



## Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 09:54 AM EDT

PDB ID : 7JGJ / pdb\_00007jgj  
EMDB ID : EMD-22328  
Title : IgA1 Protease in complex with neutralizing mAb  
Authors : Eisenmesser, E.Z.; Zheng, H.  
Deposited on : 2020-07-19  
Resolution : 4.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

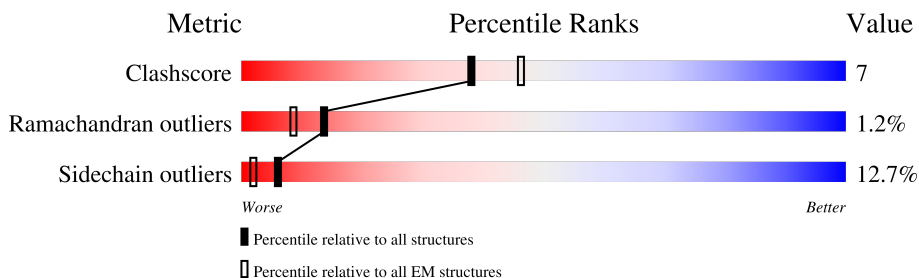
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1290	
2	L	213	
3	H	218	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13324 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 Immunoglobulin A1 protease.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1277	Total	C	N	O	S	0	0
			10070	6352	1711	1989	18		

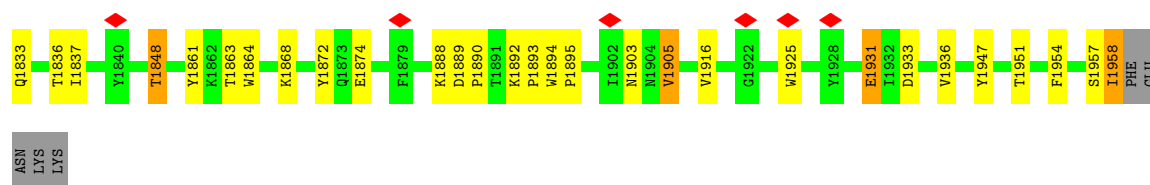
- Molecule 2 is a protein called mAB Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	212	Total	C	N	O	S	0	0
			1626	1014	267	337	8		

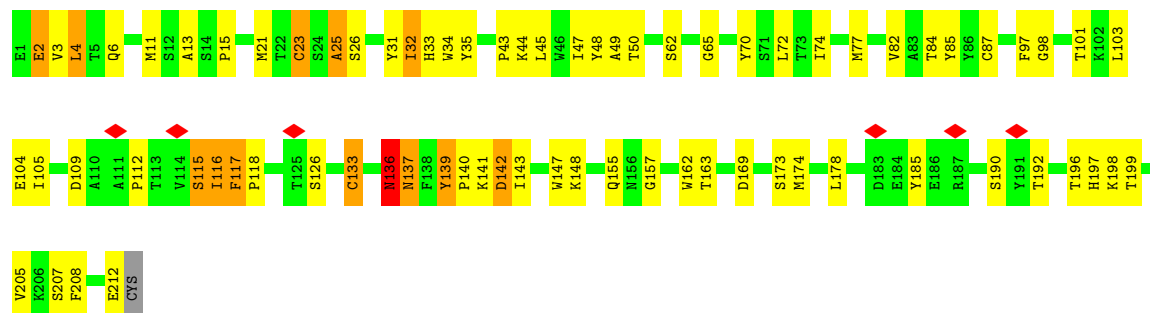
- Molecule 3 is a protein called mAB Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	218	Total	C	N	O	S	0	0
			1628	1027	261	330	10		

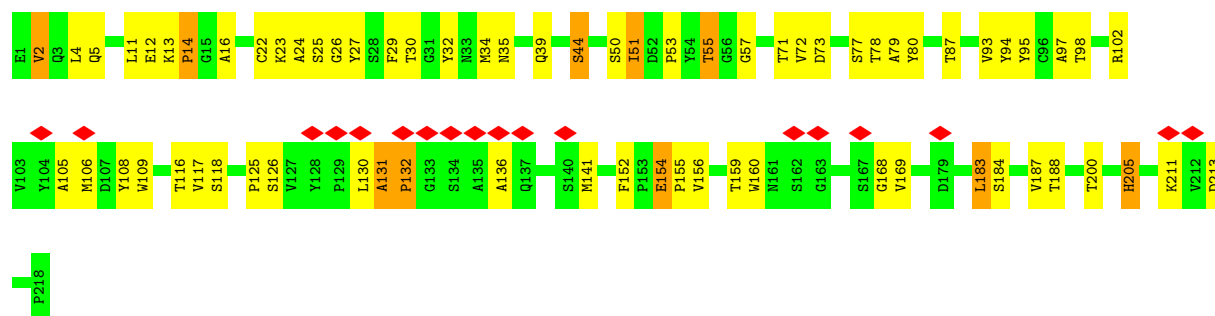




### • Molecule 2: mAB Light Chain



### • Molecule 3: mAB Heavy Chain



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64968	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.512	Depositor
Minimum map value	-0.208	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.136	Depositor
Map size (Å)	269.568, 269.568, 269.568	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	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	0.95	4/10259 (0.0%)	1.65	84/13865 (0.6%)
2	L	1.08	3/1665 (0.2%)	1.63	20/2260 (0.9%)
3	H	1.04	1/1669 (0.1%)	1.49	12/2278 (0.5%)
All	All	0.98	8/13593 (0.1%)	1.63	116/18403 (0.6%)

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	8	4
2	L	4	1
3	H	1	3
All	All	13	8

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	23	CYS	CA-C	-9.68	1.41	1.52
2	L	23	CYS	C-O	9.09	1.35	1.24
2	L	23	CYS	CA-CB	-8.38	1.40	1.53
1	A	1440	TYR	C-O	-6.64	1.16	1.24
1	A	1209	LEU	C-O	-5.41	1.16	1.23
3	H	16	ALA	C-O	-5.31	1.17	1.24
1	A	1688	PHE	C-O	-5.28	1.17	1.24
1	A	1018	THR	CB-OG1	5.06	1.51	1.43

