



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 07:18 PM UTC

PDB ID : 7X6A / pdb_00007x6a
EMDB ID : EMD-33019
Title : SARS-CoV-2 BA.2 variant spike protein in complex with Fab BD55-5840
Authors : Wang, X.; Wang, L.
Deposited on : 2022-03-07
Resolution : 3.50 Å(reported)

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
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

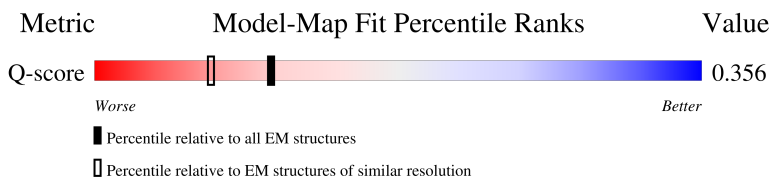
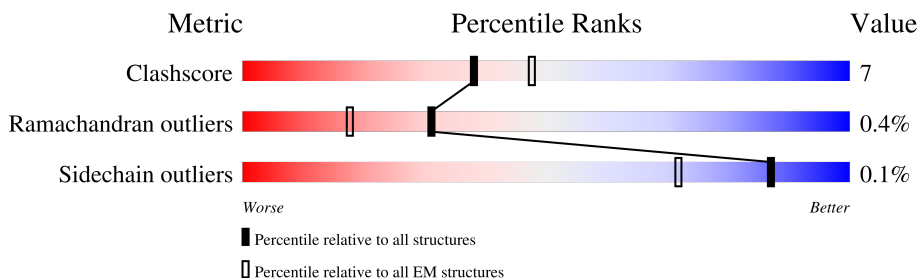
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	1270	27% 72% 14% 14%
1	B	1270	19% 73% 13% 14%
1	D	1270	38% 69% 17% 14%
2	G	119	100% 84% 16%

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Mol	Chain	Length	Quality of chain
2	H	119	
2	I	119	
3	J	109	
3	K	109	
3	L	109	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30879 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	1095	Total	C	N	O	S	0	0
			8548	5464	1424	1623	37		
1	B	1095	Total	C	N	O	S	0	0
			8548	5466	1423	1622	37		
1	D	1095	Total	C	N	O	S	0	0
			8551	5467	1424	1623	37		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	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	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	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	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	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	683	ALA	ARG	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
D	22	ILE	THR	variant	UNP P0DTC2
D	?	-	LEU	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	?	-	PRO	deletion	UNP P0DTC2
D	27	SER	ALA	variant	UNP P0DTC2
D	142	ASP	GLY	variant	UNP P0DTC2
D	213	GLY	VAL	variant	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	493	ARG	GLN	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2
D	614	GLY	ASP	variant	UNP P0DTC2
D	655	TYR	HIS	variant	UNP P0DTC2
D	679	LYS	ASN	variant	UNP P0DTC2
D	681	HIS	PRO	variant	UNP P0DTC2
D	683	ALA	ARG	variant	UNP P0DTC2
D	685	ALA	ARG	variant	UNP P0DTC2
D	764	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	796	TYR	ASP	variant	UNP P0DTC2
D	817	PRO	PHE	variant	UNP P0DTC2
D	892	PRO	ALA	variant	UNP P0DTC2
D	899	PRO	ALA	variant	UNP P0DTC2
D	942	PRO	ALA	variant	UNP P0DTC2
D	954	HIS	GLN	variant	UNP P0DTC2
D	969	LYS	ASN	variant	UNP P0DTC2
D	986	PRO	LYS	engineered mutation	UNP P0DTC2
D	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of Fab BD55-5840.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	119	Total	C	N	O	S	0	0
			927	585	157	182	3		
2	G	119	Total	C	N	O	S	0	0
			927	585	157	182	3		
2	I	119	Total	C	N	O	S	0	0
			927	585	157	182	3		

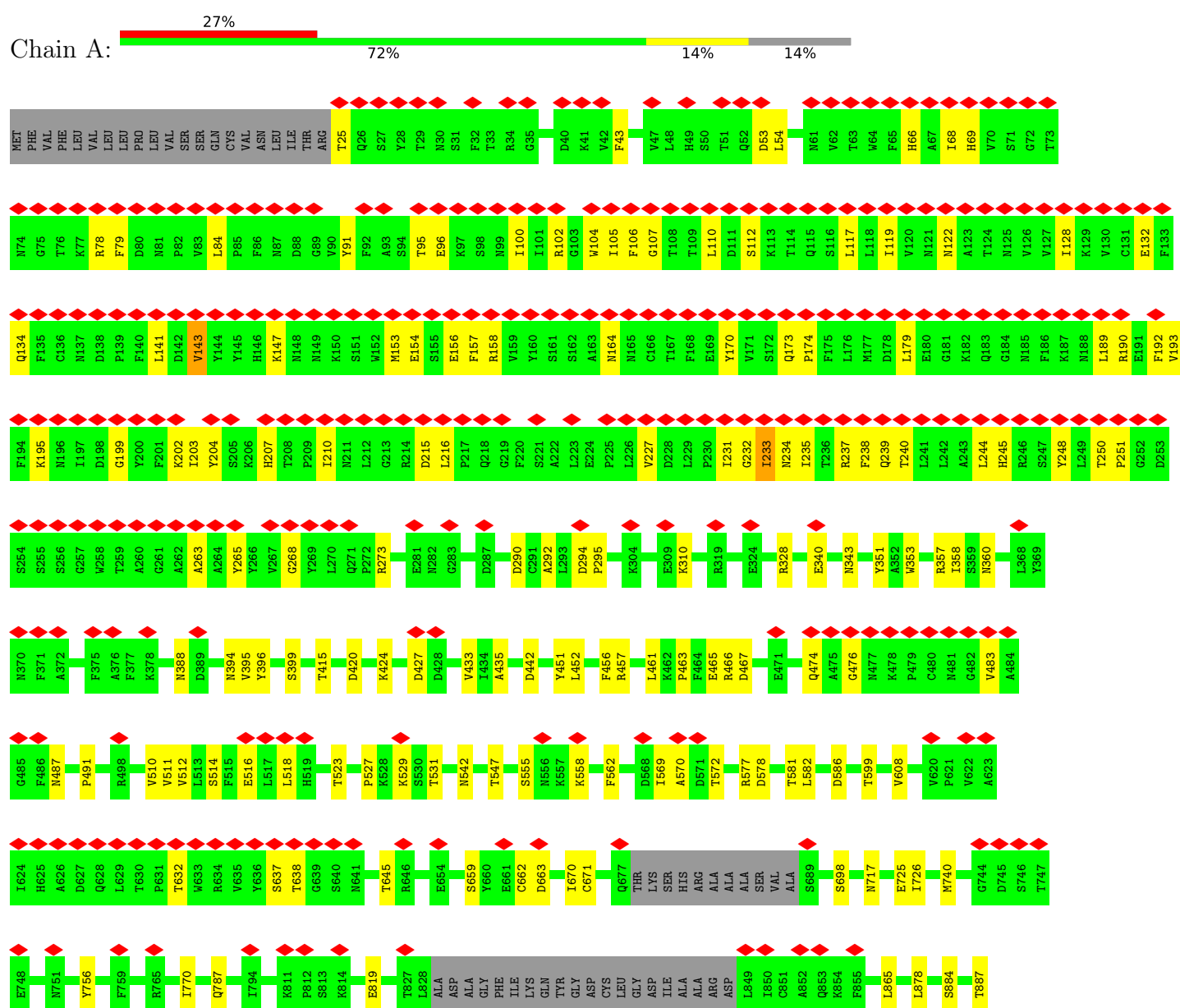
- Molecule 3 is a protein called Light chain of Fab BD55-5840.

