



Full wwPDB EM Validation Report ⓘ

Oct 10, 2026 – 10:40 am BST

PDB ID : 29SU / pdb_000029su
EMDB ID : EMD-57358
Title : BA3.2.2 SARS-CoV-2 Spike
Authors : Duyvesteyn, H.M.E.; Stuart, D.I.; Fry, E.E.
Deposited on : 2026-04-07
Resolution : 2.80 Å(reported)
Based on initial model : .

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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

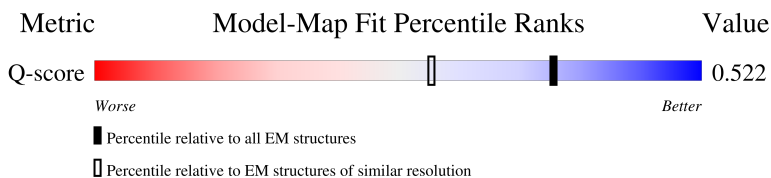
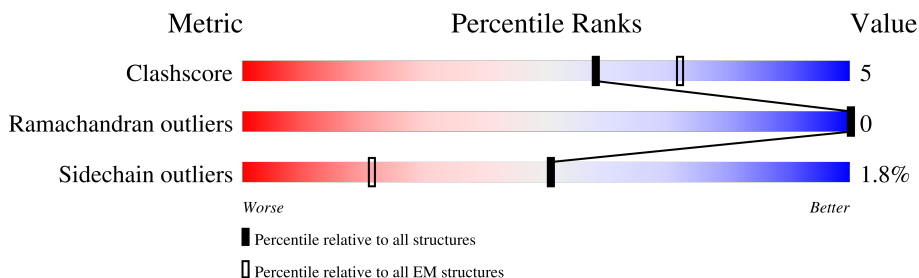
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	1144	
1	B	1144	
1	C	1144	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1001	Total	C	N	O	S	0	0
			7866	5043	1299	1489	35		
1	B	1040	Total	C	N	O	S	0	0
			8163	5230	1351	1545	37		
1	C	1023	Total	C	N	O	S	0	0
			8035	5152	1329	1518	36		

There are 198 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	LEU	PRO	conflict	UNP A0A7S6KRH9
A	21	THR	ARG	conflict	UNP A0A7S6KRH9
A	26	LEU	PRO	conflict	UNP A0A7S6KRH9
A	67	VAL	ALA	conflict	UNP A0A7S6KRH9
A	93	ILE	THR	conflict	UNP A0A7S6KRH9
A	99	THR	ILE	conflict	UNP A0A7S6KRH9
A	143	SER	PHE	conflict	UNP A0A7S6KRH9
A	150	LYS	ASN	conflict	UNP A0A7S6KRH9
A	158	PHE	SER	conflict	UNP A0A7S6KRH9
A	173	THR	LYS	conflict	UNP A0A7S6KRH9
A	198	ILE	LEU	conflict	UNP A0A7S6KRH9
A	201	ALA	-	insertion	UNP A0A7S6KRH9
A	202	SER	-	insertion	UNP A0A7S6KRH9
A	203	ASP	-	insertion	UNP A0A7S6KRH9
A	204	THR	-	insertion	UNP A0A7S6KRH9
A	219V	SER	PRO	conflict	UNP A0A7S6KRH9
A	313	VAL	ILE	conflict	UNP A0A7S6KRH9
A	326	TYR	GLY	conflict	UNP A0A7S6KRH9
A	335	PRO	ALA	conflict	UNP A0A7S6KRH9
A	343	THR	LYS	conflict	UNP A0A7S6KRH9
A	358	PHE	SER	conflict	UNP A0A7S6KRH9
A	360	PRO	SER	conflict	UNP A0A7S6KRH9
A	362	PHE	SER	conflict	UNP A0A7S6KRH9
A	390	LYS	ARG	conflict	UNP A0A7S6KRH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	392	ASN	ASP	conflict	UNP A0A7S6KRH9
A	395	SER	ARG	conflict	UNP A0A7S6KRH9
A	404	ASN	LYS	conflict	UNP A0A7S6KRH9
A	422	SER	ALA	conflict	UNP A0A7S6KRH9
A	427	ARG	ASN	conflict	UNP A0A7S6KRH9
A	432	ALA	VAL	conflict	UNP A0A7S6KRH9
A	433	ASP	GLY	conflict	UNP A0A7S6KRH9
A	439	TRP	LEU	conflict	UNP A0A7S6KRH9
A	447	LYS	ASN	conflict	UNP A0A7S6KRH9
A	464	ASN	SER	conflict	UNP A0A7S6KRH9
A	465	ASN	THR	conflict	UNP A0A7S6KRH9
A	470	VAL	ALA	conflict	UNP A0A7S6KRH9
A	471	LYS	GLU	conflict	UNP A0A7S6KRH9
A	483	SER	GLY	conflict	UNP A0A7S6KRH9
A	485	ARG	GLN	conflict	UNP A0A7S6KRH9
A	488	TYR	ASN	conflict	UNP A0A7S6KRH9
A	516	ASN	LYS	conflict	UNP A0A7S6KRH9
A	541	ASP	GLU	conflict	UNP A0A7S6KRH9
A	562	SER	ALA	conflict	UNP A0A7S6KRH9
A	570	ASP	GLU	conflict	UNP A0A7S6KRH9
A	601	GLY	ASP	conflict	UNP A0A7S6KRH9
A	612	ARG	HIS	conflict	UNP A0A7S6KRH9
A	628	LYS	ASN	conflict	UNP A0A7S6KRH9
A	629	GLY	VAL	conflict	UNP A0A7S6KRH9
A	641	LYS	GLU	conflict	UNP A0A7S6KRH9
A	642	TYR	HIS	conflict	UNP A0A7S6KRH9
A	666	ARG	ASN	conflict	UNP A0A7S6KRH9
A	668	HIS	PRO	conflict	UNP A0A7S6KRH9
A	669	GLY	ARG	conflict	UNP A0A7S6KRH9
A	670	SER	ARG	conflict	UNP A0A7S6KRH9
A	672	SER	ARG	conflict	UNP A0A7S6KRH9
A	675	ASP	ALA	conflict	UNP A0A7S6KRH9
A	691	LEU	SER	conflict	UNP A0A7S6KRH9
A	751	LYS	ASN	conflict	UNP A0A7S6KRH9
A	782	THR	LYS	conflict	UNP A0A7S6KRH9
A	783	TYR	ASP	conflict	UNP A0A7S6KRH9
A	839	LYS	ALA	conflict	UNP A0A7S6KRH9
A	926	PHE	SER	conflict	UNP A0A7S6KRH9
A	941	HIS	GLN	conflict	UNP A0A7S6KRH9
A	956	LYS	ASN	conflict	UNP A0A7S6KRH9
A	973	PRO	LYS	conflict	UNP A0A7S6KRH9
A	974	PRO	VAL	conflict	UNP A0A7S6KRH9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	9	LEU	PRO	conflict	UNP A0A7S6KRH9
B	21	THR	ARG	conflict	UNP A0A7S6KRH9
B	26	LEU	PRO	conflict	UNP A0A7S6KRH9
B	67	VAL	ALA	conflict	UNP A0A7S6KRH9
B	93	ILE	THR	conflict	UNP A0A7S6KRH9
B	99	THR	ILE	conflict	UNP A0A7S6KRH9
B	143	SER	PHE	conflict	UNP A0A7S6KRH9
B	150	LYS	ASN	conflict	UNP A0A7S6KRH9
B	158	PHE	SER	conflict	UNP A0A7S6KRH9
B	173	THR	LYS	conflict	UNP A0A7S6KRH9
B	198	ILE	LEU	conflict	UNP A0A7S6KRH9
B	201	ALA	-	insertion	UNP A0A7S6KRH9
B	202	SER	-	insertion	UNP A0A7S6KRH9
B	203	ASP	-	insertion	UNP A0A7S6KRH9
B	204	THR	-	insertion	UNP A0A7S6KRH9
B	231J	SER	PRO	conflict	UNP A0A7S6KRH9
B	313	VAL	ILE	conflict	UNP A0A7S6KRH9
B	326	TYR	GLY	conflict	UNP A0A7S6KRH9
B	335	PRO	ALA	conflict	UNP A0A7S6KRH9
B	343	THR	LYS	conflict	UNP A0A7S6KRH9
B	358	PHE	SER	conflict	UNP A0A7S6KRH9
B	360	PRO	SER	conflict	UNP A0A7S6KRH9
B	362	PHE	SER	conflict	UNP A0A7S6KRH9
B	390	LYS	ARG	conflict	UNP A0A7S6KRH9
B	392	ASN	ASP	conflict	UNP A0A7S6KRH9
B	395	SER	ARG	conflict	UNP A0A7S6KRH9
B	404	ASN	LYS	conflict	UNP A0A7S6KRH9
B	422	SER	ALA	conflict	UNP A0A7S6KRH9
B	427	ARG	ASN	conflict	UNP A0A7S6KRH9
B	432	ALA	VAL	conflict	UNP A0A7S6KRH9
B	433	ASP	GLY	conflict	UNP A0A7S6KRH9
B	439	TRP	LEU	conflict	UNP A0A7S6KRH9
B	447	LYS	ASN	conflict	UNP A0A7S6KRH9
B	464	ASN	SER	conflict	UNP A0A7S6KRH9
B	465	ASN	THR	conflict	UNP A0A7S6KRH9
B	470	VAL	ALA	conflict	UNP A0A7S6KRH9
B	471	LYS	GLU	conflict	UNP A0A7S6KRH9
B	483	SER	GLY	conflict	UNP A0A7S6KRH9
B	485	ARG	GLN	conflict	UNP A0A7S6KRH9
B	488	TYR	ASN	conflict	UNP A0A7S6KRH9
B	516	ASN	LYS	conflict	UNP A0A7S6KRH9
B	541	ASP	GLU	conflict	UNP A0A7S6KRH9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	562	SER	ALA	conflict	UNP A0A7S6KRH9
B	570	ASP	GLU	conflict	UNP A0A7S6KRH9
B	601	GLY	ASP	conflict	UNP A0A7S6KRH9
B	612	ARG	HIS	conflict	UNP A0A7S6KRH9
B	628	LYS	ASN	conflict	UNP A0A7S6KRH9
B	629	GLY	VAL	conflict	UNP A0A7S6KRH9
B	641	LYS	GLU	conflict	UNP A0A7S6KRH9
B	642	TYR	HIS	conflict	UNP A0A7S6KRH9
B	666	ARG	ASN	conflict	UNP A0A7S6KRH9
B	668	HIS	PRO	conflict	UNP A0A7S6KRH9
B	669	GLY	ARG	conflict	UNP A0A7S6KRH9
B	670	SER	ARG	conflict	UNP A0A7S6KRH9
B	672	SER	ARG	conflict	UNP A0A7S6KRH9
B	675	ASP	ALA	conflict	UNP A0A7S6KRH9
B	691	LEU	SER	conflict	UNP A0A7S6KRH9
B	751	LYS	ASN	conflict	UNP A0A7S6KRH9
B	782	THR	LYS	conflict	UNP A0A7S6KRH9
B	783	TYR	ASP	conflict	UNP A0A7S6KRH9
B	839	LYS	ALA	conflict	UNP A0A7S6KRH9
B	926	PHE	SER	conflict	UNP A0A7S6KRH9
B	941	HIS	GLN	conflict	UNP A0A7S6KRH9
B	956	LYS	ASN	conflict	UNP A0A7S6KRH9
B	973	PRO	LYS	conflict	UNP A0A7S6KRH9
B	974	PRO	VAL	conflict	UNP A0A7S6KRH9
C	9	LEU	PRO	conflict	UNP A0A7S6KRH9
C	21	THR	ARG	conflict	UNP A0A7S6KRH9
C	26	LEU	PRO	conflict	UNP A0A7S6KRH9
C	67	VAL	ALA	conflict	UNP A0A7S6KRH9
C	93	ILE	THR	conflict	UNP A0A7S6KRH9
C	99	THR	ILE	conflict	UNP A0A7S6KRH9
C	143	SER	PHE	conflict	UNP A0A7S6KRH9
C	150	LYS	ASN	conflict	UNP A0A7S6KRH9
C	158	PHE	SER	conflict	UNP A0A7S6KRH9
C	173	THR	LYS	conflict	UNP A0A7S6KRH9
C	198	ILE	LEU	conflict	UNP A0A7S6KRH9
C	201	ALA	-	insertion	UNP A0A7S6KRH9
C	202	SER	-	insertion	UNP A0A7S6KRH9
C	203	ASP	-	insertion	UNP A0A7S6KRH9
C	204	THR	-	insertion	UNP A0A7S6KRH9
C	233F	SER	PRO	conflict	UNP A0A7S6KRH9
C	313	VAL	ILE	conflict	UNP A0A7S6KRH9
C	326	TYR	GLY	conflict	UNP A0A7S6KRH9

