



# wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 05:14 PM JST

PDB ID : 7XOA  
EMDB ID : EMD-33342  
Title : SARS-CoV-2 Omicron BA.2 Variant Spike Trimer with one mouse ACE2 Bound  
Authors : Xu, Y.; Wu, C.; Liu, H.; Yin, W.; Xu, H.E.  
Deposited on : 2022-05-01  
Resolution : 3.20 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](mailto: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>.

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

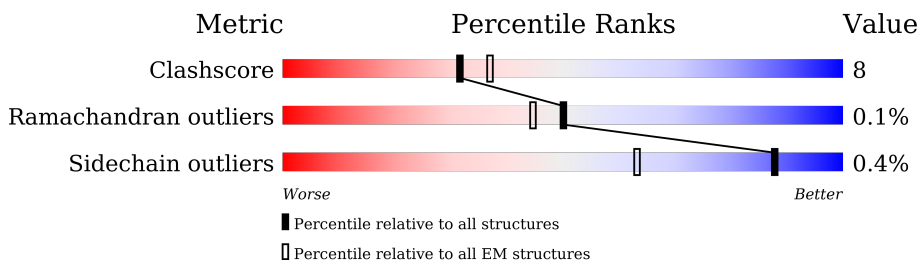
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	1270	
1	C	1270	
2	D	805	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1305	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 29202 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1026	8001	5124	1331	1511	35	0	0
1	B	1026	7950	5099	1319	1497	35	0	0
1	C	1026	7950	5099	1319	1497	35	0	0

There are 120 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	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	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
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B	478	LYS	THR	variant	UNP P0DTC2
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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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	HIS	PRO	variant	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	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	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
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
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C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2

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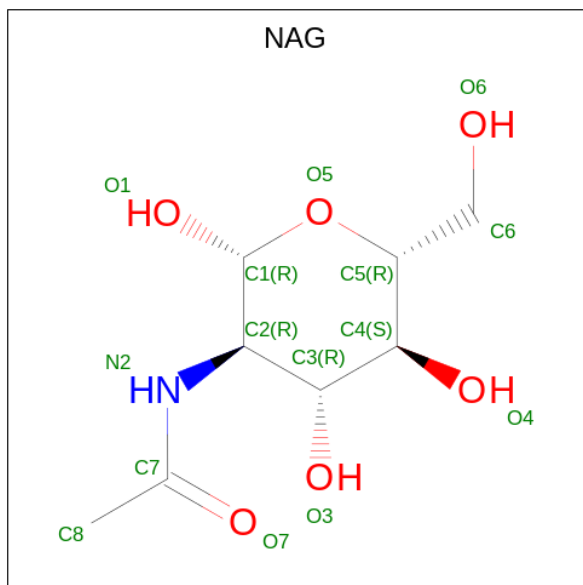
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Chain	Residue	Modelled	Actual	Comment	Reference
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	592	4824	3073	809	913	29	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	C	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0
3	D	1	Total 14	C 8	N 1	O 5	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

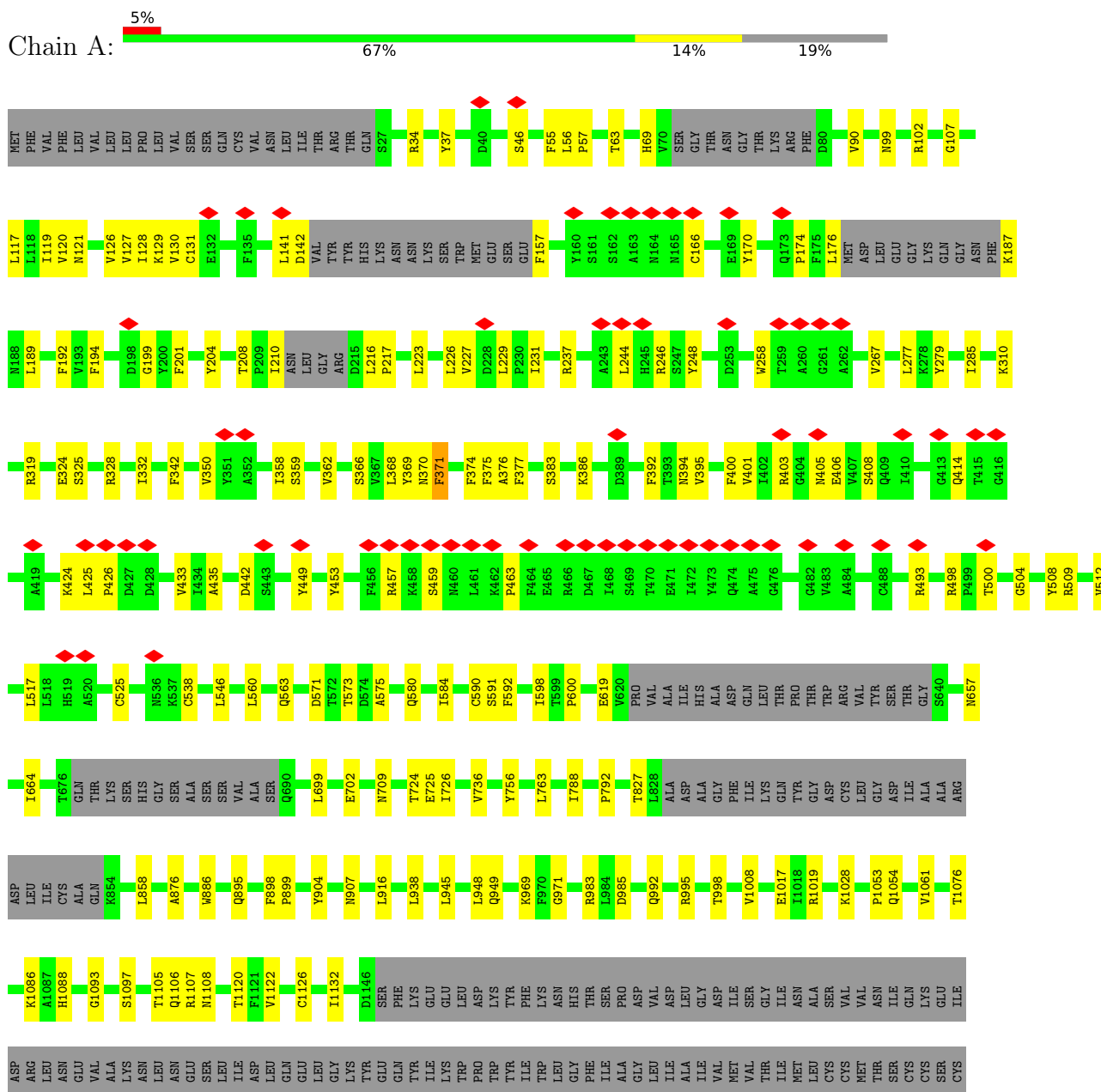
Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total 1	Zn 1	0



