



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 09:25 PM UTC

PDB ID : 7YBN / pdb_00007ybn
EMDB ID : EMD-33727
Title : SARS-CoV-2 C.1.2 variant spike (Open state)
Authors : Wang, X.; Fu, W.
Deposited on : 2022-06-29
Resolution : 3.82 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

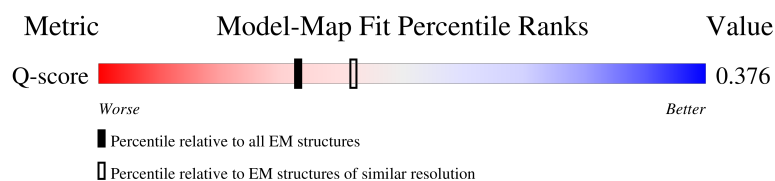
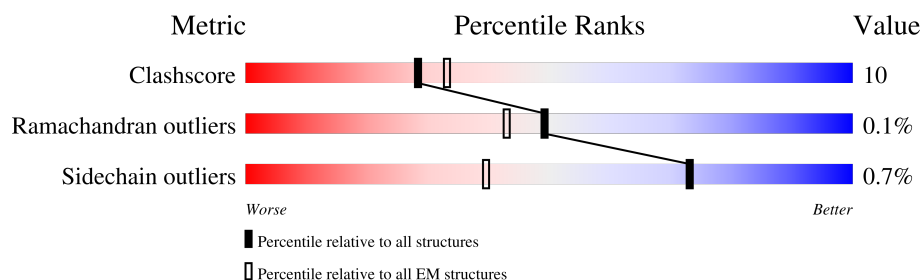
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.82 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	9152 (3.32 - 4.32)

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	1271	
1	B	1271	
1	C	1271	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25301 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	1079	Total	C	N	O	S	0	0
			8439	5395	1402	1604	38		
1	B	1077	Total	C	N	O	S	0	0
			8434	5396	1400	1601	37		
1	C	1076	Total	C	N	O	S	0	0
			8428	5391	1398	1602	37		

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PHE	LEU	variant	UNP P0DTC2
A	136	PHE	CYS	variant	UNP P0DTC2
A	190	SER	ARG	variant	UNP P0DTC2
A	215	GLY	ASP	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	447	HIS	TYR	variant	UNP P0DTC2
A	482	LYS	GLU	variant	UNP P0DTC2
A	499	TYR	ASN	variant	UNP P0DTC2
A	612	GLY	ASP	variant	UNP P0DTC2
A	653	TYR	HIS	variant	UNP P0DTC2
A	677	LYS	ASN	variant	UNP P0DTC2
A	714	ILE	THR	variant	UNP P0DTC2
A	857	ASN	THR	variant	UNP P0DTC2
A	890	PRO	ALA	engineered mutation	UNP P0DTC2
A	897	PRO	ALA	engineered mutation	UNP P0DTC2
A	940	PRO	ALA	engineered mutation	UNP P0DTC2
B	18	PHE	LEU	variant	UNP P0DTC2
B	136	PHE	CYS	variant	UNP P0DTC2
B	190	SER	ARG	variant	UNP P0DTC2
B	215	GLY	ASP	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	447	HIS	TYR	variant	UNP P0DTC2

Continued on next page...

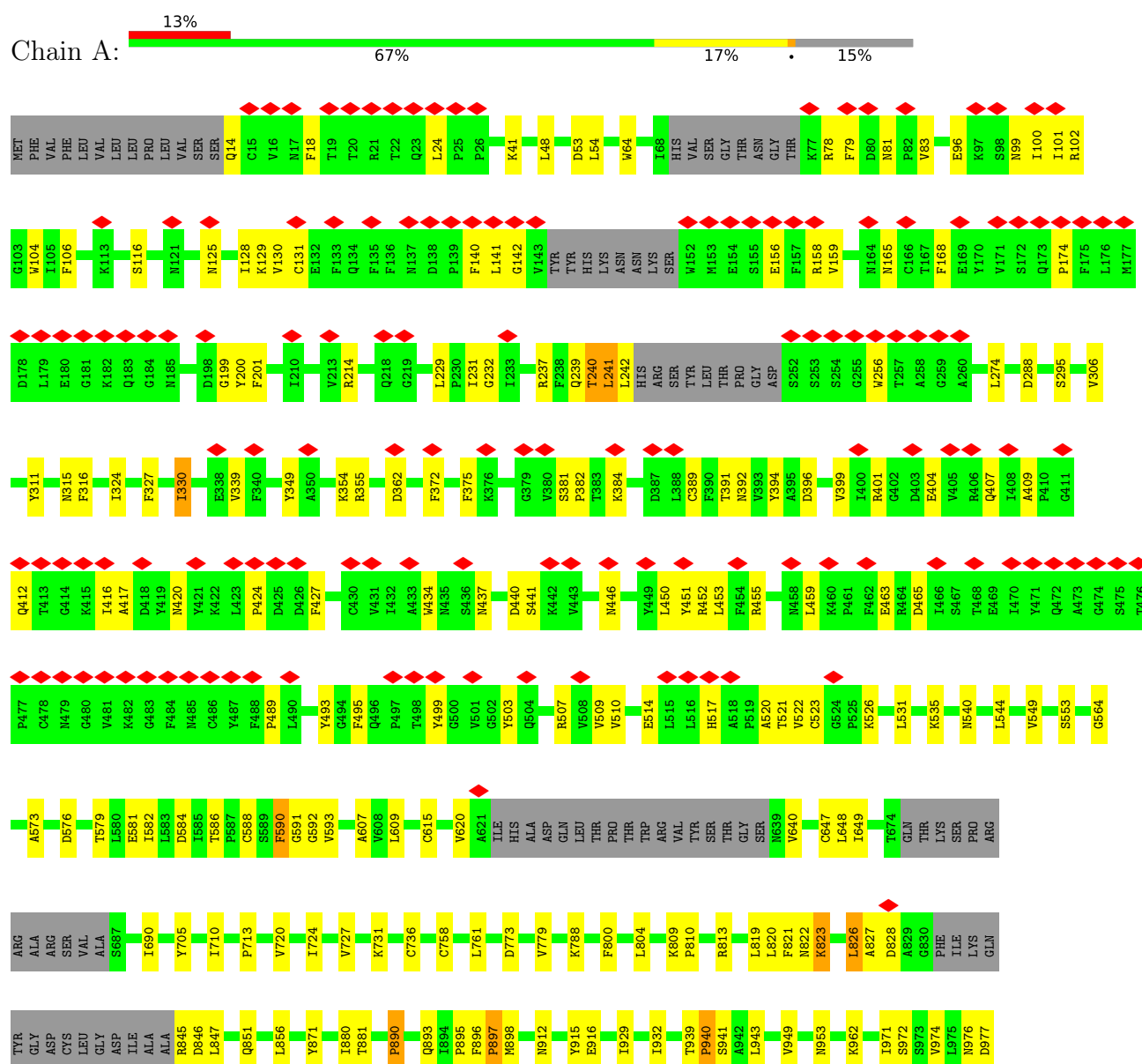
Continued from previous page...

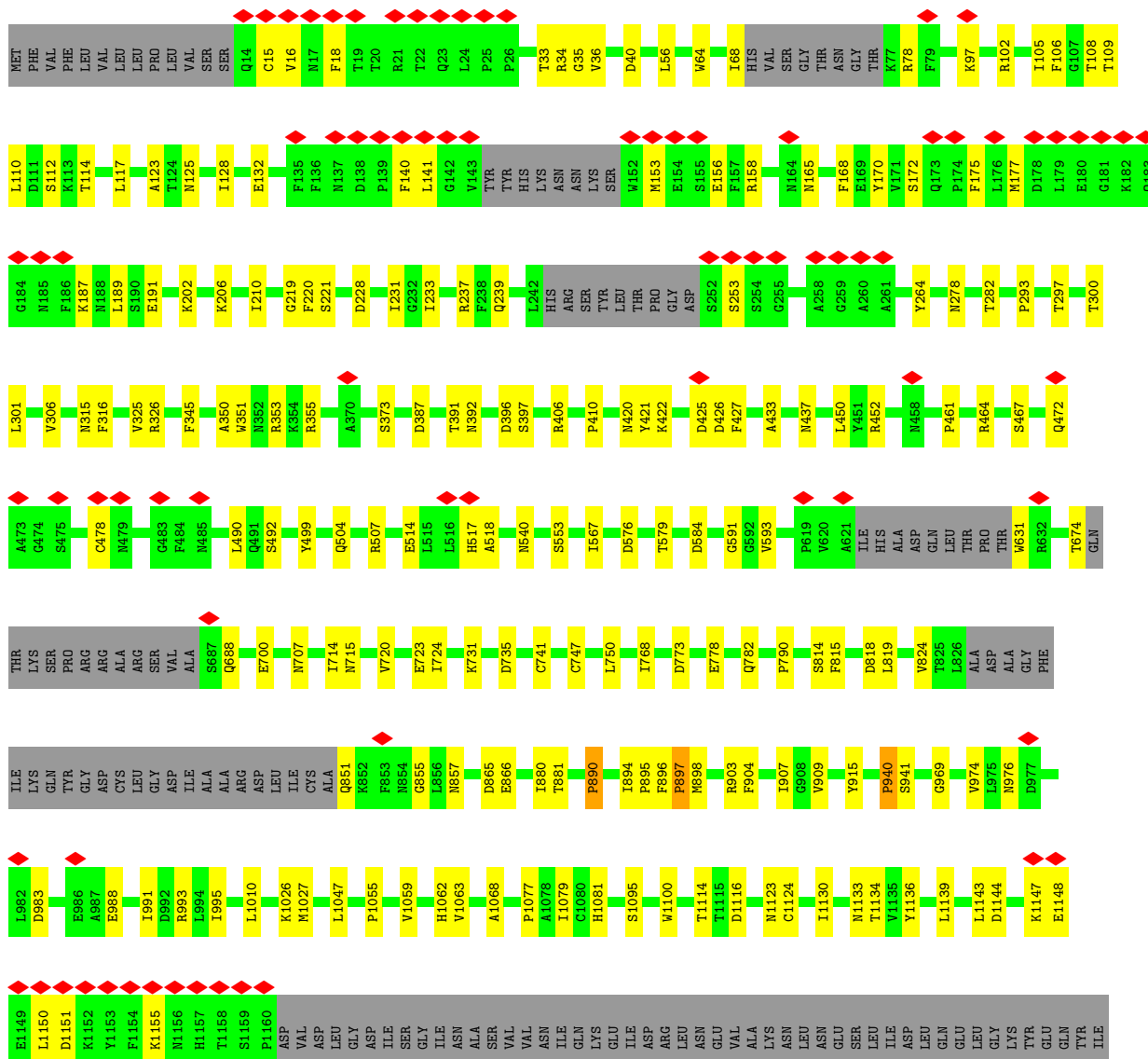
Chain	Residue	Modelled	Actual	Comment	Reference
B	482	LYS	GLU	variant	UNP P0DTC2
B	499	TYR	ASN	variant	UNP P0DTC2
B	612	GLY	ASP	variant	UNP P0DTC2
B	653	TYR	HIS	variant	UNP P0DTC2
B	677	LYS	ASN	variant	UNP P0DTC2
B	714	ILE	THR	variant	UNP P0DTC2
B	857	ASN	THR	variant	UNP P0DTC2
B	890	PRO	ALA	engineered mutation	UNP P0DTC2
B	897	PRO	ALA	engineered mutation	UNP P0DTC2
B	940	PRO	ALA	engineered mutation	UNP P0DTC2
C	18	PHE	LEU	variant	UNP P0DTC2
C	136	PHE	CYS	variant	UNP P0DTC2
C	190	SER	ARG	variant	UNP P0DTC2
C	215	GLY	ASP	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	ALA	deletion	UNP P0DTC2
C	447	HIS	TYR	variant	UNP P0DTC2
C	482	LYS	GLU	variant	UNP P0DTC2
C	499	TYR	ASN	variant	UNP P0DTC2
C	612	GLY	ASP	variant	UNP P0DTC2
C	653	TYR	HIS	variant	UNP P0DTC2
C	677	LYS	ASN	variant	UNP P0DTC2
C	714	ILE	THR	variant	UNP P0DTC2
C	857	ASN	THR	variant	UNP P0DTC2
C	890	PRO	ALA	engineered mutation	UNP P0DTC2
C	897	PRO	ALA	engineered mutation	UNP P0DTC2
C	940	PRO	ALA	engineered mutation	UNP P0DTC2

