLU:HG2	2.35	0.41
1:B:733:LYS:HE3	1:B:771:ALA:HB1	2.01	0.41
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	2.02	0.41
1:C:103:ILE:HA	1:C:242:LEU:HA	2.01	0.41
2:G:338:ASN:ND2	2:G:339:VAL:H	2.18	0.41
1:A:498:ARG:NH1	1:A:501:TYR:OH	2.50	0.41
1:A:980:ILE:HD11	1:A:996:LEU:HD11	2.02	0.41
1:C:898:PHE:N	1:C:899:PRO:HD2	2.36	0.41
1:A:770:ILE:O	1:A:774:GLN:HG2	2.20	0.41
1:B:786:LYS:H	1:B:786:LYS:HD3	1.86	0.41
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	2.03	0.41
1:A:130:ILE:HG21	1:A:229:LEU:HD21	2.03	0.41
1:A:347:PHE:CE2	1:A:509:ARG:HB3	2.56	0.41
1:B:627:ASP:OD1	1:B:627:ASP:N	2.47	0.41
1:C:290:ASP:O	1:C:297:SER:HB3	2.21	0.41
1:C:733:LYS:HE3	1:C:771:ALA:HB1	2.02	0.41
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.41
2:I:72:PHE:HA	2:I:75:GLU:HG2	2.03	0.41
1:A:121:ILE:HG22	1:A:130:ILE:HG12	2.03	0.40
1:C:87:PRO:HB2	1:C:89:ASN:HD21	1.87	0.40
1:C:97:THR:HB	1:C:190:LEU:HD13	2.02	0.40
2:H:19:SER:OG	2:H:20:THR:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:VAL:HG21	1:A:387:LEU:HD13	2.03	0.40
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.54	0.40
1:A:879:ALA:O	1:A:883:THR:OG1	2.36	0.40
1:C:85:VAL:HG11	1:C:237:ARG:NE	2.36	0.40
2:G:523:PHE:HB3	2:G:583:PRO:HB2	2.01	0.40
2:I:358:ILE:HD13	2:I:375:GLU:HB3	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	1015/1291 (79%)	991 (98%)	24 (2%)	0	100	100
1	B	1015/1291 (79%)	985 (97%)	30 (3%)	0	100	100
1	C	1015/1291 (79%)	983 (97%)	32 (3%)	0	100	100
2	G	595/742 (80%)	589 (99%)	6 (1%)	0	100	100
2	H	595/742 (80%)	588 (99%)	7 (1%)	0	100	100
2	I	595/742 (80%)	589 (99%)	6 (1%)	0	100	100
All	All	4830/6099 (79%)	4725 (98%)	105 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	912/1115 (82%)	889 (98%)	23 (2%)	42	72
1	B	912/1115 (82%)	888 (97%)	24 (3%)	41	70
1	C	912/1115 (82%)	886 (97%)	26 (3%)	37	67
2	G	527/656 (80%)	520 (99%)	7 (1%)	65	85
2	H	527/656 (80%)	520 (99%)	7 (1%)	65	85
2	I	527/656 (80%)	520 (99%)	7 (1%)	65	85
All	All	4317/5313 (81%)	4223 (98%)	94 (2%)	47	76

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	44	ASP
1	A	45	LYS
1	A	132	VAL
1	A	231	ILE
1	A	293	LEU
1	A	296	LEU
1	A	370	ASN
1	A	377	PHE
1	A	386	LYS
1	A	462	LYS
1	A	529	LYS
1	A	568	ASP
1	A	617	CYS
1	A	738	CYS
1	A	776	LYS
1	A	786	LYS
1	A	811	LYS
1	A	814	LYS
1	A	825	LYS
1	A	886	TRP
1	A	964	LYS
1	A	1148	PHE
1	B	23	VAL
1	B	45	LYS
1	B	132	VAL
1	B	296	LEU
1	B	335	LEU
1	B	338	PHE
1	B	367	VAL

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Mol	Chain	Res	Type
1	B	371	PHE
1	B	375	PHE
1	B	377	PHE
1	B	386	LYS
1	B	462	LYS
1	B	568	ASP
1	B	617	CYS
1	B	738	CYS
1	B	776	LYS
1	B	786	LYS
1	B	811	LYS
1	B	825	LYS
1	B	886	TRP
1	B	964	LYS
1	B	988	GLU
1	B	1141	LEU
1	B	1148	PHE
1	C	23	VAL
1	C	44	ASP
1	C	45	LYS
1	C	132	VAL
1	C	231	ILE
1	C	293	LEU
1	C	296	LEU
1	C	337	PRO
1	C	361	CYS
1	C	374	PHE
1	C	377	PHE
1	C	386	LYS
1	C	462	LYS
1	C	529	LYS
1	C	568	ASP
1	C	617	CYS
1	C	738	CYS
1	C	776	LYS
1	C	786	LYS
1	C	811	LYS
1	C	825	LYS
1	C	886	TRP
1	C	939	PHE
1	C	964	LYS
1	C	1141	LEU

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Mol	Chain	Res	Type
1	C	1148	PHE
2	G	78	THR
2	G	131	LYS
2	G	172	VAL
2	G	199	TYR
2	G	381	TYR
2	G	400	PHE
2	G	592	PHE
2	H	78	THR
2	H	131	LYS
2	H	172	VAL
2	H	199	TYR
2	H	381	TYR
2	H	400	PHE
2	H	592	PHE
2	I	78	THR
2	I	131	LYS
2	I	172	VAL
2	I	199	TYR
2	I	381	TYR
2	I	400	PHE
2	I	592	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	136	GLN
1	A	165	ASN
1	A	174	GLN
1	A	271	GLN
1	A	321	GLN
1	A	334	ASN
1	A	474	GLN
1	A	493	GLN
1	A	580	GLN
1	A	607	GLN
1	A	628	GLN
1	A	677	GLN
1	A	787	GLN
1	A	804	GLN
1	A	872	GLN