# 3 Residue-property plots (i)

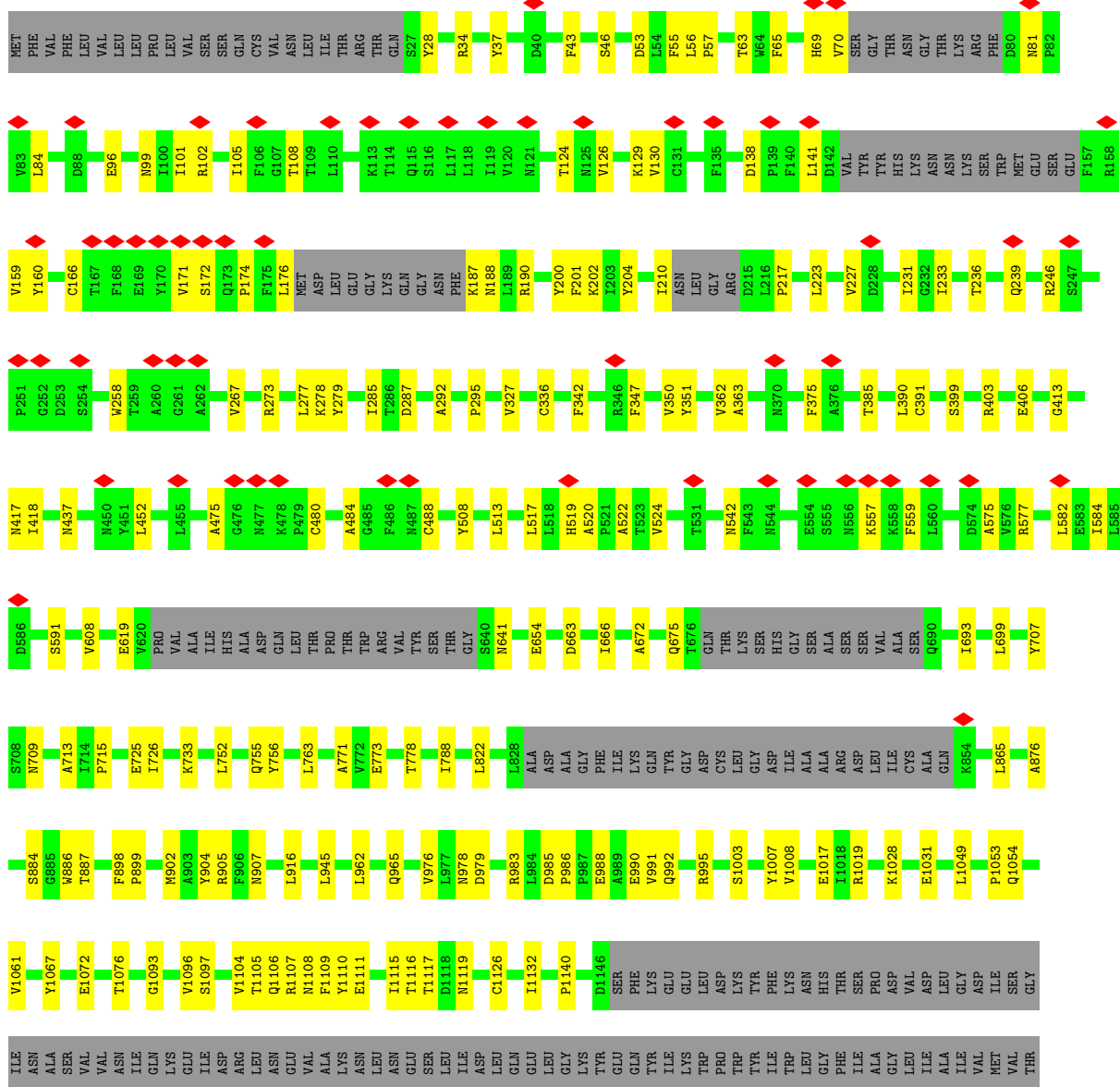
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



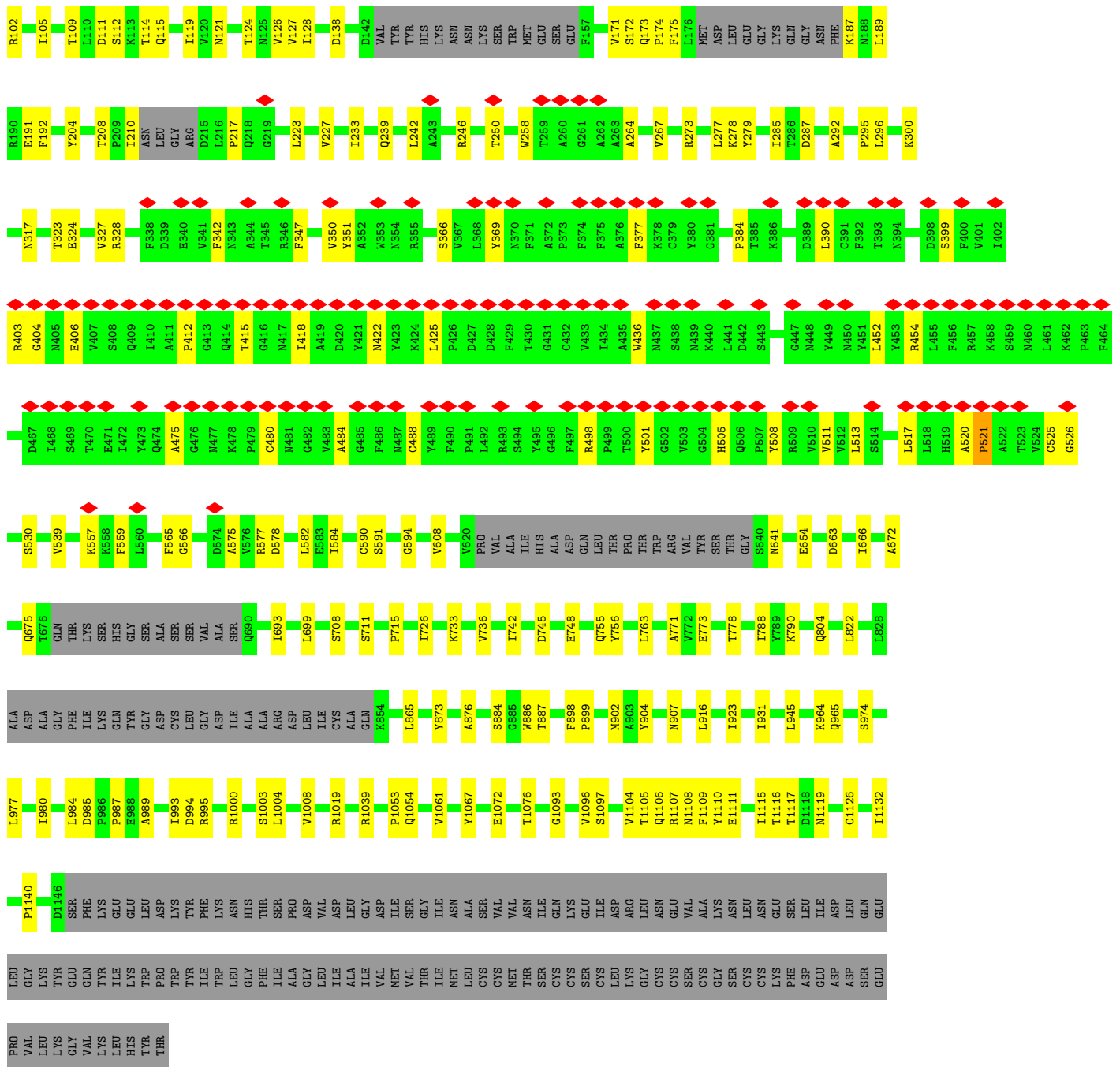
LEU  
LYS  
PHE  
GLY  
CYS  
CYS  
SER  
CYS  
CYS  
GLY  
SER  
CYS  
CYS  
PHE  
ASP  
GLU  
ASP  
ASP  
SER  
SER  
GLU  
GLU  
PRO  
VAL  
VAL  
LYS  
LYS  
GLN  
VAL  
GLY  
VAL  
LYS

