



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 08:48 PM JST

PDB ID : 7XO7
EMDB ID : EMD-33339
Title : SARS-CoV-2 Omicron BA.2 Variant Spike Trimer with two human ACE2 Bound
Authors : Xu, Y.; Wu, C.; Liu, H.; Yin, W.; Xu, H.E.
Deposited on : 2022-05-01
Resolution : 3.38 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.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

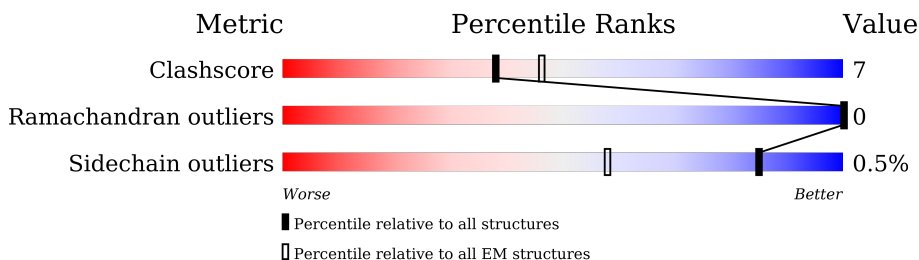
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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 ≥ 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	E	805	
2	F	805	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34209 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	1026	Total	C	N	O	S	0	0
			8001	5124	1331	1511	35		
1	B	1025	Total	C	N	O	S	0	0
			7943	5094	1318	1496	35		
1	C	1026	Total	C	N	O	S	0	0
			8001	5124	1331	1511	35		

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
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

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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
C	?	-	PRO	deletion	UNP P0DTC2
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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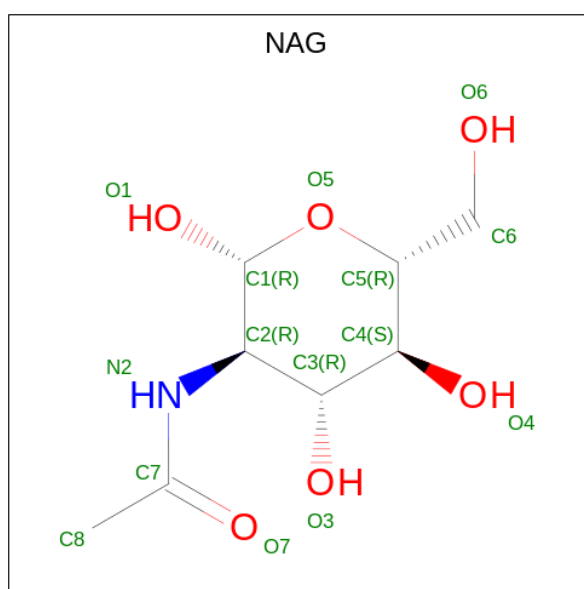
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Chain	Residue	Modelled	Actual	Comment	Reference
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
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
2	E	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	F	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		

- 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
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total	Cl	0
			1	1	
4	F	1	Total	Cl	0
			1	1	

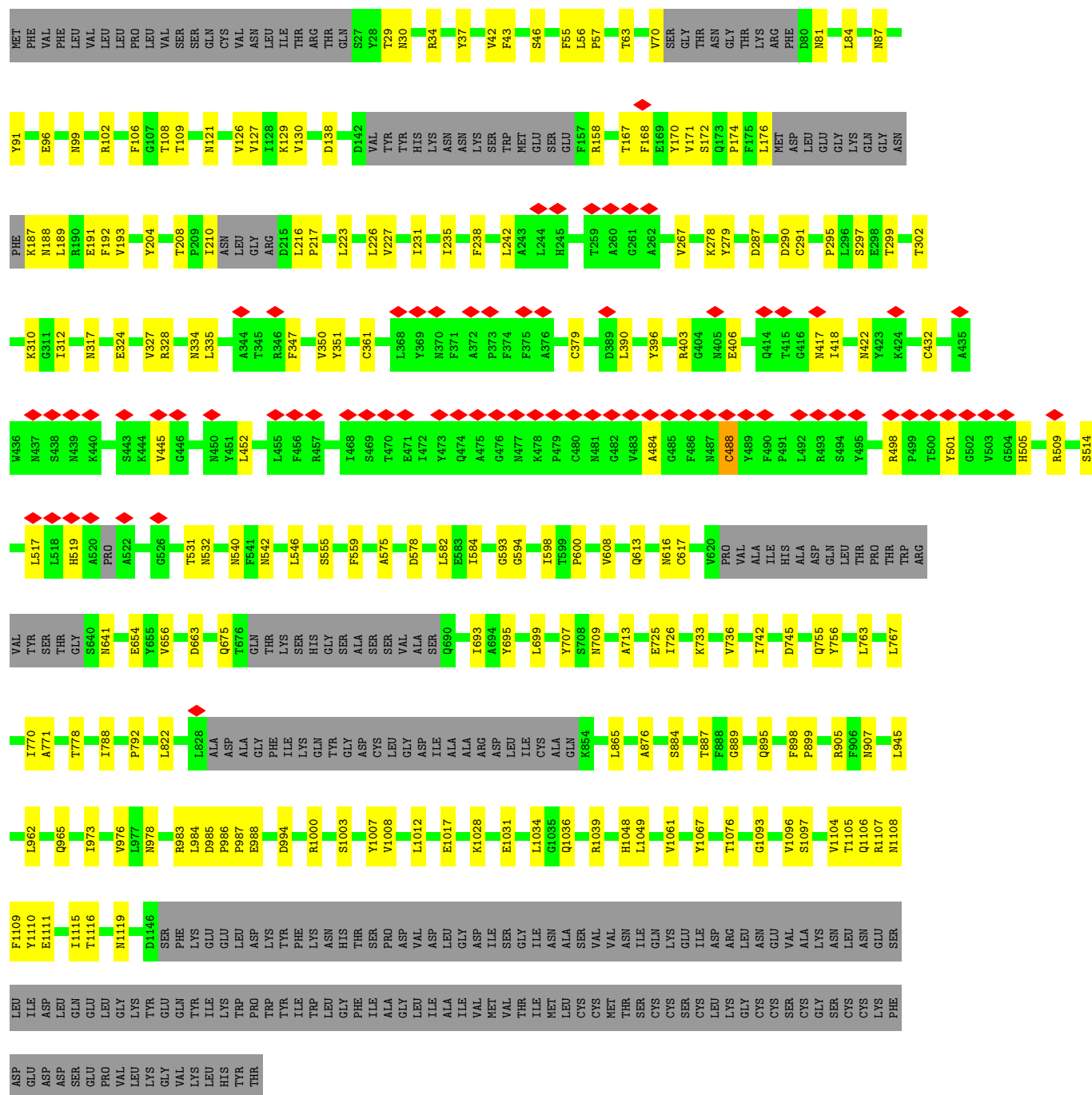
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	E	1	Total 1	Zn 1	0
5	F	1	Total 1	Zn 1	0

SER
CYS
GLY
SER
PHE
CYS
CYS
LYS
PHE
ASP
GLU
ASP
ASP
SER
SER
GLU
PRO
VAL
VAL
LEU
LYS
GLY
VAL
LYS
HIS
THR

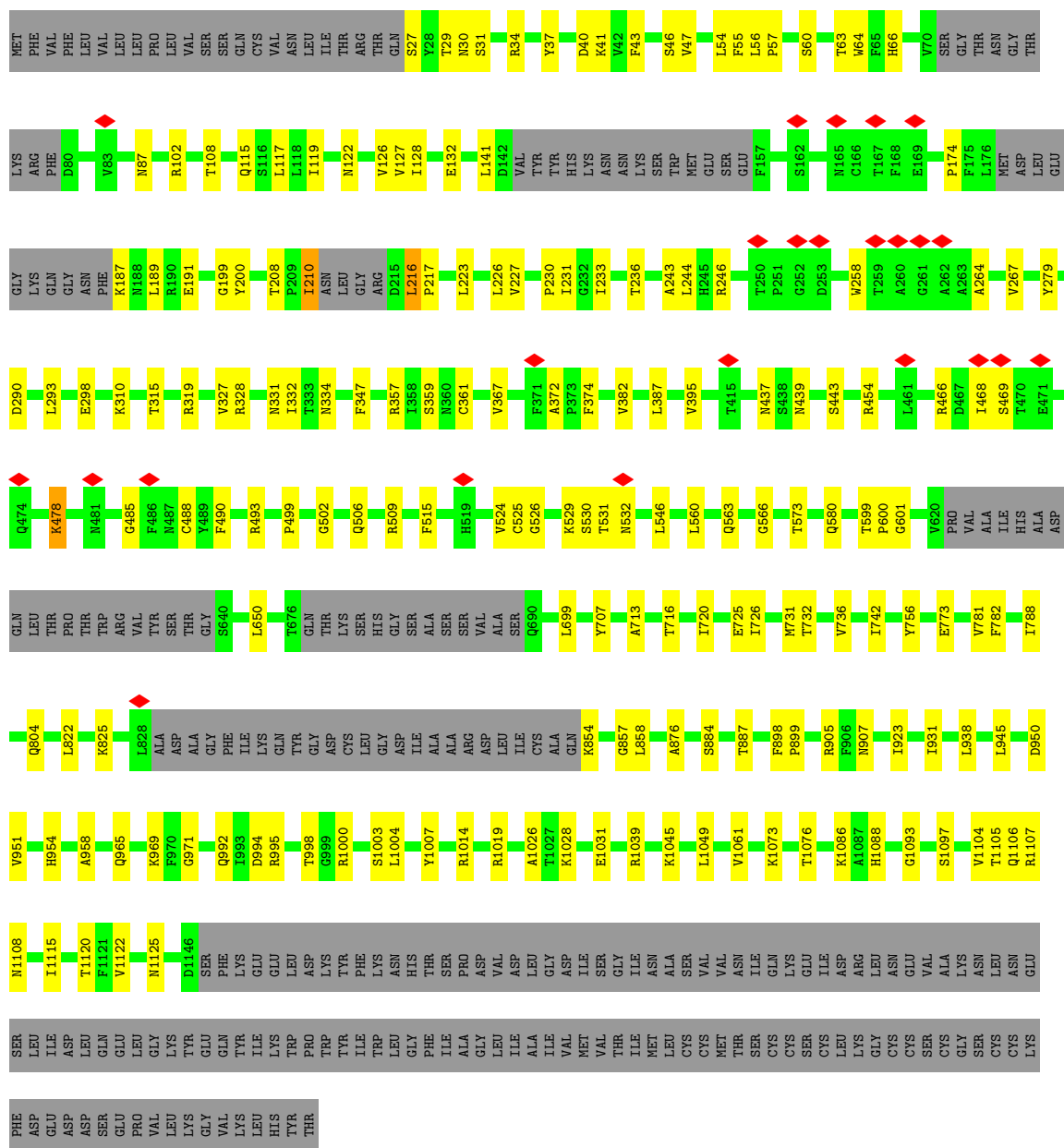
• Molecule 1: Spike glycoprotein

Chain B: 

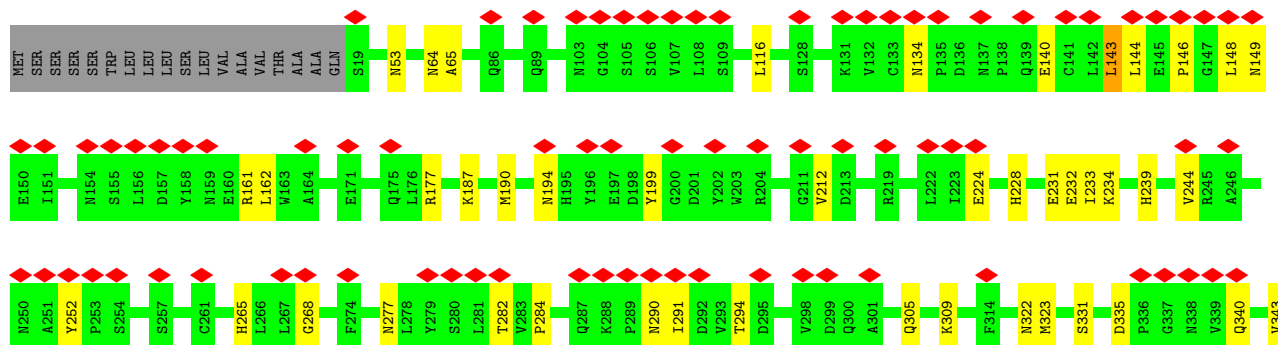


• Molecule 1: Spike glycoprotein

Chain C: 



• Molecule 2: Angiotensin-converting enzyme 2



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115739	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	2.110	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.017	Depositor
Map size (\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 (\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: CL, 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	0.24	0/8192	0.42	0/11154
1	B	0.25	0/8132	0.42	0/11076
1	C	0.25	0/8192	0.42	0/11154
2	E	0.23	0/4994	0.37	0/6785
2	F	0.23	0/4994	0.37	0/6785
All	All	0.24	0/34504	0.40	0/46954

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	7801	129	0
1	B	7943	0	7699	160	0
1	C	8001	0	7801	144	0
2	E	4857	0	4637	46	0
2	F	4857	0	4637	46	0
3	A	154	0	143	1	0
3	B	154	0	143	1	0
3	C	154	0	143	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	42	0	39	1	0
3	F	42	0	39	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	34209	0	33082	484	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.

