



## Full wwPDB EM Validation Report ⓘ

Oct 20, 2024 – 08:16 AM EDT

PDB ID : 7JGJ  
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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

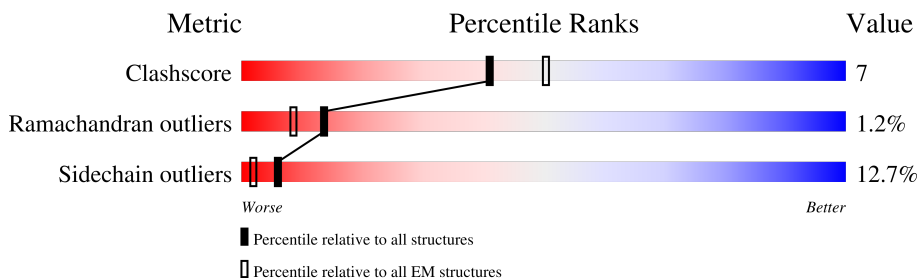
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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		

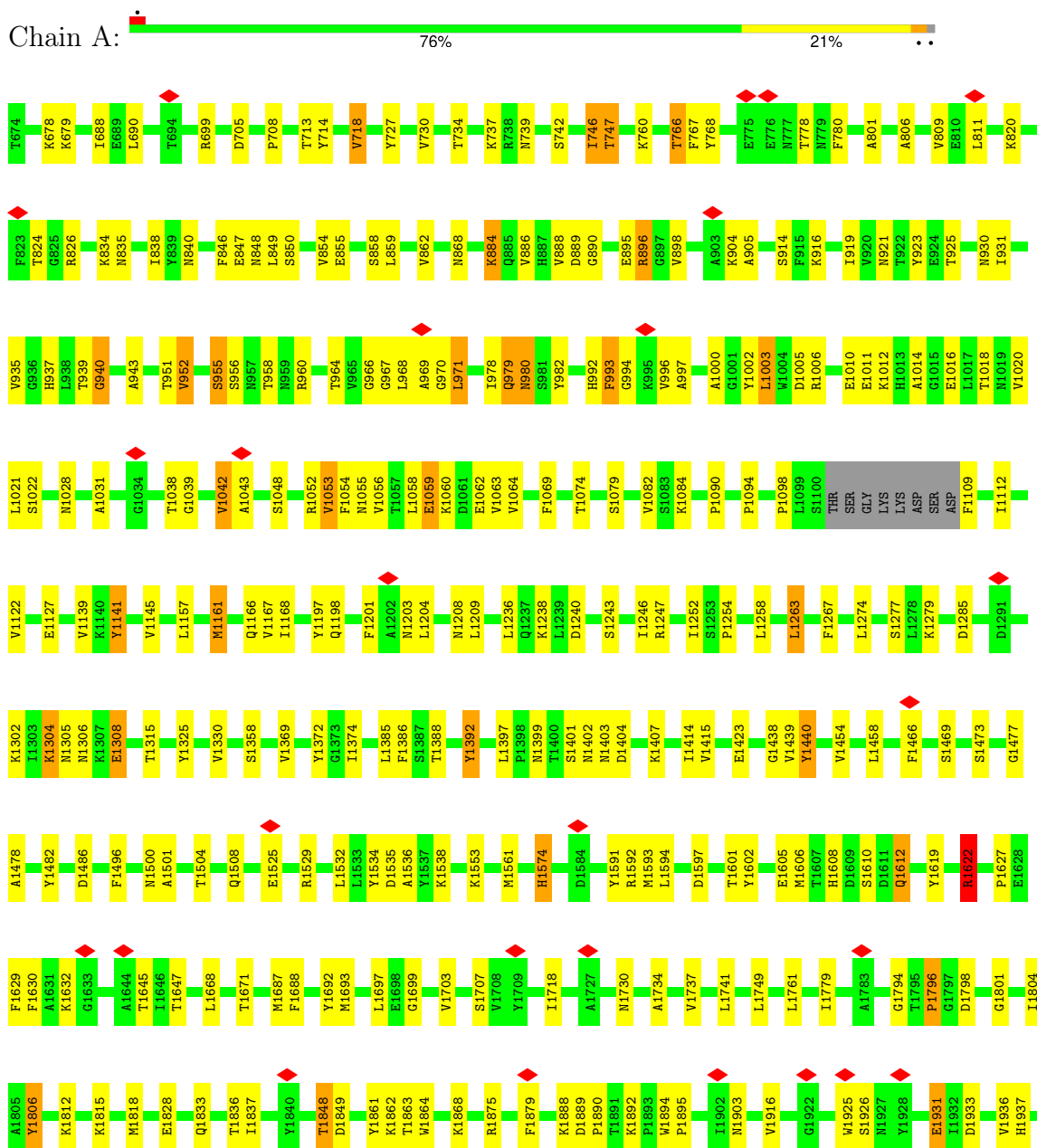
- Molecule 3 is a protein called mAB Heavy Chain.

