Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 10:10 AM EST

PDB ID	:	7KQB
EMDB ID	:	EMD-22993
Title	:	SARS-CoV-2 spike glycoprotein:Fab 5A6 complex I
Authors	:	Asarnow, D.; Charles, C.; Cheng, Y.
Deposited on	:	2020-11-14
Resolution	:	2.42 Å(reported)
Based on initial model	:	7A94

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:

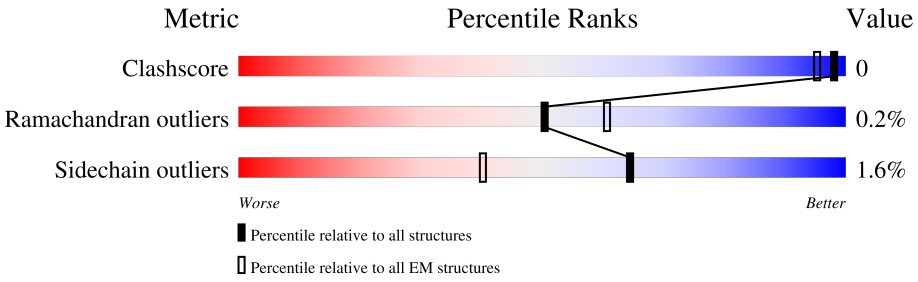
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.42 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1208	86% · 11%
1	B	1208	15% 86% · 11%
1	C	1208	86% · 11%
2	H	449	15% 47% · 51%
2	K	449	46% · 51%
3	J	214	11% 93% 6% ·
3	L	214	33% 89% 8% ·

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 63631 atoms, of which 31416 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	1080	Total	C	H	N	O	S	0	0
			16699	5397	8243	1412	1609	38		
1	B	1079	Total	C	H	N	O	S	0	0
			16677	5390	8232	1409	1608	38		
1	C	1078	Total	C	H	N	O	S	0	0
			16661	5386	8223	1408	1606	38		

There are 15 discrepancies between the modelled and reference sequences:

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

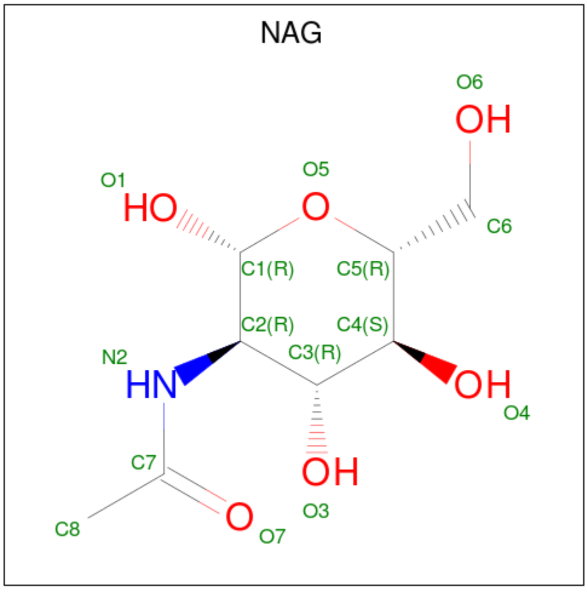
- Molecule 2 is a protein called Fab 5A6 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	220	Total	C	H	N	O	S	0	0
			3257	1034	1612	278	325	8		
2	K	220	Total	C	H	N	O	S	0	0
			3257	1034	1612	278	325	8		

- Molecule 3 is a protein called Fab 5A6 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	214	Total 3218	C 1020	H 1586	N 274	O 333	S 5	0	0
3	J	214	Total 3218	C 1020	H 1586	N 274	O 333	S 5	0	0

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



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 252	C 72	H 126	N 9	O 45	0
4	A	1	Total 252	C 72	H 126	N 9	O 45	0
4	A	1	Total 252	C 72	H 126	N 9	O 45	0
4	A	1	Total 252	C 72	H 126	N 9	O 45	0
4	A	1	Total 252	C 72	H 126	N 9	O 45	0
4	A	1	Total 252	C 72	H 126	N 9	O 45	0
4	A	1	Total 252	C 72	H 126	N 9	O 45	0
4	A	1	Total 252	C 72	H 126	N 9	O 45	0

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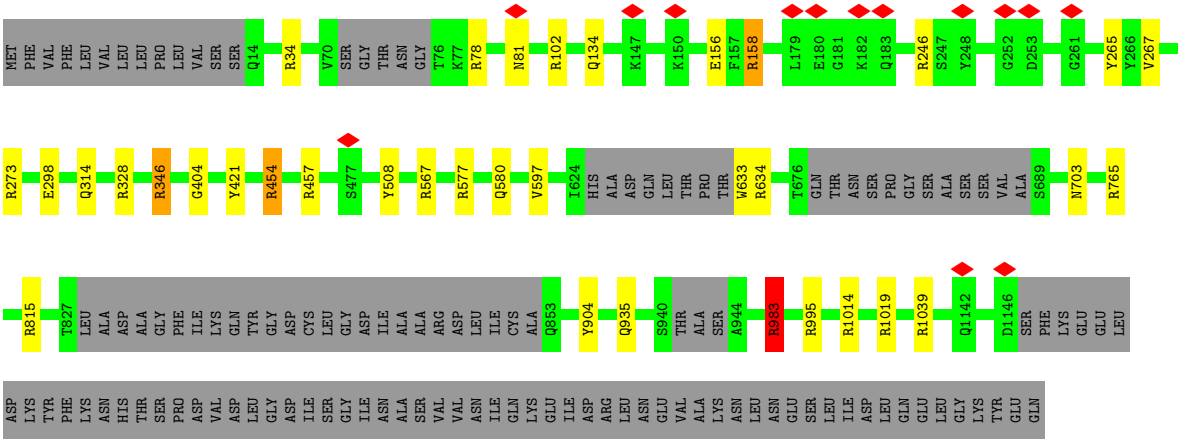
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C H N O 252 72 126 9 45	0
4	B	1	Total C H N O 168 48 84 6 30	0
4	B	1	Total C H N O 168 48 84 6 30	0
4	B	1	Total C H N O 168 48 84 6 30	0
4	B	1	Total C H N O 168 48 84 6 30	0
4	B	1	Total C H N O 168 48 84 6 30	0
4	B	1	Total C H N O 168 48 84 6 30	0
4	C	1	Total C H N O 224 64 112 8 40	0
4	C	1	Total C H N O 224 64 112 8 40	0
4	C	1	Total C H N O 224 64 112 8 40	0
4	C	1	Total C H N O 224 64 112 8 40	0
4	C	1	Total C H N O 224 64 112 8 40	0
4	C	1	Total C H N O 224 64 112 8 40	0
4	C	1	Total C H N O 224 64 112 8 40	0
4	C	1	Total C H N O 224 64 112 8 40	0

