



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 05:33 AM UTC

PDB ID : 7V2A / pdb_00007v2a
EMDB ID : EMD-31639
Title : SARS-CoV-2 Spike trimer in complex with XG014 Fab
Authors : Wang, K.; Wang, X.; Pan, L.
Deposited on : 2021-08-07
Resolution : 3.40 Å (reported)
Based on initial models : 6PZE, 6Z3P, 6VXX

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

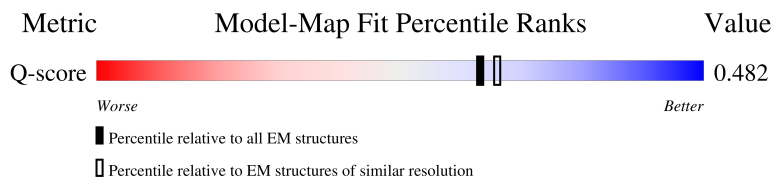
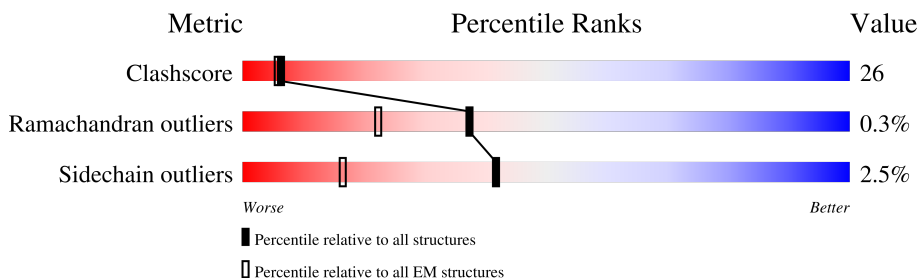
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1208	
1	B	1208	
1	C	1208	
2	D	216	

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Mol	Chain	Length	Quality of chain
2	F	216	
2	H	216	
3	E	237	
3	G	237	
3	I	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28017 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	988	Total	C	N	O	S	0	0
			7464	4774	1240	1416	34		
1	B	988	Total	C	N	O	S	0	0
			7464	4774	1240	1416	34		
1	C	988	Total	C	N	O	S	0	0
			7464	4774	1240	1416	34		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called The light chain of XG014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	111	Total	C	N	O	S	0	0
			799	496	139	162	2		
2	F	111	Total	C	N	O	S	0	0
			799	496	139	162	2		

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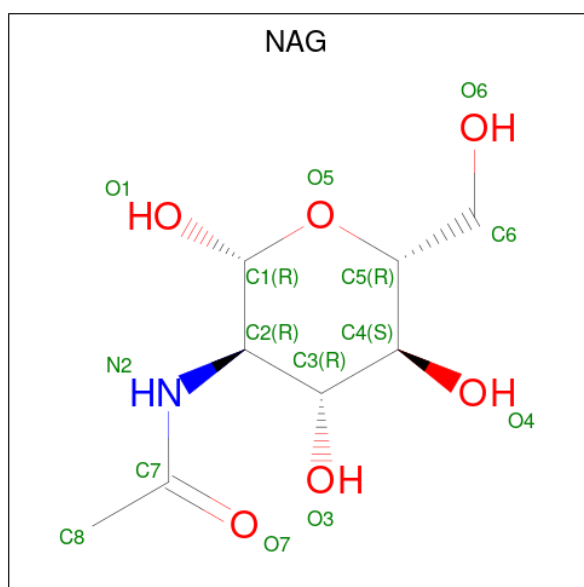
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	111	Total	C	N	O	S	0	0
			799	496	139	162	2		

- Molecule 3 is a protein called The heavy chain of XG014.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	120	Total	C	N	O	S	0	0
			964	623	153	183	5		
3	G	120	Total	C	N	O	S	0	0
			964	623	153	183	5		
3	I	120	Total	C	N	O	S	0	0
			964	623	153	183	5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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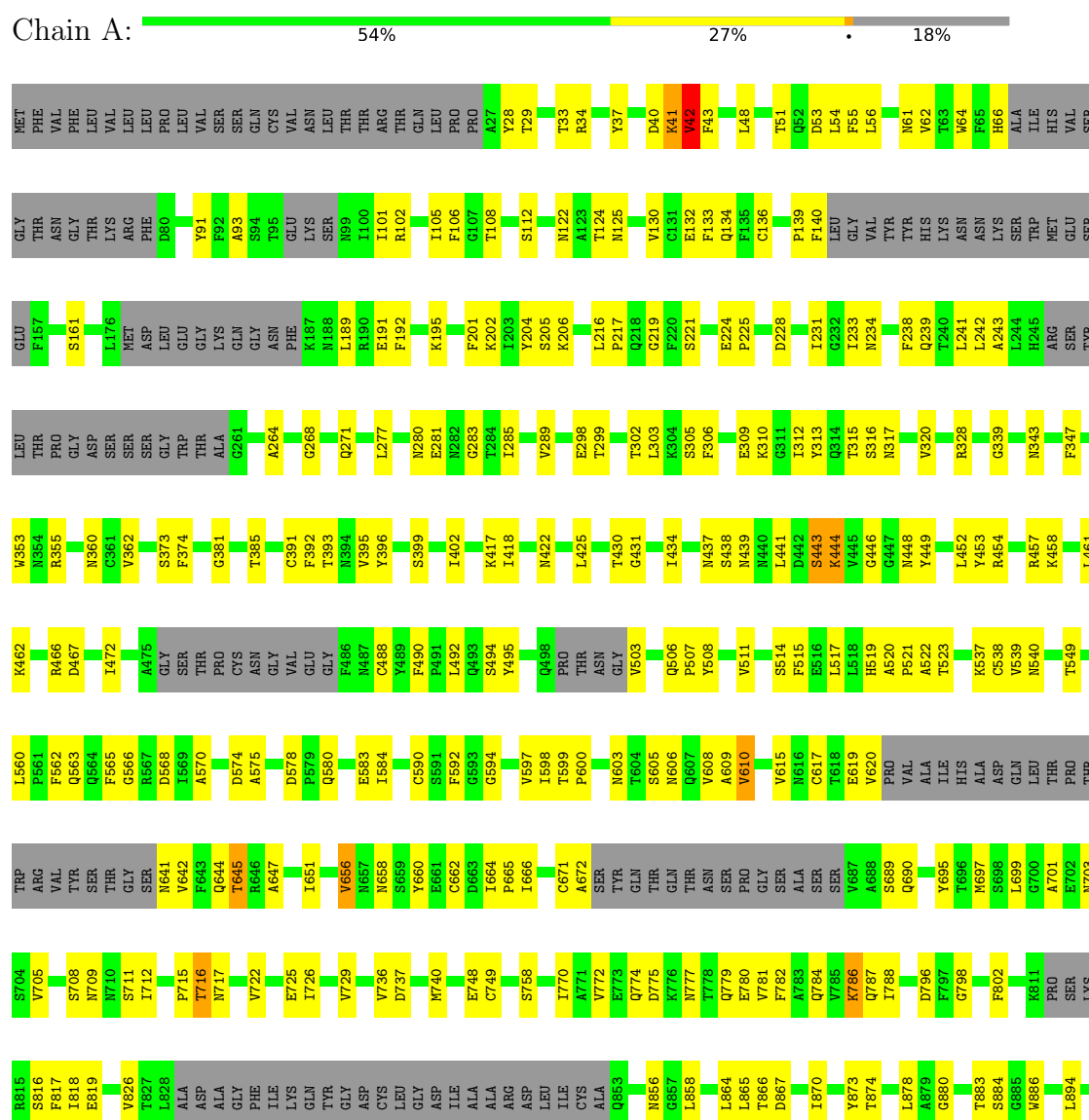
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Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total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