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1392	TYR	CA-C-O	-63.30	53.45	120.55
1	A	1392	TYR	O-C-N	-32.73	87.43	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	118	PRO	CB-CA-C	17.63	132.43	110.92
1	A	1801	GLY	CA-C-N	13.75	139.14	120.44
1	A	1801	GLY	C-N-CA	13.75	139.14	120.44
3	H	132	PRO	N-CA-C	12.71	138.64	112.47
2	L	118	PRO	N-CA-C	11.67	124.94	110.70
1	A	1141	TYR	CB-CA-C	10.53	128.26	110.79
1	A	1440	TYR	CA-C-O	-10.26	109.92	120.90
2	L	133	CYS	N-CA-CB	-10.08	93.02	111.37
1	A	1622	ARG	CB-CA-C	9.73	129.78	110.42
2	L	136	ASN	CB-CA-C	9.13	125.26	109.65
1	A	1392	TYR	CA-C-N	9.09	132.46	120.28
1	A	1392	TYR	C-N-CA	9.09	132.46	120.28
1	A	1215	LEU	CA-C-O	-9.04	110.41	121.89
1	A	1403	ASN	N-CA-C	-8.84	101.64	111.28
2	L	23	CYS	CA-C-O	-8.83	110.75	120.38
1	A	1090	PRO	N-CA-CB	8.82	111.16	103.31
2	L	133	CYS	N-CA-C	8.53	122.98	109.50
1	A	953	THR	N-CA-C	-8.25	99.11	111.81
1	A	1874	GLU	N-CA-C	-7.92	101.61	111.11
1	A	1127	GLU	N-CA-C	-7.91	102.26	112.23
1	A	1186	ASN	N-CA-C	-7.90	103.62	113.18
1	A	1094	PRO	N-CA-CB	7.87	110.20	103.35
1	A	1440	TYR	N-CA-C	-7.84	101.70	111.11
1	A	1465	VAL	N-CA-CB	7.55	121.12	111.83
2	L	23	CYS	CB-CA-C	7.52	122.73	109.72
3	H	94	TYR	CA-C-O	-7.43	112.27	121.78
1	A	1409	GLU	N-CA-C	7.42	119.16	111.14
2	L	133	CYS	CA-C-O	-7.27	112.60	121.11
1	A	777	ASN	N-CA-C	-7.23	103.40	111.28
1	A	1612	GLN	CB-CA-C	7.15	124.65	110.42
1	A	1440	TYR	N-CA-CB	7.04	120.43	109.94
1	A	979	GLN	CB-CA-C	7.00	122.95	112.03
1	A	1465	VAL	CB-CA-C	6.91	120.51	111.53
1	A	1905	VAL	N-CA-CB	6.84	119.84	110.54
2	L	173	SER	N-CA-CB	6.83	120.29	110.45
1	A	1440	TYR	O-C-N	6.82	129.18	122.09
3	H	125	PRO	CB-CA-C	-6.79	102.06	110.95
2	L	112	PRO	N-CA-C	6.78	123.00	111.68
1	A	839	TYR	CA-C-O	-6.59	113.73	120.71
1	A	1688	PHE	CA-C-O	-6.55	111.61	119.27
1	A	1475	GLY	CA-C-O	-6.52	115.71	121.58
1	A	1523	SER	N-CA-C	-6.40	105.22	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1801	GLY	CA-C-O	-6.40	114.16	120.75
1	A	1098	PRO	N-CA-CB	6.32	109.88	103.25
2	L	157	GLY	N-CA-C	-6.29	106.25	115.30
2	L	163	THR	OG1-CB-CG2	6.24	121.79	109.30
1	A	1015	GLY	CA-C-O	-6.21	116.16	122.56
1	A	1872	TYR	CA-C-O	-6.19	113.86	120.42
1	A	1437	ILE	N-CA-C	-6.15	103.20	111.44
3	H	93	VAL	N-CA-C	-6.11	101.12	109.55
1	A	1542	ASP	N-CA-C	-6.10	104.54	112.23
1	A	1394	LYS	N-CA-C	-6.07	104.67	111.28
1	A	1905	VAL	CB-CA-C	6.06	120.33	112.14
3	H	168	GLY	N-CA-C	-6.00	107.94	115.08
1	A	1578	GLY	CA-C-O	-5.96	117.50	122.33
1	A	1792	GLU	N-CA-C	-5.94	105.13	112.38
1	A	1478	ALA	CB-CA-C	5.92	119.78	110.19
3	H	125	PRO	N-CA-C	5.91	120.28	111.41
1	A	1440	TYR	CB-CA-C	-5.86	101.43	110.81
1	A	1006	ARG	N-CA-C	-5.85	104.86	112.23
3	H	205	HIS	CB-CA-C	5.83	116.64	110.17
1	A	942	ASN	N-CA-C	-5.81	105.03	111.71
2	L	115	SER	CA-C-O	-5.81	114.23	121.55
2	L	112	PRO	CB-CA-C	-5.79	102.34	110.63
1	A	1439	VAL	CA-C-O	-5.77	115.05	121.17
1	A	1291	ASP	N-CA-C	-5.74	105.10	111.71
1	A	1465	VAL	N-CA-C	5.73	114.99	106.85
1	A	1428	GLN	CB-CA-C	5.73	120.30	110.79
3	H	154	GLU	CA-C-N	5.71	126.97	119.84
3	H	154	GLU	C-N-CA	5.71	126.97	119.84
3	H	25	SER	CA-C-O	-5.71	115.33	121.38
1	A	1025	ASN	N-CA-C	-5.64	103.54	110.65
1	A	1457	LEU	CA-C-O	-5.63	114.91	120.82
1	A	1576	GLN	N-CA-C	-5.60	105.18	111.28
1	A	778	THR	CB-CA-C	5.50	118.72	109.48
1	A	1403	ASN	CB-CA-C	5.49	119.91	110.79
2	L	139	TYR	CA-C-O	-5.45	115.48	120.50
1	A	732	SER	CA-C-O	-5.42	114.09	120.60
2	L	4	LEU	CB-CA-C	5.42	119.14	109.65
1	A	1698	GLU	CA-C-O	-5.39	115.34	120.90
1	A	979	GLN	CA-C-O	-5.37	116.20	122.37
1	A	1289	ALA	N-CA-C	-5.36	106.32	112.92
1	A	1439	VAL	N-CA-C	-5.35	105.29	110.42
1	A	1187	ASP	N-CA-C	-5.31	106.06	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1379	GLN	N-CA-C	-5.30	105.08	112.45
3	H	130	LEU	CA-C-O	-5.30	114.97	120.70
1	A	1218	PRO	N-CA-C	-5.30	102.87	111.19
1	A	1524	ARG	N-CA-C	-5.27	106.69	113.01
1	A	1734	ALA	O-C-N	-5.27	116.80	123.01
1	A	1704	ASN	CA-C-O	-5.26	115.36	120.89
2	L	105	ILE	CA-C-O	-5.26	116.29	122.13
1	A	1168	ILE	N-CA-C	-5.25	107.72	112.96
1	A	1485	SER	CA-C-O	-5.23	115.43	121.19
1	A	739	ASN	N-CA-C	-5.22	102.38	109.54
1	A	1428	GLN	N-CA-C	-5.22	105.59	111.28
1	A	1626	GLY	N-CA-C	5.20	118.49	112.10
1	A	955	SER	CA-C-O	-5.19	115.88	121.38
1	A	979	GLN	N-CA-C	5.15	117.53	108.56
1	A	1954	PHE	CA-C-O	-5.15	116.18	122.41
1	A	1202	ALA	N-CA-C	-5.14	105.76	112.23
2	L	47	ILE	CA-C-O	-5.14	116.54	121.63
1	A	762	VAL	CA-C-O	-5.10	115.62	121.44
1	A	1490	GLY	CA-C-O	-5.08	116.49	120.91
1	A	1615	TYR	N-CA-C	-5.07	105.76	111.28
1	A	1037	TYR	CB-CA-C	5.04	119.32	109.35
1	A	1328	VAL	N-CA-C	5.04	114.82	107.37
1	A	1522	GLN	N-CA-C	-5.03	107.09	113.23
1	A	1629	PHE	N-CA-C	-5.03	107.14	113.28
1	A	1646	ILE	CA-C-O	-5.03	115.30	121.13
3	H	116	THR	CA-C-O	-5.02	115.57	121.44
1	A	1267	PHE	N-CA-C	-5.02	105.89	111.36
2	L	25	ALA	CA-C-O	-5.01	115.76	121.82
2	L	205	VAL	CA-C-O	-5.01	115.21	120.57
1	A	1685	HIS	O-C-N	5.00	127.22	122.07

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	979	GLN	CA
1	A	1018	THR	CB
1	A	1141	TYR	CA
1	A	1465	VAL	CA
1	A	1478	ALA	CA
1	A	1612	GLN	CA
1	A	1622	ARG	CA
1	A	1905	VAL	CA

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Mol	Chain	Res	Type	Atom
2	L	115	SER	CA
2	L	118	PRO	CA
2	L	136	ASN	CA
2	L	173	SER	CA
3	H	132	PRO	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1358	SER	Mainchain
1	A	1392	TYR	Mainchain
1	A	1627	PRO	Mainchain
1	A	940	GLY	Mainchain
3	H	105	ALA	Peptide
3	H	152	PHE	Peptide
3	H	154	GLU	Peptide
2	L	23	CYS	Mainchain