All (484) 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:168:PHE:CE1	1:C:357:ARG:HD2	1.31	1.66
1:B:168:PHE:HE1	1:C:357:ARG:CD	1.16	1.54
1:A:117:LEU:HD13	1:A:130:VAL:CG2	1.66	1.25
1:B:121:ASN:ND2	1:B:176:LEU:HD12	1.58	1.19
1:A:117:LEU:HD13	1:A:130:VAL:HG23	1.29	1.13
1:B:168:PHE:CE1	1:C:357:ARG:CD	2.02	1.12
1:B:582:LEU:HD12	1:B:582:LEU:O	1.47	1.12
1:B:121:ASN:ND2	1:B:176:LEU:CD1	2.13	1.11
1:B:121:ASN:HD22	1:B:176:LEU:CD1	1.62	1.11
1:B:531:THR:HG22	1:B:532:ASN:H	1.13	1.07
1:A:466:ARG:NH1	1:A:468:ILE:HD11	1.71	1.04
1:A:466:ARG:CZ	1:A:468:ILE:HD11	1.90	1.01
1:A:117:LEU:CD1	1:A:130:VAL:CG2	2.40	0.99
1:B:121:ASN:HD22	1:B:176:LEU:HD12	1.12	0.99
1:B:168:PHE:HE1	1:C:357:ARG:CG	1.75	0.99
1:B:985:ASP:OD2	1:B:987:PRO:HD2	1.63	0.97
1:A:117:LEU:CD1	1:A:130:VAL:HG23	1.95	0.94
1:B:327:VAL:HG23	1:B:542:ASN:HB3	1.50	0.93
1:B:531:THR:HG22	1:B:532:ASN:N	1.83	0.92
1:B:168:PHE:CZ	1:C:357:ARG:HD2	2.06	0.91
1:B:985:ASP:OD2	1:B:987:PRO:CG	2.22	0.87
1:B:985:ASP:OD2	1:B:987:PRO:CD	2.22	0.87
1:B:531:THR:CG2	1:B:532:ASN:H	1.87	0.87
1:B:121:ASN:HD22	1:B:176:LEU:CG	1.88	0.86
1:A:331:ASN:O	1:A:332:ILE:HG13	1.74	0.86
1:A:1093:GLY:HA3	1:A:1105:THR:O	1.74	0.86
1:B:168:PHE:CE1	1:C:357:ARG:CG	2.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:LEU:HD22	1:A:585:LEU:HD11	1.60	0.84
1:C:468:ILE:HG22	1:C:468:ILE:O	1.76	0.84
1:A:468:ILE:HG22	1:A:468:ILE:O	1.77	0.83
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.60	0.82
1:A:46:SER:HA	1:A:279:TYR:O	1.80	0.81
1:A:117:LEU:CD1	1:A:130:VAL:HG22	2.09	0.81
1:C:46:SER:HA	1:C:279:TYR:O	1.81	0.81
1:B:168:PHE:CE2	1:C:359:SER:HB3	2.16	0.80
1:C:1093:GLY:HA3	1:C:1105:THR:O	1.79	0.80
1:B:126:VAL:HB	1:B:174:PRO:HB3	1.64	0.79
1:C:1088:HIS:HB3	1:C:1120:THR:CG2	2.15	0.76
1:B:121:ASN:CB	1:B:176:LEU:HD12	2.15	0.76
1:B:1093:GLY:HA3	1:B:1105:THR:O	1.85	0.76
1:A:395:VAL:HG12	1:A:395:VAL:O	1.86	0.76
1:C:187:LYS:HA	1:C:210:ILE:H	1.51	0.76
1:B:121:ASN:CG	1:B:176:LEU:HD12	2.05	0.75
1:B:187:LYS:HA	1:B:210:ILE:H	1.50	0.75
1:B:755:GLN:HE22	1:C:971:GLY:H	1.33	0.75
1:C:361:CYS:O	1:C:524:VAL:HG23	1.84	0.75
1:B:985:ASP:CG	1:B:987:PRO:HD2	2.05	0.75
1:B:46:SER:HA	1:B:279:TYR:O	1.87	0.74
1:B:985:ASP:OD2	1:B:987:PRO:HG2	1.87	0.73
1:B:168:PHE:CE1	1:C:357:ARG:NE	2.57	0.72
1:B:168:PHE:CD2	1:C:359:SER:CB	2.73	0.71
1:B:168:PHE:HE1	1:C:357:ARG:NE	1.89	0.70
1:A:290:ASP:HB3	1:A:293:LEU:HD22	1.74	0.70
1:A:552:LEU:HD22	1:A:585:LEU:CD1	2.21	0.70
1:B:70:VAL:HG23	1:B:242:LEU:HD12	1.76	0.68
1:A:552:LEU:HB3	1:A:585:LEU:HD13	1.76	0.68
1:C:599:THR:HG22	1:C:601:GLY:H	1.60	0.67
1:C:29:THR:HG22	1:C:30:ASN:N	2.10	0.66
1:B:43:PHE:H	1:C:566:GLY:HA2	1.61	0.66
1:B:168:PHE:CE1	1:C:357:ARG:HG2	2.31	0.65
1:B:168:PHE:CE2	1:C:359:SER:CB	2.78	0.65
1:C:1088:HIS:HB3	1:C:1120:THR:HG21	1.79	0.65
1:C:290:ASP:HB3	1:C:293:LEU:HD22	1.79	0.65
1:B:582:LEU:O	1:B:582:LEU:CD1	2.36	0.65
1:A:699:LEU:HB2	1:C:788:ILE:HD11	1.79	0.64
1:A:69:HIS:O	1:A:70:VAL:HG12	1.98	0.64
1:B:168:PHE:CZ	1:C:359:SER:HB3	2.31	0.64
1:C:468:ILE:O	1:C:468:ILE:CG2	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:HG12	1:B:172:SER:N	2.13	0.64
1:B:788:ILE:HD11	1:C:699:LEU:HB2	1.79	0.63
1:A:907:ASN:HD22	1:B:1107:ARG:HH22	1.45	0.63
1:A:117:LEU:CB	1:A:130:VAL:HG22	2.29	0.63
1:C:466:ARG:NH1	1:C:468:ILE:HD11	2.13	0.63
1:C:31:SER:HG	1:C:60:SER:HG	1.44	0.62
1:A:466:ARG:NH2	1:A:468:ILE:HD11	2.14	0.62
1:A:117:LEU:HB2	1:A:130:VAL:HG22	1.81	0.62
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.80	0.62
1:A:468:ILE:O	1:A:468:ILE:CG2	2.45	0.61
1:C:529:LYS:NZ	1:C:580:GLN:OE1	2.34	0.61
1:B:656:VAL:HB	1:B:695:TYR:HB3	1.82	0.61
2:F:53:ASN:HB2	2:F:340:GLN:HE21	1.64	0.61
1:A:99:ASN:OD1	1:A:102:ARG:NH1	2.33	0.61
2:F:239:HIS:O	2:F:599:ASN:ND2	2.34	0.61
1:C:34:ARG:NH2	1:C:191:GLU:OE2	2.33	0.61
1:A:788:ILE:HD11	1:B:699:LEU:HB2	1.83	0.60
1:B:121:ASN:HD22	1:B:176:LEU:HG	1.65	0.60
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.83	0.60
1:A:916:LEU:HD12	1:A:923:ILE:HD12	1.84	0.60
2:E:53:ASN:HB2	2:E:340:GLN:HE21	1.67	0.60
1:A:187:LYS:HA	1:A:210:ILE:HB	1.84	0.60
1:A:34:ARG:NH2	1:A:191:GLU:OE2	2.35	0.59
1:A:367:VAL:HG12	1:A:367:VAL:O	2.01	0.59
1:B:907:ASN:HD22	1:C:1107:ARG:HH22	1.48	0.59
2:E:239:HIS:O	2:E:599:ASN:ND2	2.34	0.59
1:B:121:ASN:ND2	1:B:176:LEU:CG	2.59	0.59
1:B:575:ALA:HB1	1:B:584:ILE:HD11	1.84	0.59
1:C:367:VAL:HG12	1:C:374:PHE:HZ	1.68	0.59
1:C:367:VAL:HG12	1:C:367:VAL:O	2.03	0.59
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.84	0.59
1:B:37:TYR:H	1:B:55:PHE:HE1	1.51	0.59
1:B:34:ARG:NH2	1:B:191:GLU:OE2	2.36	0.59
2:F:224:GLU:O	2:F:228:HIS:ND1	2.36	0.59
1:B:34:ARG:HH11	1:B:217:PRO:HG2	1.68	0.58
2:F:190:MET:O	2:F:194:ASN:ND2	2.36	0.58
1:C:46:SER:CA	1:C:279:TYR:O	2.51	0.58
2:E:224:GLU:O	2:E:228:HIS:ND1	2.37	0.58
1:A:131:CYS:HA	1:A:166:CYS:HA	1.84	0.58
1:A:37:TYR:H	1:A:55:PHE:HE1	1.50	0.58
1:B:484:ALA:HB3	1:B:488:CYS:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASN:C	1:A:332:ILE:HG13	2.24	0.58
1:A:466:ARG:HH12	1:A:468:ILE:HD11	1.64	0.58
2:F:538:PRO:HD2	2:F:541:LYS:HD2	1.85	0.58
1:B:121:ASN:ND2	1:B:176:LEU:HG	2.19	0.58
2:E:190:MET:O	2:E:194:ASN:ND2	2.36	0.58
2:E:538:PRO:HD2	2:E:541:LYS:HD2	1.86	0.58
1:B:379:CYS:HA	1:B:432:CYS:HA	1.86	0.58
1:B:46:SER:CA	1:B:279:TYR:O	2.51	0.57
1:B:81:ASN:HD21	1:B:138:ASP:HB3	1.68	0.57
1:B:189:LEU:HB3	1:B:208:THR:O	2.03	0.57
1:B:763:LEU:HG	1:B:1008:VAL:HG21	1.86	0.57
1:A:1107:ARG:HH22	1:C:907:ASN:HD22	1.50	0.57
1:C:334:ASN:HD22	1:C:361:CYS:HA	1.69	0.57
1:A:466:ARG:NH2	1:A:468:ILE:CD1	2.68	0.56
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.34	0.56
1:B:130:VAL:O	1:B:167:THR:OG1	2.15	0.56
1:C:958:ALA:HB2	1:C:1014:ARG:HH22	1.70	0.56
1:C:367:VAL:HG12	1:C:374:PHE:CZ	2.40	0.56
1:B:324:GLU:O	1:B:540:ASN:ND2	2.39	0.56
1:C:226:LEU:HG	1:C:227:VAL:HG22	1.88	0.56
1:C:716:THR:OG1	1:C:1073:LYS:NZ	2.38	0.56
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.31	0.56
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.86	0.56
1:B:127:VAL:HG13	1:B:129:LYS:HE2	1.88	0.55
2:F:177:ARG:NH2	2:F:495:GLU:O	2.40	0.55
2:E:343:VAL:HG12	2:E:345:HIS:H	1.71	0.55
1:B:63:THR:HB	1:B:267:VAL:HB	1.89	0.55
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.72	0.55
1:B:158:ARG:HD2	3:B:1310:NAG:H81	1.87	0.55
2:F:343:VAL:HG12	2:F:345:HIS:H	1.71	0.55
1:A:724:THR:HG21	1:A:938:LEU:HD21	1.89	0.55
1:B:168:PHE:CG	1:C:359:SER:OG	2.54	0.55
1:B:973:ILE:HG21	1:B:983:ARG:HH12	1.71	0.55
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.39	0.55
2:F:582:ARG:O	2:F:586:ASN:ND2	2.40	0.55
2:E:177:ARG:NH2	2:E:495:GLU:O	2.40	0.55
1:B:445:VAL:HG23	1:B:445:VAL:O	2.07	0.54
1:B:1116:THR:H	1:B:1119:ASN:HD21	1.54	0.54
1:C:742:ILE:O	1:C:1000:ARG:NH2	2.41	0.54
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.88	0.54
2:E:582:ARG:O	2:E:586:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:CD2	1:C:359:SER:HB2	2.43	0.54
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.90	0.54
1:A:575:ALA:HB1	1:A:584:ILE:HD11	1.89	0.54
1:C:56:LEU:HD12	1:C:57:PRO:HD2	1.90	0.54
2:F:144:LEU:O	2:F:149:ASN:ND2	2.41	0.54
2:E:161:ARG:NH1	2:E:252:TYR:OH	2.41	0.54
2:F:305:GLN:HE21	2:F:309:LYS:HE2	1.72	0.54
1:B:965:GLN:NE2	1:B:1003:SER:OG	2.41	0.54
2:E:116:LEU:HD11	2:E:187:LYS:HE2	1.90	0.54
2:F:161:ARG:NH1	2:F:252:TYR:OH	2.41	0.53
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.91	0.53
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.90	0.53
1:B:42:VAL:O	1:C:563:GLN:NE2	2.41	0.53
1:C:720:ILE:HG13	1:C:923:ILE:HG23	1.90	0.53
2:F:116:LEU:HD11	2:F:187:LYS:HE2	1.90	0.53
1:C:29:THR:HG22	1:C:30:ASN:H	1.74	0.53
2:F:244:VAL:HG13	2:F:282:THR:HG21	1.91	0.53
1:A:566:GLY:HA2	1:C:43:PHE:H	1.74	0.53
1:A:983:ARG:HG2	1:B:390:LEU:HD21	1.90	0.53
1:B:171:VAL:CG1	1:B:172:SER:N	2.71	0.53
1:B:985:ASP:HB3	1:B:988:GLU:HG2	1.91	0.53
1:B:976:VAL:HG22	1:B:978:ASN:H	1.74	0.53
1:C:490:PHE:HB3	1:C:493:ARG:HH22	1.74	0.53
1:B:616:ASN:OD1	1:B:617:CYS:N	2.42	0.53
2:E:305:GLN:HE21	2:E:309:LYS:HE2	1.72	0.53
1:A:69:HIS:O	1:A:70:VAL:CG1	2.56	0.52
1:B:756:TYR:OH	1:B:994:ASP:OD1	2.23	0.52
1:B:226:LEU:HG	1:B:227:VAL:HG23	1.89	0.52
1:C:992:GLN:OE1	1:C:995:ARG:NH1	2.41	0.52
2:E:144:LEU:O	2:E:149:ASN:ND2	2.42	0.52
1:A:490:PHE:HB3	1:A:493:ARG:HH22	1.74	0.52
2:E:134:ASN:HD21	2:E:140:GLU:HB3	1.75	0.52
1:A:90:VAL:HG12	1:A:194:PHE:HB2	1.90	0.52
1:C:328:ARG:HH11	1:C:580:GLN:HB2	1.74	0.52
1:B:334:ASN:OD1	1:B:335:LEU:N	2.41	0.52
1:C:525:CYS:SG	1:C:526:GLY:N	2.79	0.52
2:F:134:ASN:HD21	2:F:140:GLU:HB3	1.74	0.52
1:A:1091:ARG:NH2	1:A:1120:THR:O	2.43	0.51
1:A:334:ASN:ND2	1:A:360:ASN:O	2.42	0.51
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.91	0.51
1:A:792:PRO:HG3	1:B:707:TYR:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:778:THR:HG22	1:B:865:LEU:HD12	1.91	0.51
1:A:46:SER:CA	1:A:279:TYR:O	2.53	0.51
1:B:985:ASP:OD1	1:B:986:PRO:HD2	2.10	0.51
1:C:66:HIS:HD2	1:C:264:ALA:HB2	1.76	0.51
1:A:1031:GLU:OE1	1:A:1039:ARG:NH2	2.42	0.51
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.91	0.51
1:A:331:ASN:O	1:A:332:ILE:CG1	2.53	0.51
1:C:108:THR:O	1:C:236:THR:OG1	2.28	0.51
1:A:206:LYS:HG3	1:A:208:THR:HG22	1.93	0.51
1:C:29:THR:CG2	1:C:30:ASN:N	2.73	0.51
1:C:560:LEU:HB2	1:C:563:GLN:HB2	1.93	0.51
2:E:290:ASN:OD1	2:E:291:ILE:N	2.43	0.51
1:B:555:SER:HB2	1:B:584:ILE:HG23	1.92	0.51
1:B:726:ILE:HD13	1:B:945:LEU:HD23	1.92	0.51
1:A:34:ARG:HH11	1:A:217:PRO:HG2	1.76	0.51
1:B:351:TYR:HE1	1:B:452:LEU:HB2	1.76	0.51
1:C:37:TYR:H	1:C:55:PHE:HE1	1.59	0.51
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.92	0.50
1:C:102:ARG:HB3	1:C:141:LEU:HD23	1.92	0.50
2:E:232:GLU:HB3	2:E:585:LEU:HD11	1.92	0.50
1:B:1116:THR:OG1	1:B:1119:ASN:ND2	2.45	0.50
1:C:825:LYS:NZ	1:C:938:LEU:O	2.45	0.50
2:E:394:ASN:OD1	2:E:395:GLY:N	2.43	0.50
1:A:119:ILE:HG12	1:A:128:ILE:HG23	1.94	0.50
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.94	0.50
1:C:736:VAL:HG12	1:C:858:LEU:HG	1.94	0.50
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.94	0.50
1:B:1106:GLN:HG3	1:B:1108:ASN:H	1.76	0.50
1:A:121:ASN:HD22	1:A:176:LEU:HG	1.75	0.49
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.94	0.49
1:B:531:THR:HG22	1:B:532:ASN:OD1	2.12	0.49
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.94	0.49
1:C:34:ARG:HH11	1:C:217:PRO:HG2	1.75	0.49
2:E:244:VAL:HG13	2:E:282:THR:HG21	1.93	0.49
2:F:232:GLU:HB3	2:F:585:LEU:HD11	1.93	0.49
2:F:524:GLN:HE22	2:F:570:LEU:HD21	1.78	0.49
1:A:367:VAL:HG12	1:A:374:PHE:CZ	2.47	0.49
1:A:546:LEU:HD21	1:A:573:THR:HG21	1.94	0.49
1:A:752:LEU:HD22	1:A:997:ILE:HD12	1.94	0.49
1:C:781:VAL:HG13	1:C:782:PHE:CD2	2.48	0.49
1:A:395:VAL:O	1:A:395:VAL:CG1	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:335:ASP:N	2:F:335:ASP:OD1	2.46	0.49
1:A:246:ARG:HE	1:A:248:TYR:HE1	1.60	0.49
2:E:268:GLY:O	2:E:277:ASN:ND2	2.35	0.49
1:C:40:ASP:OD1	1:C:41:LYS:N	2.44	0.49
1:B:121:ASN:ND2	1:B:176:LEU:HD11	2.20	0.49
1:C:756:TYR:OH	1:C:998:THR:OG1	2.29	0.49
1:B:1036:GLN:NE2	1:B:1048:HIS:O	2.43	0.49
1:C:439:ASN:O	1:C:443:SER:OG	2.20	0.49
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.94	0.49
1:A:500:THR:HG1	2:F:41:TYR:HH	1.60	0.49
1:A:763:LEU:HG	1:A:1008:VAL:HG21	1.95	0.49
1:C:854:LYS:N	1:C:858:LEU:O	2.46	0.48
2:F:290:ASN:OD1	2:F:291:ILE:N	2.43	0.48
2:E:143:LEU:HD23	2:E:143:LEU:H	1.78	0.48
