



Full wwPDB EM Validation Report ⓘ

Dec 6, 2025 – 03:08 PM EST

PDB ID : 9P0X / pdb_00009p0x
EMDB ID : EMD-71090
Title : Nanodisc-embedded human TF/FVIIa/XK1 in complex with 10H10 Fab (nanodisc-subtracted)
Authors : Photenhauer, A.L.; Sedzro, J.C.; Ohi, M.D.; Morrissey, J.H.
Deposited on : 2025-06-07
Resolution : 3.70 Å (reported)
Based on initial models : 4m7l, 1xka, 1iod, 1dan, 4bqd, 3th2, 12e8

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:

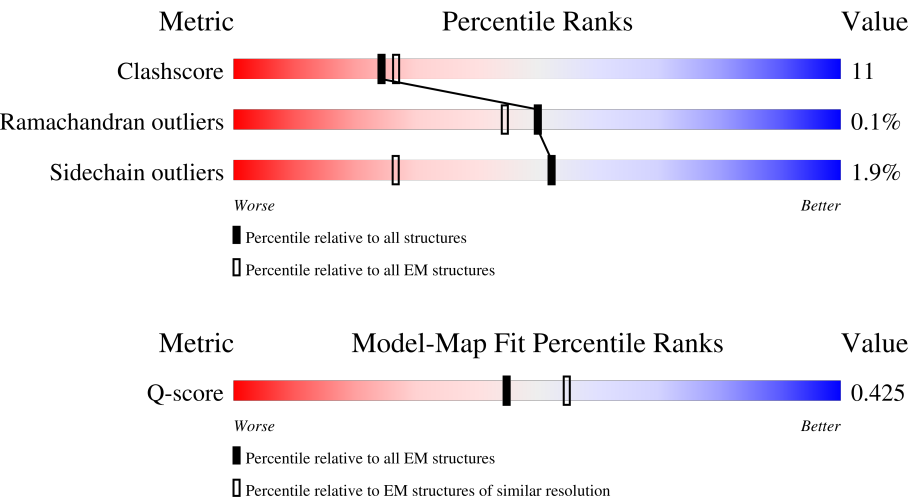
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.47

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 3.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	V	142	<div><div></div><div>71%28%.</div></div>
2	X	131	<div><div>5%</div><div>66%32%.</div></div>
3	S	254	<div><div></div><div>72%26%.</div></div>
4	T	611	<div><div></div><div>27%6%67%</div></div>

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Mol	Chain	Length	Quality of chain
5	K	68	 68% 31%
6	H	221	 77% 23%
7	L	220	 73% 27%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 9725 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 Factor VII light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	V	142	Total	C	N	O	S	0	0
			1134	683	189	247	15		

- Molecule 2 is a protein called Factor X light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	131	Total	C	N	O	S	0	0
			1055	630	170	239	16		

- Molecule 3 is a protein called Coagulation factor VII Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	254	Total	C	N	O	S	0	0
			1974	1253	351	357	13		

- Molecule 4 is a protein called Tissue factor,Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	201	Total	C	N	O	S	0	0
			1611	1021	262	323	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	245	GLY	-	linker	UNP P13726
T	246	SER	-	linker	UNP P13726
T	247	GLY	-	linker	UNP P13726
T	248	SER	-	linker	UNP P13726
T	249	GLY	-	linker	UNP P13726
T	250	MET	-	linker	UNP P13726

- Molecule 5 is a protein called Tissue factor pathway inhibitor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	68	Total	C	N	O	S	0	0
			554	349	93	103	9		

- Molecule 6 is a protein called Human 10H10 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	221	Total	C	N	O	S	0	0
			1660	1052	271	330	7		

- Molecule 7 is a protein called Human 10H10 antibody Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	220	Total	C	N	O	S	1	0
			1700	1057	281	354	8		

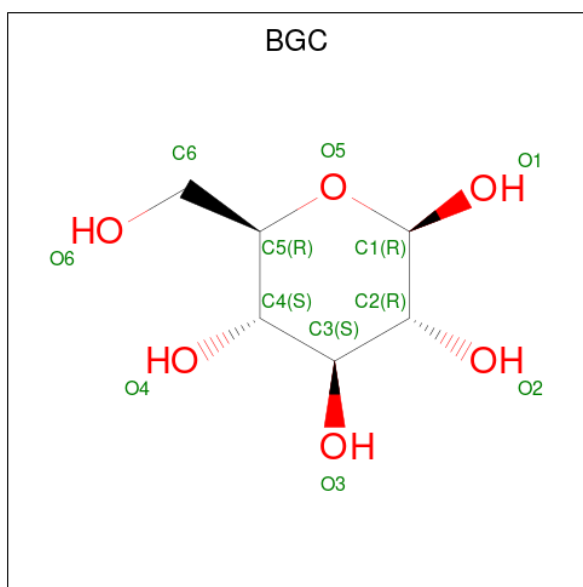
- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	V	3	Total	Mg	0
			3	3	
8	X	1	Total	Mg	0
			1	1	

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

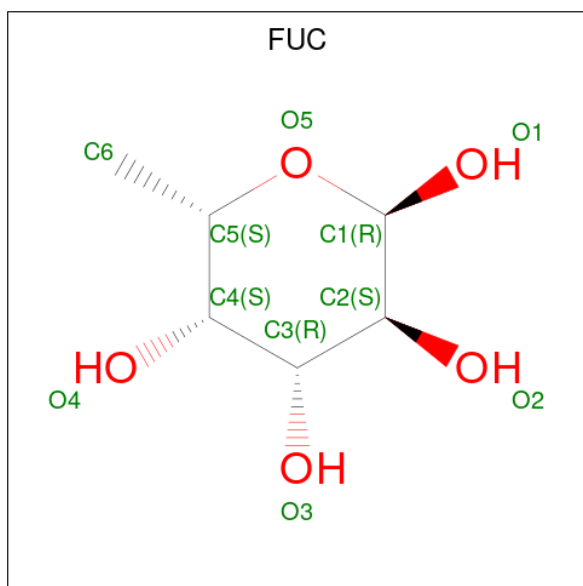
Mol	Chain	Residues	Atoms		AltConf
9	V	5	Total	Ca	0
			5	5	
9	X	6	Total	Ca	0
			6	6	
9	S	1	Total	Ca	0
			1	1	

- Molecule 10 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			AltConf
10	V	1	Total	C	O	0
			11	6	5	

- Molecule 11 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).