• Molecule 1: Spike glycoprotein

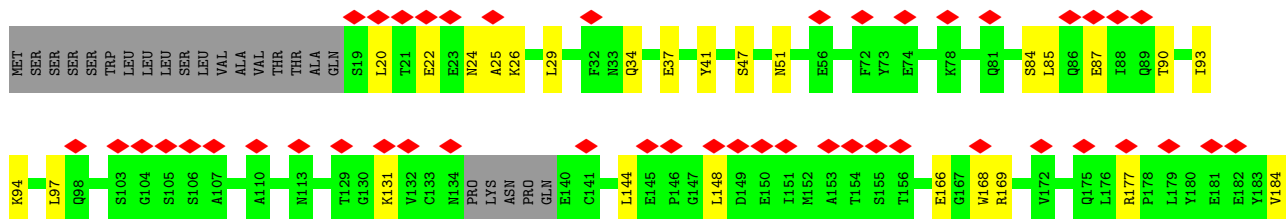


• Molecule 1: Spike glycoprotein





● Molecule 2: Angiotensin-converting enzyme 2



V185	M188	E189	M190	A191	R192	A193	M194	M195	Y196	M197	D198	Y199	G200	G205	E208	A209	E210	G211	A212	D213	G214	Y215	N216	Y217	N218	R219	N220	Q221	L222	I223	E224	E227	R228	A231	E232	L233	K234	P235	L236	Y237	E238	H239	L240	H241	A242	Y243	V244	R245	R246	K247	L248	M249	D250	T251			
Y252	P253	S254	P258	T259	G260	L267	R273	F274	L278	Y279	P280	L281	T282	V283	P284	F285	A286	Q287	K288	P289	N290	I291	D292	Q300	G301	W302	D303	A304	F314	G319	L320	P321	H322	M323	A329	D338	G339	R340	V343	C344	H345	P346	T347	A348	W349	D350											
L351	G352	H353	G354	R357	I358	K359	M360	C361	T362	K363	V364	T365	M366	D367	N368	E375	Q380	Y381	A386	R387	Q388	P389	L392	G395	E398	H401	V404	M408	P415	S420	I421	P425	S426	D427	F428	Q429	E430	D431	S432	E433	T434	E435	T436	M437	F438	L439											
Q442	I446	L450	P451	M455	L456	E457	K458	W459	R460	W461	M462	V463	F464	R465	G466	E467	I468	P469	K470	E471	Q472	W473	M474	K475	M480	K481	R482	E483	I484	W485	E489	P490	L491	P492	H493	D494	E495	T496	Y497	C498	D499	S502	H505	D509	F512	I513	R514	Y515	Y516								
T517	R518	T519	I520	Y521	Q522	F523	Q524	A532	A533	K534	Y535	N536	G537	S538	L539	H540	K541	I544	S545	Q552	K553	L554	L555	K556	M557	L558	S559	L560	G561	M562	S563	E564	P565	W566	A569	M572	V573	V574	G575	A576	R577	M578	M579	D580	V581	K582	P583	L584	L585	M586	Y587	F588	Q589	P590			
L591	F592	D593	K596	E597	Q598	N599	R600	N601	S602	F603	V604	G605	M606	N607	T608	E609	M610	S611	P612	Y613	A614	D615	GLN	SER	ILE	LYS	VAL	THR	VAL	PRO	ARG	GLY	PRO	ILE	ASN	ALA	TYR	GLU	VAL	TRP	THR	ALA	ASN	ASN	GLY	ILE	ARG	SER	SER	VAL	ALA	TYR	ALA	ALA	ALA	ALA	MET
ARG	LYS	TYR	PHE	SER	GLY	ILE	ASN	ASN	ASN	GLN	THR	VAL	VAL	ARG	VAL	VAL	ASP	ASP	TYR	LEU	LYS	GLN	PHE	ILE	ILE	LYS	THR	THR	VAL	PRO	ARG	GLY	PRO	ILE	ASN	ALA	TYR	GLU	VAL	TRP	THR	ALA	ASN	ASN	GLY	ILE	ARG	SER	SER	VAL	ALA	TYR	ALA	ALA	ALA	MET	
ASN	GLU	THR	LYS	ARG	GLU	GLU	ASN	ASN	PRO	TYR	SER	GLU	ASP	MET	ASP	ILE	GLY	LYS	GLY	GLU	SER	ASN	ASN	ALA	GLY	GLN	ASN	PRO	PRO	ASP	ASP	ASP	ALA	ALA	GLN	THR	SER	SER	PHE																		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.103	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.824, 0.824, 0.824	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, ZN

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	0.25	0/8192	0.43	0/11154
1	B	0.25	0/8141	0.44	0/11091
1	C	0.25	0/8141	0.42	0/11091
2	D	0.23	0/4956	0.37	0/6726
All	All	0.25	0/29430	0.42	0/40062

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	8001	0	7796	150	0
1	B	7950	0	7718	156	0
1	C	7950	0	7717	147	0
2	D	4824	0	4592	57	0
3	A	154	0	143	14	0
3	B	140	0	130	0	0
3	C	154	0	143	0	0
3	D	28	0	26	1	0
4	D	1	0	0	0	0
All	All	29202	0	28265	483	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 8.

The worst 5 of 483 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:375:PHE:CZ	1:B:508:TYR:HE2	1.14	1.60
1:B:375:PHE:HZ	1:B:508:TYR:CE2	1.27	1.51
1:C:577:ARG:NH2	1:C:582:LEU:CD1	1.90	1.35
1:B:375:PHE:CZ	1:B:508:TYR:CE2	2.06	1.31
1:B:336:CYS:SG	1:B:363:ALA:HA	1.76	1.25

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	1010/1270 (80%)	981 (97%)	29 (3%)	0	100	100
1	B	1010/1270 (80%)	978 (97%)	31 (3%)	1 (0%)	48	80
1	C	1010/1270 (80%)	979 (97%)	30 (3%)	1 (0%)	48	80
2	D	588/805 (73%)	577 (98%)	11 (2%)	0	100	100
All	All	3618/4615 (78%)	3515 (97%)	101 (3%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	521	PRO
1	B	520	ALA

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	890/1110 (80%)	884 (99%)	6 (1%)	81	92
1	B	875/1110 (79%)	873 (100%)	2 (0%)	92	97
1	C	875/1110 (79%)	873 (100%)	2 (0%)	92	97
2	D	516/707 (73%)	512 (99%)	4 (1%)	79	90
All	All	3156/4037 (78%)	3142 (100%)	14 (0%)	88	94

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1067	TYR
1	C	873	TYR
2	D	592	PHE
2	D	381	TYR
2	D	489	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	542	ASN
1	C	1119	ASN
1	C	641	ASN
1	C	895	GLN
2	D	60	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](#)

Of 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 for Mogul analysis.

