



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 10:22 PM JST

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

This is a 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:

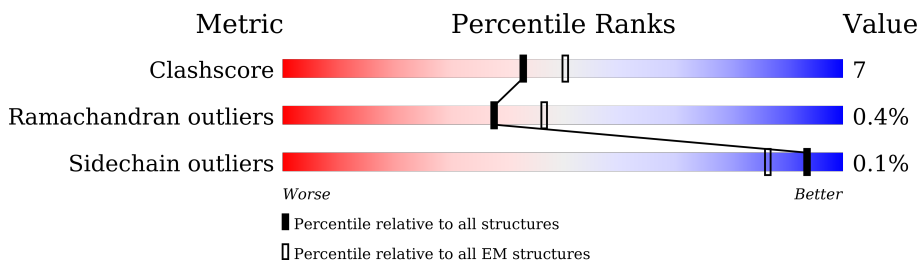
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.50 Å.

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



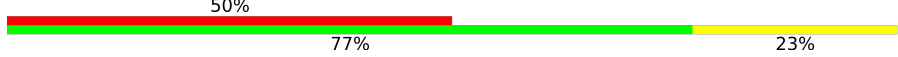
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	D	1270	
2	G	119	
2	H	119	
2	I	119	
3	J	109	
3	K	109	

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Mol	Chain	Length	Quality of chain
3	L	109	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '50%', a green segment in the middle labeled '77%', and a yellow segment on the right labeled '23%'. The segments are stacked horizontally, with the red segment starting from the left and ending at the 50% mark, the green segment starting at 50% and ending at 77%, and the yellow segment starting at 77% and ending at 100%.</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1095	8548	5464	1424	1623	37	0	0
1	B	1095	8548	5466	1423	1622	37	0	0
1	D	1095	8551	5467	1424	1623	37	0	0

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2

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

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

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

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

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

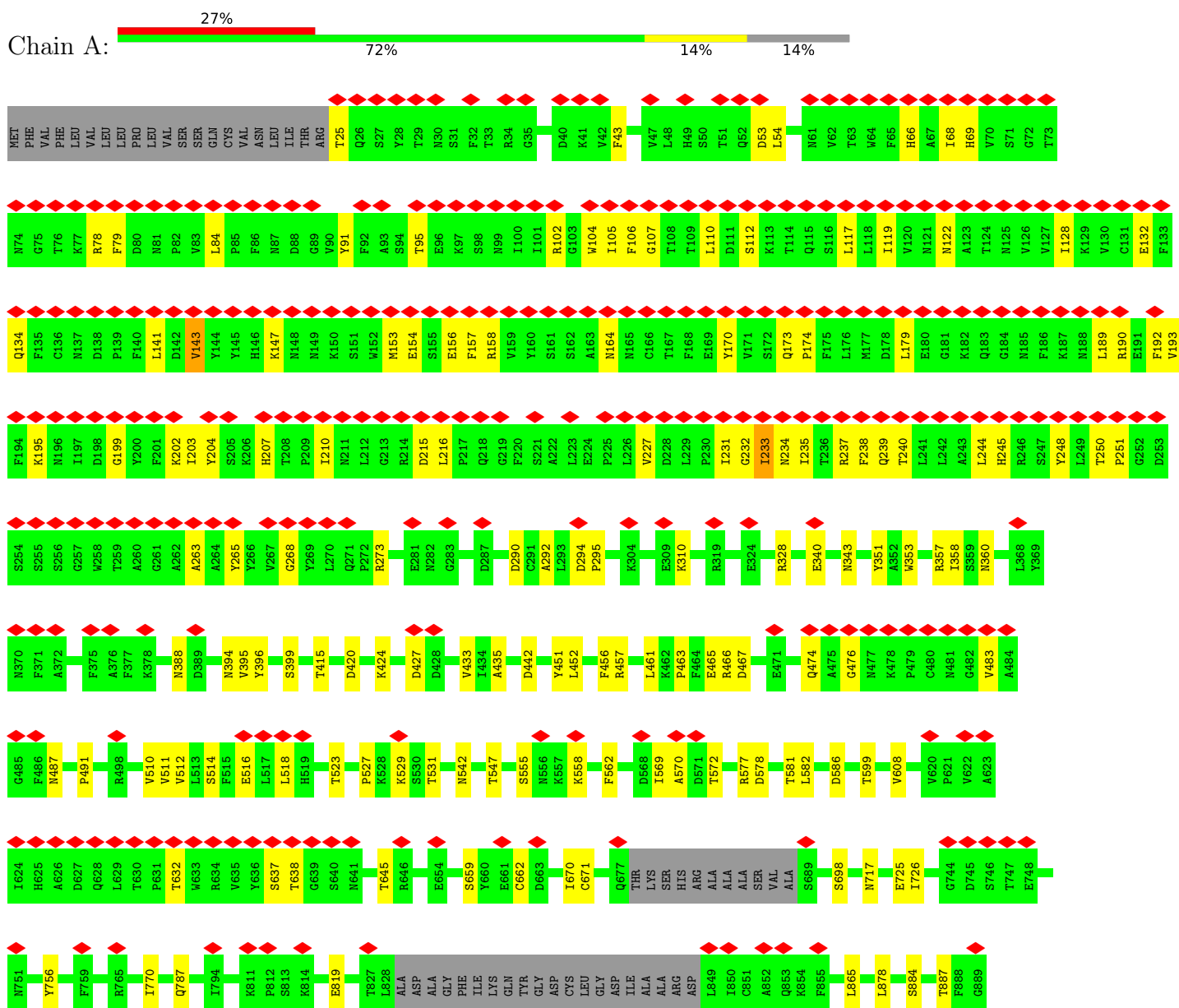
- Molecule 3 is a protein called Light chain of Fab BD55-5840.

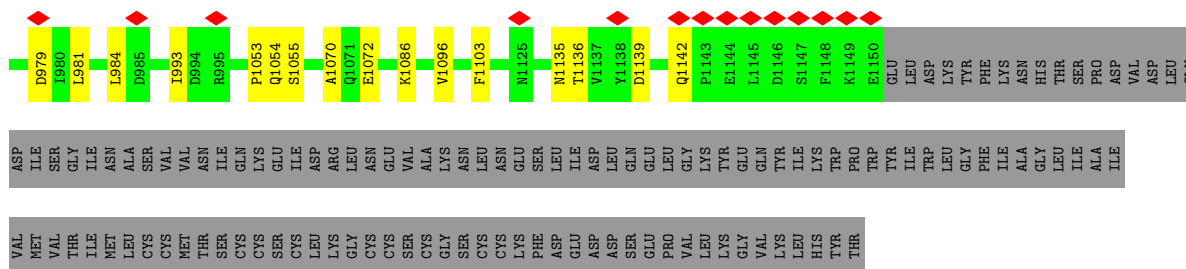
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	109	817	510	142	162	3	0	0
3	J	109	817	510	142	162	3	0	0
3	K	109	817	510	142	162	3	0	0

3 Residue-property plots

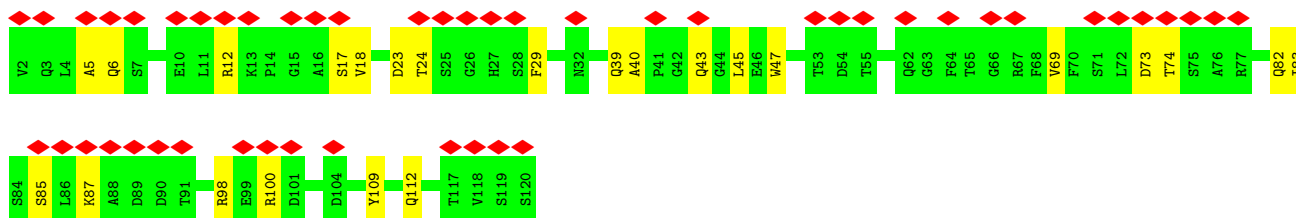
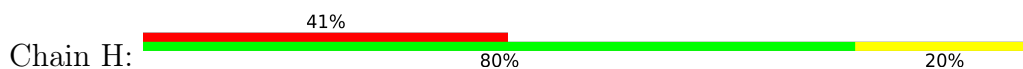
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

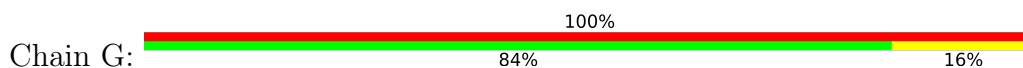




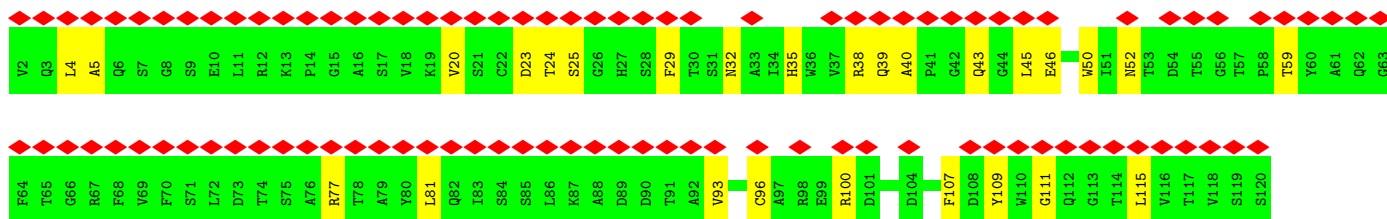
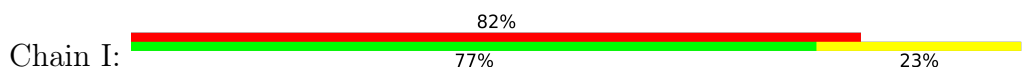
- Molecule 2: Heavy chain of Fab BD55-5840