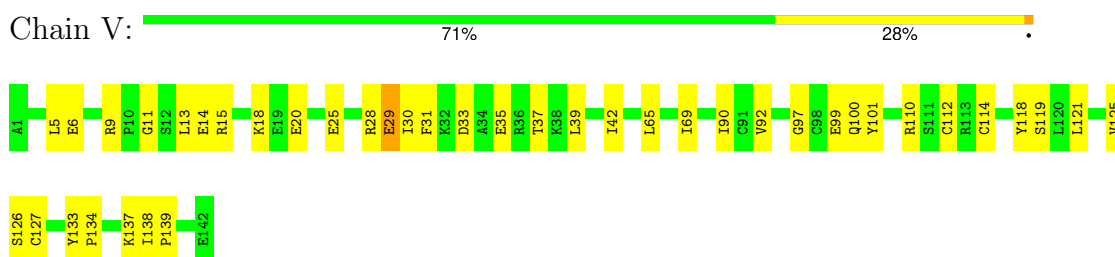


Mol	Chain	Residues	Atoms			AltConf
11	V	1	Total	C	O	0
			10	6	4	

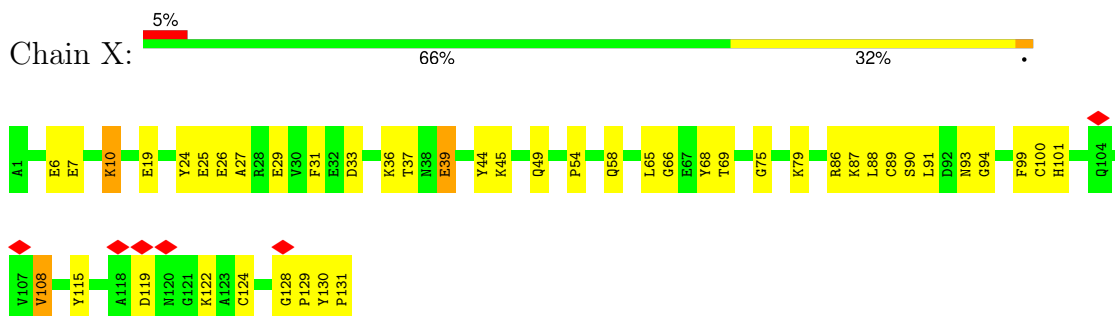
3 Residue-property plots

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.

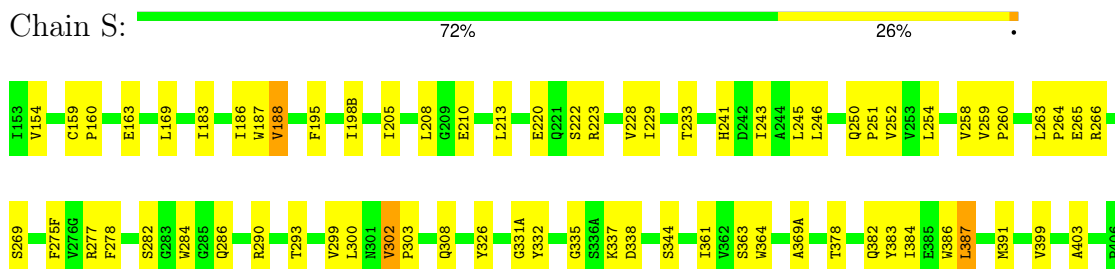
- Molecule 1: Factor VII light chain



- Molecule 2: Factor X light chain

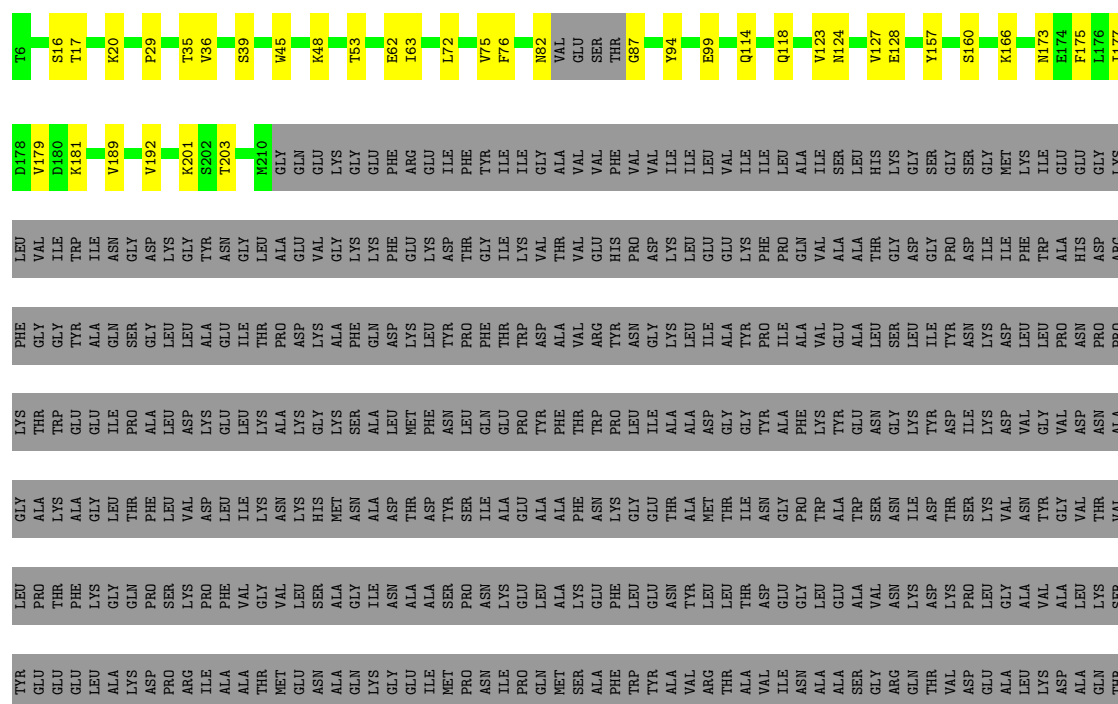


- Molecule 3: Coagulation factor VII Heavy Chain

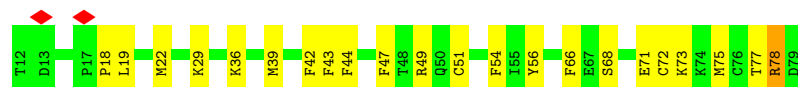


- Molecule 4: Tissue factor, Maltose/maltodextrin-binding periplasmic protein

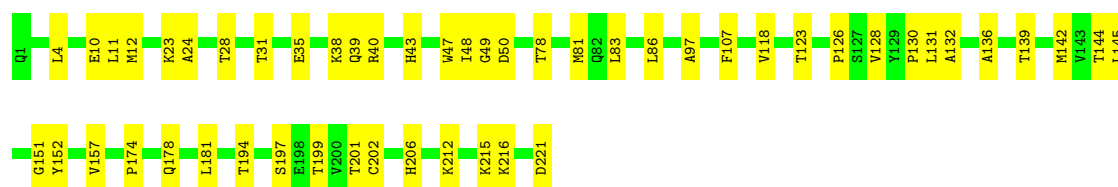
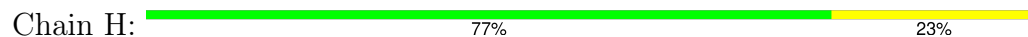




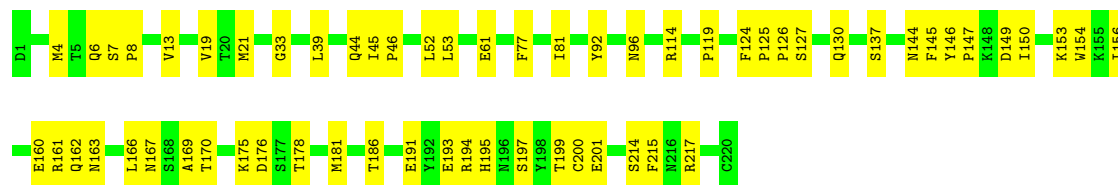
• Molecule 5: Tissue factor pathway inhibitor



• Molecule 6: Human 10H10 antibody Fab heavy chain



• Molecule 7: Human 10H10 antibody Fab light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.466	Depositor
Minimum map value	-0.236	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	350.28, 350.28, 350.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, FUC, CA, CGU, MG

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	V	0.15	0/1028	0.43	0/1374
2	X	0.14	0/933	0.40	0/1240
3	S	0.14	0/2024	0.34	0/2755
4	T	0.13	0/1646	0.34	0/2238
5	K	0.18	0/566	0.54	0/753
6	H	0.13	0/1707	0.36	0/2334
7	L	0.12	0/1740	0.31	0/2366
All	All	0.14	0/9644	0.37	0/13060

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	V	1134	0	987	29	0
2	X	1055	0	890	24	0
3	S	1974	0	1950	48	0
4	T	1611	0	1564	26	0
5	K	554	0	523	16	0
6	H	1660	0	1600	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	1700	0	1633	40	0
8	V	3	0	0	0	0
8	X	1	0	0	0	0
9	S	1	0	0	0	0
9	V	5	0	0	0	0
9	X	6	0	0	0	0
10	V	11	0	10	0	0
11	V	10	0	10	0	0
All	All	9725	0	9167	194	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 11.