## 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	10070	0	9821	114	0
2	L	1626	0	1545	42	0
3	H	1628	0	1589	37	0
All	All	13324	0	12955	188	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 (188) 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)
2:L:31:TYR:HB3	2:L:49:ALA:HA	1.47	0.96
3:H:35:ASN:HB3	3:H:97:ALA:HB3	1.49	0.92
3:H:30:THR:HA	3:H:53:PRO:HB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2:VAL:HB	3:H:27:TYR:HB3	1.67	0.77
1:A:978:ILE:O	1:A:1018:THR:HG22	1.86	0.75
1:A:1028:ASN:HA	1:A:1054:PHE:HB2	1.68	0.73
1:A:1916:VAL:HG12	1:A:1936:VAL:HG12	1.71	0.73
3:H:34:MET:HB3	3:H:51:ILE:HG23	1.71	0.73
3:H:156:VAL:HG21	3:H:183:LEU:HD21	1.75	0.68
3:H:13:LYS:HA	3:H:118:SER:O	1.96	0.65
2:L:2:GLU:HA	2:L:26:SER:OG	1.97	0.65
1:A:1247:ARG:HD3	1:A:1254:PRO:HA	1.78	0.64
2:L:34:TRP:CG	2:L:72:LEU:HD12	2.32	0.64
1:A:993:PHE:HB3	3:H:57:GLY:HA3	1.78	0.63
3:H:12:GLU:O	3:H:117:VAL:HA	2.00	0.62
1:A:1161:MET:SD	1:A:1161:MET:N	2.73	0.61
1:A:1504:THR:HG21	1:A:1594:LEU:HA	1.83	0.61
1:A:688:ILE:HG23	1:A:718:VAL:HG12	1.82	0.60
1:A:1532:LEU:HD13	1:A:1534:TYR:CD2	2.35	0.60
1:A:905:ALA:HB2	1:A:935:VAL:HG21	1.84	0.60
1:A:993:PHE:HA	3:H:55:THR:HB	1.84	0.60
1:A:997:ALA:HB3	1:A:1000:ALA:O	2.01	0.60
2:L:33:HIS:HA	2:L:48:TYR:HA	1.84	0.59
3:H:11:LEU:HD11	3:H:118:SER:HB3	1.82	0.59
1:A:780:PHE:HB3	1:A:801:ALA:HB2	1.83	0.59
1:A:1466:PHE:CE1	1:A:1594:LEU:HD13	2.36	0.59
1:A:1804:ILE:HD11	1:A:1864:TRP:CE3	2.38	0.58
3:H:27:TYR:CZ	3:H:29:PHE:HA	2.39	0.58
3:H:5:GLN:HB2	3:H:23:LYS:HB2	1.86	0.58
1:A:1304:LYS:HD2	1:A:1305:ASN:N	2.19	0.57
2:L:3:VAL:O	2:L:25:ALA:HA	2.04	0.57
2:L:117:PHE:CZ	3:H:131:ALA:HB3	2.40	0.57
1:A:690:LEU:HD11	1:A:730:VAL:HG11	1.86	0.57
1:A:980:ASN:H	1:A:1018:THR:CG2	2.17	0.57
3:H:13:LYS:HD3	3:H:13:LYS:C	2.31	0.56
2:L:15:PRO:HA	2:L:77:MET:HE3	1.86	0.56
2:L:147:TRP:CD2	2:L:178:LEU:HB2	2.41	0.56
1:A:1053:VAL:HB	1:A:1063:VAL:HG22	1.88	0.56
1:A:1501:ALA:HA	1:A:1594:LEU:HD11	1.86	0.56
1:A:958:THR:HB	1:A:994:GLY:HA3	1.87	0.56
1:A:1402:ASN:OD1	1:A:1403:ASN:N	2.39	0.55
1:A:940:GLY:HA3	1:A:943:ALA:HB3	1.87	0.55
3:H:35:ASN:HA	3:H:50:SER:HA	1.87	0.55
2:L:6:GLN:HE22	2:L:85:TYR:C	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:TYR:HE2	3:H:32:TYR:HB2	1.72	0.54
1:A:1308:GLU:CD	1:A:1308:GLU:H	2.14	0.54
2:L:34:TRP:CD2	2:L:72:LEU:HD12	2.42	0.53
1:A:1439:VAL:O	1:A:1440:TYR:C	2.50	0.53
1:A:1304:LYS:HD2	1:A:1304:LYS:C	2.34	0.52
1:A:1688:PHE:O	1:A:1692:TYR:CG	2.63	0.52
1:A:858:SER:C	1:A:859:LEU:HD22	2.34	0.52
1:A:1240:ASP:HB2	1:A:1243:SER:HB2	1.92	0.52
2:L:34:TRP:CE2	2:L:72:LEU:HB2	2.45	0.52
2:L:148:LYS:HB2	2:L:192:THR:HB	1.91	0.52
3:H:156:VAL:HG21	3:H:183:LEU:CD2	2.39	0.51
3:H:12:GLU:O	3:H:118:SER:N	2.43	0.51
1:A:690:LEU:HD12	1:A:714:TYR:HB3	1.93	0.51
1:A:1079:SER:O	1:A:1082:VAL:HG22	2.09	0.51
1:A:1236:LEU:HD12	1:A:1274:LEU:HD13	1.93	0.51
2:L:13:ALA:O	2:L:77:MET:HE2	2.10	0.51
1:A:746:ILE:HD12	1:A:747:THR:N	2.25	0.51
1:A:1031:ALA:HB3	1:A:1069:PHE:HB3	1.91	0.51
1:A:1957:SER:O	1:A:1958:ILE:C	2.53	0.50
2:L:35:TYR:CE2	2:L:43:PRO:HB2	2.45	0.50
1:A:1003:LEU:HD13	1:A:1014:ALA:HB1	1.94	0.50
1:A:1779:ILE:HG21	1:A:1806:TYR:CE2	2.46	0.50
1:A:980:ASN:H	1:A:1018:THR:HG22	1.76	0.50
2:L:140:PRO:O	2:L:141:LYS:C	2.55	0.50
2:L:136:ASN:O	2:L:137:ASN:C	2.53	0.50
3:H:11:LEU:HD11	3:H:118:SER:CB	2.42	0.50
1:A:1386:PHE:HE1	1:A:1454:VAL:HG11	1.76	0.50
3:H:13:LYS:HD3	3:H:14:PRO:N	2.26	0.49
1:A:951:THR:O	1:A:952:VAL:HG13	2.12	0.49
1:A:1730:ASN:HD22	1:A:1837:ILE:HG13	1.76	0.49
2:L:141:LYS:HD2	2:L:142:ASP:N	2.27	0.49
3:H:27:TYR:CE2	3:H:32:TYR:HB2	2.48	0.49
1:A:1263:LEU:O	1:A:1267:PHE:N	2.45	0.49
2:L:34:TRP:CZ2	2:L:87:CYS:HB3	2.48	0.49
2:L:117:PHE:CE1	3:H:131:ALA:HB3	2.48	0.49
1:A:1058:LEU:O	1:A:1059:GLU:C	2.56	0.48
2:L:4:LEU:CB	2:L:98:GLY:HA2	2.43	0.48
3:H:39:GLN:CD	3:H:95:TYR:HD2	2.22	0.48
3:H:160:TRP:CD1	3:H:169:VAL:HG21	2.49	0.48
2:L:141:LYS:C	2:L:141:LYS:HD2	2.39	0.48
1:A:992:HIS:HB2	1:A:1054:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ALA:HB2	1:A:838:ILE:HG22	1.96	0.47
1:A:1500:ASN:O	1:A:1504:THR:HG23	2.15	0.47
2:L:77:MET:SD	2:L:103:LEU:HD21	2.55	0.47
1:A:1236:LEU:CD1	1:A:1274:LEU:HD13	2.45	0.47
1:A:1372:TYR:CE2	1:A:1385:LEU:HA	2.49	0.47
2:L:35:TYR:CZ	2:L:43:PRO:HB2	2.49	0.47
2:L:34:TRP:CE2	2:L:87:CYS:HB3	2.50	0.47
3:H:71:THR:OG1	3:H:80:TYR:HB2	2.15	0.47
1:A:1386:PHE:CE1	1:A:1454:VAL:HG11	2.49	0.46
2:L:34:TRP:CZ2	2:L:72:LEU:HB2	2.50	0.46
2:L:162:TRP:HA	2:L:174:MET:SD	2.55	0.46
1:A:859:LEU:HD22	1:A:859:LEU:N	2.30	0.46
2:L:141:LYS:O	2:L:142:ASP:C	2.58	0.46
3:H:98:THR:HB	3:H:108:TYR:H	1.81	0.46
1:A:980:ASN:N	1:A:1018:THR:CG2	2.78	0.46
1:A:1021:LEU:HD23	1:A:1022:SER:N	2.31	0.46
3:H:24:ALA:HB1	3:H:27:TYR:HE1	1.80	0.46
1:A:809:VAL:HG13	1:A:811:LEU:HD22	1.97	0.46
3:H:72:VAL:HA	3:H:79:ALA:HA	1.98	0.46
1:A:916:LYS:HA	1:A:951:THR:O	2.15	0.46
2:L:4:LEU:HB2	2:L:98:GLY:HA2	1.97	0.46
1:A:690:LEU:HD11	1:A:730:VAL:CG1	2.46	0.46
2:L:109:ASP:CB	2:L:199:THR:HG22	2.46	0.45
1:A:898:VAL:HG11	1:A:919:ILE:HG21	1.98	0.45
1:A:1000:ALA:HB1	1:A:1003:LEU:HD23	1.98	0.45
2:L:32:ILE:HG22	2:L:50:THR:HA	1.99	0.45
2:L:116:ILE:O	2:L:116:ILE:HG23	2.16	0.45
1:A:1403:ASN:O	1:A:1407:LYS:HG3	2.16	0.45
3:H:132:PRO:CB	3:H:136:ALA:HB3	2.47	0.45
1:A:1591:TYR:CG	1:A:1601:THR:HG21	2.52	0.45
1:A:868:ASN:HA	1:A:896:ARG:HE	1.81	0.45
1:A:937:HIS:HA	1:A:971:LEU:HB3	1.99	0.45
1:A:955:SER:O	1:A:956:SER:HB3	2.16	0.45
1:A:1010:GLU:C	1:A:1012:LYS:N	2.73	0.45
1:A:1161:MET:HA	1:A:1167:VAL:HG12	1.99	0.45
1:A:1397:LEU:N	1:A:1397:LEU:HD12	2.32	0.45
1:A:966:GLY:HA3	1:A:970:GLY:CA	2.46	0.44
1:A:1482:TYR:CD1	1:A:1482:TYR:N	2.84	0.44
1:A:1236:LEU:HD13	1:A:1274:LEU:HD22	2.00	0.44
2:L:45:LEU:HD21	2:L:48:TYR:HB3	1.98	0.44
1:A:966:GLY:HA3	1:A:970:GLY:HA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:LEU:H	1:A:1258:LEU:HD12	1.83	0.44
1:A:884:LYS:O	1:A:885:GLN:C	2.60	0.44
1:A:966:GLY:O	1:A:968:LEU:N	2.50	0.44
1:A:1734:ALA:HB3	1:A:1796:PRO:HA	2.00	0.44
1:A:1893:PRO:O	1:A:1894:TRP:C	2.61	0.44
1:A:1466:PHE:CZ	1:A:1477:GLY:HA3	2.53	0.44
1:A:980:ASN:OD1	1:A:1018:THR:HG23	2.18	0.43
2:L:192:THR:HG23	2:L:207:SER:OG	2.17	0.43
1:A:898:VAL:O	1:A:931:ILE:HA	2.18	0.43
1:A:1055:ASN:HA	1:A:1063:VAL:HA	2.00	0.43
1:A:1532:LEU:C	1:A:1532:LEU:HD12	2.43	0.43
3:H:73:ASP:HB2	3:H:80:TYR:HE1	1.83	0.43
1:A:859:LEU:HD23	1:A:888:VAL:HG22	1.99	0.43
1:A:979:GLN:CB	1:A:1018:THR:HG21	2.48	0.43
1:A:1536:ALA:HB1	1:A:1538:LYS:HD2	2.01	0.43
2:L:212:GLU:N	2:L:212:GLU:OE1	2.52	0.43
1:A:1561:MET:SD	1:A:1561:MET:C	3.02	0.43
3:H:102:ARG:O	3:H:102:ARG:HG2	2.18	0.43
1:A:1621:ARG:O	1:A:1622:ARG:C	2.61	0.43
2:L:72:LEU:HD22	2:L:74:ILE:HD11	2.00	0.43
3:H:131:ALA:HB1	3:H:132:PRO:CD	2.48	0.43
1:A:1718:ILE:HD12	1:A:1737:VAL:O	2.19	0.43
1:A:1699:GLY:O	1:A:1703:VAL:HG22	2.19	0.42
3:H:12:GLU:N	3:H:12:GLU:OE1	2.52	0.42
1:A:747:THR:HA	1:A:766:THR:HA	2.01	0.42
1:A:1011:GLU:OE1	1:A:1039:GLY:HA3	2.19	0.42
1:A:862:VAL:HG22	1:A:890:GLY:HA3	2.01	0.42
1:A:1031:ALA:HB2	1:A:1052:ARG:HG2	1.99	0.42
1:A:1263:LEU:HD12	1:A:1315:THR:HG22	2.00	0.42
2:L:139:TYR:CG	2:L:140:PRO:HA	2.54	0.42
1:A:1003:LEU:HD22	1:A:1003:LEU:HA	1.84	0.42
1:A:1688:PHE:O	1:A:1692:TYR:CD2	2.72	0.42
1:A:1404:ASP:HA	1:A:1407:LYS:HE2	2.02	0.42
1:A:1894:TRP:HB3	1:A:1895:PRO:HD3	2.01	0.42
1:A:1056:VAL:HG22	1:A:1062:GLU:O	2.20	0.41
2:L:4:LEU:HD12	2:L:97:PHE:C	2.45	0.41
1:A:971:LEU:HD13	1:A:1002:TYR:HB3	2.02	0.41
1:A:1403:ASN:OD1	1:A:1440:TYR:CB	2.69	0.41
1:A:1611:ASP:O	1:A:1612:GLN:C	2.63	0.41
1:A:1693:MET:SD	1:A:1697:LEU:HD12	2.60	0.41
2:L:43:PRO:HD2	3:H:109:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:4:LEU:HB3	3:H:22:CYS:SG	2.61	0.41
1:A:826:ARG:NH1	1:A:850:SER:O	2.53	0.41
1:A:884:LYS:O	1:A:886:VAL:HG13	2.21	0.41
3:H:29:PHE:CD2	3:H:77:SER:HA	2.56	0.41
1:A:1122:VAL:CG1	1:A:1145:VAL:HG21	2.51	0.41
1:A:1414:ILE:HG21	1:A:1439:VAL:HG21	2.02	0.41
1:A:707:ILE:O	1:A:708:PRO:C	2.63	0.41
1:A:895:GLU:HA	1:A:923:TYR:CD1	2.56	0.41
1:A:1010:GLU:O	1:A:1011:GLU:C	2.63	0.41
1:A:1042:VAL:O	1:A:1043:ALA:HB3	2.21	0.41
1:A:1947:TYR:CZ	1:A:1951:THR:HG21	2.56	0.41
2:L:148:LYS:CB	2:L:192:THR:HB	2.49	0.41
2:L:169:ASP:OD1	2:L:169:ASP:C	2.62	0.41
1:A:992:HIS:HA	1:A:1028:ASN:HB3	2.03	0.40
1:A:1536:ALA:HB1	1:A:1538:LYS:CD	2.52	0.40
2:L:65:GLY:HA3	2:L:70:TYR:CD2	2.56	0.40
1:A:1112:ILE:HG21	1:A:1139:VAL:HG21	2.03	0.40
1:A:1794:GLY:HA2	1:A:1848:THR:HA	2.04	0.40
3:H:23:LYS:HD3	3:H:78:THR:OG1	2.22	0.40
2:L:133:CYS:SG	2:L:147:TRP:CZ2	3.15	0.40
1:A:846:PHE:CG	1:A:849:LEU:HD21	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1273/1290 (99%)	1163 (91%)	99 (8%)	11 (1%)	14	50
2	L	210/213 (99%)	196 (93%)	10 (5%)	4 (2%)	6	32
3	H	216/218 (99%)	197 (91%)	13 (6%)	6 (3%)	4	24
All	All	1699/1721 (99%)	1556 (92%)	122 (7%)	21 (1%)	14	44