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



P897	E1031	M1135	GLN
F898	G1035	T1136	GLU
A899	Q1036	E1144	LEU
N900	Q1037	L1145	GLY
Q901	K1038	D1146	LYS
M902	R1039	SER	TYR
N903	V1040	PHE	GLU
Y904	D1041	LYS	GLN
R905	F1042	GLU	
		GLU	
		GLU	
		LEU	
		ASP	
		ASP	
		LYS	
		TYR	
		PHE	
		GLY	
		LYS	
		ASN	
		HIS	
		THR	
		SER	
		PRO	
		ASP	
		VAL	
		ASP	
		LEU	
		GLY	
		ASP	
		ILE	
		ILE	
		SER	
		GLY	
		ILE	
		ASN	
		ALA	
		ALA	
		SER	
		F1087	
		H1088	
		VAL	
		VAL	
		ASN	
		TLE	
		GLN	
		LYS	
		GLU	
		ILE	
		ASP	
		ARG	
		LEU	
		ASN	
		GLU	
		VAL	
		ALA	
		LYS	
		ASN	
		LEU	
		ALA	
		ASN	
		GLU	
		SER	
		ILE	
		TLE	
		ASP	
		N1134	

• Molecule 1: Spike glycoprotein

Chain B:  54% 27% 18%

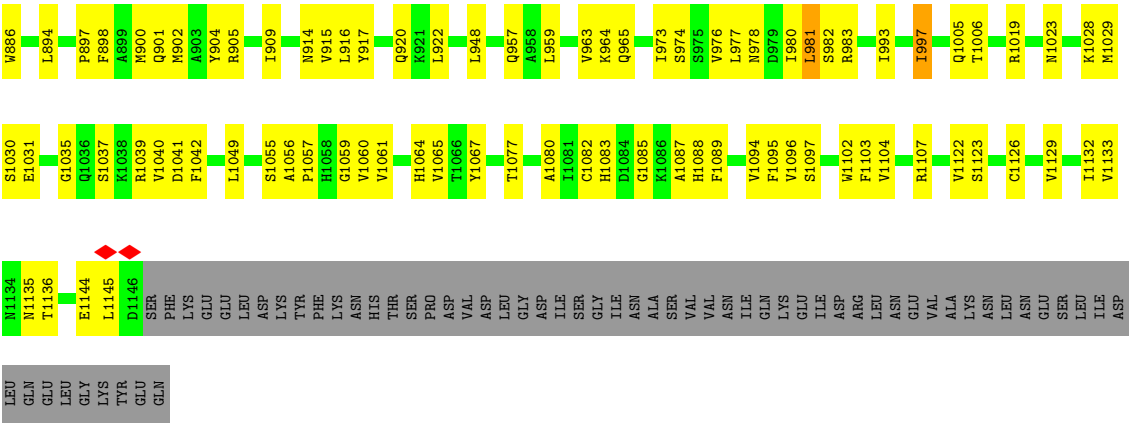
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PHE	GLY	L176	ASP	N362	GLY	A574	F643	I716	T827
VAL	THR	MET	SER	V362	THR	D574	Q644	N717	L828
LEU	LYS	ASP	SER	S373	CYS	A575	T645	V722	ALA
VAL	PHE	LEU	TRP	F374	ASN	D578	R646	E725	ASP
LEU	D80	GLY	THR	G381	GLY	F579	A647	I726	ALA
PRO	Y91	LYS	ALA	G385	VAL	Q580	T651	V729	GLY
LEU	F92	GLN	G261	T385	GLY	E583	V656	V736	PHE
PRO	A93	ASN	A264	C391	GLY	I584	N657	D737	ILE
VAL	S94	PHE	F486	F392	N487	C488	N658	V740	GLN
SER	T95	GLU	G268	F393	C489	C590	S659	M740	TYR
GLN	LYS	LYS	Q271	T394	F490	S591	E661	M740	GLY
CYS	VAL	SER	L189	N394	P491	F592	C662	E748	ASP
ASN	ASN	R99	L277	V395	L492	G593	D663	C749	CYS
LEU	THR	I101	N280	S399	N493	G594	I664	S758	LEU
THR	ARG	R102	E281	S399	S494	V697	P665		ASP
ARG	THR	F106	N282	I402	S495	I698	T666		ILE
THR	GLN	G107	G283	L402	Q498	T599	C671		ALA
LEU	LEU	T108	T284	I418	PRO	P600	A672		ALA
PRO	PRO	S112	T285	N422	ASN	N603	SER		ARG
ASP	ASP	M122	V289	L425	GLY	T604	THR		ASP
GLY	GLY	T29	E298	L425	V503	S605	GLN		LEU
ILE	ILE	T29	E298	L425	V503	N606	THR		ILE
SER	SER	T33	T299	T430	Q506	Q607	GLN		CYS
GLY	GLY	R34	T302	G431	P507	V610	ASN		ALA
ILE	ASN	D40	L303	T434	Y508	V611	SER		K853
ASN	ALA	K41	K304	N437	V511	N615	THR		K854
ALA	VAL	V42	F220	S438	S514	C617	GLY		K855
VAL	VAL	F43	F306	N439	F515	T618	PRO		N856
ASN	ASN	L48	E309	N440	E516	E620	GLY		G857
TLE	TLE	T51	K310	L441	L517	V620	THR		L858
GLN	LYS	Q52	G311	D442	L518	PRO	SER		L864
LYS	GLY	D53	I312	S443	H519	VAL	THR		L865
ILE	ILE	F55	I313	K444	A520	ALA	GLN		T866
ASP	ASP	L56	Q314	V445	P521	ILE	LEU		D867
LEU	LEU	N61	T233	G446	A522	HIS	THR		I870
ASN	ASN	V62	N234	G447	T523	ASP	PRO		Y873
VAL	VAL	T63	T235	N449	K537	ALA	THR		T874
ALA	ALA	W64	F238	Y449	V539	HIS	LEU		L878
LYS	LYS	H66	L241	L452	N540	ASP	GLN		A879
ASN	ASN	F65	L242	Y453	V539	LEU	THR		G880
LEU	LEU	H66	A243	R454	N540	PRO	PRO		T883
ASN	ASN	ILE	L244	L461	T549	THR	THR		S884
SER	SER	VAL	H245	K462	T549	TRP	TRP		G885
GLU	GLU	HIS	ARG	L462	V560	ARG	VAL		W886
LEU	LEU	VAL	TYR	R466	P561	TYR	VAL		L894
ASP	ASP	THR	THR	D467	F562	THR	SER		P897
			THR	I472	Q563	GLY	THR		F898
			PRO		Q564	LEU	GLY		A899
					S566		SER		M900