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

TRP	TRP	M898	V783	L648	H517	A261	F175	S98	MET
TYR	TYR	R903	K784	M656	C536	A262	L176	N99	PHE
TRP	TRP	I786	I786	I664	G546	T272	M177	I100	VAL
GLY	GLY	F925	F800	I664	G546	D288	D178	R102	PHE
PHE	PHE	I332	S801	A670	N554	C289	L179	G103	VAL
ILE	ILE	Q933	Q802	T674	N554	C289	E180	M104	LEU
ALA	ALA	L936	I803	G1N	E404	A290	G181	I105	LEU
GLY	GLY	S937	S937	THR	F560	L291	G182	F106	PRO
LEU	LEU	S937	S937	THR	Q561	E296	G107	T108	VAL
ASP	ASP	P810	P810	LYS	F567	T297	Q183	SER	SER
ALA	ALA	K823	K823	SER	K422	K298	G184	SER	SER
ILE	ILE	P940	V824	PRO	M437	C299	N185	L117	Q14
VAL	VAL	S941	T825	ARG	Q472	T500	F186	L118	C15
MET	MET	GLY	LEU	ARG	L450	L301	K187	V120	C15
VAL	VAL	K945	ALA	ALA	L450	E307	N188	V16	N17
THR	THR	V949	ASP	ARG	Y451	E307	N188	N121	F18
ILE	ILE	N953	ALA	VAL	R452	L310	L189	N122	F18
MET	MET	GLY	VAL	ALA	R455	Y311	I197	A123	T19
LEU	LEU	PHE	S687	ALA	R455	Y311	I197	T124	T20
CYS	CYS	ILE	ILE	ILE	C588	Q319	F201	N125	R21
CYS	CYS	K962	LYS	LYS	S594	P320	K202	I128	T22
THR	THR	V974	GLN	GLN	R464	P320	I203	K129	Q23
SER	SER	D977	TYR	L697	R464	P320	I203	V130	Q23
CYS	CYS	V1006	GLY	M701	D465	E322	F220	F133	P25
ASN	ASN	V1006	ASP	S702	L603	E322	F220	F133	P25
GLN	GLN	V1006	CYS	S702	L603	E322	F220	F133	P25
LYS	LYS	L1047	LEU	S709	Y610	P328	L223	N137	G35
GLY	GLY	M1048	GLY	S709	Y610	P328	L223	N137	V36
GLY	GLY	S1048	ILE	V720	N613	I330	L226	D138	Q52
CYS	CYS	F1050	ALA	V720	N613	I330	L226	D138	Q52
ASP	ASP	H1062	ALA	E723	C515	P335	D228	P139	D53
LEU	LEU	V1063	ALA	V727	E617	E338	D228	P139	D53
ASN	ASN	V1063	ARG	V727	E617	E338	D228	P139	D53
GLU	GLU	V1063	ASP	V727	E617	E338	D228	P139	D53
VAL	VAL	I1079	LEU	D735	V618	N341	L229	G142	L56
CYS	CYS	H1086	CYS	C736	P619	A342	L229	G142	L56
LYS	LYS	F1087	ALA	C736	V620	A342	L229	G142	L56
ASN	ASN	S1095	GLN	I740	ALA	F345	M234	TRR	W64
ASP	ASP	W1100	LYS	C741	ASP	A350	ASN	HIS	I68
GLU	GLU	N1133	F853	C747	GLN	V351	ASN	VAL	HIS
ASP	ASP	W1100	A874	L751	LEU	T566	LYS	GLY	VAL
SER	SER	N1133	L875	L751	T628	T566	THR	THR	THR
GLU	GLU	Q1140	L876	L761	P629	V360	ARG	GLY	ASN
VAL	VAL	L1143	A877	I768	T630	A361	THR	THR	THR
LYS	LYS	D1144	T879	Q772	W631	D362	TRR	TRR	K77
GLY	GLY	S1145	I880	Q772	W631	D362	TRR	TRR	K77
VAL	VAL	F1146	T881	Q772	W631	D362	TRR	TRR	K77
LYS	LYS	K1147	S882	Q777	T636	V366	PR0	L366	F79
LEU	LEU	E1148	S882	E778	Q504	V367	GLY	V159	D80
HIS	HIS	E1149	P895	E778	Q504	V367	GLY	V159	D80
TYR	TYR	L1150	P897	F780	S633	N368	ASP	Y160	V83
THR	THR	D1151	P897	Q782	V640	A370	S253	N165	P85

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212138	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 ($e^-/\text{\AA}^2$)	60.00	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.19	0/8635	0.38	3/11745 (0.0%)
1	B	0.13	0/8633	0.33	3/11744 (0.0%)
1	C	0.20	0/8628	0.39	3/11740 (0.0%)
All	All	0.18	0/25896	0.37	9/35229 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	940	PRO	CA-N-CD	-9.13	99.22	112.00
1	C	897	PRO	CA-N-CD	-9.10	99.26	112.00
1	A	940	PRO	CA-N-CD	-9.08	99.28	112.00
1	A	897	PRO	CA-N-CD	-9.08	99.29	112.00
1	B	897	PRO	CA-N-CD	-9.00	99.40	112.00
1	C	940	PRO	CA-N-CD	-9.00	99.40	112.00
1	C	890	PRO	CA-N-CD	-8.76	99.74	112.00
1	A	890	PRO	CA-N-CD	-8.74	99.76	112.00
1	B	890	PRO	CA-N-CD	-8.72	99.80	112.00

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	8439	0	8247	181	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8434	0	8236	146	0
1	C	8428	0	8226	173	0
All	All	25301	0	24709	475	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 10.