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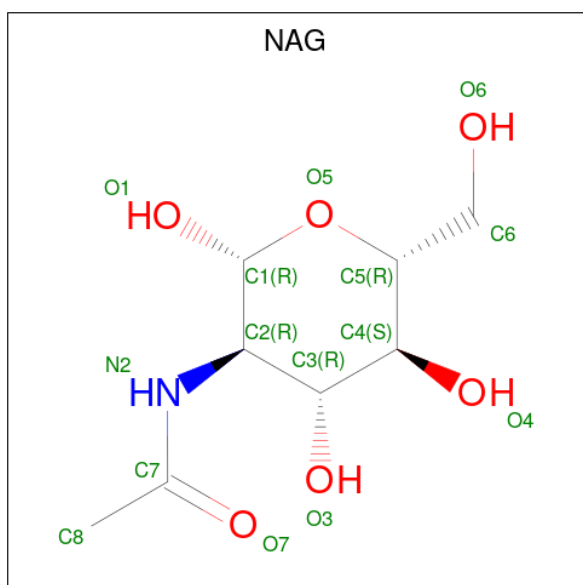
Chain	Residue	Modelled	Actual	Comment	Reference
C	335	PRO	ALA	conflict	UNP A0A7S6KRH9
C	343	THR	LYS	conflict	UNP A0A7S6KRH9
C	358	PHE	SER	conflict	UNP A0A7S6KRH9
C	360	PRO	SER	conflict	UNP A0A7S6KRH9
C	362	PHE	SER	conflict	UNP A0A7S6KRH9
C	390	LYS	ARG	conflict	UNP A0A7S6KRH9
C	392	ASN	ASP	conflict	UNP A0A7S6KRH9
C	395	SER	ARG	conflict	UNP A0A7S6KRH9
C	404	ASN	LYS	conflict	UNP A0A7S6KRH9
C	422	SER	ALA	conflict	UNP A0A7S6KRH9
C	427	ARG	ASN	conflict	UNP A0A7S6KRH9
C	432	ALA	VAL	conflict	UNP A0A7S6KRH9
C	433	ASP	GLY	conflict	UNP A0A7S6KRH9
C	439	TRP	LEU	conflict	UNP A0A7S6KRH9
C	447	LYS	ASN	conflict	UNP A0A7S6KRH9
C	464	ASN	SER	conflict	UNP A0A7S6KRH9
C	465	ASN	THR	conflict	UNP A0A7S6KRH9
C	470	VAL	ALA	conflict	UNP A0A7S6KRH9
C	471	LYS	GLU	conflict	UNP A0A7S6KRH9
C	483	SER	GLY	conflict	UNP A0A7S6KRH9
C	485	ARG	GLN	conflict	UNP A0A7S6KRH9
C	488	TYR	ASN	conflict	UNP A0A7S6KRH9
C	516	ASN	LYS	conflict	UNP A0A7S6KRH9
C	541	ASP	GLU	conflict	UNP A0A7S6KRH9
C	562	SER	ALA	conflict	UNP A0A7S6KRH9
C	570	ASP	GLU	conflict	UNP A0A7S6KRH9
C	601	GLY	ASP	conflict	UNP A0A7S6KRH9
C	612	ARG	HIS	conflict	UNP A0A7S6KRH9
C	628	LYS	ASN	conflict	UNP A0A7S6KRH9
C	629	GLY	VAL	conflict	UNP A0A7S6KRH9
C	641	LYS	GLU	conflict	UNP A0A7S6KRH9
C	642	TYR	HIS	conflict	UNP A0A7S6KRH9
C	666	ARG	ASN	conflict	UNP A0A7S6KRH9
C	668	HIS	PRO	conflict	UNP A0A7S6KRH9
C	669	GLY	ARG	conflict	UNP A0A7S6KRH9
C	670	SER	ARG	conflict	UNP A0A7S6KRH9
C	672	SER	ARG	conflict	UNP A0A7S6KRH9
C	675	ASP	ALA	conflict	UNP A0A7S6KRH9
C	691	LEU	SER	conflict	UNP A0A7S6KRH9
C	751	LYS	ASN	conflict	UNP A0A7S6KRH9
C	782	THR	LYS	conflict	UNP A0A7S6KRH9
C	783	TYR	ASP	conflict	UNP A0A7S6KRH9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	839	LYS	ALA	conflict	UNP A0A7S6KRH9
C	926	PHE	SER	conflict	UNP A0A7S6KRH9
C	941	HIS	GLN	conflict	UNP A0A7S6KRH9
C	956	LYS	ASN	conflict	UNP A0A7S6KRH9
C	973	PRO	LYS	conflict	UNP A0A7S6KRH9
C	974	PRO	VAL	conflict	UNP A0A7S6KRH9

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	

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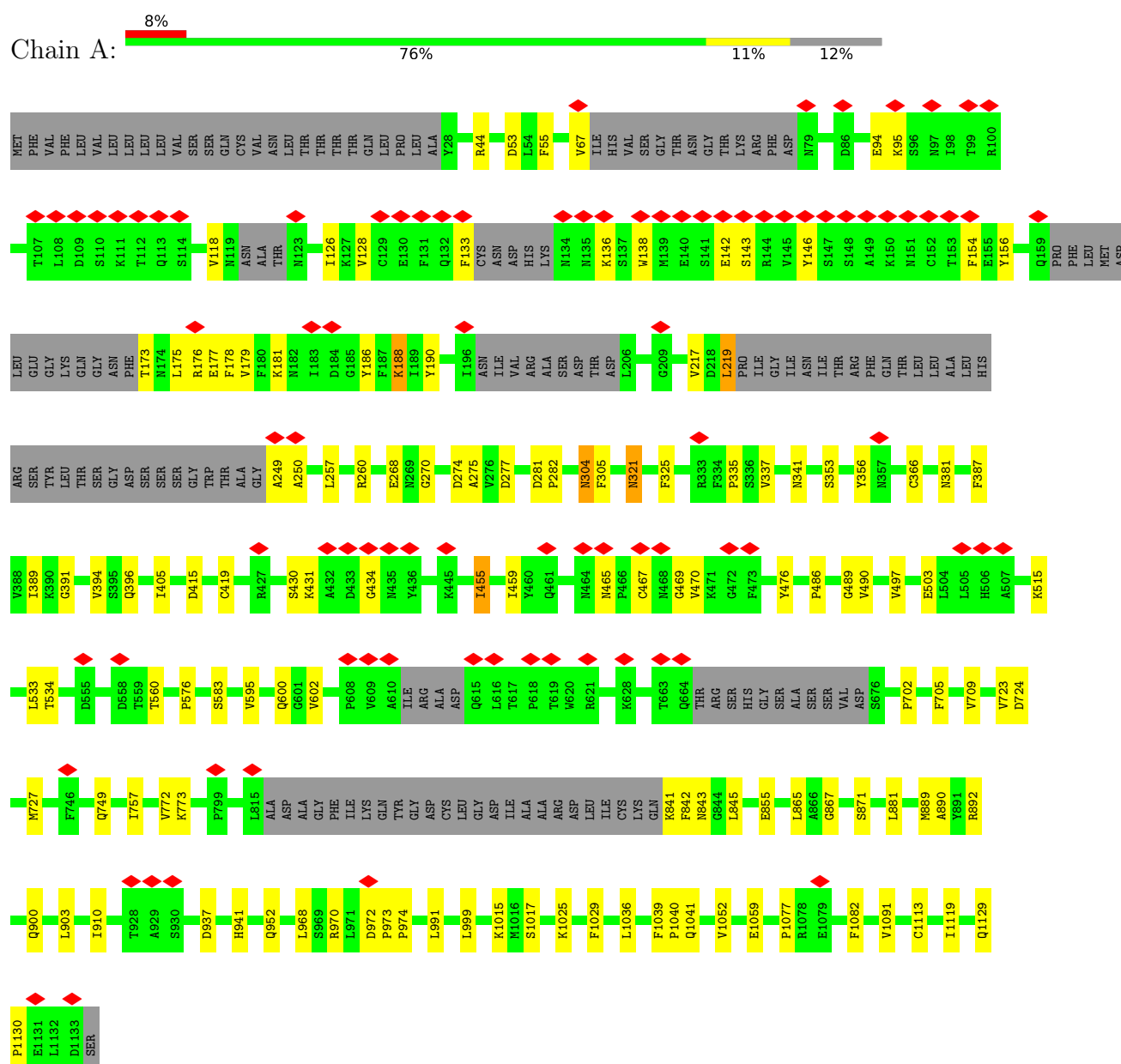
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Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

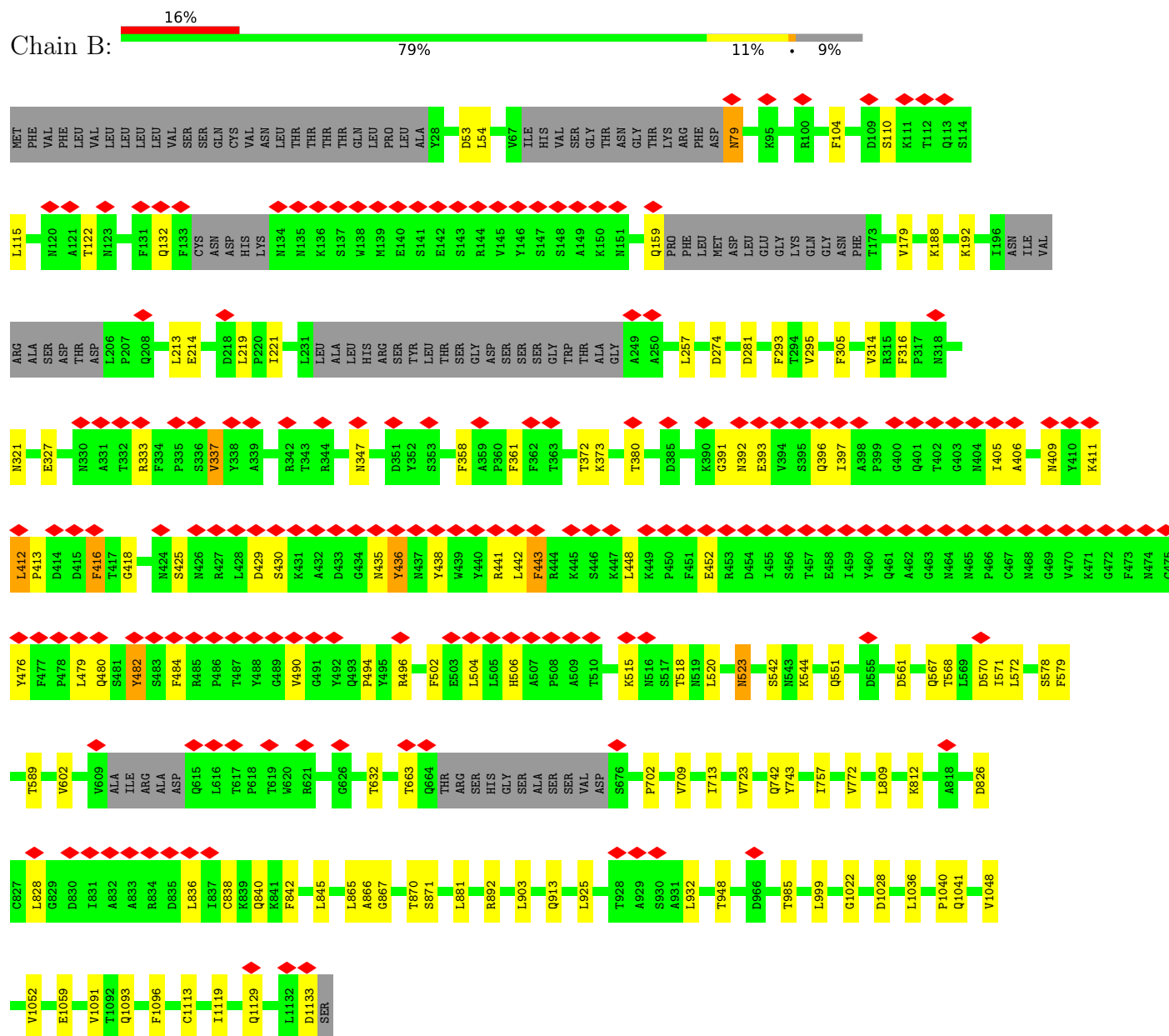
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