Q901	S1037	L1145	LYS
R902	K1038	D1146	TYR
A903	R1039	SER	GLN
Y904	V1040	PHE	
R905	D1041	LYS	
	F1042	GLU	
I909		LEU	
	L1049	LEU	
N914	S1055	ASP	
V915	A1056	LYS	
L916	P1057	TYR	
Y917	H1058	PHE	
	G1059	LYS	
Q920	V1060	ASN	
R921	V1061	HIS	
L922		THR	
	H1064	SER	
A942	V1065	PRO	
S943	T1066	ASP	
	Y1067	VAL	
L949		ASP	
	T1077	LEU	
Q957		GLY	
A958	A1080	ASP	
L959	I1081	ILE	
	C1082	SER	
Y963	H1083	GLY	
K964	D1084	ILE	
Q965	G1085	ASN	
	K1086	ALA	
I973	A1087	SER	
S974	H1088	VAL	
S975	V976	VAL	
L977	F1089	ASN	
N978		ILE	
D979	V1094	GLN	
F1095	F1095	LYS	
V1096	V1096	GLU	
S1097		ILE	
	W1102	ARG	
F1103	F1103	ASP	
V1104		LEU	
		ASN	
	R1107	GLU	
		VAL	
Q1005	V1122	ALA	
T1006	S1123	LYS	
		ASN	
	C1126	LEU	
R1019		ASN	
		GLU	
N1023	V1129	GLU	
		SER	
K1028	I1132	LEU	
M1029	V1133	ILE	
S1030	W1134	ASP	
E1031	N1135	LEU	
	T1136	GLN	
G1035		LEU	
Q1036	E1144	GLY	

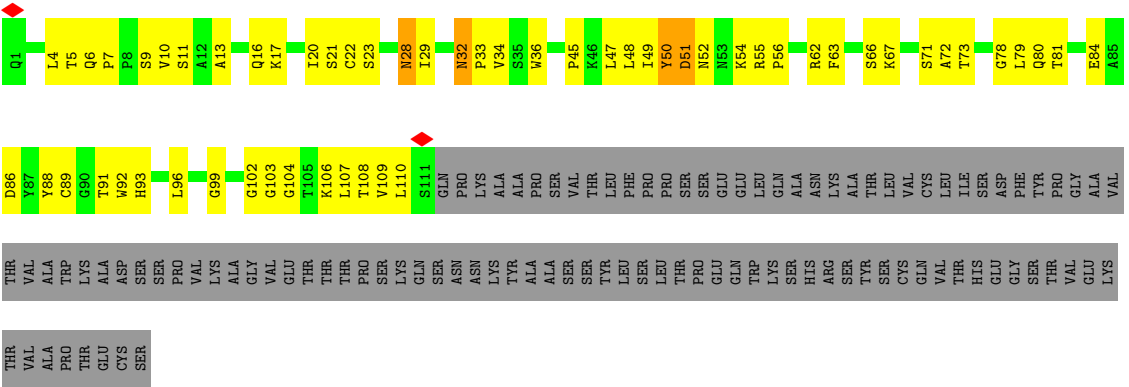
• Molecule 1: Spike glycoprotein

Chain C:  53% 27% 18%

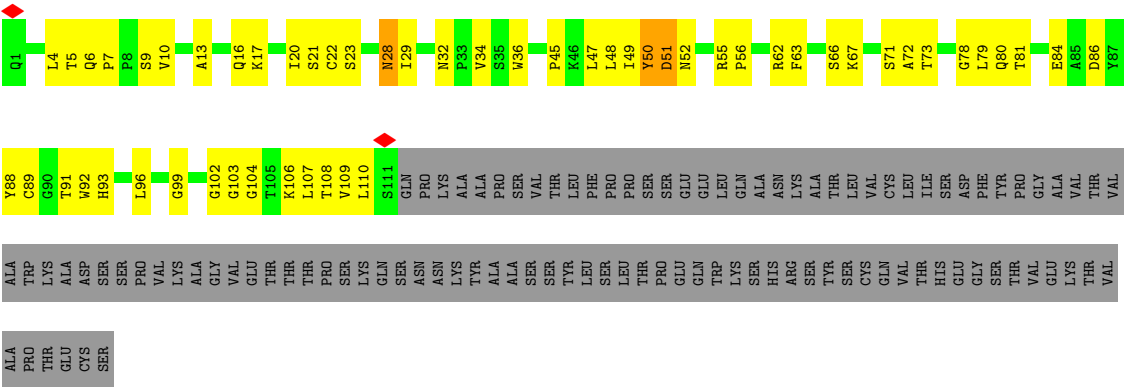
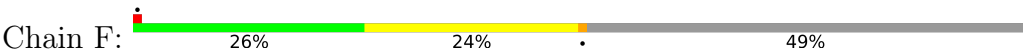
MET	THR	L176	SER	K360	A475	R567	THR	W710	PRO
PHE	LYS	MET	GLY	C361	GLY	D568	GLY	S711	SER
VAL	ARG	ASP	THR	V362	SER	A570	THR	I712	LYS
PHE	PHE	LEU	ALA	F374	PRO	T571	THR	P715	R815
LEU	D80	GLU	G261	G381	CYS	D572	F643	T716	S816
LEU	Y91	LYS	A264	G385	ASN	T573	Q644	N717	I818
LEU	F92	GLN	G268	T385	VAL	A575	T645	V722	E819
PRO	S94	GLY	G271	C391	GLY	D578	R646	E725	V826
LEU	T95	ASN	L277	F392	F486	P579	A647	I726	L828
VAL	GLU	PHE	L277	T393	M487	Q580	I651	V729	ALA
SER	LYS	N188	L277	F394	C488	Q580	V656		ASP
GLN	SER	N188	L277	V395	F489	I584	R657		ALA
CYS	N99	R189	N280	V396	F490	I584	N658	V736	GLY
ASN	I101	E191	E281	Y396	P491	I584	S659	D737	PHE
LEU	R102	F192	N282	S399	L492	C590	V660	M740	ILE
THR			T284		O493	S591	F661		LYS
THR	I105		T284		S494	F592	C662		GLN
ARG	F106		I285		Y495	G593	D663	E748	TYR
GLN	T108		V289		Q498	G594	I664	C749	GLY
LEU	S112		D294		PRO	V597	I666	L754	ASP
PRO	N122		T295		THR	I598	C671	S758	CYS
ASP	A123		L296		ASN	T599	A672		GLY
THR	N125		S297		V503	P600	SER	L767	ASP
Y37			L216			N603	TYR		ILE
			P217			S605	GLN	I770	ALA
						N606	THR	A771	ALA
						Q607	GLN	V772	ARG
						V608	THR	E773	ASP
						A609	ASN	Q774	LEU
						V610	SER	D775	ILE
							PRO	K776	CYS
							GLY	N777	ALA
							SER	V778	Q853
							ALA	Q779	K854
							ALA	Q780	F855
							SER	E781	N856
							SER	F782	Q857
							GLY	A783	L858
							PRO	Q784	L864
							SER	V785	L865
							ALA	K786	L866
							ALA	I788	D867
							ASP		I870
							GLN	D796	Y873
							LEU	F797	T874
							THR	Q799	G798
							THR	E702	L878
							PRO	N801	A879
							THR	F802	G880
							ARG		
							VAL	L806	T883
							TYR	F565	S884
							SER	K811	G885