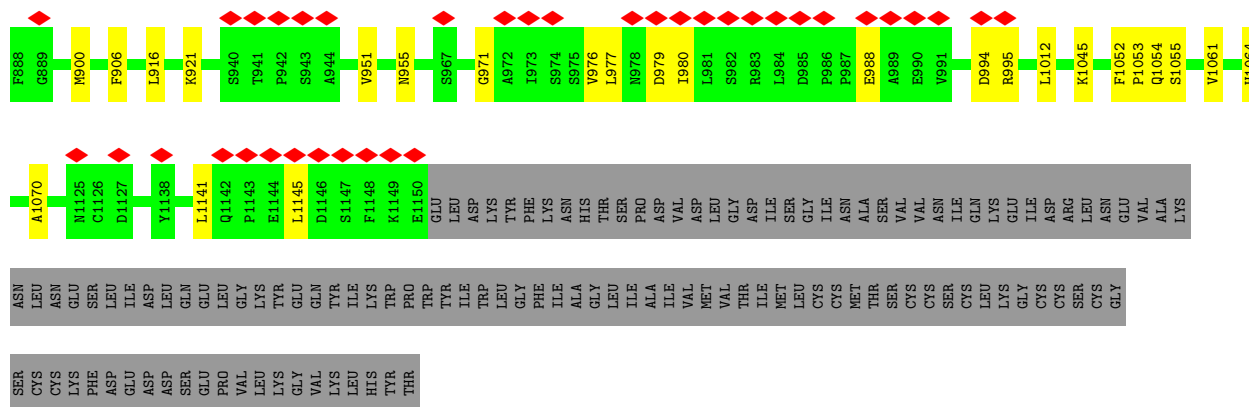
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	109	Total	C	N	O	S	0	0
			817	510	142	162	3		
3	J	109	Total	C	N	O	S	0	0
			817	510	142	162	3		
3	K	109	Total	C	N	O	S	0	0
			817	510	142	162	3		

3 Residue-property plots

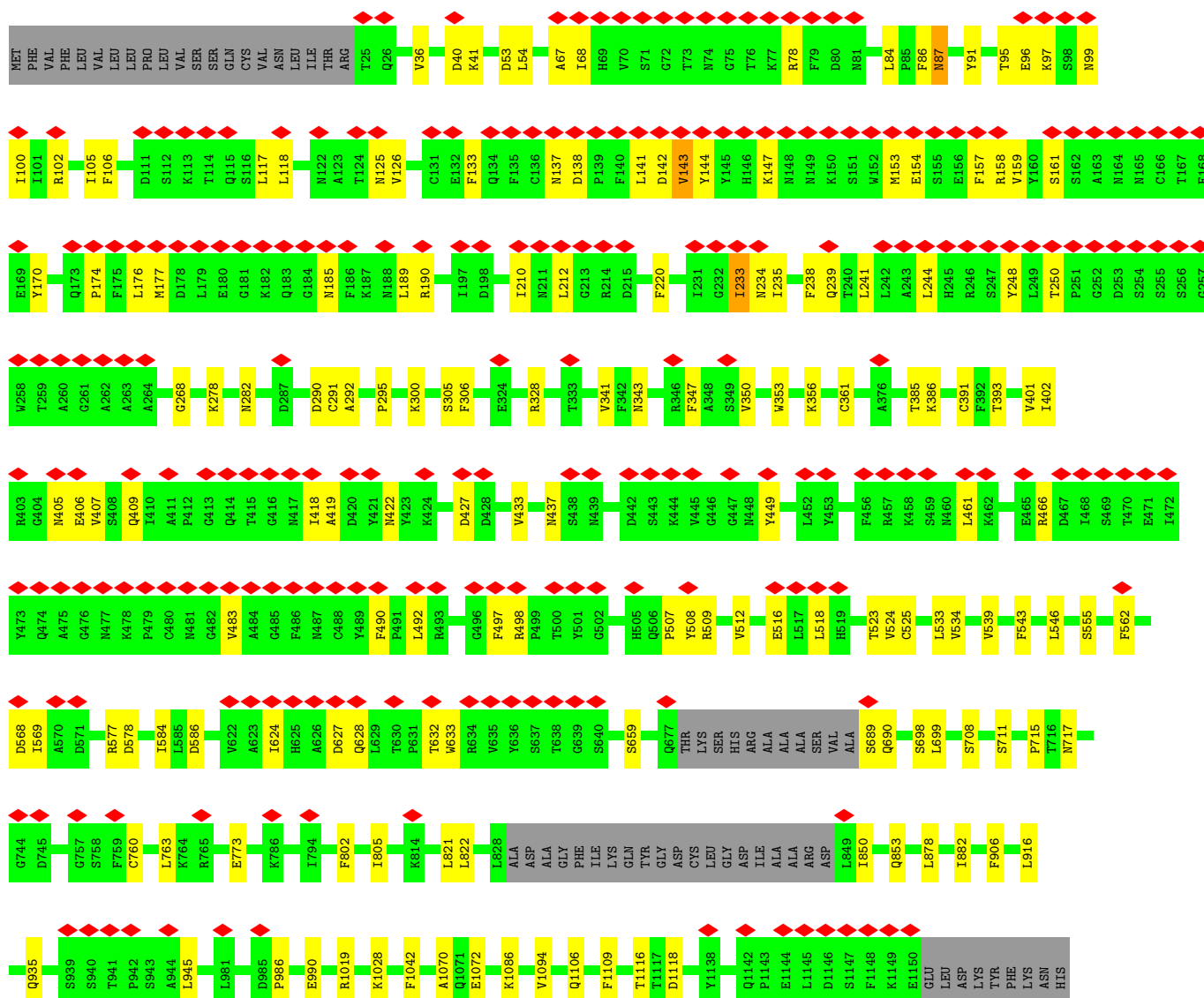
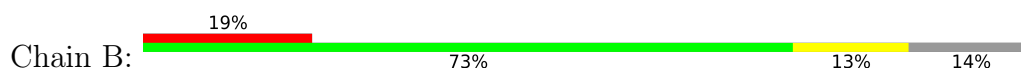
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