All (194) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:188:VAL:HG12	3:S:246:LEU:HB2	1.69	0.75
2:X:24:TYR:O	2:X:27:ALA:HB3	1.86	0.75
6:H:199:THR:HG23	6:H:216:LYS:HG3	1.69	0.74
6:H:126:PRO:HB3	6:H:152:TYR:HB3	1.70	0.73
3:S:275(F):PHE:HB3	4:T:45:TRP:HB2	1.70	0.72
2:X:115:TYR:HB3	2:X:124:CYS:HB3	1.72	0.71
4:T:179:VAL:HG23	4:T:181:LYS:H	1.56	0.71
7:L:153:LYS:HB3	7:L:201:GLU:HB2	1.77	0.66
6:H:151:GLY:HA2	6:H:181:LEU:HD13	1.79	0.65
4:T:157:TYR:CE1	4:T:177:ILE:HG21	2.32	0.65
3:S:363:SER:HG	3:S:364:TRP:CD1	2.15	0.63
5:K:71:GLU:O	5:K:75:MET:HG2	1.97	0.63
7:L:119:PRO:HB3	7:L:145:PHE:HB3	1.81	0.63
1:V:121:LEU:HD13	1:V:127:CYS:HA	1.81	0.62
2:X:65:LEU:HD12	2:X:66:GLY:H	1.65	0.61
1:V:13:LEU:H	4:T:160:SER:HB2	1.67	0.60
5:K:49:ARG:H	5:K:49:ARG:NH1	2.00	0.59
2:X:101:HIS:HB2	2:X:108:VAL:HG13	1.84	0.59
5:K:44:PHE:HA	5:K:51:CYS:HA	1.84	0.59
1:V:11:GLY:HA2	1:V:15:ARG:HH21	1.68	0.58
2:X:10:LYS:HD3	2:X:10:LYS:H	1.69	0.58
3:S:282:SER:HB2	3:S:299:VAL:HG23	1.86	0.57
6:H:86:LEU:HB3	6:H:118:VAL:HG21	1.86	0.57
6:H:97:ALA:HB1	6:H:107:PHE:HB3	1.86	0.57
1:V:65:LEU:HD22	4:T:203:THR:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:93:ASN:HB2	2:X:99:PHE:HA	1.86	0.56
6:H:81:MET:HE2	6:H:83:LEU:HD21	1.86	0.56
6:H:10:GLU:HB3	6:H:12:MET:SD	2.47	0.56
6:H:132:ALA:HB3	6:H:221:ASP:HB3	1.87	0.55
3:S:254:LEU:HD22	3:S:260:PRO:HD3	1.87	0.55
7:L:126:PRO:HB3	7:L:130:GLN:HG2	1.86	0.55
2:X:36:LYS:O	2:X:39:CGU:HB3	2.06	0.55
7:L:191:GLU:HG3	7:L:194:ARG:HH21	1.72	0.54
3:S:183:ILE:O	3:S:260:PRO:HB2	2.07	0.54
3:S:277:ARG:O	3:S:303:PRO:HA	2.07	0.54
3:S:264:PRO:HG2	3:S:269:SER:HB2	1.88	0.54
2:X:44:TYR:HB3	2:X:45:LYS:HZ2	1.73	0.54
6:H:31:THR:HG22	6:H:31:THR:O	2.08	0.54
7:L:161:ARG:HD2	7:L:163:ASN:H	1.73	0.54
4:T:157:TYR:CE2	4:T:166:LYS:HB2	2.43	0.53
6:H:131:LEU:HD12	7:L:124:PHE:HB3	1.89	0.53
6:H:142:MET:HA	6:H:142:MET:HE2	1.90	0.53
4:T:35:THR:HG23	4:T:76:PHE:HD2	1.74	0.53
7:L:137:SER:HA	7:L:186:THR:HA	1.90	0.53
7:L:145:PHE:HE1	7:L:181:MET:H	1.57	0.52
4:T:82:ASN:HD22	4:T:87:GLY:HA2	1.74	0.52
4:T:157:TYR:HE1	4:T:177:ILE:HG21	1.74	0.52
4:T:29:PRO:HG3	4:T:53:THR:O	2.10	0.52
1:V:69:ILE:HD11	4:T:17:THR:HB	1.92	0.51
7:L:45:ILE:HG22	7:L:46:PRO:HD2	1.92	0.51
3:S:160:PRO:HB2	3:S:163:GLU:HG3	1.93	0.51
7:L:199:THR:HG23	7:L:214:SER:HB2	1.92	0.51
6:H:39:GLN:HE22	7:L:44:GLN:HE22	1.59	0.51
3:S:266:ARG:HA	3:S:384:ILE:HD12	1.92	0.51
7:L:19:VAL:HG22	7:L:81:ILE:HB	1.92	0.51
4:T:118:GLN:HG2	4:T:123:VAL:HG12	1.92	0.51
5:K:78:ARG:NE	5:K:78:ARG:H	2.09	0.50
4:T:127:VAL:HG22	4:T:189:VAL:HG11	1.94	0.50
5:K:68:SER:O	5:K:72:CYS:HB2	2.11	0.50
4:T:72:LEU:HD13	4:T:99:GLU:HG2	1.92	0.50
6:H:201:THR:HA	6:H:216:LYS:HA	1.93	0.50
3:S:290:ARG:NE	3:S:290:ARG:HA	2.26	0.50
4:T:76:PHE:CD1	4:T:94:TYR:HB3	2.47	0.50
1:V:13:LEU:HA	1:V:30:ILE:HD13	1.94	0.49
1:V:14:CGU:HA	1:V:18:LYS:HB2	1.93	0.49
6:H:38:LYS:HB2	6:H:48:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:36:VAL:HB	4:T:75:VAL:HG22	1.94	0.49
2:X:94:GLY:HA3	2:X:100:CYS:HB2	1.94	0.49
7:L:4:MET:HE1	7:L:39:LEU:HD12	1.95	0.49
3:S:159:CYS:HB2	3:S:299:VAL:HB	1.95	0.49
7:L:114:ARG:HH22	7:L:146:TYR:HB2	1.78	0.49
3:S:205:ILE:HD11	3:S:222:SER:OG	2.13	0.49
1:V:134:PRO:HG2	1:V:137:LYS:HB3	1.93	0.48
3:S:208:LEU:HD11	3:S:252:VAL:HG21	1.95	0.48
3:S:386:TRP:HZ2	3:S:403:ALA:HB3	1.79	0.48
1:V:33:ASP:O	1:V:37:THR:HG23	2.13	0.48
7:L:161:ARG:HD2	7:L:162:GLN:N	2.29	0.48
6:H:47:TRP:CZ2	6:H:49:GLY:HA2	2.49	0.48
6:H:130:PRO:O	7:L:127:SER:HB2	2.14	0.48
7:L:52:LEU:HD23	7:L:53:LEU:N	2.29	0.47
3:S:286:GLN:HA	3:S:293:THR:HA	1.96	0.47
3:S:263:LEU:HD21	3:S:387:LEU:HD23	1.96	0.47
1:V:139:PRO:HD3	3:S:259:VAL:HG21	1.96	0.47
3:S:154:VAL:HG22	3:S:338:ASP:O	2.15	0.47
3:S:300:LEU:HD11	3:S:337:LYS:HB3	1.95	0.47
1:V:101:TYR:HE1	3:S:265:GLU:H	1.63	0.47
7:L:39:LEU:HD13	7:L:77:PHE:CD2	2.50	0.47
2:X:88:LEU:HB3	2:X:90:SER:H	1.80	0.47
7:L:175:LYS:HG3	7:L:176:ASP:H	1.79	0.46
3:S:302:VAL:HG22	3:S:303:PRO:HD2	1.97	0.46
5:K:42:PHE:HB2	5:K:66:PHE:HB2	1.98	0.46
7:L:176:ASP:HB3	7:L:178:THR:HG22	1.96	0.46
2:X:89:CYS:HB3	2:X:100:CYS:HB3	1.57	0.46
1:V:39:LEU:O	1:V:42:ILE:HG12	2.16	0.46
1:V:133:TYR:HB3	3:S:259:VAL:HG22	1.97	0.46
1:V:138:ILE:HG21	3:S:163:GLU:HA	1.97	0.46
1:V:101:TYR:HD2	1:V:114:CYS:HA	1.80	0.45
6:H:194:THR:C	6:H:197:SER:HB2	2.41	0.45
1:V:9:ARG:HG2	1:V:15:ARG:HH22	1.81	0.45
1:V:97:GLY:HA3	1:V:110:ARG:HH21	1.82	0.45
1:V:137:LYS:O	3:S:259:VAL:HG11	2.17	0.45
2:X:75:GLY:H	2:X:87:LYS:HZ1	1.65	0.45
3:S:187:TRP:CD1	3:S:391:MET:HG3	2.52	0.45
3:S:361:ILE:HG13	3:S:378:THR:HB	1.99	0.45
4:T:39:SER:HB3	4:T:45:TRP:HA	1.97	0.45
2:X:69:THR:HA	2:X:79:LYS:HE3	1.99	0.45
4:T:48:LYS:HD2	4:T:62:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:25:CGU:O	1:V:29:CGU:HG	2.16	0.44
3:S:303:PRO:HD3	3:S:332:TYR:CE1	2.52	0.44
7:L:147:PRO:HG2	7:L:149:ASP:OD1	2.17	0.44
7:L:52:LEU:HD22	7:L:61:GLU:HB2	1.99	0.44
1:V:28:ARG:HA	1:V:37:THR:HG21	1.99	0.44
3:S:326:TYR:HA	3:S:382:GLN:HG3	1.99	0.44
3:S:335:GLY:HA2	3:S:369(A):ALA:HB1	2.00	0.44
3:S:228:VAL:HG12	3:S:246:LEU:HG	2.00	0.44
6:H:4:LEU:HD23	6:H:24:ALA:HA	1.99	0.44
2:X:129:PRO:HG2	2:X:130:TYR:CD1	2.53	0.44
5:K:43:PHE:CD1	5:K:54:PHE:HB3	2.53	0.44
1:V:31:PHE:HB2	1:V:37:THR:HG22	2.00	0.44
1:V:35:CGU:O	1:V:39:LEU:HG	2.18	0.44
2:X:68:TYR:O	2:X:68:TYR:CG	2.71	0.44
3:S:223:ARG:HD2	3:S:250:GLN:HB2	2.00	0.44
4:T:124:ASN:HA	4:T:175:PHE:O	2.18	0.43
3:S:344:SER:HB2	5:K:36:LYS:O	2.17	0.43
6:H:178:GLN:HB2	7:L:166:LEU:HD22	2.00	0.43
1:V:118:TYR:CZ	1:V:134:PRO:HB2	2.53	0.43
6:H:23:LYS:HG3	6:H:78:THR:HG22	1.99	0.43
3:S:302:VAL:HG22	3:S:331(A):GLY:HA2	2.01	0.43
5:K:43:PHE:CE1	5:K:54:PHE:HB3	2.53	0.43
6:H:212:LYS:HD2	6:H:212:LYS:HA	1.74	0.43
3:S:229:ILE:HG22	3:S:245:LEU:HB3	1.99	0.43
6:H:157:VAL:HG12	6:H:206:HIS:HA	2.00	0.43
7:L:169:ALA:HB2	7:L:181:MET:SD	2.58	0.43
7:L:191:GLU:HA	7:L:194:ARG:NE	2.34	0.43
1:V:90:ILE:HD11	1:V:92:VAL:HG12	2.00	0.43
2:X:122:LYS:HD2	2:X:122:LYS:HA	1.82	0.43
2:X:130:TYR:N	2:X:131:PRO:HD3	2.34	0.43
3:S:254:LEU:HD23	3:S:258:VAL:HG12	2.01	0.43
2:X:31:PHE:CB	2:X:37:THR:HG22	2.49	0.42
5:K:73:LYS:HE3	5:K:77:THR:OG1	2.18	0.42
1:V:119:SER:O	1:V:127:CYS:HB2	2.19	0.42
4:T:76:PHE:HD1	4:T:94:TYR:HB3	1.84	0.42
5:K:39:MET:HG3	5:K:56:TYR:HB3	2.01	0.42
5:K:49:ARG:H	5:K:49:ARG:HH11	1.65	0.42
3:S:169:LEU:HB2	3:S:284:TRP:CZ3	2.53	0.42
4:T:114:GLN:HB2	4:T:128:GLU:HB2	2.01	0.42
7:L:13:VAL:HG11	7:L:19:VAL:HG11	2.02	0.42
7:L:154:TRP:CZ3	7:L:200:CYS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:167:ASN:HB3	7:L:181:MET:HE3	2.01	0.42
1:V:99:GLU:HB3	1:V:126:SER:HA	2.00	0.42
3:S:213:LEU:HD23	3:S:213:LEU:HA	1.92	0.42
5:K:29:LYS:HB2	5:K:29:LYS:NZ	2.33	0.42
6:H:144:THR:C	6:H:145:LEU:HD12	2.45	0.42
5:K:47:PHE:CD1	5:K:47:PHE:N	2.85	0.42
5:K:18:PRO:O	5:K:19:LEU:HB3	2.20	0.42
7:L:13:VAL:HG21	7:L:19:VAL:HG12	2.01	0.42
7:L:156:ILE:HD12	7:L:197:SER:O	2.20	0.41
7:L:193:GLU:HA	7:L:217:ARG:CZ	2.50	0.41
4:T:192:VAL:HG22	4:T:201:LYS:HG2	2.02	0.41
7:L:153:LYS:NZ	7:L:160:GLU:HG3	2.34	0.41
6:H:48:ILE:HD13	6:H:81:MET:HE1	2.01	0.41
7:L:7[A]:SER:HB2	7:L:8:PRO:HD3	2.02	0.41
3:S:186:ILE:HG22	3:S:251:PRO:HA	2.01	0.41
3:S:241:HIS:HA	3:S:383:TYR:OH	2.20	0.41
3:S:308:GLN:HB3	4:T:94:TYR:HE1	1.84	0.41
7:L:21:MET:HE1	7:L:92:TYR:HB2	2.01	0.41
1:V:101:TYR:OH	3:S:264:PRO:HA	2.21	0.41
4:T:16:SER:HA	4:T:20:LYS:O	2.20	0.41
3:S:243:ILE:HD11	3:S:387:LEU:HD21	2.03	0.41
1:V:100:GLN:CB	1:V:114:CYS:HB2	2.51	0.41
1:V:112:CYS:SG	1:V:125:VAL:HA	2.61	0.41
2:X:33:ASP:O	2:X:37:THR:HG23	2.21	0.41
3:S:382:GLN:HB2	3:S:383:TYR:CE1	2.56	0.41
6:H:174:PRO:HD3	7:L:170:THR:HG22	2.02	0.41
2:X:128:GLY:H	2:X:131:PRO:HG3	1.86	0.41
6:H:130:PRO:HD3	6:H:215:LYS:HG2	2.03	0.41
2:X:54:PRO:HB2	2:X:68:TYR:OH	2.21	0.41
4:T:173:ASN:OD1	7:L:33:GLY:HA3	2.21	0.41
6:H:35:GLU:OE1	6:H:50:ASP:HB3	2.21	0.41
2:X:49:GLN:HG2	2:X:66:GLY:HA2	2.03	0.41
3:S:308:GLN:HB3	4:T:94:TYR:CE1	2.56	0.41
3:S:210:GLU:HA	3:S:220:GLU:HG3	2.02	0.40
6:H:10:GLU:OE2	6:H:10:GLU:N	2.55	0.40
6:H:136:ALA:O	6:H:139:THR:HG23	2.21	0.40
3:S:383:TYR:CD1	3:S:383:TYR:N	2.90	0.40
7:L:125:PRO:HG3	7:L:215:PHE:CG	2.57	0.40
7:L:145:PHE:CD2	7:L:150:ILE:HD12	2.56	0.40
2:X:86:ARG:NH1	2:X:91:LEU:HB3	2.37	0.40
7:L:195:HIS:C	7:L:217:ARG:HH21	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:58:GLN:CD	2:X:58:GLN:N	2.79	0.40
3:S:286:GLN:HG2	3:S:293:THR:HG22	2.03	0.40
5:K:22:MET:H	5:K:22:MET:HG3	1.70	0.40
6:H:40:ARG:HH21	6:H:43:HIS:CE1	2.39	0.40
7:L:144:ASN:HA	7:L:178:THR:HG21	2.04	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	V	130/142 (92%)	118 (91%)	11 (8%)	1 (1%)	16	49
2	X	118/131 (90%)	95 (80%)	23 (20%)	0	100	100
3	S	252/254 (99%)	234 (93%)	18 (7%)	0	100	100
4	T	197/611 (32%)	186 (94%)	11 (6%)	0	100	100
5	K	66/68 (97%)	59 (89%)	7 (11%)	0	100	100
6	H	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
7	L	219/220 (100%)	208 (95%)	11 (5%)	0	100	100
All	All	1201/1647 (73%)	1102 (92%)	98 (8%)	1 (0%)	50	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	V	5	LEU