All (475) 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:C:18:PHE:CE2	1:C:140:PHE:CE1	1.81	1.68
1:A:18:PHE:CZ	1:A:140:PHE:CE1	1.77	1.66
1:B:18:PHE:HE2	1:B:140:PHE:CE1	1.27	1.52
1:C:18:PHE:CZ	1:C:140:PHE:CZ	2.11	1.37
1:A:18:PHE:HZ	1:A:140:PHE:CZ	1.46	1.33
1:B:18:PHE:CE2	1:B:140:PHE:CE1	2.18	1.31
1:A:18:PHE:HZ	1:A:140:PHE:CE1	1.22	1.30
1:C:18:PHE:CE2	1:C:140:PHE:HE1	1.29	1.29
1:C:18:PHE:CE2	1:C:140:PHE:CZ	2.26	1.19
1:A:18:PHE:CE2	1:A:140:PHE:HE1	1.61	1.17
1:A:315:ASN:HA	1:A:592:GLY:HA2	1.28	1.12
1:A:18:PHE:CE2	1:A:140:PHE:CE1	2.37	1.08
1:A:940:PRO:HD2	1:A:941:SER:H	1.15	1.07
1:A:18:PHE:CZ	1:A:140:PHE:CZ	2.29	1.07
1:C:18:PHE:CZ	1:C:140:PHE:HZ	1.60	1.05
1:C:940:PRO:HD2	1:C:941:SER:H	1.24	1.02
1:C:897:PRO:HD2	1:C:898:MET:H	1.25	0.99
1:B:18:PHE:CE2	1:B:140:PHE:CZ	2.53	0.97
1:A:18:PHE:CZ	1:A:140:PHE:HE1	1.38	0.95
1:C:895:PRO:C	1:C:897:PRO:HD3	1.92	0.95
1:C:18:PHE:CD2	1:C:140:PHE:CE1	2.56	0.92
1:C:18:PHE:HZ	1:C:140:PHE:HZ	1.17	0.91
1:B:897:PRO:HD2	1:B:898:MET:H	1.36	0.89
1:A:81:ASN:HD21	1:A:242:LEU:HD22	1.36	0.89
1:A:897:PRO:HD2	1:A:898:MET:H	1.34	0.87
1:B:18:PHE:CZ	1:B:140:PHE:CZ	2.62	0.87
1:A:940:PRO:HD2	1:A:941:SER:N	1.91	0.86
1:A:895:PRO:C	1:A:897:PRO:HD3	2.05	0.81
1:B:18:PHE:HE2	1:B:140:PHE:CD1	1.97	0.81
1:A:83:VAL:HG12	1:A:237:ARG:HG2	1.61	0.81
1:C:896:PHE:N	1:C:897:PRO:HD3	1.97	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:OE2	1:A:517:HIS:ND1	2.14	0.79
1:C:895:PRO:C	1:C:897:PRO:CD	2.55	0.78
1:A:104:TRP:HA	1:A:240:THR:HA	1.65	0.78
1:C:895:PRO:HB2	1:C:897:PRO:HD3	1.65	0.78
1:C:18:PHE:HE2	1:C:140:PHE:CE1	1.57	0.77
1:B:895:PRO:C	1:B:897:PRO:HD3	2.10	0.77
1:B:896:PHE:N	1:B:897:PRO:HD3	2.01	0.77
1:A:897:PRO:HD2	1:A:898:MET:N	2.00	0.76
1:A:896:PHE:N	1:A:897:PRO:HD3	2.00	0.76
1:B:897:PRO:HD2	1:B:898:MET:N	2.00	0.76
1:C:18:PHE:HZ	1:C:158:ARG:HH11	1.34	0.75
1:C:897:PRO:HD2	1:C:898:MET:N	1.96	0.75
1:C:450:LEU:HD12	1:C:490:LEU:HB3	1.68	0.75
1:A:895:PRO:HB2	1:A:897:PRO:CD	2.18	0.73
1:B:18:PHE:CE2	1:B:140:PHE:CD1	2.76	0.72
1:B:68:ILE:H	1:B:78:ARG:HB2	1.54	0.72
1:B:1079:ILE:HD11	1:B:1133:ASN:HB3	1.71	0.72
1:C:18:PHE:HE2	1:C:140:PHE:HE1	0.77	0.71
1:A:1150:LEU:HD13	1:C:1150:LEU:HD11	1.71	0.71
1:C:895:PRO:HB2	1:C:897:PRO:CD	2.20	0.71
1:A:99:ASN:O	1:A:102:ARG:NH1	2.24	0.70
1:A:940:PRO:CD	1:A:941:SER:H	1.98	0.70
1:A:949:VAL:O	1:A:953:ASN:ND2	2.23	0.70
1:C:940:PRO:HD2	1:C:941:SER:N	1.94	0.70
1:C:1079:ILE:HD11	1:C:1133:ASN:HB3	1.73	0.70
1:C:940:PRO:CD	1:C:941:SER:H	2.03	0.70
1:A:324:ILE:HD11	1:A:531:LEU:HA	1.73	0.69
1:A:590:PHE:CZ	1:B:855:GLY:HA2	2.27	0.69
1:C:18:PHE:HZ	1:C:158:ARG:NH1	1.89	0.69
1:A:130:VAL:HG12	1:A:168:PHE:HB3	1.75	0.69
1:A:895:PRO:HB2	1:A:897:PRO:HD3	1.74	0.69
1:B:450:LEU:HD12	1:B:490:LEU:HG	1.75	0.69
1:A:315:ASN:HA	1:A:592:GLY:CA	2.16	0.68
1:A:895:PRO:C	1:A:897:PRO:CD	2.66	0.68
1:A:420:ASN:HB3	1:A:452:ARG:HD2	1.76	0.68
1:B:895:PRO:C	1:B:897:PRO:CD	2.67	0.68
1:A:1079:ILE:HD11	1:A:1133:ASN:HB3	1.77	0.67
1:C:401:ARG:HH22	1:C:494:GLY:H	1.41	0.67
1:A:731:LYS:NZ	1:A:773:ASP:OD2	2.29	0.66
1:A:823:LYS:HG3	1:A:943:LEU:HD22	1.78	0.66
1:A:381:SER:H	1:A:384:LYS:HE3	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:PRO:CD	1:C:898:MET:H	2.06	0.66
1:B:301:LEU:HD22	1:B:306:VAL:HG12	1.78	0.66
1:C:391:THR:OG1	1:C:514:GLU:OE2	2.12	0.66
1:C:450:LEU:HB3	1:C:490:LEU:HD12	1.77	0.66
1:A:553:SER:HB2	1:A:584:ASP:HB2	1.77	0.66
1:C:949:VAL:O	1:C:953:ASN:ND2	2.29	0.66
1:B:18:PHE:HZ	1:B:140:PHE:CZ	2.14	0.65
1:A:389:CYS:HA	1:A:523:CYS:HB3	1.77	0.65
1:A:315:ASN:CA	1:A:592:GLY:HA2	2.18	0.65
1:A:813:ARG:HD2	1:A:821:PHE:CE2	2.32	0.65
1:B:1114:THR:OG1	1:B:1116:ASP:OD1	2.15	0.65
1:A:14:GLN:HB2	1:A:158:ARG:HG2	1.79	0.65
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.78	0.64
1:B:350:ALA:HA	1:B:464:ARG:HD3	1.79	0.64
1:C:68:ILE:H	1:C:78:ARG:HB2	1.62	0.64
1:A:288:ASP:O	1:A:295:SER:OG	2.13	0.64
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.80	0.64
1:C:351:TRP:O	1:C:464:ARG:NH1	2.31	0.64
1:B:778:GLU:O	1:B:782:GLN:NE2	2.31	0.64
1:A:890:PRO:HD2	1:A:890:PRO:O	1.98	0.63
1:C:628:THR:O	1:C:631:TRP:HD1	1.81	0.63
1:C:940:PRO:CD	1:C:941:SER:N	2.61	0.63
1:B:897:PRO:CD	1:B:898:MET:H	2.11	0.63
1:C:890:PRO:HD2	1:C:890:PRO:O	1.99	0.63
1:B:890:PRO:HD2	1:B:890:PRO:O	1.98	0.63
1:A:940:PRO:CD	1:A:941:SER:N	2.60	0.63
1:A:48:LEU:HD23	1:A:274:LEU:HD21	1.80	0.62
1:C:903:ARG:NH1	1:C:1047:LEU:O	2.32	0.62
1:B:903:ARG:NH1	1:B:1047:LEU:O	2.33	0.62
1:B:472:GLN:HG3	1:B:478:CYS:HB3	1.81	0.62
1:C:1140:GLN:O	1:C:1144:ASP:N	2.29	0.62
1:A:897:PRO:CD	1:A:898:MET:H	2.10	0.62
1:B:851:GLN:N	1:B:857:ASN:OD1	2.33	0.61
1:B:593:VAL:HG11	1:B:631:TRP:HZ2	1.65	0.61
1:A:96:GLU:OE2	1:A:100:ILE:N	2.24	0.61
1:C:896:PHE:N	1:C:897:PRO:CD	2.63	0.61
1:B:108:THR:HG23	1:B:109:THR:HG23	1.81	0.61
1:A:1114:THR:OG1	1:A:1117:ASN:OD1	2.19	0.61
1:A:375:PHE:HE2	1:A:382:PRO:HB3	1.66	0.60
1:B:450:LEU:HB3	1:B:490:LEU:HD11	1.82	0.60
1:B:896:PHE:N	1:B:897:PRO:CD	2.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG13	1:A:241:LEU:HD13	1.82	0.60
1:C:22:THR:O	1:C:78:ARG:NH2	2.35	0.60
1:C:100:ILE:O	1:C:102:ARG:NH1	2.35	0.60
1:C:99:ASN:HB2	1:C:179:LEU:HG	1.85	0.59
1:A:896:PHE:N	1:A:897:PRO:CD	2.65	0.59
1:A:1124:CYS:HB2	1:A:1130:ILE:HD13	1.85	0.59
1:B:974:VAL:HG12	1:B:976:ASN:H	1.66	0.59
1:A:897:PRO:CD	1:A:898:MET:N	2.66	0.59
1:A:609:LEU:HB2	1:A:648:LEU:HD13	1.83	0.59
1:B:406:ARG:NH2	1:C:373:SER:O	2.32	0.59
1:A:821:PHE:HE1	1:A:1054:ALA:HA	1.68	0.59
1:B:156:GLU:HB3	1:B:158:ARG:HG3	1.84	0.59
1:C:620:VAL:HA	1:C:632:ARG:HH22	1.66	0.58
1:C:897:PRO:CD	1:C:898:MET:N	2.64	0.58
1:A:851:GLN:HB2	1:A:856:LEU:HD12	1.84	0.58
1:A:452:ARG:NH2	1:A:465:ASP:O	2.37	0.58
1:C:809:LYS:HD3	1:C:810:PRO:HD2	1.86	0.58
1:B:1144:ASP:O	1:B:1148:GLU:N	2.31	0.57
1:A:229:LEU:HB3	1:A:231:ILE:HG12	1.86	0.57
1:A:880:ILE:HG13	1:A:881:THR:HG23	1.85	0.57
1:C:125:ASN:HD21	1:C:171:VAL:HG13	1.70	0.57
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.86	0.57
1:C:637:GLY:C	1:C:639:ASN:H	2.13	0.57
1:A:440:ASP:O	1:A:446:ASN:ND2	2.38	0.57
1:B:897:PRO:CD	1:B:898:MET:N	2.66	0.56
1:C:619:PRO:HB2	1:C:631:TRP:CH2	2.41	0.56
1:B:345:PHE:HD1	1:B:397:SER:HB2	1.70	0.56
1:C:21:ARG:HH11	1:C:80:ASP:HA	1.70	0.56
1:C:575:ARG:HH21	1:C:580:LEU:HD11	1.71	0.56
1:B:326:ARG:NH2	1:B:576:ASP:OD2	2.37	0.56
1:A:81:ASN:OD1	1:A:242:LEU:HD13	2.06	0.56
1:C:895:PRO:CB	1:C:897:PRO:HD3	2.36	0.56
1:C:64:TRP:HE1	1:C:262:ALA:HB1	1.71	0.55
1:B:768:ILE:HD11	1:B:1010:LEU:HD22	1.87	0.55
1:C:367:TYR:HE1	1:C:382:PRO:HB2	1.71	0.55
1:A:81:ASN:HD21	1:A:242:LEU:CD2	2.15	0.55
1:A:813:ARG:HD2	1:A:821:PHE:HE2	1.71	0.55
1:A:809:LYS:HD2	1:A:810:PRO:HD2	1.89	0.55
1:C:83:VAL:HG12	1:C:237:ARG:HE	1.72	0.55
1:A:459:LEU:HD13	1:A:463:GLU:HB3	1.88	0.54
1:C:18:PHE:CZ	1:C:158:ARG:NH1	2.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ASP:C	1:C:290:ALA:H	2.15	0.54
1:B:420:ASN:HD21	1:B:452:ARG:HB2	1.72	0.54
1:A:404:GLU:HG3	1:A:416:ILE:HD13	1.90	0.54
1:C:561:GLN:O	1:C:575:ARG:NH1	2.39	0.54
1:A:156:GLU:OE1	1:A:158:ARG:NH1	2.41	0.53
1:A:1048:MET:HE3	1:A:1050:PHE:HZ	1.73	0.53
1:C:472:GLN:HG2	1:C:478:CYS:HB3	1.90	0.53
1:A:1048:MET:HE3	1:A:1050:PHE:CZ	2.44	0.53
1:B:988:GLU:HA	1:B:991:ILE:HG12	1.90	0.53
1:C:802:GLN:OE1	1:C:933:GLN:NE2	2.41	0.53
1:B:108:THR:O	1:B:237:ARG:NH2	2.41	0.53
1:A:727:VAL:HG21	1:A:779:VAL:HG11	1.90	0.53
1:C:119:ILE:HG22	1:C:128:ILE:HG23	1.90	0.53
1:C:803:ILE:HD12	1:C:876:LEU:HD11	1.89	0.53
1:B:300:THR:HG23	1:B:301:LEU:HD12	1.90	0.53
1:C:103:GLY:HA3	1:C:241:LEU:HD22	1.91	0.52
1:C:471:TYR:CE2	1:C:473:ALA:HB2	2.44	0.52
1:C:823:LYS:NZ	1:C:936:LEU:O	2.41	0.52
1:A:939:THR:HG22	1:A:940:PRO:CD	2.39	0.52
1:B:724:ILE:HG13	1:B:1059:VAL:HG22	1.90	0.52
1:C:720:VAL:HG12	1:C:1063:VAL:HG22	1.92	0.52
1:C:777:GLN:O	1:C:781:ALA:HB3	2.09	0.52
1:A:102:ARG:HG2	1:A:141:LEU:HB2	1.91	0.52
1:A:140:PHE:HA	1:A:242:LEU:C	2.34	0.52
1:A:142:GLY:HA3	1:A:156:GLU:HB2	1.91	0.52
1:A:788:LYS:HE3	1:C:702:SER:HB2	1.92	0.52
1:B:345:PHE:CD1	1:B:397:SER:HB2	2.43	0.52
1:A:41:LYS:HE3	1:C:560:PHE:HB2	1.90	0.52
1:A:407:GLN:HB3	1:A:417:ALA:HB2	1.91	0.52
1:B:895:PRO:CB	1:B:897:PRO:HD3	2.40	0.52
1:A:845:ARG:HG2	1:A:846:ASP:H	1.75	0.52
1:B:425:ASP:OD1	1:B:426:ASP:N	2.42	0.52
1:B:1139:LEU:HG	1:B:1143:LEU:HD23	1.92	0.52
1:C:86:PHE:HE1	1:C:90:VAL:HG22	1.74	0.52
1:C:723:GLU:OE1	1:C:1062:HIS:NE2	2.41	0.52
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.36	0.51
1:A:974:VAL:HG13	1:A:977:ASP:HB2	1.91	0.51
1:B:97:LYS:HD3	1:B:187:LYS:H	1.75	0.51
1:A:240:THR:O	1:A:241:LEU:C	2.53	0.51
1:B:175:PHE:HE2	1:B:177:MET:HE2	1.76	0.51
1:C:356:ILE:HB	1:C:393:VAL:HB	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1079:ILE:O	1:C:1086:HIS:N	2.37	0.51
1:A:437:ASN:OD1	1:A:441:SER:OG	2.17	0.51
1:C:35:GLY:HA3	1:C:56:LEU:HB3	1.93	0.51
1:A:392:ASN:ND2	1:A:394:TYR:OH	2.44	0.51
1:B:33:THR:OG1	1:B:219:GLY:O	2.25	0.51
1:C:610:TYR:HB3	1:C:613:VAL:HG23	1.93	0.51
1:B:437:ASN:HB3	1:B:504:GLN:HB3	1.93	0.51
1:B:567:ILE:HD11	1:C:962:LYS:HD3	1.92	0.50
1:A:962:LYS:NZ	1:C:567:ILE:O	2.38	0.50
1:C:159:VAL:HG13	1:C:160:TYR:HD1	1.77	0.50
1:C:1143:LEU:O	1:C:1147:LYS:HG3	2.10	0.50
1:A:81:ASN:ND2	1:A:242:LEU:HD22	2.16	0.50
1:A:96:GLU:HG3	1:A:101:ILE:HG12	1.93	0.50
1:A:1137:ASP:OD1	1:A:1137:ASP:N	2.44	0.50
1:C:204:TYR:HB3	1:C:223:LEU:HG	1.93	0.50
1:A:24:LEU:HD23	1:A:78:ARG:HG3	1.93	0.50
1:A:391:THR:HA	1:A:520:ALA:HA	1.94	0.50
1:C:736:CYS:O	1:C:740:ILE:HG12	2.12	0.50
1:A:434:TRP:HZ3	1:A:509:VAL:HG12	1.77	0.49
1:A:705:TYR:HB3	1:B:790:PRO:HG2	1.94	0.49
1:C:656:ASN:HD22	1:C:656:ASN:C	2.15	0.49
1:B:315:ASN:ND2	1:C:735:ASP:OD2	2.44	0.49
1:B:940:PRO:HD2	1:B:941:SER:N	2.26	0.49
1:A:199:GLY:HA2	1:A:232:GLY:HA2	1.93	0.49
1:C:419:TYR:CD1	1:C:455:ARG:HB2	2.46	0.49
1:A:446:ASN:HD21	1:A:495:PHE:HD2	1.60	0.49
1:A:64:TRP:HH2	1:A:214:ARG:HE	1.61	0.49
1:B:396:ASP:OD2	1:B:421:TYR:OH	2.31	0.49
1:A:83:VAL:HG22	1:A:239:GLN:HB2	1.94	0.49
1:A:1143:LEU:O	1:A:1147:LYS:N	2.36	0.49
1:B:723:GLU:OE2	1:B:1026:LYS:NZ	2.44	0.49
1:B:818:ASP:OD1	1:B:819:LEU:N	2.45	0.49
1:C:119:ILE:HG22	1:C:128:ILE:HD12	1.94	0.49
1:A:521:THR:HG23	1:A:522:VAL:HG23	1.94	0.49
1:A:895:PRO:CB	1:A:897:PRO:HD3	2.42	0.49
1:B:123:ALA:HA	1:B:177:MET:HB3	1.94	0.49
1:B:231:ILE:HD12	1:B:233:ILE:HG12	1.94	0.49
1:B:316:PHE:N	1:B:591:GLY:O	2.38	0.49
1:B:206:LYS:NZ	1:B:221:SER:OG	2.46	0.49
1:C:631:TRP:CD1	1:C:632:ARG:HG3	2.47	0.49
1:C:875:LEU:O	1:C:879:THR:OG1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:LYS:HG3	1:B:461:PRO:HA	1.95	0.49
1:A:362:ASP:OD1	1:A:362:ASP:N	2.46	0.49