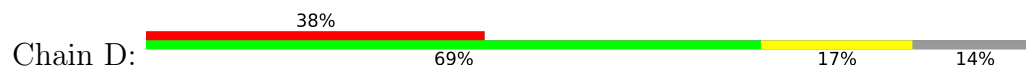


• Molecule 1: Spike glycoprotein

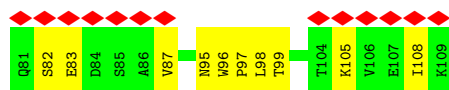


THR	SER	PRO	ASP	VAL	ASP	LEU	GLY	ASP	ILE	LEU	GLY	ASP	THR	GLY	ASN	ALA	SER	VAL	ASN	THR	ILE	GLN	CYS	LYS	GLY	ASP	ARG	LEU	ASN	CYS	GLU	SER	VAL	ALA	LYS	ASN	CYS	ASN	GLU	GLY	SER	LEU	ASP	ILE	ASP	GLU	ASP	ASP	GLN	GLY	PRO	VAL	GLY	LYS	TYR	GLY	VAL	GLN	TYR	ILE	LYS	TRP	PRO	THR	TYR	ILE	THR	LEU	GLY
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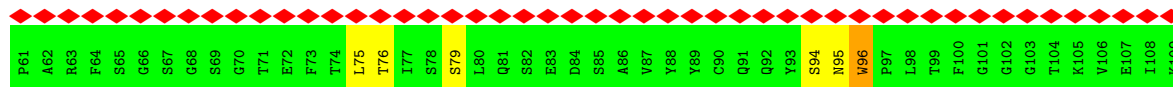
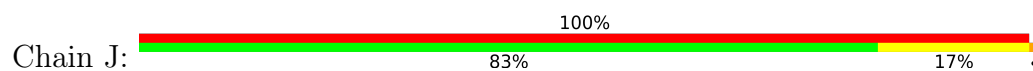
● Molecule 1: Spike glycoprotein



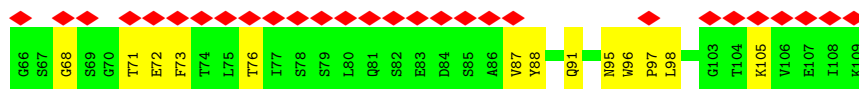
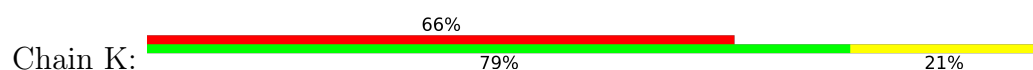
MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	LEU	VAL	SER	SER	GLN	VAL	ASN	LEU	ILE	THR	ARG	T25	Q26	T33	V36	Y37	D40	K41	D53	L54	F65	H66	A67	I68	H69	V70	S71	G72	T73	N74	G75	T76	K77	R78	F79	D80	N81	P82	Y83	L84	F85	F86	N87	D88						
Y91	S94	T95	E96	K97	S98	N99	I100	I101	R102	I105	F106	G107	T108	T109	L110	D111	S112	K113	T114	Q115	S116	L117	L118	I119	V120	M121	N122	A123	T124	I128	K129	V130	E132	F133	Q134	F135	C136	N137	D138	P139	F140	L141	D142	V143	Y144	H146	K147	N148	K149	K150	S151	M152	M153	E154				
S155	E156	F157	R158	V159	Y160	S161	A162	A163	M164	M165	C166	T167	F168	E169	Q173	P174	F175	L176	M177	D178	L179	E180	G181	K182	V184	Q183	G184	N185	F186	K187	N188	L189	R190	E191	F192	K195	N196	I197	D198	G199	Y200	F201	K202	L203	H207	T208	P209	I210	N211	L212	Q213	R214	D215	L216	P217	Q218	G219	
F220	L223	L226	V227	D228	P230	T231	G232	T233	N234	T235	T236	R237	F238	Q239	T240	L241	L242	A243	L244	H245	R246	S247	Y248	L249	T250	P251	G252	D253	S254	S255	S256	Q257	Q258	T259	A260	G261	A262	A263	Y265	Y266	V267	G268	Y269	L270	Q271	P272	R273	L276	L277	K278	E281	P285						
K304	S305	F306	N317	F318	R319	V320	Q321	P322	T323	E324	S325	I326	V327	R328	F329	P330	N331	I332	N334	L335	C336	P337	F338	D339	E340	V341	F342	N343	A344	T345	R346	F347	A348	S349	V350	Y351	A352	K353	N354	R355	K356	R357	I358	S359	N360	C361	V362	A363	D364	Y365	S366	L368	Y369	F371				
A372	P373	F374	F375	A376	F377	K378	C379	Y380	G381	V382	S383	P384	T385	K386	L387	N388	D389	L390	C391	F392	N394	V395	Y396	A397	D398	S399	F400	V401	I402	R403	G404	N405	E406	V407	S408	Q409	I410	A411	P412	G413	Q414	T415	Q416	Q417	N417	L418	A419	D420	Y421	N422	Y423	K424	L425	P426	D427	F428	T430	G431
C432	V433	I434	A435	W436	N437	S438	N439	K440	L441	D442	S443	V444	V445	G446	G447	N448	Y449	M450	Y451	L452	R454	L455	F456	R457	K458	S459	M460	L461	K462	P463	F464	E465	R466	D467	I468	S469	T470	E471	I472	G473	Q474	A475	G476	N477	K478	P479	C480	N481	G482	V483	A484	G485	F486	N487	C488	F489	P491	
L492	R493	S494	Y495	G496	F497	R498	P499	T500	Y501	F502	G503	V504	H505	Q506	P507	Y508	R509	V510	V511	V512	S514	F515	E516	L517	L518	H519	A520	P521	A522	T523	V524	C525	G526	P527	K528	K529	S530	T531	N532	L533	V534	K535	N536	K537	C538	V539	N540	F541	N542	F543	N544	G545	L546	T547	G548	T549	L552	
T553	E554	S555	N556	K557	K558	F559	L560	P561	F562	Q563	Q564	F565	G566	H567	D568	I569	A570	D571	T572	T573	D574	A575	V576	R577	D578	P579	Q580	T581	L582	E583	I584	L585	D586	I587	T588	P589	C590	S591	F592	T599	V608	N616	C617	T618	E619	V620	P621	V622	A623	I624	H625	A626	D627	Q628	L629	T630		
P631	T632	W633	R634	V635	W636	S637	T638	G639	S640	N641	V642	L650	I651	S659	T676	Q677	THR	LYS	SER	ARG	HIS	ARG	ALA	ALA	ALA	VAL	ALA	S689	S698	E702	N703	S708	S711	P715	T716	N717	G744	D745	L752	F759	L763	Q804	D808	K811														
P812	S813	K814	E819	L828	ALA	ASP	ALA	GLY	PHE	ILE	LYS	GLN	TYR	GLY	ASP	CYS	LEU	GLY	ASP	ILE	ALA	ALA	ASP	L849	Q853	L865	M869	S884	T887	M900	F906	L916	Q935	D936	S939	S940	T941	P942	S943	A944	V951	N955	G971															