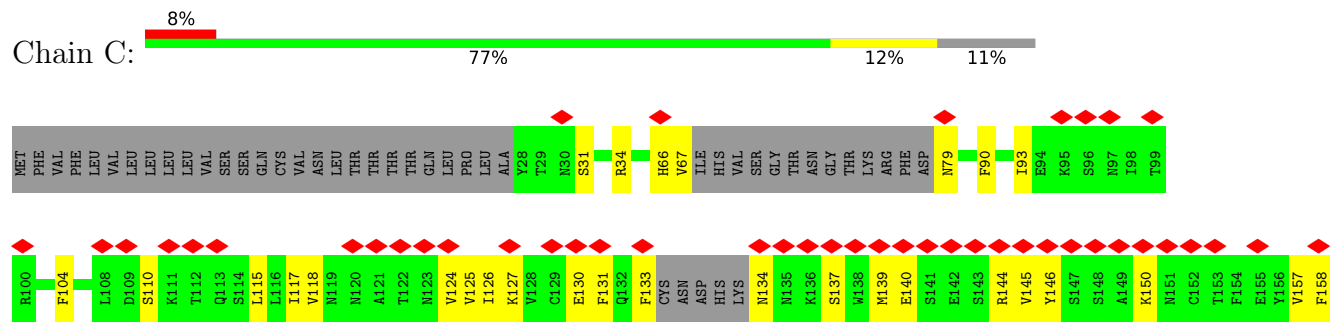
• Molecule 1: Spike glycoprotein

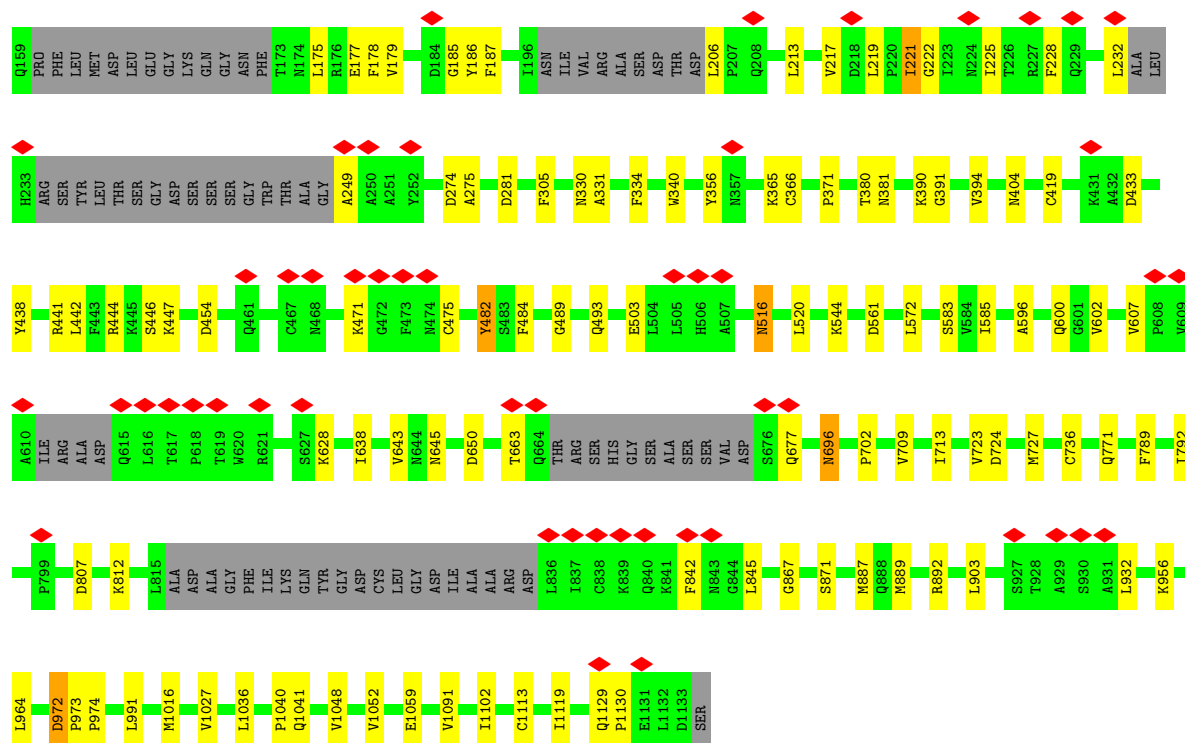
Chain B:



• Molecule 1: Spike glycoprotein

Chain C:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28786	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.778	Depositor
Minimum map value	-0.439	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.125	Depositor
Map size (Å)	408.96802, 408.96802, 408.96802	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7303, 0.7303, 0.7303	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.12	0/8054	0.25	0/10960
1	B	0.12	0/8357	0.26	0/11373
1	C	0.12	0/8226	0.26	0/11196
All	All	0.12	0/24637	0.26	0/33529

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	7866	0	7667	81	0
1	B	8163	0	7969	78	0
1	C	8035	0	7853	83	0
2	A	112	0	104	2	0
2	B	112	0	104	1	0
2	C	112	0	104	0	0
All	All	24400	0	23801	227	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 5.