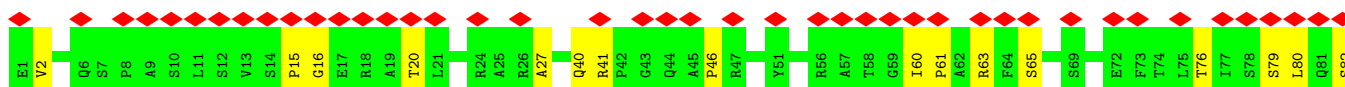
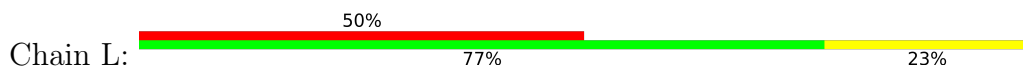
- Molecule 2: Heavy chain of Fab BD55-5840

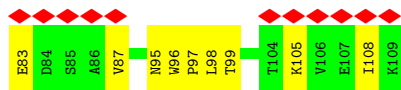


- Molecule 2: Heavy chain of Fab BD55-5840

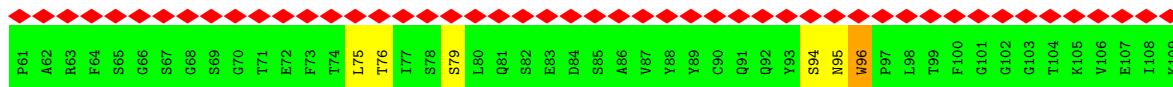
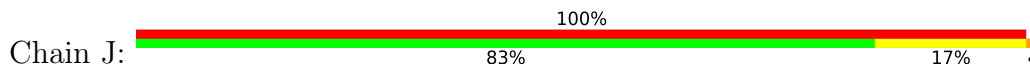


- Molecule 3: Light chain of Fab BD55-5840

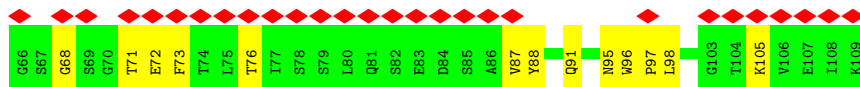
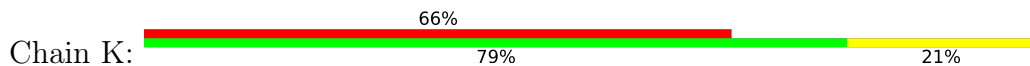




• Molecule 3: Light chain of Fab BD55-5840



• Molecule 3: Light chain of Fab BD55-5840



4 Experimental information

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/8758	0.47	0/11930
1	B	0.25	0/8758	0.47	0/11930
1	D	0.25	0/8761	0.48	0/11934
2	G	0.24	0/952	0.48	0/1295
2	H	0.25	0/952	0.53	0/1295
2	I	0.25	0/952	0.49	0/1295
3	J	0.24	0/834	0.51	0/1133
3	K	0.25	0/834	0.52	0/1133
3	L	0.25	0/834	0.54	0/1133
All	All	0.25	0/31635	0.48	0/43078