• Molecule 3: Light chain of Fab BD55-5840



• Molecule 3: Light chain of Fab BD55-5840



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	355445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.043	Depositor
Minimum map value	-1.849	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.558	Depositor
Map size ($\text{\AA}$)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.11	0/8758	0.30	0/11930
1	B	0.11	0/8758	0.28	0/11930
1	D	0.12	0/8761	0.30	0/11934
2	G	0.08	0/952	0.23	0/1295
2	H	0.11	0/952	0.31	0/1295
2	I	0.10	0/952	0.27	0/1295
3	J	0.10	0/834	0.28	0/1133
3	K	0.10	0/834	0.28	0/1133
3	L	0.11	0/834	0.33	0/1133
All	All	0.11	0/31635	0.29	0/43078

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
3	J	0	1
3	K	0	1
3	L	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	96	TRP	Peptide
3	K	96	TRP	Peptide
3	L	96	TRP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8548	0	8314	123	0
1	B	8548	0	8319	107	0
1	D	8551	0	8323	157	0
2	G	927	0	862	11	0
2	H	927	0	862	15	0
2	I	927	0	862	15	0
3	J	817	0	802	13	0
3	K	817	0	802	14	0
3	L	817	0	802	15	0
All	All	30879	0	29948	447	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 7.

The worst 5 of 447 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:D:185:ASN:HB2	1:D:212:LEU:CD2	1.38	1.50
1:B:185:ASN:O	1:B:212:LEU:HD23	1.36	1.24
1:D:185:ASN:CB	1:D:212:LEU:CD2	2.25	1.15
1:B:185:ASN:O	1:B:212:LEU:CD2	1.98	1.12
1:D:185:ASN:HB2	1:D:212:LEU:HD21	1.27	1.11

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1089/1270 (86%)	1023 (94%)	62 (6%)	4 (0%)	30	62
1	B	1089/1270 (86%)	1024 (94%)	60 (6%)	5 (0%)	24	57
1	D	1089/1270 (86%)	1007 (92%)	77 (7%)	5 (0%)	24	57
2	G	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
2	H	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
2	I	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
3	J	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
3	K	107/109 (98%)	97 (91%)	10 (9%)	0	100	100
3	L	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
All	All	3939/4494 (88%)	3682 (94%)	243 (6%)	14 (0%)	31	62

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ILE
1	B	143	VAL
1	B	233	ILE
1	D	143	VAL
1	D	233	ILE

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	950/1109 (86%)	950 (100%)	0	100	100
1	B	950/1109 (86%)	949 (100%)	1 (0%)	88	87
1	D	951/1109 (86%)	950 (100%)	1 (0%)	88	87
2	G	98/98 (100%)	98 (100%)	0	100	100
2	H	98/98 (100%)	98 (100%)	0	100	100
2	I	98/98 (100%)	98 (100%)	0	100	100
3	J	88/88 (100%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	88/88 (100%)	88 (100%)	0	100	100
3	L	88/88 (100%)	88 (100%)	0	100	100
All	All	3409/3885 (88%)	3407 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	D	87	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	82	GLN
2	G	3	GLN
2	I	43	GLN
1	B	1106	GLN
1	B	965	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.

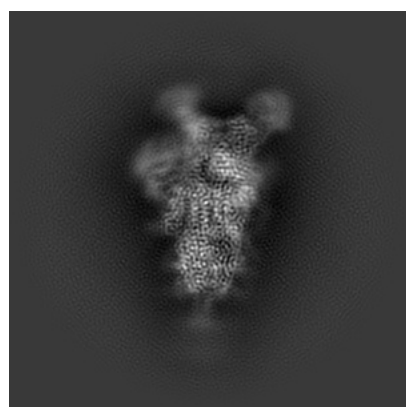
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33019. These allow visual inspection of the internal detail of the map and identification of artifacts.

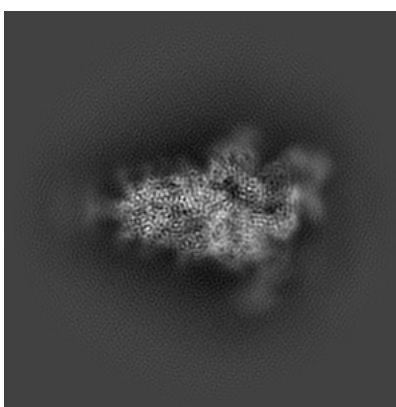
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