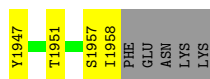
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	218	Total	C	N	O	S	0	0
			1628	1027	261	330	10		

### 3 Residue-property plots

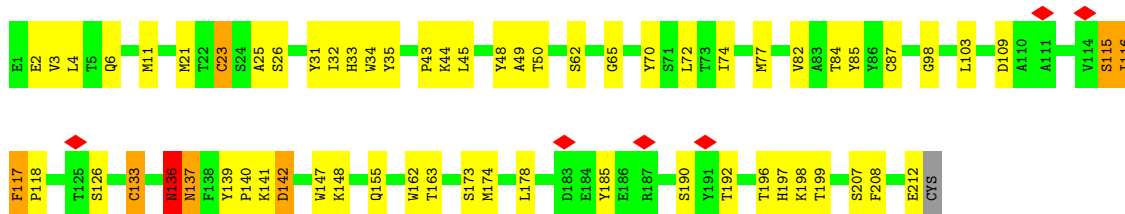
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Immunoglobulin A1 protease

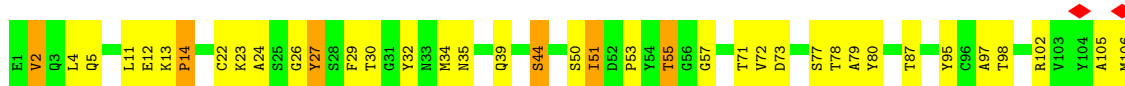




• Molecule 2: mAB Light Chain



• 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

### 5.1 Standard geometry

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	0.62	0/10259	0.98	14/13865 (0.1%)
2	L	0.71	2/1665 (0.1%)	1.08	11/2260 (0.5%)
3	H	0.67	0/1669	0.93	1/2278 (0.0%)
All	All	0.64	2/13593 (0.0%)	0.99	26/18403 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	23	CYS	C-O	6.14	1.35	1.23
2	L	23	CYS	CA-CB	-5.99	1.40	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1392	TYR	CA-C-O	-31.74	53.45	120.10
1	A	1392	TYR	O-C-N	-22.05	87.43	122.70
1	A	1392	TYR	CA-C-N	10.70	140.73	117.20
3	H	132	PRO	N-CA-C	10.21	138.64	112.10
2	L	133	CYS	N-CA-CB	-9.77	93.02	110.60
1	A	1622	ARG	CB-CA-C	9.69	129.78	110.40
1	A	1141	TYR	CB-CA-C	8.93	128.26	110.40
2	L	118	PRO	CB-CA-C	8.17	132.43	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	136	ASN	CB-CA-C	7.43	125.26	110.40
1	A	1612	GLN	CB-CA-C	7.12	124.65	110.40
1	A	1801	GLY	C-N-CA	6.98	139.14	121.70
2	L	173	SER	CB-CA-C	6.66	122.76	110.10
2	L	133	CYS	CA-CB-SG	6.60	125.88	114.00
1	A	1090	PRO	N-CA-CB	6.55	111.16	103.30
2	L	173	SER	N-CA-CB	6.53	120.29	110.50
1	A	1478	ALA	CB-CA-C	6.46	119.78	110.10
1	A	979	GLN	CB-CA-C	6.28	122.95	110.40
2	L	23	CYS	CB-CA-C	6.16	122.73	110.40
2	L	115	SER	CB-CA-C	5.83	121.19	110.10
1	A	1094	PRO	N-CA-CB	5.75	110.20	103.30
1	A	1478	ALA	N-CA-CB	5.61	117.96	110.10
1	A	1098	PRO	N-CA-CB	5.49	109.88	103.30
1	A	1440	TYR	N-CA-CB	5.46	120.43	110.60
2	L	163	THR	CA-CB-CG2	-5.30	104.98	112.40
2	L	115	SER	N-CA-CB	5.20	118.30	110.50
2	L	163	THR	OG1-CB-CG2	5.12	121.79	110.00

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
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

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Mol	Chain	Res	Type	Group
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 ⓘ

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	106	0
2	L	1626	0	1545	38	0
3	H	1628	0	1589	37	0
All	All	13324	0	12955	176	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 (176) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:H:27:TYR:HE2	3:H:32:TYR:HB2	1.72	0.54
2:L:34:TRP:CD2	2:L:72:LEU:HD12	2.42	0.53
1:A:1688:PHE:O	1:A:1692:TYR:CG	2.63	0.52
3:H:13:LYS:HD3	3:H:13:LYS:C	2.31	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
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
2:L:35:TYR:CE2	2:L:43:PRO:HB2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:LEU:HD13	1:A:1014:ALA:HB1	1.94	0.50
1:A:1308:GLU:CD	1:A:1308:GLU:H	2.14	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
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
2:L:6:GLN:HE22	2:L:85:TYR:C	2.15	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:1439:VAL:O	1:A:1440:TYR:C	2.50	0.48
2:L:4:LEU:CB	2:L:98:GLY:HA2	2.43	0.48
3:H:160:TRP:CD1	3:H:169:VAL:HG21	2.49	0.48
1:A:858:SER:C	1:A:859:LEU:HD22	2.34	0.48
1:A:1304:LYS:HD2	1:A:1304:LYS:C	2.34	0.48
1:A:992:HIS:HB2	1:A:1054:PHE:HD2	1.79	0.47
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
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
1:A:1957:SER:O	1:A:1958:ILE:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:140:PRO:O	2:L:141:LYS:C	2.55	0.45
2:L:136:ASN:O	2:L:137:ASN:C	2.53	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: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
1:A:1258:LEU:H	1:A:1258:LEU:HD12	1.83	0.44
1:A:966:GLY:O	1:A:968:LEU:N	2.50	0.44
1:A:1058:LEU:O	1:A:1059:GLU:C	2.56	0.44
1:A:1734:ALA:HB3	1:A:1796:PRO:HA	2.00	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
3:H:39:GLN:CD	3:H:95:TYR:HD2	2.22	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
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:141:LYS:HD2	2:L:141:LYS:C	2.39	0.43
2:L:212:GLU:N	2:L:212:GLU:OE1	2.52	0.43
3:H:102:ARG:O	3:H:102:ARG:HG2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:141:LYS:O	2:L:142:ASP:C	2.58	0.41
1:A:1056:VAL:HG22	1:A:1062:GLU:O	2.20	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: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
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:895:GLU:HA	1:A:923:TYR:CD1	2.56	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
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
1:A:1010:GLU:C	1:A:1012:LYS:N	2.73	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%)	927 (86%)	151 (14%)	3	14
2	L	186/187 (100%)	170 (91%)	16 (9%)	8	27
3	H	187/187 (100%)	170 (91%)	17 (9%)	7	24
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	678	LYS
1	A	679	LYS
1	A	699	ARG
1	A	705	ASP
1	A	708	PRO
1	A	713	THR
1	A	718	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	767	PHE
1	A	768	TYR
1	A	778	THR
1	A	820	LYS
1	A	824	THR
1	A	834	LYS
1	A	835	ASN
1	A	847	GLU
1	A	848	ASN
1	A	854	VAL