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Mol	Chain	Res	Type
1	A	913	GLN
1	A	935	GLN
1	A	1002	GLN
1	A	1010	GLN
1	A	1071	GLN
1	A	1142	GLN
1	B	89	ASN
1	B	136	GLN
1	B	165	ASN
1	B	174	GLN
1	B	271	GLN
1	B	321	GLN
1	B	474	GLN
1	B	493	GLN
1	B	607	GLN
1	B	628	GLN
1	B	677	GLN
1	B	787	GLN
1	B	804	GLN
1	B	872	GLN
1	B	913	GLN
1	B	935	GLN
1	B	1002	GLN
1	B	1010	GLN
1	B	1071	GLN
1	B	1142	GLN
1	C	89	ASN
1	C	123	ASN
1	C	136	GLN
1	C	165	ASN
1	C	174	GLN
1	C	271	GLN
1	C	321	GLN
1	C	474	GLN
1	C	493	GLN
1	C	580	GLN
1	C	607	GLN
1	C	628	GLN
1	C	677	GLN
1	C	787	GLN
1	C	804	GLN
1	C	872	GLN

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Mol	Chain	Res	Type
1	C	913	GLN
1	C	935	GLN
1	C	1002	GLN
1	C	1010	GLN
1	C	1071	GLN
1	C	1142	GLN
2	G	58	ASN
2	G	239	HIS
2	G	338	ASN
2	G	340	GLN
2	G	508	ASN
2	G	524	GLN
2	H	58	ASN
2	H	239	HIS
2	H	338	ASN
2	H	340	GLN
2	H	508	ASN
2	H	524	GLN
2	I	58	ASN
2	I	239	HIS
2	I	338	ASN
2	I	340	GLN
2	I	508	ASN
2	I	524	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.

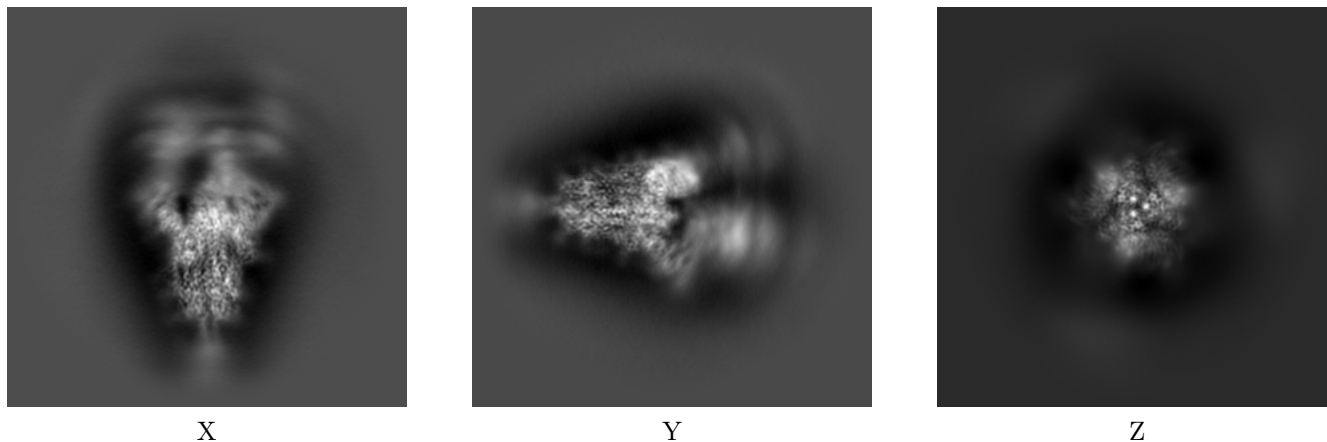
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39689. These allow visual inspection of the internal detail of the map and identification of artifacts.

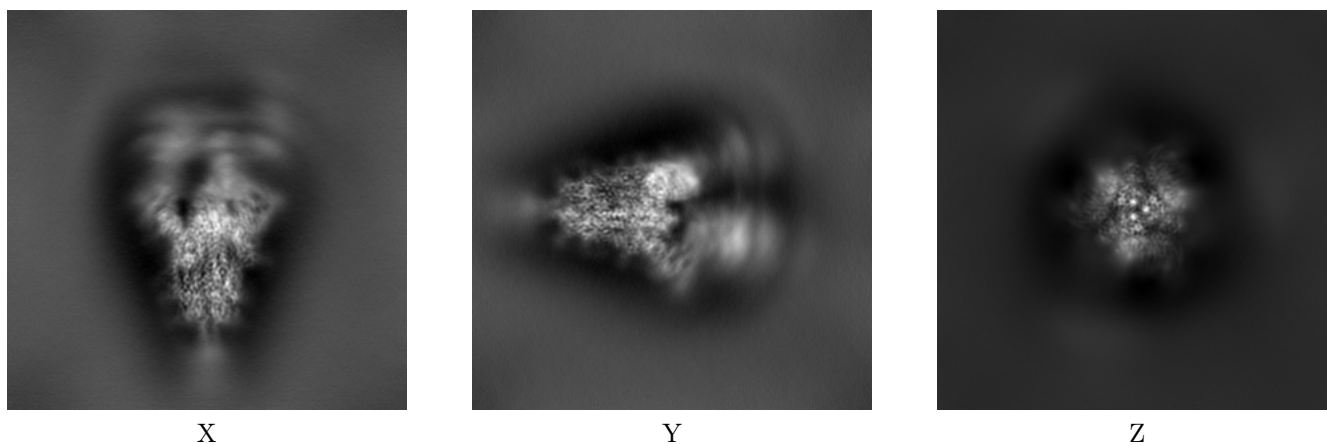
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