All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	840	ASN
2	L	116	ILE
3	H	44	SER
1	A	1438	GLY
1	A	1574	HIS
2	L	137	ASN
3	H	26	GLY
1	A	967	GLY
1	A	1612	GLN
1	A	969	ALA
1	A	1622	ARG
1	A	1890	PRO
1	A	1931	GLU
2	L	142	ASP
1	A	1796	PRO
1	A	1059	GLU
3	H	14	PRO
3	H	155	PRO
3	H	187	VAL
3	H	131	ALA
2	L	82	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1078/1112 (97%)	931 (86%)	147 (14%)	3	14
2	L	186/187 (100%)	165 (89%)	21 (11%)	4	18
3	H	187/187 (100%)	171 (91%)	16 (9%)	8	27
All	All	1451/1486 (98%)	1267 (87%)	184 (13%)	6	15

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	679	LYS
1	A	699	ARG
1	A	708	PRO
1	A	713	THR
1	A	718	VAL
1	A	726	VAL
1	A	727	TYR
1	A	734	THR
1	A	737	LYS
1	A	739	ASN
1	A	742	SER
1	A	746	ILE
1	A	747	THR
1	A	760	LYS
1	A	766	THR
1	A	768	TYR
1	A	778	THR
1	A	824	THR
1	A	834	LYS
1	A	835	ASN
1	A	838	ILE
1	A	847	GLU
1	A	848	ASN
1	A	854	VAL
1	A	855	GLU
1	A	859	LEU
1	A	889	ASP
1	A	896	ARG
1	A	904	LYS
1	A	914	SER
1	A	920	VAL
1	A	925	THR
1	A	926	THR
1	A	930	ASN
1	A	939	THR
1	A	952	VAL
1	A	955	SER
1	A	963	GLN
1	A	964	THR
1	A	971	LEU
1	A	972	VAL
1	A	977	HIS
1	A	980	ASN