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Mol	Chain	Res	Type
1	A	855	GLU
1	A	884	LYS
1	A	889	ASP
1	A	896	ARG
1	A	904	LYS
1	A	914	SER
1	A	921	ASN
1	A	925	THR
1	A	930	ASN
1	A	939	THR
1	A	952	VAL
1	A	955	SER
1	A	960	ARG
1	A	964	THR
1	A	971	LEU
1	A	980	ASN
1	A	982	TYR
1	A	993	PHE
1	A	996	VAL
1	A	1003	LEU
1	A	1005	ASP
1	A	1006	ARG
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	1064	VAL
1	A	1074	THR
1	A	1084	LYS
1	A	1109	PHE
1	A	1127	GLU
1	A	1141	TYR
1	A	1157	LEU
1	A	1161	MET
1	A	1166	GLN
1	A	1168	ILE
1	A	1197	TYR
1	A	1198	GLN
1	A	1201	PHE

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Mol	Chain	Res	Type
1	A	1203	ASN
1	A	1204	LEU
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	1277	SER
1	A	1279	LYS
1	A	1285	ASP
1	A	1302	LYS
1	A	1304	LYS
1	A	1306	ASN
1	A	1308	GLU
1	A	1325	TYR
1	A	1330	VAL
1	A	1369	VAL
1	A	1374	ILE
1	A	1388	THR
1	A	1399	ASN
1	A	1401	SER
1	A	1415	VAL
1	A	1423	GLU
1	A	1458	LEU
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	1529	ARG
1	A	1535	ASP
1	A	1553	LYS
1	A	1561	MET
1	A	1574	HIS
1	A	1592	ARG
1	A	1593	MET
1	A	1597	ASP
1	A	1602	TYR
1	A	1605	GLU
1	A	1606	MET

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Mol	Chain	Res	Type
1	A	1608	HIS
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	1741	LEU
1	A	1749	LEU
1	A	1761	LEU
1	A	1798	ASP
1	A	1806	TYR
1	A	1812	LYS
1	A	1815	LYS
1	A	1818	MET
1	A	1828	GLU
1	A	1833	GLN
1	A	1836	THR
1	A	1848	THR
1	A	1849	ASP
1	A	1861	TYR
1	A	1862	LYS
1	A	1863	THR
1	A	1868	LYS
1	A	1875	ARG
1	A	1879	PHE
1	A	1888	LYS
1	A	1889	ASP
1	A	1892	LYS
1	A	1903	ASN
1	A	1925	TRP
1	A	1926	SER
1	A	1931	GLU
1	A	1933	ASP
1	A	1937	HIS
2	L	11	MET

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Mol	Chain	Res	Type
2	L	21	MET
2	L	44	LYS
2	L	62	SER
2	L	84	THR
2	L	115	SER
2	L	117	PHE
2	L	126	SER
2	L	136	ASN
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
3	H	27	TYR
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	161	ASN
3	H	183	LEU
3	H	184	SER
3	H	188	THR
3	H	211	LYS
3	H	213	ASP
3	H	215	LYS

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	921	ASN
1	A	930	ASN
1	A	1686	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

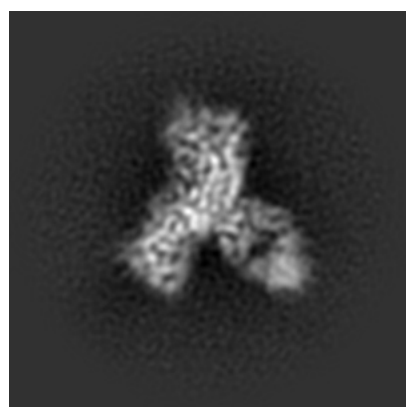
## 6 Map visualisation [i](#)

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

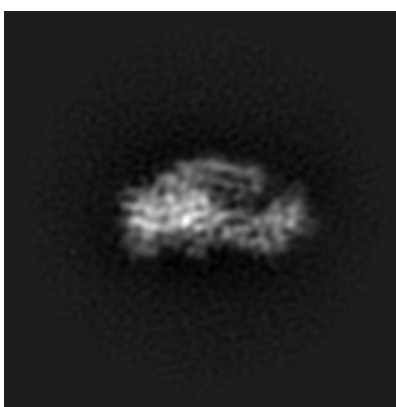
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