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	V	114/114 (100%)	114 (100%)	0	100	100
2	X	103/104 (99%)	100 (97%)	3 (3%)	37	59
3	S	216/216 (100%)	208 (96%)	8 (4%)	29	54
4	T	185/514 (36%)	184 (100%)	1 (0%)	86	92
5	K	61/61 (100%)	60 (98%)	1 (2%)	58	74
6	H	185/185 (100%)	180 (97%)	5 (3%)	40	61
7	L	197/196 (100%)	195 (99%)	2 (1%)	73	82
All	All	1061/1390 (76%)	1041 (98%)	20 (2%)	52	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	10	LYS
2	X	108	VAL
2	X	119	ASP
3	S	188	VAL
3	S	195	PHE
3	S	198(B)	ILE
3	S	233	THR
3	S	278	PHE
3	S	302	VAL
3	S	387	LEU
3	S	399	VAL
4	T	63	ILE
5	K	78	ARG
6	H	11	LEU
6	H	28	THR
6	H	123	THR
6	H	128	VAL
6	H	202	CYS
7	L	6	GLN
7	L	96	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	S	250	GLN
4	T	31	ASN
4	T	110	GLN
4	T	124	ASN
4	T	199	ASN
6	H	39	GLN
7	L	44	GLN
7	L	48	GLN
7	L	95	GLN
7	L	96	ASN
7	L	130	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