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	$\# Z  > 2$
3	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	C	1309	1	14,14,15	0.44	0	17,19,21	0.44	0
3	NAG	C	1302	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	A	1305	-	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	C	1307	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	B	1304	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	A	1308	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	B	1310	1	14,14,15	0.48	0	17,19,21	1.25	1 (5%)
3	NAG	C	1305	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	1311	1	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
3	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.40	0
3	NAG	C	1303	1	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	A	1310	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	A	1306	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	B	1308	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	C	1304	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	1310	1	14,14,15	0.31	0	17,19,21	0.38	0
3	NAG	B	1303	1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	A	1311	1	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	C	1306	1	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	D	902	2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	B	1309	1	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	D	903	2	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.45	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
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	-	-	3/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	D	902	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	D	903	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1310	NAG	C1-O5-C5	4.78	118.66	112.19
3	C	1311	NAG	C1-O5-C5	2.10	115.03	112.19

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1311	NAG	C8-C7-N2-C2
3	C	1311	NAG	O7-C7-N2-C2
3	B	1307	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1305	NAG	14	0
3	D	903	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

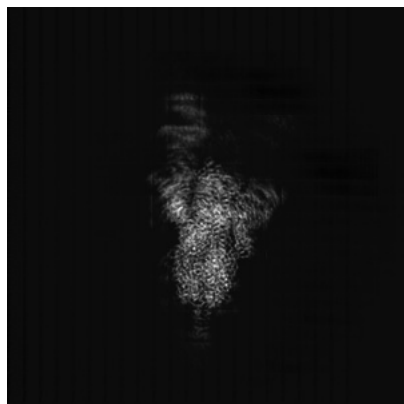
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33342. These allow visual inspection of the internal detail of the map and identification of artifacts.

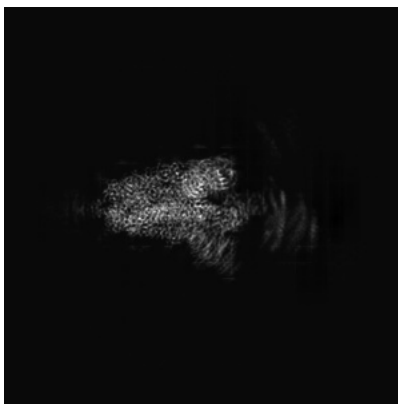
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

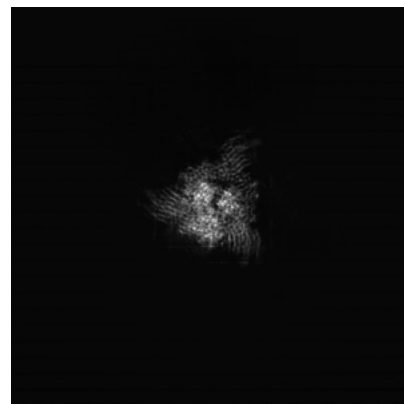
#### 6.1.1 Primary map



X

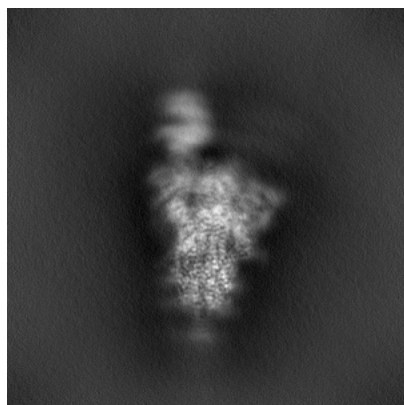


Y

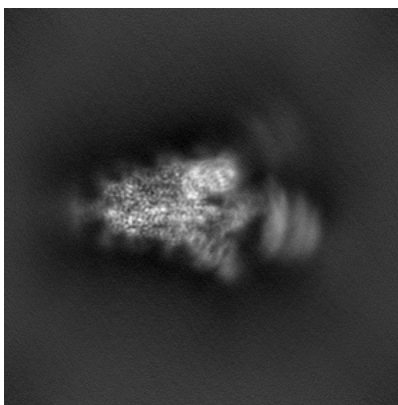


Z

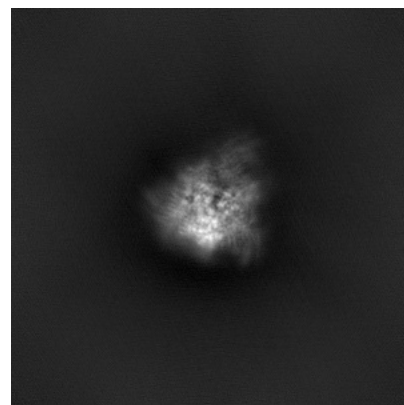
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

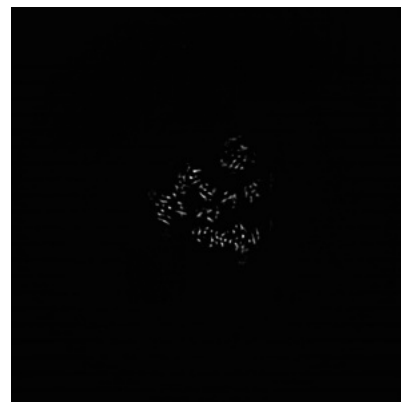
### 6.2.1 Primary map



X Index: 240



Y Index: 240

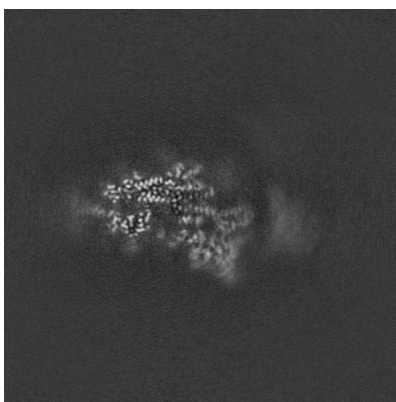


Z Index: 240

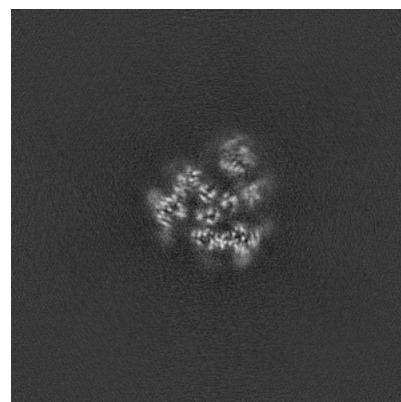
### 6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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: 229