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
3	K	0	1
3	L	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8548	0	8314	117	0
1	B	8548	0	8319	102	0
1	D	8551	0	8323	152	0
2	G	927	0	862	11	0
2	H	927	0	862	14	0
2	I	927	0	862	15	0
3	J	817	0	802	13	0
3	K	817	0	802	14	0
3	L	817	0	802	14	0
All	All	30879	0	29948	433	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 (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ASN:HB2	1:D:212:LEU:CD2	1.38	1.50
1:B:185:ASN:O	1:B:212:LEU:HD23	1.36	1.24
1:D:185:ASN:CB	1:D:212:LEU:CD2	2.25	1.15
1:B:185:ASN:O	1:B:212:LEU:CD2	1.98	1.12
1:D:185:ASN:HB2	1:D:212:LEU:HD21	1.27	1.11
1:D:185:ASN:CB	1:D:212:LEU:HD22	1.79	1.10
1:D:185:ASN:HB2	1:D:212:LEU:HD22	1.08	1.06
1:A:153:MET:O	1:A:154:GLU:HG3	1.63	0.96
1:D:153:MET:O	1:D:154:GLU:HG3	1.72	0.89
1:B:153:MET:O	1:B:154:GLU:HG3	1.74	0.87
1:D:552:LEU:HD11	1:D:587:ILE:HD13	1.61	0.80
1:A:542:ASN:ND2	1:A:547:THR:HG22	1.98	0.79
1:A:1141:LEU:HG	1:A:1145:LEU:HD12	1.64	0.78
1:D:564:GLN:HB3	1:D:577:ARG:HB2	1.69	0.74
2:I:40:ALA:HB3	2:I:43:GLN:HB2	1.70	0.74
1:D:659:SER:HB3	1:D:698:SER:HB3	1.74	0.70
1:B:86:PHE:HB2	1:B:238:PHE:HB2	1.72	0.70
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:PHE:HB2	1:D:238:PHE:HB2	1.74	0.69
2:I:39:GLN:HB2	2:I:45:LEU:HD23	1.74	0.69
1:A:233:ILE:HG22	1:A:234:ASN:H	1.58	0.69
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.75	0.69
1:D:394:ASN:ND2	1:D:516:GLU:OE2	2.27	0.68
1:A:555:SER:HB3	1:A:586:ASP:HB2	1.75	0.67
1:A:542:ASN:HD22	1:A:547:THR:HG22	1.60	0.67
1:B:141:LEU:HG	1:B:143:VAL:H	1.60	0.67
1:B:233:ILE:HG22	1:B:234:ASN:H	1.60	0.66
1:D:546:LEU:HG	1:D:576:VAL:HG22	1.77	0.66
1:D:629:LEU:HG	1:D:631:PRO:HD2	1.77	0.66
1:D:87:ASN:ND2	1:D:87:ASN:O	2.29	0.66
2:H:100:ARG:NH1	2:H:109:TYR:OH	2.28	0.66
1:B:87:ASN:ND2	1:B:87:ASN:O	2.28	0.65
2:H:6:GLN:H	2:H:112:GLN:HE22	1.44	0.65
1:D:185:ASN:CA	1:D:212:LEU:CD2	2.75	0.65
1:D:185:ASN:CB	1:D:212:LEU:HD21	2.14	0.64
1:A:988:GLU:N	1:A:988:GLU:OE2	2.31	0.64
1:A:415:THR:HG22	1:B:385:THR:HG23	1.79	0.64
1:B:555:SER:HB2	1:B:586:ASP:HB2	1.80	0.64
2:I:20:VAL:HB	2:I:81:LEU:HB3	1.79	0.64
1:A:132:GLU:HB3	1:A:164:ASN:HB2	1.80	0.63
1:D:153:MET:O	1:D:154:GLU:CG	2.46	0.63
1:A:43:PHE:HB2	1:D:563:GLN:HB3	1.81	0.62
1:B:402:ILE:HD12	1:B:406:GLU:HG3	1.81	0.62
1:D:405:ASN:N	1:D:504:GLY:O	2.32	0.62
1:A:153:MET:O	1:A:154:GLU:CG	2.42	0.62
2:H:85:SER:O	2:H:87:LYS:NZ	2.31	0.62
1:B:659:SER:HB3	1:B:698:SER:HB3	1.81	0.61
1:B:78:ARG:HD2	1:B:244:LEU:HD13	1.82	0.61
1:D:574:ASP:HA	1:D:587:ILE:HB	1.80	0.61
3:K:68:GLY:HA3	3:K:73:PHE:HA	1.83	0.61
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.65	0.61
2:H:69:VAL:HB	2:H:82:GLN:HB3	1.82	0.60
3:J:56:ARG:NH1	3:J:60:ILE:O	2.34	0.60
1:A:717:ASN:HB3	1:A:1070:ALA:HB3	1.83	0.60
1:B:153:MET:O	1:B:154:GLU:CG	2.49	0.60
1:B:158:ARG:HH12	1:B:161:SER:HA	1.67	0.60
1:A:351:TYR:HE1	1:A:452:LEU:HB2	1.67	0.60
1:A:360:ASN:H	1:A:523:THR:HG22	1.66	0.59
1:B:174:PRO:HG2	1:B:177:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:63:ARG:NH1	3:L:79:SER:O	2.35	0.59
1:A:119:ILE:HD12	1:A:119:ILE:H	1.67	0.59
1:A:461:LEU:HD12	1:A:465:GLU:HB2	1.84	0.59
1:A:66:HIS:HE2	1:A:250:THR:HA	1.68	0.59
1:D:454:ARG:NH2	1:D:469:SER:O	2.36	0.59
1:B:386:LYS:NZ	1:D:981:LEU:O	2.29	0.58
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.36	0.58
1:B:393:THR:O	1:B:523:THR:OG1	2.20	0.58
1:B:717:ASN:HB3	1:B:1070:ALA:HB3	1.85	0.58
3:L:16:GLY:H	3:L:80:LEU:HB3	1.66	0.58
3:K:33:THR:HB	3:K:53:ALA:HB2	1.85	0.58
1:D:456:PHE:HB2	1:D:491:PRO:HB3	1.86	0.58
1:A:569:ILE:HD11	1:B:853:GLN:HE22	1.69	0.58
1:A:819:GLU:OE1	1:A:1055:SER:OG	2.21	0.57
3:K:71:THR:HG23	3:K:72:GLU:HG2	1.86	0.57
1:A:110:LEU:HD13	1:A:237:ARG:HG2	1.86	0.57
1:D:677:GLN:NE2	1:D:689:SER:O	2.37	0.57
1:A:107:GLY:H	1:A:235:ILE:HG23	1.69	0.57
1:B:292:ALA:O	1:B:632:THR:OG1	2.18	0.57
1:D:564:GLN:HG3	1:D:577:ARG:HD3	1.86	0.57
2:G:69:VAL:HB	2:G:82:GLN:HB2	1.87	0.57
1:A:105:ILE:HB	1:A:239:GLN:HB3	1.85	0.57
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.37	0.57
1:A:358:ILE:HB	1:A:395:VAL:HB	1.87	0.57
1:B:568:ASP:HB2	1:D:853:GLN:HE21	1.69	0.57
1:A:141:LEU:HD13	1:A:245:HIS:HA	1.86	0.57
1:A:195:LYS:HB3	1:A:202:LYS:HD3	1.87	0.57
1:A:343:ASN:O	3:K:95:ASN:ND2	2.32	0.56
3:J:16:GLY:HA2	3:J:79:SER:HA	1.87	0.56
1:A:637:SER:OG	1:A:638:THR:N	2.37	0.56
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.38	0.56
3:J:31:ILE:HG22	3:J:34:ASP:HB2	1.86	0.56
1:A:112:SER:HB3	1:A:134:GLN:HG3	1.86	0.56
1:D:53:ASP:OD1	1:D:54:LEU:N	2.36	0.56
1:D:343:ASN:O	3:J:95:ASN:ND2	2.37	0.56
3:L:60:ILE:HD12	3:L:61:PRO:HD2	1.87	0.56
1:A:95:THR:HG23	1:A:189:LEU:HD13	1.86	0.56
1:D:403:ARG:NH1	1:D:406:GLU:OE2	2.38	0.56
1:A:53:ASP:OD1	1:A:54:LEU:N	2.36	0.56
1:A:474:GLN:NE2	1:A:476:GLY:O	2.37	0.56
1:D:357:ARG:NH1	1:D:395:VAL:O	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD23	1:A:119:ILE:HD11	1.88	0.55
3:J:31:ILE:HG23	3:J:94:SER:HB2	1.89	0.55
1:D:84:LEU:HB2	1:D:238:PHE:HB3	1.87	0.55
1:D:137:ASN:OD1	1:D:138:ASP:N	2.36	0.55
1:B:68:ILE:HG13	1:B:68:ILE:O	2.07	0.55
1:B:391:CYS:HA	1:B:525:CYS:CB	2.36	0.55
1:D:141:LEU:HG	1:D:143:VAL:H	1.71	0.55
3:L:65:SER:OG	3:L:76:THR:OG1	2.24	0.54
1:D:378:LYS:O	1:D:433:VAL:N	2.34	0.54
1:D:566:GLY:H	1:D:575:ALA:HB3	1.72	0.54
1:D:819:GLU:OE1	1:D:1055:SER:OG	2.24	0.54
1:A:951:VAL:O	1:A:955:ASN:ND2	2.32	0.54
1:B:361:CYS:H	1:B:524:VAL:HG12	1.73	0.54
2:I:25:SER:HA	2:I:77:ARG:HH21	1.73	0.54
1:A:415:THR:OG1	1:A:420:ASP:OD2	2.25	0.54
1:D:346:ARG:HH22	1:D:450:ASN:HB3	1.72	0.54
2:G:96:CYS:O	2:G:111:GLY:N	2.37	0.54
1:A:976:VAL:HG12	1:A:979:ASP:H	1.73	0.53
3:K:20:THR:HG22	3:K:76:THR:HG22	1.89	0.53
1:A:95:THR:CG2	1:A:189:LEU:HD13	2.38	0.53
1:D:173:GLN:HG2	1:D:174:PRO:HD2	1.89	0.53
1:A:156:GLU:HG3	1:A:157:PHE:H	1.73	0.53
1:D:715:PRO:HA	1:D:1072:GLU:HA	1.91	0.53
1:D:717:ASN:HB3	1:D:1070:ALA:HB3	1.89	0.53
3:J:20:THR:HG22	3:J:76:THR:HG22	1.90	0.53
3:K:2:VAL:H	3:K:97:PRO:HG3	1.72	0.53
1:B:99:ASN:HB2	1:B:102:ARG:HH12	1.73	0.53
1:D:78:ARG:HG2	1:D:79:PHE:N	2.23	0.53
2:G:31:SER:HG	2:G:98:ARG:HE	1.57	0.53
1:A:25:THR:HB	1:A:66:HIS:HB3	1.90	0.53
1:A:233:ILE:HG22	1:A:234:ASN:N	2.23	0.53
1:B:67:ALA:O	1:B:250:THR:OG1	2.18	0.52
1:D:117:LEU:HD13	1:D:235:ILE:HD11	1.90	0.52
1:A:117:LEU:HD11	1:A:231:ILE:HG21	1.92	0.52
1:D:98:SER:O	1:D:190:ARG:NH2	2.42	0.52
1:A:68:ILE:O	1:A:68:ILE:HG13	2.08	0.52
1:B:185:ASN:O	1:B:212:LEU:HD21	2.03	0.52
1:B:878:LEU:O	1:B:882:ILE:HG12	2.09	0.52
1:D:458:LYS:HD2	1:D:473:TYR:HE1	1.74	0.52
1:D:474:GLN:NE2	1:D:478:LYS:O	2.31	0.52
1:D:474:GLN:NE2	1:D:476:GLY:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:12:ARG:HE	2:G:18:VAL:HA	1.75	0.52
1:A:102:ARG:NH2	1:A:122:ASN:O	2.43	0.52
1:D:66:HIS:ND1	1:D:262:ALA:O	2.42	0.52