21 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CGU	V	26	9,8,1	9,11,12	1.18	0	10,14,16	1.08	0
2	CGU	X	6	9,2	9,11,12	1.19	0	10,14,16	1.31	1 (10%)
2	CGU	X	14	2,8	9,11,12	1.16	0	10,14,16	1.23	0
2	CGU	X	16	9,2	9,11,12	1.17	0	10,14,16	1.23	0
2	CGU	X	7	9,2	9,11,12	1.19	0	10,14,16	0.99	1 (10%)
2	CGU	X	29	9,2	9,11,12	1.16	0	10,14,16	1.33	1 (10%)
1	CGU	V	25	8,1	9,11,12	1.15	0	10,14,16	1.12	0
2	CGU	X	20	9,2	9,11,12	1.18	0	10,14,16	1.15	0
1	CGU	V	14	8,1	9,11,12	1.16	0	10,14,16	1.15	0
2	CGU	X	39	2	9,11,12	1.17	0	10,14,16	1.31	1 (10%)
2	CGU	X	25	9,2	9,11,12	1.16	0	10,14,16	1.45	2 (20%)
1	CGU	V	29	9,8,1	9,11,12	1.18	0	10,14,16	1.23	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CGU	V	19	8,1	9,11,12	1.19	0	10,14,16	1.20	0
2	CGU	X	26	9,2	9,11,12	1.15	0	10,14,16	1.20	1 (10%)
2	CGU	X	19	2,8	9,11,12	1.16	0	10,14,16	1.26	1 (10%)
2	CGU	X	32	2	9,11,12	1.20	0	10,14,16	1.10	0
1	CGU	V	20	9,1	9,11,12	1.19	0	10,14,16	1.39	1 (10%)
1	CGU	V	16	9,8,1	9,11,12	1.18	0	10,14,16	1.25	0
1	CGU	V	6	9,1	9,11,12	1.16	0	10,14,16	1.36	1 (10%)
1	CGU	V	35	1	9,11,12	1.23	0	10,14,16	1.17	0
1	CGU	V	7	9,8,1	9,11,12	1.19	0	10,14,16	1.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CGU	V	26	9,8,1	-	6/13/14/16	-
2	CGU	X	6	9,2	-	6/13/14/16	-
2	CGU	X	14	2,8	-	5/13/14/16	-
2	CGU	X	16	9,2	-	3/13/14/16	-
2	CGU	X	7	9,2	-	4/13/14/16	-
2	CGU	X	29	9,2	-	6/13/14/16	-
1	CGU	V	25	8,1	-	1/13/14/16	-
2	CGU	X	20	9,2	-	2/13/14/16	-
1	CGU	V	14	8,1	-	5/13/14/16	-
2	CGU	X	39	2	-	1/13/14/16	-
2	CGU	X	25	9,2	-	5/13/14/16	-
1	CGU	V	29	9,8,1	-	5/13/14/16	-
1	CGU	V	19	8,1	-	3/13/14/16	-
2	CGU	X	26	9,2	-	2/13/14/16	-
2	CGU	X	19	2,8	-	2/13/14/16	-
2	CGU	X	32	2	-	7/13/14/16	-
1	CGU	V	20	9,1	-	4/13/14/16	-
1	CGU	V	16	9,8,1	-	3/13/14/16	-
1	CGU	V	6	9,1	-	3/13/14/16	-
1	CGU	V	35	1	-	3/13/14/16	-
1	CGU	V	7	9,8,1	-	8/13/14/16	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	6	CGU	CB-CG-CD1	-2.84	107.35	113.11
2	X	25	CGU	CB-CG-CD2	-2.70	107.64	113.11
1	V	20	CGU	CB-CG-CD2	-2.59	107.86	113.11
2	X	29	CGU	CB-CG-CD2	-2.31	108.42	113.11
2	X	6	CGU	CB-CG-CD1	-2.28	108.47	113.11
2	X	19	CGU	CB-CG-CD2	-2.28	108.47	113.11
2	X	26	CGU	CB-CG-CD2	-2.22	108.61	113.11
2	X	39	CGU	CB-CG-CD1	-2.21	108.63	113.11
2	X	25	CGU	CB-CG-CD1	-2.09	108.86	113.11
1	V	29	CGU	CB-CG-CD1	-2.06	108.92	113.11
2	X	7	CGU	OE22-CD2-OE21	-2.05	119.43	124.08