3 Residue-property plots (i)

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

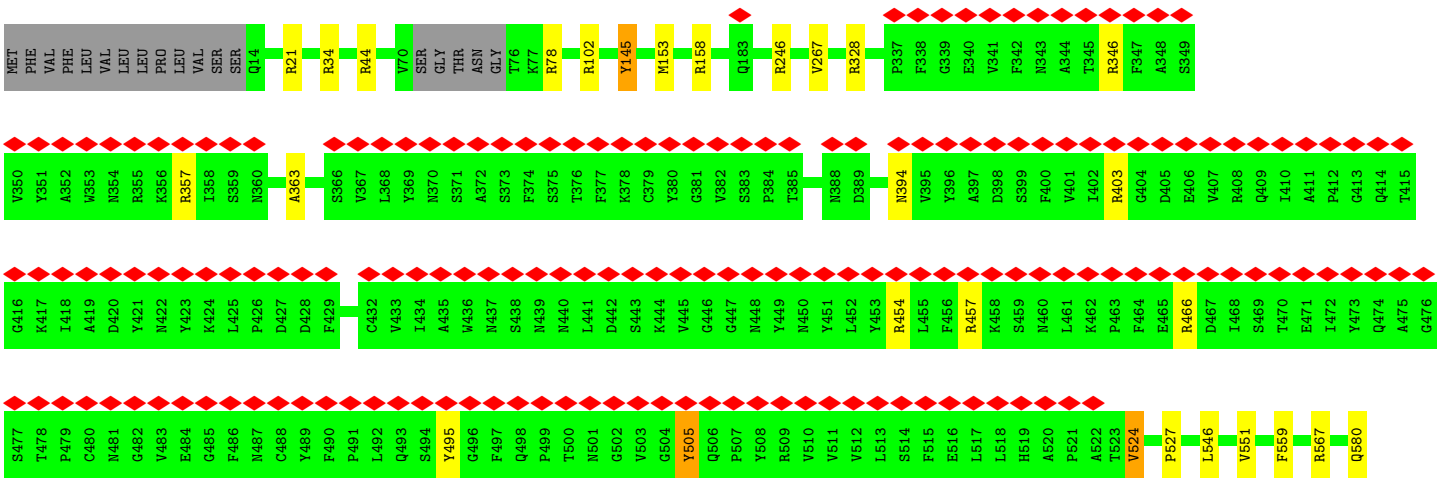
• Molecule 1: Spike glycoprotein

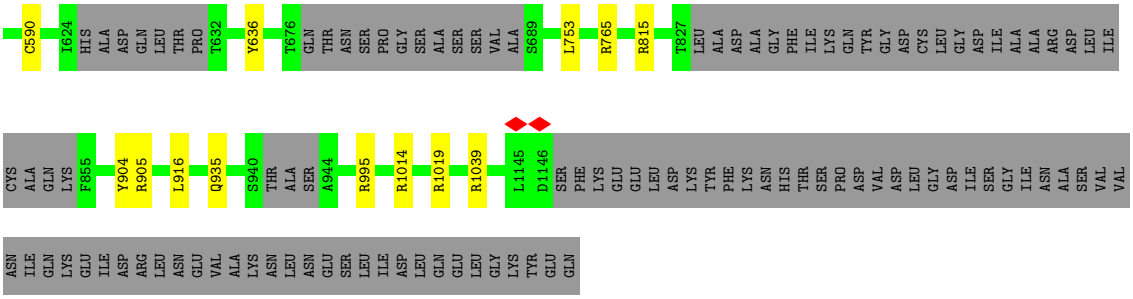
Chain A:



• Molecule 1: Spike glycoprotein

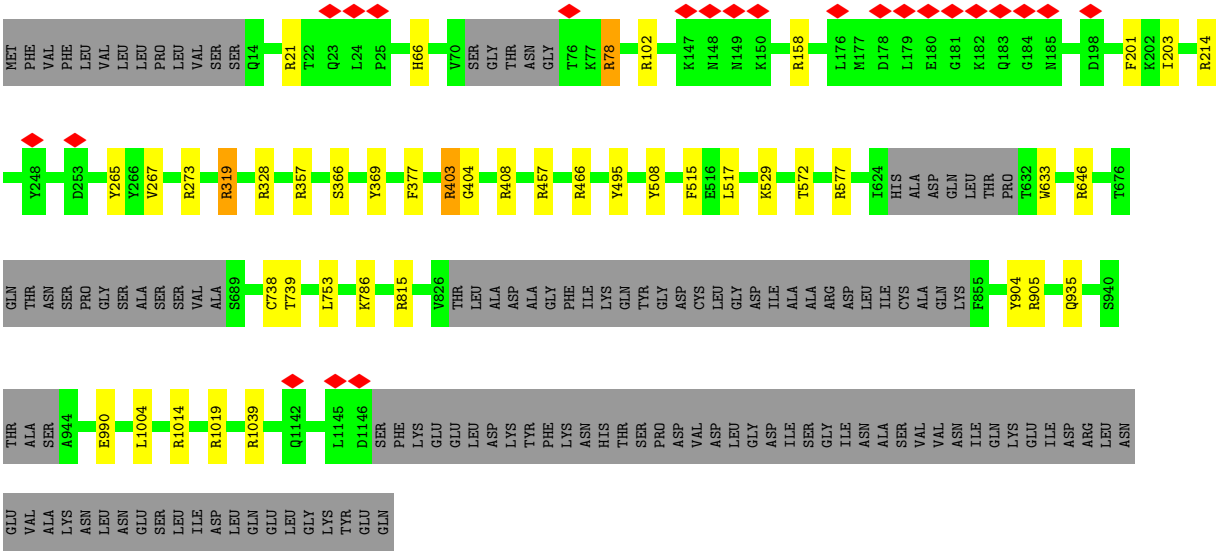
Chain B:





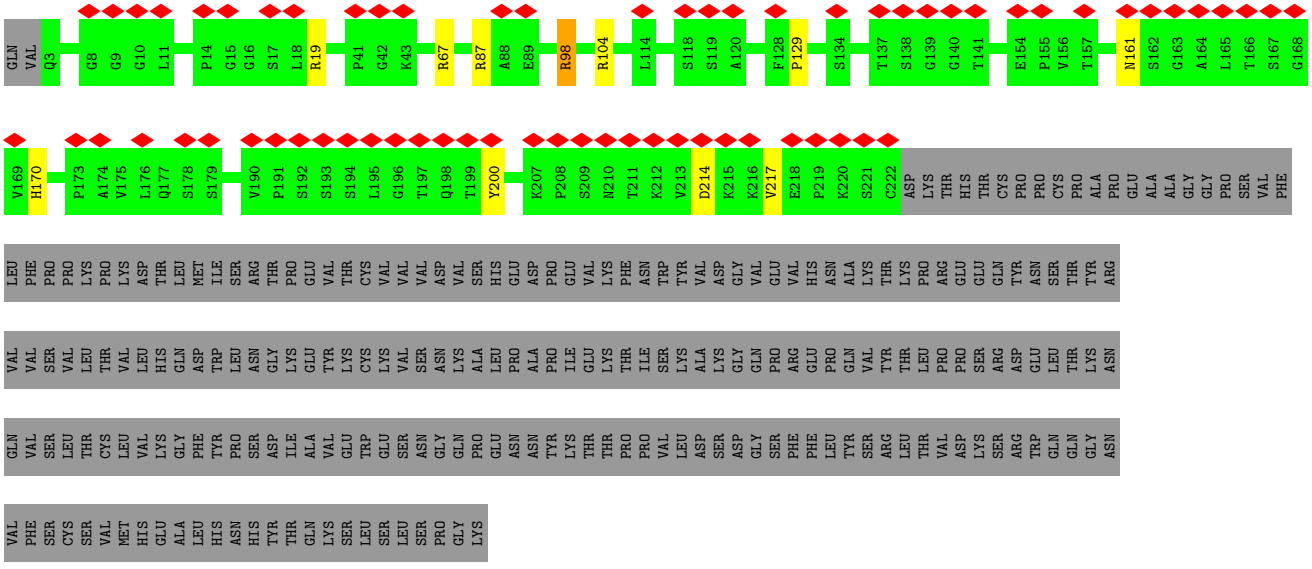
• Molecule 1: Spike glycoprotein

Chain C:



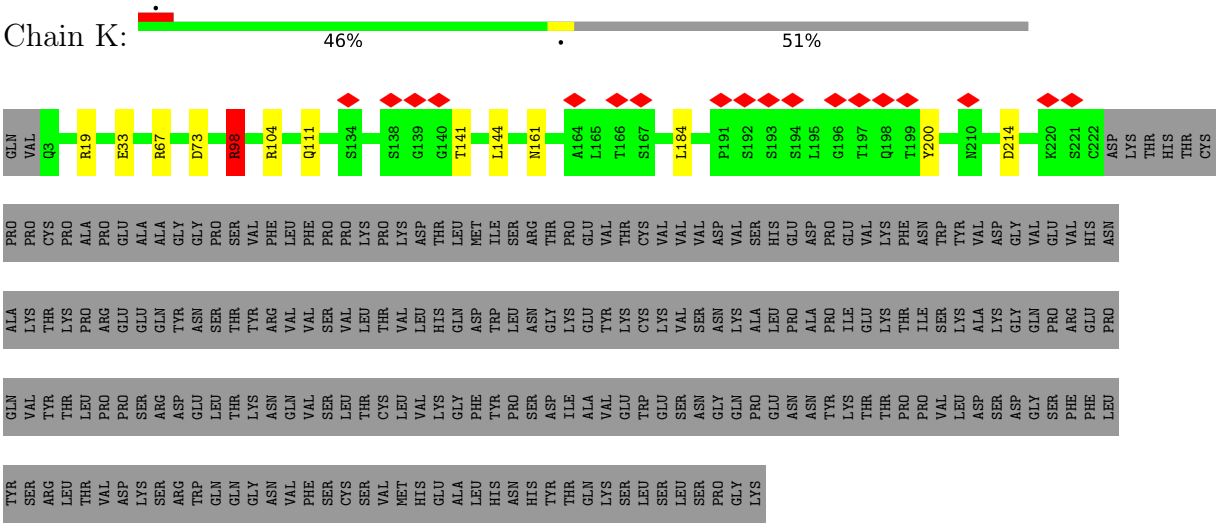
• Molecule 2: Fab 5A6 heavy chain

Chain H:



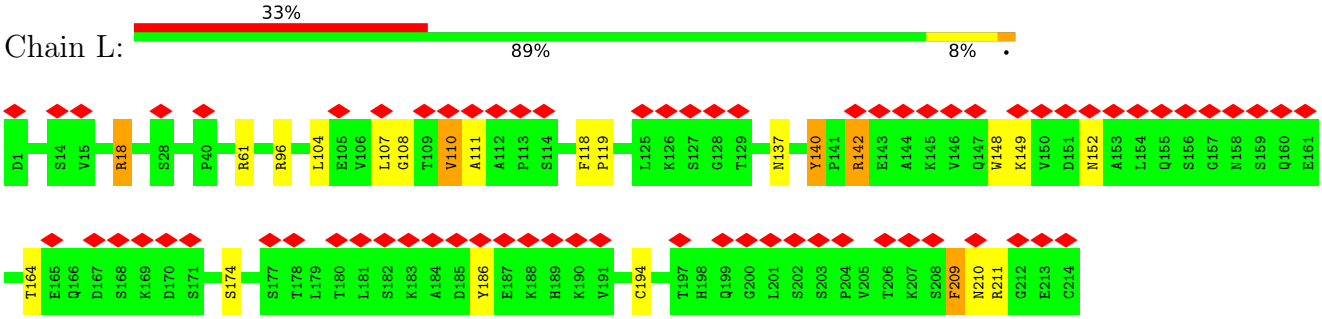
• Molecule 2: Fab 5A6 heavy chain

Chain K:



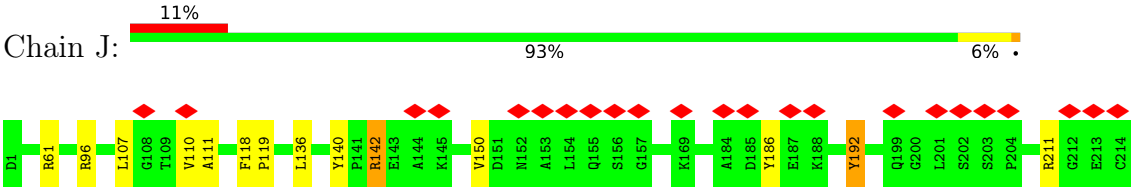
• Molecule 3: Fab 5A6 light chain

Chain L:



• Molecule 3: Fab 5A6 light chain

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	380163	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.869	Depositor
Minimum map value	-0.563	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	427.52158, 427.52158, 427.52158	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.18756, 1.18756, 1.18756	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.64	0/8654	0.96	25/11779 (0.2%)
1	B	0.65	0/8643	0.96	29/11766 (0.2%)
1	C	0.65	0/8636	0.96	25/11756 (0.2%)
2	H	0.65	0/1682	1.04	5/2287 (0.2%)
2	K	0.63	0/1682	1.04	4/2287 (0.2%)
3	J	0.62	0/1667	1.02	4/2263 (0.2%)
3	L	0.64	0/1667	1.04	7/2263 (0.3%)
All	All	0.64	0/32631	0.97	99/44401 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	4
2	H	0	1
2	K	0	1
3	J	0	2
3	L	0	2
All	All	0	14

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	98	ARG	NE-CZ-NH2	8.85	124.72	120.30
1	A	158	ARG	NE-CZ-NH1	8.29	124.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	995	ARG	NE-CZ-NH1	8.21	124.41	120.30
2	K	98	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	C	158	ARG	NE-CZ-NH1	7.87	124.23	120.30
3	L	96	ARG	NE-CZ-NH2	7.85	124.22	120.30
3	L	142	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	A	904	TYR	CB-CG-CD2	-7.70	116.38	121.00
1	C	905	ARG	NE-CZ-NH1	7.66	124.13	120.30
3	J	211	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	B	904	TYR	CB-CG-CD2	-7.57	116.46	121.00
1	B	905	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	454	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	B	158	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	246	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	246	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	457	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	273	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	C	904	TYR	CB-CG-CD2	-6.81	116.92	121.00
1	B	102	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	K	104	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	457	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	815	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	403	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	C	577	ARG	NE-CZ-NH1	6.62	123.61	120.30
3	J	61	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	319	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	21	ARG	NE-CZ-NH1	6.32	123.46	120.30
3	L	61	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	1014	ARG	NE-CZ-NH1	6.26	123.43	120.30
3	L	211	ARG	NE-CZ-NH2	6.25	123.43	120.30
1	A	577	ARG	NE-CZ-NH1	6.18	123.39	120.30
2	K	67	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	K	19	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	102	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	1039	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	44	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	1019	ARG	NE-CZ-NH1	6.03	123.32	120.30
2	H	67	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	357	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	B	1019	ARG	NE-CZ-NH1	5.96	123.28	120.30
3	J	142	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	C	1039	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	1039	ARG	NE-CZ-NH1	5.91	123.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	567	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	B	357	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	C	815	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	815	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	995	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	C	214	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	567	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	B	457	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	765	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	21	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	C	328	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	145	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	457	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	158	ARG	CD-NE-CZ	5.62	131.47	123.60
1	A	78	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	983	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	78	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	636	TYR	CB-CG-CD2	-5.58	117.65	121.00
2	H	98	ARG	NH1-CZ-NH2	-5.57	113.28	119.40
1	A	328	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	466	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	815	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	765	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	457	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	403	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	C	466	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	L	18	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	346	ARG	NE-CZ-NH2	5.42	123.01	120.30
3	L	209	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	C	1039	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	C	408	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	C	1014	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	421	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	273	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	1014	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	328	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	505	TYR	CB-CG-CD2	-5.33	117.81	121.00
1	A	1019	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	1039	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	454	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	B	158	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	34	ARG	NE-CZ-NH1	5.29	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	634	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	815	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	815	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	102	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	78	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	1039	ARG	NE-CZ-NH2	-5.17	117.71	120.30
3	L	140	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	C	646	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	H	87	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	H	19	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	34	ARG	NE-CZ-NH1	5.07	122.84	120.30
3	J	96	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	B	559	PHE	CB-CG-CD2	-5.00	117.30	120.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	TYR	Sidechain
1	A	454	ARG	Sidechain
1	A	983	ARG	Sidechain
1	B	495	TYR	Sidechain
1	C	265	TYR	Sidechain
1	C	319	ARG	Sidechain
1	C	403	ARG	Sidechain
1	C	495	TYR	Sidechain
2	H	104	ARG	Sidechain
3	J	140	TYR	Sidechain
3	J	192	TYR	Sidechain
2	K	98	ARG	Sidechain
3	L	118	PHE	Sidechain
3	L	140	TYR	Sidechain

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	8456	8243	8237	3	0
1	B	8445	8232	8226	3	0
1	C	8438	8223	8217	5	0
2	H	1645	1612	1611	3	0
2	K	1645	1612	1611	1	0
3	J	1632	1586	1586	4	0
3	L	1632	1586	1586	5	0
4	A	126	126	117	0	0
4	B	84	84	78	0	0
4	C	112	112	104	0	0
All	All	32215	31416	31373	20	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 0.

All (20) 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)
3:J:110:VAL:HG22	3:J:111:ALA:H	1.71	0.55
1:C:201:PHE:CD2	1:C:203:ILE:HD11	2.42	0.55
1:A:983:ARG:HD3	1:C:517:LEU:HD13	1.90	0.52
3:L:110:VAL:HG22	3:L:111:ALA:H	1.74	0.51
3:L:148:TRP:CZ3	3:L:194:CYS:SG	3.07	0.47
2:H:170:HIS:CE1	3:L:174:SER:HG	2.32	0.47
2:H:129:PRO:HB3	2:H:217:VAL:HG22	1.96	0.46
1:A:983:ARG:CD	1:C:517:LEU:HD13	2.47	0.44
3:L:119:PRO:HA	3:L:209:PHE:CD2	2.54	0.43
3:J:107:LEU:H	3:J:107:LEU:HD12	1.82	0.43
3:J:118:PHE:CG	3:J:119:PRO:HD2	2.54	0.43
1:B:363:ALA:HB2	1:B:524:VAL:HG12	2.01	0.43
3:J:150:VAL:HG22	3:J:192:TYR:CD2	2.53	0.43
1:C:366:SER:HA	1:C:369:TYR:CZ	2.55	0.42
2:H:170:HIS:CD2	3:L:137:ASN:HD21	2.37	0.42
1:A:404:GLY:HA2	1:A:508:TYR:CD1	2.55	0.42
2:K:144:LEU:HD22	2:K:200:TYR:CG	2.55	0.42
1:B:551:VAL:HG23	1:B:590:CYS:HB2	2.03	0.41
1:B:546:LEU:C	1:B:546:LEU:HD23	2.42	0.40
1:C:404:GLY:HA2	1:C:508:TYR:CD1	2.56	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	1068/1208 (88%)	1027 (96%)	41 (4%)	0	100 100
1	B	1067/1208 (88%)	1004 (94%)	61 (6%)	2 (0%)	47 61
1	C	1066/1208 (88%)	1016 (95%)	49 (5%)	1 (0%)	51 67
2	H	218/449 (49%)	202 (93%)	15 (7%)	1 (0%)	29 40
2	K	218/449 (49%)	206 (94%)	12 (6%)	0	100 100
3	J	212/214 (99%)	192 (91%)	20 (9%)	0	100 100
3	L	212/214 (99%)	188 (89%)	19 (9%)	5 (2%)	6 5
All	All	4061/4950 (82%)	3835 (94%)	217 (5%)	9 (0%)	50 61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	633	TRP
3	L	108	GLY
3	L	110	VAL
3	L	107	LEU
1	B	527	PRO
2	H	200	TYR
3	L	210	ASN
3	L	152	ASN
1	B	524	VAL