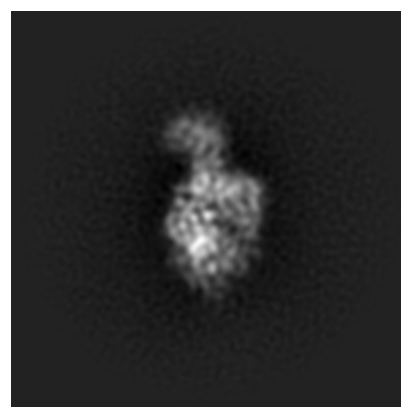
#### 6.1.1 Primary map



X



Y

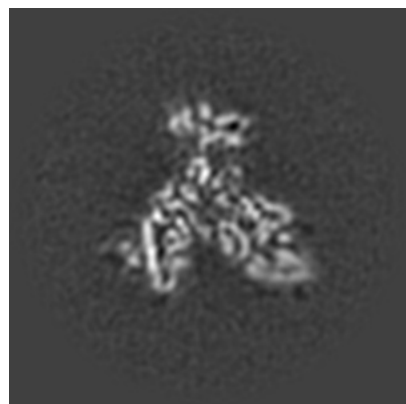


Z

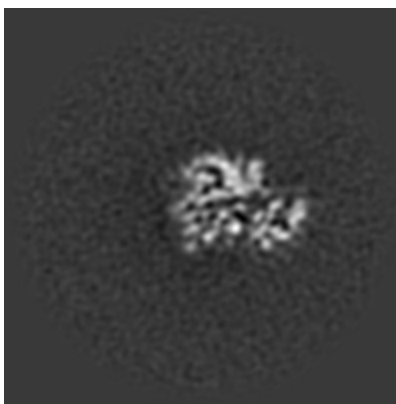
The images above show the map projected in three orthogonal directions.

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

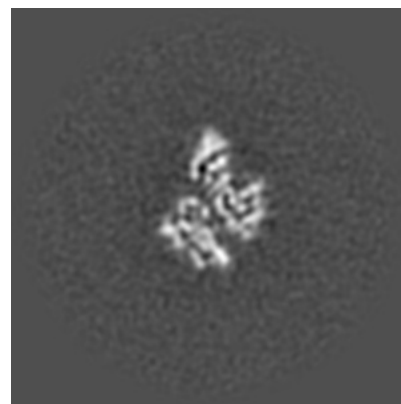
#### 6.2.1 Primary map



X Index: 162



Y Index: 162

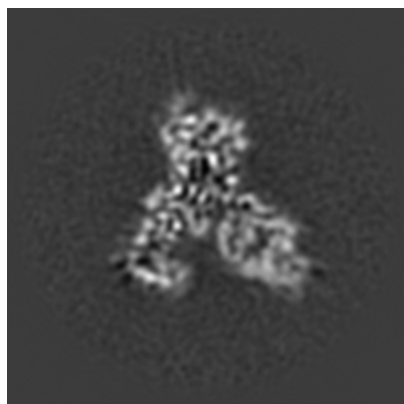


Z Index: 162

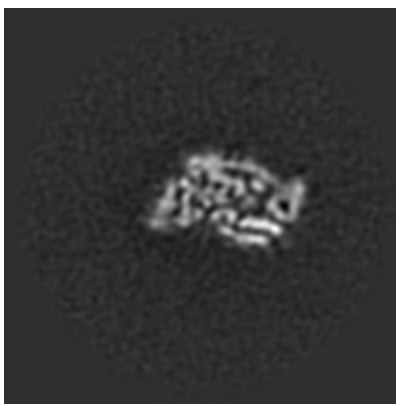
The images above show central slices of the map in three orthogonal directions.

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

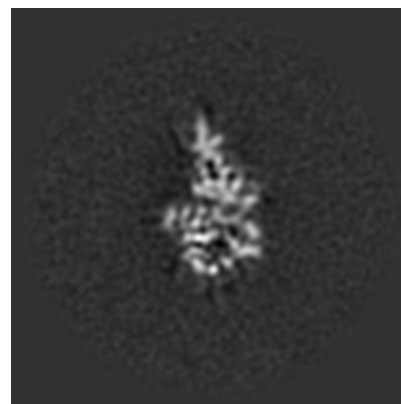
### 6.3.1 Primary map



X Index: 153



Y Index: 179

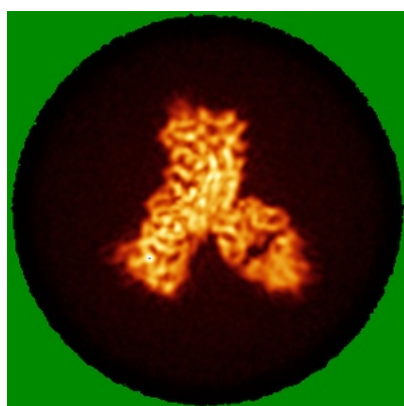


Z Index: 147

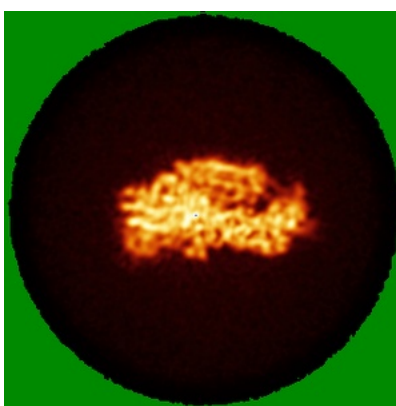
The images above show the largest variance slices of the map in three orthogonal directions.