2:H:12:ARG:HG3	2:H:18:VAL:HG22	1.91	0.52
1:A:442:ASP:OD1	1:A:451:TYR:OH	2.26	0.52
1:D:117:LEU:HD11	1:D:231:ILE:HG21	1.91	0.52
1:A:570:ALA:HB3	1:A:572:THR:HG22	1.92	0.52
1:D:752:LEU:HD22	1:D:993:ILE:HD11	1.92	0.52
2:G:93:VAL:HG22	2:G:115:LEU:HD13	1.92	0.52
1:A:542:ASN:ND2	1:A:547:THR:CG2	2.72	0.51
1:B:627:ASP:O	1:B:628:GLN:NE2	2.44	0.51
2:G:58:PRO:HB3	2:G:70:PHE:HB2	1.92	0.51
1:A:328:ARG:NH1	1:A:531:THR:O	2.42	0.51
1:D:453:TYR:OH	1:D:493:ARG:NH1	2.44	0.51
1:D:91:TYR:N	1:D:268:GLY:O	2.37	0.51
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.26	0.51
1:B:708:SER:HB3	1:B:711:SER:HB2	1.90	0.51
1:D:466:ARG:HH21	1:D:468:ILE:HG21	1.74	0.51
1:A:66:HIS:CE1	1:A:251:PRO:HD2	2.46	0.50
2:I:5:ALA:HB3	2:I:23:ASP:HB3	1.93	0.50
1:D:147:LYS:HD3	1:D:248:TYR:HB2	1.92	0.50
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.94	0.50
1:D:67:ALA:O	1:D:250:THR:OG1	2.20	0.50
1:B:562:PHE:HD2	1:D:41:LYS:HD2	1.77	0.50
1:B:699:LEU:HD21	1:D:869:MET:HB3	1.94	0.50
2:I:32:ASN:ND2	2:I:52:ASN:OD1	2.41	0.50
1:B:353:TRP:O	1:B:466:ARG:NH2	2.36	0.50
1:D:951:VAL:O	1:D:955:ASN:ND2	2.44	0.50
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.36	0.50
1:D:132:GLU:HB2	1:D:164:ASN:HB2	1.94	0.50
3:L:41:ARG:NE	3:L:83:GLU:O	2.43	0.50
2:I:4:LEU:HD11	2:I:29:PHE:HZ	1.76	0.50
1:D:383:SER:HB3	1:D:386:LYS:HG2	1.92	0.50
3:L:15:PRO:HG3	3:L:108:ILE:HG23	1.93	0.50
3:L:97:PRO:O	3:L:99:THR:HG23	2.11	0.50
1:A:119:ILE:HG13	1:A:128:ILE:HG23	1.92	0.50
1:D:340:GLU:HG2	3:J:29:LEU:HB2	1.93	0.50
1:A:476:GLY:HA3	1:A:487:ASN:HB3	1.93	0.49
3:K:56:ARG:NH1	3:K:62:ALA:HA	2.27	0.49
1:D:1053:PRO:O	1:D:1054:GLN:NE2	2.43	0.49
1:D:119:ILE:HG13	1:D:128:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:ARG:NH1	1:D:357:ARG:HA	2.27	0.49
1:D:599:THR:HB	1:D:608:VAL:HG12	1.93	0.49
1:A:66:HIS:ND1	1:A:263:ALA:HA	2.26	0.49
3:K:87:VAL:HG22	3:K:105:LYS:HG3	1.93	0.49
1:A:351:TYR:CE1	1:A:452:LEU:HB2	2.46	0.49
1:A:399:SER:HB3	1:A:511:VAL:HG23	1.95	0.49
1:D:185:ASN:CA	1:D:212:LEU:HD23	2.41	0.49
1:D:328:ARG:HD2	1:D:579:PRO:HG2	1.95	0.49
1:D:353:TRP:O	1:D:466:ARG:NH1	2.46	0.49
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.94	0.49
1:A:558:LYS:HE2	1:B:282:ASN:HB3	1.95	0.49
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.95	0.48
1:A:173:GLN:HG2	1:A:174:PRO:HD2	1.95	0.48
1:D:158:ARG:O	1:D:158:ARG:HG3	2.13	0.48
1:A:141:LEU:HG	1:A:143:VAL:H	1.78	0.48
1:A:577:ARG:HD3	1:A:582:LEU:HD13	1.93	0.48
1:D:324:GLU:HB2	1:D:539:VAL:HG23	1.95	0.48
1:D:457:ARG:NE	1:D:467:ASP:OD2	2.45	0.48
1:A:119:ILE:HG23	1:A:128:ILE:HG12	1.95	0.48
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.37	0.48
1:D:327:VAL:HG13	1:D:542:ASN:HB3	1.94	0.48
1:D:140:PHE:CZ	1:D:158:ARG:HG2	2.48	0.48
1:D:340:GLU:HB2	3:J:29:LEU:HD12	1.96	0.48
1:D:624:ILE:HD11	1:D:637:SER:HA	1.94	0.48
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.96	0.48
1:D:66:HIS:HE1	1:D:251:PRO:HD2	1.78	0.48
1:D:396:TYR:HB2	1:D:514:SER:HB3	1.94	0.48
1:B:427:ASP:OD1	1:B:427:ASP:N	2.47	0.48
1:D:185:ASN:HA	1:D:212:LEU:HD23	1.96	0.48
2:I:35:HIS:CD2	2:I:107:PHE:HE2	2.32	0.48
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.47	0.48
1:D:884:SER:O	1:D:884:SER:OG	2.33	0.47
3:L:20:THR:HG22	3:L:76:THR:HG22	1.96	0.47
1:A:91:TYR:N	1:A:268:GLY:O	2.41	0.47
1:D:66:HIS:CG	1:D:263:ALA:HA	2.49	0.47
1:D:105:ILE:HD12	1:D:241:LEU:HD21	1.96	0.47
2:H:73:ASP:OD1	2:H:74:THR:N	2.46	0.47
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.96	0.47
1:B:99:ASN:O	1:B:102:ARG:NH2	2.48	0.47
1:D:99:ASN:ND2	1:D:102:ARG:HH12	2.12	0.47
1:A:569:ILE:HG13	1:A:569:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:ILE:HG13	1:A:1061:VAL:HG22	1.95	0.47
1:B:84:LEU:HB2	1:B:238:PHE:HB3	1.97	0.47
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.80	0.47
1:B:569:ILE:HG13	1:B:569:ILE:O	2.15	0.47
1:D:81:ASN:O	1:D:239:GLN:NE2	2.42	0.47
1:D:295:PRO:HB2	1:D:608:VAL:HG21	1.96	0.47
1:D:319:ARG:HH11	1:D:592:PHE:HB3	1.80	0.47
1:D:560:LEU:HG	1:D:561:PRO:HD2	1.96	0.47
2:H:23:ASP:OD1	2:H:24:THR:N	2.47	0.47
1:A:645:THR:HG23	1:A:670:ILE:HG13	1.97	0.47
1:D:99:ASN:HD22	1:D:102:ARG:HH12	1.60	0.47
1:D:529:LYS:NZ	1:D:580:GLN:HE21	2.13	0.47
1:B:95:THR:CG2	1:B:189:LEU:HD13	2.45	0.47
1:D:100:ILE:HG22	1:D:242:LEU:HD11	1.97	0.47
1:D:552:LEU:HG	1:D:586:ASP:O	2.15	0.47
1:D:804:GLN:NE2	1:D:935:GLN:OE1	2.43	0.47
1:A:84:LEU:HB2	1:A:238:PHE:HD2	1.80	0.46
1:A:294:ASP:OD2	1:A:295:PRO:HD2	2.15	0.46
1:A:353:TRP:O	1:A:466:ARG:NH2	2.36	0.46
1:B:328:ARG:HH11	1:B:533:LEU:HD13	1.80	0.46
1:D:215:ASP:N	1:D:215:ASP:OD1	2.49	0.46
1:D:318:PHE:CE1	1:D:629:LEU:HD11	2.50	0.46
1:D:642:VAL:HG22	1:D:651:ILE:HD12	1.97	0.46
2:I:93:VAL:HG22	2:I:115:LEU:HD13	1.97	0.46
1:A:157:PHE:CG	1:A:158:ARG:N	2.83	0.46
3:J:21:LEU:HD13	3:J:75:LEU:HD23	1.98	0.46
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.97	0.46
1:B:67:ALA:HB1	1:B:244:LEU:HD21	1.98	0.46
1:D:106:PHE:HB2	1:D:117:LEU:HB2	1.96	0.46
1:D:332:ILE:HD12	1:D:362:VAL:HG22	1.98	0.46
2:H:5:ALA:HB3	2:H:23:ASP:HB3	1.96	0.46
1:D:334:ASN:O	1:D:362:VAL:N	2.49	0.46
1:D:619:GLU:OE1	1:D:619:GLU:N	2.48	0.46
1:B:137:ASN:OD1	1:B:138:ASP:N	2.45	0.46
1:A:884:SER:OG	1:A:887:THR:OG1	2.34	0.46
1:D:251:PRO:HG2	1:D:262:ALA:HB3	1.97	0.46
1:D:616:ASN:OD1	1:D:617:CYS:N	2.49	0.46
1:D:630:THR:HB	1:D:631:PRO:HD3	1.98	0.46
1:D:1139:ASP:HB3	1:D:1142:GLN:HG2	1.97	0.46
1:A:179:LEU:HD11	1:A:207:HIS:HB3	1.97	0.46
1:A:878:LEU:HD21	1:A:1052:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:100:ARG:HB2	2:I:109:TYR:HE1	1.81	0.45
1:A:190:ARG:HB3	1:A:192:PHE:HE1	1.81	0.45
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.82	0.45
1:D:102:ARG:HG2	1:D:121:ASN:HB3	1.99	0.45
1:D:153:MET:C	1:D:154:GLU:HG3	2.36	0.45
2:G:12:ARG:HH21	2:G:19:LYS:H	1.64	0.45
2:I:24:THR:OG1	2:I:77:ARG:O	2.22	0.45
1:B:409:GLN:HG2	1:B:419:ALA:HB2	1.98	0.45
1:B:106:PHE:HB3	1:B:235:ILE:HG21	1.97	0.45
1:D:68:ILE:HG13	1:D:68:ILE:O	2.16	0.45
1:D:276:LEU:HD11	1:D:304:LYS:HA	1.98	0.45
1:A:427:ASP:N	1:A:427:ASP:OD1	2.46	0.45
3:J:8:PRO:HD2	3:J:11:LEU:HD11	1.98	0.45
1:A:240:THR:HG21	1:A:265:TYR:HE2	1.82	0.45
1:B:36:VAL:HG11	1:B:220:PHE:CZ	2.52	0.45
1:B:105:ILE:HG23	1:B:239:GLN:HB3	1.98	0.45
1:D:884:SER:OG	1:D:887:THR:OG1	2.35	0.45
1:D:117:LEU:HD23	1:D:119:ILE:HD11	1.99	0.45
1:D:808:ASP:HB3	1:D:811:LYS:HD2	1.99	0.45
3:L:40:GLN:HG3	3:L:46:PRO:HG3	1.98	0.44
1:A:147:LYS:HD3	1:A:248:TYR:HB2	2.00	0.44
1:A:424:LYS:HB3	1:A:463:PRO:HA	1.98	0.44
1:B:153:MET:C	1:B:154:GLU:HG3	2.36	0.44
1:B:850:ILE:O	1:B:853:GLN:HG2	2.16	0.44
1:D:146:HIS:CE1	1:D:148:ASN:HB2	2.52	0.44
1:A:921:LYS:HB3	1:A:921:LYS:HE2	1.60	0.44
1:B:125:ASN:OD1	1:B:126:VAL:N	2.51	0.44
1:B:343:ASN:O	3:L:95:ASN:ND2	2.50	0.44
1:B:461:LEU:H	1:B:461:LEU:HD23	1.81	0.44