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Mol	Chain	Res	Type
1	A	993	PHE
1	A	996	VAL
1	A	1003	LEU
1	A	1005	ASP
1	A	1016	GLU
1	A	1020	VAL
1	A	1038	THR
1	A	1042	VAL
1	A	1048	SER
1	A	1053	VAL
1	A	1060	LYS
1	A	1063	VAL
1	A	1064	VAL
1	A	1074	THR
1	A	1109	PHE
1	A	1126	ILE
1	A	1127	GLU
1	A	1141	TYR
1	A	1157	LEU
1	A	1166	GLN
1	A	1168	ILE
1	A	1177	THR
1	A	1198	GLN
1	A	1201	PHE
1	A	1204	LEU
1	A	1206	GLU
1	A	1208	ASN
1	A	1209	LEU
1	A	1238	LYS
1	A	1246	ILE
1	A	1252	ILE
1	A	1263	LEU
1	A	1274	LEU
1	A	1277	SER
1	A	1279	LYS
1	A	1282	LEU
1	A	1285	ASP
1	A	1302	LYS
1	A	1306	ASN
1	A	1308	GLU
1	A	1330	VAL
1	A	1353	ILE

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Mol	Chain	Res	Type
1	A	1369	VAL
1	A	1374	ILE
1	A	1388	THR
1	A	1399	ASN
1	A	1401	SER
1	A	1414	ILE
1	A	1415	VAL
1	A	1423	GLU
1	A	1434	LYS
1	A	1458	LEU
1	A	1465	VAL
1	A	1469	SER
1	A	1473	SER
1	A	1486	ASP
1	A	1496	PHE
1	A	1508	GLN
1	A	1525	GLU
1	A	1527	LEU
1	A	1535	ASP
1	A	1561	MET
1	A	1574	HIS
1	A	1592	ARG
1	A	1593	MET
1	A	1594	LEU
1	A	1597	ASP
1	A	1602	TYR
1	A	1606	MET
1	A	1610	SER
1	A	1619	TYR
1	A	1622	ARG
1	A	1629	PHE
1	A	1630	PHE
1	A	1632	LYS
1	A	1645	THR
1	A	1647	THR
1	A	1668	LEU
1	A	1671	THR
1	A	1687	MET
1	A	1707	SER
1	A	1737	VAL
1	A	1741	LEU
1	A	1749	LEU

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Mol	Chain	Res	Type
1	A	1761	LEU
1	A	1789	LEU
1	A	1798	ASP
1	A	1812	LYS
1	A	1818	MET
1	A	1833	GLN
1	A	1836	THR
1	A	1848	THR
1	A	1861	TYR
1	A	1863	THR
1	A	1868	LYS
1	A	1888	LYS
1	A	1889	ASP
1	A	1892	LYS
1	A	1903	ASN
1	A	1905	VAL
1	A	1925	TRP
1	A	1931	GLU
1	A	1933	ASP
1	A	1958	ILE
2	L	2	GLU
2	L	11	MET
2	L	21	MET
2	L	32	ILE
2	L	44	LYS
2	L	62	SER
2	L	84	THR
2	L	101	THR
2	L	104	GLU
2	L	115	SER
2	L	117	PHE
2	L	126	SER
2	L	136	ASN
2	L	143	ILE
2	L	155	GLN
2	L	185	TYR
2	L	190	SER
2	L	196	THR
2	L	197	HIS
2	L	198	LYS
2	L	208	PHE
3	H	2	VAL

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Mol	Chain	Res	Type
3	H	44	SER
3	H	51	ILE
3	H	55	THR
3	H	87	THR
3	H	106	MET
3	H	126	SER
3	H	141	MET
3	H	159	THR
3	H	183	LEU
3	H	184	SER
3	H	188	THR
3	H	200	THR
3	H	205	HIS
3	H	211	LYS
3	H	213	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	701	HIS
1	A	779	ASN
1	A	793	ASN
1	A	799	HIS
1	A	868	ASN
1	A	921	ASN
1	A	937	HIS
1	A	974	GLN
1	A	977	HIS
1	A	1114	HIS
1	A	1176	GLN
1	A	1266	GLN
1	A	1362	ASN
1	A	1379	GLN
1	A	1563	ASN
1	A	1686	ASN
1	A	1710	GLN
1	A	1873	GLN
2	L	36	GLN
2	L	144	ASN
2	L	155	GLN
2	L	156	ASN
3	H	62	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](#)

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.

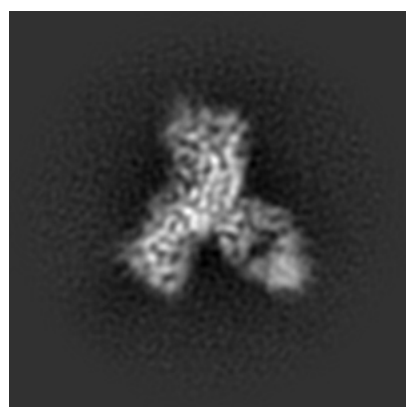
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22328. These allow visual inspection of the internal detail of the map and identification of artifacts.

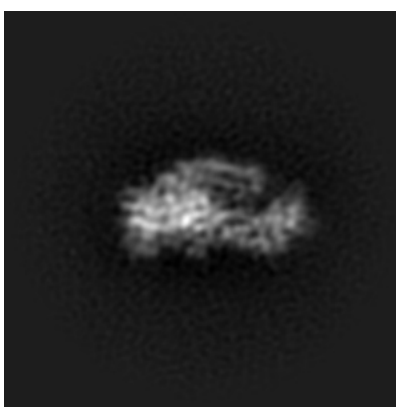
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

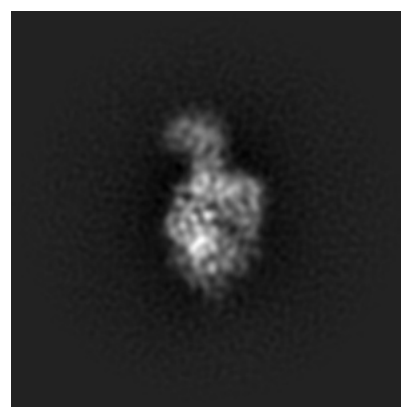
#### 6.1.1 Primary map



X



Y

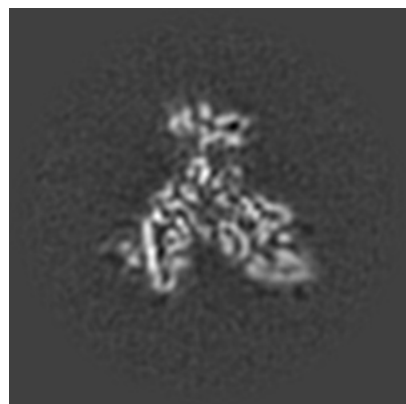


Z

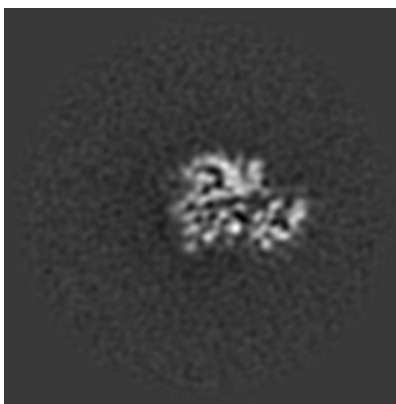
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

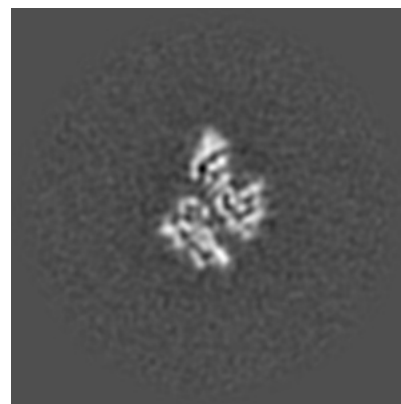
#### 6.2.1 Primary map



X Index: 162



Y Index: 162



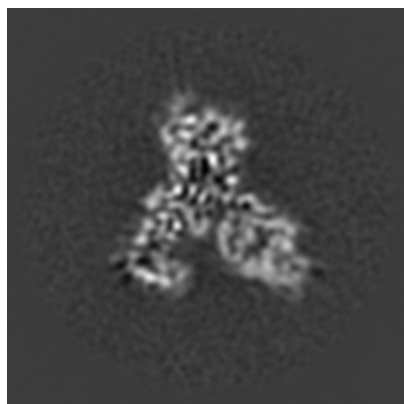
Z Index: 162



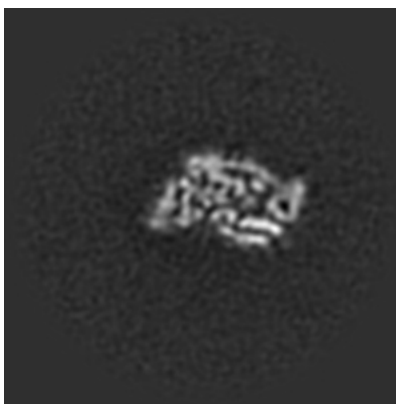
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