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	945/1053 (90%)	932 (99%)	13 (1%)	67	81
1	B	944/1053 (90%)	934 (99%)	10 (1%)	73	86
1	C	943/1053 (90%)	929 (98%)	14 (2%)	65	79
2	H	184/394 (47%)	181 (98%)	3 (2%)	62	78
2	K	184/394 (47%)	176 (96%)	8 (4%)	29	44
3	J	187/187 (100%)	184 (98%)	3 (2%)	62	78
3	L	187/187 (100%)	181 (97%)	6 (3%)	39	57
All	All	3574/4321 (83%)	3517 (98%)	57 (2%)	64	78

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	134	GLN
1	A	156	GLU
1	A	158	ARG
1	A	267	VAL
1	A	298	GLU
1	A	314	GLN
1	A	346	ARG
1	A	580	GLN
1	A	597	VAL
1	A	633	TRP
1	A	703	ASN
1	A	935	GLN
1	B	145	TYR
1	B	153	MET
1	B	267	VAL
1	B	346	ARG
1	B	394	ASN
1	B	505	TYR
1	B	580	GLN
1	B	753	LEU
1	B	916	LEU
1	B	935	GLN
1	C	66	HIS
1	C	78	ARG
1	C	267	VAL
1	C	377	PHE
1	C	515	PHE
1	C	529	LYS

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Mol	Chain	Res	Type
1	C	572	THR
1	C	738	CYS
1	C	739	THR
1	C	753	LEU
1	C	786	LYS
1	C	935	GLN
1	C	990	GLU
1	C	1004	LEU
2	H	98	ARG
2	H	161	ASN
2	H	214	ASP
3	L	18	ARG
3	L	104	LEU
3	L	142	ARG
3	L	149	LYS
3	L	164	THR
3	L	186	TYR
2	K	33	GLU
2	K	73	ASP
2	K	98	ARG
2	K	111	GLN
2	K	141	THR
2	K	161	ASN
2	K	184	LEU
2	K	214	ASP
3	J	136	LEU
3	J	142	ARG
3	J	186	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	824	ASN
1	A	1023	ASN
1	B	125	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	1304	1	14,14,15	1.19	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	A	1307	1	14,14,15	1.02	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	B	1301	1	14,14,15	1.28	2 (14%)	17,19,21	0.77	0
4	NAG	A	1303	1	14,14,15	1.23	2 (14%)	17,19,21	1.14	2 (11%)
4	NAG	C	1307	1	14,14,15	1.06	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	C	1306	1	14,14,15	1.20	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	B	1305	1	14,14,15	1.05	1 (7%)	17,19,21	1.10	1 (5%)
4	NAG	A	1302	1	14,14,15	1.19	1 (7%)	17,19,21	0.60	0
4	NAG	A	1308	1	14,14,15	1.10	1 (7%)	17,19,21	1.04	2 (11%)
4	NAG	B	1304	1	14,14,15	1.11	1 (7%)	17,19,21	0.55	0
4	NAG	B	1303	1	14,14,15	1.25	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	C	1302	1	14,14,15	1.24	1 (7%)	17,19,21	0.88	1 (5%)
4	NAG	A	1305	1	14,14,15	0.90	0	17,19,21	1.17	1 (5%)
4	NAG	A	1306	1	14,14,15	1.13	1 (7%)	17,19,21	0.70	0
4	NAG	A	1304	1	14,14,15	0.90	1 (7%)	17,19,21	0.90	1 (5%)
4	NAG	C	1303	1	14,14,15	1.03	1 (7%)	17,19,21	1.10	2 (11%)
4	NAG	B	1306	1	14,14,15	1.20	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	A	1301	1	14,14,15	1.21	1 (7%)	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	C	1305	1	14,14,15	1.01	1 (7%)	17,19,21	0.94	1 (5%)
4	NAG	C	1308	1	14,14,15	1.18	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	B	1302	1	14,14,15	1.20	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	A	1309	1	14,14,15	1.20	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	C	1301	1	14,14,15	1.28	2 (14%)	17,19,21	0.87	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1302	NAG	O5-C5	2.78	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1306	NAG	O5-C5	2.75	1.49	1.43
4	C	1304	NAG	O5-C5	2.67	1.48	1.43
4	C	1308	NAG	O5-C5	2.66	1.48	1.43
4	B	1303	NAG	O5-C5	2.66	1.48	1.43
4	B	1306	NAG	O5-C5	2.65	1.48	1.43
4	A	1309	NAG	O5-C5	2.65	1.48	1.43
4	B	1302	NAG	O5-C5	2.64	1.48	1.43
4	A	1301	NAG	O5-C5	2.61	1.48	1.43
4	B	1301	NAG	O5-C5	2.58	1.48	1.43
4	A	1303	NAG	O5-C5	2.56	1.48	1.43
4	B	1305	NAG	O5-C5	2.55	1.48	1.43
4	A	1306	NAG	O5-C5	2.50	1.48	1.43
4	A	1308	NAG	O5-C5	2.48	1.48	1.43
4	A	1307	NAG	O5-C5	2.45	1.48	1.43
4	C	1305	NAG	O5-C5	2.45	1.48	1.43
4	C	1301	NAG	O5-C5	2.42	1.48	1.43
4	A	1302	NAG	O5-C5	2.41	1.48	1.43
4	C	1307	NAG	O5-C5	2.36	1.48	1.43
4	B	1304	NAG	O5-C5	2.35	1.48	1.43
4	A	1304	NAG	O5-C5	2.32	1.48	1.43
4	A	1303	NAG	C1-C2	2.09	1.55	1.52
4	C	1303	NAG	C1-C2	2.01	1.55	1.52
4	C	1301	NAG	C1-C2	2.00	1.55	1.52
4	B	1301	NAG	C1-C2	2.00	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1305	NAG	C1-O5-C5	3.71	117.22	112.19
4	C	1307	NAG	C1-O5-C5	3.21	116.54	112.19
4	C	1308	NAG	C1-O5-C5	3.15	116.46	112.19
4	C	1306	NAG	C1-O5-C5	3.14	116.45	112.19
4	B	1302	NAG	C1-O5-C5	3.12	116.42	112.19
4	A	1307	NAG	C1-O5-C5	3.03	116.30	112.19
4	C	1304	NAG	C1-O5-C5	2.91	116.14	112.19
4	B	1303	NAG	C1-O5-C5	2.85	116.06	112.19
4	C	1305	NAG	C1-O5-C5	2.83	116.02	112.19
4	A	1301	NAG	C1-O5-C5	2.81	116.00	112.19
4	B	1306	NAG	C1-O5-C5	2.81	116.00	112.19
4	A	1309	NAG	C1-O5-C5	2.72	115.88	112.19
4	A	1304	NAG	C1-O5-C5	2.63	115.76	112.19
4	C	1303	NAG	C1-O5-C5	2.57	115.67	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1308	NAG	C1-O5-C5	2.55	115.64	112.19
4	A	1305	NAG	C2-N2-C7	2.43	126.37	122.90
4	C	1302	NAG	C1-O5-C5	2.37	115.41	112.19
4	A	1308	NAG	C3-C4-C5	2.18	114.14	110.24
4	A	1303	NAG	C1-O5-C5	2.18	115.15	112.19
4	C	1303	NAG	O4-C4-C3	-2.07	105.55	110.35
4	A	1303	NAG	C1-C2-N2	2.03	113.95	110.49

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1305	NAG	C1-C2-N2-C7
4	A	1308	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	C	1301	NAG	C1-C2-N2-C7
4	B	1301	NAG	C1-C2-N2-C7
4	C	1303	NAG	C1-C2-N2-C7
4	A	1303	NAG	C3-C2-N2-C7
4	A	1305	NAG	C3-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	C	1301	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

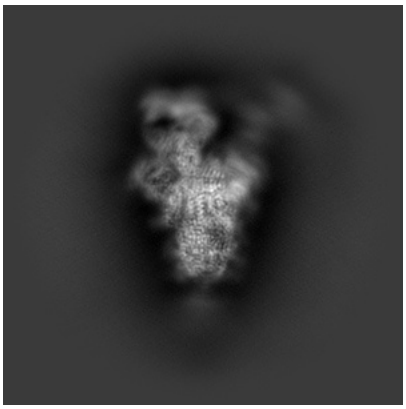
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22993. These allow visual inspection of the internal detail of the map and identification of artifacts.