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	V	6	CGU	CA-CB-CG-CD1
1	V	6	CGU	CA-CB-CG-CD2
1	V	7	CGU	CA-CB-CG-CD1
1	V	7	CGU	CA-CB-CG-CD2
1	V	7	CGU	OE11-CD1-CG-CB
1	V	7	CGU	OE12-CD1-CG-CB
1	V	7	CGU	OE12-CD1-CG-CD2
1	V	14	CGU	CA-CB-CG-CD1
1	V	14	CGU	CA-CB-CG-CD2
1	V	14	CGU	OE12-CD1-CG-CD2
1	V	16	CGU	N-CA-CB-CG
1	V	19	CGU	C-CA-CB-CG
1	V	19	CGU	CA-CB-CG-CD1
1	V	20	CGU	N-CA-CB-CG
1	V	20	CGU	C-CA-CB-CG
1	V	25	CGU	C-CA-CB-CG
1	V	26	CGU	N-CA-CB-CG
1	V	26	CGU	C-CA-CB-CG
1	V	26	CGU	CA-CB-CG-CD2
2	X	6	CGU	CA-CB-CG-CD1
2	X	6	CGU	CA-CB-CG-CD2
2	X	14	CGU	C-CA-CB-CG
2	X	14	CGU	CA-CB-CG-CD1
2	X	14	CGU	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
2	X	20	CGU	N-CA-CB-CG
2	X	20	CGU	C-CA-CB-CG
2	X	25	CGU	C-CA-CB-CG
2	X	25	CGU	CA-CB-CG-CD1
2	X	25	CGU	CA-CB-CG-CD2
2	X	25	CGU	OE22-CD2-CG-CD1
2	X	29	CGU	N-CA-CB-CG
2	X	29	CGU	C-CA-CB-CG
2	X	32	CGU	CA-CB-CG-CD2
2	X	39	CGU	O-C-CA-CB
1	V	35	CGU	CA-CB-CG-CD2
2	X	32	CGU	CA-CB-CG-CD1
1	V	7	CGU	N-CA-CB-CG
1	V	26	CGU	OE21-CD2-CG-CB
1	V	26	CGU	OE22-CD2-CG-CB
1	V	29	CGU	OE21-CD2-CG-CB
1	V	29	CGU	OE22-CD2-CG-CB
2	X	6	CGU	OE21-CD2-CG-CB
2	X	6	CGU	OE22-CD2-CG-CB
2	X	26	CGU	OE11-CD1-CG-CB
2	X	26	CGU	OE12-CD1-CG-CB
2	X	29	CGU	OE21-CD2-CG-CB
2	X	29	CGU	OE22-CD2-CG-CB
2	X	32	CGU	OE21-CD2-CG-CB
2	X	32	CGU	OE22-CD2-CG-CB
1	V	6	CGU	OE21-CD2-CG-CD1
1	V	7	CGU	OE11-CD1-CG-CD2
2	X	14	CGU	OE21-CD2-CG-CD1
2	X	14	CGU	OE22-CD2-CG-CD1
2	X	16	CGU	OE21-CD2-CG-CD1
2	X	19	CGU	OE21-CD2-CG-CD1
2	X	19	CGU	OE22-CD2-CG-CD1
2	X	25	CGU	OE21-CD2-CG-CD1
2	X	32	CGU	OE21-CD2-CG-CD1
2	X	32	CGU	OE22-CD2-CG-CD1
1	V	7	CGU	C-CA-CB-CG
1	V	16	CGU	C-CA-CB-CG
2	X	6	CGU	C-CA-CB-CG
1	V	26	CGU	CA-CB-CG-CD1
1	V	19	CGU	N-CA-CB-CG
2	X	6	CGU	N-CA-CB-CG
2	X	7	CGU	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	X	32	CGU	N-CA-CB-CG
1	V	29	CGU	OE11-CD1-CG-CB
1	V	29	CGU	OE12-CD1-CG-CB
1	V	35	CGU	OE11-CD1-CG-CB
1	V	35	CGU	OE12-CD1-CG-CB
2	X	7	CGU	OE21-CD2-CG-CB
2	X	7	CGU	OE22-CD2-CG-CB
1	V	14	CGU	OE11-CD1-CG-CD2
1	V	14	CGU	OE21-CD2-CG-CD1
1	V	16	CGU	OE21-CD2-CG-CD1
1	V	20	CGU	OE21-CD2-CG-CD1
1	V	20	CGU	OE22-CD2-CG-CD1
1	V	29	CGU	OE22-CD2-CG-CD1
2	X	7	CGU	OE11-CD1-CG-CD2
2	X	16	CGU	OE11-CD1-CG-CD2
2	X	16	CGU	OE22-CD2-CG-CD1
2	X	29	CGU	OE21-CD2-CG-CD1
2	X	29	CGU	OE22-CD2-CG-CD1

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	V	25	CGU	1	0
1	V	14	CGU	1	0
2	X	39	CGU	1	0
1	V	29	CGU	1	0
1	V	35	CGU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 16 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	BGC	V	208	1	11,11,12	1.68	3 (27%)	15,15,17	0.93	0
11	FUC	V	209	1	10,10,11	1.73	3 (30%)	14,14,16	1.12	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BGC	V	208	1	-	2/2/19/22	0/1/1/1
11	FUC	V	209	1	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	V	208	BGC	O5-C1	4.24	1.50	1.43
11	V	209	FUC	O5-C1	4.14	1.50	1.43
11	V	209	FUC	C2-C3	-2.51	1.48	1.52
10	V	208	BGC	C2-C3	-2.48	1.48	1.52
11	V	209	FUC	O5-C5	2.11	1.47	1.43
10	V	208	BGC	O5-C5	2.02	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	209	FUC	C6-C5-C4	-2.63	108.27	113.08

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	V	208	BGC	C4-C5-C6-O6
10	V	208	BGC	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

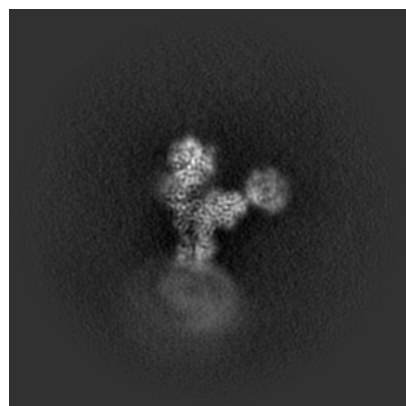
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71090. These allow visual inspection of the internal detail of the map and identification of artifacts.