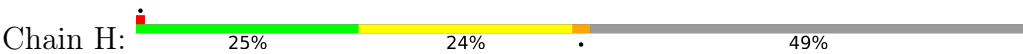
• Molecule 2: The light chain of XG014 Fab



• Molecule 2: The light chain of XG014 Fab



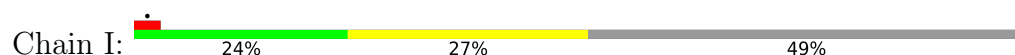
• Molecule 2: The light chain of XG014 Fab

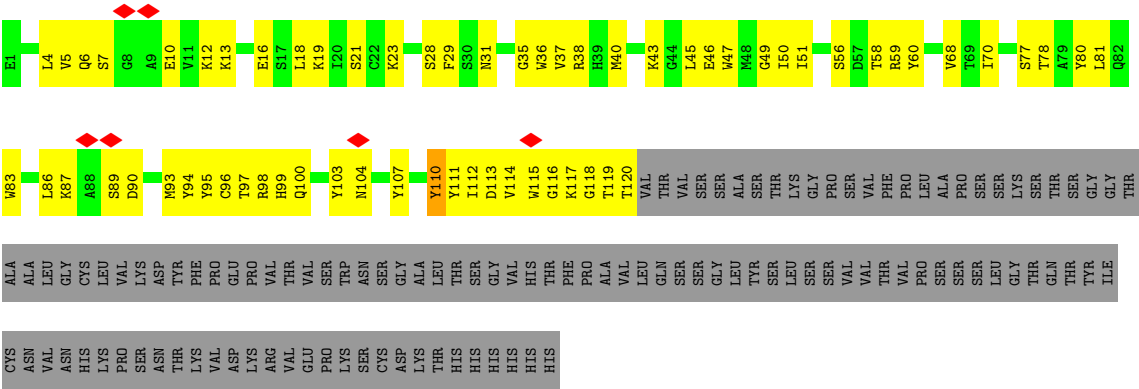


- Molecule 3: The heavy chain of XG014

- Molecule 3: The heavy chain of XG014

- Molecule 3: The heavy chain of XG014





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	414922	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	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)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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	0.54	1/7625 (0.0%)	0.58	1/10400 (0.0%)
1	B	0.54	1/7625 (0.0%)	0.57	1/10400 (0.0%)
1	C	0.54	1/7625 (0.0%)	0.58	2/10400 (0.0%)
2	D	0.40	0/817	0.61	1/1113 (0.1%)
2	F	0.40	0/817	0.61	1/1113 (0.1%)
2	H	0.41	0/817	0.62	1/1113 (0.1%)
3	E	0.43	0/996	0.60	0/1352
3	G	0.42	0/996	0.65	1/1352 (0.1%)
3	I	0.45	0/996	0.67	1/1352 (0.1%)
All	All	0.52	3/28314 (0.0%)	0.59	9/38595 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
2	D	0	1
2	F	0	1
2	H	0	1
3	E	0	1
3	G	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1088	HIS	C-N	-5.80	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1088	HIS	C-N	-5.78	1.21	1.33
1	B	1088	HIS	C-N	-5.77	1.21	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	110	TYR	CB-CA-C	-8.09	95.26	112.82
3	I	110	TYR	CB-CA-C	-8.03	95.39	112.82
1	B	41	LYS	N-CA-C	-5.48	107.59	114.56
1	A	41	LYS	N-CA-C	-5.42	106.60	113.43
1	C	324	GLU	CB-CA-C	-5.38	100.98	114.11

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	443	SER	Peptide
1	B	443	SER	Peptide
1	C	443	SER	Peptide
2	D	50	TYR	Peptide
3	E	104	ASN	Peptide

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	7464	0	7087	422	0
1	B	7464	0	7087	423	0
1	C	7464	0	7087	431	0
2	D	799	0	782	58	0
2	F	799	0	782	56	0
2	H	799	0	782	50	0
3	E	964	0	904	64	0
3	G	964	0	904	69	0
3	I	964	0	904	63	0
4	A	112	0	104	3	0
4	B	112	0	104	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	112	0	104	4	0
All	All	28017	0	26631	1394	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 26.

The worst 5 of 1394 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:697:MET:CE	1:C:864:LEU:HD11	1.11	1.56
1:A:697:MET:CE	1:B:864:LEU:HD11	1.13	1.54
1:A:864:LEU:HD11	1:C:697:MET:CE	1.11	1.51
1:A:864:LEU:CD1	1:C:697:MET:CE	1.90	1.48
1:B:697:MET:CE	1:C:864:LEU:CD1	1.90	1.46

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	964/1208 (80%)	872 (90%)	90 (9%)	2 (0%)	43	71
1	B	964/1208 (80%)	872 (90%)	90 (9%)	2 (0%)	43	71
1	C	964/1208 (80%)	871 (90%)	91 (9%)	2 (0%)	43	71
2	D	109/216 (50%)	96 (88%)	12 (11%)	1 (1%)	14	42
2	F	109/216 (50%)	96 (88%)	12 (11%)	1 (1%)	14	42
2	H	109/216 (50%)	96 (88%)	12 (11%)	1 (1%)	14	42
3	E	118/237 (50%)	107 (91%)	11 (9%)	0	100	100
3	G	118/237 (50%)	106 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	118/237 (50%)	107 (91%)	11 (9%)	0	100	100
All	All	3573/4983 (72%)	3223 (90%)	341 (10%)	9 (0%)	37	65

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	B	42	VAL
1	C	42	VAL
1	A	444	LYS
2	D	51	ASP

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	796/1053 (76%)	774 (97%)	22 (3%)	38	60
1	B	796/1053 (76%)	774 (97%)	22 (3%)	38	60
1	C	796/1053 (76%)	775 (97%)	21 (3%)	40	61
2	D	89/181 (49%)	88 (99%)	1 (1%)	65	74
2	F	89/181 (49%)	88 (99%)	1 (1%)	65	74
2	H	89/181 (49%)	88 (99%)	1 (1%)	65	74
3	E	102/205 (50%)	100 (98%)	2 (2%)	48	65
3	G	102/205 (50%)	100 (98%)	2 (2%)	48	65
3	I	102/205 (50%)	100 (98%)	2 (2%)	48	65
All	All	2961/4317 (69%)	2887 (98%)	74 (2%)	42	62

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	716	THR
3	G	89	SER

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Mol	Chain	Res	Type
1	C	786	LYS
1	C	997	ILE
3	E	89	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	751	ASN
3	I	39	HIS
1	C	901	GLN
2	F	31	ASN
3	E	39	HIS

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](#)