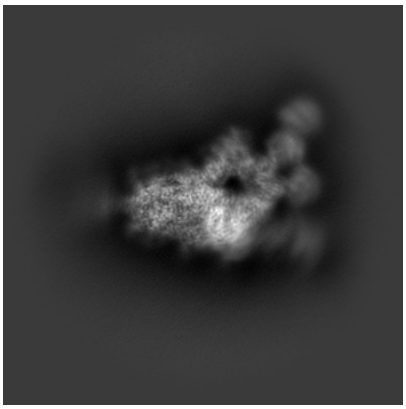
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

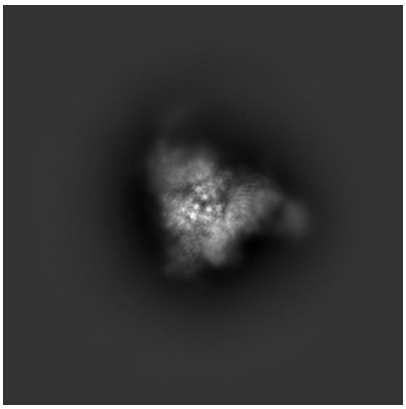
6.1.1 Primary map



X

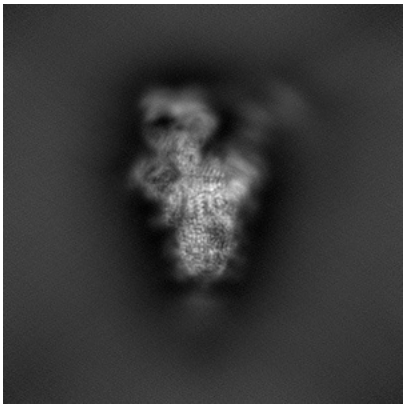


Y

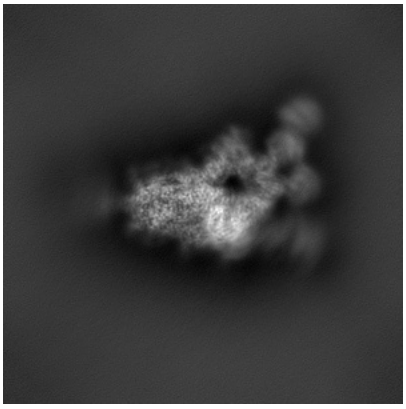


Z

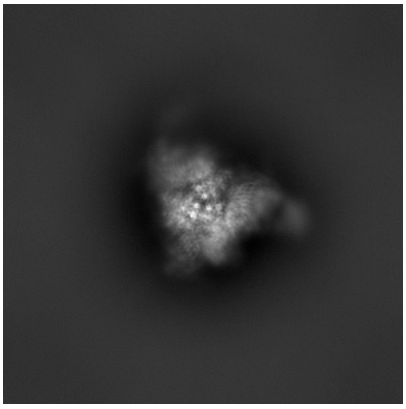
6.1.2 Raw map



X



Y

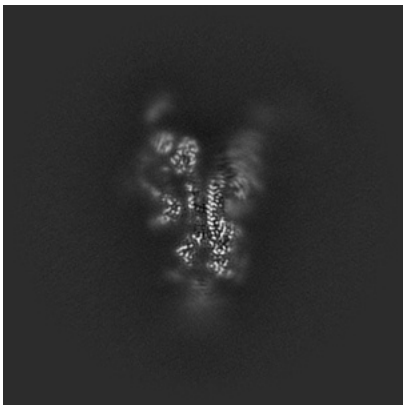


Z

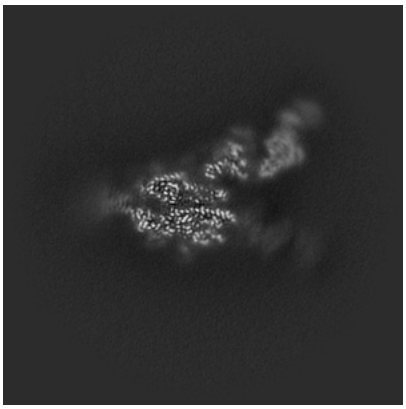
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

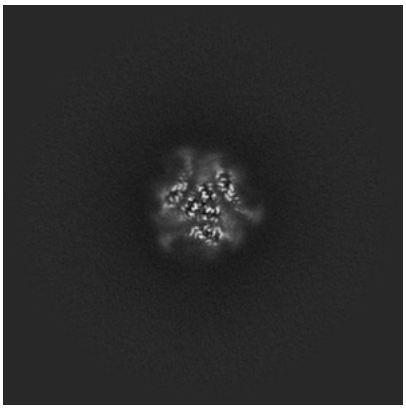
6.2.1 Primary map



X Index: 180

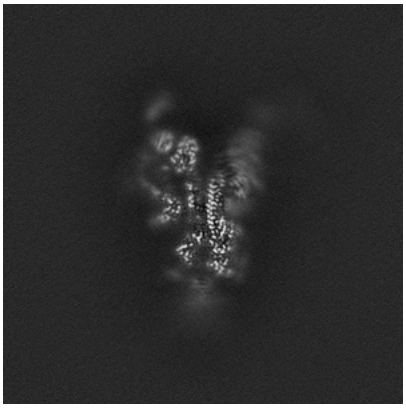


Y Index: 180

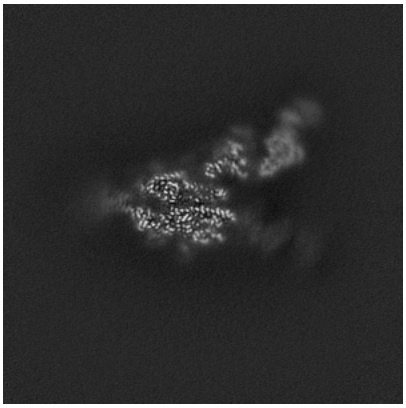


Z Index: 180

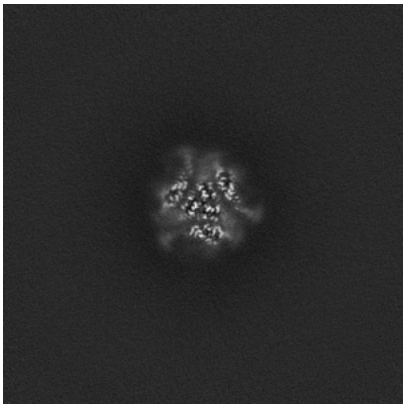
6.2.2 Raw map



X Index: 180



Y Index: 180

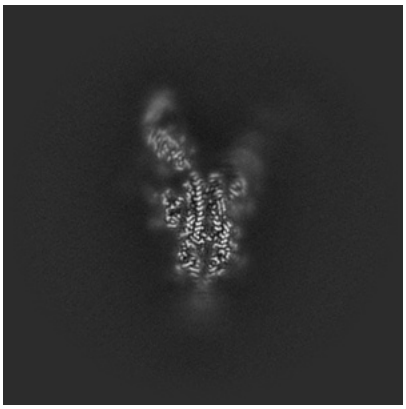


Z Index: 180

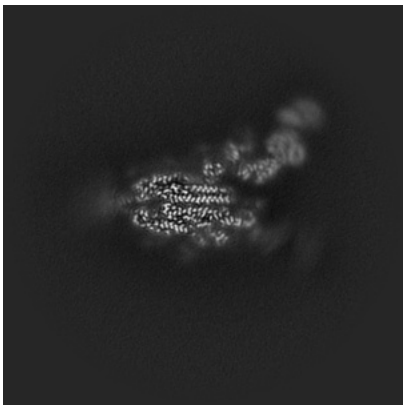
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