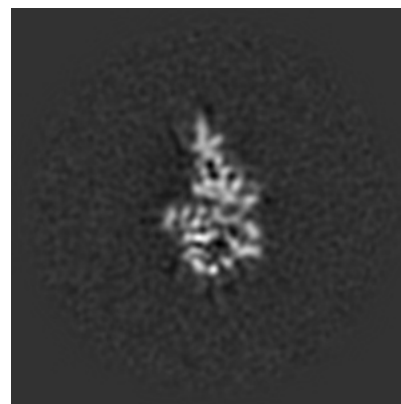
### 6.3.1 Primary map



X Index: 153



Y Index: 179

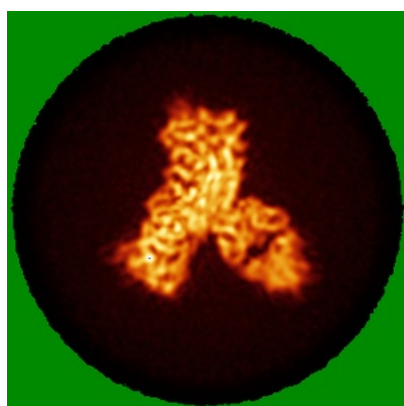


Z Index: 147

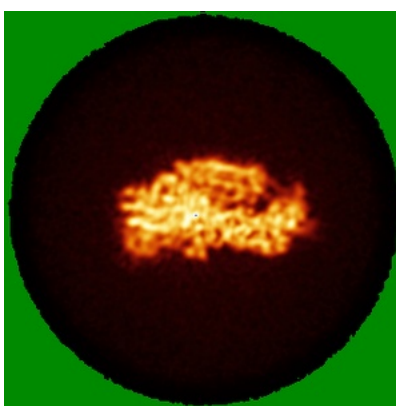
The images above show the largest variance slices of the map in three orthogonal directions.

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

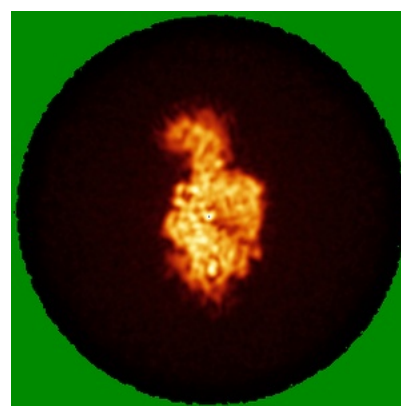
### 6.4.1 Primary map



X



Y

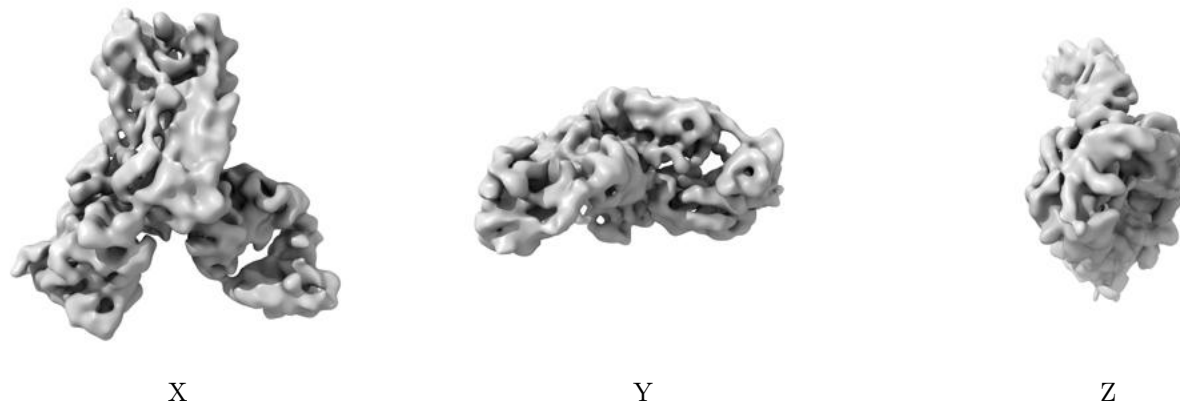


Z

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

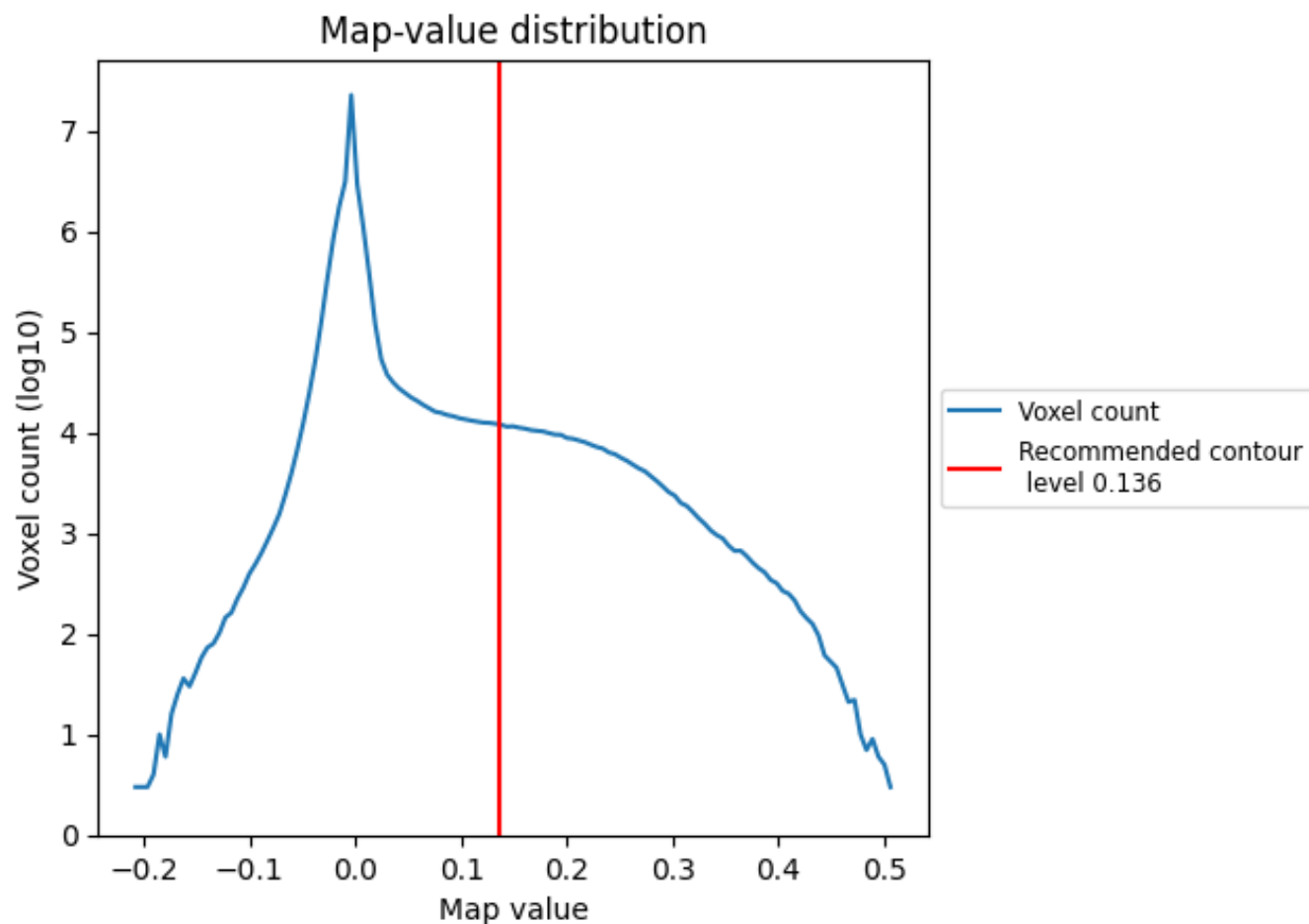
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