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	$\# Z > 2$
4	NAG	C	1305	1	14,14,15	0.43	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1303	1	14,14,15	0.31	0	17,19,21	0.59	0
4	NAG	B	1303	1	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.51	0
4	NAG	B	1307	1	14,14,15	0.35	0	17,19,21	0.37	0
4	NAG	A	1301	1	14,14,15	0.41	0	17,19,21	0.40	0
4	NAG	C	1303	1	14,14,15	0.31	0	17,19,21	0.58	0
4	NAG	B	1301	1	14,14,15	0.41	0	17,19,21	0.40	0
4	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.50	0
4	NAG	B	1302	1	14,14,15	0.34	0	17,19,21	0.60	0
4	NAG	C	1308	1	14,14,15	0.40	0	17,19,21	1.87	4 (23%)
4	NAG	B	1308	1	14,14,15	0.37	0	17,19,21	1.56	1 (5%)
4	NAG	A	1302	1	14,14,15	0.34	0	17,19,21	0.60	0
4	NAG	A	1305	1	14,14,15	0.44	0	17,19,21	0.66	1 (5%)
4	NAG	B	1306	1	14,14,15	0.18	0	17,19,21	0.60	0
4	NAG	A	1306	1	14,14,15	0.19	0	17,19,21	0.59	0
4	NAG	C	1306	1	14,14,15	0.18	0	17,19,21	0.59	0
4	NAG	B	1305	1	14,14,15	0.44	0	17,19,21	0.65	1 (5%)
4	NAG	C	1301	1	14,14,15	0.39	0	17,19,21	0.41	0
4	NAG	A	1307	1	14,14,15	0.35	0	17,19,21	0.38	0
4	NAG	A	1308	1	14,14,15	0.37	0	17,19,21	1.59	1 (5%)
4	NAG	C	1302	1	14,14,15	0.33	0	17,19,21	0.60	0
4	NAG	C	1307	1	14,14,15	0.35	0	17,19,21	0.38	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
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1308	NAG	C1-O5-C5	5.10	119.02	112.19
4	C	1308	NAG	C1-O5-C5	5.09	119.00	112.19
4	B	1308	NAG	C1-O5-C5	5.05	118.96	112.19
4	C	1308	NAG	C2-N2-C7	-3.49	118.22	122.90
4	C	1308	NAG	O5-C5-C6	2.65	112.82	107.66

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1308	NAG	C3-C2-N2-C7
4	A	1308	NAG	C8-C7-N2-C2
4	A	1308	NAG	O7-C7-N2-C2
4	B	1308	NAG	C3-C2-N2-C7
4	B	1308	NAG	C8-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1305	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1307	NAG	1	0
4	A	1305	NAG	1	0
4	B	1306	NAG	1	0
4	A	1306	NAG	1	0
4	C	1306	NAG	1	0
4	B	1305	NAG	1	0
4	A	1307	NAG	1	0
4	C	1307	NAG	2	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.

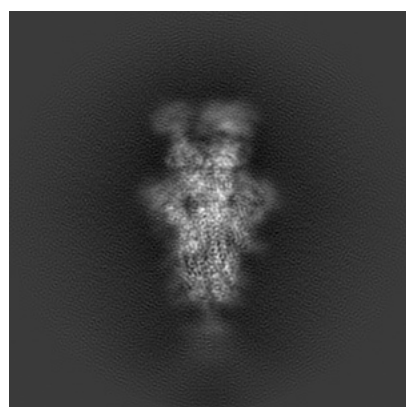
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31639. These allow visual inspection of the internal detail of the map and identification of artifacts.

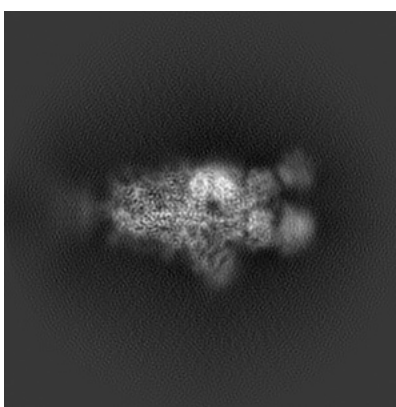
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

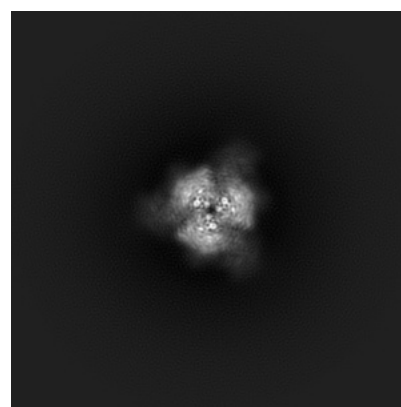
6.1.1 Primary map



X



Y

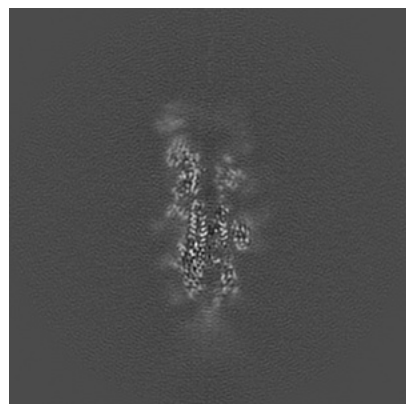


Z

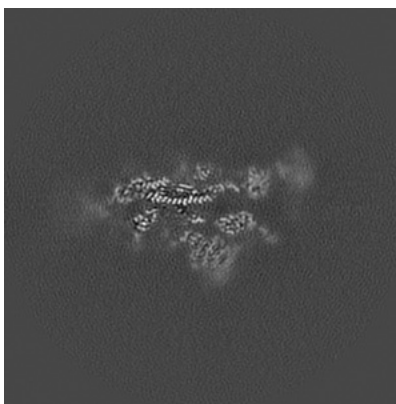
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

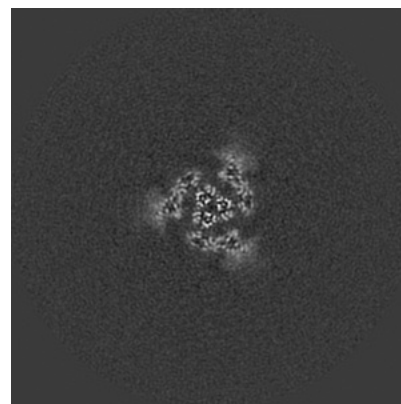
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

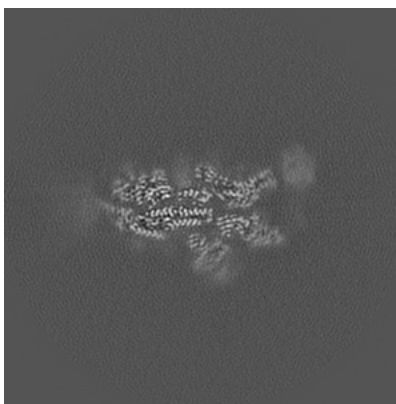
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