1:C:342:ALA:HB3	1:C:345:PHE:HE1	1.78	0.49
1:C:142:GLY:O	1:C:155:SER:N	2.45	0.48
1:B:351:TRP:HZ3	1:B:353:ARG:HB2	1.77	0.48
1:B:1147:LYS:HD3	1:C:1146:PHE:HE1	1.79	0.48
1:B:714:ILE:HG22	1:B:714:ILE:O	2.12	0.48
1:B:355:ARG:NH1	1:B:392:ASN:HB2	2.29	0.48
1:A:758:CYS:HA	1:A:761:LEU:HD13	1.93	0.48
1:C:236:THR:HG22	1:C:237:ARG:HG3	1.96	0.48
1:C:783:VAL:HG22	1:C:785:GLN:H	1.79	0.48
1:B:16:VAL:HG21	1:B:253:SER:HB2	1.94	0.48
1:B:969:GLY:O	1:B:993:ARG:NH1	2.46	0.48
1:B:1077:PRO:HA	1:C:898:MET:HE3	1.96	0.48
1:B:189:LEU:HD22	1:B:210:ILE:HD13	1.95	0.48
1:B:720:VAL:HG12	1:B:1063:VAL:HG22	1.95	0.48
1:C:226:LEU:HG	1:C:227:VAL:HG23	1.96	0.48
1:A:131:CYS:HB3	1:A:165:ASN:O	2.14	0.47
1:A:389:CYS:HA	1:A:523:CYS:CB	2.44	0.47
1:A:349:TYR:CE1	1:A:450:LEU:HB2	2.49	0.47
1:A:590:PHE:CE1	1:B:855:GLY:HA2	2.48	0.47
1:B:880:ILE:HG23	1:B:881:THR:HG23	1.95	0.47
1:B:895:PRO:HB2	1:B:897:PRO:CD	2.44	0.47
1:C:201:PHE:HB3	1:C:229:LEU:HB2	1.96	0.47
1:C:761:LEU:HD22	1:C:1006:VAL:HG21	1.96	0.47
1:C:629:PRO:O	1:C:633:VAL:HG22	2.14	0.47
1:A:330:ILE:HG13	1:A:330:ILE:O	2.15	0.47
1:C:594:SER:HB2	1:C:609:LEU:HB3	1.96	0.47
1:A:564:GLY:HA3	1:A:573:ALA:HB3	1.97	0.47
1:B:814:SER:OG	1:B:815:PHE:N	2.47	0.47
1:A:1150:LEU:HD21	1:B:1150:LEU:HD13	1.94	0.47
1:B:890:PRO:O	1:B:890:PRO:CD	2.63	0.47
1:C:451:TYR:HB3	1:C:493:TYR:CE2	2.50	0.47
1:C:648:LEU:HD23	1:C:648:LEU:H	1.80	0.47
1:A:1146:PHE:O	1:A:1150:LEU:N	2.40	0.47
1:B:741:CYS:HB3	1:B:747:CYS:HB3	1.64	0.47
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.48	0.46
1:B:824:VAL:HG21	1:B:1055:PRO:HG2	1.98	0.46
1:C:664:ILE:HD11	1:C:670:ALA:HB2	1.97	0.46
1:A:451:TYR:HB3	1:A:493:TYR:CE1	2.51	0.46
1:A:590:PHE:HZ	1:B:855:GLY:HA2	1.76	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:VAL:HG21	1:A:1130:ILE:HD12	1.97	0.46
1:B:387:ASP:OD1	1:B:387:ASP:N	2.46	0.46
1:B:1124:CYS:HB2	1:B:1130:ILE:HD13	1.96	0.46
1:B:1133:ASN:OD1	1:B:1134:THR:N	2.47	0.46
1:C:468:THR:HG22	1:C:468:THR:O	2.15	0.46
1:A:724:ILE:HG13	1:A:1059:VAL:HG22	1.96	0.46
1:A:890:PRO:O	1:A:890:PRO:CD	2.64	0.46
1:B:865:ASP:OD1	1:B:866:GLU:N	2.49	0.46
1:C:298:LYS:HE2	1:C:298:LYS:HB3	1.61	0.46
1:A:720:VAL:HG12	1:A:1063:VAL:HG22	1.96	0.46
1:B:391:THR:HB	1:B:518:ALA:HB3	1.96	0.46
1:B:715:ASN:HB3	1:B:1068:ALA:HB3	1.98	0.46
1:C:630:THR:HA	1:C:634:TYR:CE1	2.50	0.46
1:A:821:PHE:HD1	1:A:1055:PRO:HD3	1.80	0.46
1:A:736:CYS:HB3	1:A:758:CYS:HB2	1.75	0.46
1:A:327:PHE:CD2	1:A:526:LYS:HB3	2.51	0.46
1:A:540:ASN:HA	1:A:544:LEU:O	2.15	0.46
1:A:455:ARG:HH12	1:A:459:LEU:HD23	1.81	0.45
1:A:1114:THR:OG1	1:A:1116:ASP:OD1	2.34	0.45
1:B:35:GLY:HA3	1:B:56:LEU:HB3	1.98	0.45
1:C:727:VAL:HG13	1:C:779:VAL:HG21	1.98	0.45
1:B:64:TRP:HD1	1:B:264:TYR:CE1	2.34	0.45
1:B:64:TRP:HD1	1:B:264:TYR:HE1	1.63	0.45
1:B:904:PHE:HB3	1:B:909:VAL:HG13	1.98	0.45
1:A:424:PRO:HD2	1:A:427:PHE:HD1	1.81	0.45
1:B:410:PRO:HG3	1:B:427:PHE:HD2	1.81	0.45
1:A:53:ASP:OD1	1:A:54:LEU:N	2.42	0.45
1:B:674:THR:HA	1:B:688:GLN:HA	1.99	0.45
1:C:437:ASN:HA	1:C:505:PRO:HG2	1.98	0.45
1:B:1123:ASN:OD1	1:B:1124:CYS:N	2.50	0.45
1:C:142:GLY:HA3	1:C:156:GLU:HB2	1.97	0.45
1:A:576:ASP:HB3	1:A:579:THR:O	2.16	0.45
1:B:297:THR:HA	1:B:300:THR:HG22	1.98	0.45
1:B:895:PRO:CB	1:B:897:PRO:CD	2.95	0.45
1:C:100:ILE:HD13	1:C:261:ALA:HB2	1.97	0.45
1:C:320:PRO:HA	1:C:536:CYS:O	2.16	0.45
1:A:316:PHE:H	1:A:591:GLY:C	2.25	0.45
1:C:401:ARG:NH2	1:C:494:GLY:H	2.12	0.45
1:C:701:ASN:OD1	1:C:702:SER:N	2.50	0.45
1:A:83:VAL:HG13	1:A:239:GLN:HB2	1.98	0.45
1:B:452:ARG:NH2	1:B:467:SER:O	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:PHE:HZ	1:C:158:ARG:HH11	1.63	0.45
1:B:983:ASP:OD1	1:B:983:ASP:N	2.50	0.44
1:A:125:ASN:HB3	1:A:174:PRO:HA	1.99	0.44
1:A:1127:VAL:HG12	1:B:915:TYR:HB3	1.99	0.44
1:B:68:ILE:N	1:B:78:ARG:HB2	2.28	0.44
1:C:178:ASP:OD1	1:C:178:ASP:N	2.46	0.44
1:C:890:PRO:O	1:C:890:PRO:CD	2.64	0.44
1:A:939:THR:HG22	1:A:940:PRO:HD2	2.00	0.44
1:B:450:LEU:HD13	1:B:492:SER:HB2	1.99	0.44
1:C:1095:SER:HB2	1:C:1100:TRP:CD2	2.51	0.44
1:A:106:PHE:O	1:A:116:SER:OG	2.29	0.44
1:B:114:THR:C	1:B:132:GLU:HG3	2.41	0.44
1:C:974:VAL:HG12	1:C:977:ASP:H	1.83	0.44
1:A:549:VAL:HG22	1:A:586:THR:O	2.17	0.44
1:B:112:SER:HA	1:B:132:GLU:HB3	2.00	0.44
1:B:1081:HIS:ND1	1:B:1134:THR:HA	2.33	0.44
1:B:1151:ASP:O	1:B:1155:LYS:HG2	2.18	0.44
1:C:400:ILE:HD12	1:C:404:GLU:HG3	2.00	0.44
1:C:188:ASN:OD1	1:C:189:LEU:N	2.51	0.44
1:A:200:TYR:OH	1:C:392:ASN:ND2	2.51	0.44
1:C:878:GLY:O	1:C:882:SER:OG	2.30	0.44
1:A:713:PRO:HA	1:A:1070:GLU:HA	1.98	0.44
1:C:139:PRO:HB2	1:C:159:VAL:HA	2.00	0.44
1:C:880:ILE:HG13	1:C:881:THR:HG23	1.99	0.44
1:A:409:ALA:HB3	1:A:412:GLN:HG3	2.00	0.43
1:A:710:ILE:HG22	1:B:894:ILE:HG13	1.99	0.43
1:C:499:TYR:HB3	1:C:503:TYR:HB2	1.99	0.43
1:A:535:LYS:HB3	1:A:535:LYS:HE2	1.87	0.43
1:A:615:CYS:HB3	1:A:647:CYS:HB3	1.94	0.43
1:B:325:VAL:HG12	1:B:540:ASN:HB3	2.00	0.43
1:C:310:ILE:HD11	1:C:594:SER:HB3	2.00	0.43
1:B:895:PRO:HB2	1:B:897:PRO:HD2	1.99	0.43
1:B:1095:SER:HB2	1:B:1100:TRP:CE3	2.53	0.43
1:A:1080:CYS:HB3	1:A:1124:CYS:HB3	1.84	0.43
1:B:125:ASN:ND2	1:B:172:SER:O	2.29	0.43
1:B:499:TYR:O	1:B:504:GLN:NE2	2.52	0.43
1:A:18:PHE:CE1	1:A:140:PHE:CZ	2.98	0.43
1:A:499:TYR:HB3	1:A:503:TYR:HB2	2.00	0.43
1:C:130:VAL:HG11	1:C:231:ILE:HG21	1.99	0.43
1:A:452:ARG:HD3	1:A:455:ARG:HG3	2.01	0.43
1:A:553:SER:HB3	1:A:582:ILE:HG22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:LYS:NZ	1:B:773:ASP:OD2	2.37	0.43
1:C:328:PRO:HG3	1:C:577:PRO:HB2	2.01	0.43
1:A:372:PHE:HD1	1:A:434:TRP:HB3	1.83	0.43
1:A:607:ALA:HB2	1:A:690:ILE:HD12	2.01	0.43
1:C:85:PRO:HD3	1:C:237:ARG:HH22	1.84	0.43
1:C:97:LYS:HD3	1:C:187:LYS:H	1.84	0.43
1:C:365:VAL:HG23	1:C:366:LEU:HD12	2.00	0.43
1:C:484:PHE:O	1:C:485:ASN:ND2	2.52	0.43
1:A:800:PHE:HB3	1:A:804:LEU:HD23	2.01	0.43
1:A:929:ILE:O	1:A:932:ILE:HG22	2.19	0.43
1:A:1100:TRP:HB2	1:A:1133:ASN:HD22	1.83	0.43
1:A:1139:LEU:HD11	1:B:1139:LEU:HD13	2.01	0.43
1:B:293:PRO:HD3	1:B:631:TRP:HB2	2.01	0.43
1:C:291:LEU:H	1:C:296:GLU:CD	2.26	0.43
1:A:396:ASP:HB2	1:A:510:VAL:HG12	2.00	0.42
1:A:821:PHE:CD1	1:A:1055:PRO:HD3	2.54	0.42
1:A:1133:ASN:OD1	1:A:1134:THR:N	2.47	0.42
1:B:34:ARG:HA	1:B:34:ARG:HD3	1.86	0.42
1:B:40:ASP:OD1	1:B:40:ASP:N	2.52	0.42
1:C:615:CYS:HB3	1:C:647:CYS:HB3	1.52	0.42
1:A:640:VAL:HG12	1:A:649:ILE:HG22	2.02	0.42
1:B:707:ASN:HA	1:C:895:PRO:HB3	2.01	0.42
1:C:105:ILE:HG13	1:C:241:LEU:HD11	2.00	0.42
1:C:330:ILE:HG22	1:C:360:VAL:HG23	2.01	0.42
1:C:1151:ASP:O	1:C:1155:LYS:HG2	2.19	0.42
1:A:581:GLU:OE1	1:A:581:GLU:HA	2.20	0.42
1:A:820:LEU:C	1:A:822:ASN:H	2.27	0.42
1:C:422:LYS:NZ	1:C:461:PRO:HG3	2.34	0.42
1:A:79:PHE:HB2	1:A:256:TRP:CZ2	2.55	0.42
1:A:316:PHE:HZ	1:A:620:VAL:HB	1.84	0.42
1:A:453:LEU:N	1:A:489:PRO:O	2.42	0.42
1:B:373:SER:OG	1:B:433:ALA:O	2.31	0.42
1:C:106:PHE:HD2	1:C:117:LEU:HD22	1.83	0.42
1:C:307:GLU:O	1:C:311:TYR:OH	2.33	0.42
1:A:826:LEU:HD13	1:A:826:LEU:HA	1.83	0.42
1:B:907:ILE:HG13	1:B:909:VAL:HG12	2.00	0.42
1:C:108:THR:HA	1:C:236:THR:HB	2.01	0.42
1:C:637:GLY:C	1:C:639:ASN:N	2.78	0.42
1:C:800:PHE:HE1	1:C:925:PHE:HE2	1.65	0.42
1:C:786:ILE:HG13	1:C:874:ALA:HB2	2.01	0.42
1:C:1048:MET:HE2	1:C:1050:PHE:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:TYR:HD2	1:C:1087:PHE:HE2	1.68	0.42
1:B:991:ILE:O	1:B:995:ILE:HG12	2.19	0.42
1:C:741:CYS:HB3	1:C:747:CYS:HB3	1.90	0.42
1:A:446:ASN:OD1	1:A:446:ASN:N	2.53	0.42
1:A:1007:THR:O	1:A:1011:ILE:HG12	2.20	0.42
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.54	0.42
1:B:576:ASP:HB3	1:B:579:THR:O	2.20	0.42
1:A:896:PHE:HZ	1:A:1048:MET:HE1	1.84	0.42
1:B:106:PHE:O	1:B:117:LEU:N	2.52	0.42
1:C:58:PHE:HB2	1:C:291:LEU:HD21	2.02	0.42
1:C:452:ARG:HH22	1:C:466:ILE:HA	1.85	0.42
1:C:656:ASN:C	1:C:656:ASN:ND2	2.78	0.42
1:A:991:ILE:O	1:A:995:ILE:HG12	2.20	0.41
1:A:1088:PRO:HA	1:A:1118:THR:HG22	2.01	0.41
1:B:1114:THR:HA	1:B:1136:TYR:O	2.20	0.41
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.55	0.41
1:C:631:TRP:HE1	1:C:632:ARG:CZ	2.33	0.41
1:A:821:PHE:CE1	1:A:1054:ALA:HA	2.52	0.41
1:B:278:ASN:OD1	1:B:282:THR:N	2.52	0.41
1:B:700:GLU:HA	1:C:786:ILE:HG23	2.02	0.41
1:A:813:ARG:HD2	1:A:821:PHE:CD2	2.55	0.41
1:A:912:ASN:O	1:A:916:GLU:HG2	2.21	0.41
1:C:52:GLN:HG3	1:C:272:THR:HG22	2.02	0.41
1:C:367:TYR:CE1	1:C:382:PRO:HB2	2.54	0.41
1:A:971:ILE:HG13	1:A:972:SER:N	2.35	0.41
1:A:1140:GLN:O	1:A:1144:ASP:N	2.39	0.41
1:B:102:ARG:HE	1:B:141:LEU:HD22	1.85	0.41
1:C:768:ILE:O	1:C:772:GLN:HG2	2.19	0.41
1:B:153:MET:SD	1:B:153:MET:N	2.93	0.41
1:B:514:GLU:OE2	1:B:517:HIS:ND1	2.49	0.41
1:C:488:PHE:CE2	1:C:490:LEU:HB2	2.55	0.41
1:C:607:ALA:HB2	1:C:690:ILE:HD12	2.02	0.41
1:A:355:ARG:NH2	1:A:392:ASN:HD22	2.18	0.41
1:A:893:GLN:HE22	1:C:709:SER:C	2.29	0.41
1:B:15:CYS:SG	1:B:158:ARG:HB3	2.61	0.41
1:B:278:ASN:ND2	1:B:282:THR:OG1	2.54	0.41
1:B:714:ILE:O	1:B:714:ILE:CG2	2.68	0.41
1:A:306:VAL:HG13	1:A:311:TYR:HE2	1.85	0.41
1:A:399:VAL:HG22	1:A:507:ARG:HG2	2.02	0.41
1:A:845:ARG:HH22	1:A:847:LEU:HD23	1.86	0.41
1:B:345:PHE:HE2	1:B:507:ARG:CZ	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:HD2	1:C:97:LYS:HA	1.94	0.41
1:C:720:VAL:HG23	1:C:932:ILE:HD11	2.03	0.41
1:C:740:ILE:HD11	1:C:751:LEU:HD22	2.02	0.41
1:B:105:ILE:HG12	1:B:239:GLN:HB3	2.03	0.41
1:B:132:GLU:OE1	1:B:165:ASN:HB3	2.21	0.41
1:B:1027:MET:HE2	1:B:1027:MET:HB2	1.95	0.41
1:C:335:PRO:HB2	1:C:338:GLU:HB2	2.02	0.41
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.56	0.41
1:C:340:PHE:CE1	1:C:509:VAL:HG21	2.56	0.41
1:C:554:ASN:OD1	1:C:554:ASN:N	2.53	0.41
1:C:1079:ILE:HG23	1:C:1086:HIS:HB2	2.03	0.41
1:A:128:ILE:C	1:A:129:LYS:HD3	2.46	0.41
1:A:401:ARG:HD3	1:A:495:PHE:HE1	1.86	0.41
1:A:819:LEU:O	1:A:823:LYS:HG2	2.21	0.41
1:A:962:LYS:HA	1:A:962:LYS:HD3	1.91	0.41
1:A:1090:GLU:OE2	1:A:1105:ARG:NH1	2.53	0.41
1:C:106:PHE:HB3	1:C:235:ILE:HD11	2.02	0.41
1:C:128:ILE:HG12	1:C:170:TYR:HD2	1.86	0.41
1:C:536:CYS:HB3	1:C:588:CYS:HB3	1.98	0.41
1:A:339:VAL:HG22	1:A:354:LYS:NZ	2.36	0.40
1:B:553:SER:HB2	1:B:584:ASP:HB2	2.02	0.40
1:B:723:GLU:OE1	1:B:1062:HIS:NE2	2.54	0.40
1:C:945:LYS:HE3	1:C:945:LYS:HB3	1.92	0.40
1:C:83:VAL:HG12	1:C:237:ARG:NE	2.36	0.40
1:C:875:LEU:HD23	1:C:875:LEU:HA	1.95	0.40
1:A:976:ASN:HD22	1:C:546:GLY:HA2	1.87	0.40
1:A:1116:ASP:OD1	1:A:1116:ASP:N	2.53	0.40
1:A:315:ASN:ND2	1:B:735:ASP:OD1	2.42	0.40
1:B:750:LEU:HD21	1:B:988:GLU:HB2	2.04	0.40
1:B:1095:SER:HB2	1:B:1100:TRP:CD2	2.57	0.40
1:C:451:TYR:HB3	1:C:493:TYR:CZ	2.56	0.40
1:A:871:TYR:HE1	1:C:697:LEU:HB3	1.86	0.40
1:B:105:ILE:HD12	1:B:110:LEU:HD22	2.03	0.40
1:C:609:LEU:HD22	1:C:664:ILE:HG23	2.04	0.40