All (227) 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:A:335:PRO:HG3	1:A:341:ASN:HB2	1.69	0.74
1:B:1113:CYS:HB2	1:B:1119:ILE:HD13	1.71	0.73
1:C:438:TYR:HB2	1:C:482:TYR:HE1	1.55	0.72
1:A:467:CYS:HB3	1:A:470:VAL:HG22	1.74	0.70
1:A:305:PHE:HZ	1:A:602:VAL:HG21	1.57	0.68
1:A:126:ILE:HD13	1:A:219:LEU:HD22	1.76	0.68
1:C:404:ASN:HD21	1:C:442:LEU:HA	1.60	0.67
1:C:104:PHE:HB2	1:C:115:LEU:HB3	1.75	0.66
1:A:723:VAL:HG11	1:A:991:LEU:HD21	1.76	0.66
1:A:1113:CYS:HB2	1:A:1119:ILE:HD13	1.77	0.65
1:A:95:LYS:HE2	1:A:173:THR:HG23	1.76	0.65
1:B:544:LYS:NZ	1:B:561:ASP:OD1	2.29	0.65
1:C:972:ASP:OD1	1:C:972:ASP:N	2.29	0.65
1:B:438:TYR:HA	1:B:482:TYR:HB2	1.78	0.65
1:B:405:ILE:HA	1:B:409:ASN:HB2	1.79	0.64
1:B:412:LEU:HD23	1:B:413:PRO:HD2	1.80	0.64
1:C:1113:CYS:HB2	1:C:1119:ILE:HD13	1.79	0.63
1:B:812:LYS:HD3	1:B:932:LEU:HD12	1.78	0.63
1:C:137:SER:HB2	1:C:232:LEU:HD12	1.81	0.63
1:C:444:ARG:NH1	1:C:446:SER:O	2.30	0.63
1:C:179:VAL:HG23	1:C:213:LEU:HD22	1.82	0.62
1:B:425:SER:HB2	1:B:494:PRO:HB2	1.81	0.61
1:B:1040:PRO:O	1:B:1041:GLN:NE2	2.34	0.61
1:C:723:VAL:HG11	1:C:991:LEU:HD21	1.83	0.60
1:B:484:PHE:HB3	1:B:494:PRO:HG3	1.82	0.60
1:A:67:VAL:O	1:A:249:ALA:N	2.36	0.59
1:A:515:LYS:HA	2:A:1201:NAG:H82	1.84	0.59
1:C:117:ILE:HG23	1:C:124:VAL:HG13	1.83	0.59
1:C:544:LYS:NZ	1:C:561:ASP:OD1	2.36	0.59
1:B:104:PHE:HB2	1:B:115:LEU:HB3	1.84	0.58
1:C:892:ARG:NH1	1:C:1036:LEU:O	2.35	0.58
1:C:390:LYS:HA	1:C:484:PHE:HE1	1.67	0.58
1:C:133:PHE:HA	1:C:146:TYR:HA	1.86	0.58
1:C:1040:PRO:O	1:C:1041:GLN:NE2	2.34	0.57
1:A:304:ASN:N	1:A:304:ASN:OD1	2.38	0.57
1:A:128:VAL:HB	1:A:154:PHE:HB3	1.85	0.56
1:B:314:VAL:N	1:B:518:THR:OG1	2.35	0.56
1:C:67:VAL:O	1:C:249:ALA:N	2.37	0.56
1:C:643:VAL:HG12	1:C:645:ASN:H	1.70	0.56
1:A:430:SER:O	1:A:434:GLY:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLY:HA3	1:B:490:VAL:HG12	1.86	0.56
1:A:181:LYS:HE2	1:A:190:TYR:HE1	1.71	0.56
1:A:217:VAL:HG12	1:A:219:LEU:H	1.71	0.56
1:B:568:THR:HG23	1:B:570:ASP:H	1.70	0.56
1:A:1015:LYS:NZ	1:A:1029:PHE:O	2.36	0.55
1:C:1091:VAL:HG23	1:C:1102:ILE:HG12	1.87	0.55
1:C:140:GLU:H	1:C:144:ARG:HD2	1.71	0.55
1:A:415:ASP:OD1	1:A:415:ASP:N	2.38	0.54
1:B:743:TYR:OH	1:B:985:THR:OG1	2.25	0.54
1:A:321:ASN:OD1	1:A:321:ASN:N	2.40	0.54
1:A:353:SER:HA	1:A:356:TYR:HD2	1.71	0.54
1:B:409:ASN:OD1	1:B:441:ARG:N	2.34	0.54
1:A:459:ILE:HD12	1:A:469:GLY:HA2	1.89	0.54
1:B:333:ARG:HH12	1:B:435:ASN:HB2	1.73	0.53
1:C:438:TYR:HB2	1:C:482:TYR:CE1	2.40	0.53
1:C:187:PHE:HB3	1:C:219:LEU:HB2	1.91	0.53
1:A:118:VAL:HG11	1:A:142:GLU:HB2	1.90	0.52
1:B:709:VAL:HG22	1:B:1052:VAL:HG22	1.92	0.52
1:C:127:LYS:HB3	1:C:131:PHE:HZ	1.74	0.52
1:A:126:ILE:HD12	1:A:156:TYR:HD2	1.75	0.52
1:A:889:MET:HE1	1:A:1036:LEU:HD13	1.90	0.52
1:B:110:SER:HB3	1:B:132:GLN:HB2	1.91	0.52
1:B:337:VAL:HB	1:B:409:ASN:HB3	1.91	0.51
1:C:104:PHE:O	1:C:115:LEU:N	2.42	0.51
1:A:260:ARG:NH1	1:A:277:ASP:OD2	2.38	0.51
1:C:305:PHE:HZ	1:C:602:VAL:HG21	1.75	0.51
1:A:305:PHE:CZ	1:A:602:VAL:HG21	2.43	0.51
1:C:125:VAL:HG13	1:C:157:VAL:HG22	1.93	0.51
1:A:489:GLY:N	1:C:489:GLY:O	2.43	0.51
1:A:1040:PRO:O	1:A:1041:GLN:NE2	2.38	0.51
1:B:393:GLU:OE1	1:B:482:TYR:OH	2.27	0.50
1:B:520:LEU:HD21	1:B:572:LEU:HD11	1.92	0.50
1:A:186:TYR:HB2	1:A:188:LYS:HZ2	1.77	0.50
1:A:867:GLY:O	1:A:871:SER:OG	2.24	0.50
1:B:53:ASP:OD1	1:B:54:LEU:N	2.41	0.50
1:C:812:LYS:HD2	1:C:932:LEU:HD12	1.94	0.50
1:A:381:ASN:OD1	1:C:186:TYR:OH	2.29	0.50
1:A:968:LEU:O	1:B:373:LYS:NZ	2.44	0.50
1:B:122:THR:HG22	1:B:159:GLN:HE21	1.76	0.50
1:B:372:THR:HG21	1:C:447:LYS:HE3	1.93	0.50
1:C:356:TYR:OH	1:C:371:PRO:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:ILE:HG13	1:C:1048:VAL:HG22	1.94	0.50
1:A:268:GLU:HB2	2:A:1202:NAG:H82	1.94	0.49
1:B:702:PRO:HA	1:B:1059:GLU:HA	1.93	0.49
1:B:866:ALA:O	1:B:870:THR:OG1	2.26	0.49
1:A:749:GLN:HG3	1:B:948:THR:HG21	1.93	0.49
1:B:442:LEU:HB2	1:B:480:GLN:HB2	1.94	0.49
1:B:429:ASP:HA	1:B:494:PRO:HG2	1.95	0.49
1:C:583:SER:OG	1:C:600:GLN:NE2	2.46	0.49
1:B:425:SER:OG	1:B:496:ARG:N	2.44	0.48
1:B:713:ILE:HG13	1:B:1048:VAL:HG22	1.94	0.48
1:C:118:VAL:HG23	1:C:125:VAL:HB	1.95	0.48
1:C:390:LYS:HA	1:C:484:PHE:CE1	2.46	0.48
1:A:757:ILE:HD11	1:A:999:LEU:HD23	1.95	0.48
1:C:31:SER:HA	1:C:206:LEU:HD12	1.94	0.48
1:C:471:LYS:O	1:C:475:CYS:HB2	2.14	0.48
1:A:337:VAL:HA	1:A:387:PHE:HB2	1.95	0.48
1:A:533:LEU:HD21	1:A:560:THR:HG21	1.95	0.48
1:B:913:GLN:NE2	2:B:1208:NAG:O6	2.46	0.48
1:B:1129:GLN:NE2	1:B:1133:ASP:OD2	2.47	0.48
1:B:79:ASN:N	1:B:79:ASN:HD22	2.12	0.48
1:C:110:SER:HB2	1:C:150:LYS:HD2	1.96	0.48
1:A:465:ASN:HD22	1:A:465:ASN:H	1.61	0.48
1:B:396:GLN:HB3	1:B:406:ALA:HB2	1.96	0.48
1:B:881:LEU:HD13	1:C:702:PRO:HD3	1.95	0.48
1:C:130:GLU:HB2	1:C:150:LYS:HB2	1.95	0.48
1:C:380:THR:HB	1:C:503:GLU:HB2	1.95	0.47
1:B:219:LEU:HD22	1:B:221:ILE:HG22	1.96	0.47
1:C:789:PHE:HD1	1:C:792:ILE:HD11	1.80	0.47
1:A:723:VAL:HG22	1:A:845:LEU:HD22	1.96	0.47
1:B:380:THR:HG21	1:B:506:HIS:HB2	1.96	0.47
1:A:1129:GLN:HB3	1:A:1130:PRO:HD3	1.96	0.47
1:B:396:GLN:HB2	1:B:405:ILE:HD11	1.96	0.47
1:C:340:TRP:H	1:C:340:TRP:CD1	2.33	0.47
1:A:274:ASP:OD1	1:A:275:ALA:N	2.47	0.47
1:A:881:LEU:HD13	1:B:702:PRO:HD3	1.96	0.47
1:C:134:ASN:ND2	1:C:144:ARG:O	2.48	0.47
1:C:331:ALA:HB3	1:C:334:PHE:HE1	1.80	0.47
1:C:516:ASN:OD1	1:C:516:ASN:N	2.49	0.47
1:B:441:ARG:HG2	1:B:479:LEU:HD23	1.97	0.46
1:A:937:ASP:O	1:A:941:HIS:ND1	2.46	0.46
1:C:274:ASP:OD1	1:C:275:ALA:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ASN:ND2	1:C:330:ASN:O	2.48	0.46
1:A:176:ARG:HB3	1:A:178:PHE:HE2	1.80	0.46
1:A:455:ILE:HD13	1:A:455:ILE:H	1.79	0.46
1:B:430:SER:HB2	1:B:436:TYR:HA	1.98	0.46
1:C:696:ASN:OD1	1:C:696:ASN:N	2.47	0.46
1:A:970:ARG:CZ	1:B:504:LEU:HD13	2.45	0.46
1:B:179:VAL:HG13	1:B:257:LEU:HD11	1.98	0.46
1:C:93:ILE:HG12	1:C:175:LEU:HD13	1.98	0.46
1:C:104:PHE:HB3	1:C:225:ILE:HD13	1.97	0.46
1:A:855:GLU:N	1:A:855:GLU:OE1	2.49	0.46
1:B:418:GLY:HA2	1:B:502:PHE:CD2	2.51	0.46
1:A:972:ASP:OD1	1:A:972:ASP:N	2.41	0.46
1:C:281:ASP:OD1	1:C:281:ASP:N	2.46	0.45
1:C:709:VAL:HG22	1:C:1052:VAL:HG22	1.98	0.45
1:B:295:VAL:HB	1:B:589:THR:HG23	1.97	0.45
1:B:723:VAL:HG22	1:B:845:LEU:HD23	1.97	0.45
1:A:136:LYS:HD3	1:A:138:TRP:CZ3	2.51	0.45
1:B:742:GLN:HE21	1:C:956:LYS:HB2	1.82	0.45
1:A:179:VAL:HG13	1:A:257:LEU:HD11	1.98	0.45
1:C:221:ILE:H	1:C:221:ILE:HG13	1.53	0.44
1:C:1129:GLN:HB3	1:C:1130:PRO:HD3	1.99	0.44
1:C:139:MET:HG2	1:C:145:VAL:HG22	1.98	0.44
1:C:305:PHE:CZ	1:C:602:VAL:HG21	2.52	0.44
1:C:724:ASP:HB3	1:C:727:MET:HB3	2.00	0.44
1:A:705:PHE:CE1	1:A:910:ILE:HG12	2.53	0.44
1:A:181:LYS:HE2	1:A:190:TYR:CE1	2.51	0.44
1:A:381:ASN:HB2	1:A:503:GLU:HG3	1.99	0.44
1:A:94:GLU:HG2	1:A:250:ALA:HB1	1.99	0.44
1:A:396:GLN:HE22	1:A:405:ILE:H	1.64	0.44
1:B:281:ASP:N	1:B:281:ASP:OD1	2.51	0.44
1:B:523:ASN:N	1:B:523:ASN:OD1	2.51	0.44
1:A:709:VAL:HG22	1:A:1052:VAL:HG22	1.99	0.44
1:A:175:LEU:HG	1:A:177:GLU:HG3	2.00	0.44
1:B:413:PRO:HG2	1:B:416:PHE:HB3	2.00	0.44
1:B:1093:GLN:HG3	1:B:1096:PHE:O	2.18	0.44
1:B:305:PHE:CE1	1:B:602:VAL:HG21	2.54	0.43
1:B:316:PHE:O	1:B:567:GLN:NE2	2.52	0.43
1:B:321:ASN:ND2	1:B:347:ASN:O	2.41	0.43
1:C:702:PRO:HA	1:C:1059:GLU:HA	2.01	0.43
1:C:771:GLN:HG3	1:C:1016:MET:HG2	1.99	0.43
1:B:443:PHE:HZ	1:B:476:TYR:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLY:HA2	1:A:394:VAL:HG23	1.99	0.43
1:B:448:LEU:HD22	1:B:452:GLU:HB3	2.00	0.43
1:C:126:ILE:HD12	1:C:219:LEU:HD11	2.00	0.43
1:B:327:GLU:OE1	1:B:327:GLU:N	2.50	0.43
1:C:663:THR:HB	1:C:677:GLN:HG2	2.00	0.43
1:C:391:GLY:HA2	1:C:394:VAL:HG23	2.00	0.43
1:A:133:PHE:HA	1:A:146:TYR:HA	2.01	0.43
1:A:702:PRO:HA	1:A:1059:GLU:HA	2.00	0.43
1:B:406:ALA:O	1:B:411:LYS:HD3	2.19	0.43
1:A:366:CYS:HA	1:A:419:CYS:HA	2.00	0.42
1:B:865:LEU:HD11	1:B:1041:GLN:HE22	1.83	0.42
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.80	0.42
1:C:185:GLY:HA2	1:C:222:GLY:HA2	2.01	0.42
1:A:724:ASP:HB3	1:A:727:MET:HB3	2.01	0.42
1:B:809:LEU:HD21	1:B:925:LEU:HD13	2.02	0.42
1:B:826:ASP:OD1	1:B:842:PHE:HB2	2.19	0.42
1:B:867:GLY:O	1:B:871:SER:OG	2.31	0.42
1:C:585:ILE:HB	1:C:596:ALA:HB3	2.02	0.42
1:A:583:SER:OG	1:A:600:GLN:OE1	2.36	0.42
1:A:773:LYS:H	1:A:773:LYS:HG3	1.60	0.42
1:A:841:LYS:HB2	1:B:579:PHE:CZ	2.55	0.42
1:B:757:ILE:HD11	1:B:999:LEU:HD23	2.02	0.42
1:A:576:PRO:HG2	1:C:842:PHE:CG	2.55	0.42
1:B:515:LYS:HE2	1:B:515:LYS:HB3	1.93	0.42
1:C:124:VAL:HB	1:C:158:PHE:CE1	2.55	0.42
1:A:389:ILE:HD11	1:A:497:VAL:HG21	2.02	0.42
1:A:892:ARG:NH1	1:A:1036:LEU:O	2.50	0.42
1:C:520:LEU:HD21	1:C:572:LEU:HD11	2.01	0.42
1:A:431:LYS:HG3	1:A:486:PRO:HD2	2.02	0.41
1:B:274:ASP:HB3	1:B:293:PHE:HE2	1.86	0.41
1:C:441:ARG:NH2	1:C:454:ASP:O	2.48	0.41
1:A:973:PRO:N	1:A:974:PRO:HD2	2.36	0.41
1:A:890:ALA:HB1	1:A:900:GLN:HB2	2.02	0.41
1:A:865:LEU:HD21	1:A:1039:PHE:HB3	2.02	0.41
1:C:433:ASP:OD1	1:C:433:ASP:N	2.53	0.41
1:C:867:GLY:O	1:C:871:SER:OG	2.29	0.41
1:A:705:PHE:HE1	1:A:910:ILE:HG12	1.86	0.41
1:C:366:CYS:HA	1:C:419:CYS:HA	2.03	0.41
1:C:736:CYS:HB2	1:C:964:LEU:HD21	2.03	0.41
1:C:887:MET:HE2	1:C:887:MET:HB3	1.90	0.41
1:A:1025:LYS:HE3	1:A:1025:LYS:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:828:LEU:HD21	1:B:840:GLN:HE21	1.85	0.41
1:C:973:PRO:N	1:C:974:PRO:HD2	2.36	0.41
1:A:282:PRO:HB2	1:A:595:VAL:HG21	2.02	0.41
1:B:221:ILE:HD12	1:B:221:ILE:HA	1.97	0.41
1:B:892:ARG:NH1	1:B:1036:LEU:O	2.52	0.41
1:C:90:PHE:O	1:C:178:PHE:N	2.48	0.41
1:C:131:PHE:HB2	1:C:133:PHE:CZ	2.56	0.41
1:B:192:LYS:HB3	1:B:213:LEU:HD22	2.02	0.40
1:B:358:PHE:HB2	1:B:361:PHE:CE1	2.56	0.40
1:A:281:ASP:OD1	1:A:281:ASP:N	2.53	0.40
1:A:490:VAL:HG21	1:B:392:ASN:CG	2.46	0.40
1:A:1077:PRO:HD3	1:A:1082:PHE:CE2	2.56	0.40
1:C:889:MET:HE1	1:C:1036:LEU:HD13	2.03	0.40
1:A:44:ARG:O	1:A:270:GLY:HA2	2.22	0.40
1:A:143:SER:HA	1:A:146:TYR:CE2	2.56	0.40
1:C:34:ARG:HD2	1:C:177:GLU:OE2	2.21	0.40
1:C:381:ASN:HB3	1:C:503:GLU:HG3	2.03	0.40
1:C:607:VAL:HG11	1:C:638:ILE:HD11	2.03	0.40
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.57	0.40
1:A:841:LYS:HE3	1:B:578:SER:HA	2.04	0.40
1:A:1017:SER:HB3	1:B:1028:ASP:HB2	2.04	0.40
1:B:542:SER:HB3	1:B:571:ILE:HG13	2.03	0.40
1:B:1022:GLY:HA3	1:C:1027:VAL:HG21	2.03	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	983/1144 (86%)	962 (98%)	21 (2%)	0	100	100
1	B	1026/1144 (90%)	994 (97%)	32 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1007/1144 (88%)	984 (98%)	23 (2%)	0	100	100
All	All	3016/3432 (88%)	2940 (98%)	76 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	880/1000 (88%)	866 (98%)	14 (2%)	55	83
1	B	911/1000 (91%)	892 (98%)	19 (2%)	47	79
1	C	899/1000 (90%)	883 (98%)	16 (2%)	51	82
All	All	2690/3000 (90%)	2641 (98%)	49 (2%)	51	82