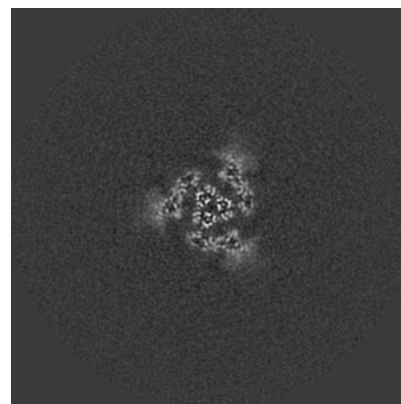
6.3.1 Primary map



X Index: 196



Y Index: 207

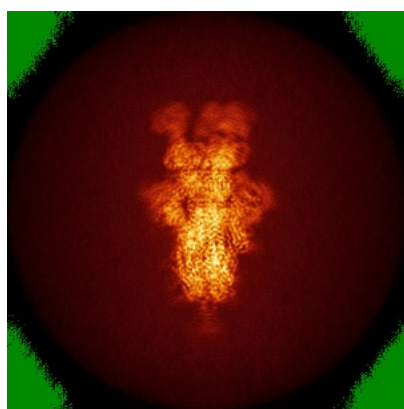


Z Index: 200

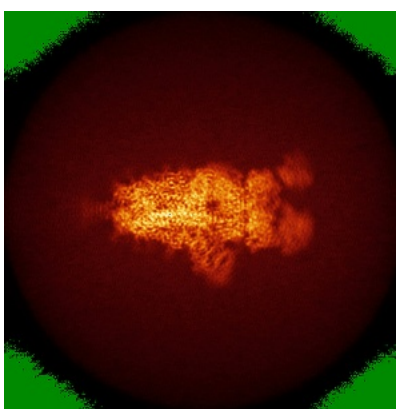
The images above show the largest variance slices of the map in three orthogonal directions.

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

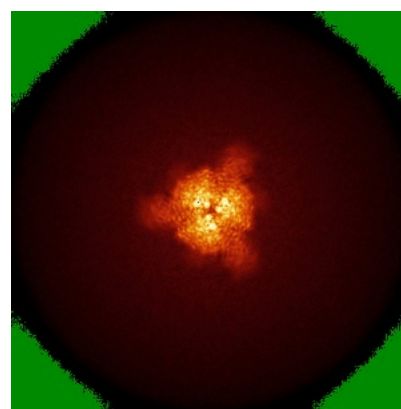
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