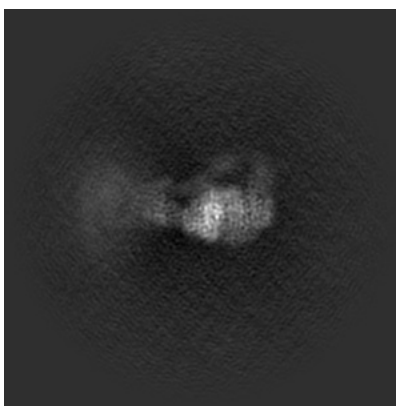
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

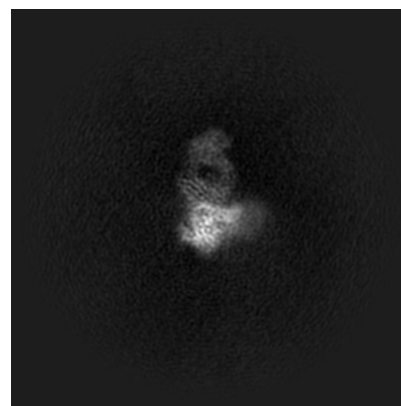
6.1.1 Primary map



X

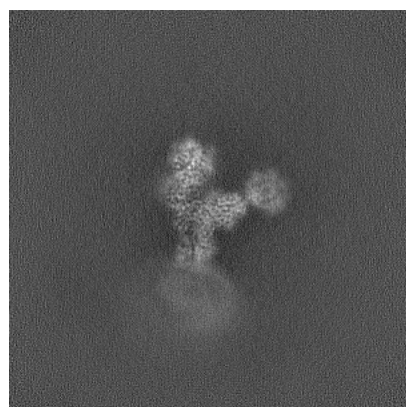


Y

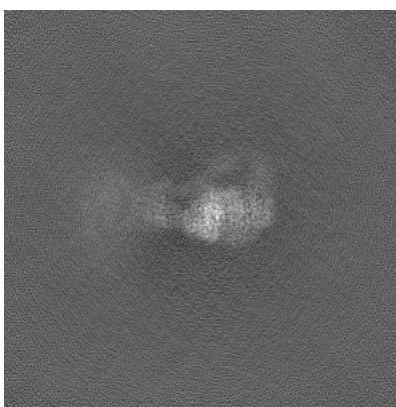


Z

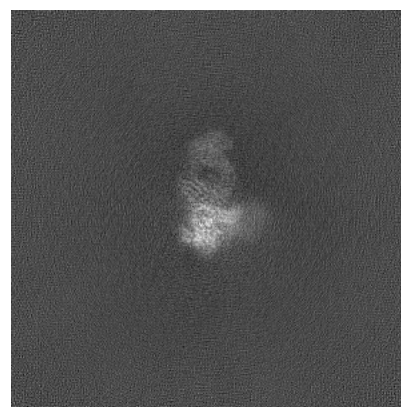
6.1.2 Raw map



X



Y

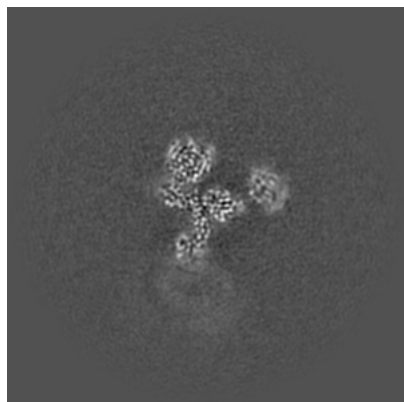


Z

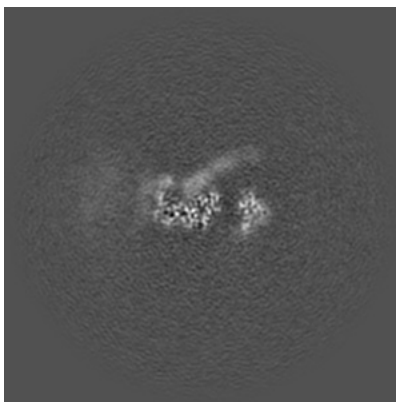
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