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	1065/1271 (84%)	1024 (96%)	39 (4%)	2 (0%)	43	73
1	B	1063/1271 (84%)	1030 (97%)	33 (3%)	0	100	100
1	C	1062/1271 (84%)	1021 (96%)	41 (4%)	0	100	100
All	All	3190/3813 (84%)	3075 (96%)	113 (4%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ILE
1	A	827	ALA

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	943/1112 (85%)	935 (99%)	8 (1%)	73	75
1	B	943/1112 (85%)	943 (100%)	0	100	100
1	C	944/1112 (85%)	932 (99%)	12 (1%)	61	71
All	All	2830/3336 (85%)	2810 (99%)	20 (1%)	73	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	241	LEU
1	A	588	CYS
1	A	590	PHE
1	A	593	VAL
1	A	823	LYS
1	A	826	LEU
1	A	828	ASP
1	C	297	THR
1	C	298	LYS
1	C	300	THR
1	C	301	LEU
1	C	617	GLU
1	C	628	THR
1	C	630	THR
1	C	631	TRP
1	C	635	SER
1	C	639	ASN
1	C	640	VAL
1	C	656	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	165	ASN
1	A	312	GLN
1	A	392	ASN
1	A	562	GLN
1	A	642	GLN
1	A	822	ASN
1	A	893	GLN
1	A	976	ASN
1	A	1021	ASN
1	A	1062	HIS
1	B	137	ASN
1	B	438	ASN
1	B	538	ASN
1	B	951	ASN
1	B	990	GLN
1	C	99	ASN
1	C	115	GLN
1	C	329	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	447	HIS
1	C	785	GLN
1	C	976	ASN

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.

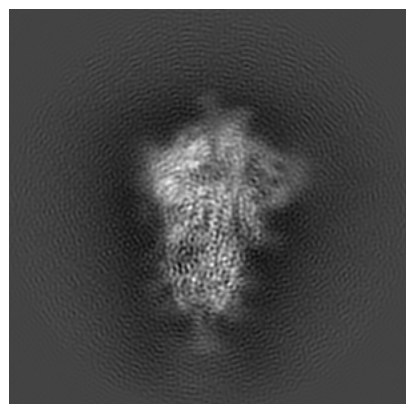
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33727. These allow visual inspection of the internal detail of the map and identification of artifacts.

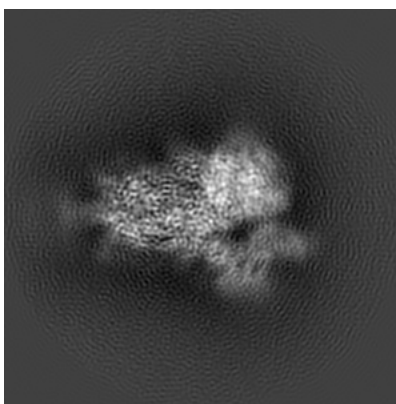
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