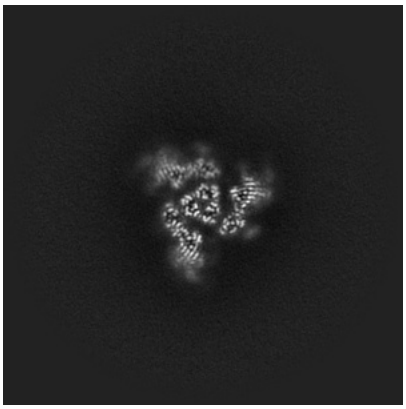
6.3.1 Primary map



X Index: 186

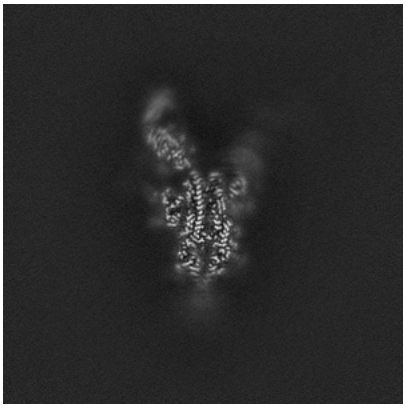


Y Index: 176

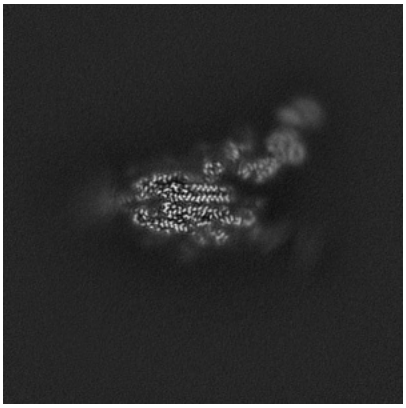


Z Index: 196

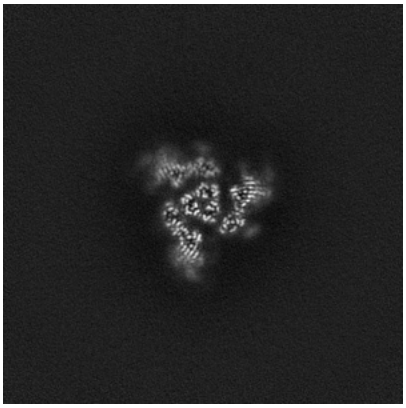
6.3.2 Raw map



X Index: 186



Y Index: 176



Z Index: 196

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

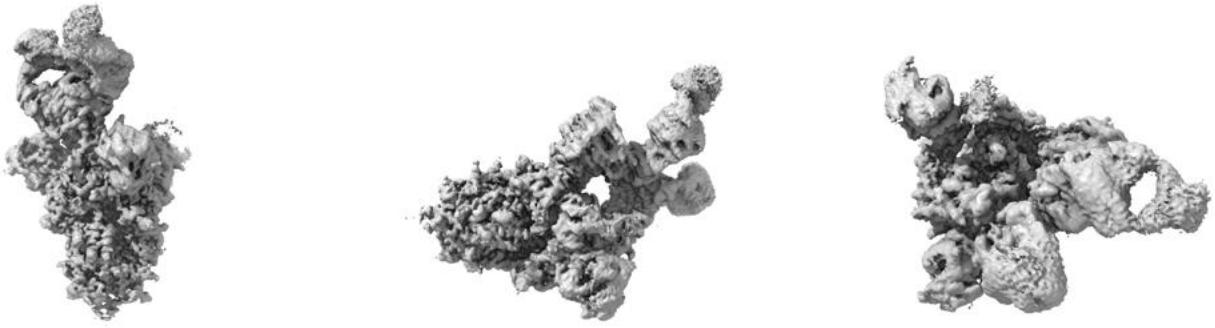
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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.

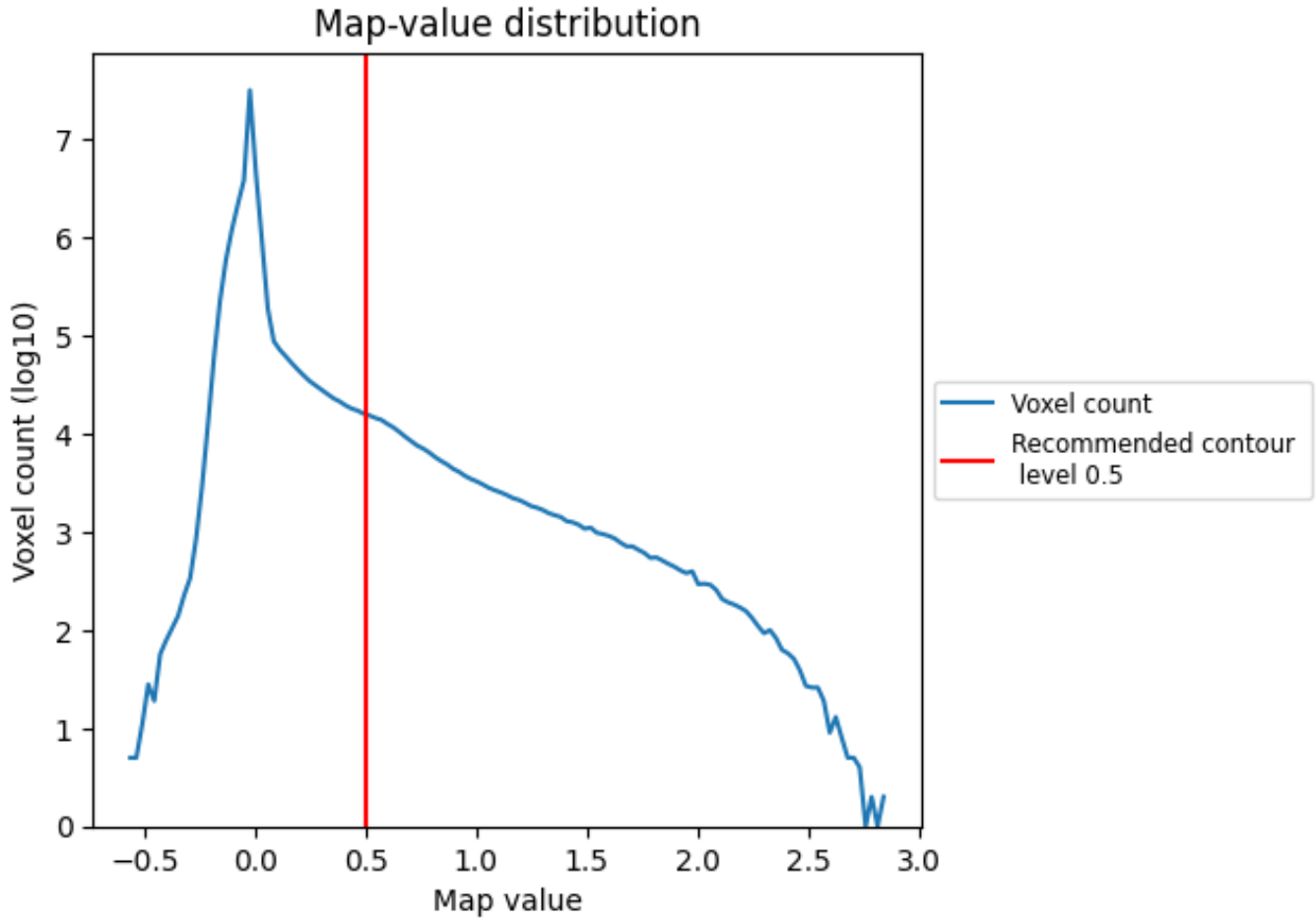
6.5 Mask visualisation (i)

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

7 Map analysis

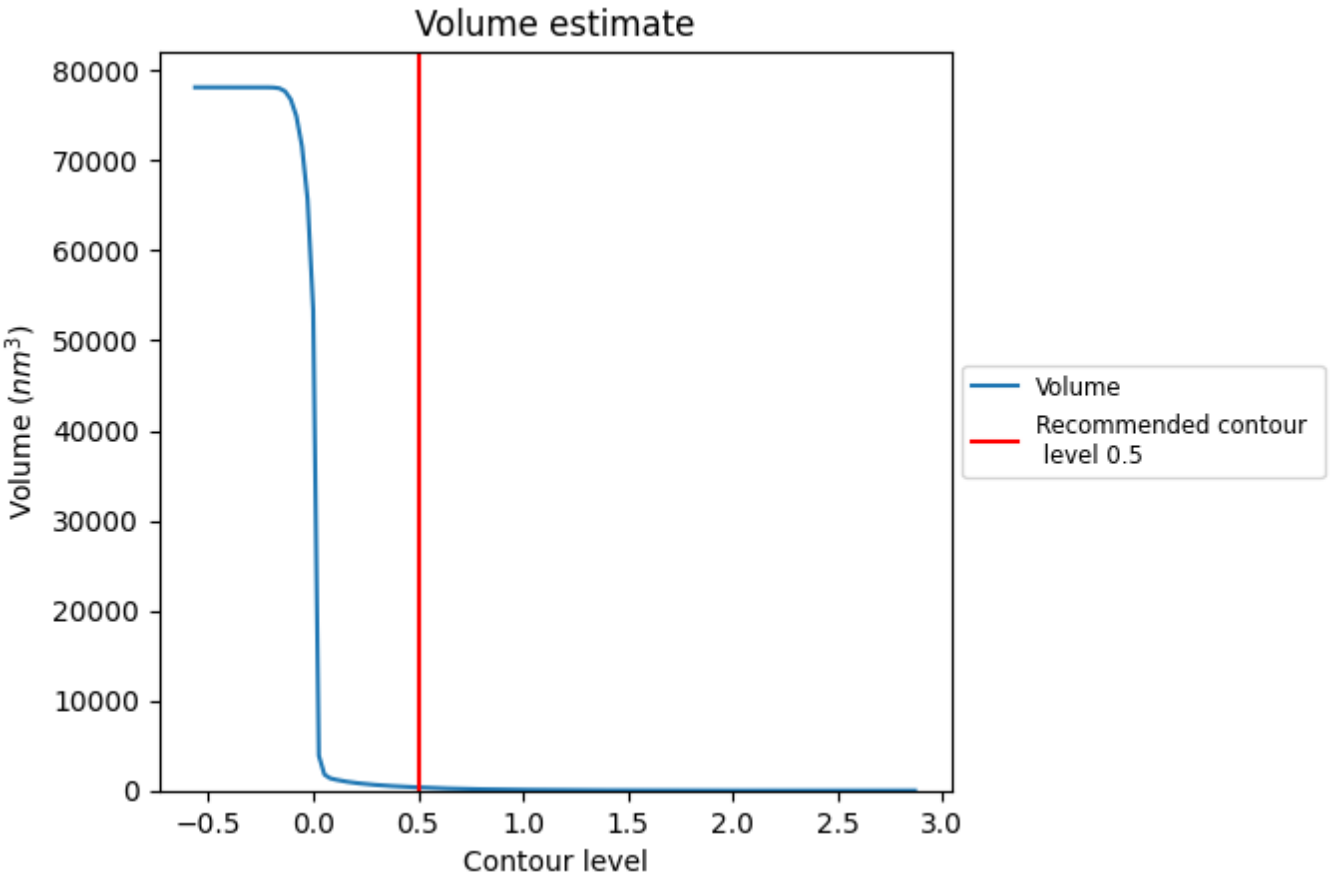
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