2:F:143:LEU:HD23	2:F:143:LEU:H	1.78	0.48
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.95	0.48
1:A:916:LEU:CD1	1:A:923:ILE:HD12	2.43	0.48
1:B:334:ASN:HB3	1:B:361:CYS:HA	1.94	0.48
1:B:501:TYR:HB3	1:B:505:HIS:HB2	1.95	0.48
2:E:335:ASP:OD1	2:E:335:ASP:N	2.45	0.48
1:B:884:SER:OG	1:B:887:THR:OG1	2.31	0.48
1:A:331:ASN:OD1	1:A:580:GLN:NE2	2.46	0.48
1:B:290:ASP:OD1	1:B:291:CYS:N	2.44	0.48
2:E:488:VAL:HG21	2:E:611:SER:HA	1.95	0.48
2:E:527:GLU:OE2	2:E:531:GLN:NE2	2.47	0.48
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.22	0.48
1:A:102:ARG:HB3	1:A:141:LEU:HD23	1.95	0.48
1:A:391:CYS:HB2	1:A:522:ALA:HB1	1.95	0.48
1:A:437:ASN:ND2	1:A:506:GLN:OE1	2.45	0.48
1:C:332:ILE:HG13	1:C:529:LYS:HE2	1.96	0.48
1:C:490:PHE:O	1:C:493:ARG:NH2	2.47	0.48
2:F:488:VAL:HG21	2:F:611:SER:HA	1.96	0.48
2:E:457:GLU:OE2	2:E:460:ARG:NH2	2.47	0.48
1:A:187:LYS:HA	1:A:210:ILE:H	1.78	0.47
1:A:1106:GLN:HG3	1:A:1108:ASN:H	1.79	0.47
1:B:96:GLU:O	1:B:188:ASN:ND2	2.47	0.47
1:B:350:VAL:HG21	1:B:418:ILE:HD12	1.96	0.47
1:B:742:ILE:O	1:B:1000:ARG:NH2	2.47	0.47
1:A:466:ARG:CZ	1:A:468:ILE:CD1	2.79	0.47
1:A:490:PHE:O	1:A:493:ARG:NH2	2.46	0.47
2:F:457:GLU:OE2	2:F:460:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HB	1:A:598:ILE:HG12	1.97	0.47
1:C:115:GLN:NE2	1:C:132:GLU:OE2	2.48	0.47
1:A:246:ARG:HD2	1:A:258:TRP:HE3	1.79	0.47
1:C:804:GLN:NE2	1:C:931:ILE:O	2.46	0.47
1:A:656:VAL:HA	3:A:1305:NAG:H82	1.96	0.47
1:A:742:ILE:O	1:A:1000:ARG:NH2	2.47	0.47
1:A:1019:ARG:NH2	1:B:1017:GLU:OE1	2.48	0.47
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.33	0.47
2:E:231:GLU:HA	2:E:234:LYS:HE2	1.97	0.47
1:A:726:ILE:HD13	1:A:945:LEU:HD23	1.96	0.47
1:A:827:THR:OG1	1:A:949:GLN:NE2	2.48	0.47
1:B:905:ARG:NH2	1:B:1049:LEU:O	2.44	0.47
1:A:895:GLN:HG2	1:B:713:ALA:HB2	1.97	0.47
2:E:560:LEU:HD13	2:E:564:GLU:HG3	1.97	0.47
2:F:560:LEU:HD13	2:F:564:GLU:HG3	1.97	0.47
1:A:905:ARG:NH2	1:A:1049:LEU:O	2.47	0.47
1:A:1126:CYS:HB3	1:A:1132:ILE:HD13	1.97	0.47
1:C:965:GLN:NE2	1:C:1003:SER:OG	2.48	0.47
1:C:781:VAL:HG23	1:C:1026:ALA:HA	1.97	0.46
1:A:478:LYS:NZ	1:A:488:CYS:SG	2.87	0.46
1:A:1031:GLU:OE2	1:B:1039:ARG:NH1	2.45	0.46
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.79	0.46
1:C:437:ASN:ND2	1:C:506:GLN:OE1	2.44	0.46
2:E:143:LEU:HG	2:E:146:PRO:HD2	1.97	0.46
2:E:331:SER:OG	2:E:358:ILE:O	2.32	0.46
1:A:119:ILE:HG23	1:A:128:ILE:HG13	1.97	0.46
2:F:529:LEU:HD22	2:F:550:ALA:HB1	1.97	0.46
1:B:983:ARG:HE	1:B:984:LEU:HG	1.80	0.46
1:C:822:LEU:HD21	1:C:938:LEU:HD13	1.98	0.46
2:E:524:GLN:HE22	2:E:570:LEU:HD21	1.79	0.46
1:A:367:VAL:HG12	1:A:374:PHE:HZ	1.80	0.46
1:C:478:LYS:NZ	1:C:488:CYS:SG	2.88	0.46
2:F:331:SER:OG	2:F:358:ILE:O	2.32	0.46
1:B:70:VAL:CG2	1:B:242:LEU:HD12	2.44	0.46
1:C:531:THR:OG1	1:C:532:ASN:N	2.45	0.46
1:C:905:ARG:NH2	1:C:1049:LEU:O	2.44	0.46
1:A:552:LEU:HB3	1:A:585:LEU:HD22	1.98	0.46
1:B:328:ARG:NH2	1:B:578:ASP:OD2	2.49	0.46
1:C:244:LEU:HD22	1:C:258:TRP:HE3	1.81	0.46
1:C:1106:GLN:HG3	1:C:1108:ASN:H	1.81	0.46
1:A:367:VAL:O	1:A:367:VAL:CG1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HG23	1:A:876:ALA:HB2	1.98	0.46
2:F:231:GLU:HA	2:F:234:LYS:HE2	1.97	0.46
1:A:290:ASP:OD1	1:A:291:CYS:N	2.44	0.46
1:C:395:VAL:HG23	1:C:515:PHE:HE1	1.81	0.46
2:E:294:THR:HG22	2:E:366:MET:H	1.81	0.46
1:A:454:ARG:NH2	1:A:469:SER:O	2.40	0.45
1:B:138:ASP:OD1	1:B:138:ASP:N	2.49	0.45
1:B:327:VAL:O	1:B:327:VAL:HG13	2.16	0.45
1:C:29:THR:CG2	1:C:30:ASN:H	2.28	0.45
1:C:117:LEU:HD11	1:C:233:ILE:HD12	1.97	0.45
1:A:1086:LYS:HD2	1:A:1122:VAL:HG21	1.97	0.45
1:B:778:THR:HG22	1:B:778:THR:O	2.15	0.45
2:E:402:GLU:HB2	2:E:518:ARG:HG3	1.98	0.45
2:F:143:LEU:HG	2:F:146:PRO:HD2	1.98	0.45
1:B:108:THR:HG22	1:B:109:THR:HG23	1.99	0.45
1:B:675:GLN:HB3	1:B:693:ILE:HD13	1.98	0.45
2:F:187:LYS:HB3	2:F:199:TYR:CG	2.52	0.45
2:F:322:ASN:OD1	2:F:323:MET:N	2.47	0.45
1:B:84:LEU:HB2	1:B:238:PHE:HB3	1.98	0.45
1:C:189:LEU:HB2	1:C:210:ILE:HG22	1.98	0.45
2:F:161:ARG:NE	2:F:265:HIS:O	2.49	0.45
1:C:216:LEU:H	1:C:216:LEU:HG	1.60	0.45
1:C:958:ALA:HB1	1:C:1007:TYR:HE1	1.81	0.45
2:F:501:ALA:O	2:F:507:SER:OG	2.35	0.45
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.99	0.45
1:B:403:ARG:HB2	1:B:406:GLU:HB2	1.98	0.45
2:E:161:ARG:NE	2:E:265:HIS:O	2.49	0.45
1:A:983:ARG:HD2	1:B:517:LEU:HD13	1.99	0.45
1:C:189:LEU:HB3	1:C:208:THR:O	2.16	0.45
1:C:331:ASN:OD1	1:C:580:GLN:NE2	2.50	0.45
2:E:187:LYS:HB3	2:E:199:TYR:CG	2.52	0.45
1:A:120:VAL:HG23	1:A:127:VAL:HB	1.99	0.45
1:B:709:ASN:OD1	1:B:709:ASN:N	2.49	0.45
2:E:322:ASN:OD1	2:E:323:MET:N	2.47	0.45
2:F:402:GLU:HB2	2:F:518:ARG:HG3	1.98	0.45
1:B:168:PHE:CD1	1:C:357:ARG:NE	2.85	0.45
2:E:212:VAL:O	2:E:212:VAL:HG13	2.16	0.45
2:F:268:GLY:O	2:F:277:ASN:ND2	2.36	0.45
1:A:69:HIS:C	1:A:70:VAL:HG12	2.37	0.44
1:A:83:VAL:HG22	1:A:237:ARG:HH22	1.82	0.44
1:A:552:LEU:HB3	1:A:585:LEU:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:ARG:CZ	1:C:468:ILE:HD11	2.46	0.44
2:F:394:ASN:OD1	2:F:395:GLY:N	2.43	0.44
1:C:485:GLY:H	1:C:488:CYS:HB2	1.82	0.44
2:E:284:PRO:HG3	2:E:440:LEU:HD13	1.99	0.44
2:F:144:LEU:HD12	2:F:148:LEU:HD23	1.99	0.44
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.99	0.44
2:E:144:LEU:HD12	2:E:148:LEU:HD23	1.98	0.44
1:B:733:LYS:HE3	1:B:771:ALA:HB1	1.99	0.44
2:F:212:VAL:HG13	2:F:212:VAL:O	2.18	0.44
2:F:294:THR:HG22	2:F:366:MET:H	1.82	0.44
1:C:736:VAL:HG21	1:C:1004:LEU:HD11	1.99	0.44
1:C:950:ASP:OD1	1:C:951:VAL:N	2.48	0.44
2:F:284:PRO:HG3	2:F:440:LEU:HD13	1.99	0.44
1:A:962:LEU:HD11	1:A:1007:TYR:HB2	1.99	0.44
2:E:501:ALA:O	2:E:507:SER:OG	2.35	0.44
1:A:552:LEU:CB	1:A:585:LEU:HD13	2.44	0.44
1:B:295:PRO:HB2	1:B:608:VAL:HG21	2.00	0.44
1:C:454:ARG:NH2	1:C:469:SER:O	2.41	0.44
1:C:884:SER:OG	1:C:887:THR:OG1	2.36	0.44
1:A:439:ASN:O	1:A:443:SER:OG	2.21	0.44
2:F:450:LEU:HD21	2:F:519:THR:HG21	2.00	0.44
1:B:962:LEU:HD11	1:B:1007:TYR:HB2	1.99	0.44
1:B:87:ASN:N	1:B:87:ASN:OD1	2.50	0.43
1:A:439:ASN:HD21	1:A:499:PRO:HA	1.82	0.43
1:B:593:GLY:HA3	1:B:613:GLN:O	2.18	0.43
1:A:372:ALA:O	1:A:374:PHE:N	2.50	0.43
2:E:233:ILE:HD13	2:E:450:LEU:HD13	2.00	0.43
1:A:382:VAL:HG11	1:A:387:LEU:HD13	1.99	0.43
1:C:246:ARG:HH11	1:C:246:ARG:HA	1.82	0.43
1:C:327:VAL:O	1:C:530:SER:HB3	2.18	0.43
1:C:372:ALA:O	1:C:374:PHE:N	2.51	0.43
2:F:233:ILE:HD13	2:F:450:LEU:HD13	2.00	0.43
1:B:641:ASN:HD22	1:B:654:GLU:HA	1.83	0.43
2:E:529:LEU:HD22	2:E:550:ALA:HB1	1.99	0.43
1:C:63:THR:OG1	1:C:267:VAL:HB	2.19	0.43
1:C:298:GLU:HG2	1:C:315:THR:HB	2.01	0.43
1:A:127:VAL:HG12	1:A:129:LYS:HG2	2.00	0.43
1:A:756:TYR:OH	1:A:998:THR:OG1	2.32	0.43
1:B:895:GLN:HG2	1:C:713:ALA:HB2	2.00	0.43
1:C:87:ASN:OD1	1:C:87:ASN:N	2.51	0.43
1:C:1086:LYS:HD2	1:C:1122:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ILE:HB	1:B:598:ILE:HG12	2.00	0.43
1:B:417:ASN:O	1:B:422:ASN:ND2	2.49	0.43
1:C:546:LEU:HD21	1:C:573:THR:HG21	2.01	0.43
1:C:788:ILE:HG23	1:C:876:ALA:HB2	2.00	0.43
1:C:439:ASN:HD21	1:C:499:PRO:HA	1.84	0.43
1:C:1088:HIS:HB3	1:C:1120:THR:HG22	1.97	0.43
2:E:64:ASN:OD1	2:E:65:ALA:N	2.52	0.43
2:F:64:ASN:OD1	2:F:65:ALA:N	2.52	0.43
1:B:663:ASP:OD1	1:B:663:ASP:N	2.51	0.42
1:B:745:ASP:OD1	1:C:319:ARG:NH1	2.51	0.42
1:C:37:TYR:OH	1:C:54:LEU:O	2.31	0.42
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.54	0.42
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	2.00	0.42
1:A:902:MET:HB2	1:A:916:LEU:HD21	2.00	0.42
1:B:171:VAL:CG1	1:B:172:SER:H	2.31	0.42
2:E:450:LEU:HD21	2:E:519:THR:HG21	2.01	0.42
1:B:519:HIS:HD2	1:B:546:LEU:HD23	1.84	0.42
1:B:1031:GLU:OE1	1:B:1039:ARG:NH2	2.43	0.42
1:C:127:VAL:HG11	3:C:1310:NAG:H81	2.01	0.42
2:F:503:LEU:HD23	2:F:506:VAL:HG23	2.01	0.42
1:B:299:THR:HA	1:B:302:THR:HG22	2.00	0.42
1:B:792:PRO:HG3	1:C:707:TYR:HB3	2.01	0.42
2:E:503:LEU:HD23	2:E:506:VAL:HG23	2.01	0.42
1:A:466:ARG:NH1	1:A:468:ILE:CD1	2.62	0.42
1:C:731:MET:HG2	1:C:732:THR:H	1.83	0.42
1:C:951:VAL:O	1:C:954:HIS:HB2	2.19	0.42
1:A:1039:ARG:NH1	1:C:1031:GLU:OE2	2.50	0.42
1:B:1031:GLU:OE2	1:C:1039:ARG:NH1	2.47	0.42
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	2.02	0.42
1:C:199:GLY:O	1:C:231:ILE:N	2.53	0.42
1:C:382:VAL:HG11	1:C:387:LEU:HD13	2.01	0.42
2:E:539:LEU:HD23	2:E:587:TYR:HB2	2.02	0.42
1:A:744:GLY:H	1:A:977:LEU:HD12	1.84	0.42
1:B:29:THR:OG1	1:B:30:ASN:N	2.52	0.42
1:B:290:ASP:O	1:B:297:SER:HB3	2.20	0.42
1:B:898:PHE:N	1:B:899:PRO:HD2	2.35	0.42
1:C:102:ARG:HG2	1:C:243:ALA:HB2	2.02	0.42
1:A:117:LEU:HD12	1:A:130:VAL:CG2	2.40	0.41
1:B:327:VAL:CG2	1:B:542:ASN:HB3	2.37	0.41
1:C:66:HIS:CD2	1:C:264:ALA:HB2	2.55	0.41
1:C:898:PHE:N	1:C:899:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ILE:HD13	1:C:47:VAL:HB	2.02	0.41
1:B:34:ARG:HD2	1:B:216:LEU:HD23	2.03	0.41
1:C:126:VAL:HB	1:C:174:PRO:HA	2.02	0.41
1:A:592:PHE:HZ	1:C:857:GLY:HA2	1.84	0.41
1:A:1109:PHE:HD1	1:A:1111:GLU:HG3	1.85	0.41
1:B:99:ASN:OD1	1:B:102:ARG:NH2	2.52	0.41
1:C:367:VAL:CG1	1:C:374:PHE:HZ	2.31	0.41
1:A:822:LEU:HD22	1:A:945:LEU:HD21	2.00	0.41
1:B:559:PHE:CE1	1:B:584:ILE:HG12	2.55	0.41
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.93	0.41
2:E:545:SER:HB2	3:E:904:NAG:H82	2.03	0.41
1:B:317:ASN:HA	1:B:594:GLY:HA2	2.03	0.41
1:B:788:ILE:HG23	1:B:876:ALA:HB2	2.02	0.41
1:B:1109:PHE:HD1	1:B:1111:GLU:HG3	1.85	0.41
1:A:485:GLY:H	1:A:488:CYS:HB2	1.86	0.41
1:A:37:TYR:OH	1:A:54:LEU:O	2.30	0.41
1:A:244:LEU:HD13	1:A:258:TRP:HB3	2.03	0.41
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.02	0.41
1:C:119:ILE:HG23	1:C:128:ILE:HG13	2.03	0.41
1:C:122:ASN:HB3	3:C:1310:NAG:O5	2.20	0.41
1:A:650:LEU:HD23	1:A:650:LEU:H	1.86	0.41
1:A:902:MET:CB	1:A:916:LEU:HD21	2.51	0.41
1:B:396:TYR:HB2	1:B:514:SER:HB3	2.03	0.41
1:B:755:GLN:NE2	1:C:969:LYS:HB2	2.36	0.41
1:C:27:SER:N	1:C:64:TRP:O	2.53	0.41
1:C:650:LEU:HD23	1:C:650:LEU:H	1.84	0.41
2:E:162:LEU:HD13	2:E:265:HIS:CE1	2.56	0.41
2:F:162:LEU:HD13	2:F:265:HIS:CE1	2.56	0.41
1:A:898:PHE:N	1:A:899:PRO:HD2	2.35	0.41
1:B:91:TYR:HD1	1:B:193:VAL:HG22	1.86	0.41
1:C:502:GLY:O	1:C:506:GLN:HG3	2.20	0.41
1:B:498:ARG:NH2	1:B:501:TYR:OH	2.54	0.40
2:F:535:HIS:NE2	2:F:538:PRO:O	2.54	0.40
2:F:539:LEU:HD23	2:F:587:TYR:HB2	2.03	0.40
1:A:192:PHE:HA	1:A:204:TYR:O	2.22	0.40
1:A:502:GLY:O	1:A:506:GLN:HG3	2.21	0.40
1:A:945:LEU:HD22	1:A:948:LEU:HD12	2.04	0.40
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.57	0.40
1:B:889:GLY:HA3	1:B:1034:LEU:HD23	2.03	0.40
1:C:200:TYR:HD1	1:C:230:PRO:HA	1.86	0.40
1:B:278:LYS:HE2	1:B:287:ASP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:557:MET:HG2	2:F:569:ALA:HB1	2.03	0.40
1:B:170:TYR:OH	1:B:231:ILE:HB	2.21	0.40
1:B:736:VAL:HG22	1:B:767:LEU:HD11	2.04	0.40
1:B:192:PHE:HA	1:B:204:TYR:O	2.22	0.40
1:B:1096:VAL:HG21	1:B:1110:TYR:HE1	1.87	0.40
2:E:535:HIS:NE2	2:E:538:PRO:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1010/1270 (80%)	989 (98%)	21 (2%)	0	100	100
1	B	1007/1270 (79%)	976 (97%)	31 (3%)	0	100	100
1	C	1010/1270 (80%)	985 (98%)	25 (2%)	0	100	100
2	E	593/805 (74%)	590 (100%)	3 (0%)	0	100	100
2	F	593/805 (74%)	590 (100%)	3 (0%)	0	100	100
All	All	4213/5420 (78%)	4130 (98%)	83 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	886 (100%)	4 (0%)	89	93
1	B	874/1110 (79%)	872 (100%)	2 (0%)	92	96
1	C	890/1110 (80%)	885 (99%)	5 (1%)	84	91
2	E	526/711 (74%)	522 (99%)	4 (1%)	79	88
2	F	526/711 (74%)	523 (99%)	3 (1%)	84	91
All	All	3706/4752 (78%)	3688 (100%)	18 (0%)	85	92