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

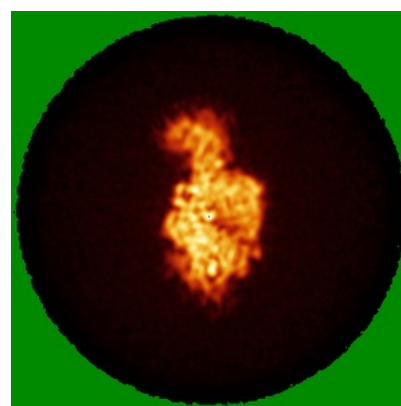
### 6.4.1 Primary map



X



Y

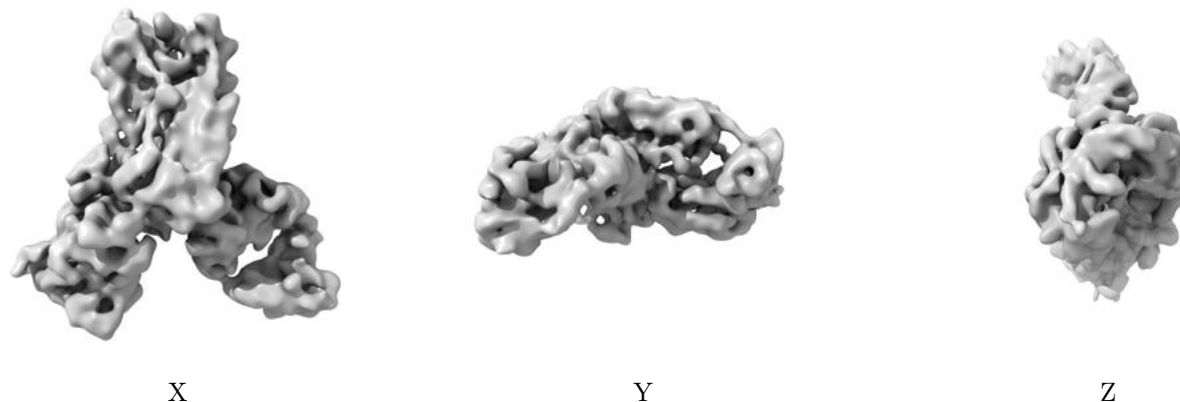


Z

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.

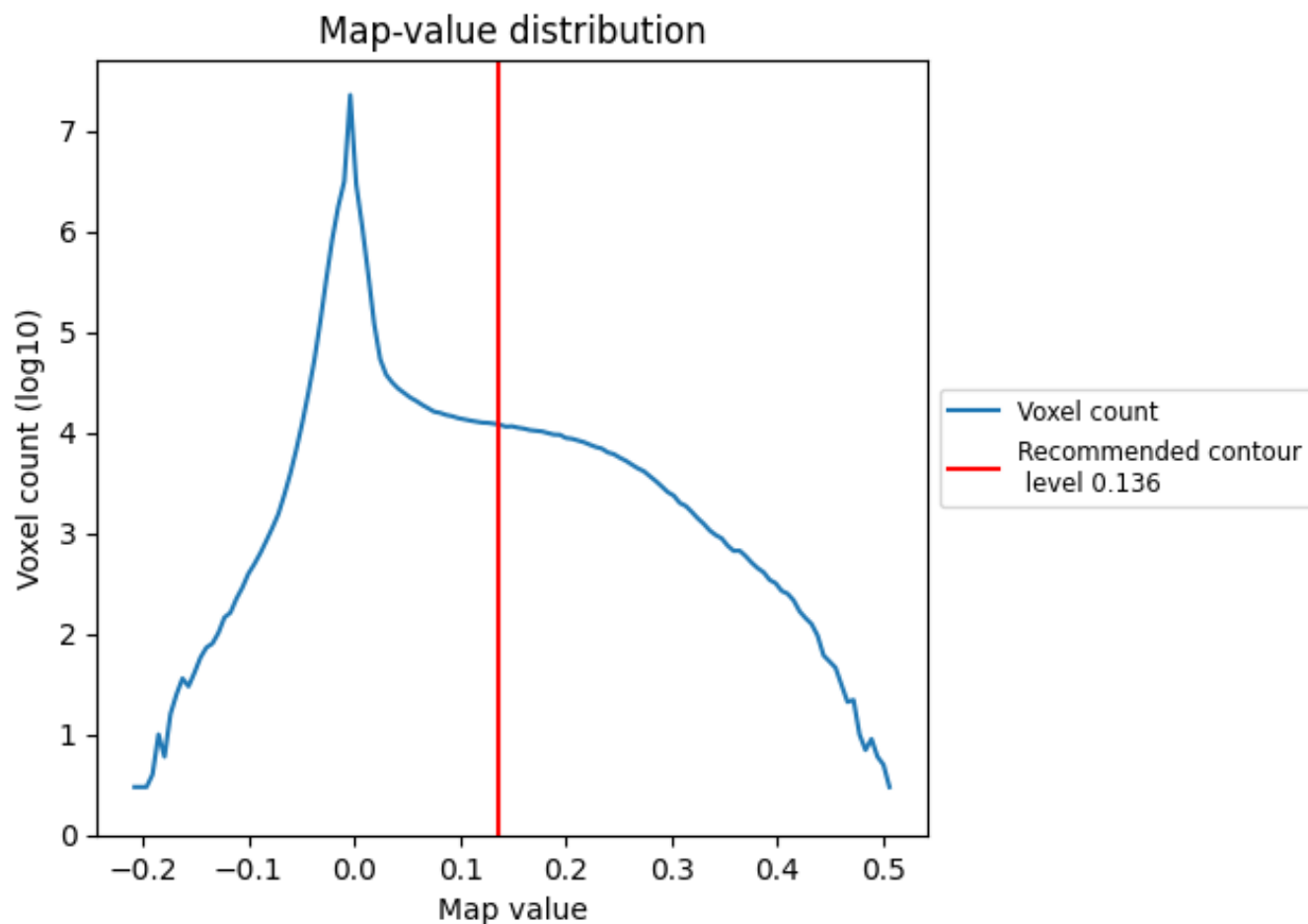
## 6.6 Mask visualisation [i](#)

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.