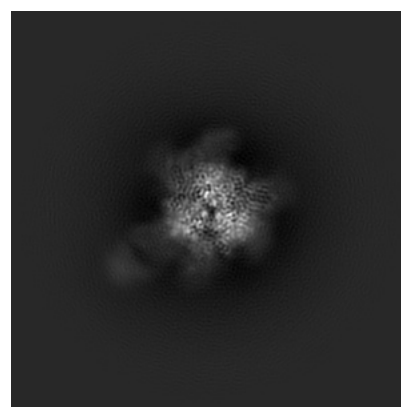
6.1.1 Primary map



X



Y

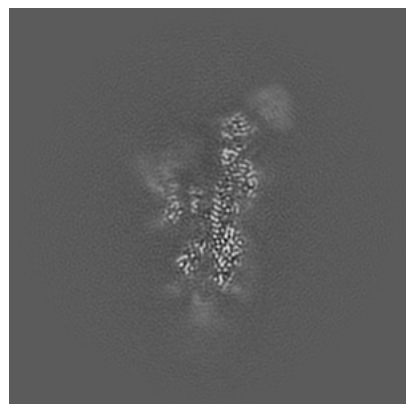


Z

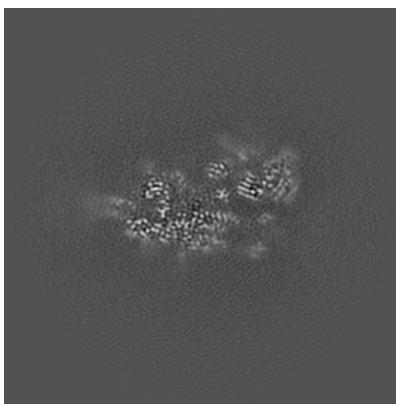
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

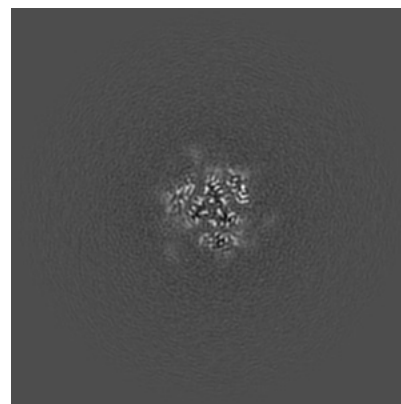
6.2.1 Primary map



X Index: 180



Y Index: 180

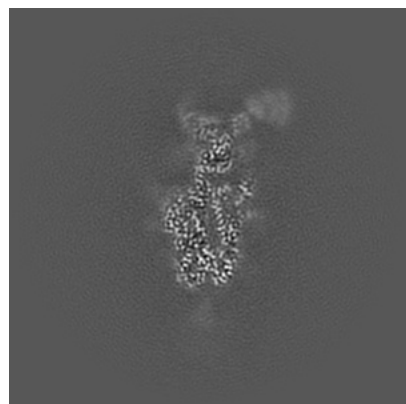


Z Index: 180

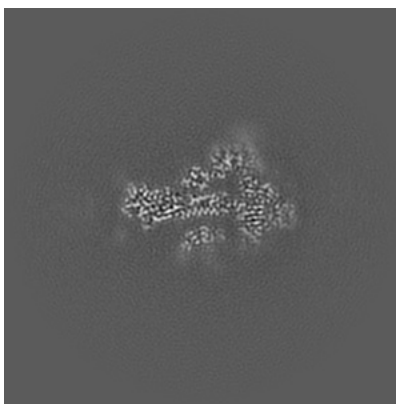
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

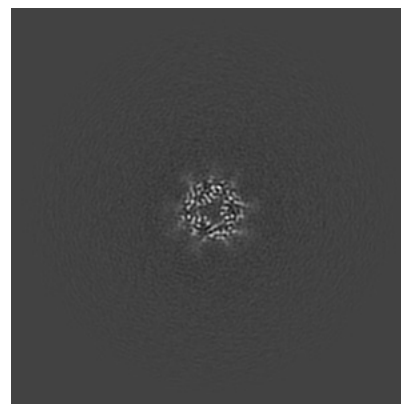
6.3.1 Primary map



X Index: 192



Y Index: 195



Z Index: 129

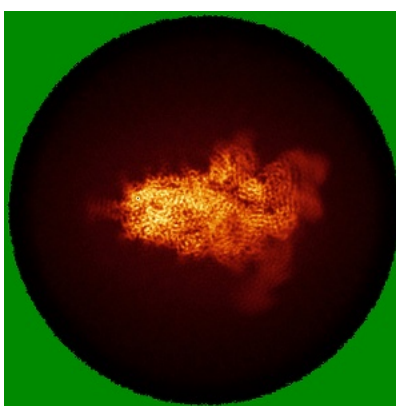
The images above show the largest variance slices of the map in three orthogonal directions.

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

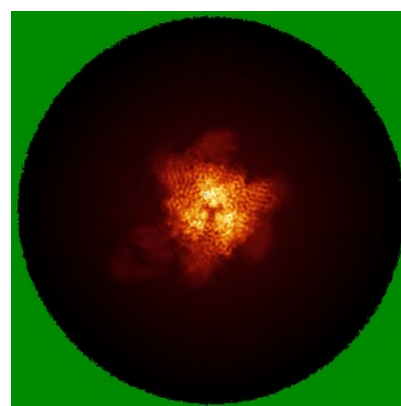
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.558. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