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	THR
1	A	428	ASP
1	A	478	LYS
1	A	538	CYS
1	B	488	CYS
1	B	1067	TYR
1	C	210	ILE
1	C	216	LEU
1	C	478	LYS
1	C	1045	LYS
1	C	1125	ASN
2	E	143	LEU
2	E	381	TYR
2	E	400	PHE
2	E	592	PHE
2	F	143	LEU
2	F	381	TYR
2	F	592	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	314	GLN
1	A	360	ASN
1	A	439	ASN
1	A	474	GLN
1	A	580	GLN
1	A	607	GLN
1	A	755	GLN

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Mol	Chain	Res	Type
1	A	895	GLN
1	A	907	ASN
1	A	949	GLN
1	A	953	ASN
1	A	965	GLN
1	A	1005	GLN
1	A	1106	GLN
1	B	52	GLN
1	B	81	ASN
1	B	121	ASN
1	B	173	GLN
1	B	282	ASN
1	B	394	ASN
1	B	519	HIS
1	B	580	GLN
1	B	641	ASN
1	B	703	ASN
1	B	755	GLN
1	B	895	GLN
1	B	907	ASN
1	B	965	GLN
1	B	1005	GLN
1	B	1106	GLN
1	B	1119	ASN
1	B	1125	ASN
1	C	52	GLN
1	C	66	HIS
1	C	239	GLN
1	C	314	GLN
1	C	334	ASN
1	C	439	ASN
1	C	474	GLN
1	C	607	GLN
1	C	895	GLN
1	C	907	ASN
1	C	965	GLN
1	C	1106	GLN
1	C	1119	ASN
2	E	51	ASN
2	E	60	GLN
2	E	81	GLN
2	E	239	HIS