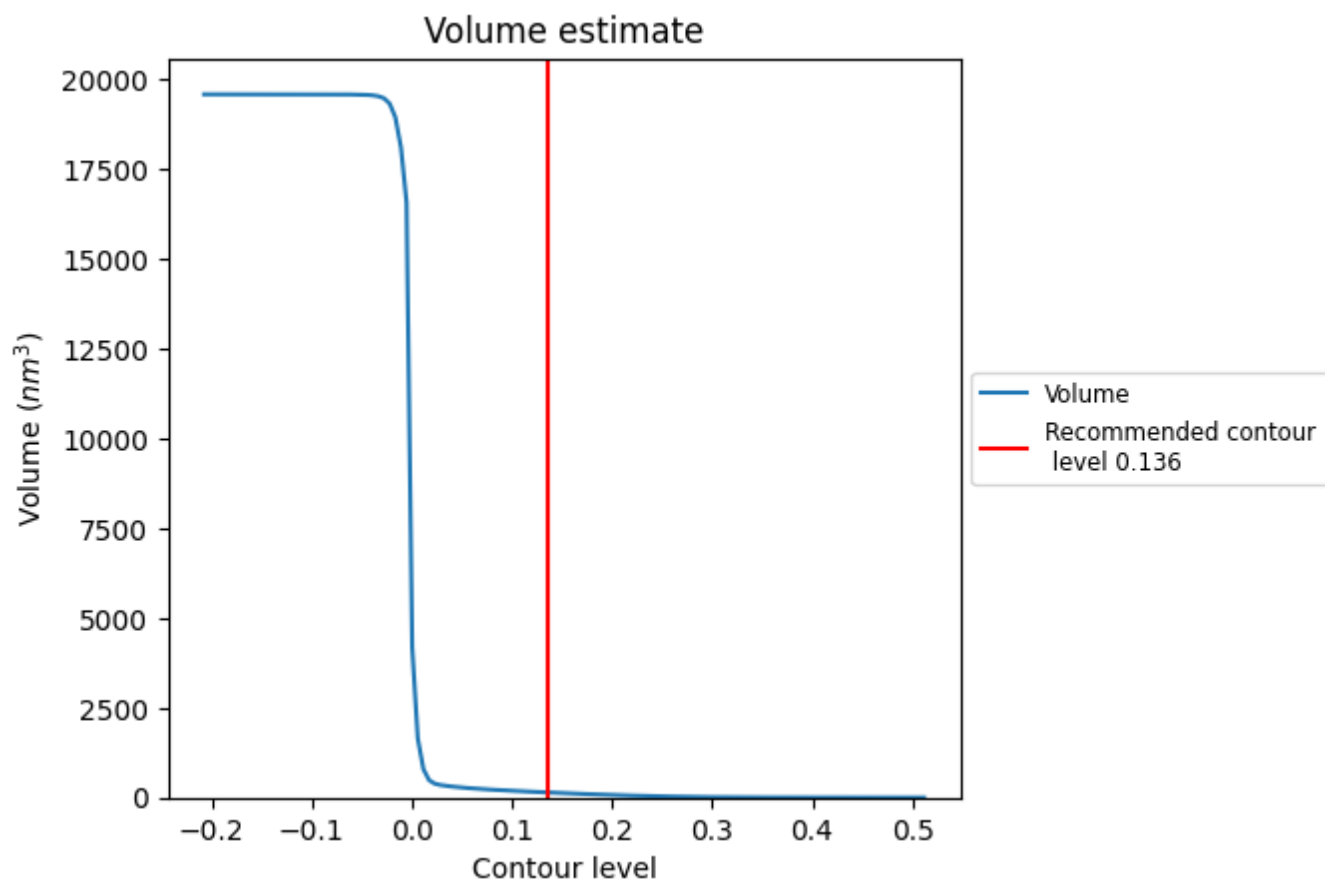
### 7.1 Map-value distribution [i](#)



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.



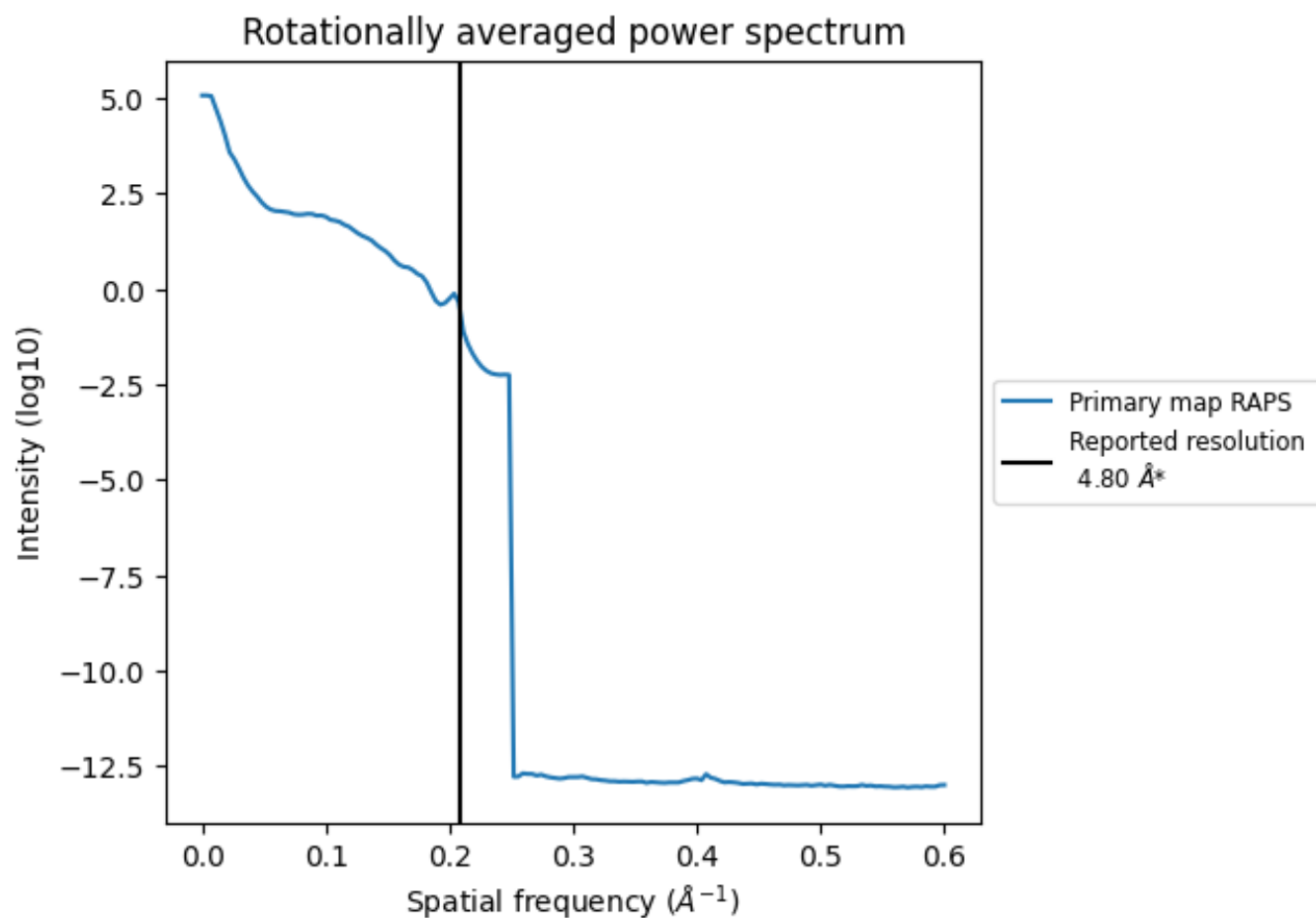
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141  $\text{nm}^3$ ; 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  $\text{\AA}^{-1}$