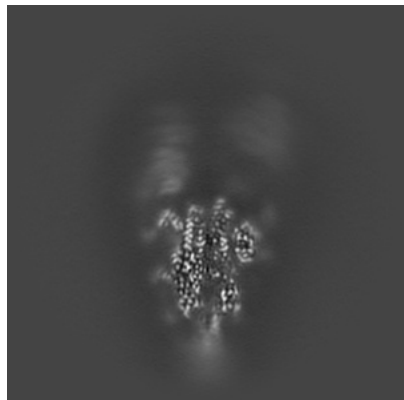
6.1.2 Raw map



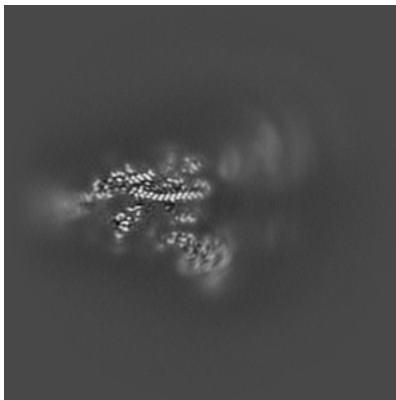
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

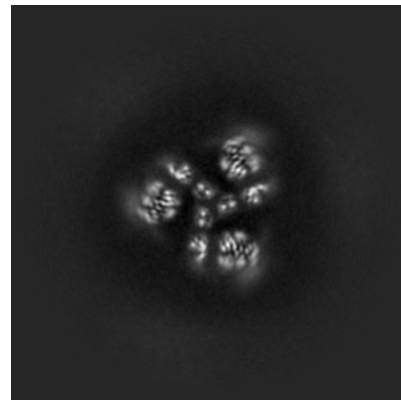
6.2.1 Primary map



X Index: 160

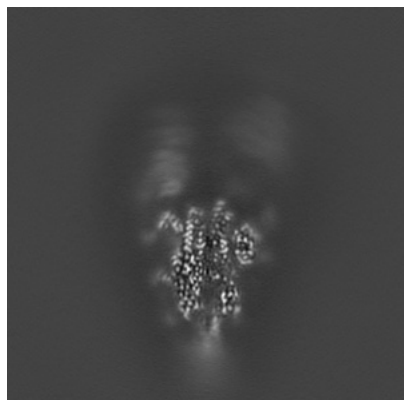


Y Index: 160

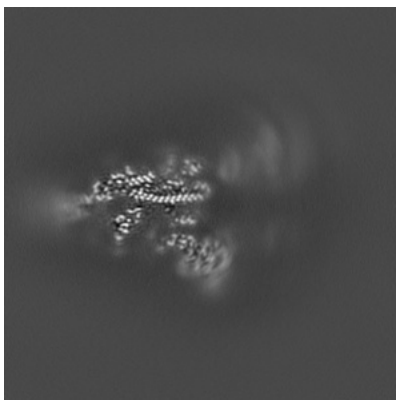


Z Index: 160

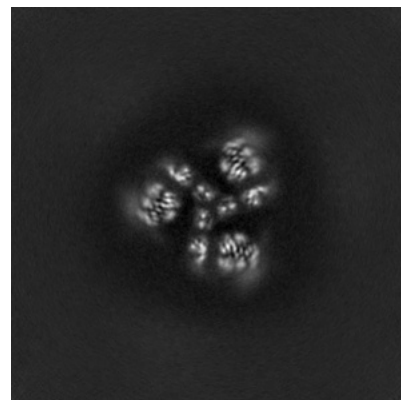
6.2.2 Raw map



X Index: 160



Y Index: 160

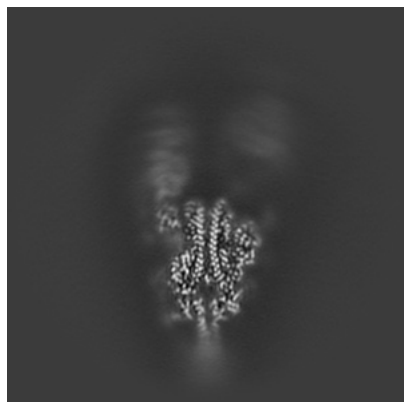


Z Index: 160

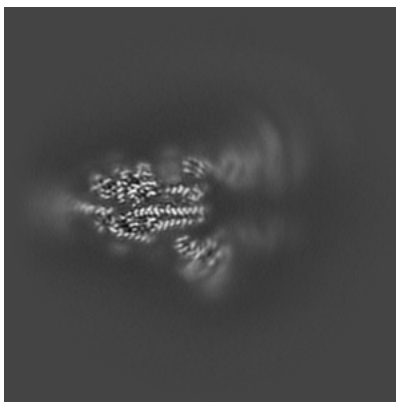
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