1:D:534:VAL:HG11	1:D:537:LYS:HB2	1.99	0.44
1:D:552:LEU:HD23	1:D:585:LEU:HB3	2.00	0.44
1:B:689:SER:OG	1:B:690:GLN:N	2.51	0.44
1:B:986:PRO:O	1:B:990:GLU:HG2	2.17	0.44
1:D:36:VAL:HG21	1:D:220:PHE:CE2	2.53	0.44
1:A:153:MET:C	1:A:154:GLU:HG3	2.35	0.44
1:A:599:THR:HB	1:A:608:VAL:HG12	2.00	0.44
1:B:347:PHE:CZ	1:B:509:ARG:HD3	2.52	0.44
1:A:215:ASP:N	1:A:215:ASP:OD1	2.50	0.44
3:L:87:VAL:HG22	3:L:105:LYS:HD2	2.00	0.44
1:D:105:ILE:HG13	1:D:241:LEU:HD11	2.00	0.44
1:D:445:VAL:HA	1:D:499:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.50	0.43
1:A:529:LYS:HA	1:A:529:LYS:HD2	1.72	0.43
1:A:659:SER:HB3	1:A:698:SER:HB3	2.00	0.43
1:D:112:SER:HB3	1:D:134:GLN:HG3	2.00	0.43
2:G:104:ASP:HB3	2:G:106:PHE:CE2	2.53	0.43
1:A:435:ALA:HB2	1:A:510:VAL:HG23	2.01	0.43
1:B:437:ASN:HA	1:B:508:TYR:CD1	2.53	0.43
1:B:821:LEU:HD22	1:B:935:GLN:HG3	2.00	0.43
1:D:141:LEU:HD13	1:D:245:HIS:HA	2.00	0.43
3:K:4:MET:HA	3:K:25:ALA:HA	1.99	0.43
1:A:433:VAL:HG23	1:A:512:VAL:HB	2.00	0.43
1:B:159:VAL:HG21	1:B:241:LEU:HD23	2.00	0.43
1:D:344:ALA:HB3	1:D:347:PHE:CE1	2.53	0.43
1:D:759:PHE:O	1:D:763:LEU:HD13	2.19	0.43
1:A:971:GLY:O	1:A:995:ARG:NH1	2.41	0.43
1:B:40:ASP:OD1	1:B:41:LYS:N	2.41	0.43
1:D:226:LEU:HD23	1:D:227:VAL:HB	2.00	0.43
3:L:82:SER:HA	3:L:108:ILE:HG21	1.99	0.43
1:B:577:ARG:HH21	1:B:584:ILE:HD11	1.82	0.43
1:D:66:HIS:CE1	1:D:250:THR:HA	2.53	0.43
1:D:357:ARG:HA	1:D:357:ARG:HH11	1.82	0.43
3:J:25:ALA:HB3	3:J:31:ILE:HD11	2.00	0.43
2:I:4:LEU:HB2	2:I:111:GLY:HA2	2.00	0.43
2:G:18:VAL:HG21	2:G:116:VAL:HG11	2.01	0.43
3:K:39:GLN:HG3	3:K:88:TYR:HE1	1.84	0.43
1:A:456:PHE:HD2	1:A:491:PRO:HA	1.84	0.43
2:I:96:CYS:O	2:I:111:GLY:N	2.50	0.43
1:B:300:LYS:HG2	1:B:305:SER:O	2.19	0.43
1:B:350:VAL:HG21	1:B:418:ILE:HD11	2.01	0.43
1:B:497:PHE:CZ	1:B:507:PRO:HB3	2.54	0.43
3:J:33:THR:HB	3:J:53:ALA:HB2	2.01	0.43
1:A:104:TRP:HD1	1:A:238:PHE:HE1	1.66	0.43
1:A:433:VAL:HA	1:A:512:VAL:HA	2.00	0.43
1:B:401:VAL:HG12	1:B:509:ARG:HA	2.00	0.43
1:D:708:SER:HB3	1:D:711:SER:HB2	2.01	0.43
1:D:865:LEU:HD23	1:D:865:LEU:HA	1.91	0.43
1:D:1086:LYS:HE3	1:D:1086:LYS:HB2	1.88	0.43
3:K:105:LYS:HE3	3:K:105:LYS:HB2	1.86	0.43
1:A:233:ILE:CG2	1:A:234:ASN:H	2.29	0.42
1:A:461:LEU:HD23	1:A:461:LEU:H	1.84	0.42
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:THR:OG1	1:D:219:GLY:O	2.29	0.42
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.89	0.42
1:A:310:LYS:HE2	1:A:310:LYS:HB3	1.82	0.42
1:A:906:PHE:CD2	1:A:916:LEU:HB2	2.54	0.42
1:B:91:TYR:N	1:B:268:GLY:O	2.48	0.42
1:B:386:LYS:NZ	1:D:984:LEU:O	2.43	0.42
1:B:433:VAL:HG22	1:B:512:VAL:HG23	2.00	0.42
1:B:822:LEU:HD22	1:B:945:LEU:HD21	2.01	0.42
1:D:276:LEU:HD23	1:D:276:LEU:O	2.19	0.42
1:A:388:ASN:HB3	1:A:527:PRO:HD2	2.00	0.42
1:B:295:PRO:HG3	1:B:633:TRP:CE3	2.54	0.42
1:B:407:VAL:HG21	1:B:508:TYR:HD2	1.83	0.42
3:K:35:LEU:HD12	3:K:91:GLN:O	2.18	0.42
1:B:624:ILE:H	1:B:624:ILE:HD12	1.85	0.42
1:D:344:ALA:HB3	1:D:347:PHE:HE1	1.83	0.42
2:H:17:SER:HB2	2:H:82:GLN:NE2	2.34	0.42
1:A:662:CYS:HB2	1:A:671:CYS:HB3	1.63	0.42
1:A:977:LEU:O	1:A:980:ILE:HG22	2.20	0.42
1:D:327:VAL:HA	1:D:542:ASN:HB3	2.01	0.42
1:B:516:GLU:O	1:B:516:GLU:HG2	2.20	0.42
1:D:278:LYS:HD2	1:D:306:PHE:CE2	2.54	0.42
1:A:578:ASP:OD1	1:A:581:THR:N	2.40	0.42
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.55	0.42
1:D:1135:ASN:OD1	1:D:1136:THR:N	2.52	0.42
2:G:4:LEU:HB2	2:G:111:GLY:HA2	2.02	0.42
2:G:37:VAL:HG21	2:G:110:TRP:CH2	2.55	0.42
1:A:69:HIS:HB3	1:A:244:LEU:HD22	2.02	0.42
1:B:176:LEU:HD13	1:B:190:ARG:HH22	1.85	0.42
1:D:334:ASN:OD1	1:D:334:ASN:N	2.51	0.42
1:D:1096:VAL:O	1:D:1103:PHE:N	2.43	0.42
1:A:787:GLN:OE1	1:D:703:ASN:ND2	2.40	0.41
1:A:193:VAL:HG12	1:A:204:TYR:HB2	2.01	0.41
1:A:203:ILE:HB	1:A:227:VAL:HG12	2.02	0.41
1:D:406:GLU:HB3	1:D:418:ILE:HG21	2.02	0.41
1:D:578:ASP:HB2	1:D:583:GLU:O	2.20	0.41
2:H:47:TRP:CE3	3:L:98:LEU:HB2	2.55	0.41
1:B:97:LYS:HG2	1:B:100:ILE:HD11	2.02	0.41
1:B:170:TYR:HD1	1:B:170:TYR:O	2.04	0.41
1:D:91:TYR:HE1	1:D:191:GLU:OE2	2.03	0.41
1:D:142:ASP:C	1:D:144:TYR:H	2.24	0.41
1:A:357:ARG:CZ	1:A:394:ASN:HD22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:HD23	1:A:518:LEU:H	1.86	0.41
2:H:29:PHE:CE2	2:H:98:ARG:HG2	2.55	0.41
1:A:1045:LYS:HE3	1:A:1045:LYS:HB3	1.77	0.41
1:B:405:ASN:OD1	1:B:406:GLU:N	2.53	0.41
1:D:278:LYS:HD2	1:D:306:PHE:HE2	1.86	0.41
1:D:317:ASN:OD1	1:D:318:PHE:N	2.52	0.41
1:D:343:ASN:HD21	3:J:96:TRP:HB2	1.85	0.41
1:B:341:VAL:HG22	1:B:356:LYS:HD2	2.02	0.41
1:B:278:LYS:HD2	1:B:306:PHE:HE2	1.85	0.41
1:B:543:PHE:O	1:B:546:LEU:HD23	2.20	0.41
1:D:357:ARG:NH2	1:D:394:ASN:HB2	2.36	0.41
1:D:416:GLY:N	1:D:420:ASP:OD2	2.41	0.41
1:A:562:PHE:HB2	1:B:41:LYS:NZ	2.36	0.41
1:B:147:LYS:HD3	1:B:248:TYR:HB2	2.02	0.41
1:B:760:CYS:HA	1:B:763:LEU:HB2	2.03	0.41
1:D:323:THR:O	1:D:539:VAL:HA	2.21	0.41
2:I:38:ARG:O	2:I:46:GLU:N	2.45	0.41
1:A:199:GLY:HA2	1:A:232:GLY:HA2	2.03	0.41
1:A:292:ALA:HB1	1:A:632:THR:OG1	2.21	0.41
1:A:516:GLU:O	1:A:516:GLU:HG2	2.21	0.41
1:A:865:LEU:HD23	1:A:865:LEU:HA	1.93	0.41
1:B:105:ILE:HG13	1:B:117:LEU:O	2.20	0.41
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.56	0.41
1:B:850:ILE:HG23	1:B:853:GLN:NE2	2.36	0.41
1:D:37:TYR:HA	1:D:223:LEU:H	1.86	0.41
1:D:528:LYS:HE3	1:D:528:LYS:HB3	1.85	0.41
3:K:98:LEU:HD23	3:K:98:LEU:HA	1.92	0.41
1:B:233:ILE:HG22	1:B:234:ASN:N	2.33	0.41
1:B:518:LEU:H	1:B:518:LEU:HD23	1.87	0.40
1:D:906:PHE:CD2	1:D:916:LEU:HB2	2.55	0.40
1:B:449:TYR:OH	1:B:498:ARG:NH2	2.54	0.40
1:A:340:GLU:HA	3:K:95:ASN:ND2	2.37	0.40
1:B:250:THR:HG23	1:B:250:THR:O	2.21	0.40
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.56	0.40
1:D:650:LEU:H	1:D:650:LEU:HD23	1.86	0.40
1:D:976:VAL:HG12	1:D:979:ASP:H	1.85	0.40
1:D:253:ASP:N	1:D:253:ASP:OD1	2.55	0.40
1:D:560:LEU:HD21	1:D:562:PHE:CE1	2.57	0.40
2:H:18:VAL:HB	2:H:83:ILE:HG22	2.03	0.40
1:A:78:ARG:HG3	1:A:79:PHE:H	1.86	0.40
1:B:118:LEU:HD22	1:B:133:PHE:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ASP:OD1	1:B:291:CYS:N	2.55	0.40
1:B:1086:LYS:HB2	1:B:1086:LYS:HE3	1.93	0.40
1:D:616:ASN:HB3	1:D:619:GLU:OE1	2.22	0.40
3:L:2:VAL:HG22	3:L:27:ALA:HB2	2.02	0.40
2:I:50:TRP:CD1	2:I:59:THR:HB	2.57	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	1089/1270 (86%)	1023 (94%)	62 (6%)	4 (0%)	34	72
1	B	1089/1270 (86%)	1024 (94%)	60 (6%)	5 (0%)	29	68
1	D	1089/1270 (86%)	1007 (92%)	77 (7%)	5 (0%)	29	68
2	G	117/119 (98%)	116 (99%)	1 (1%)	0	100	100
2	H	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
2	I	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
3	J	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
3	K	107/109 (98%)	97 (91%)	10 (9%)	0	100	100
3	L	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
All	All	3939/4494 (88%)	3682 (94%)	243 (6%)	14 (0%)	38	72