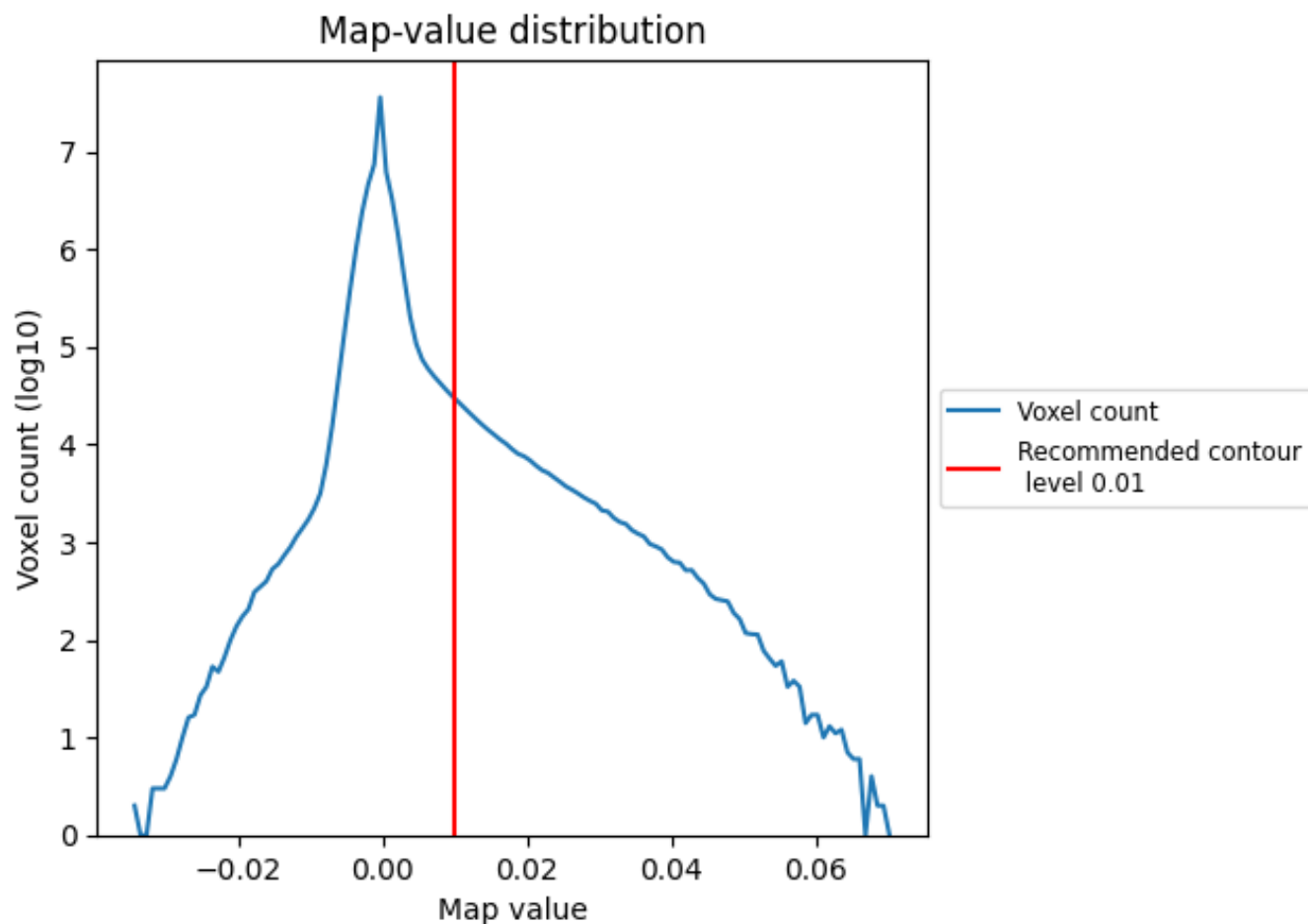
6.6 Mask visualisation

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

7 Map analysis [i](#)

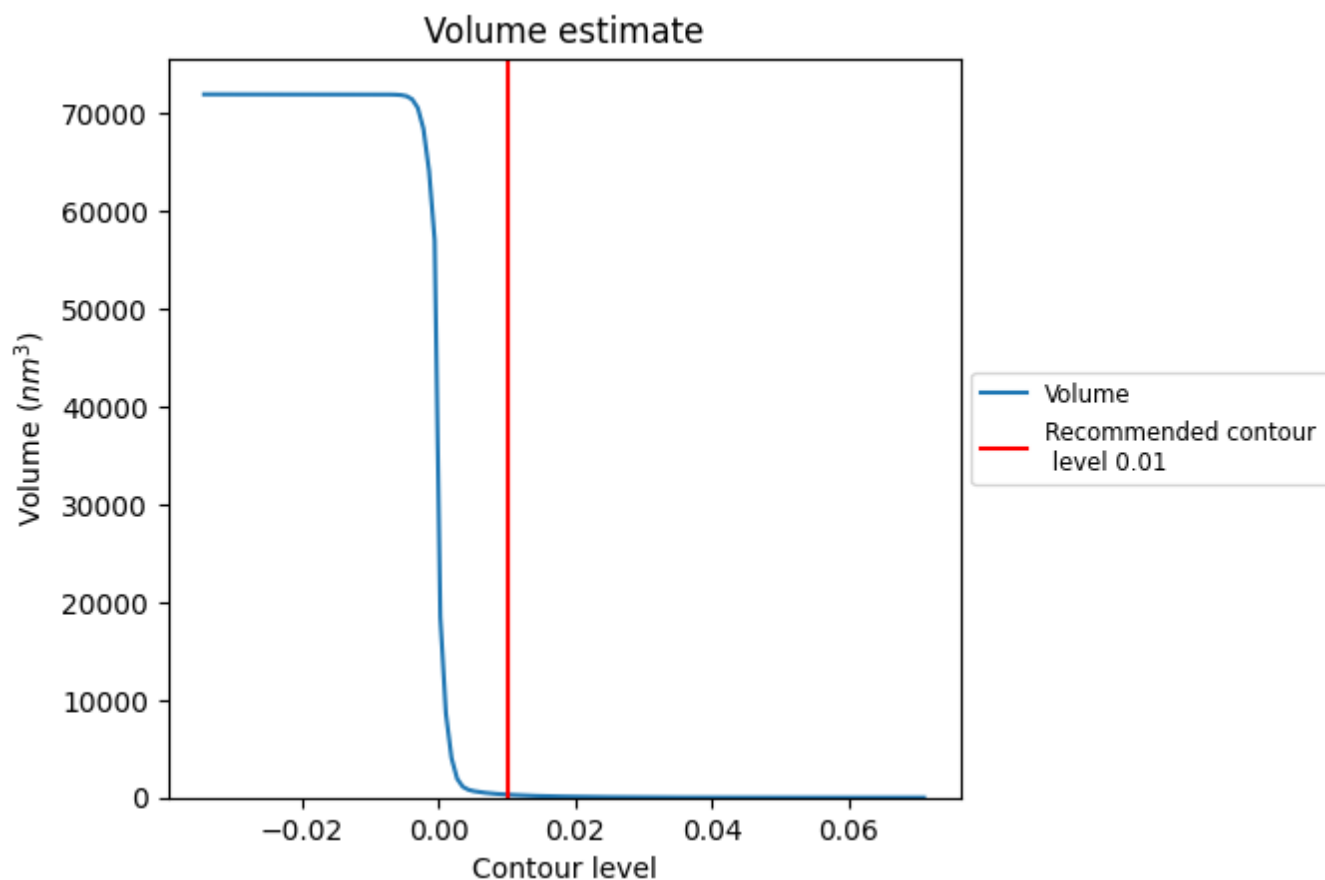
This section contains the results of statistical analysis of the map.

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.

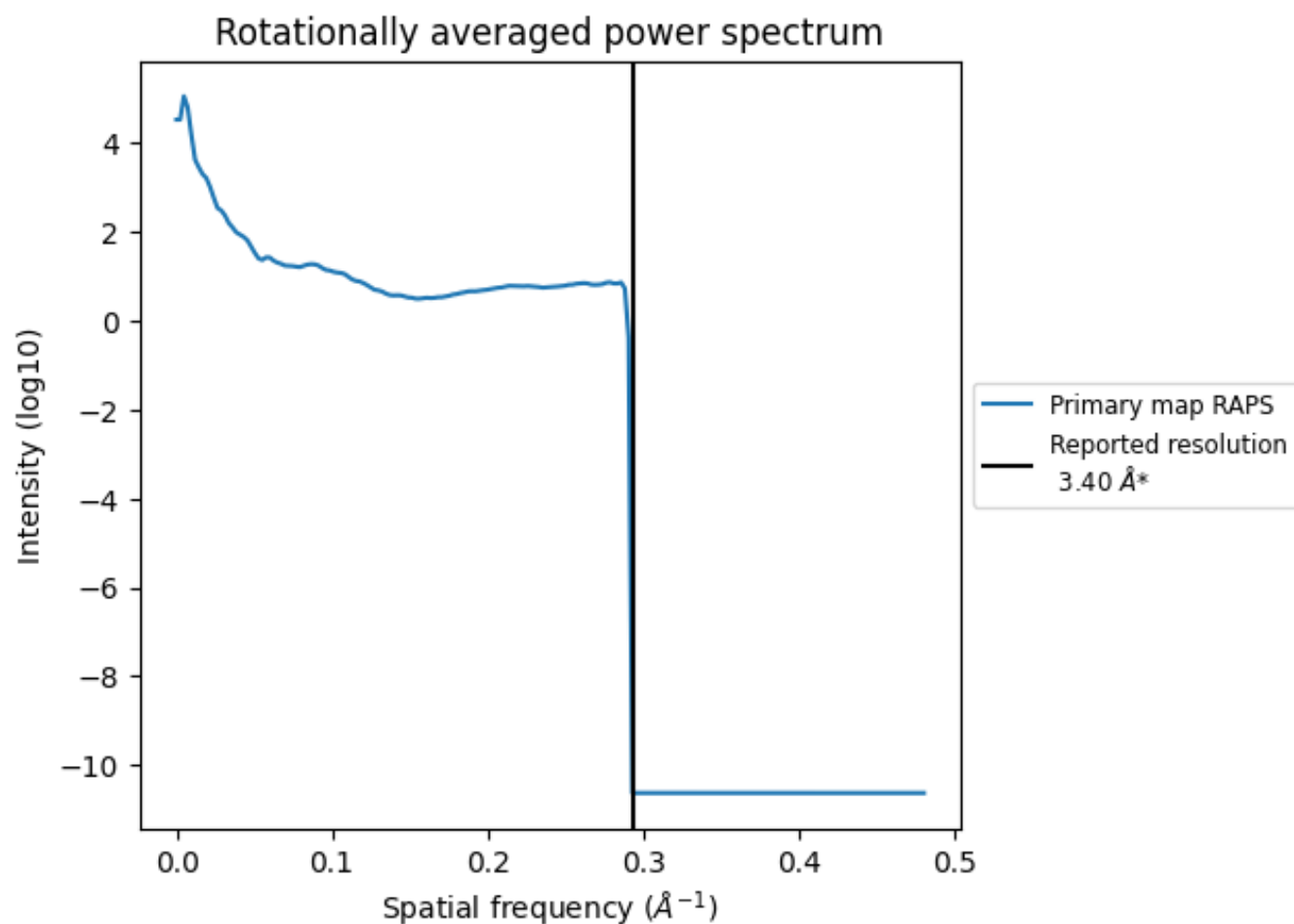
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm³; this corresponds to an approximate mass of 271 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 0.294 Å⁻¹