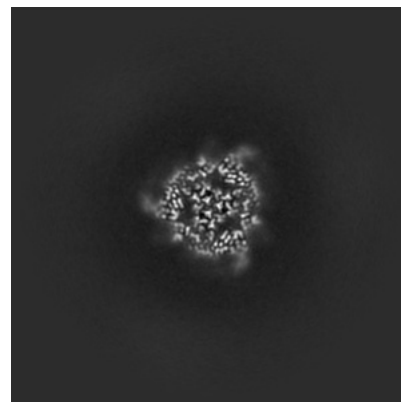
6.3.1 Primary map



X Index: 156

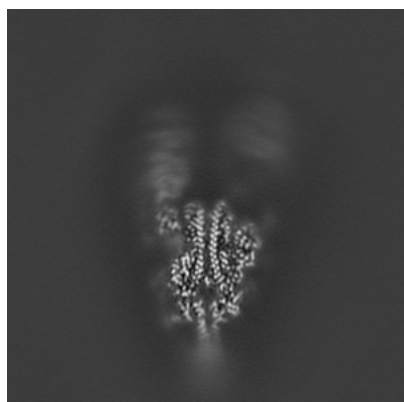


Y Index: 166

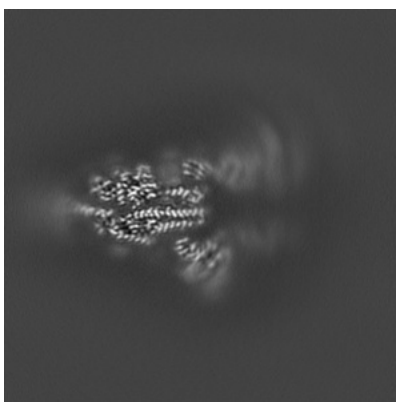


Z Index: 143

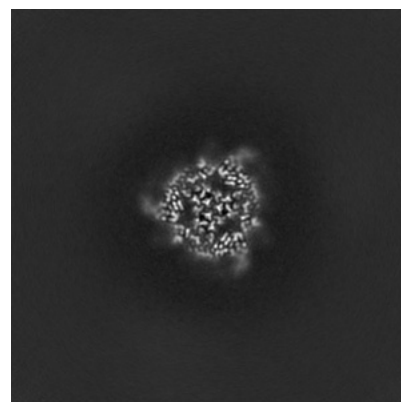
6.3.2 Raw map



X Index: 156



Y Index: 166

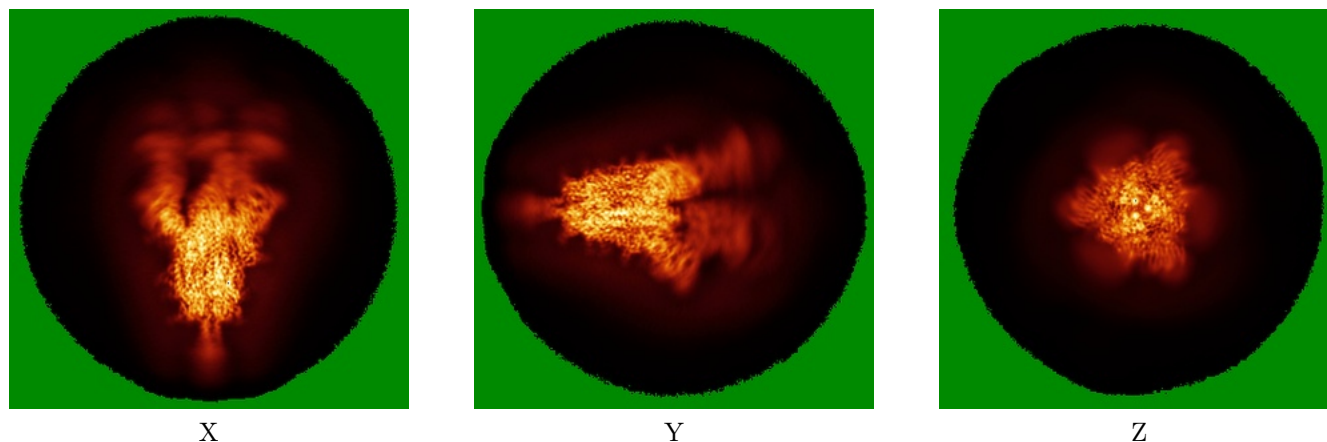


Z Index: 143

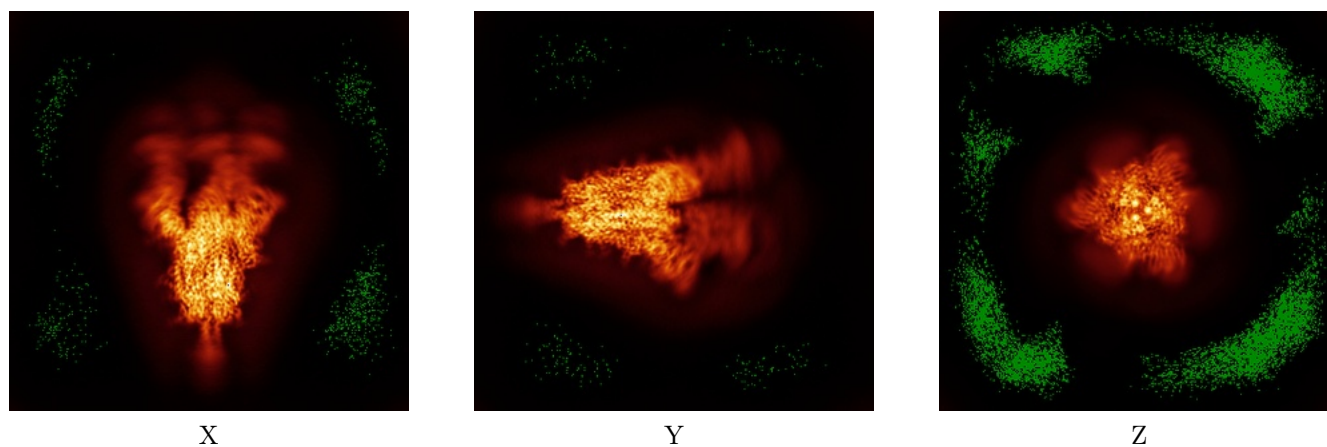
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



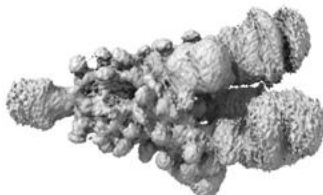
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