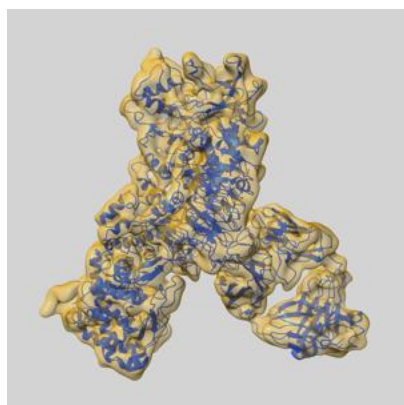
## 8 Fourier-Shell correlation

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

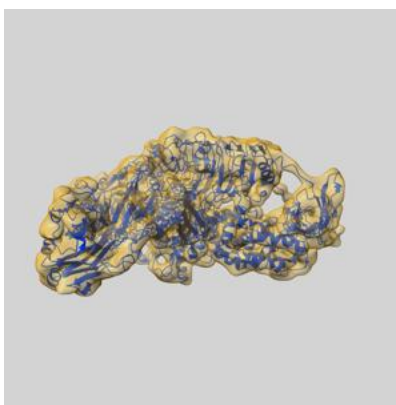
## 9 Map-model fit [i](#)

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](#).

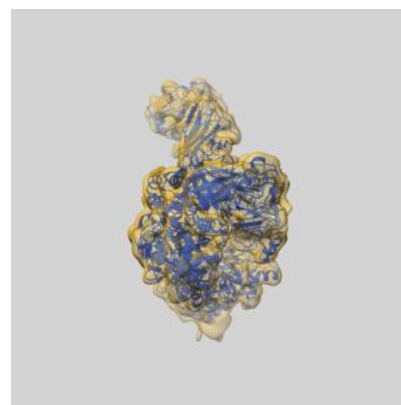
### 9.1 Map-model overlay [i](#)