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	LYS
1	A	219	LEU
1	A	304	ASN
1	A	321	ASN
1	A	325	PHE
1	A	455	ILE
1	A	476	TYR
1	A	534	THR
1	A	772	VAL
1	A	842	PHE
1	A	843	ASN
1	A	903	LEU
1	A	952	GLN
1	A	1091	VAL
1	B	79	ASN
1	B	188	LYS
1	B	214	GLU

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Mol	Chain	Res	Type
1	B	337	VAL
1	B	397	ILE
1	B	412	LEU
1	B	416	PHE
1	B	436	TYR
1	B	443	PHE
1	B	482	TYR
1	B	523	ASN
1	B	551	GLN
1	B	632	THR
1	B	663	THR
1	B	772	VAL
1	B	836	LEU
1	B	838	CYS
1	B	903	LEU
1	B	1091	VAL
1	C	66	HIS
1	C	79	ASN
1	C	217	VAL
1	C	221	ILE
1	C	228	PHE
1	C	365	LYS
1	C	482	TYR
1	C	493	GLN
1	C	516	ASN
1	C	628	LYS
1	C	650	ASP
1	C	696	ASN
1	C	807	ASP
1	C	845	LEU
1	C	903	LEU
1	C	972	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	182	ASN
1	A	396	GLN
1	A	465	ASN
1	A	474	ASN
1	A	594	GLN

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Mol	Chain	Res	Type
1	A	749	GLN
1	A	761	GLN
1	A	952	GLN
1	A	1070	HIS
1	A	1075	HIS
1	B	113	GLN
1	B	159	GLN
1	B	229	GLN
1	B	401	GLN
1	B	506	HIS
1	B	531	ASN
1	B	594	GLN
1	B	615	GLN
1	B	631	GLN
1	B	664	GLN
1	B	742	GLN
1	B	766	GLN
1	B	774	GLN
1	B	840	GLN
1	B	913	GLN
1	B	989	GLN
1	C	49	HIS
1	C	66	HIS
1	C	119	ASN
1	C	174	ASN
1	C	182	ASN
1	C	404	ASN
1	C	426	ASN
1	C	749	GLN
1	C	894	ASN
1	C	900	GLN
1	C	989	GLN
1	C	1075	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	C	1204	1	14,14,15	0.76	0	17,19,21	1.00	1 (5%)
2	NAG	B	1201	1	14,14,15	0.73	0	17,19,21	2.28	3 (17%)
2	NAG	C	1202	1	14,14,15	0.74	0	17,19,21	1.00	1 (5%)
2	NAG	C	1203	1	14,14,15	0.76	0	17,19,21	0.91	0
2	NAG	A	1208	1	14,14,15	0.71	0	17,19,21	1.36	1 (5%)
2	NAG	C	1207	1	14,14,15	0.70	0	17,19,21	1.15	1 (5%)
2	NAG	B	1202	1	14,14,15	0.69	0	17,19,21	1.16	1 (5%)
2	NAG	C	1205	1	14,14,15	0.73	0	17,19,21	0.92	0
2	NAG	B	1203	1	14,14,15	0.73	0	17,19,21	0.81	0
2	NAG	B	1207	1	14,14,15	0.73	0	17,19,21	0.85	0
2	NAG	A	1207	1	14,14,15	0.75	0	17,19,21	0.91	0
2	NAG	A	1204	1	14,14,15	0.77	0	17,19,21	0.89	0
2	NAG	A	1206	1	14,14,15	0.72	0	17,19,21	0.93	0
2	NAG	B	1208	1	14,14,15	0.74	0	17,19,21	0.91	0
2	NAG	B	1204	1	14,14,15	0.78	0	17,19,21	0.85	0
2	NAG	C	1201	1	14,14,15	0.69	0	17,19,21	1.19	1 (5%)
2	NAG	C	1206	1	14,14,15	0.74	0	17,19,21	0.87	0
2	NAG	A	1201	1	14,14,15	0.72	0	17,19,21	0.77	0
2	NAG	A	1205	1	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
2	NAG	A	1202	1	14,14,15	0.71	0	17,19,21	0.81	0
2	NAG	B	1206	1	14,14,15	0.72	0	17,19,21	0.89	0
2	NAG	A	1203	1	14,14,15	0.77	0	17,19,21	1.12	1 (5%)
2	NAG	C	1208	1	14,14,15	0.71	0	17,19,21	1.31	2 (11%)
2	NAG	B	1205	1	14,14,15	0.76	0	17,19,21	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1204	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1201	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1202	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1203	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1208	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1207	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1202	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1203	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1207	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1207	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1204	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1204	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1201	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1205	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1202	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1206	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1208	1	-	1/6/23/26	0/1/1/1
2	NAG	B	1205	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	NAG	C2-N2-C7	8.06	134.38	122.90
2	A	1208	NAG	C2-N2-C7	4.05	128.68	122.90
2	C	1201	NAG	C2-N2-C7	3.17	127.41	122.90
2	B	1202	NAG	C2-N2-C7	3.13	127.36	122.90
2	C	1208	NAG	C2-N2-C7	3.11	127.33	122.90
2	A	1203	NAG	C2-N2-C7	3.02	127.20	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1207	NAG	C2-N2-C7	2.97	127.14	122.90
2	B	1201	NAG	C8-C7-N2	2.50	120.34	116.10
2	C	1202	NAG	C2-N2-C7	2.44	126.38	122.90
2	C	1204	NAG	C2-N2-C7	2.22	126.07	122.90
2	B	1201	NAG	C1-C2-N2	2.16	114.17	110.49
2	C	1208	NAG	C1-O5-C5	2.09	115.02	112.19
2	A	1205	NAG	C2-N2-C7	2.08	125.87	122.90

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1205	NAG	C4-C5-C6-O6
2	A	1205	NAG	O5-C5-C6-O6
2	A	1203	NAG	C1-C2-N2-C7
2	A	1205	NAG	C8-C7-N2-C2
2	A	1205	NAG	O7-C7-N2-C2
2	A	1206	NAG	C8-C7-N2-C2
2	A	1206	NAG	O7-C7-N2-C2
2	A	1207	NAG	C8-C7-N2-C2
2	A	1207	NAG	O7-C7-N2-C2
2	B	1201	NAG	C8-C7-N2-C2
2	B	1201	NAG	O7-C7-N2-C2
2	B	1205	NAG	C8-C7-N2-C2
2	B	1205	NAG	O7-C7-N2-C2
2	B	1206	NAG	C8-C7-N2-C2
2	B	1206	NAG	O7-C7-N2-C2
2	B	1207	NAG	C8-C7-N2-C2
2	B	1207	NAG	O7-C7-N2-C2
2	B	1208	NAG	C8-C7-N2-C2
2	B	1208	NAG	O7-C7-N2-C2
2	C	1204	NAG	C8-C7-N2-C2
2	C	1204	NAG	O7-C7-N2-C2
2	C	1205	NAG	C8-C7-N2-C2
2	C	1205	NAG	O7-C7-N2-C2
2	C	1206	NAG	C8-C7-N2-C2
2	C	1206	NAG	O7-C7-N2-C2
2	C	1202	NAG	C1-C2-N2-C7
2	A	1208	NAG	C1-C2-N2-C7
2	B	1201	NAG	O5-C5-C6-O6
2	B	1202	NAG	O5-C5-C6-O6
2	A	1202	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	1203	NAG	C3-C2-N2-C7
2	B	1202	NAG	C3-C2-N2-C7
2	C	1208	NAG	C3-C2-N2-C7
2	B	1202	NAG	C1-C2-N2-C7
2	B	1203	NAG	C1-C2-N2-C7
2	B	1201	NAG	C3-C2-N2-C7
2	C	1201	NAG	C3-C2-N2-C7
2	C	1202	NAG	C3-C2-N2-C7
2	C	1207	NAG	C3-C2-N2-C7
2	C	1201	NAG	C1-C2-N2-C7
2	C	1207	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1208	NAG	1	0
2	A	1201	NAG	1	0
2	A	1202	NAG	1	0

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.

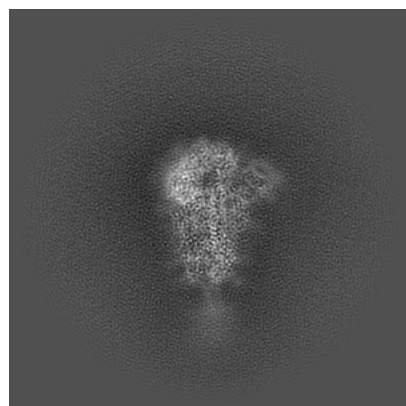
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57358. These allow visual inspection of the internal detail of the map and identification of artifacts.

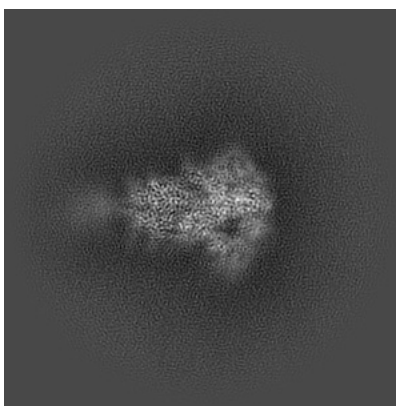
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

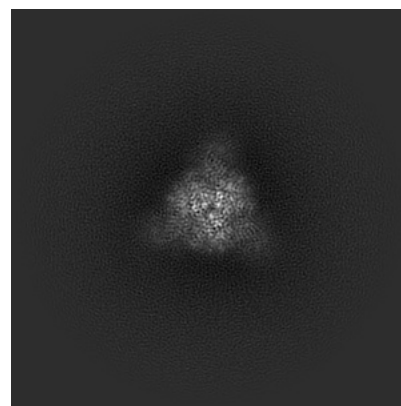
6.1.1 Primary map



X

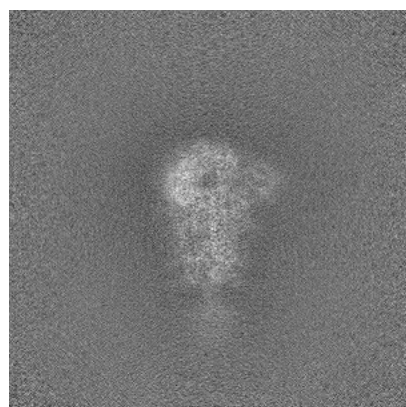


Y

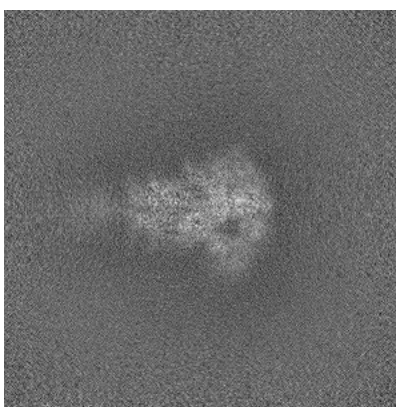


Z

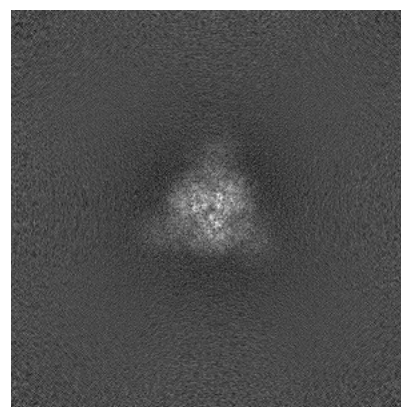
6.1.2 Raw map



X



Y

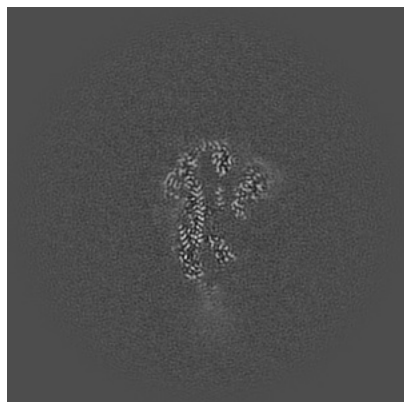


Z

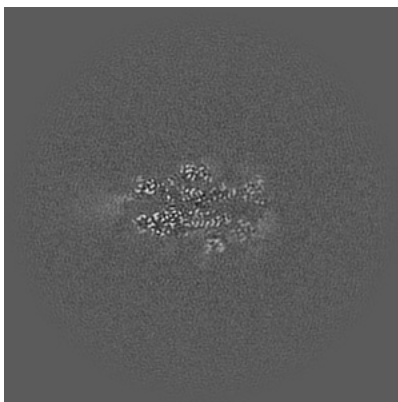
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