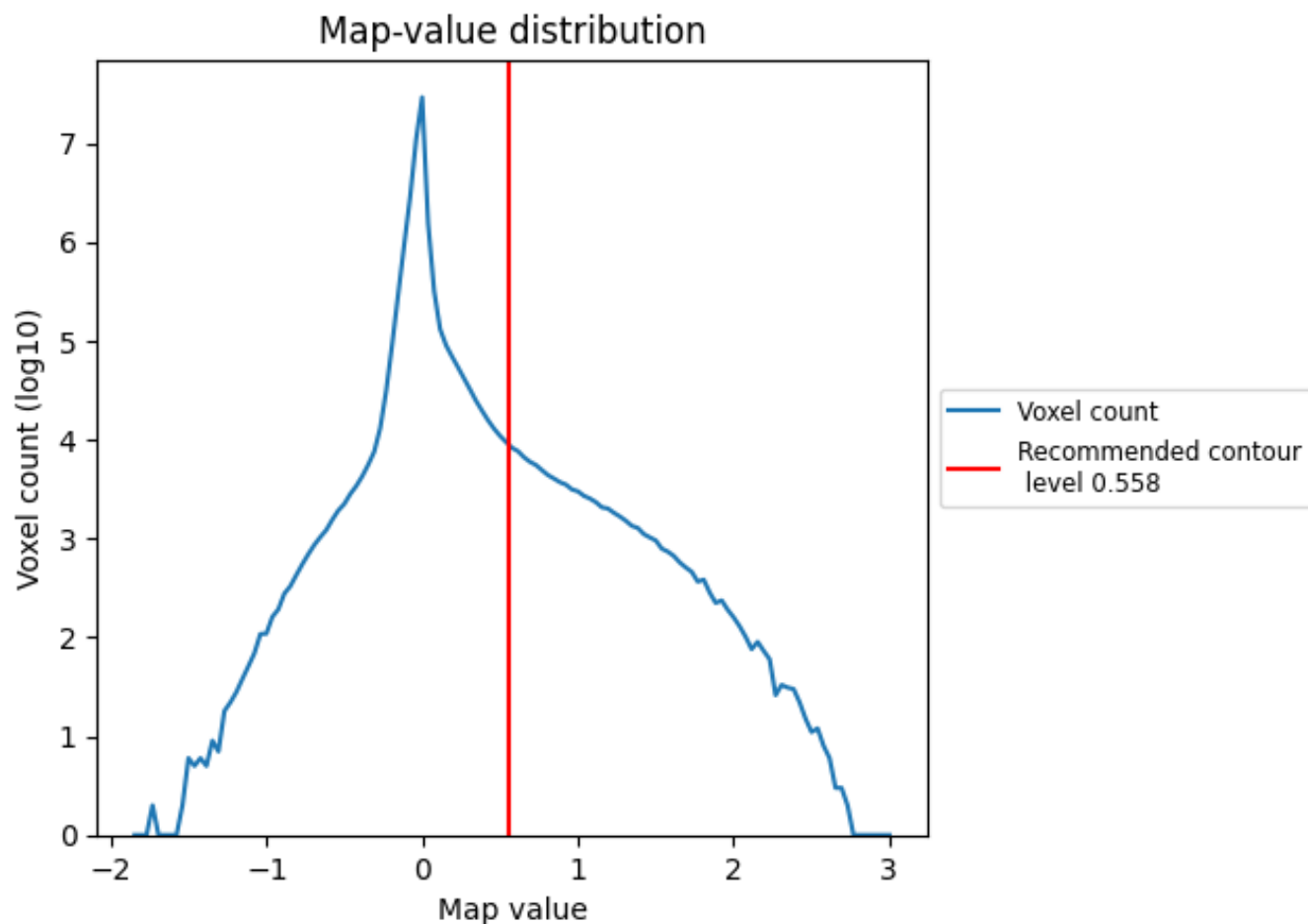
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

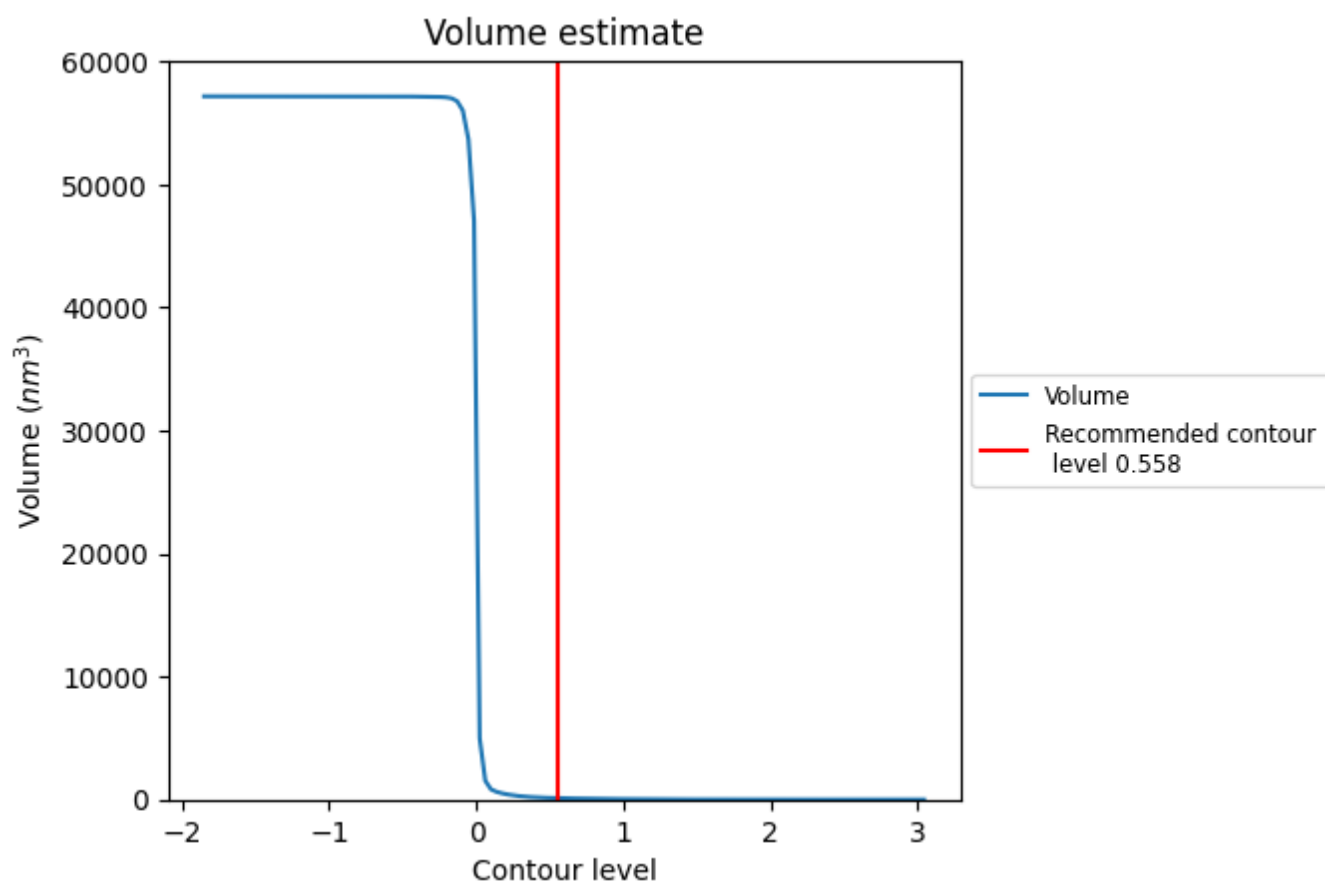
This section contains the results of statistical analysis of the map.

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.