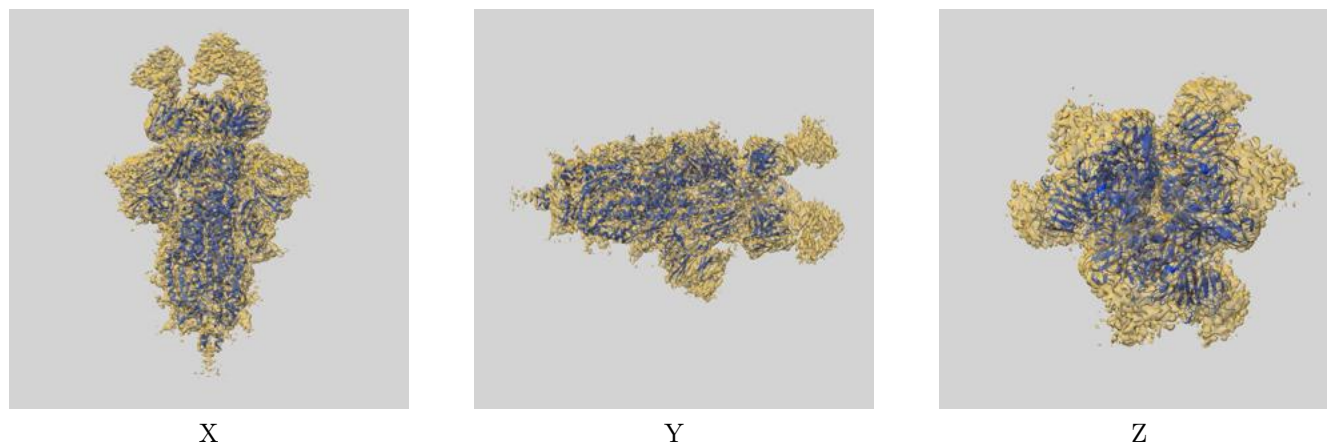
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

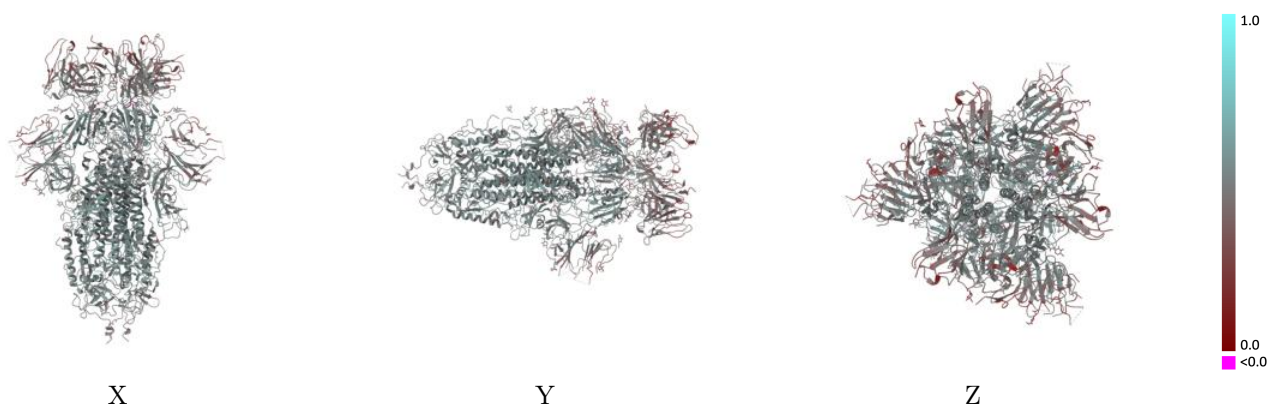
This section contains information regarding the fit between EMDB map EMD-31639 and PDB model 7V2A. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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](#)



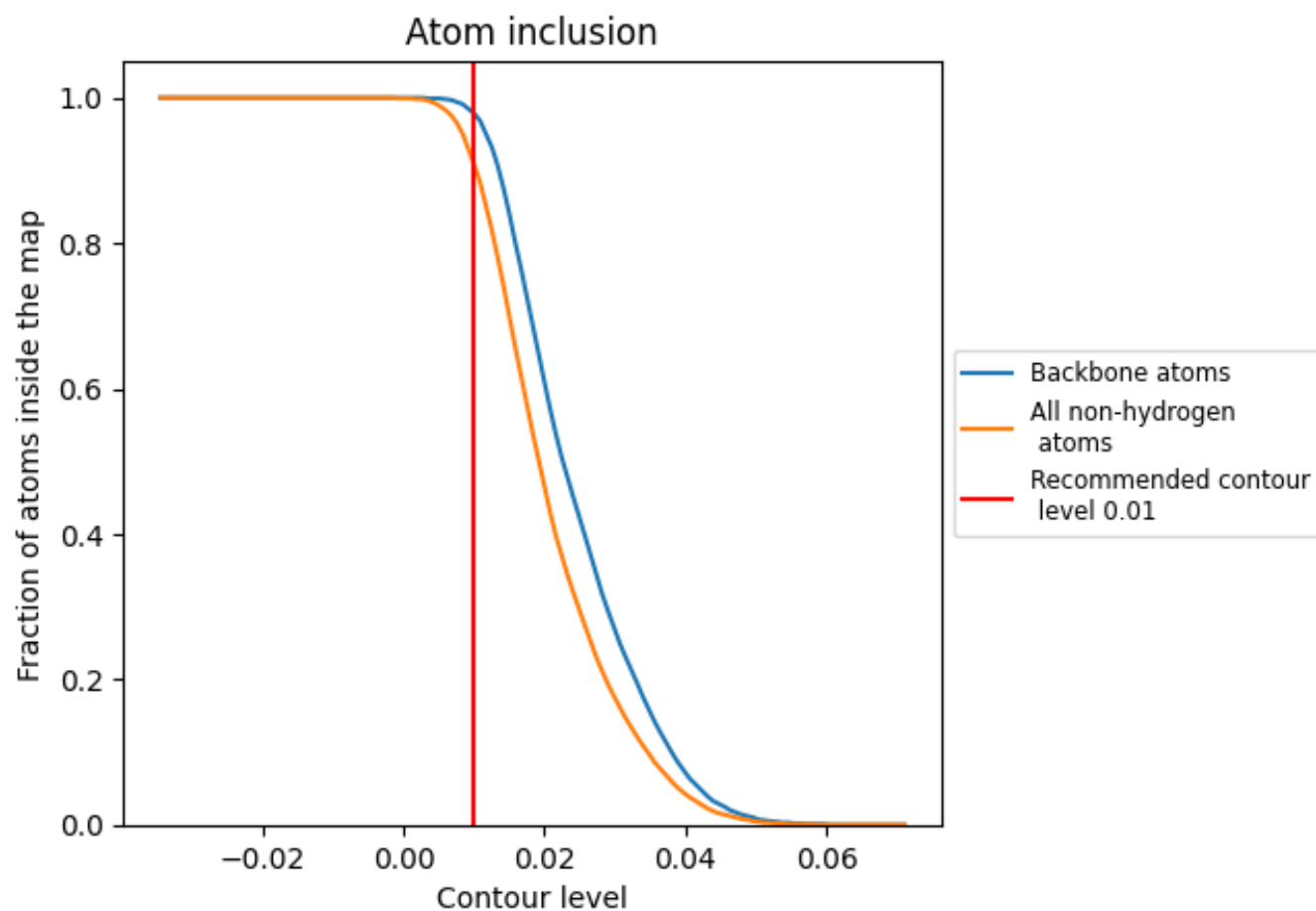
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9100	0.4820
A	0.9180	0.5010
B	0.9170	0.4990
C	0.9170	0.4990
D	0.8770	0.4070
E	0.8800	0.4040
F	0.8730	0.4050
G	0.8810	0.4100
H	0.8740	0.4070
I	0.8770	0.4010

1.0

0.0

<0.0