All (14) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	D	143	VAL
1	D	233	ILE
1	D	527	PRO
1	A	143	VAL
1	A	483	VAL
1	B	157	PHE
1	D	483	VAL
1	B	483	VAL
1	B	210	ILE
1	A	210	ILE
1	D	210	ILE

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	950/1109 (86%)	950 (100%)	0	100	100
1	B	950/1109 (86%)	948 (100%)	2 (0%)	93	98
1	D	951/1109 (86%)	949 (100%)	2 (0%)	93	98
2	G	98/98 (100%)	98 (100%)	0	100	100
2	H	98/98 (100%)	98 (100%)	0	100	100
2	I	98/98 (100%)	98 (100%)	0	100	100
3	J	88/88 (100%)	88 (100%)	0	100	100
3	K	88/88 (100%)	88 (100%)	0	100	100
3	L	88/88 (100%)	88 (100%)	0	100	100
All	All	3409/3885 (88%)	3405 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	B	646	ARG
1	D	78	ARG

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Mol	Chain	Res	Type
1	D	87	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	ASN
1	A	542	ASN
1	B	66	HIS
1	B	173	GLN
1	B	853	GLN
1	D	87	ASN
1	D	580	GLN
2	G	112	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

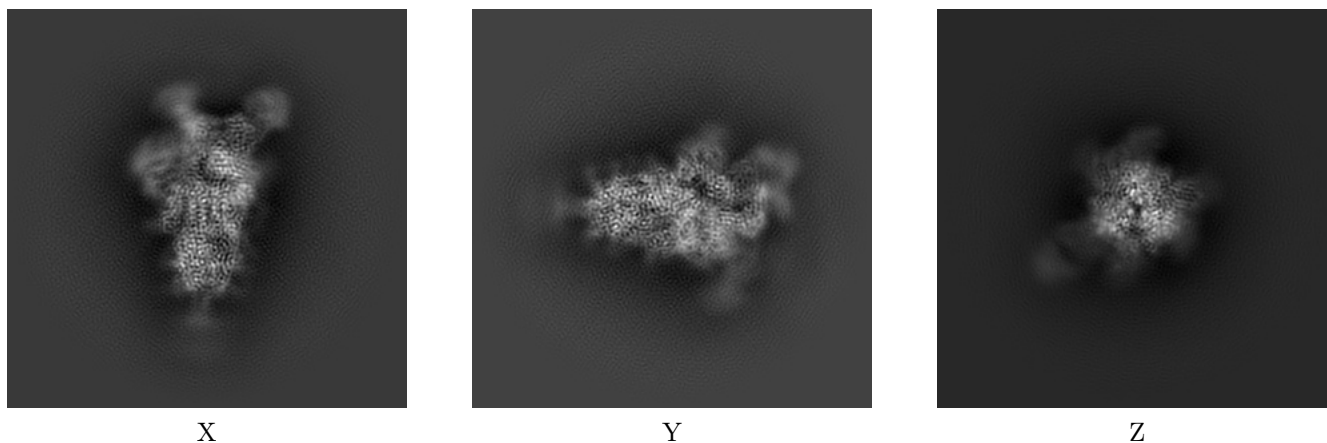
6 Map visualisation [i](#)

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

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

6.1 Orthogonal projections [i](#)

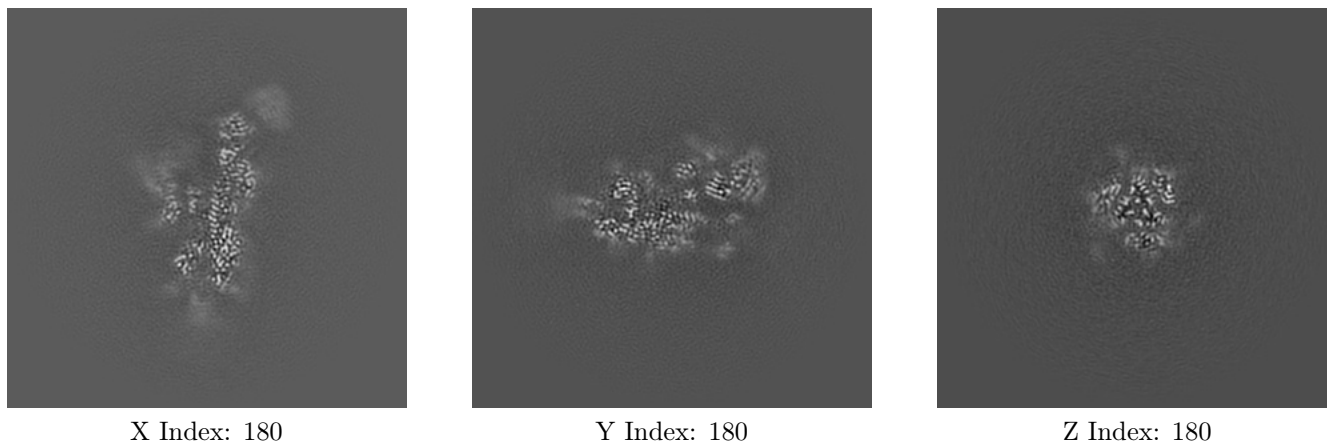
6.1.1 Primary map



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

6.2 Central slices [i](#)

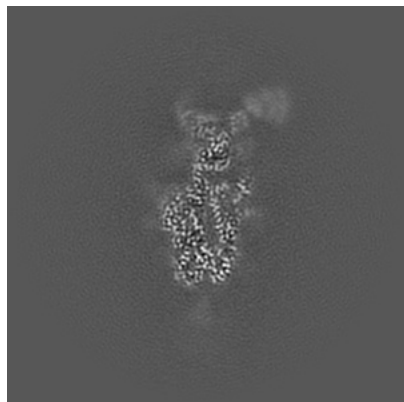
6.2.1 Primary map



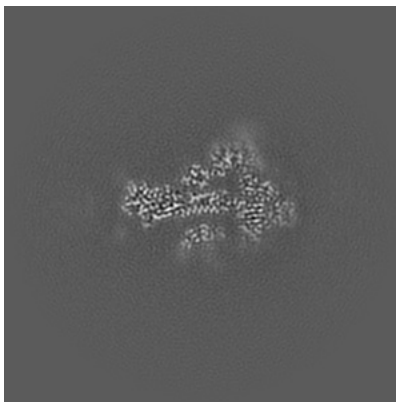
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

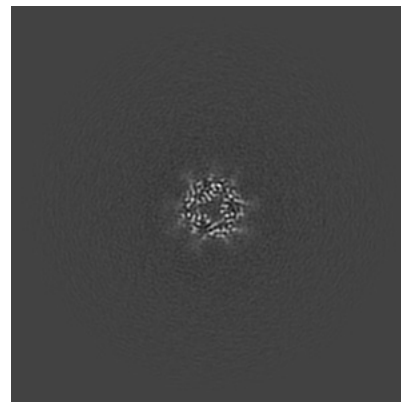
6.3.1 Primary map



X Index: 192



Y Index: 195

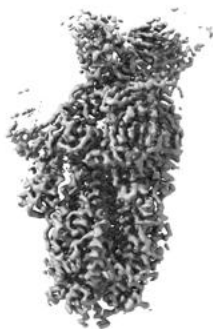


Z Index: 129

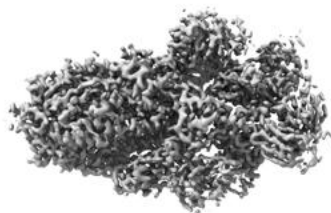
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal 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 0.558. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