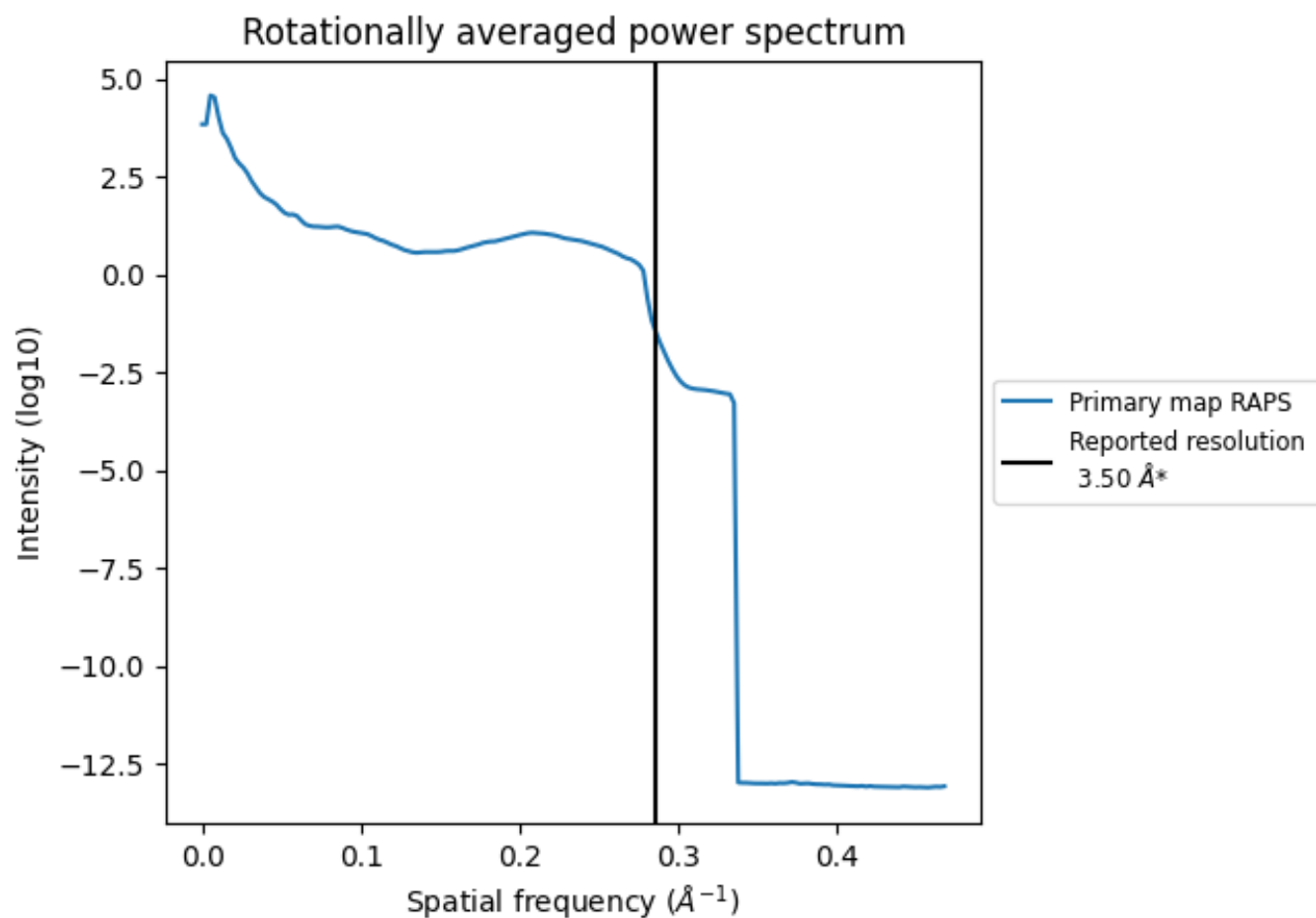
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 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 0.286 Å⁻¹

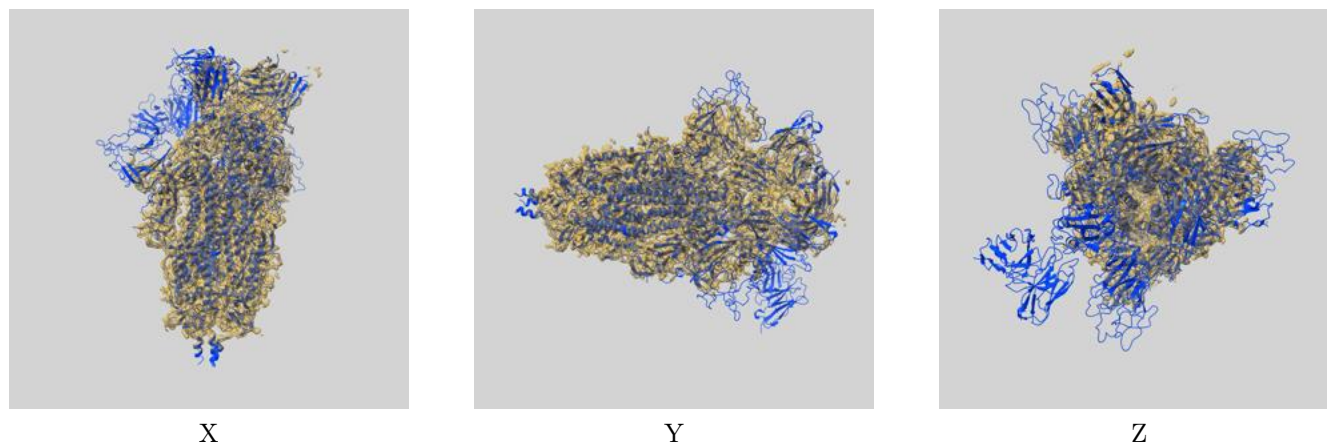
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

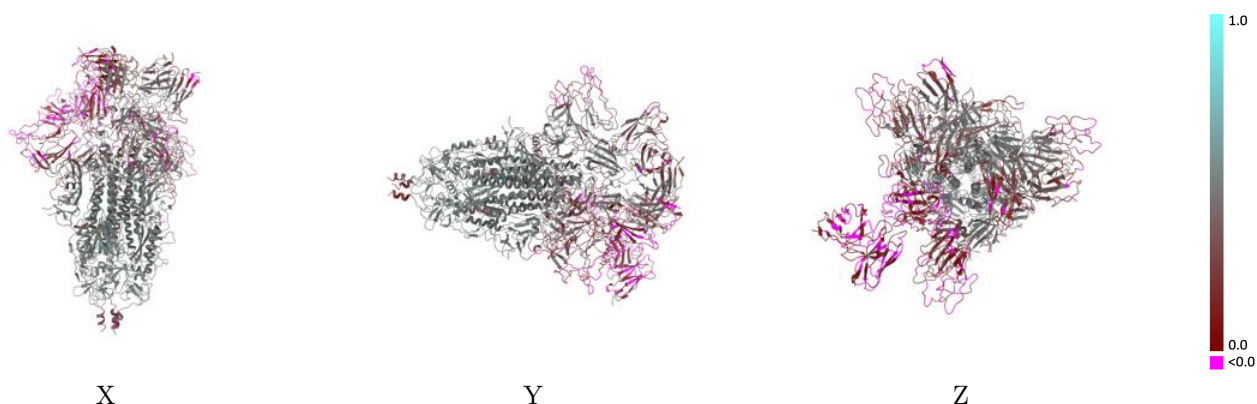
This section contains information regarding the fit between EMDB map EMD-33019 and PDB model 7X6A. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