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Mol	Chain	Res	Type
2	E	300	GLN
2	E	305	GLN
2	E	325	GLN
2	E	340	GLN
2	E	429	GLN
2	E	493	HIS
2	E	524	GLN
2	E	586	ASN
2	F	51	ASN
2	F	60	GLN
2	F	81	GLN
2	F	239	HIS
2	F	300	GLN
2	F	305	GLN
2	F	325	GLN
2	F	340	GLN
2	F	429	GLN
2	F	493	HIS
2	F	524	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 43 ligands modelled in this entry, 4 are monoatomic - leaving 39 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	B	1307	1	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	C	1310	1	14,14,15	0.36	0	17,19,21	0.43	0
3	NAG	F	905	2	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	B	1305	1	14,14,15	0.22	0	17,19,21	0.40	0
3	NAG	E	905	2	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	1302	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	B	1310	1	14,14,15	0.26	0	17,19,21	0.40	0
3	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	F	903	2	14,14,15	0.38	0	17,19,21	0.52	0
3	NAG	F	904	2	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	C	1309	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	E	904	2	14,14,15	0.27	0	17,19,21	0.44	0
3	NAG	A	1307	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	B	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	A	1310	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.45	0
3	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	E	903	2	14,14,15	0.36	0	17,19,21	0.42	0
3	NAG	A	1311	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	C	1305	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	C	1308	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	B	1308	1	14,14,15	0.21	0	17,19,21	0.42	0
3	NAG	C	1301	1	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	A	1305	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	C	1311	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	B	1301	1	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	B	1311	1	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	C	1303	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	A	1309	1	14,14,15	0.23	0	17,19,21	0.41	0
3	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	1304	1	14,14,15	0.21	0	17,19,21	0.43	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	B	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	F	905	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	E	905	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	1/6/23/26	0/1/1/1
3	NAG	F	903	2	-	3/6/23/26	0/1/1/1
3	NAG	F	904	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	E	904	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
3	NAG	E	903	2	-	1/6/23/26	0/1/1/1
3	NAG	A	1311	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	1302	1	-	1/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	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	1304	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1309	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	B	1311	NAG	O5-C5-C6-O6
3	A	1307	NAG	C4-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	C	1307	NAG	O5-C5-C6-O6
3	F	903	NAG	O5-C5-C6-O6
3	B	1309	NAG	C4-C5-C6-O6
3	B	1311	NAG	C4-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	F	904	NAG	C4-C5-C6-O6
3	B	1307	NAG	O5-C5-C6-O6
3	C	1311	NAG	O5-C5-C6-O6
3	F	904	NAG	O5-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	A	1305	NAG	O5-C5-C6-O6
3	A	1307	NAG	O5-C5-C6-O6
3	B	1308	NAG	O5-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1310	NAG	C4-C5-C6-O6
3	F	903	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	B	1308	NAG	C4-C5-C6-O6
3	C	1311	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	1307	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	C	1311	NAG	C8-C7-N2-C2
3	C	1311	NAG	O7-C7-N2-C2
3	A	1306	NAG	C4-C5-C6-O6
3	B	1310	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1305	NAG	C4-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	E	903	NAG	O5-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1305	NAG	O5-C5-C6-O6
3	C	1305	NAG	C4-C5-C6-O6
3	C	1302	NAG	O5-C5-C6-O6
3	A	1306	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6
3	B	1302	NAG	O5-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	B	1306	NAG	C4-C5-C6-O6
3	F	903	NAG	C3-C2-N2-C7
3	A	1304	NAG	C4-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	E	904	NAG	C4-C5-C6-O6
3	E	904	NAG	O5-C5-C6-O6
3	C	1302	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1310	NAG	2	0
3	B	1310	NAG	1	0
3	E	904	NAG	1	0
3	A	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

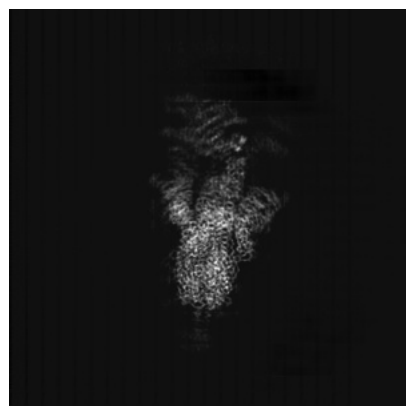
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33339. These allow visual inspection of the internal detail of the map and identification of artifacts.