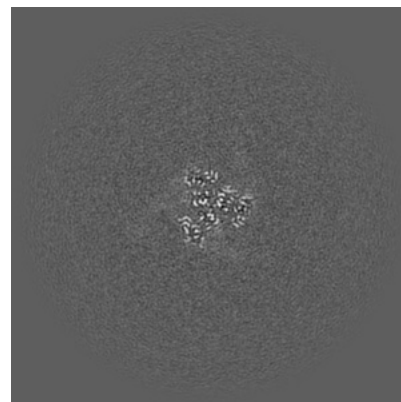
6.2.1 Primary map



X Index: 280

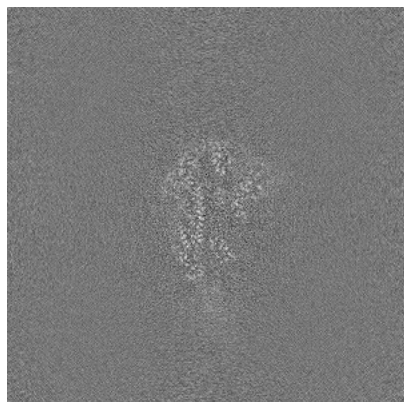


Y Index: 280

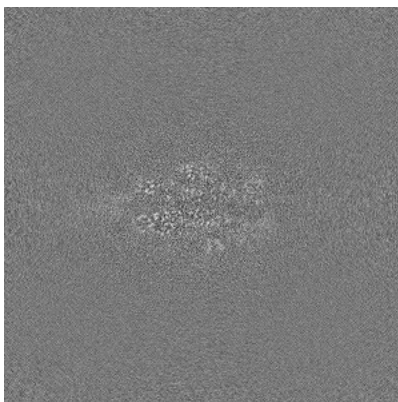


Z Index: 280

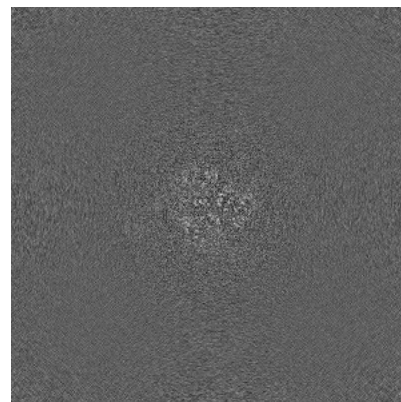
6.2.2 Raw map



X Index: 280



Y Index: 280

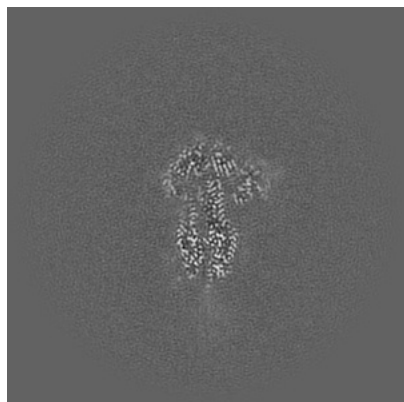


Z Index: 280

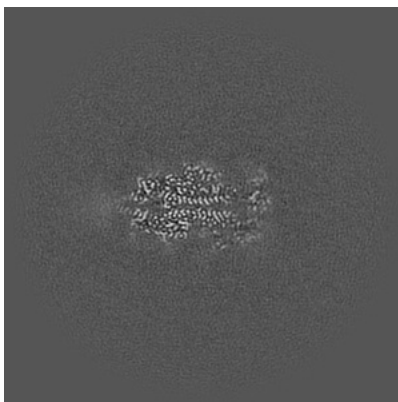
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

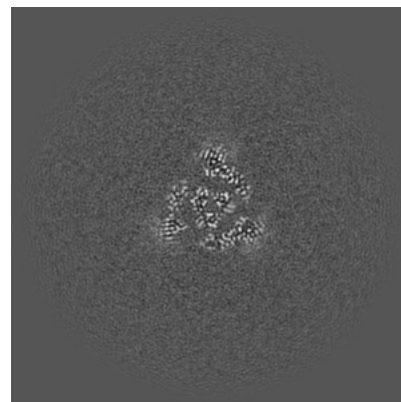
6.3.1 Primary map



X Index: 294

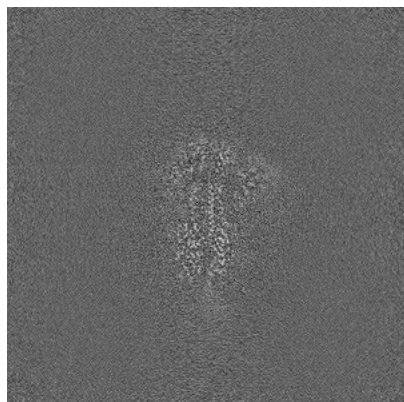


Y Index: 287

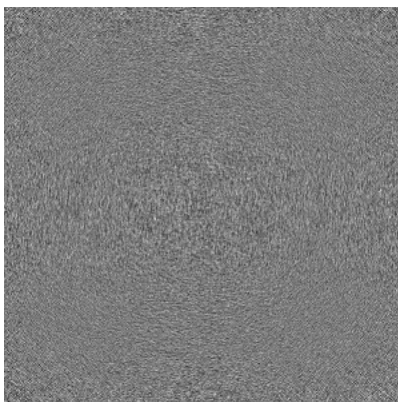


Z Index: 307

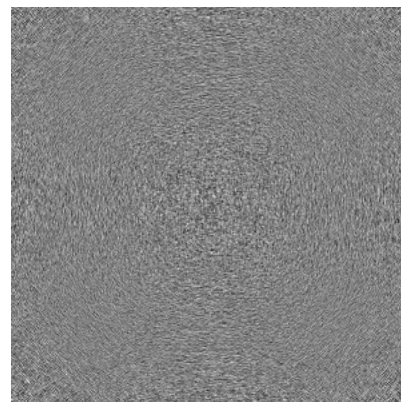
6.3.2 Raw map



X Index: 289



Y Index: 0

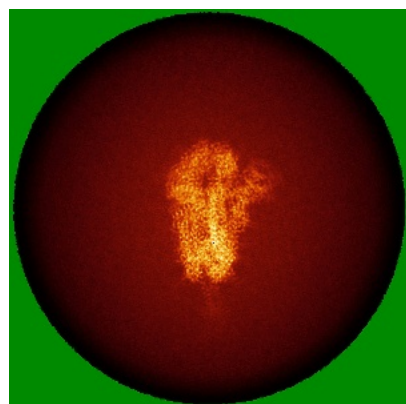


Z Index: 0

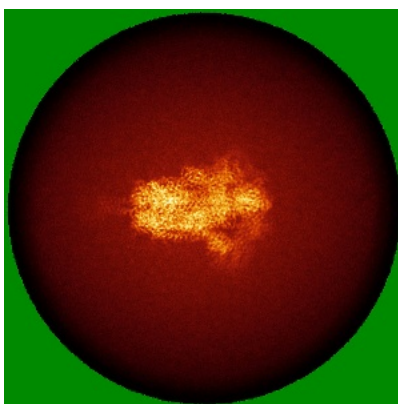
The images above show the largest variance slices of the map in three orthogonal directions.

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

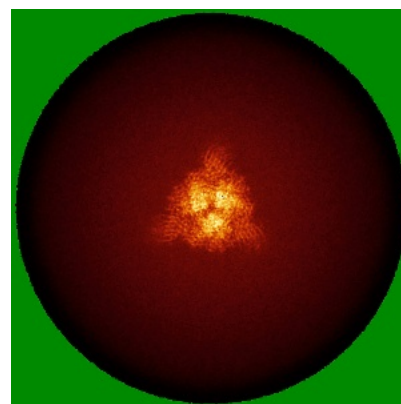
6.4.1 Primary map



X

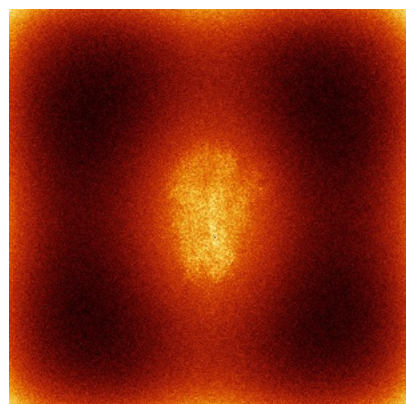


Y

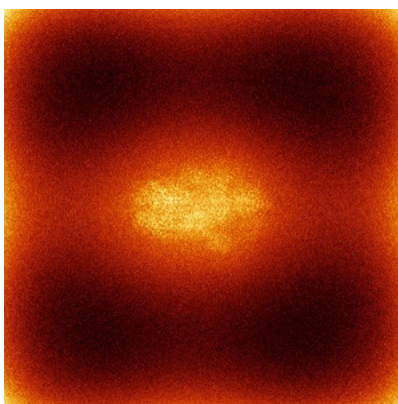


Z

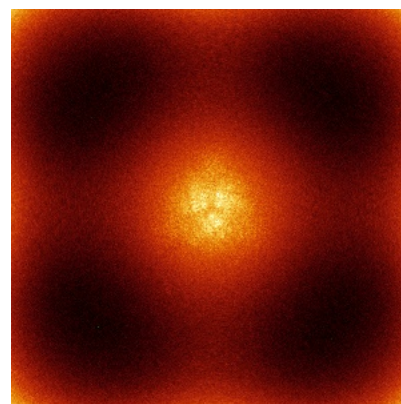
6.4.2 Raw map



X



Y

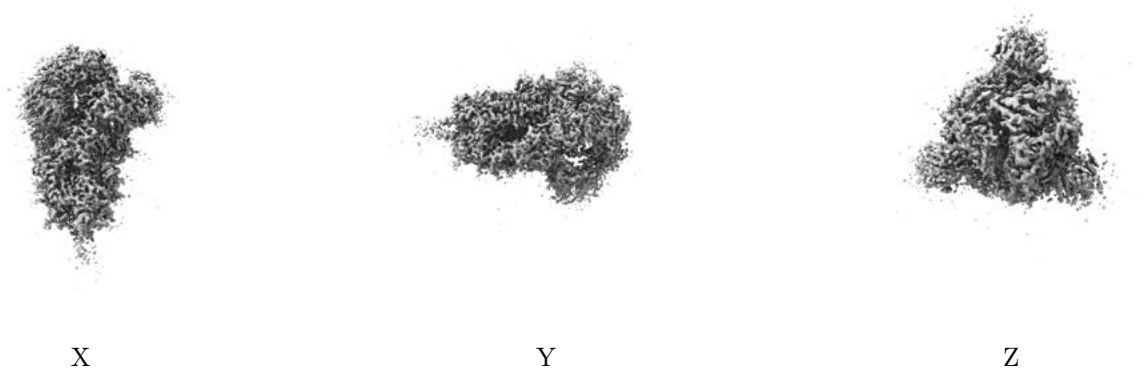


Z

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.

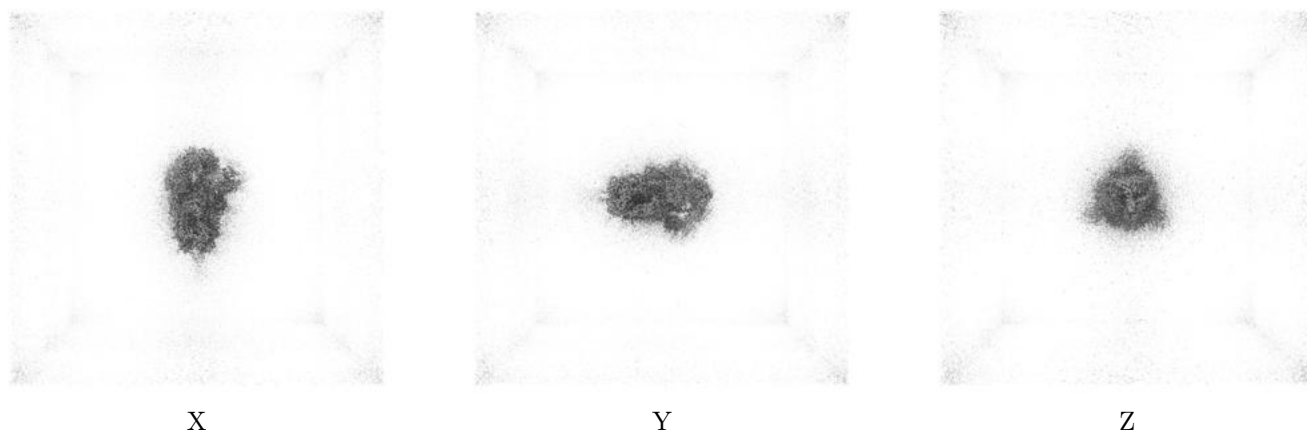
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.125. 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.