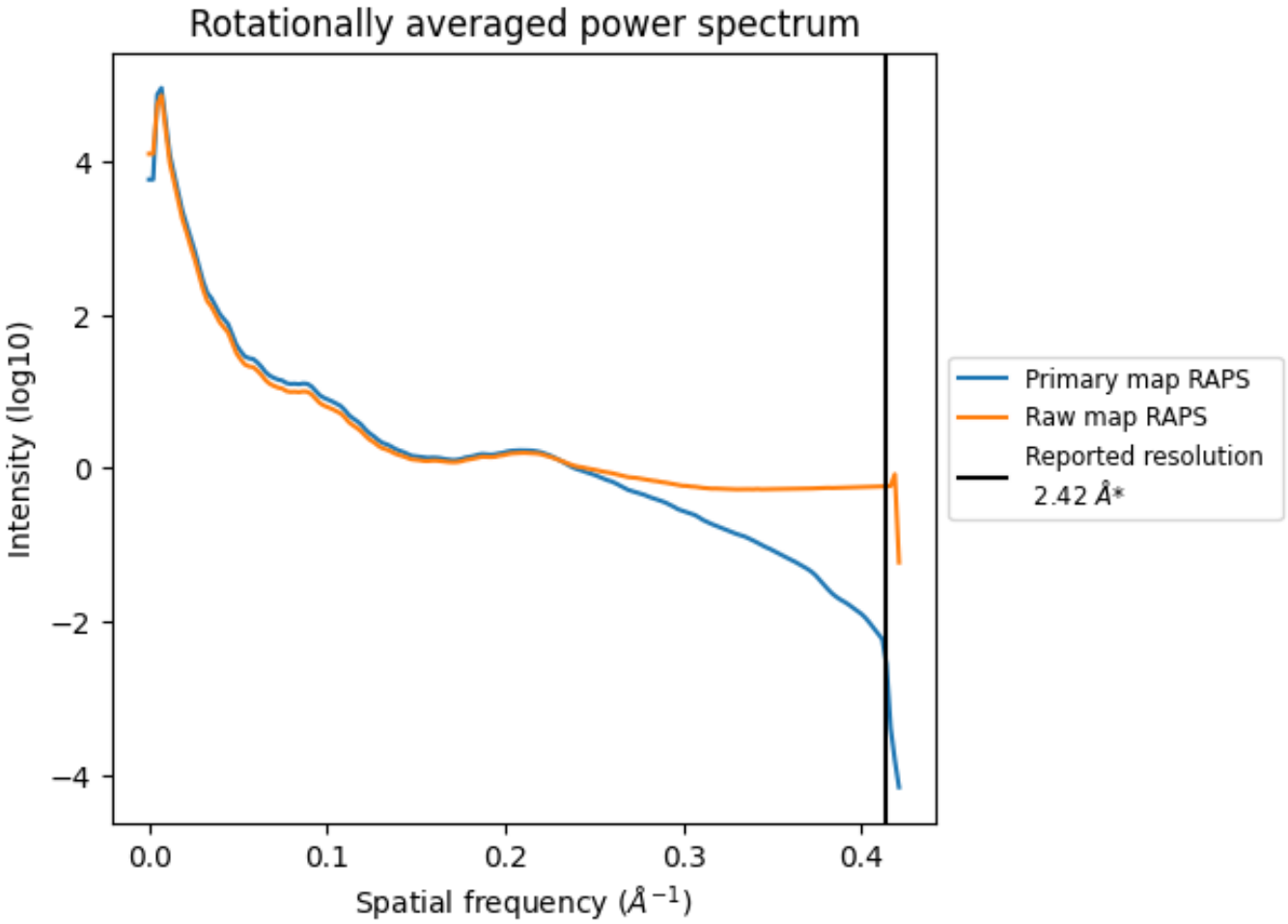
7.2 Volume estimate (i)



The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 321 kDa.

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

7.3 Rotationally averaged power spectrum (i)

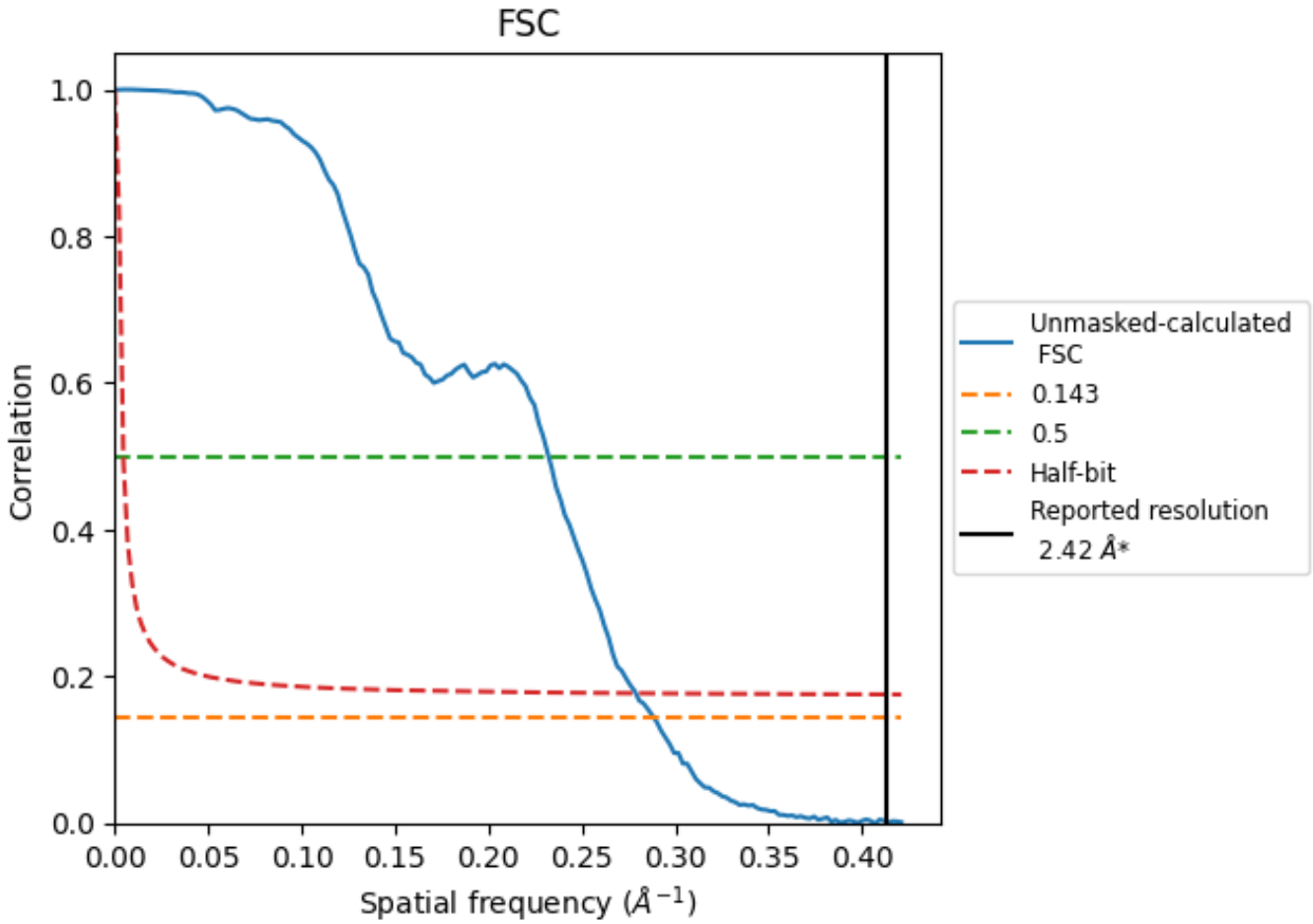


*Reported resolution corresponds to spatial frequency of 0.413 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.413 Å^{-1}

8.2 Resolution estimates (i)

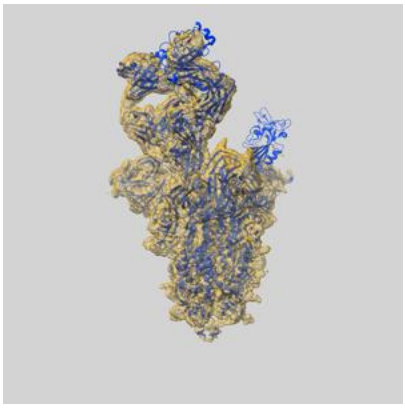
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.42	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.47	4.31	3.59

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 2.42 by more than 10 %

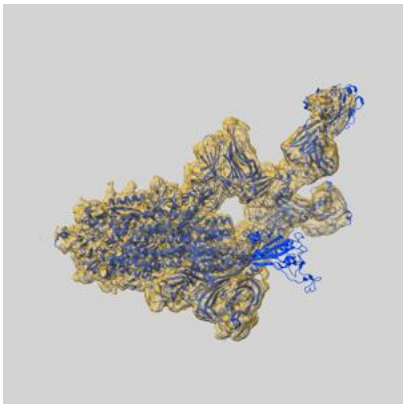
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22993 and PDB model 7KQB. Per-residue inclusion information can be found in section 3 on page 6.