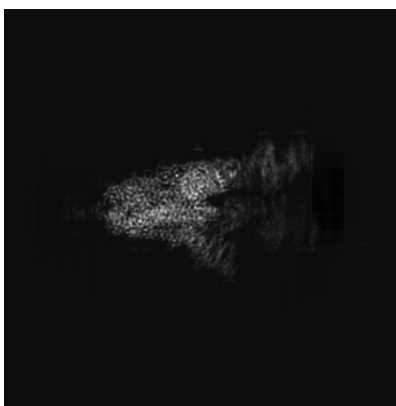
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

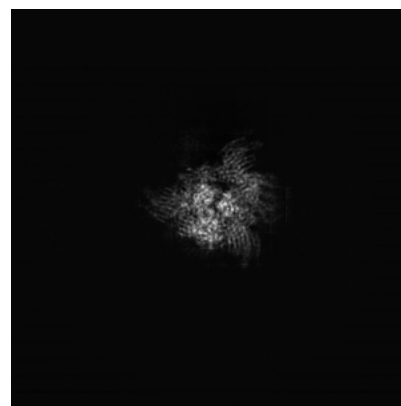
6.1.1 Primary map



X

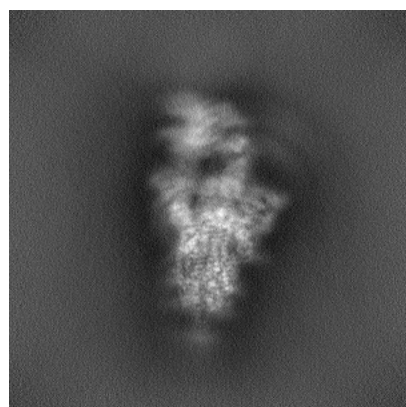


Y

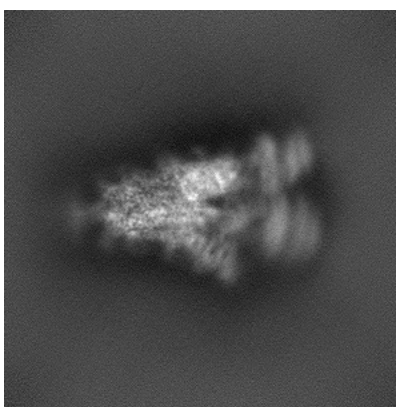


Z

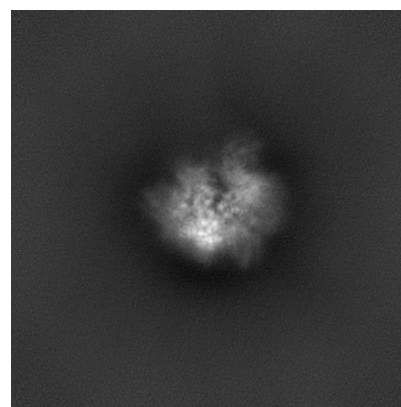
6.1.2 Raw map



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

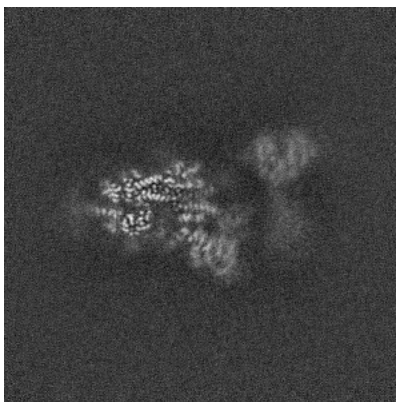


Z Index: 240

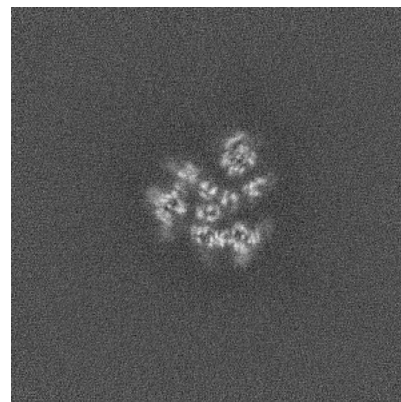
6.2.2 Raw map



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: 239

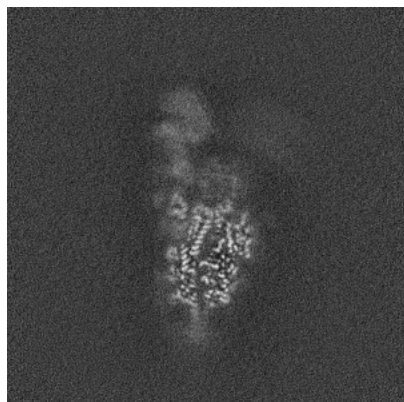


Y Index: 248

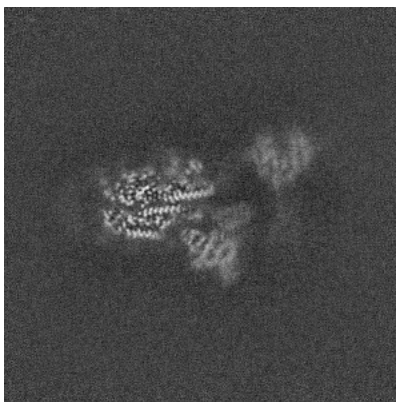


Z Index: 223

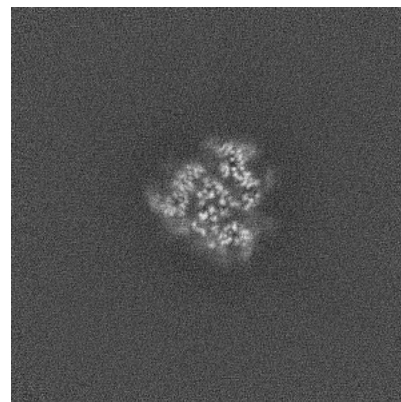
6.3.2 Raw map



X Index: 229



Y Index: 246

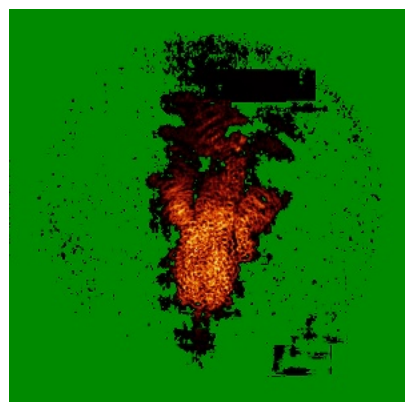


Z Index: 228

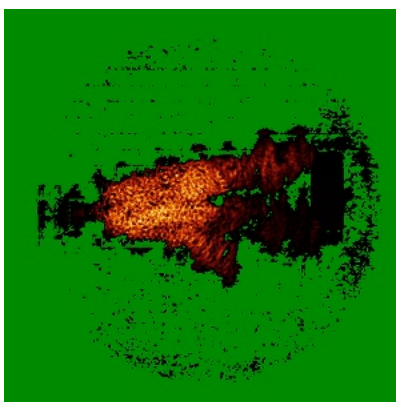
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

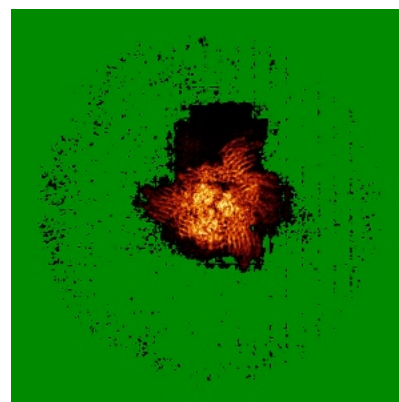
6.4.1 Primary map



X

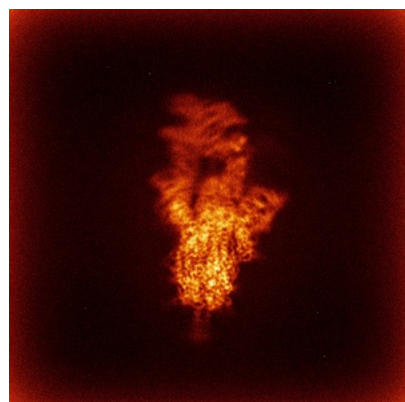


Y

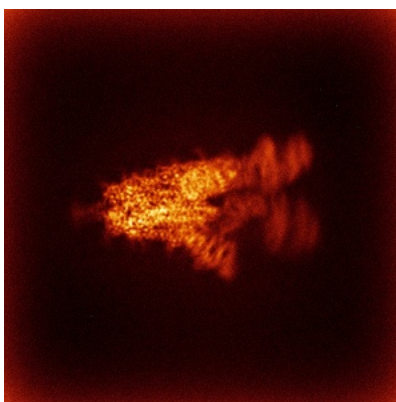


Z

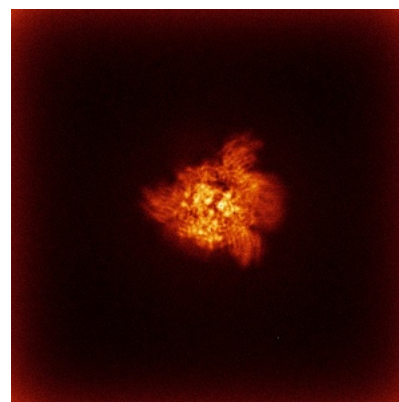
6.4.2 Raw map



X



Y

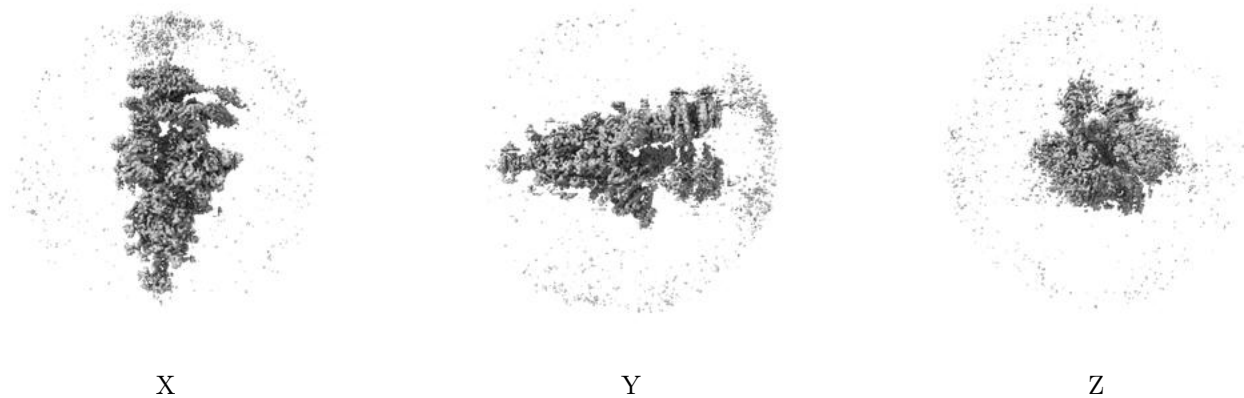


Z

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.

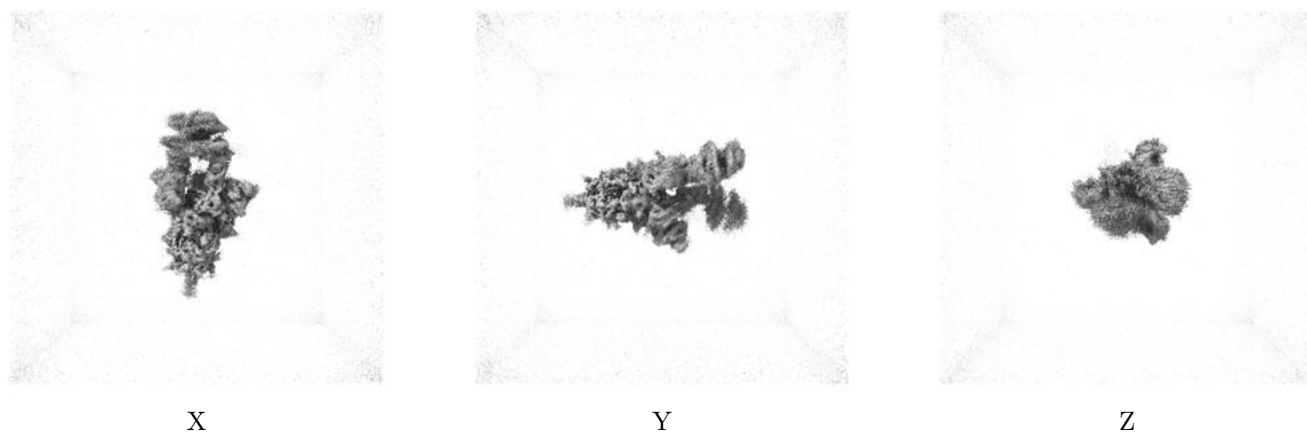
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. 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.