Y Index: 244

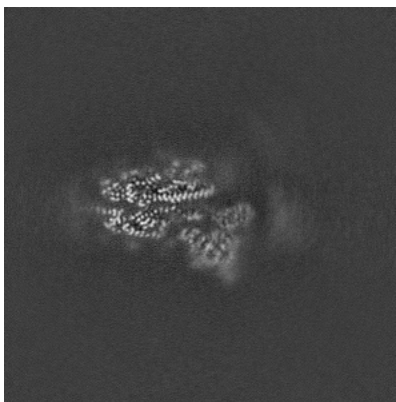


Z Index: 235

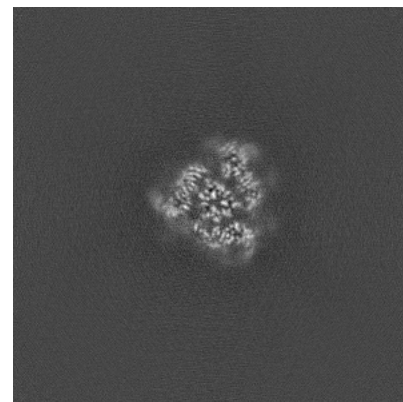
### 6.3.2 Raw map



X Index: 238



Y Index: 244



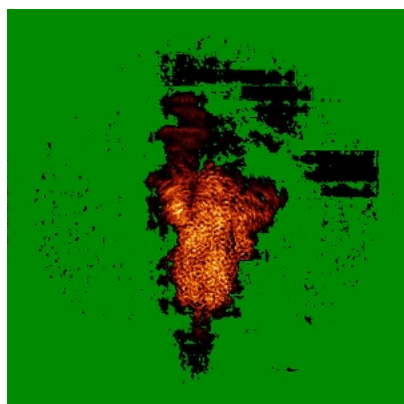
Z Index: 229

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

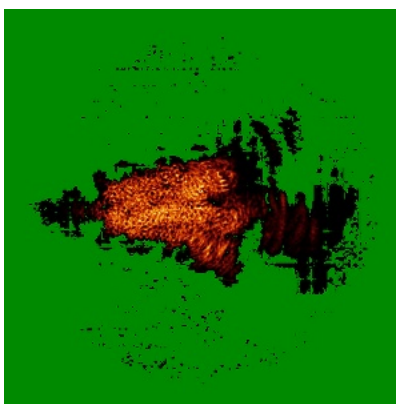


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

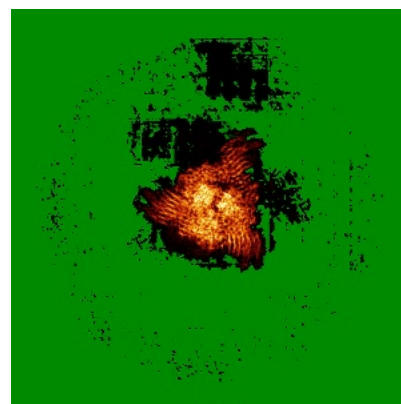
### 6.4.1 Primary map



X



Y

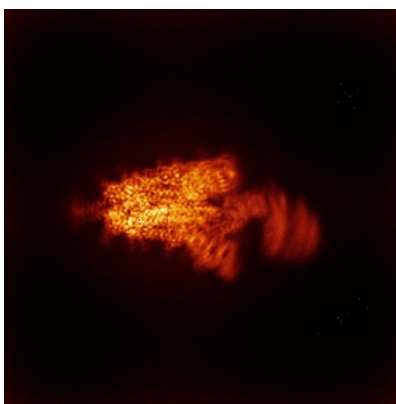


Z

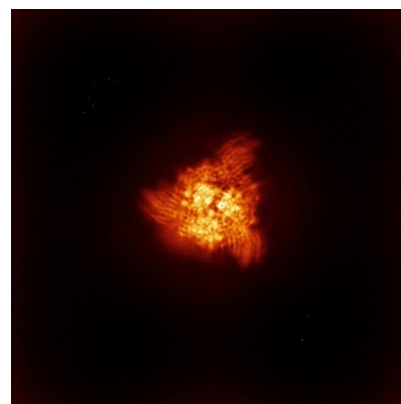
### 6.4.2 Raw map



X



Y



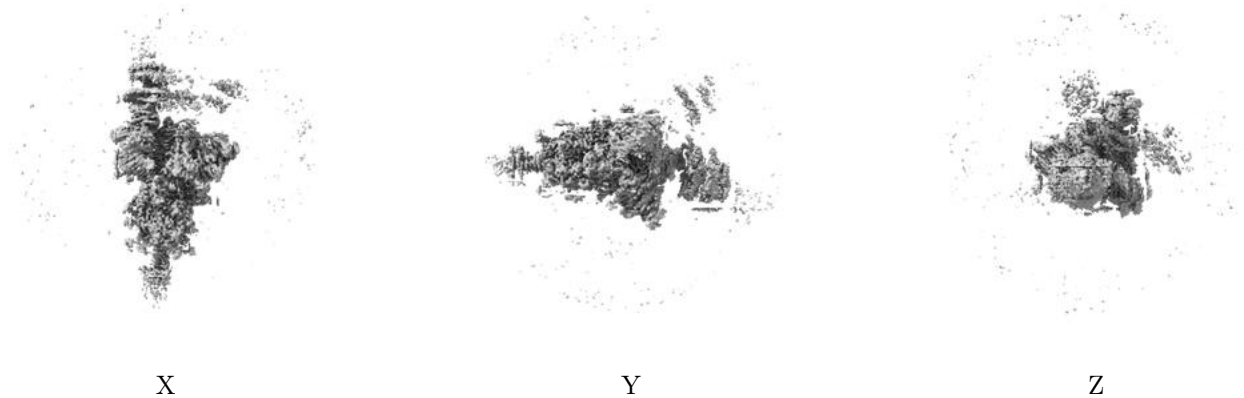
Z

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.



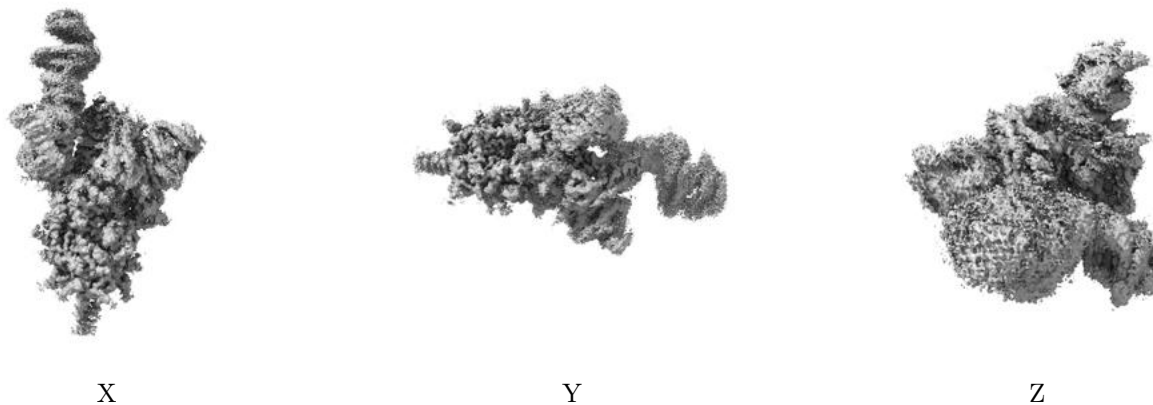
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