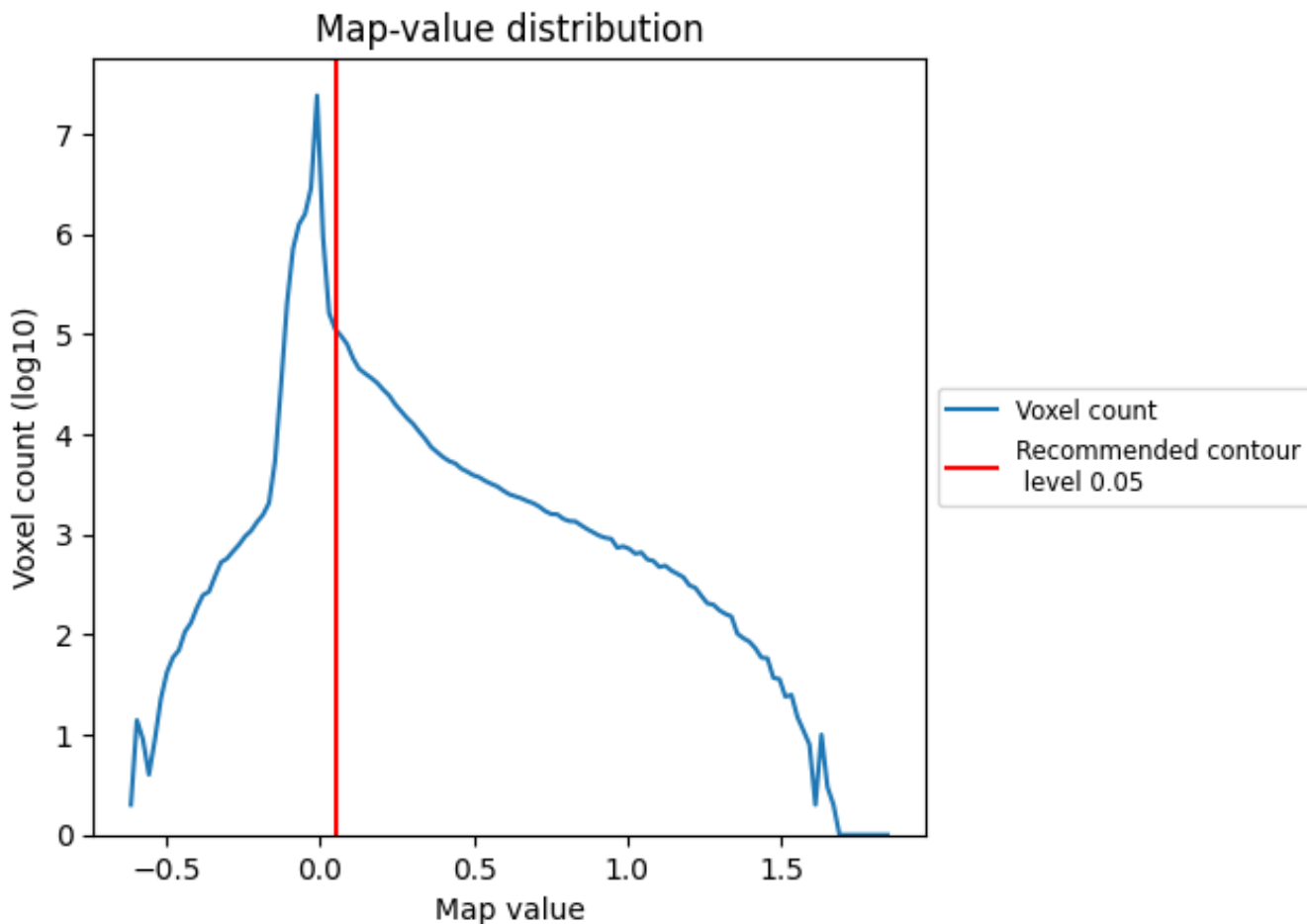
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

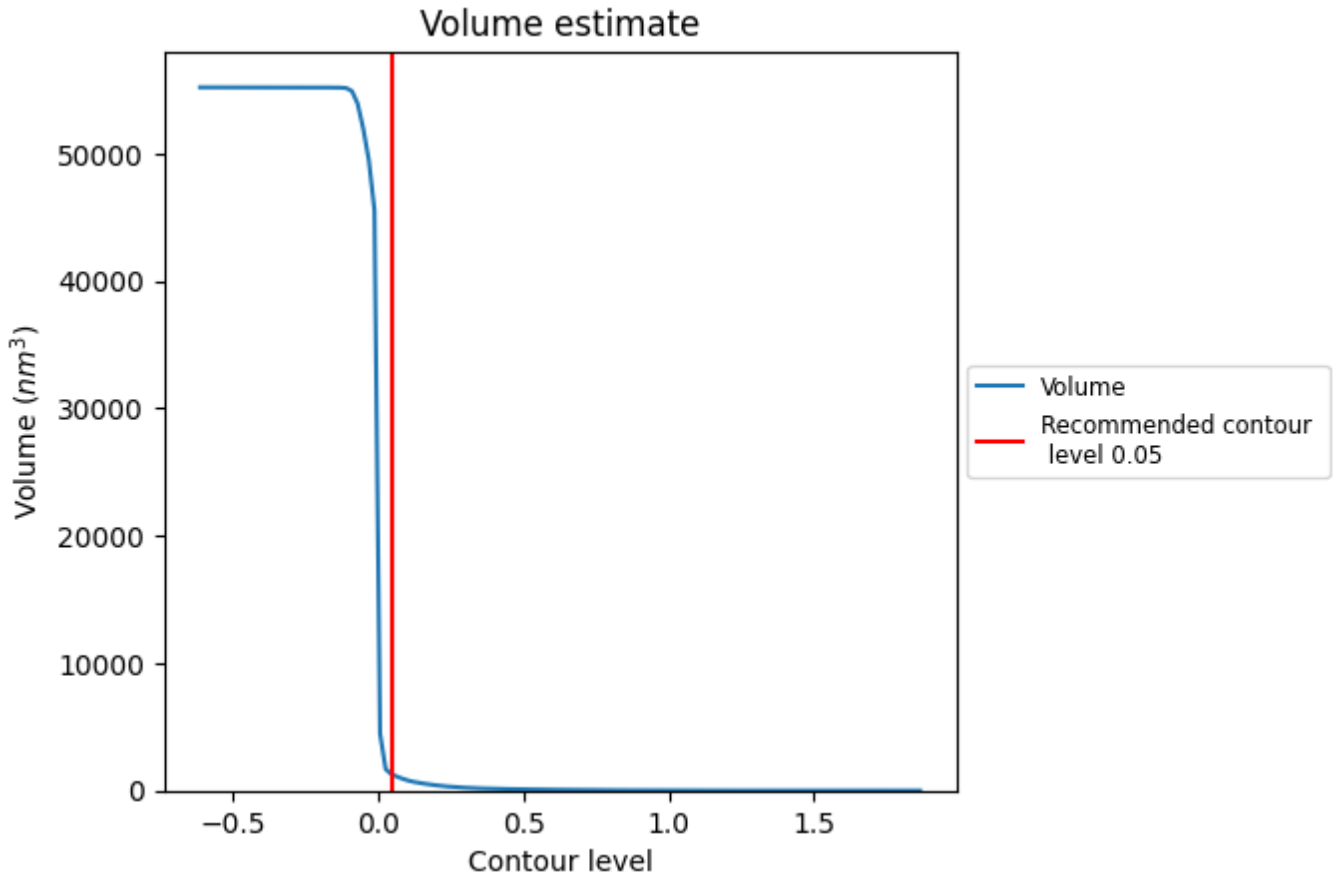
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