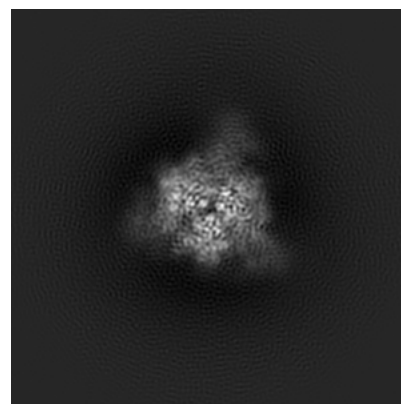
6.1.1 Primary map



X

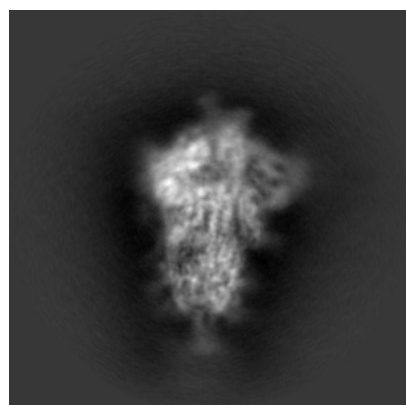


Y

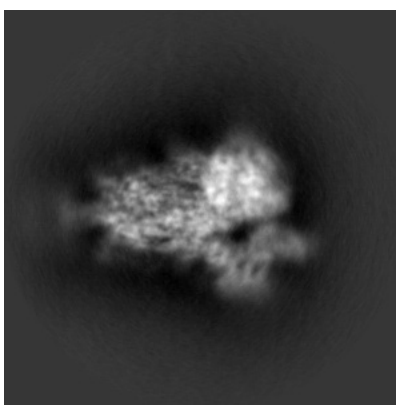


Z

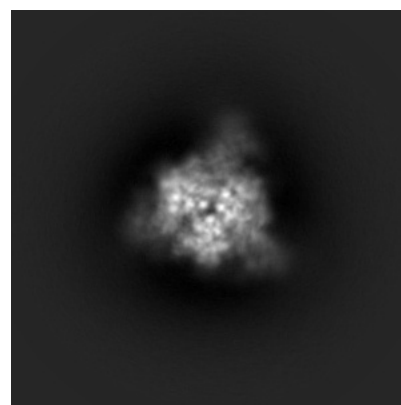
6.1.2 Raw map



X



Y

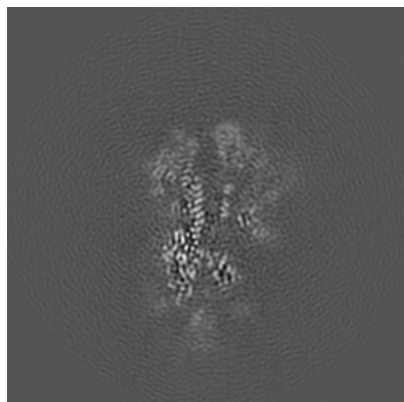


Z

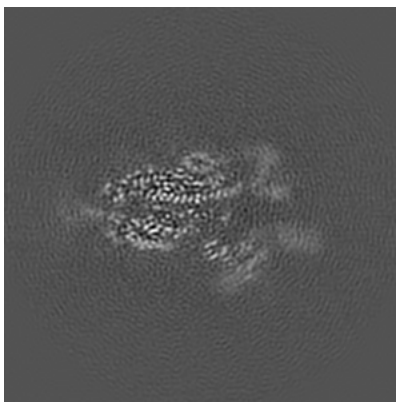
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

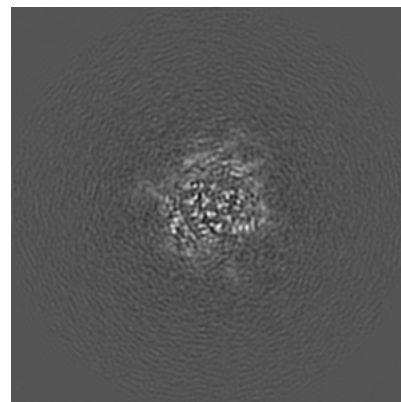
6.2.1 Primary map



X Index: 150

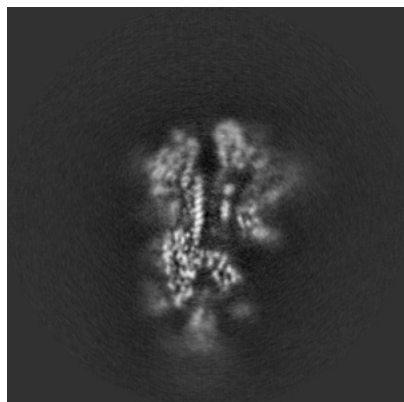


Y Index: 150

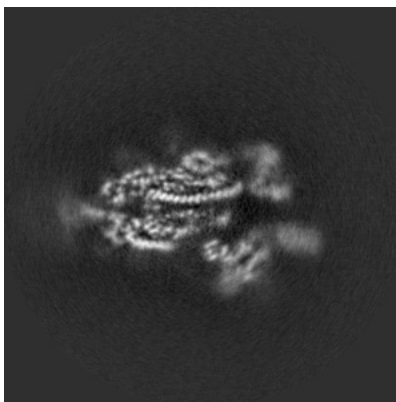


Z Index: 150

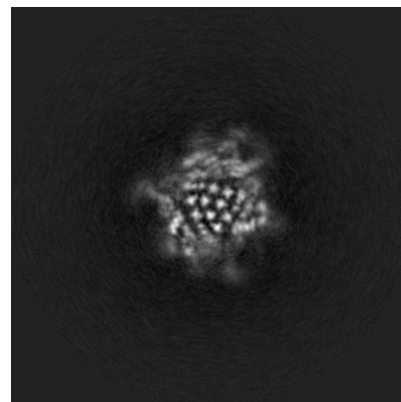
6.2.2 Raw map



X Index: 150



Y Index: 150

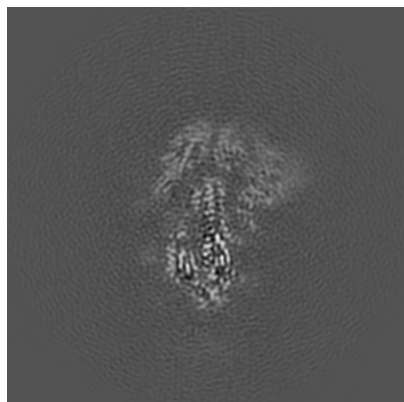


Z Index: 150

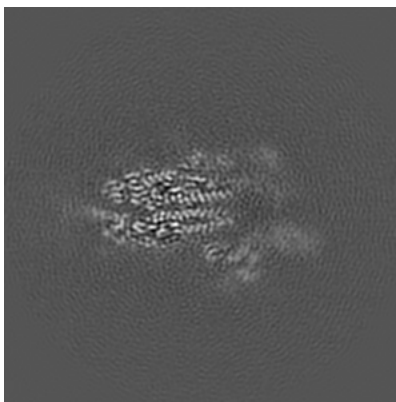
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

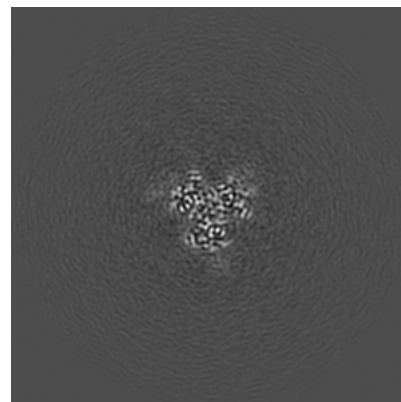
6.3.1 Primary map



X Index: 159

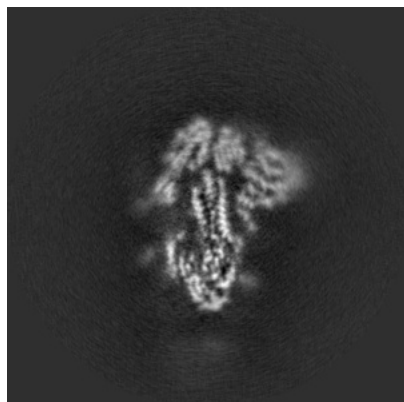


Y Index: 153

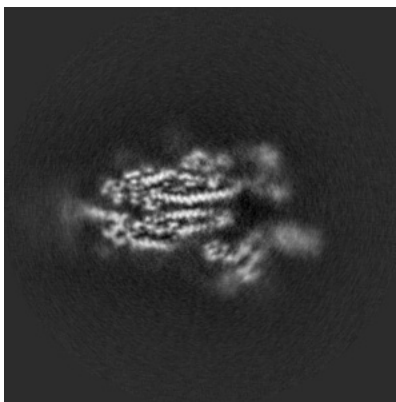


Z Index: 113

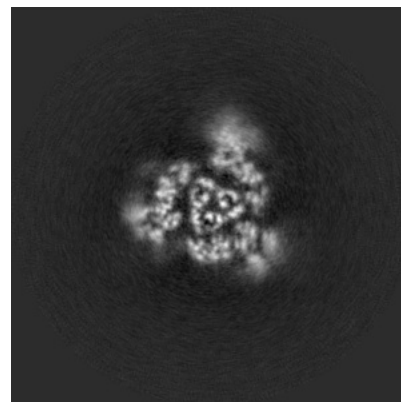
6.3.2 Raw map



X Index: 161



Y Index: 152

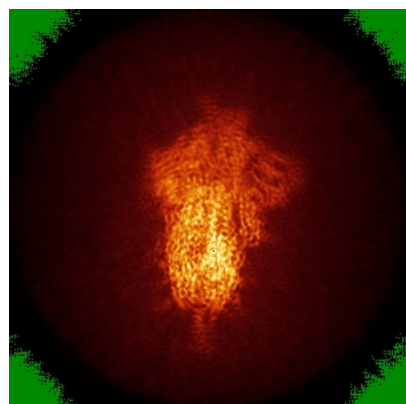


Z Index: 164

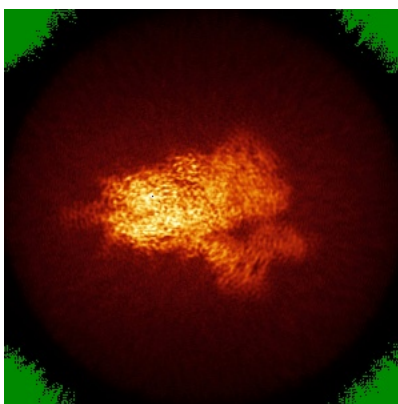
The images above show the largest variance slices of the map in three orthogonal directions.

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

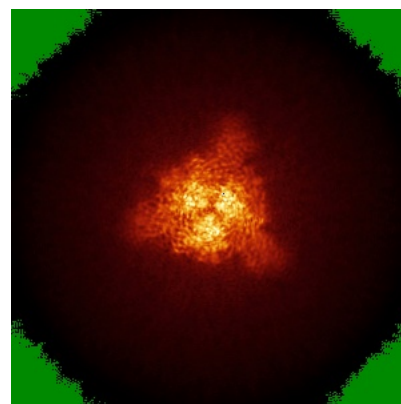
6.4.1 Primary map



X



Y

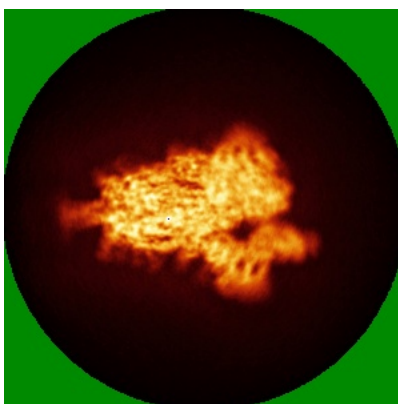


Z

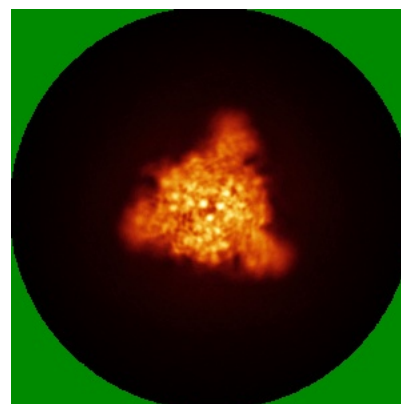
6.4.2 Raw map



X



Y

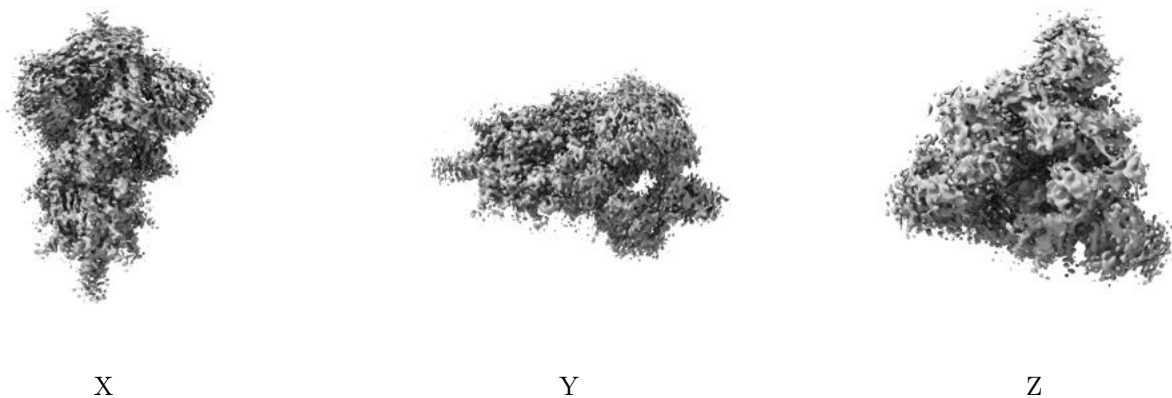


Z

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 0.015. 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.