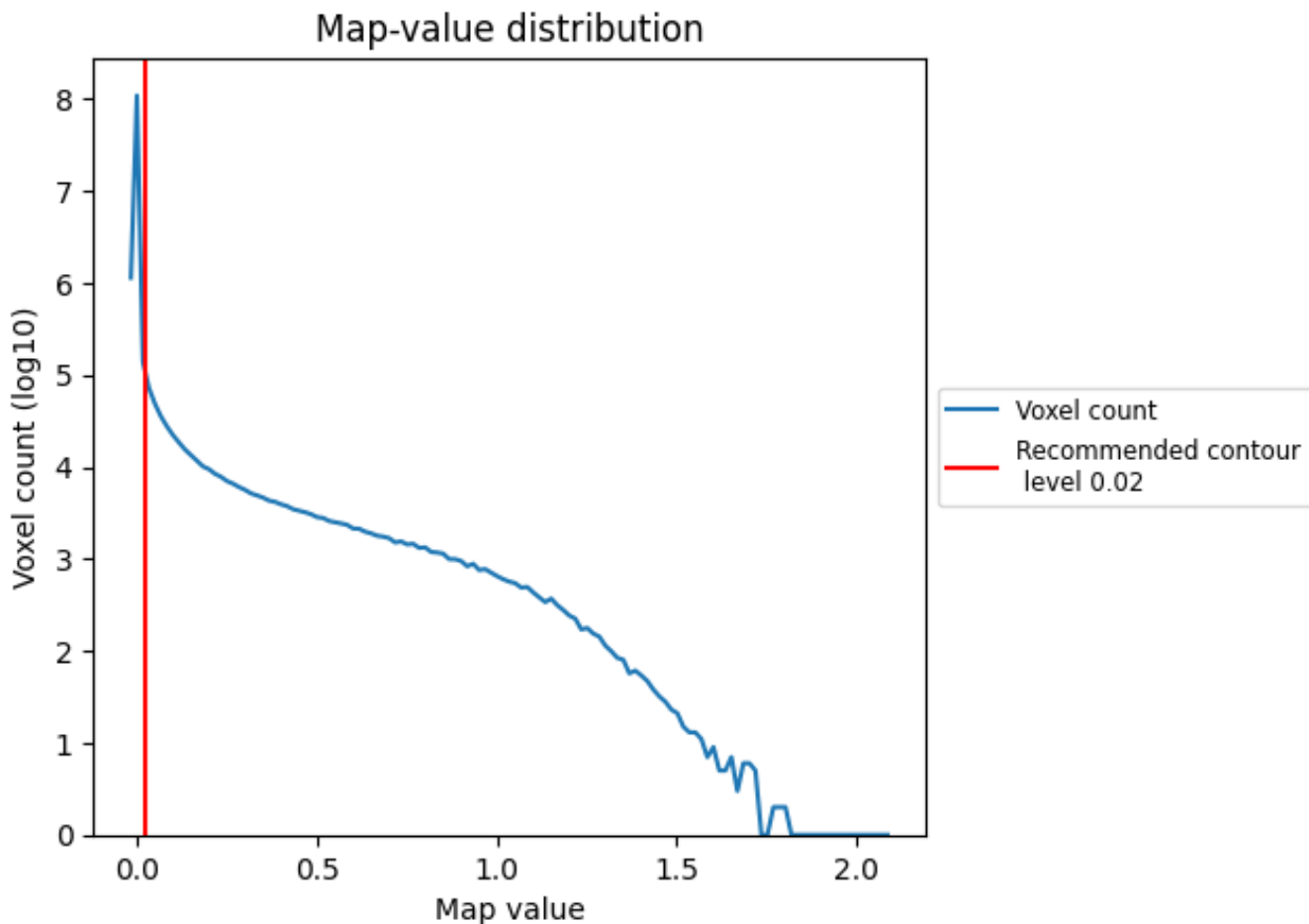
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

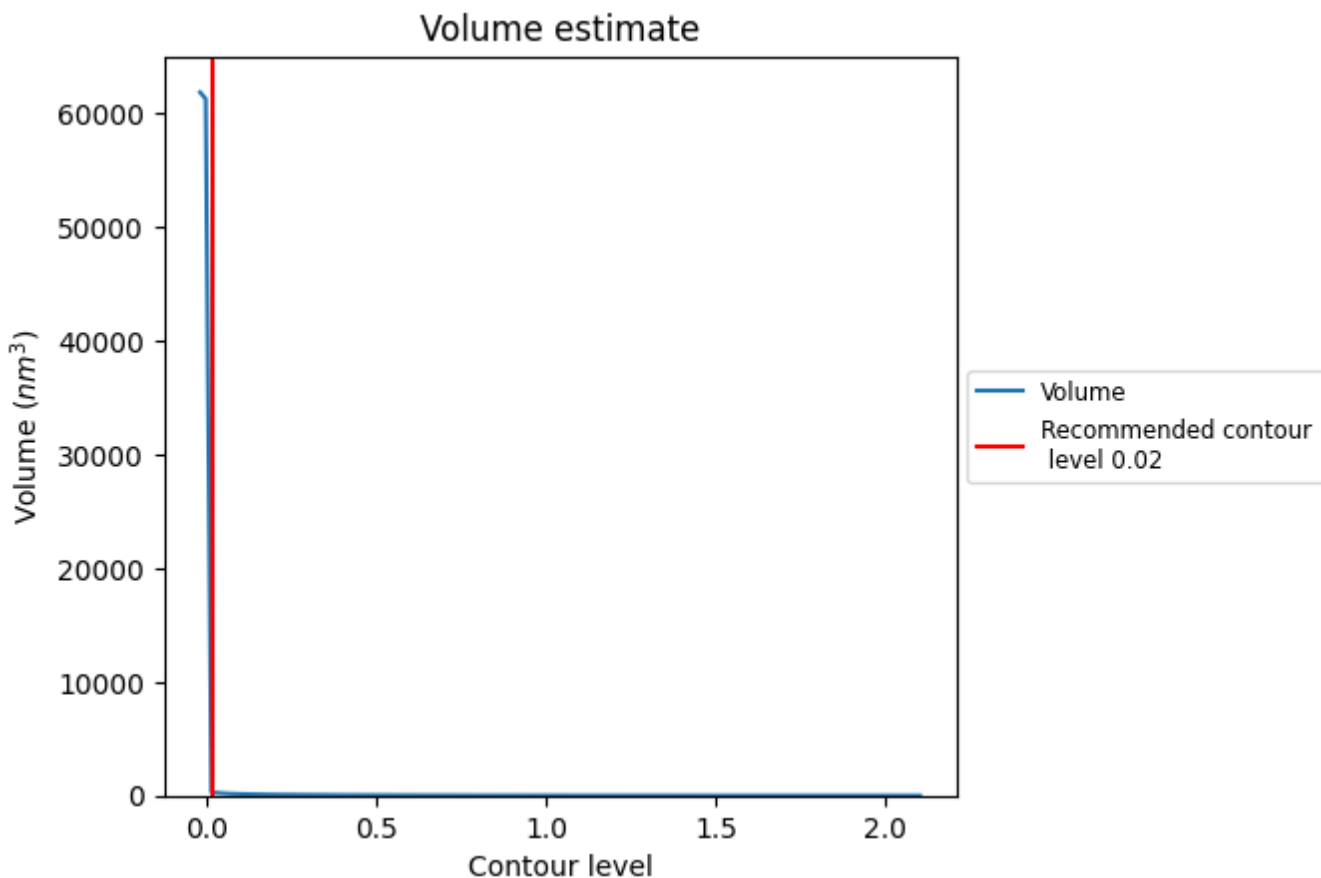
This section contains the results of statistical analysis of the map.