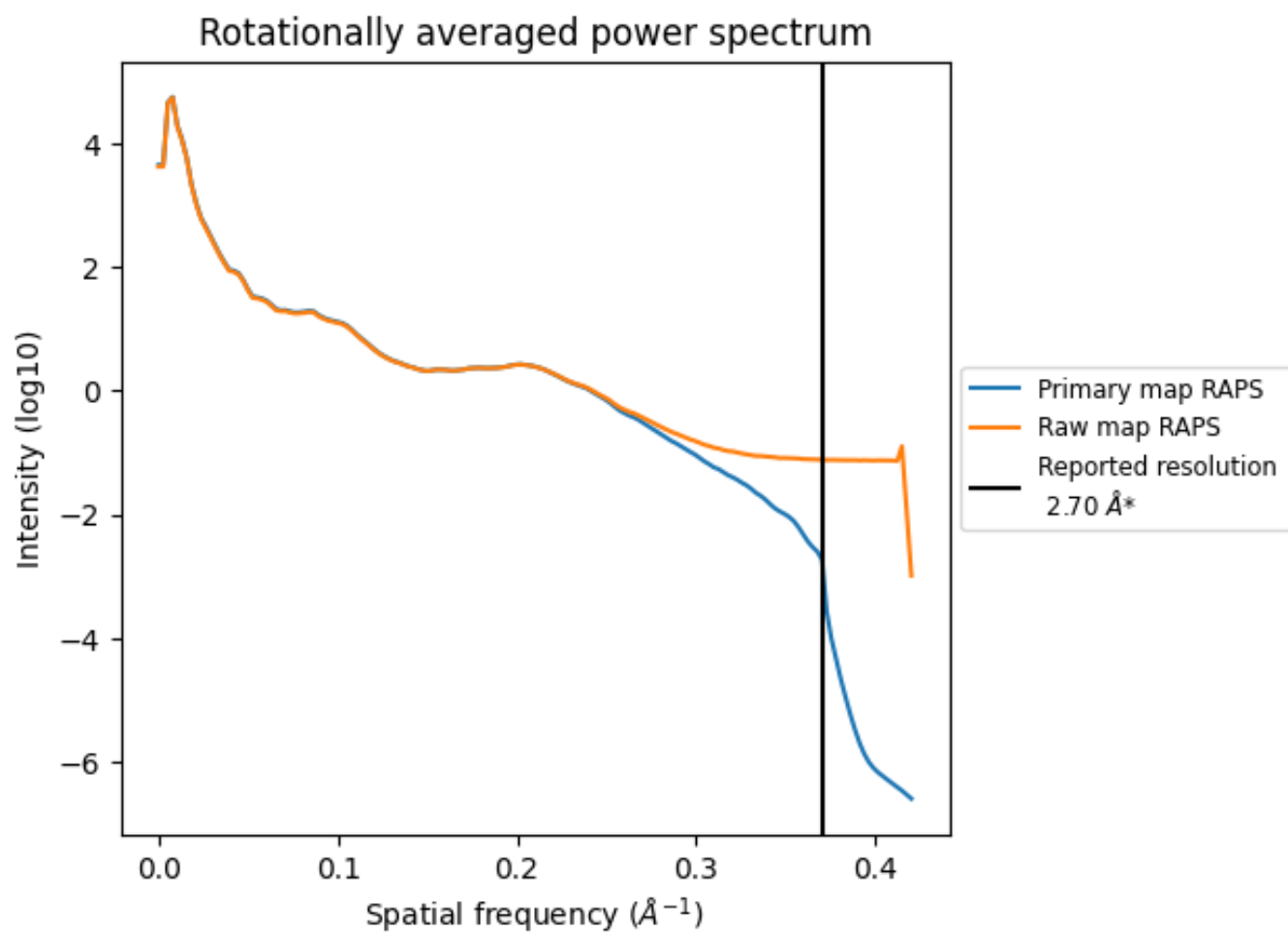
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1236 nm³; this corresponds to an approximate mass of 1116 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