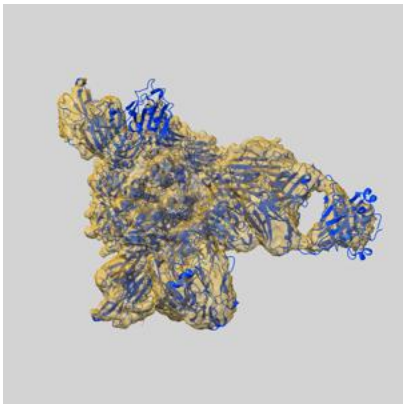
9.1 Map-model overlay



X



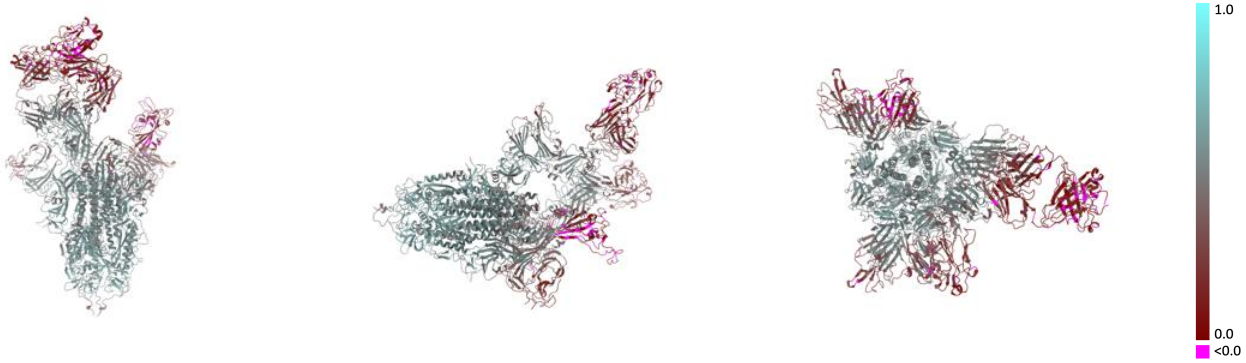
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

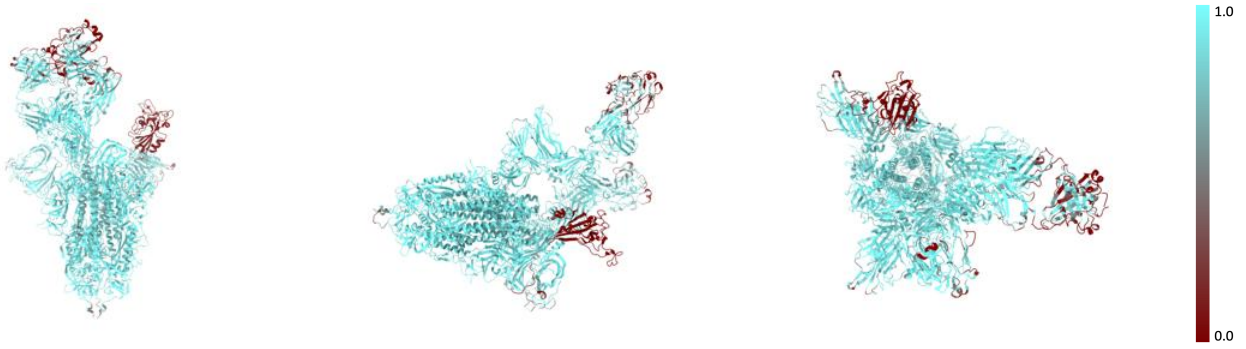
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

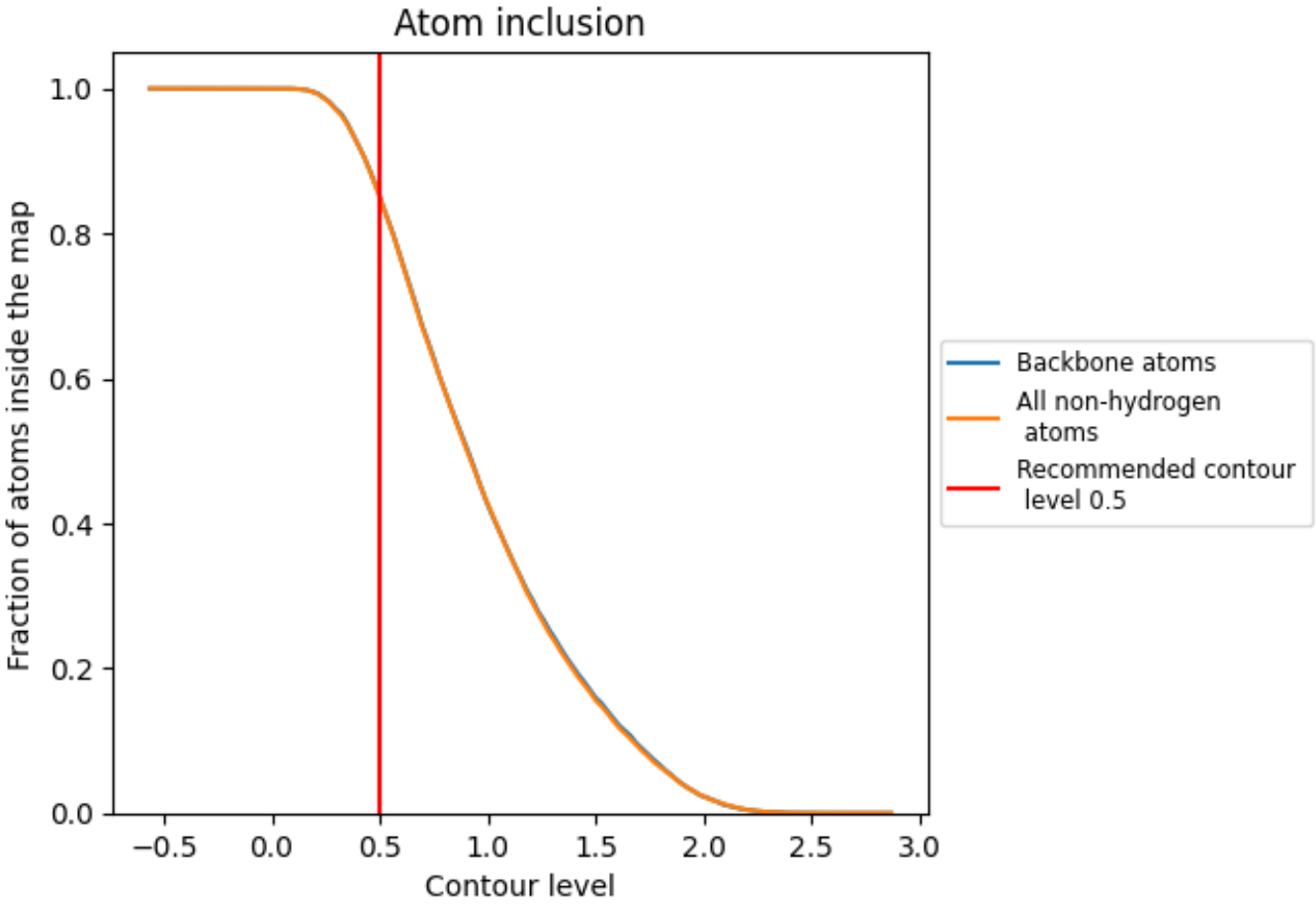
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8507	0.4370
A	0.9386	0.5100
B	0.7927	0.4460
C	0.9236	0.4950
H	0.6658	0.1730
J	0.8277	0.3340
K	0.8781	0.3600
L	0.6057	0.1500