### 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.

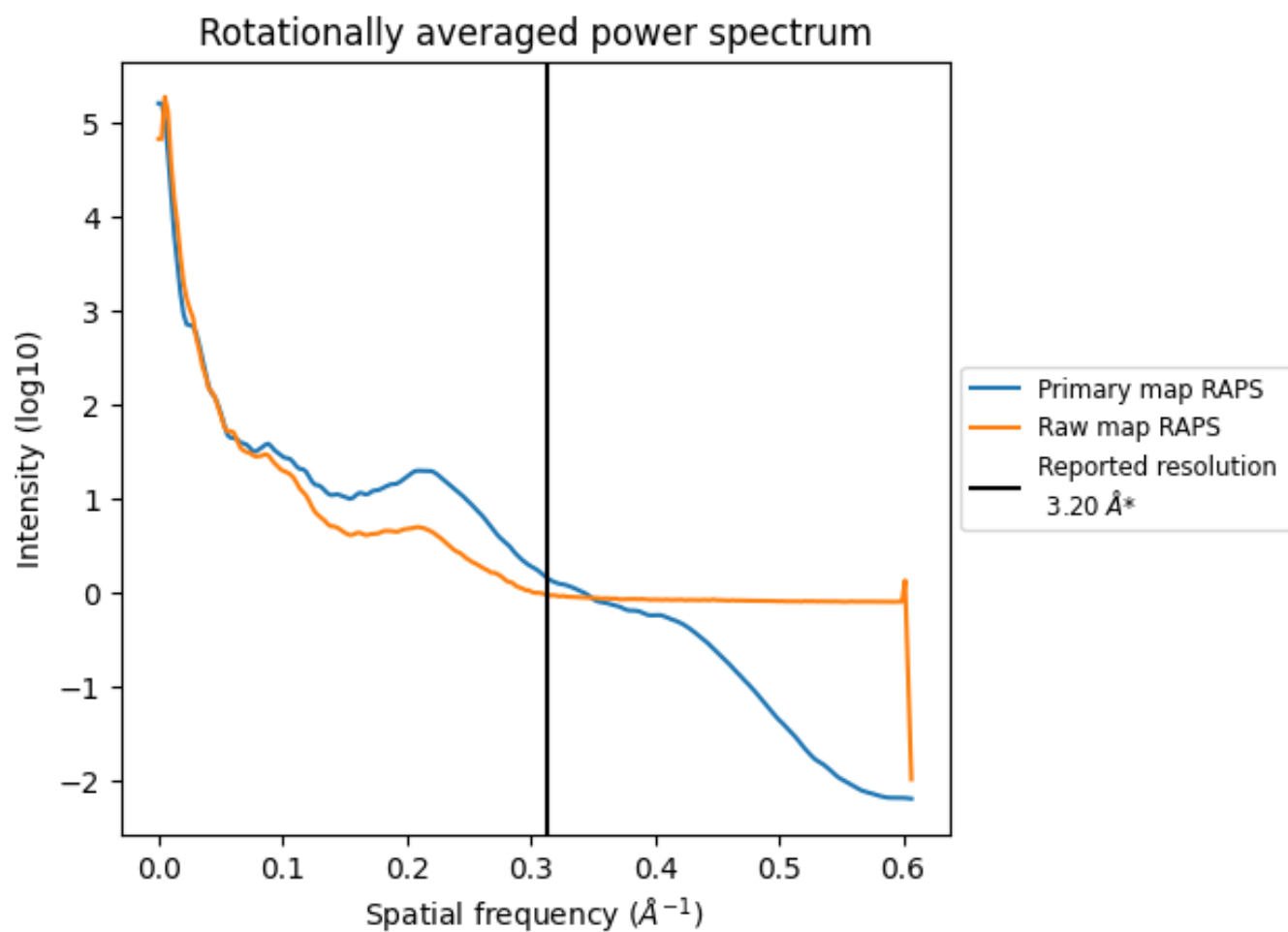
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm<sup>3</sup>; this corresponds to an approximate mass of 264 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

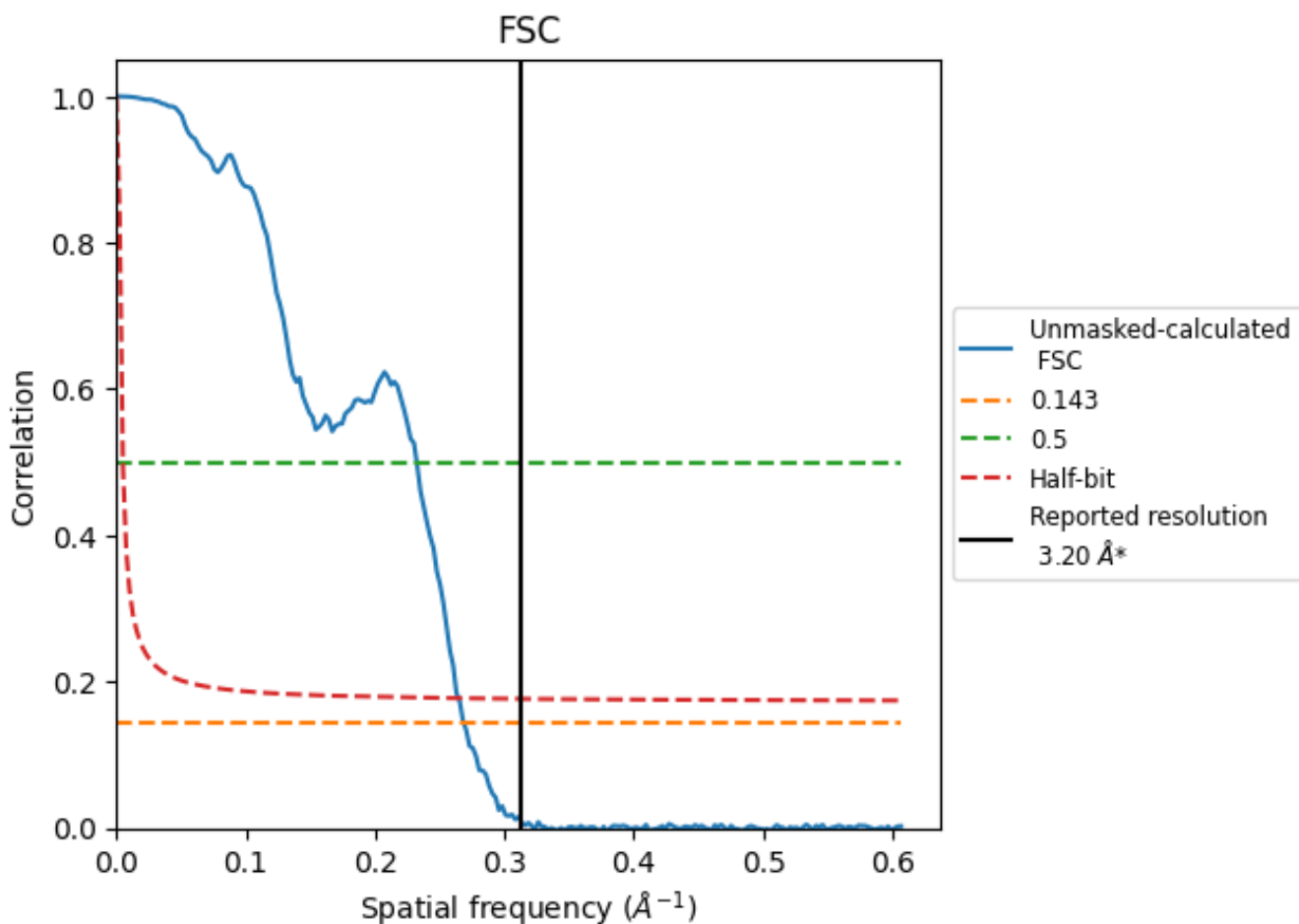


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.31	3.78

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.72 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