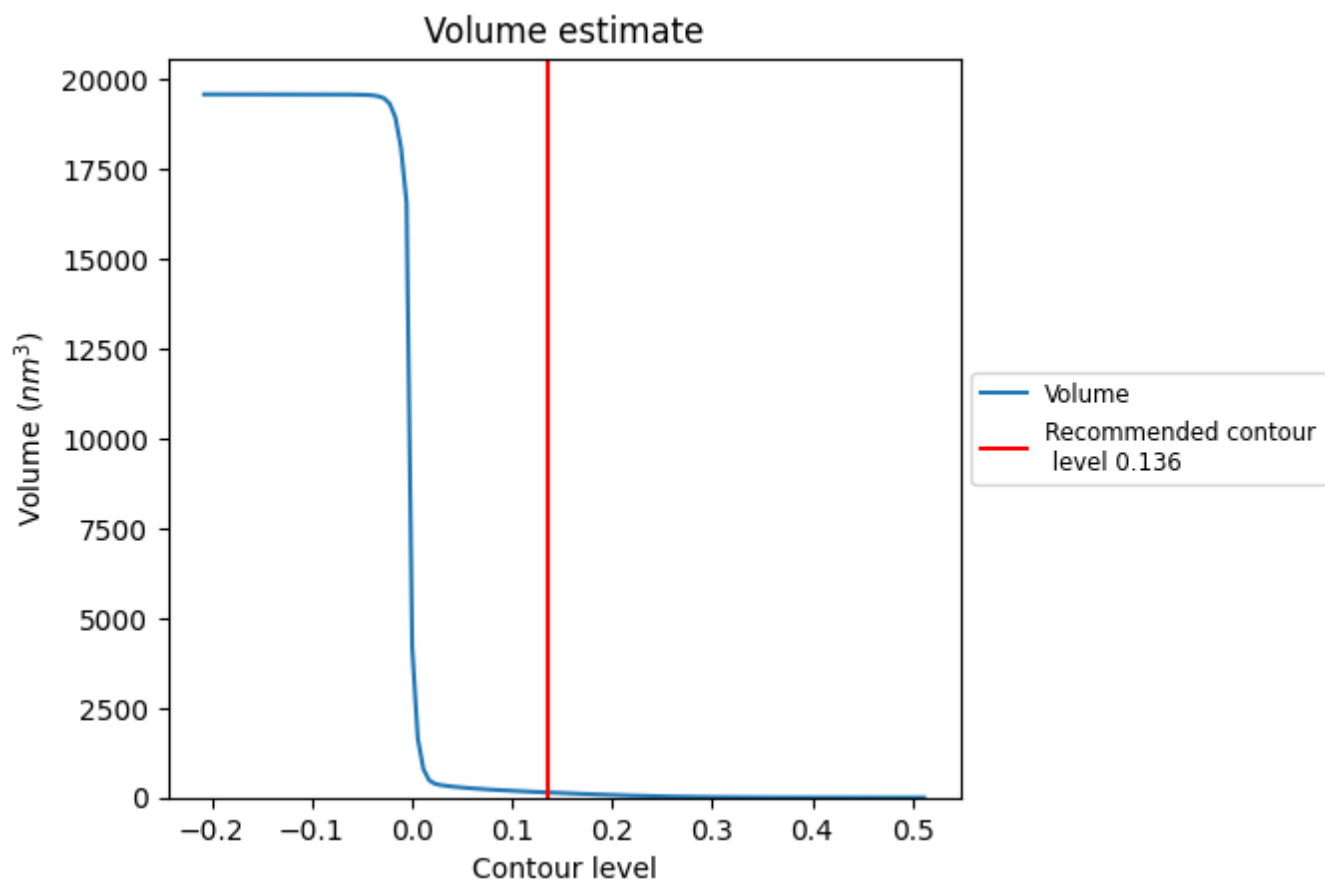
This section contains the results of statistical analysis of the map.

### 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.

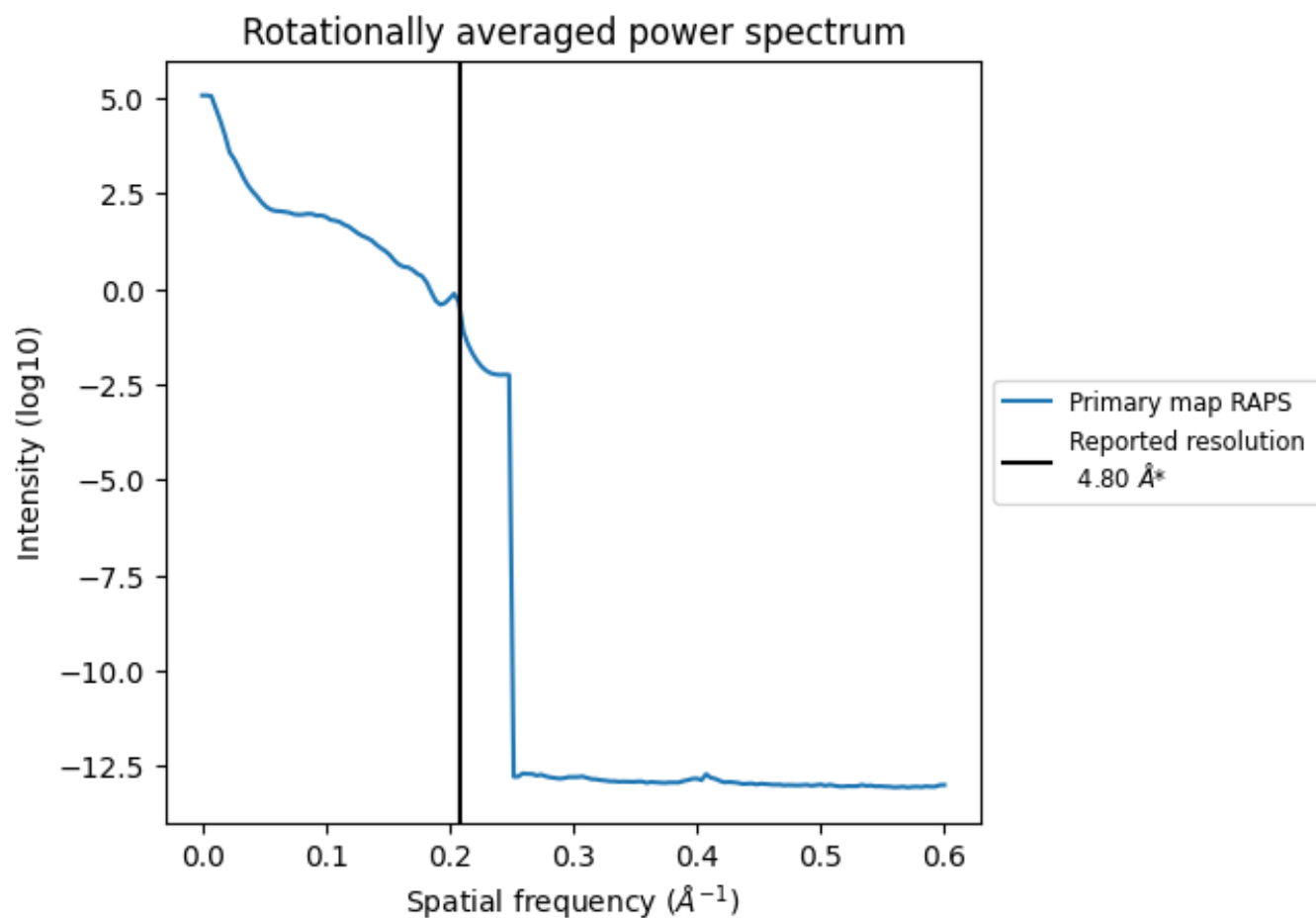
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm<sup>3</sup>; this corresponds to an approximate mass of 128 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 0.208  $\text{\AA}^{-1}$

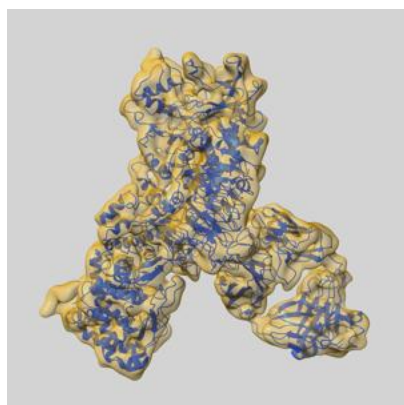
## 8 Fourier-Shell correlation ⓘ

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

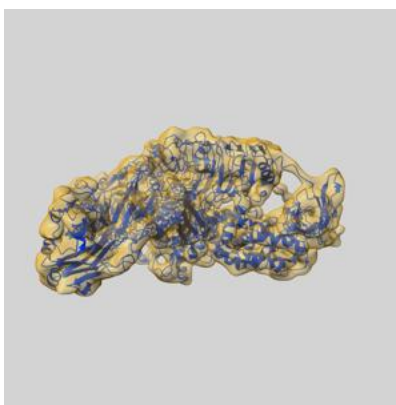
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22328 and PDB model 7JGJ. Per-residue inclusion information can be found in section [3](#) on page [4](#).