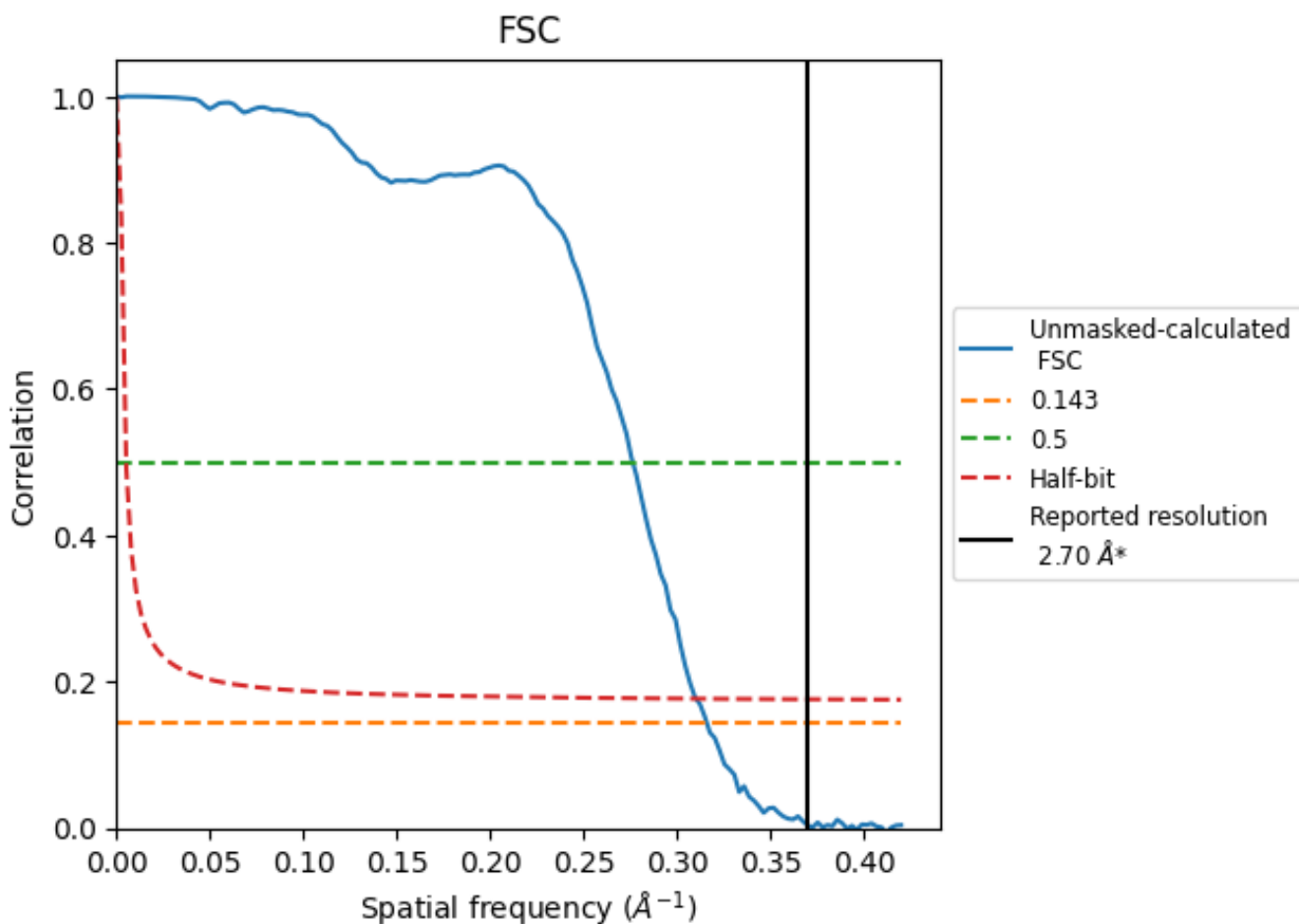


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

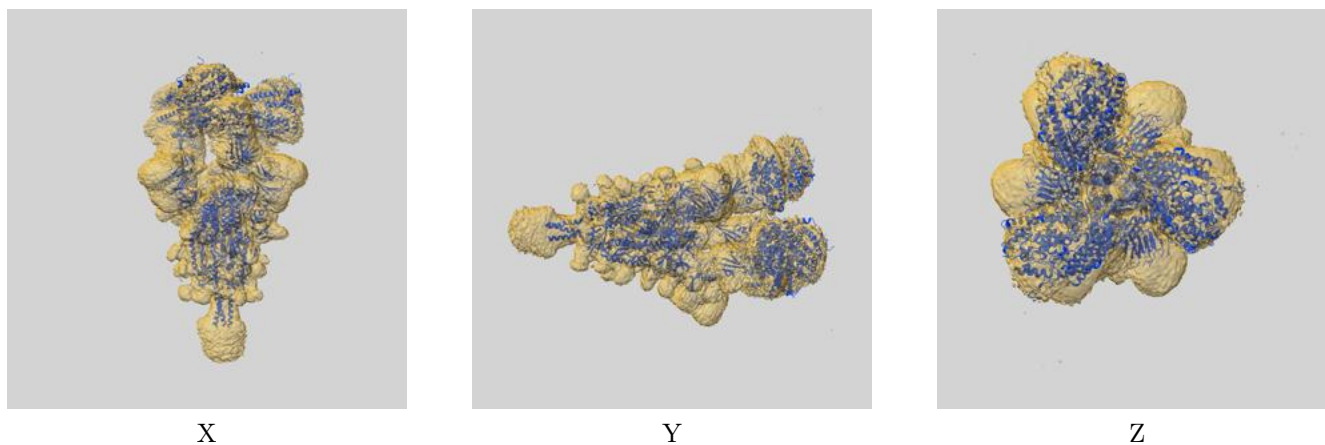
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	3.62	3.22

*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 3.16 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

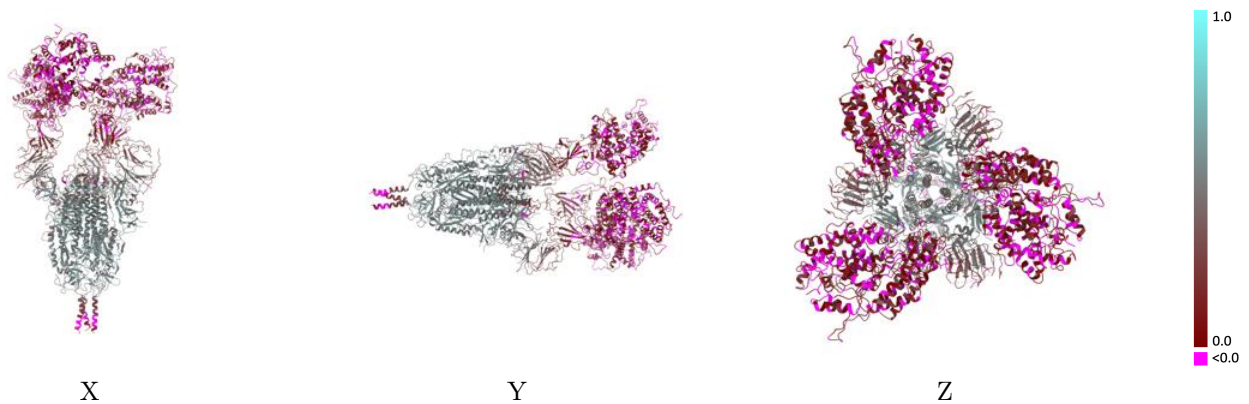
This section contains information regarding the fit between EMDB map EMD-39689 and PDB model 8YZC. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