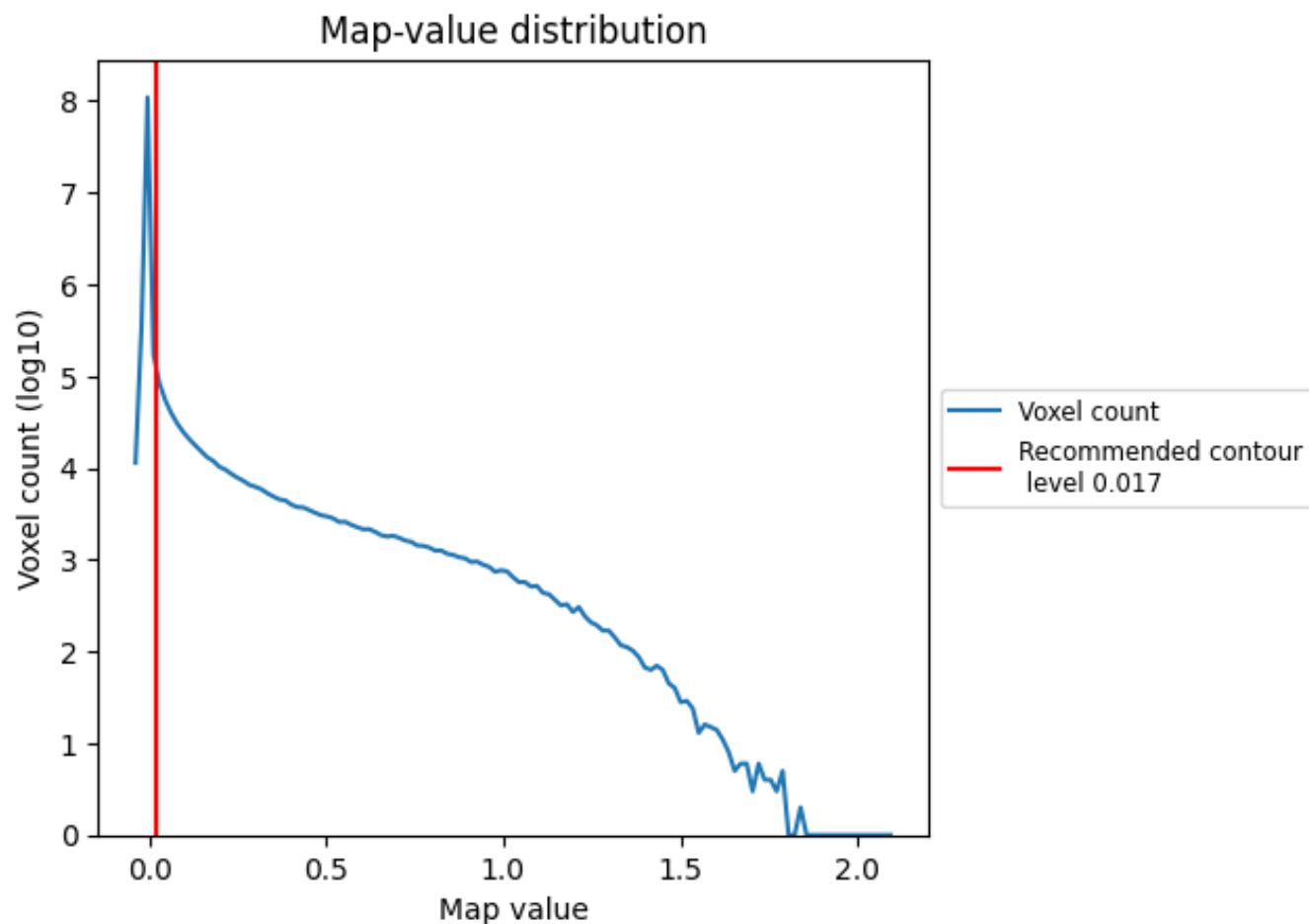
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

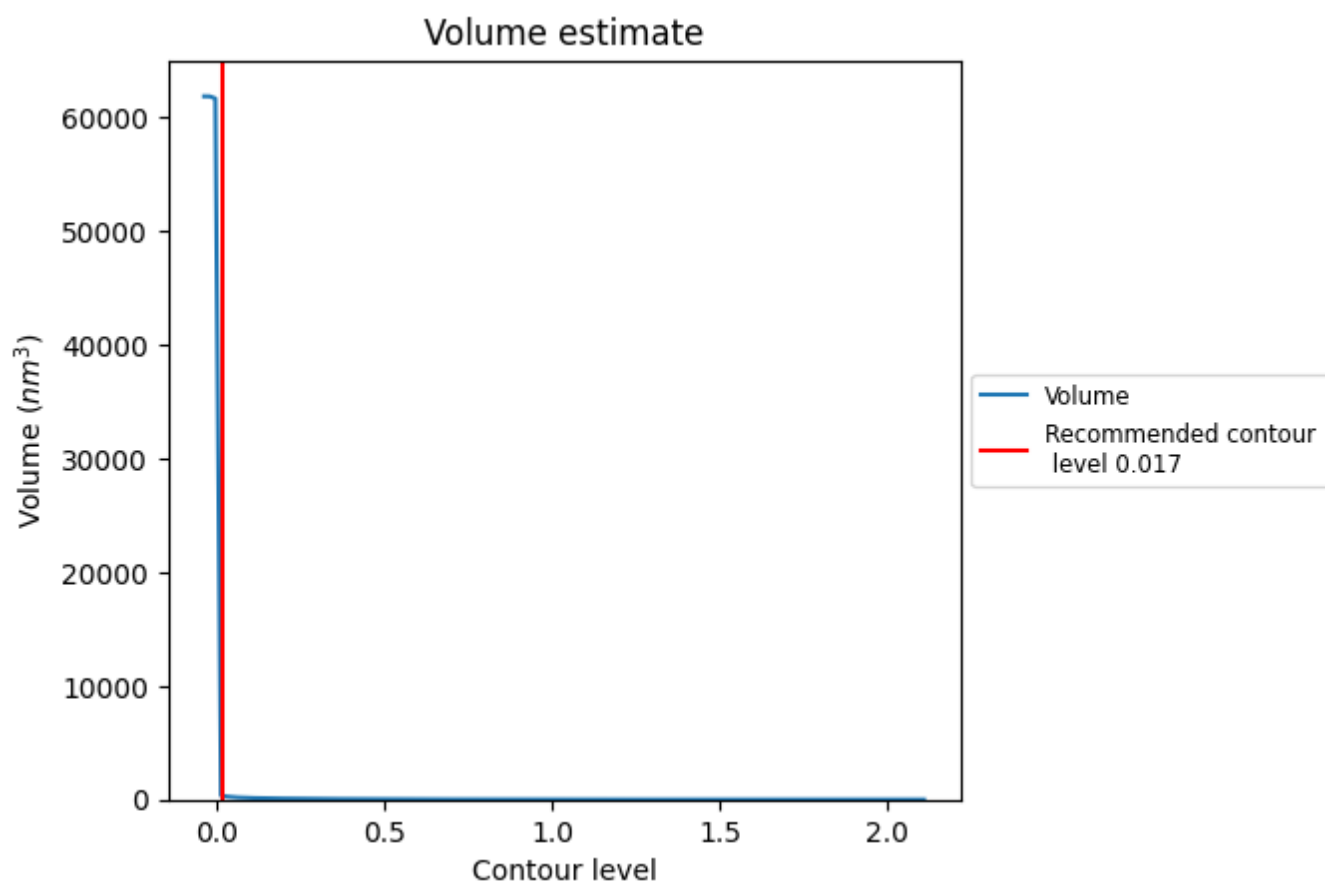
This section contains the results of statistical analysis of the map.

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.

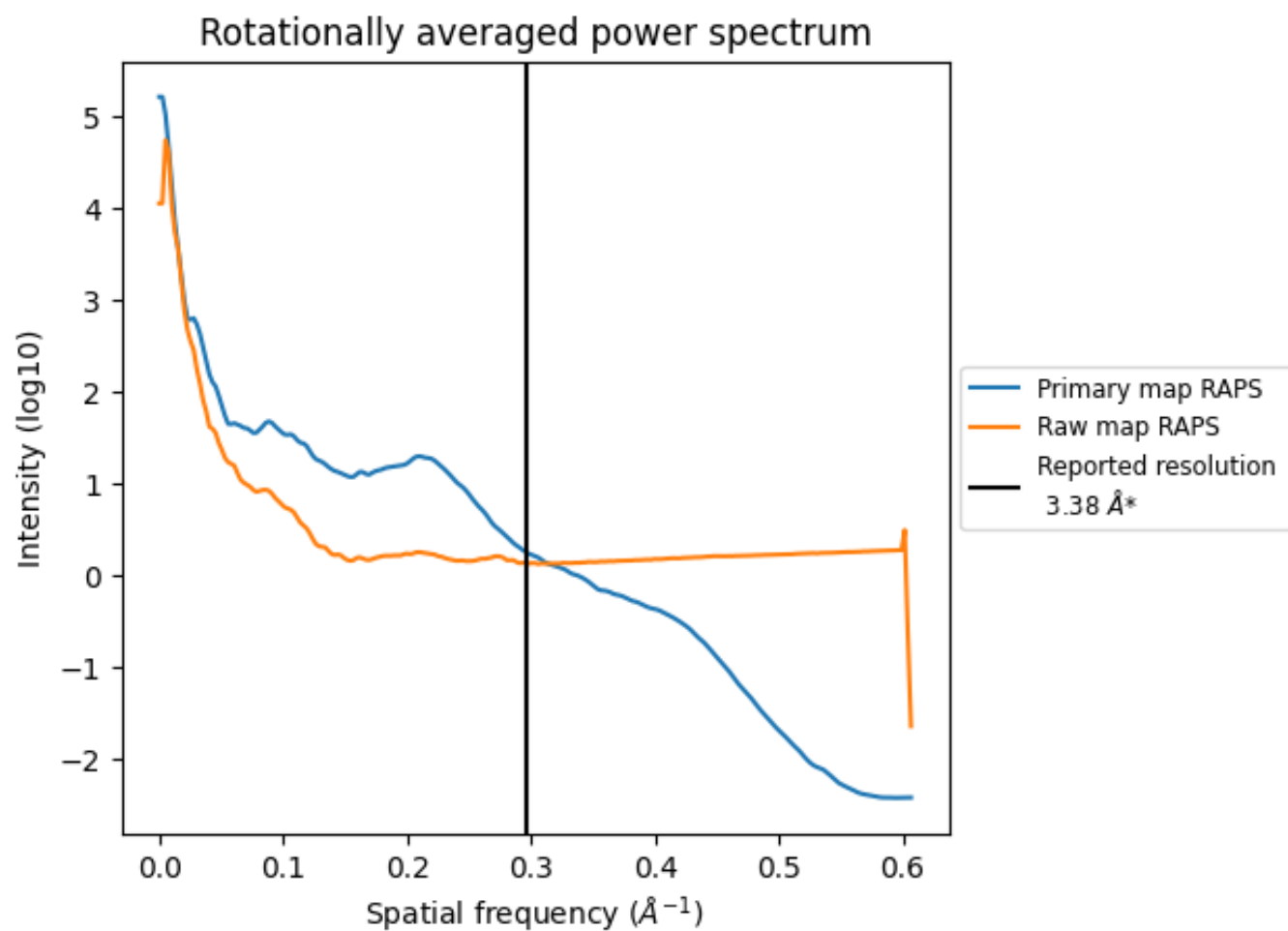
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 334 nm^3 ; this corresponds to an approximate mass of 301 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 ⓘ