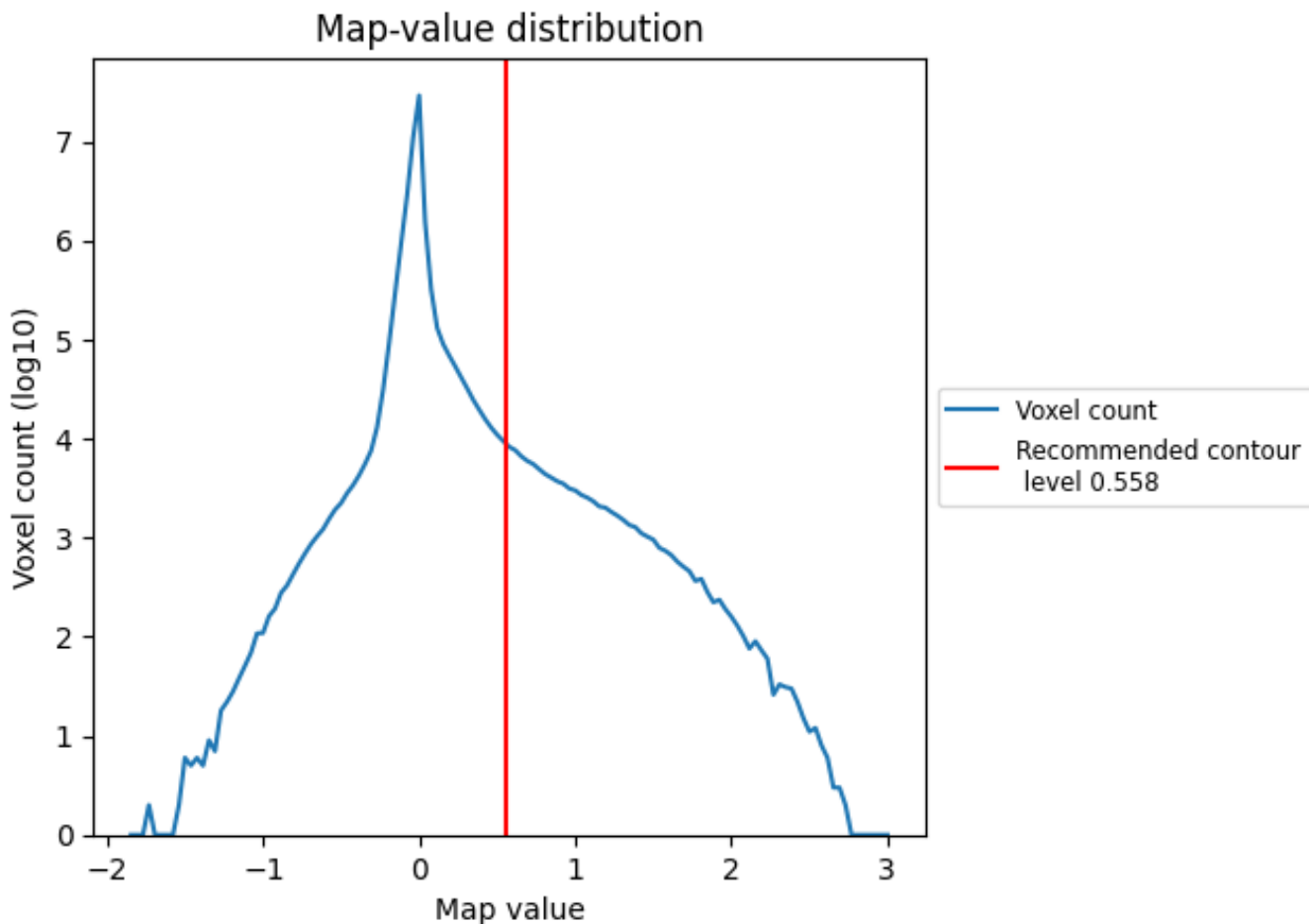
6.5 Mask visualisation

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

7 Map analysis [i](#)

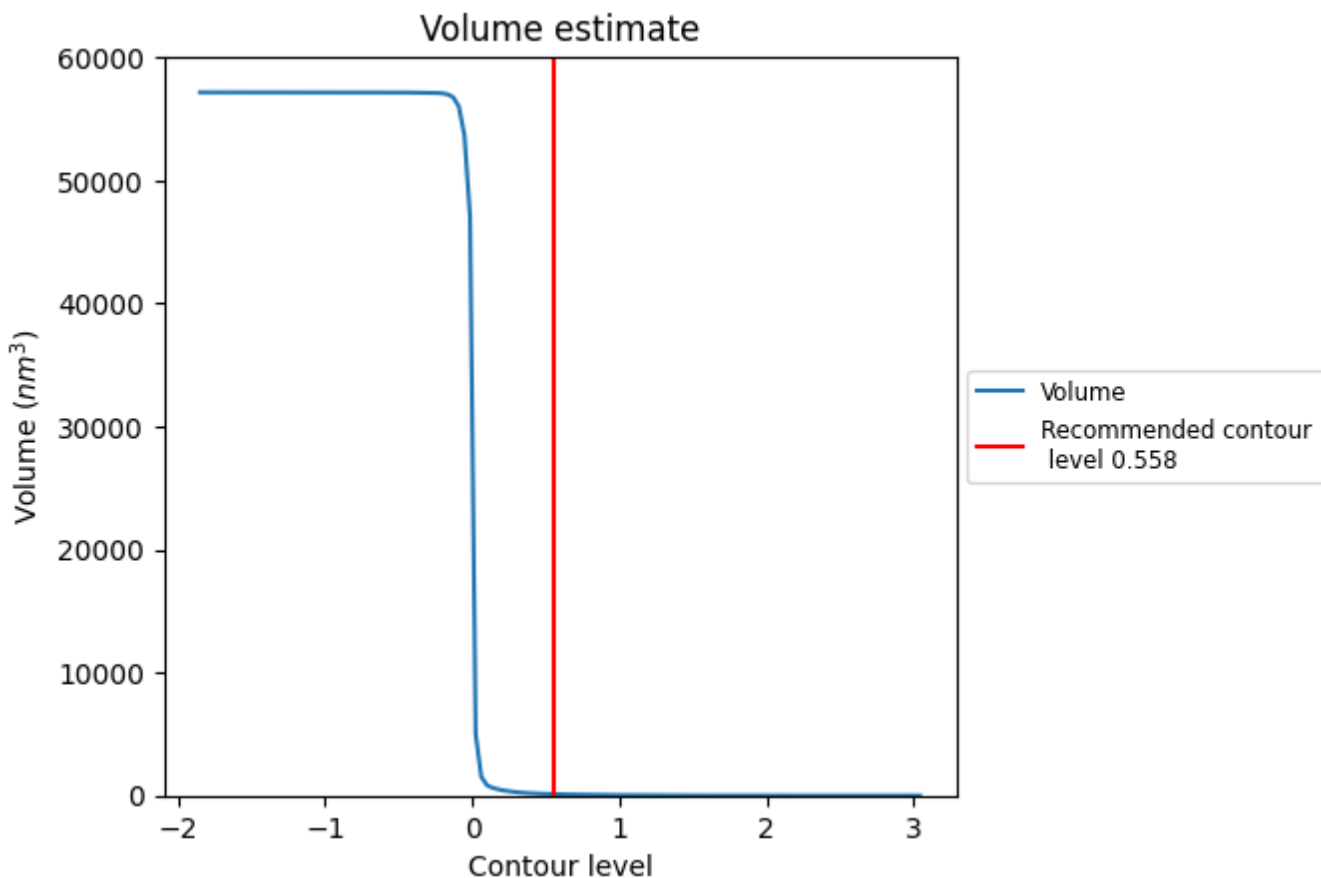
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

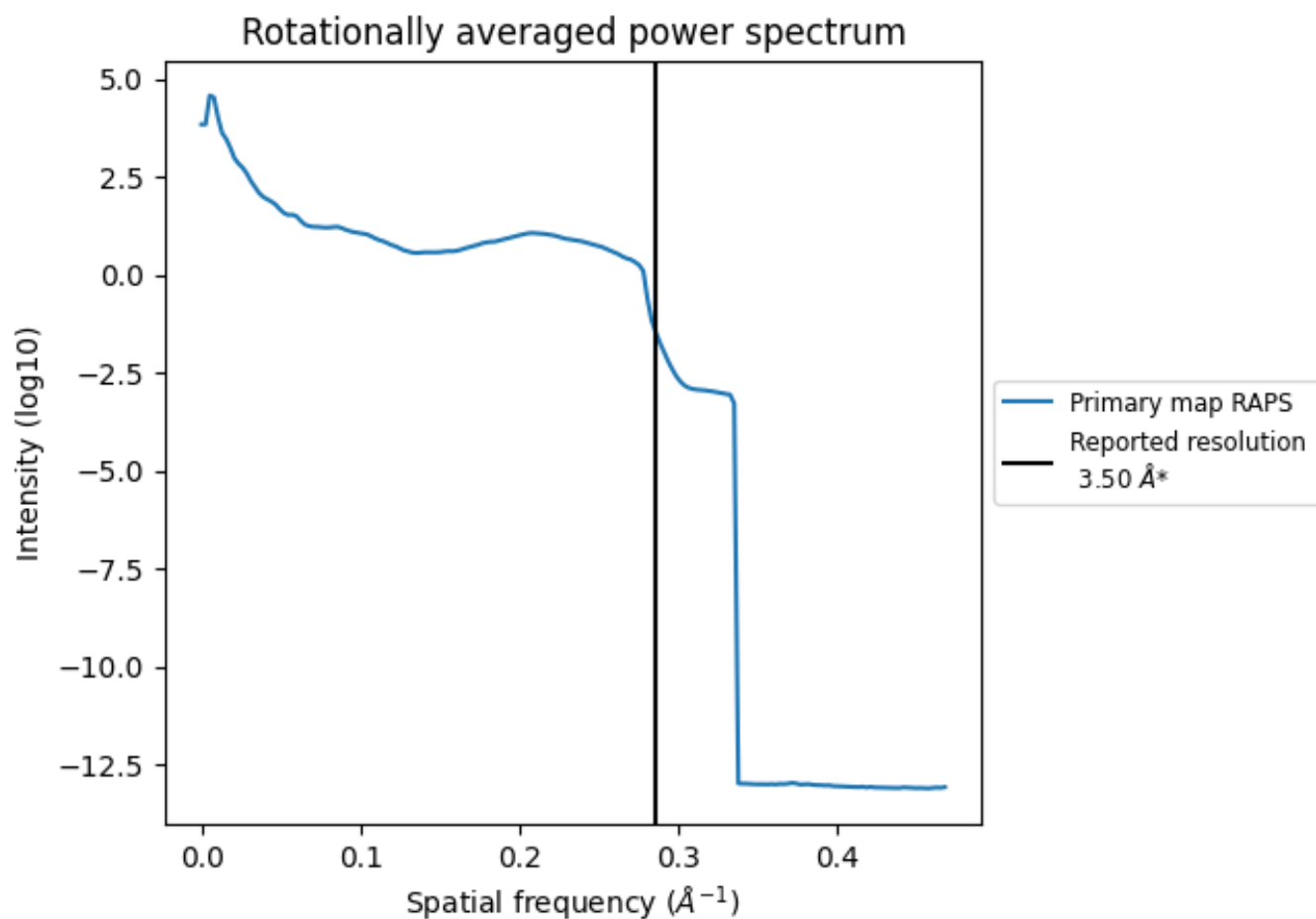
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 115 nm³; this corresponds to an approximate mass of 104 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