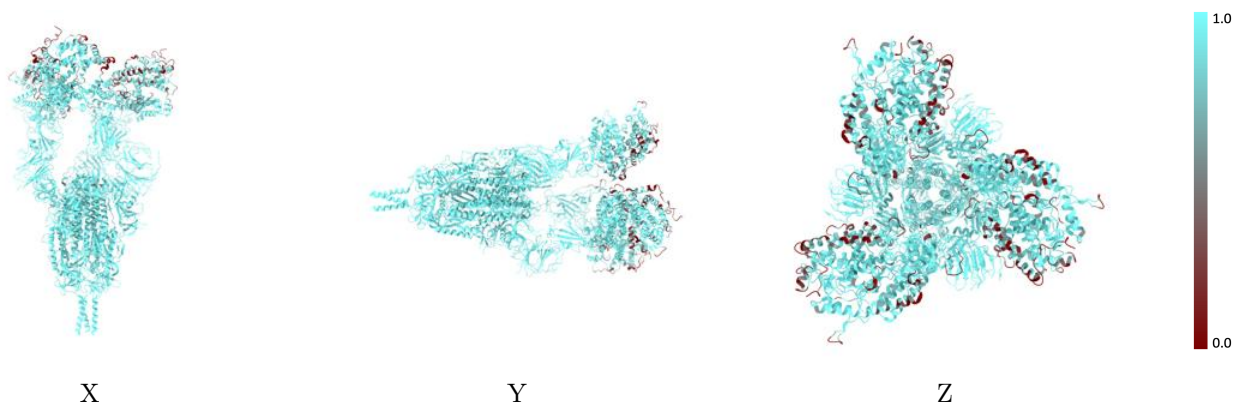
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



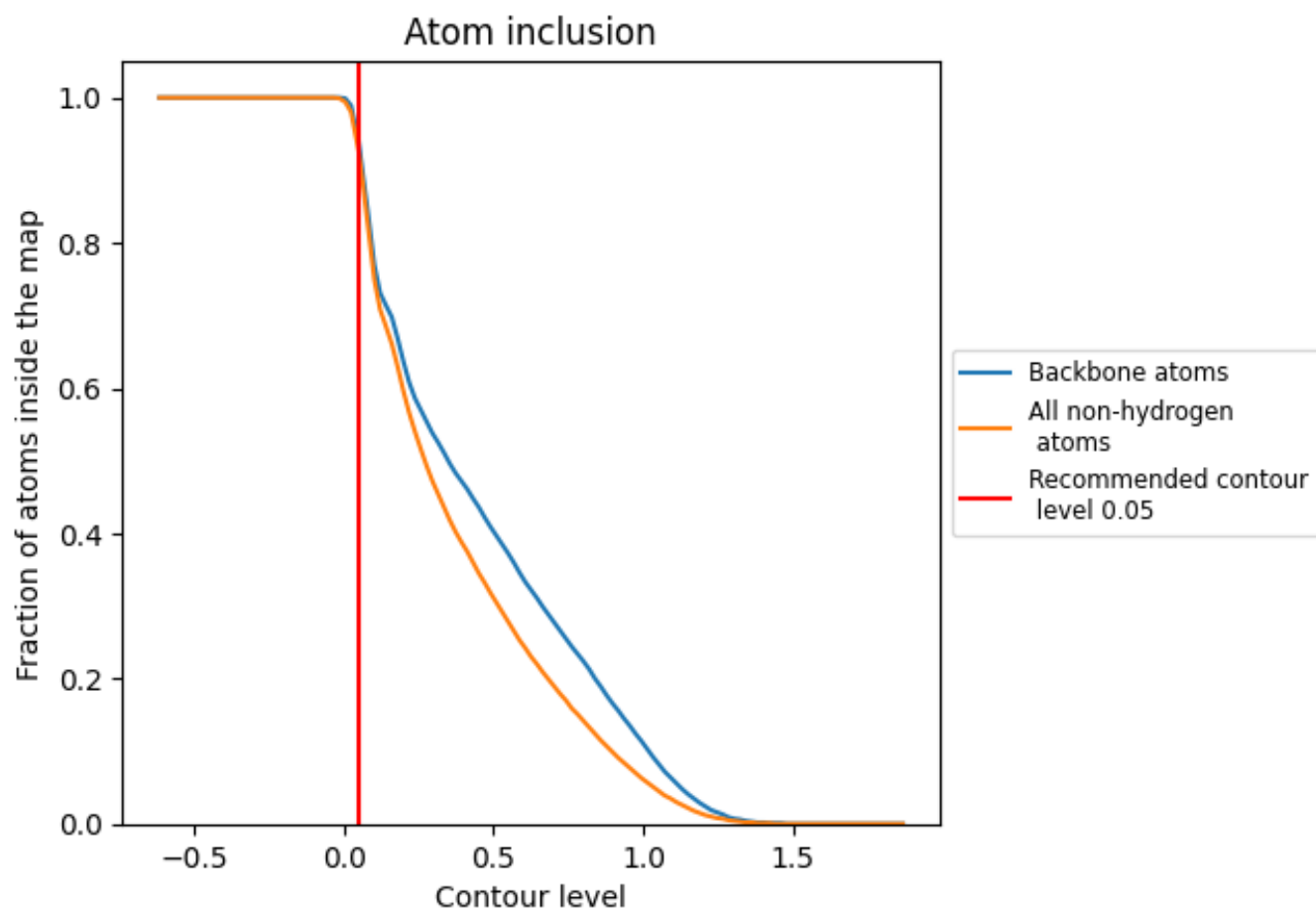
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).















9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.2670
A	 0.9870	 0.3950
B	 0.9880	 0.3920
C	 0.9880	 0.3940
G	 0.8220	 0.0600
H	 0.8310	 0.0590
I	 0.8160	 0.0520