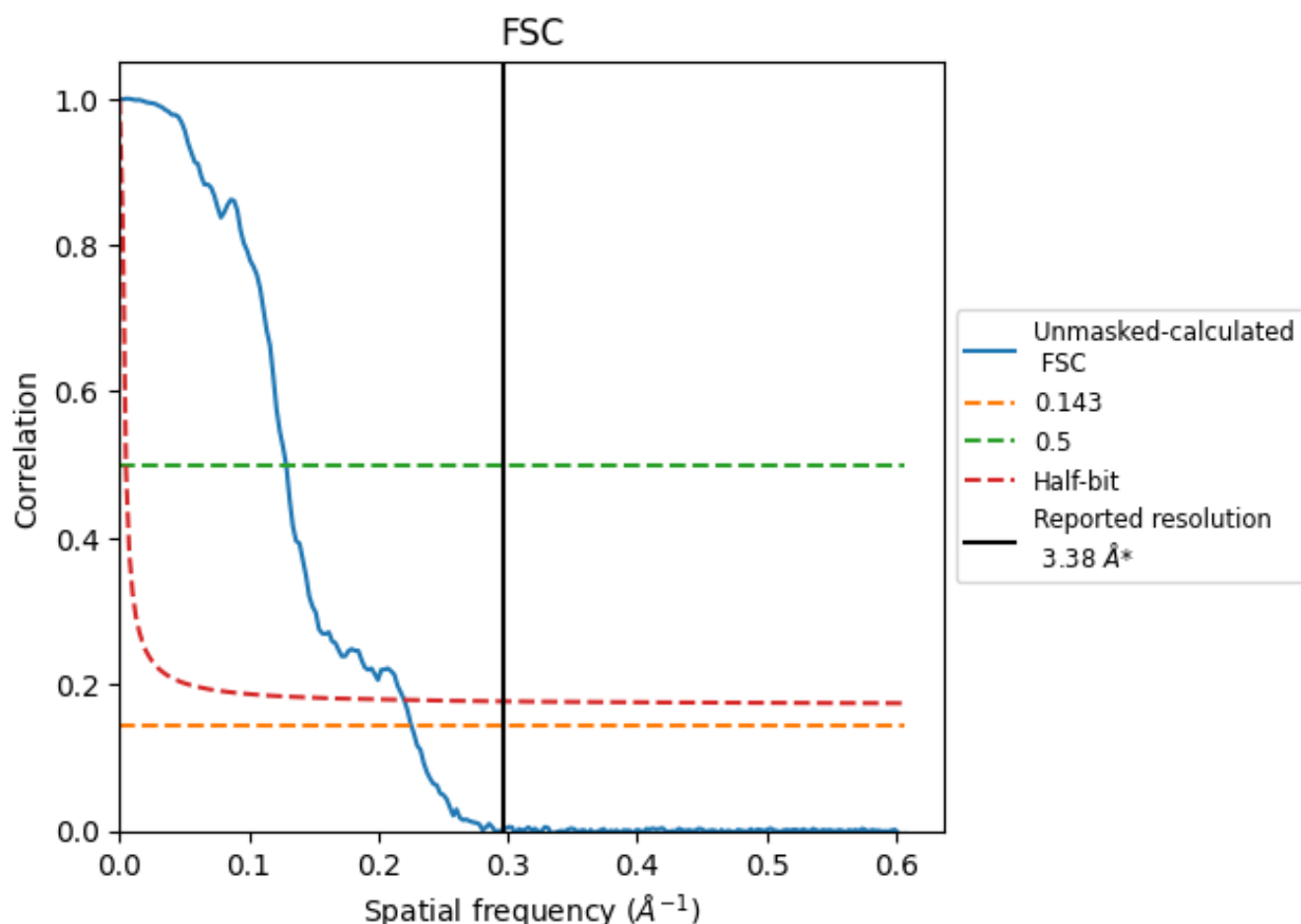


*Reported resolution corresponds to spatial frequency of 0.296 \AA^{-1}

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 0.296 \AA^{-1}

8.2 Resolution estimates [i](#)

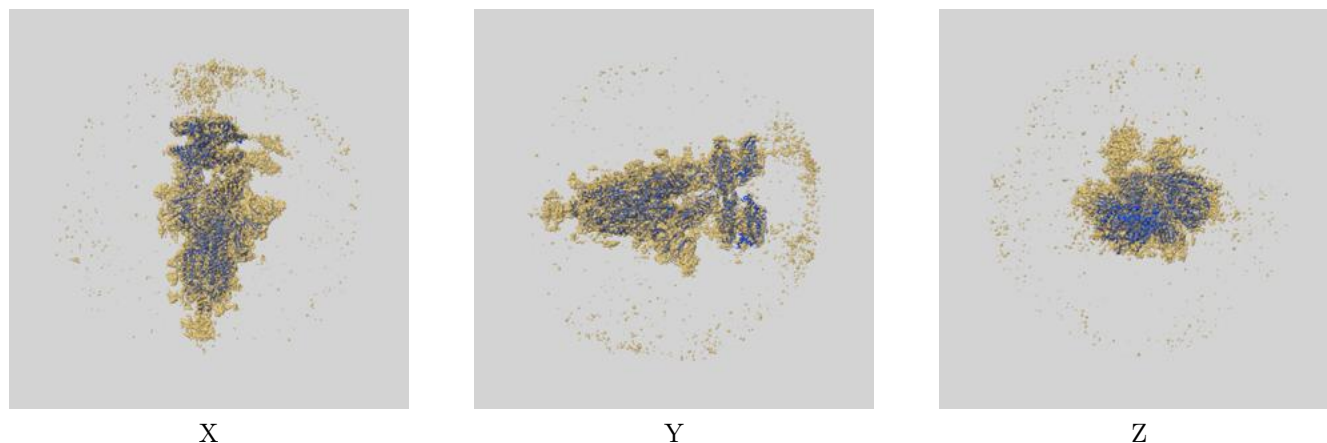
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.43	7.76	4.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 3.38 by more than 10 %

9 Map-model fit [i](#)

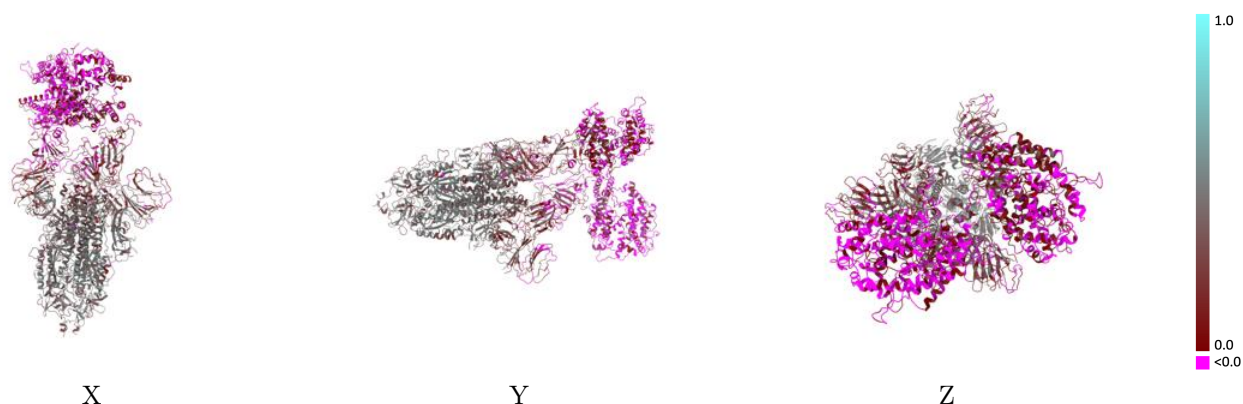
This section contains information regarding the fit between EMDB map EMD-33339 and PDB model 7XO7. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



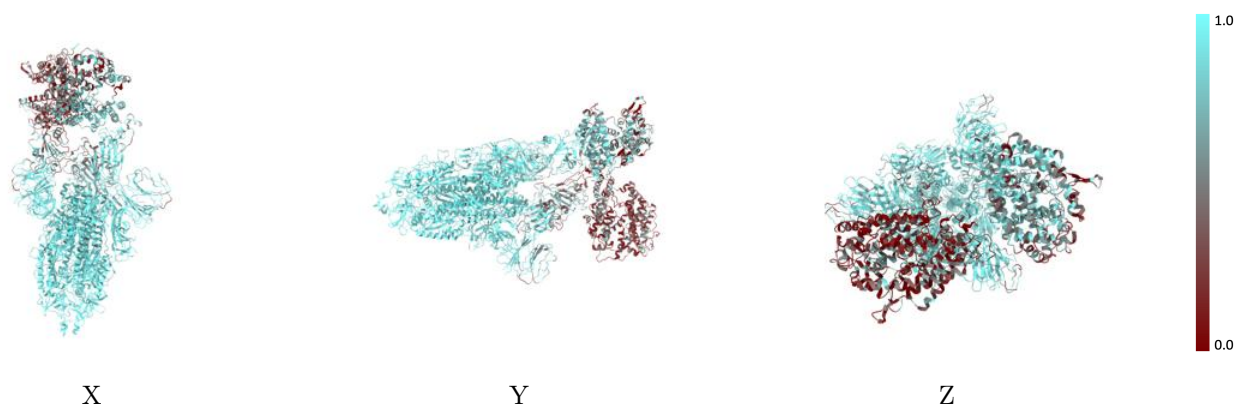
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



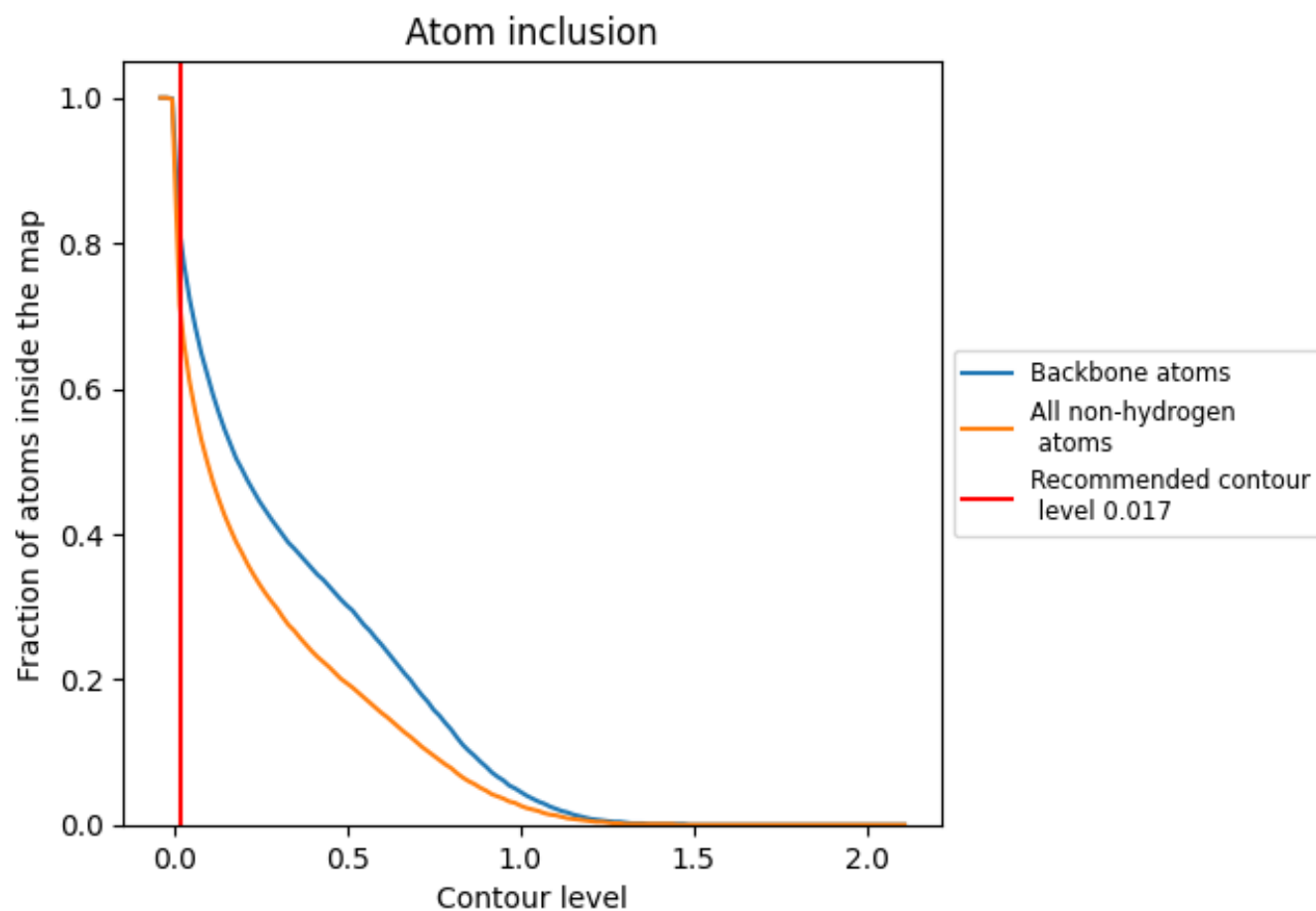
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7150	<div></div> 0.2190
A	<div></div> 0.8110	<div></div> 0.2970
B	<div></div> 0.8260	<div></div> 0.3120
C	<div></div> 0.8710	<div></div> 0.3240
E	<div></div> 0.5760	<div></div> 0.0380
F	<div></div> 0.2470	<div></div> -0.0550