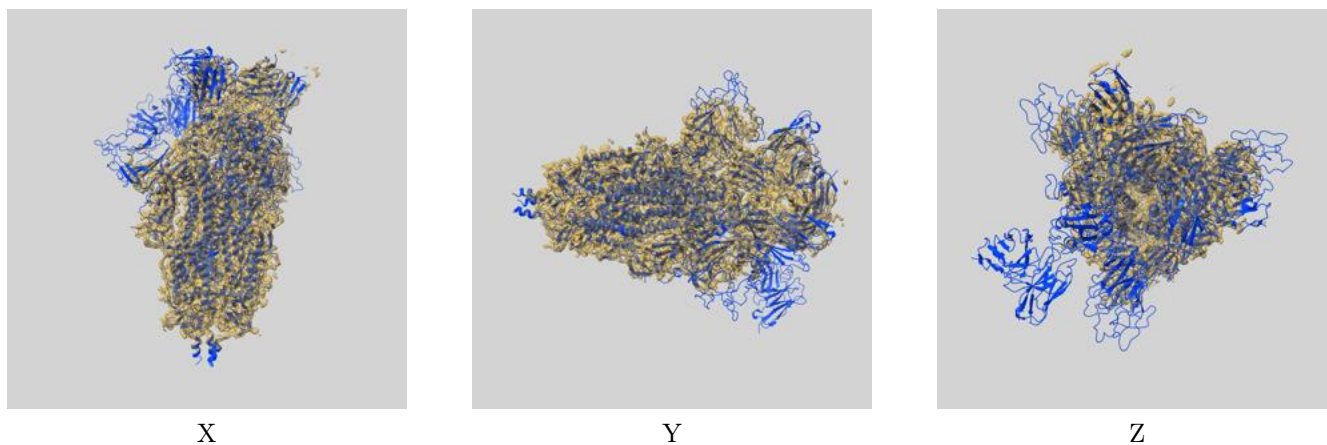
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

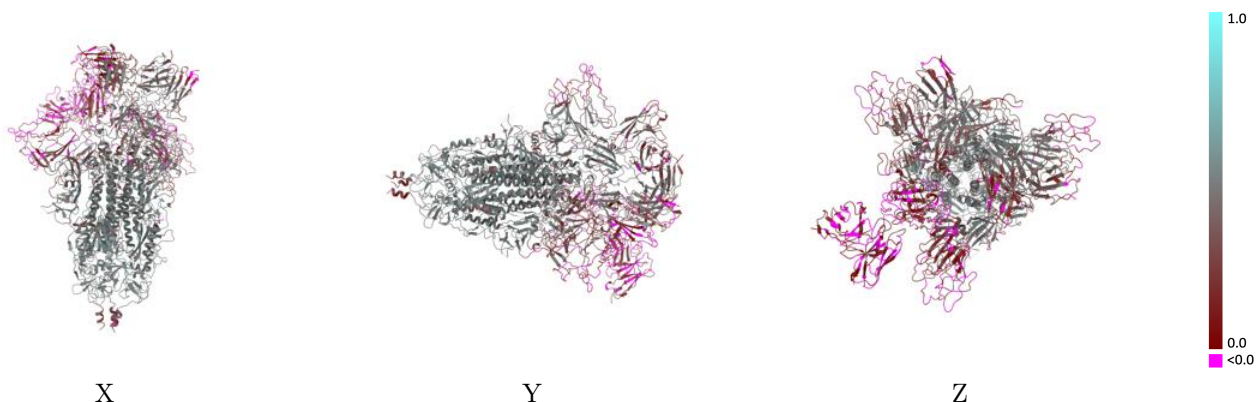
This section contains information regarding the fit between EMDB map EMD-33019 and PDB model 7X6A. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



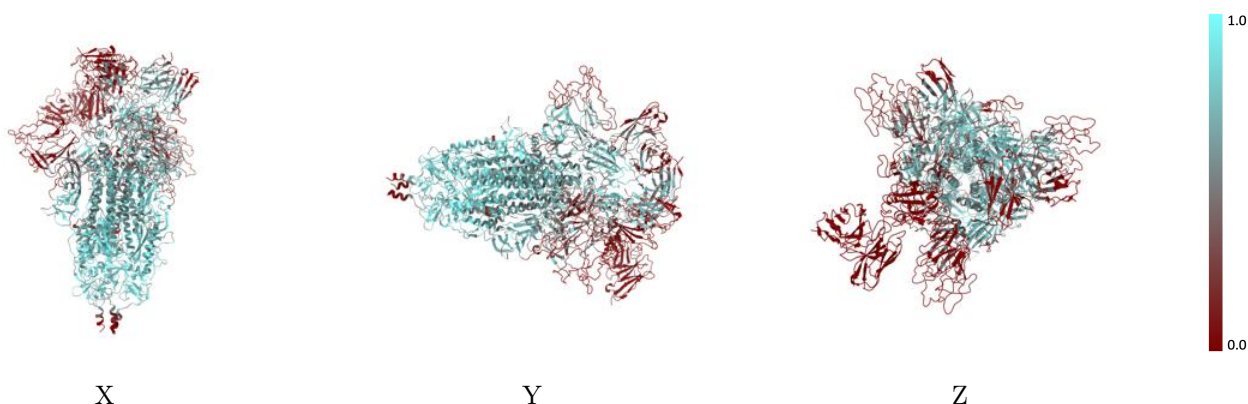
The images above show the 3D surface view of the map at the recommended contour level 0.558 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



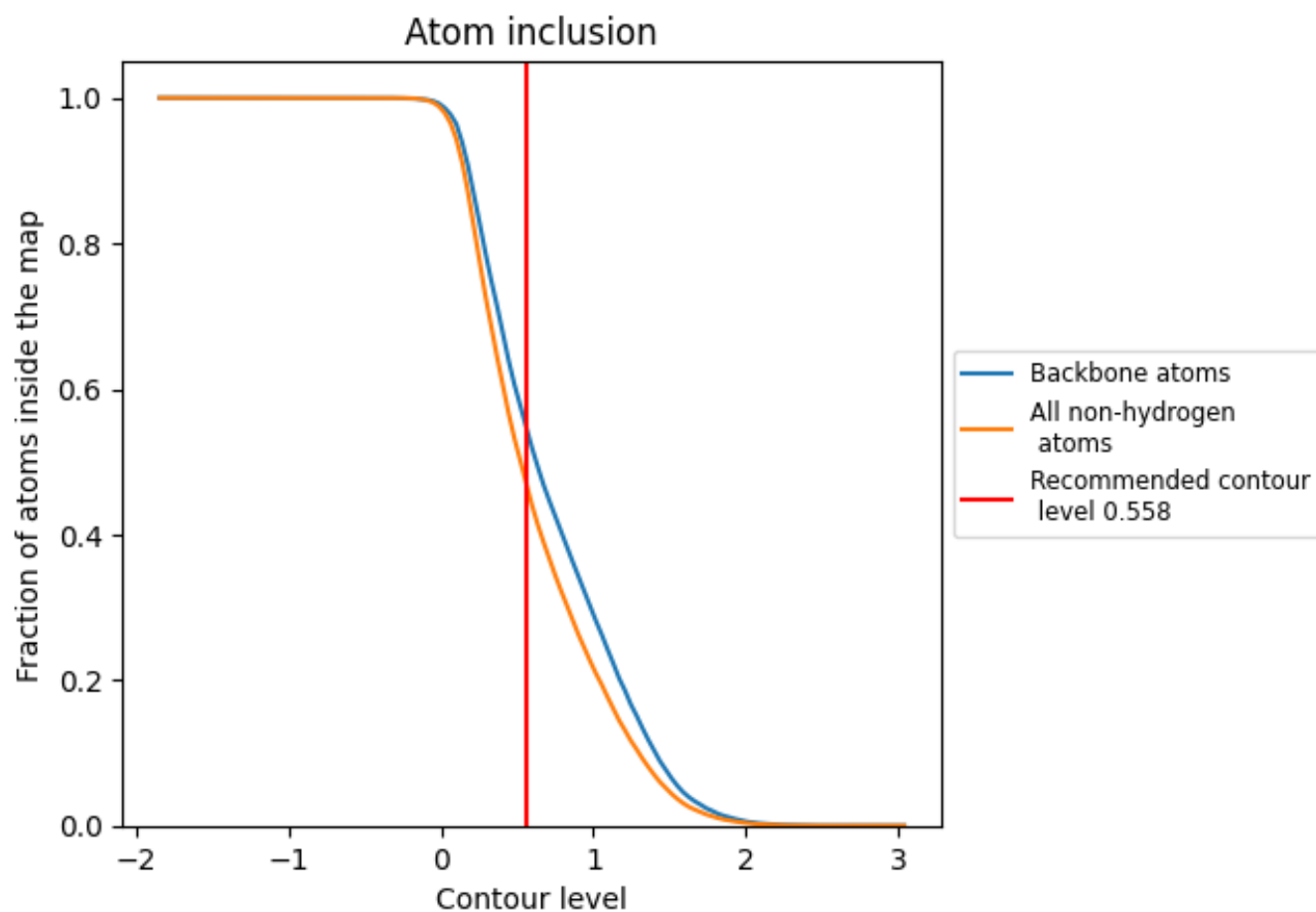
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.558).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.558) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4709	 0.3560
A	 0.5285	 0.3920
B	 0.5961	 0.4180
D	 0.4376	 0.3340
G	 0.0000	 0.0540
H	 0.4685	 0.3850
I	 0.1867	 0.2420
J	 0.0000	 0.0480
K	 0.2864	 0.3250
L	 0.4058	 0.3150