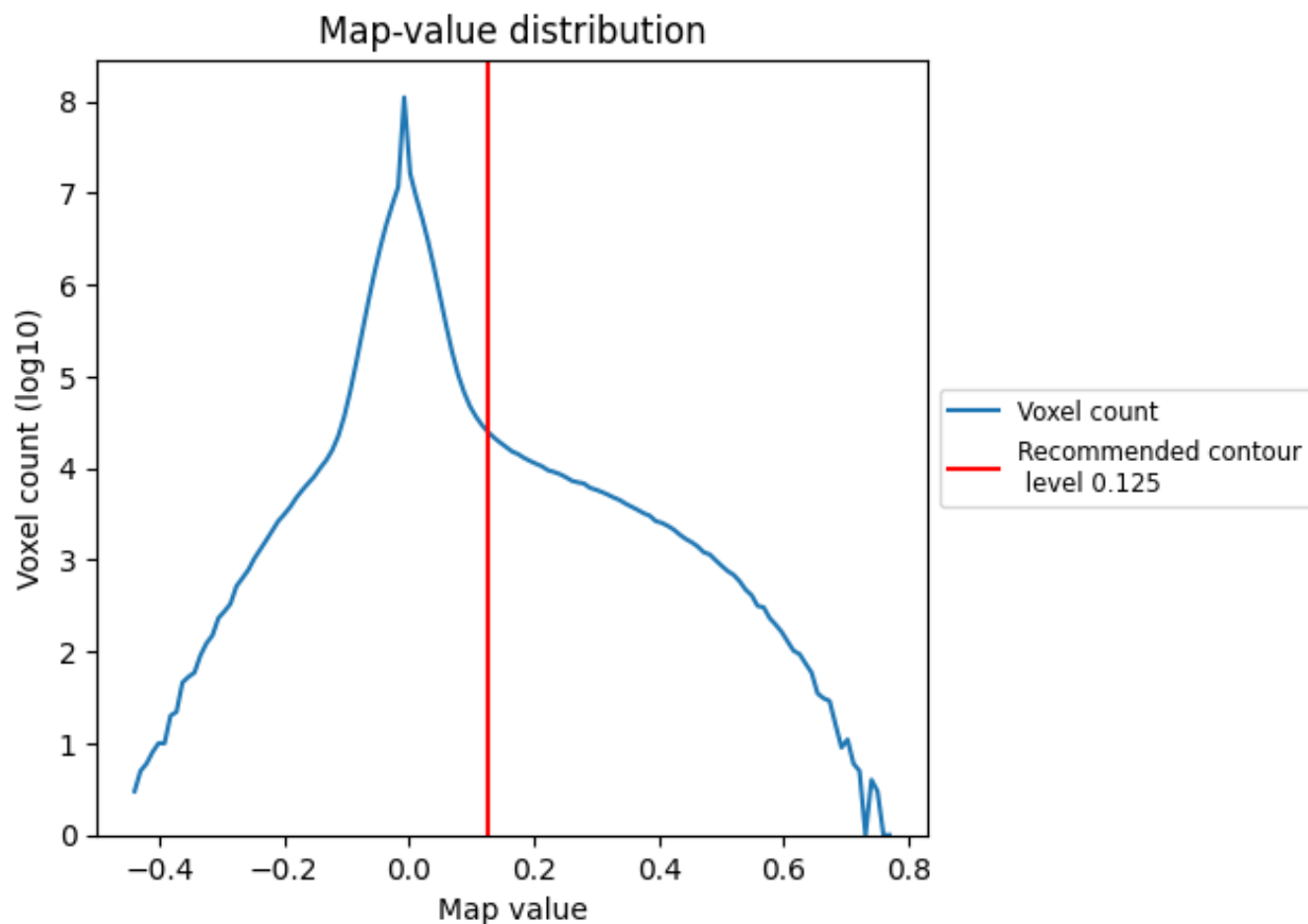
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

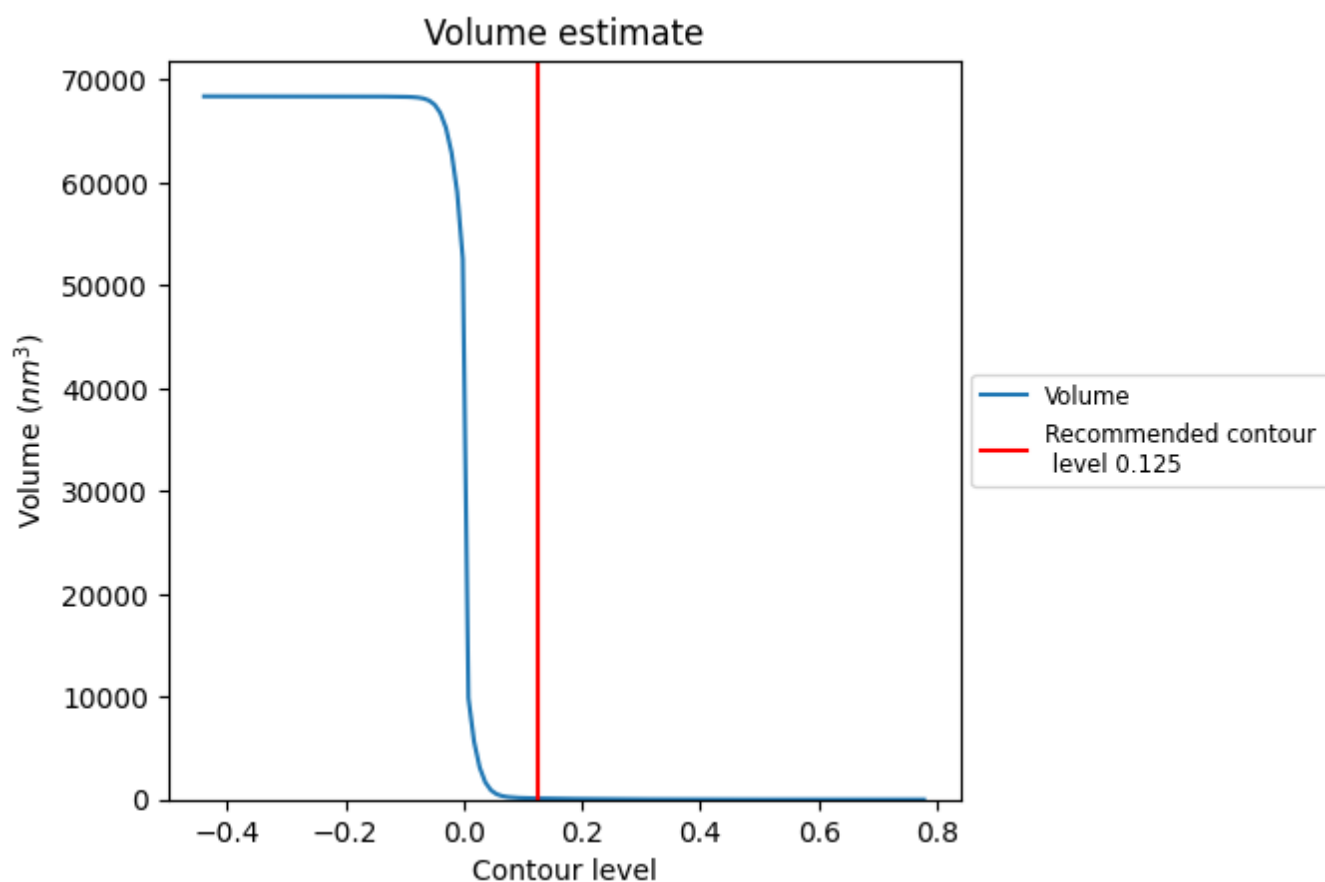
This section contains the results of statistical analysis of the map.

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.

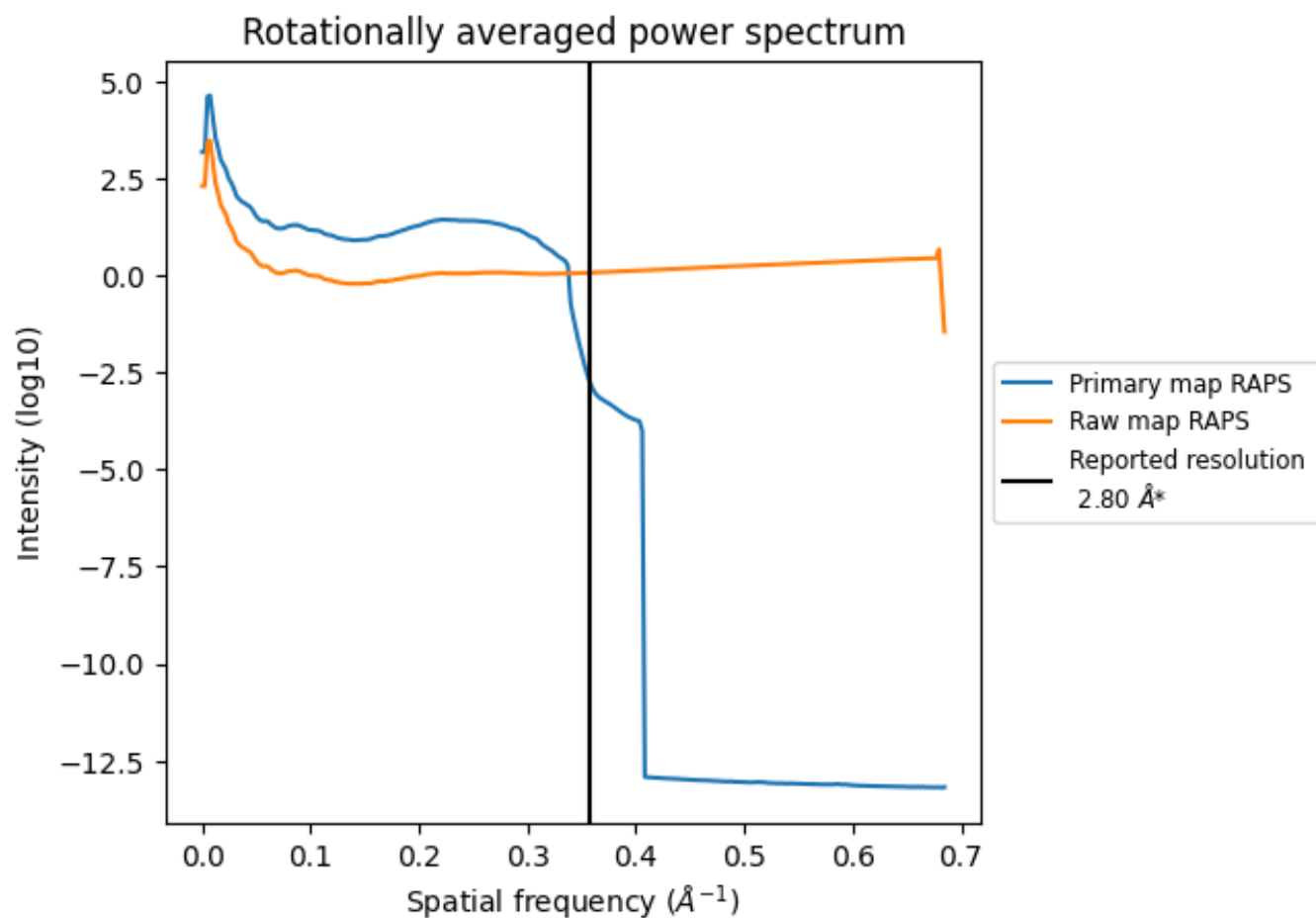
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 114 nm³; this corresponds to an approximate mass of 103 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