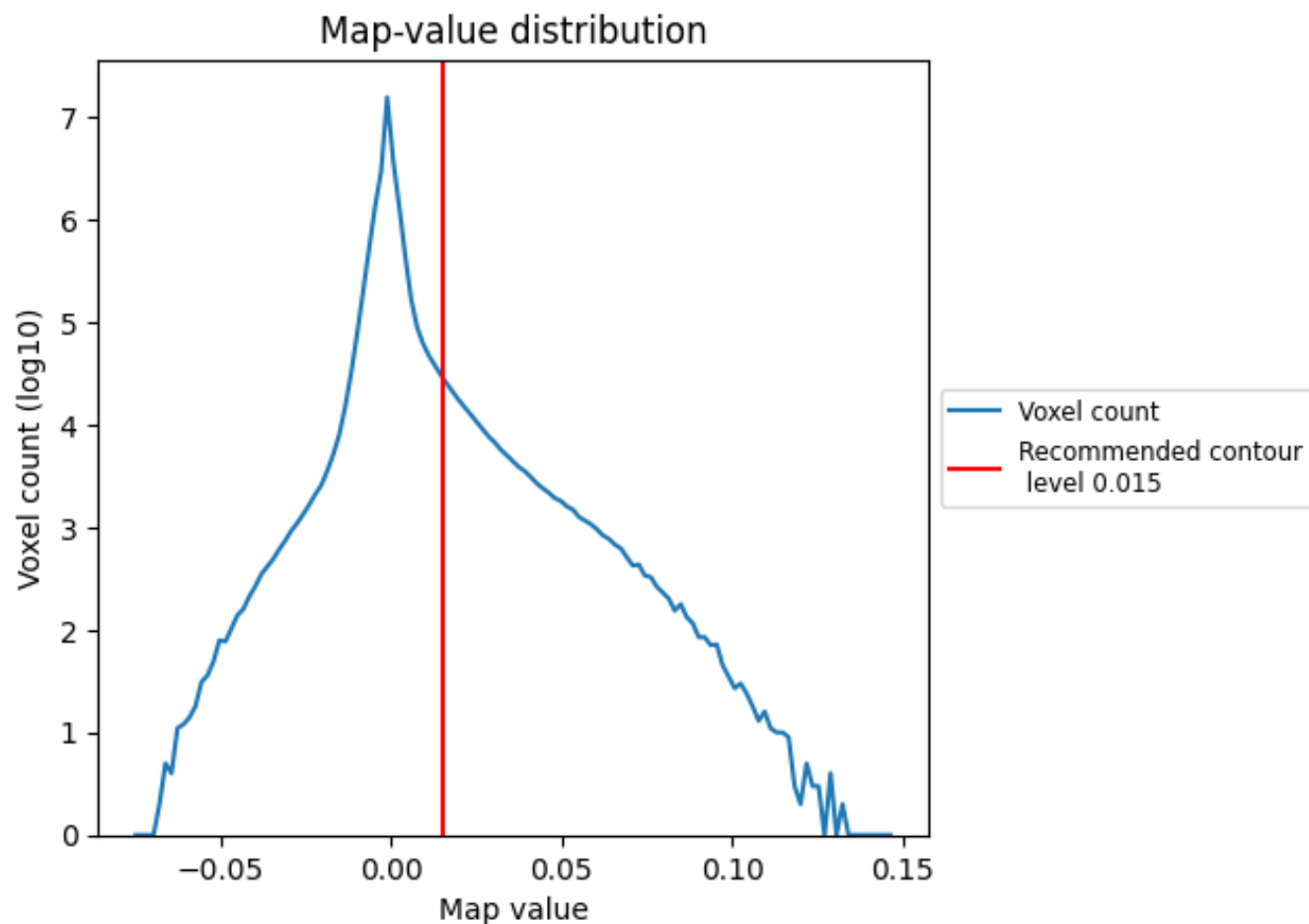
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

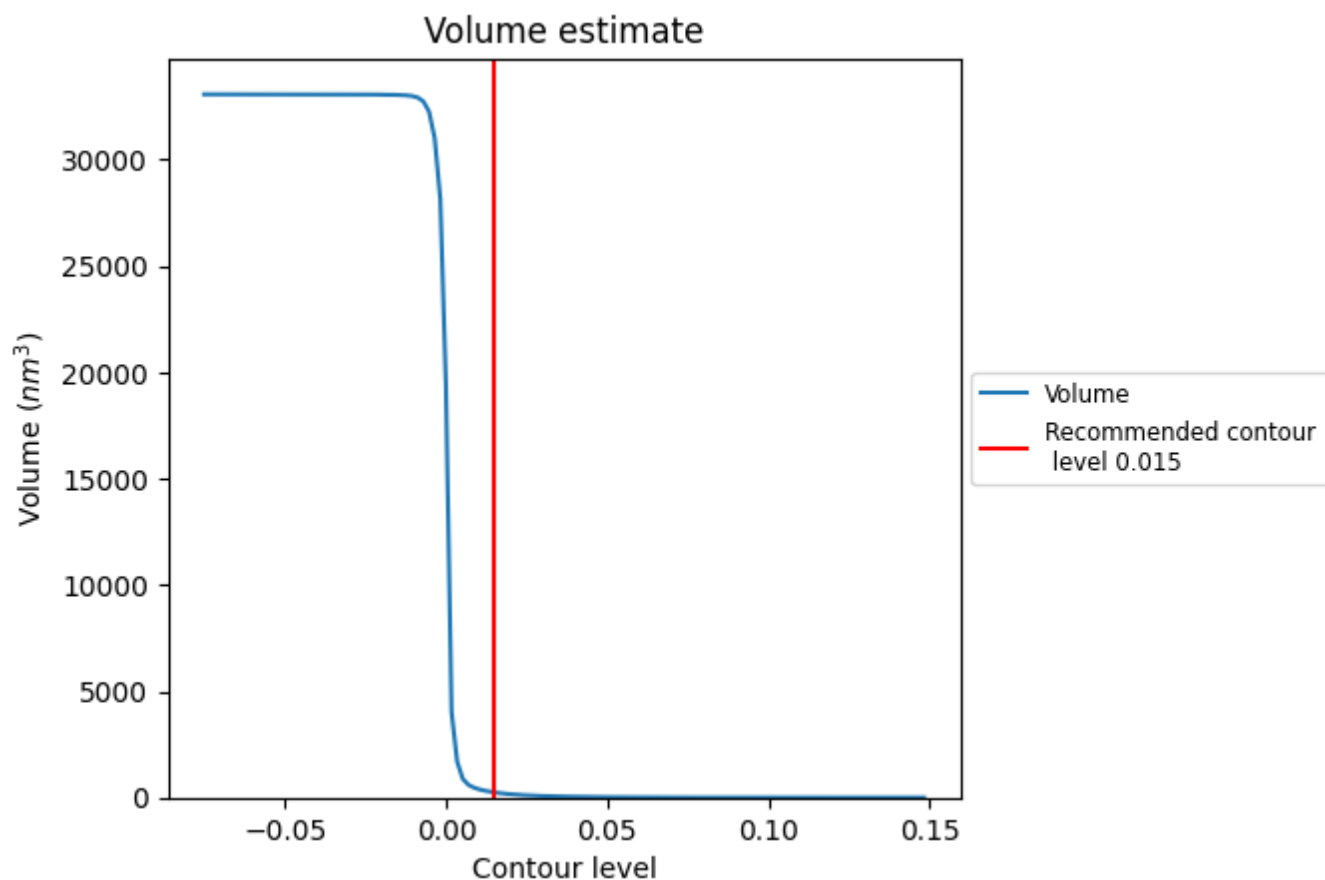
This section contains the results of statistical analysis of the map.

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.

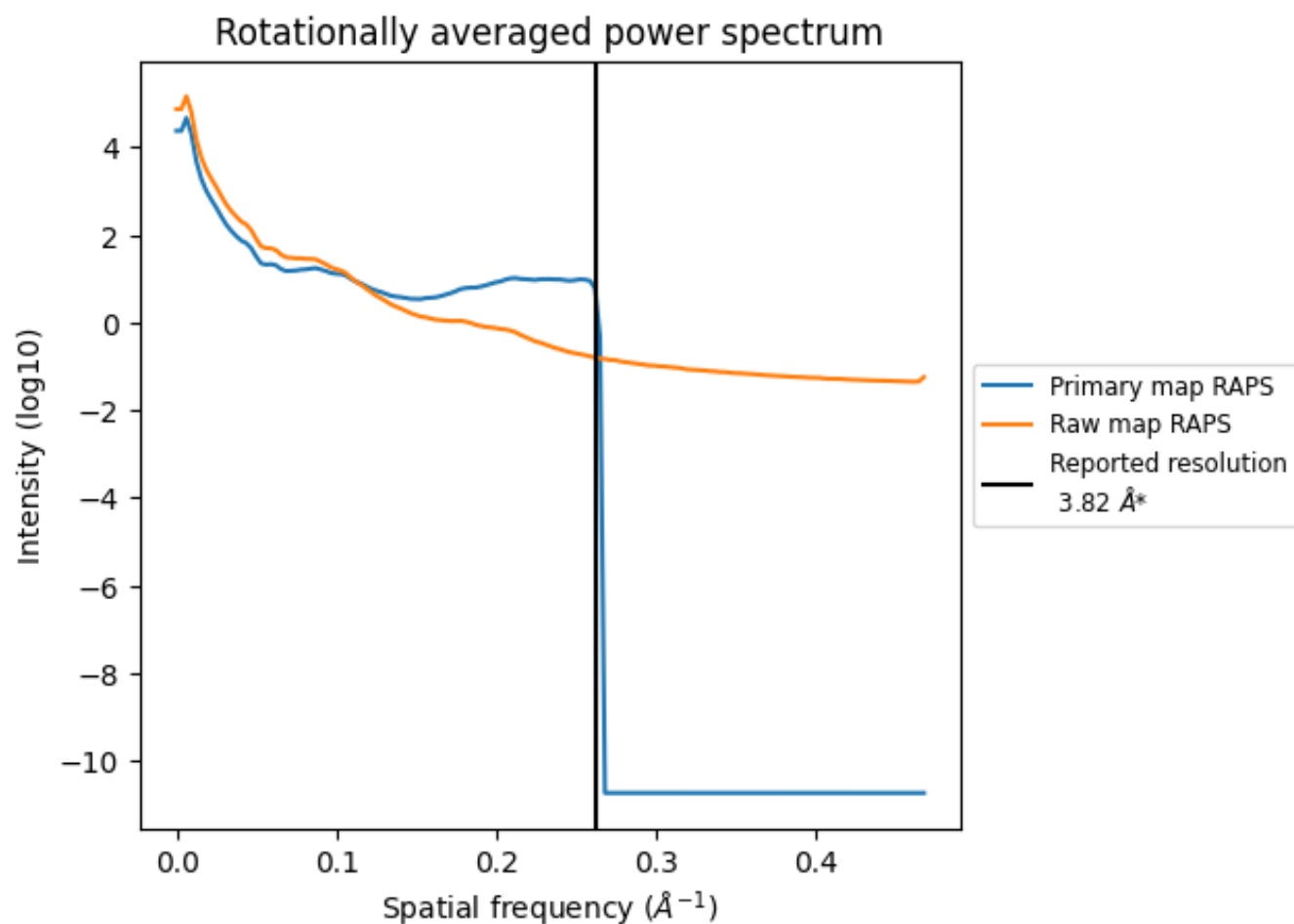
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 243 nm³; this corresponds to an approximate mass of 219 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 ⓘ