X



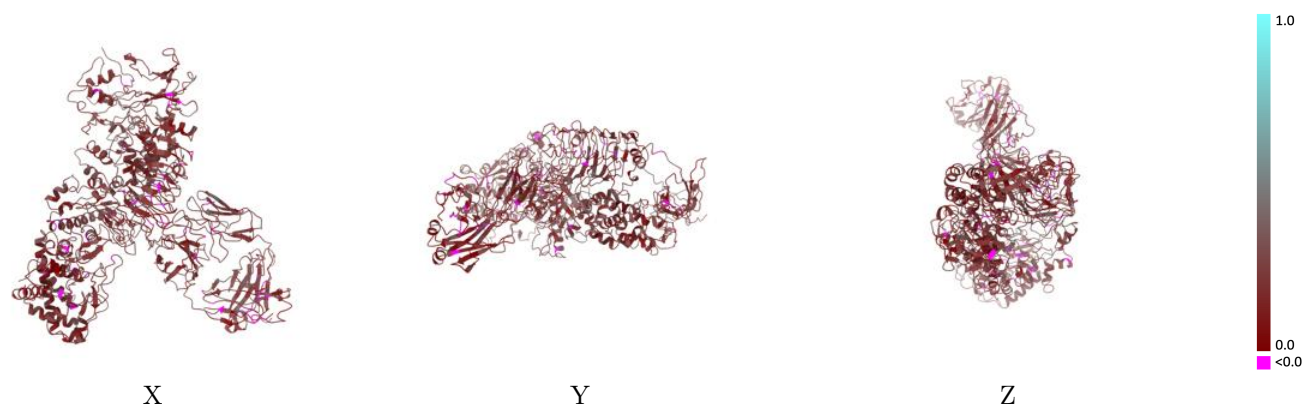
Y



Z

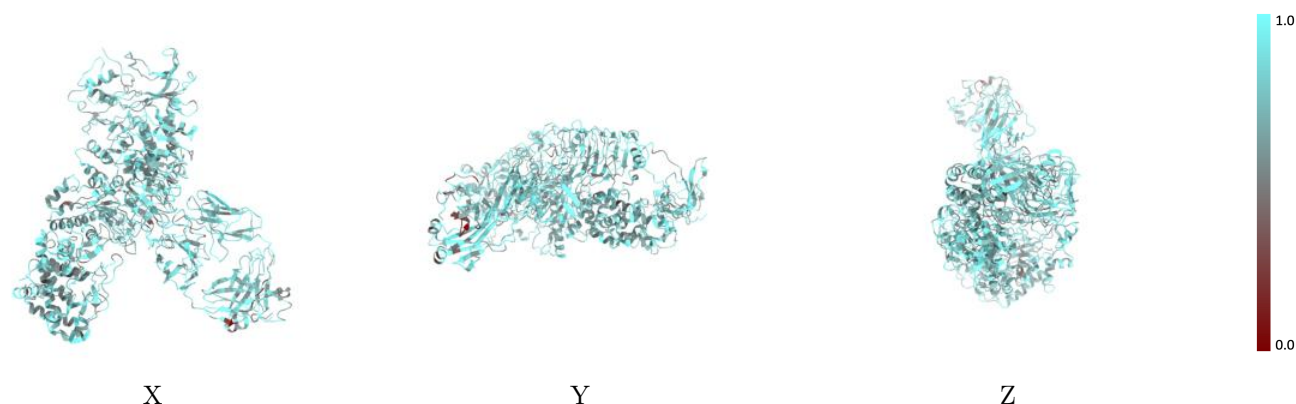
The images above show the 3D surface view of the map at the recommended contour level 0.136 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



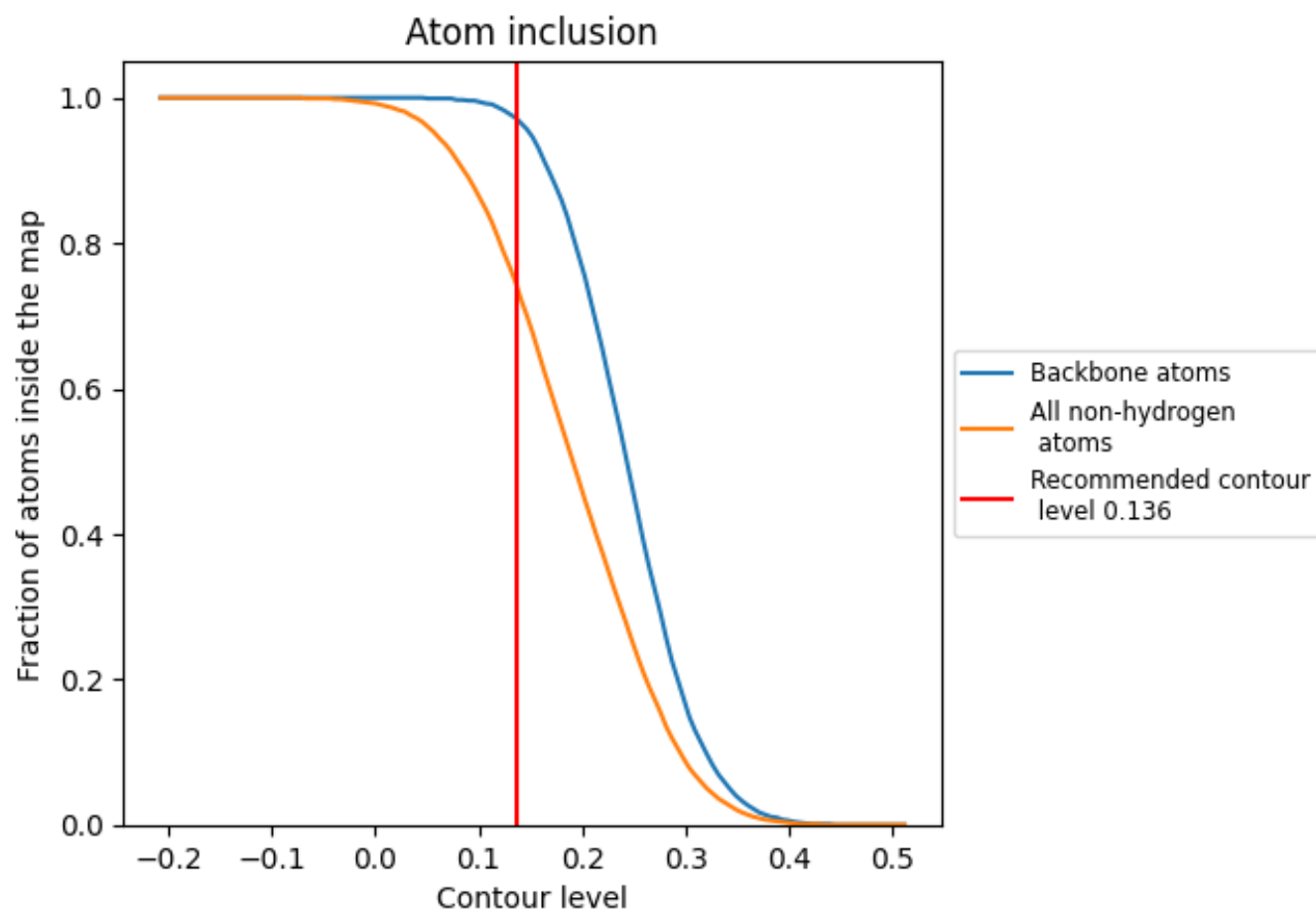
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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> 0.7450	<div></div> 0.2000
A	<div></div> 0.7370	<div></div> 0.2030
H	<div></div> 0.7400	<div></div> 0.1830
L	<div></div> 0.7980	<div></div> 0.1970