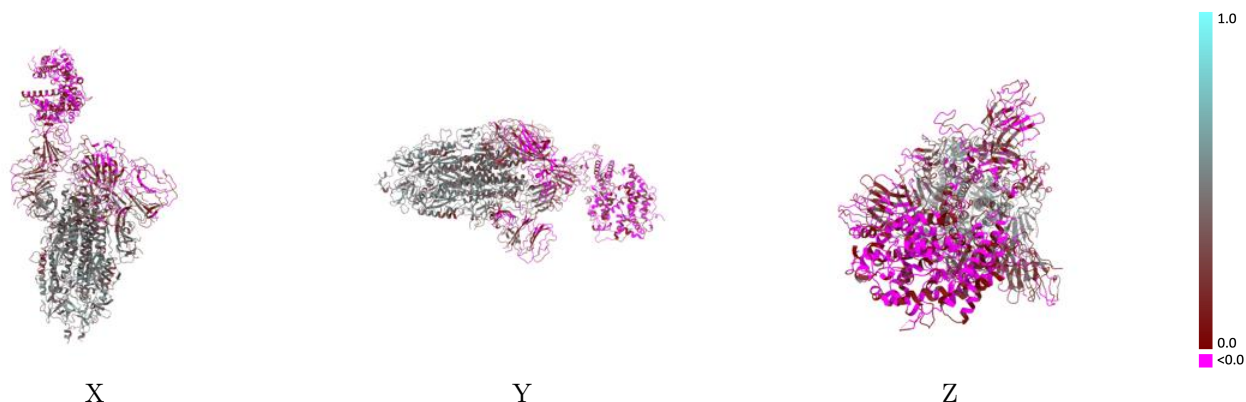
This section contains information regarding the fit between EMDB map EMD-33342 and PDB model 7XOA. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



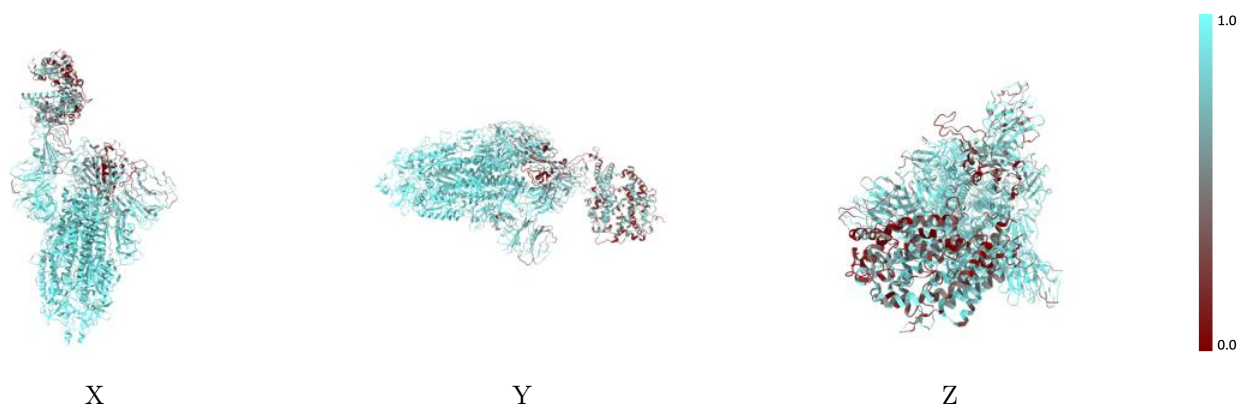
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

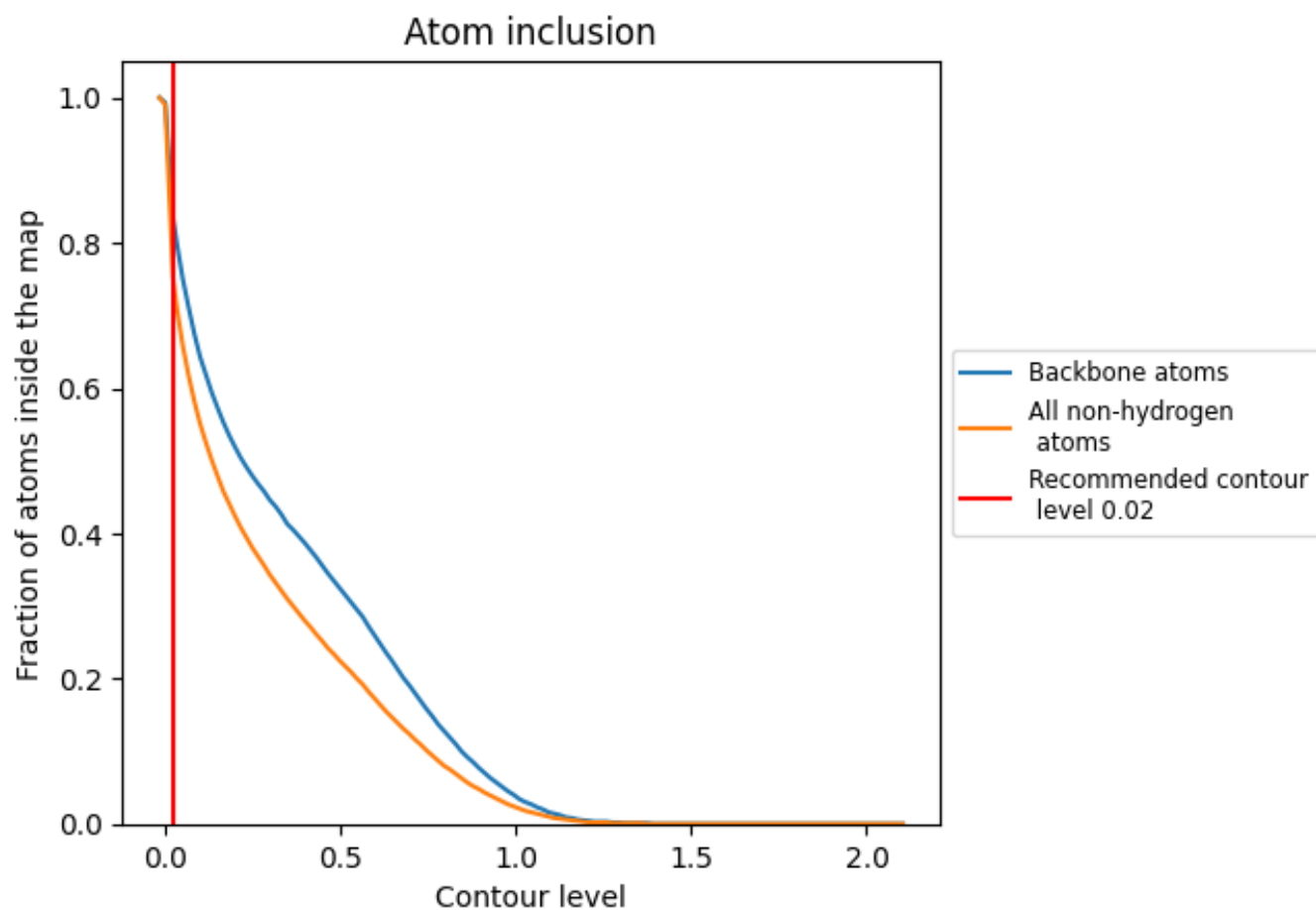
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



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 (0.02).













## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7520	 0.2530
A	 0.8140	 0.2940
B	 0.8310	 0.3120
C	 0.7730	 0.3060
D	 0.4810	 -0.0030