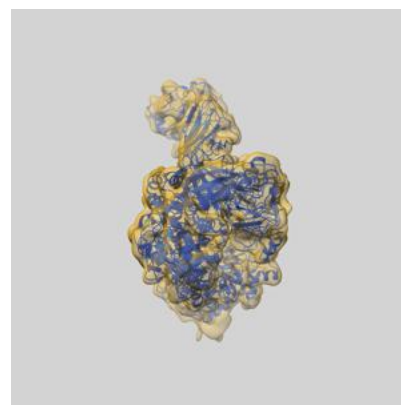
### 9.1 Map-model overlay [i](#)



X



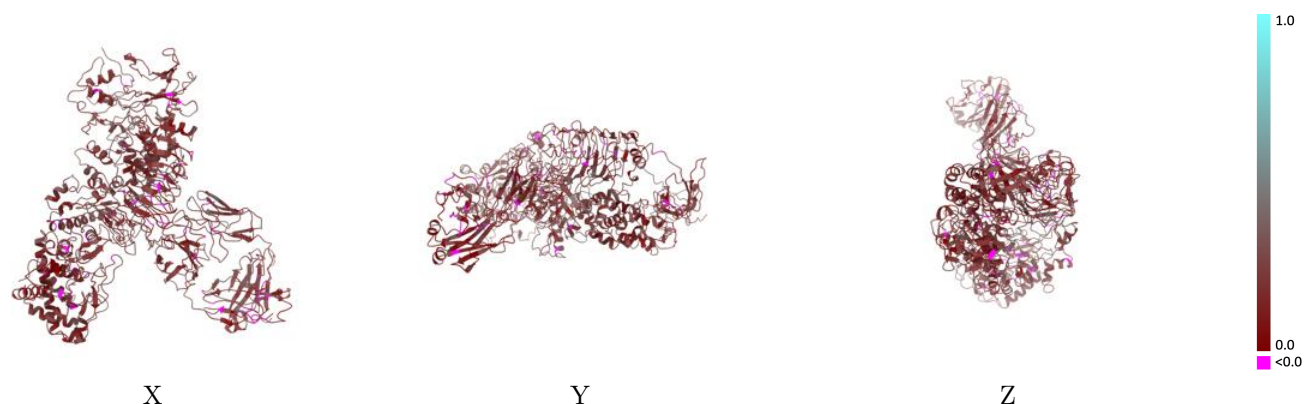
Y



Z

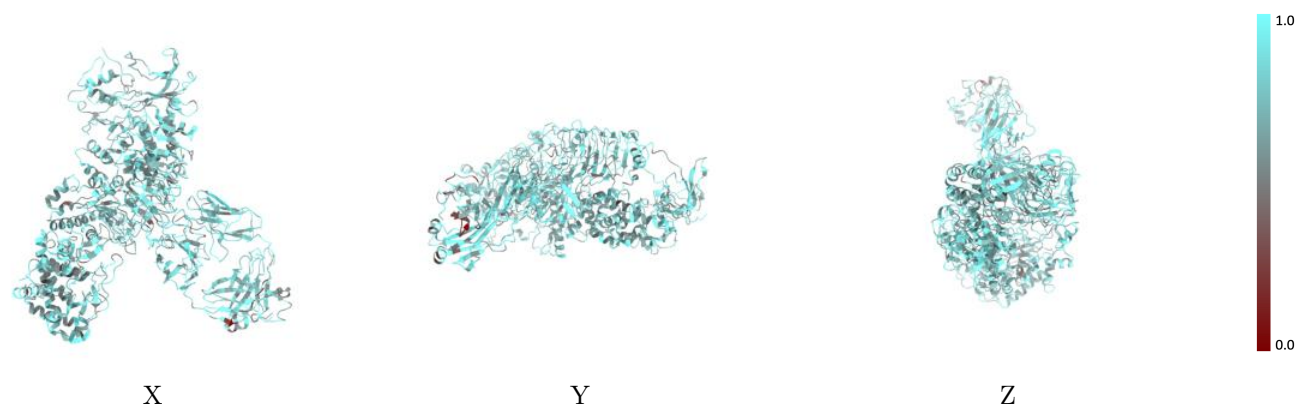
The images above show the 3D surface view of the map at the recommended contour level 0.136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

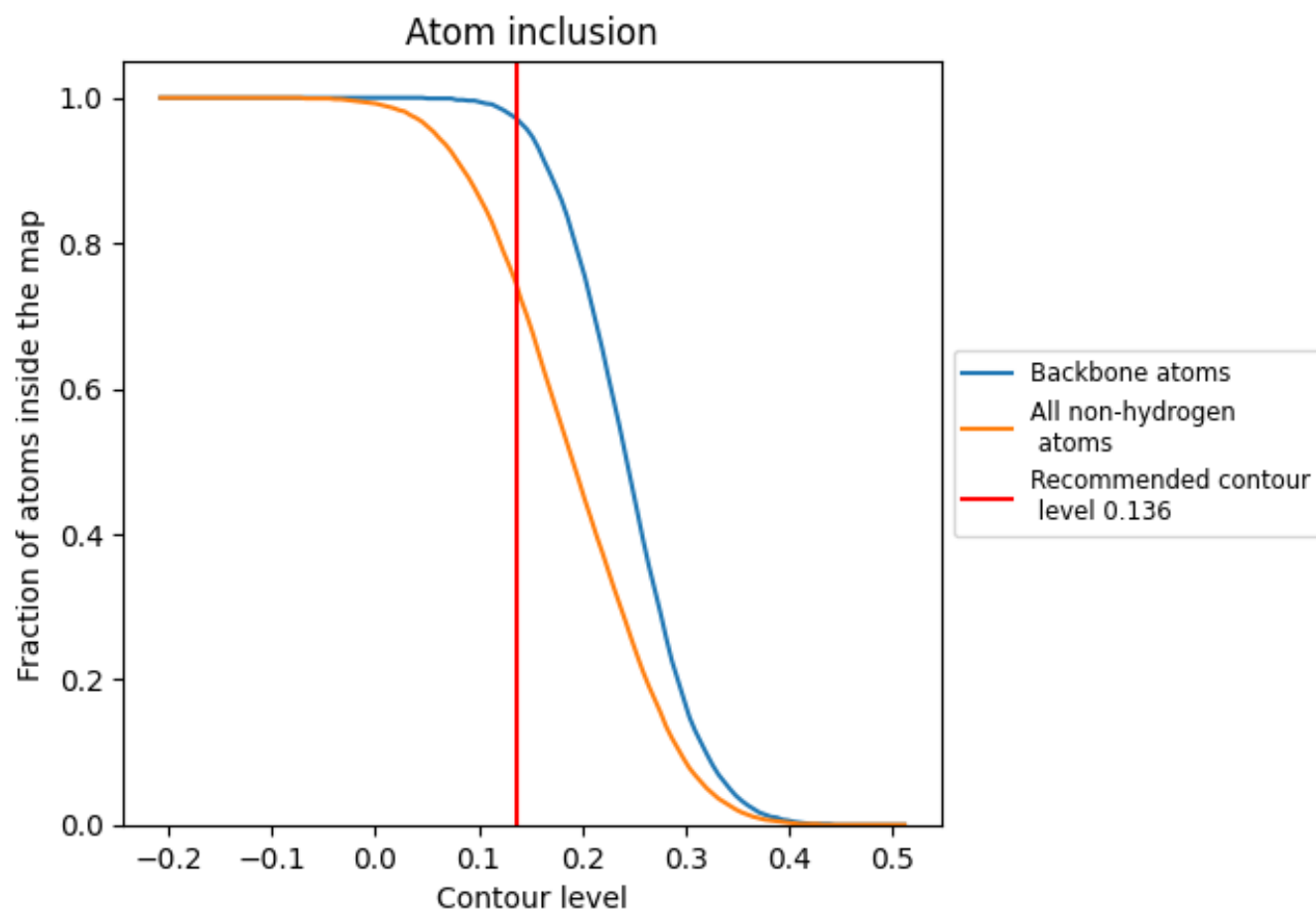
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.136).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 74% 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 (0.136) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.7450</div>	<div><div></div>0.2000</div>
A	<div><div></div>0.7370</div>	<div><div></div>0.2030</div>
H	<div><div></div>0.7400</div>	<div><div></div>0.1830</div>
L	<div><div></div>0.7980</div>	<div><div></div>0.1970</div>