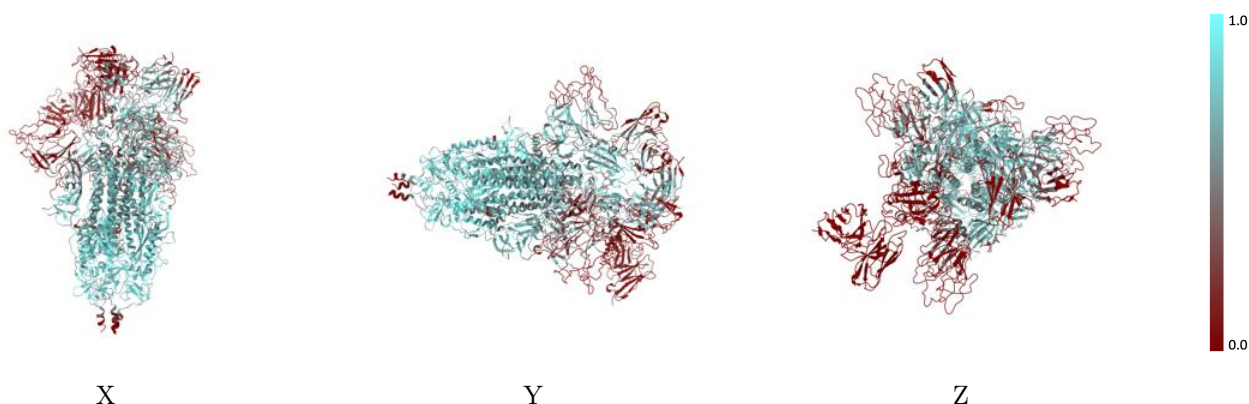
The images above show the 3D surface view of the map at the recommended contour level 0.558 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



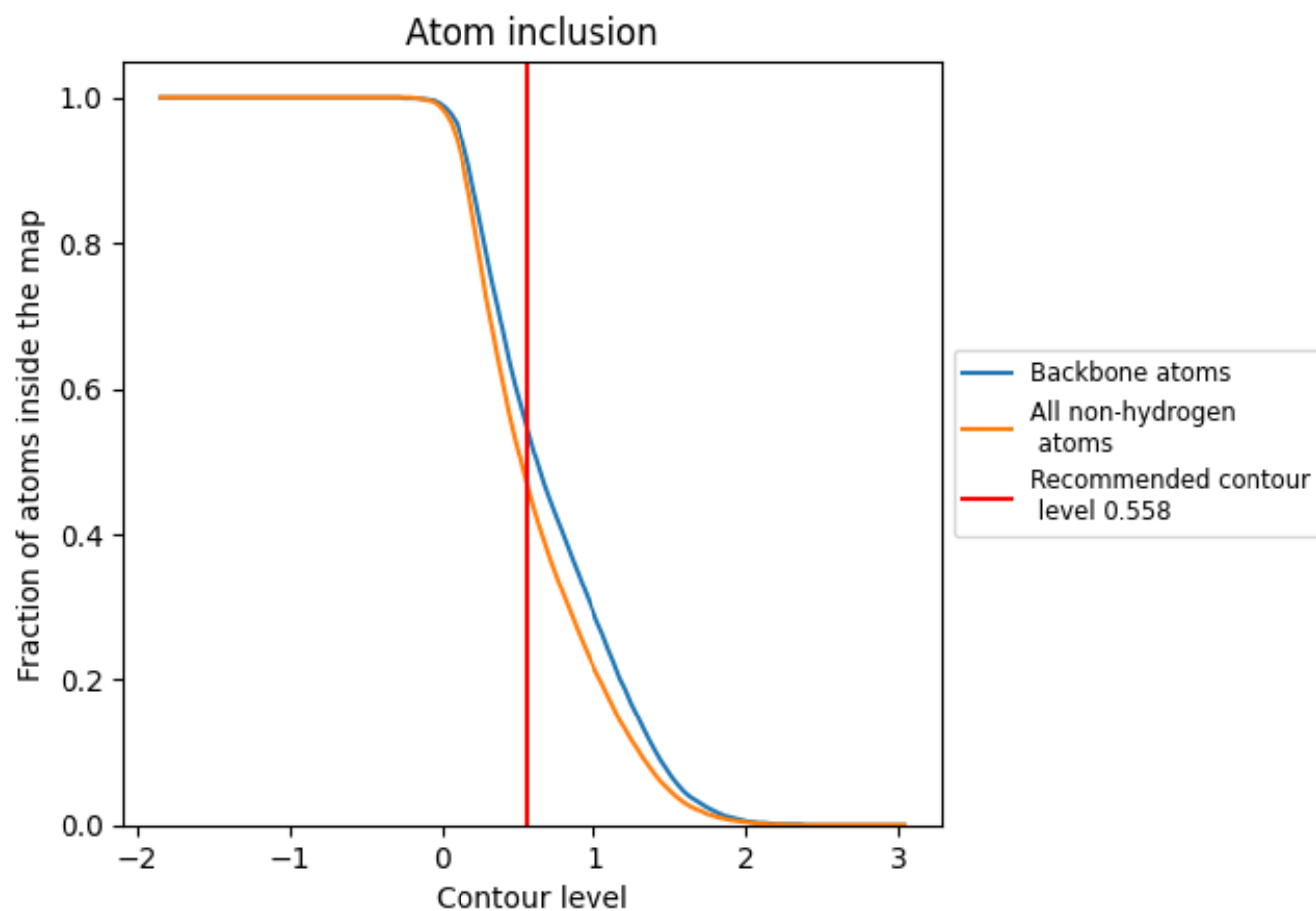
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.558).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 47% 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 (0.558) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4710	0.3560
A	0.5280	0.3920
B	0.5960	0.4180
D	0.4380	0.3340
G	0.0000	0.0540
H	0.4690	0.3850
I	0.1870	0.2420
J	0.0000	0.0480
K	0.2860	0.3250
L	0.4060	0.3150

1.0

0.0

<0.0