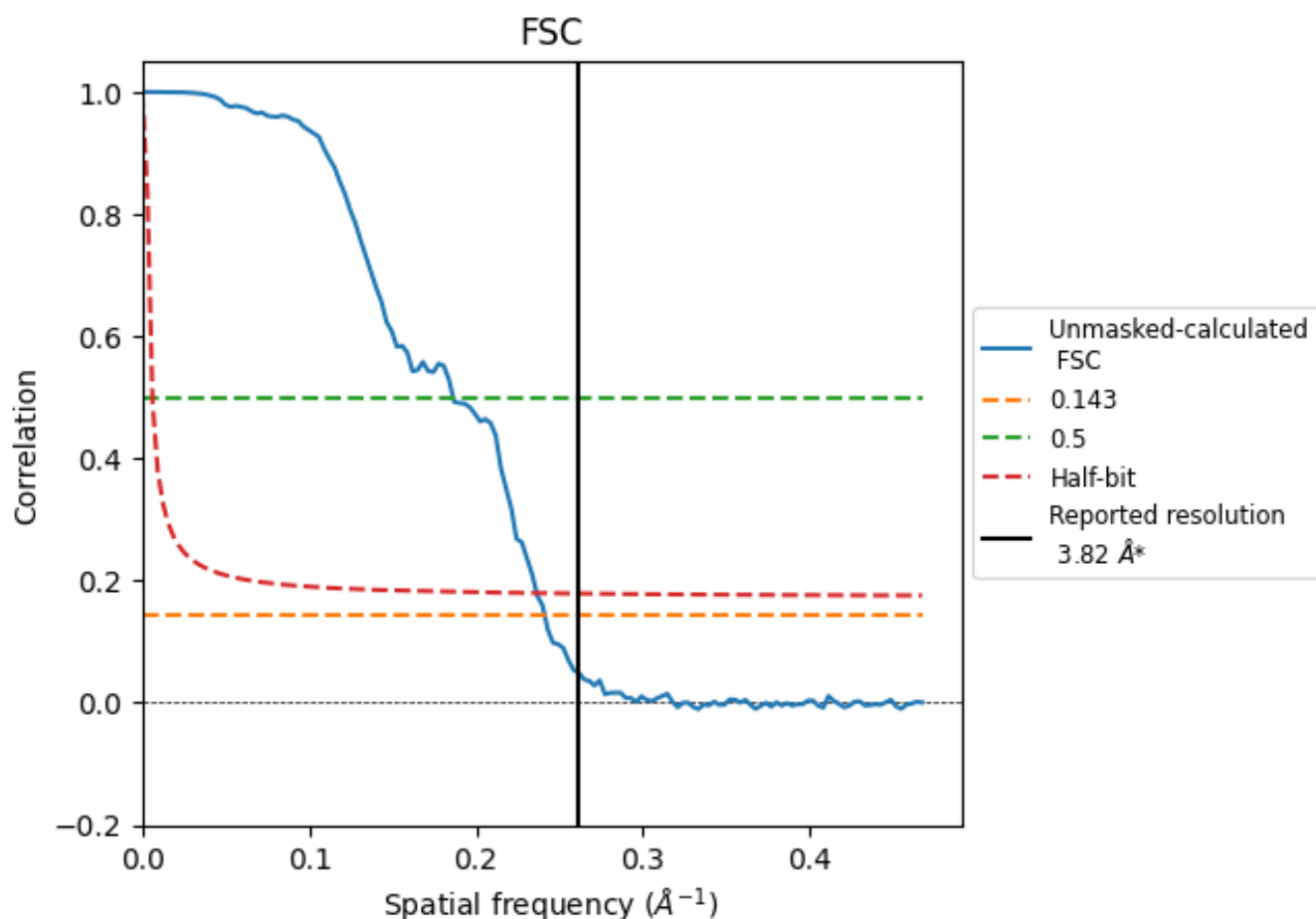


*Reported resolution corresponds to spatial frequency of 0.262 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.262 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

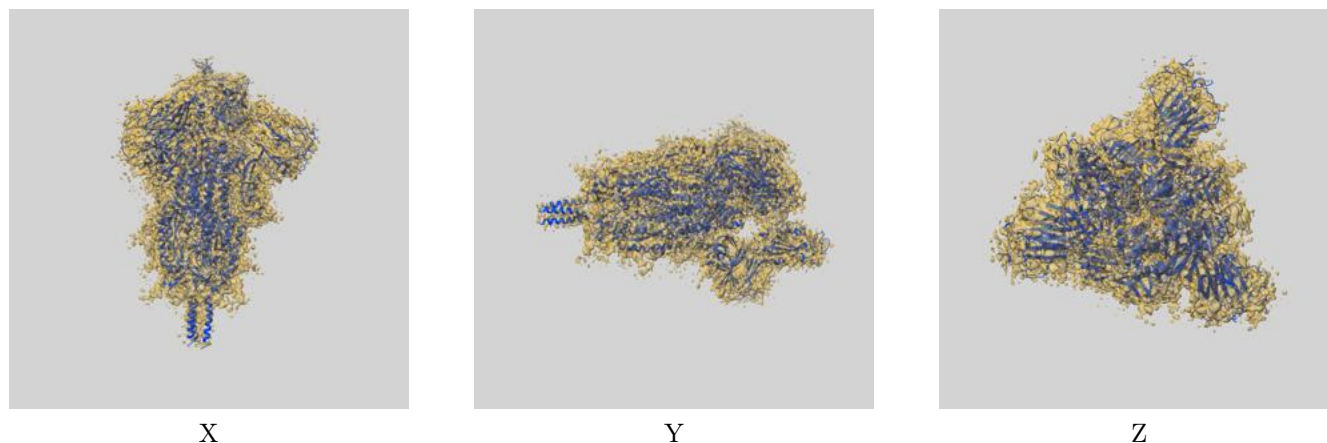
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	5.37	4.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

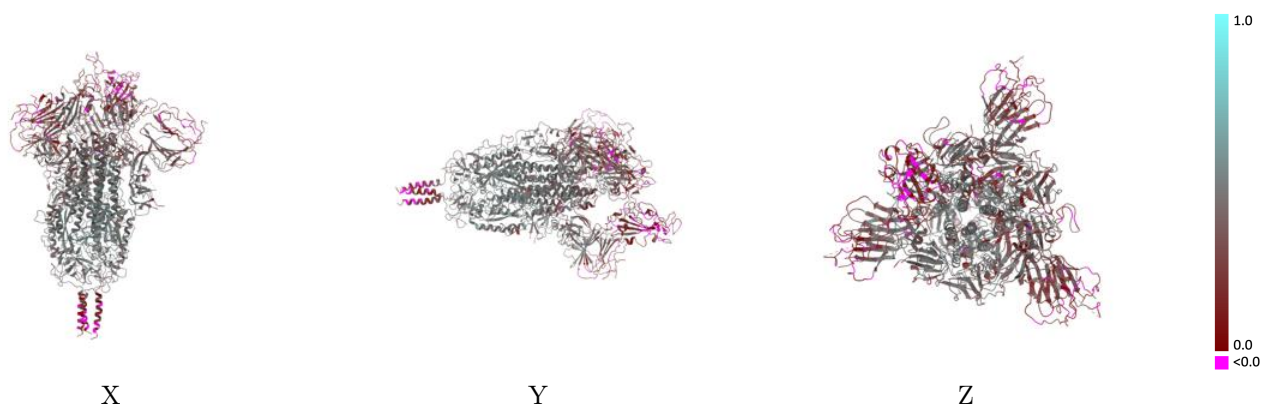
This section contains information regarding the fit between EMDB map EMD-33727 and PDB model 7YBN. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



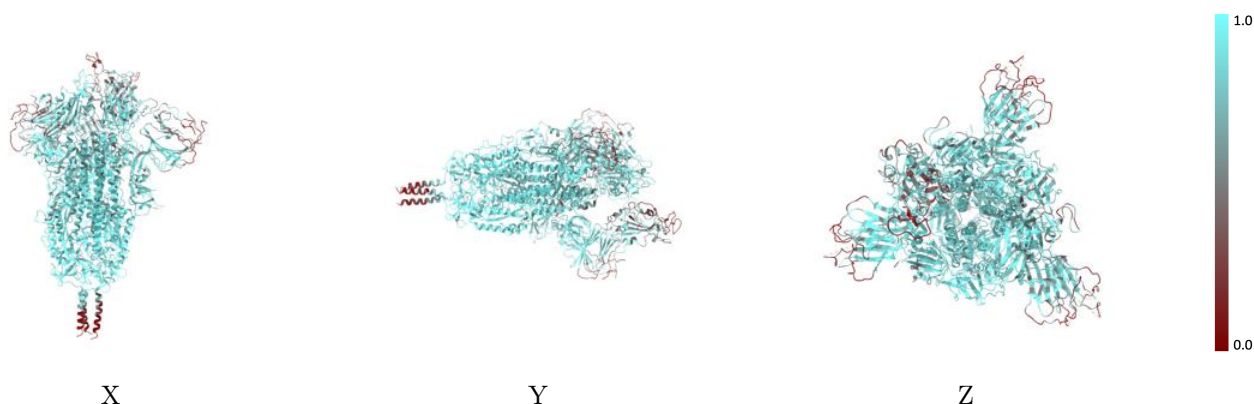
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



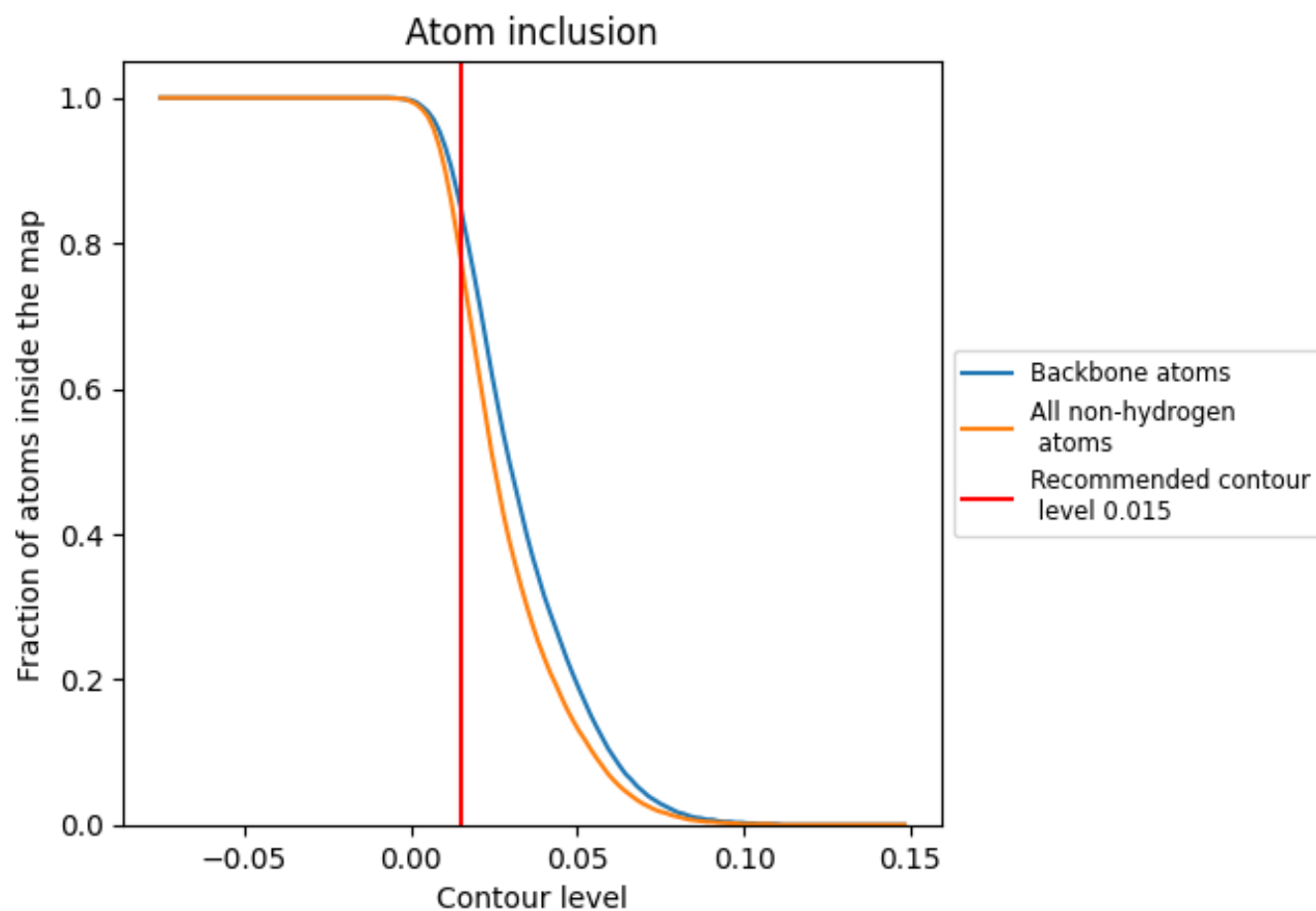
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7800	0.3760
A	0.7330	0.3520
B	0.8200	0.4000
C	0.7880	0.3740