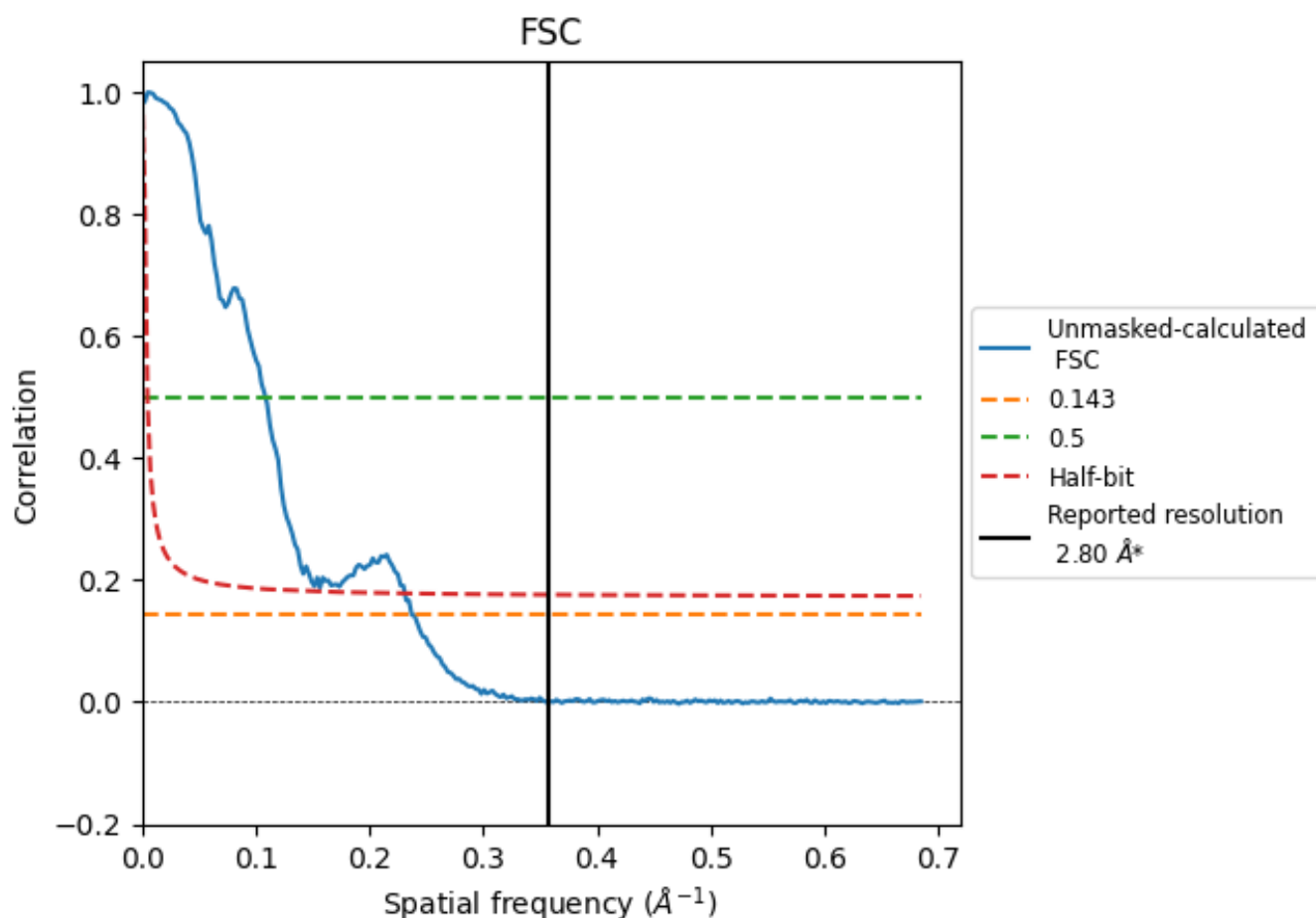


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

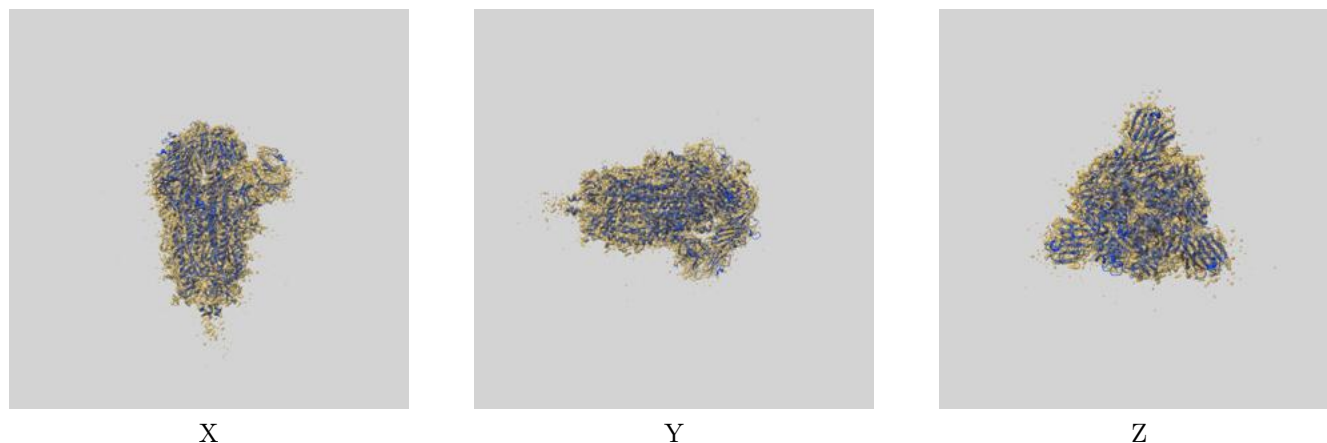
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.22	9.22	4.33

*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 4.22 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

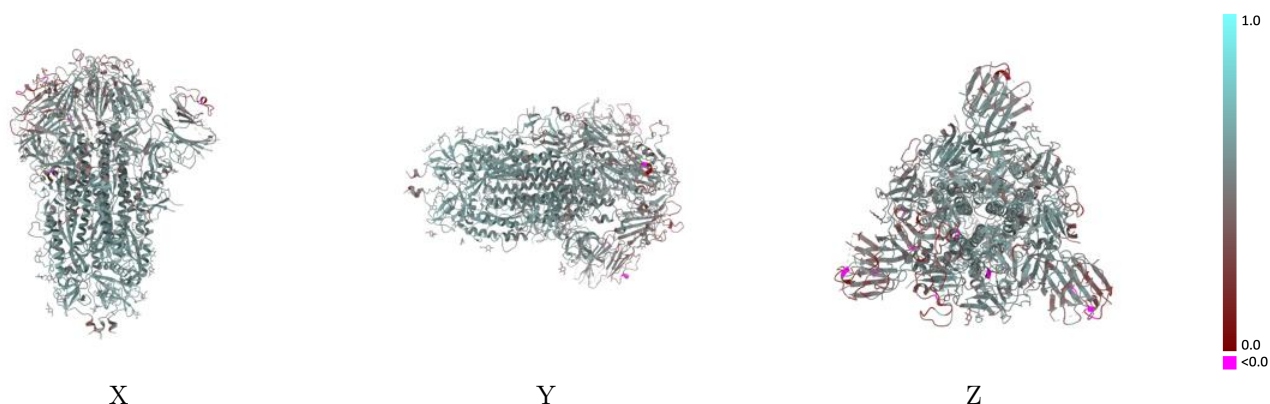
This section contains information regarding the fit between EMDB map EMD-57358 and PDB model 29SU. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



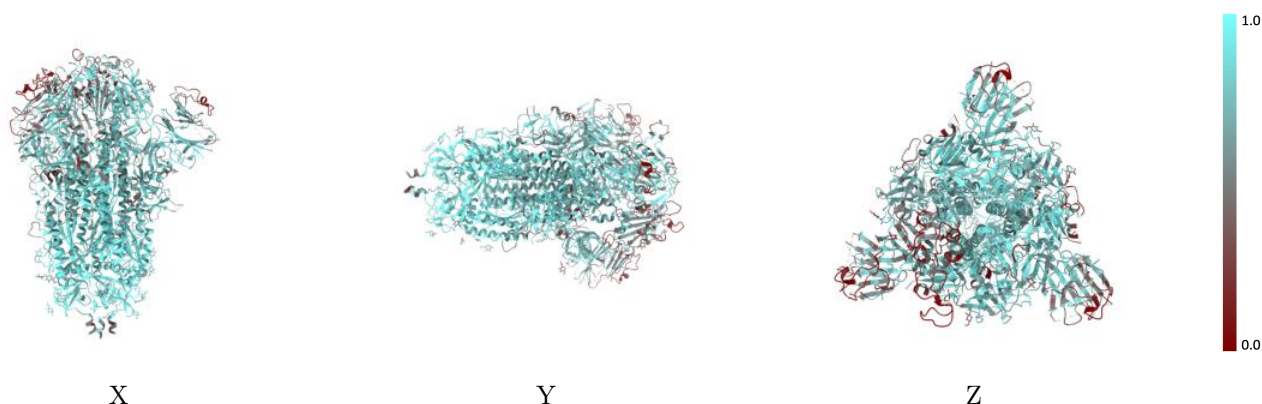
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



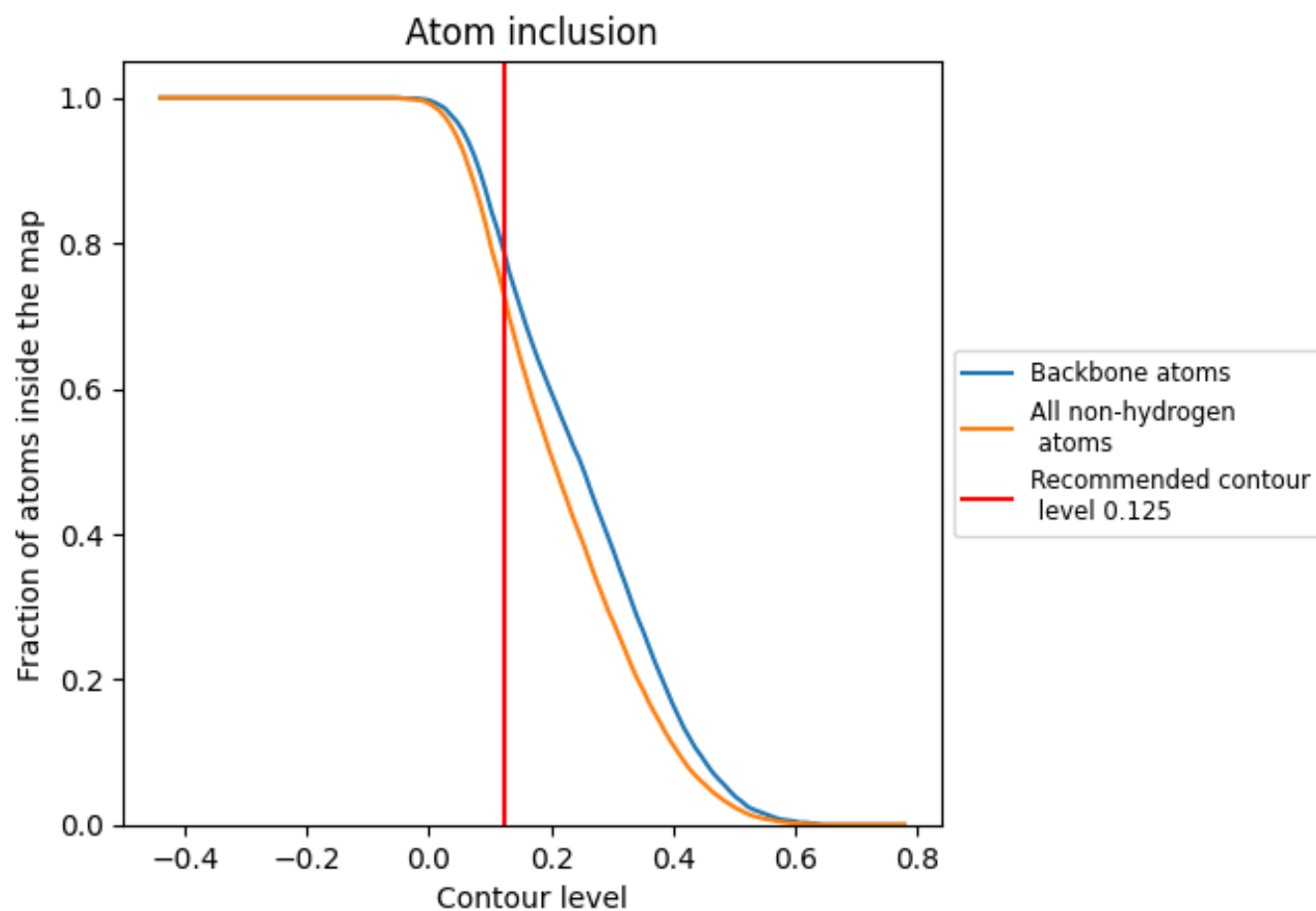
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7220	0.5220
A	0.7370	0.5270
B	0.6830	0.5110
C	0.7470	0.5270