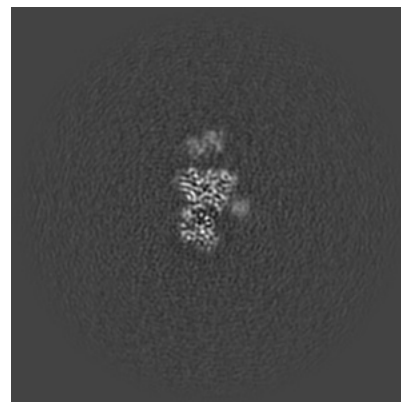
6.2.1 Primary map



X Index: 210

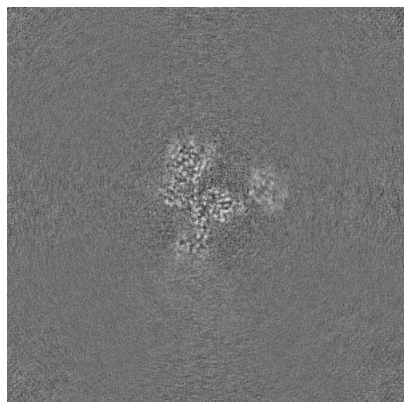


Y Index: 210

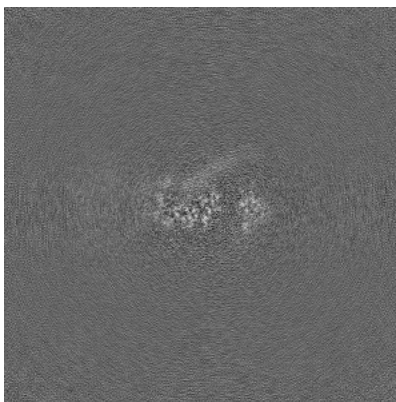


Z Index: 210

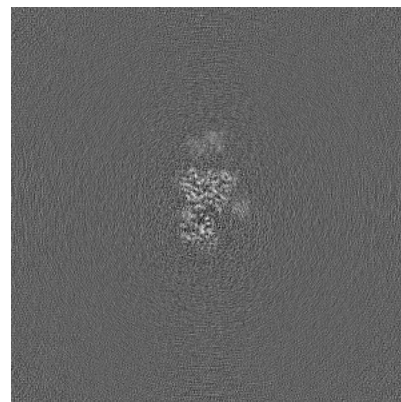
6.2.2 Raw map



X Index: 210



Y Index: 210

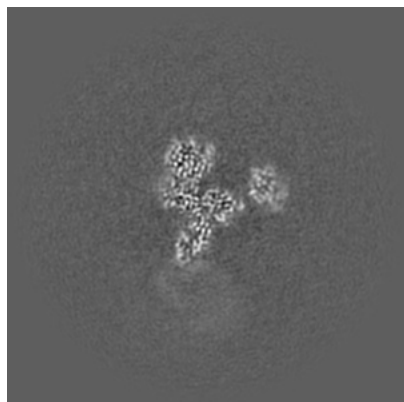


Z Index: 210

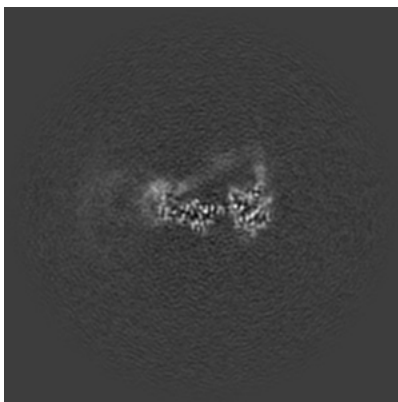
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

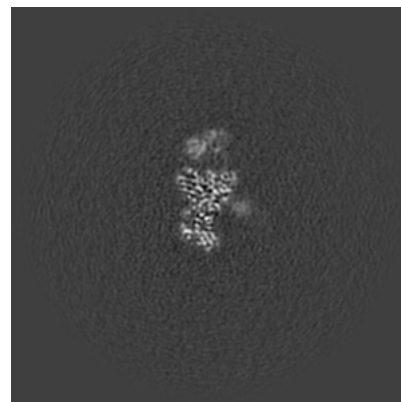
6.3.1 Primary map



X Index: 208

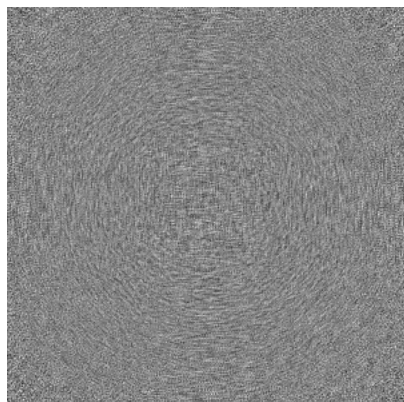


Y Index: 198

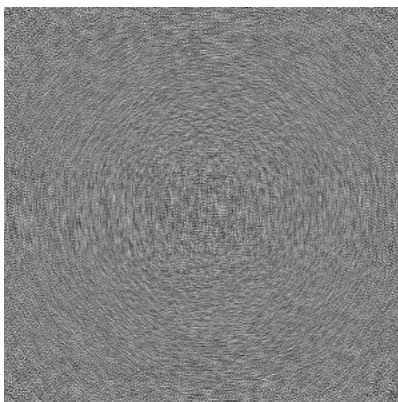


Z Index: 212

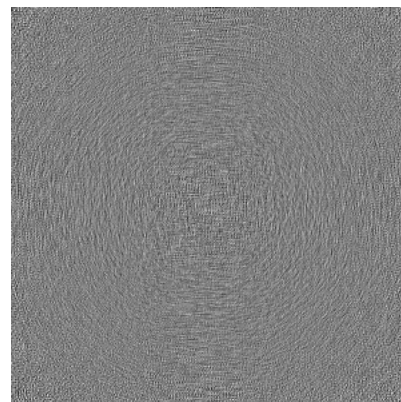
6.3.2 Raw map



X Index: 0



Y Index: 0

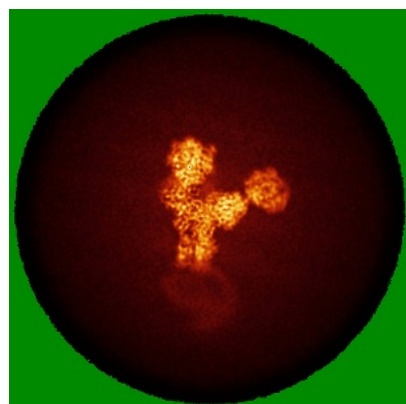


Z Index: 419

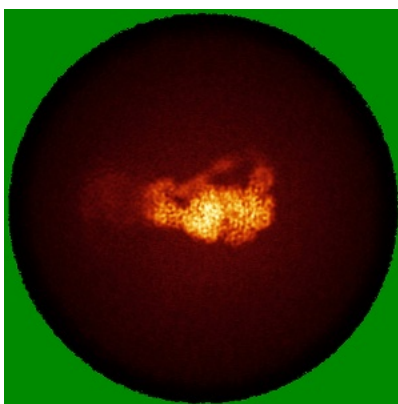
The images above show the largest variance slices of the map in three orthogonal directions.

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

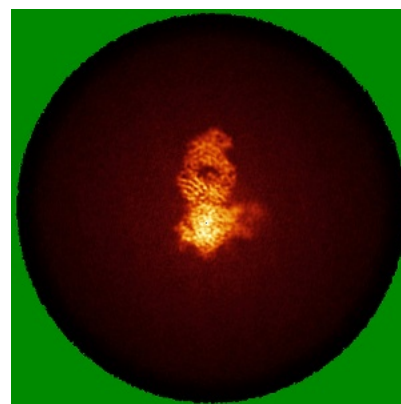
6.4.1 Primary map



X

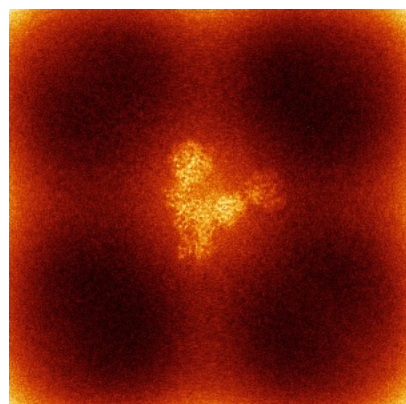


Y

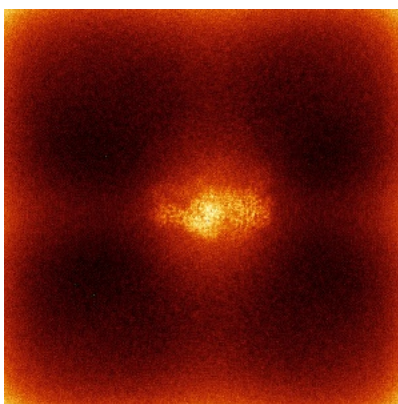


Z

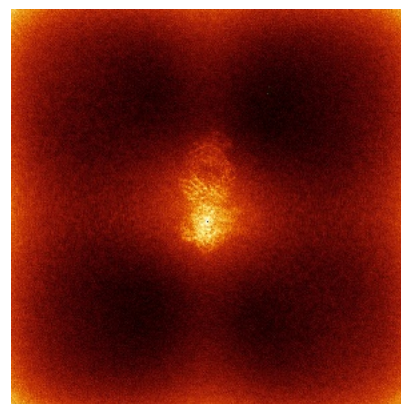
6.4.2 Raw map



X



Y

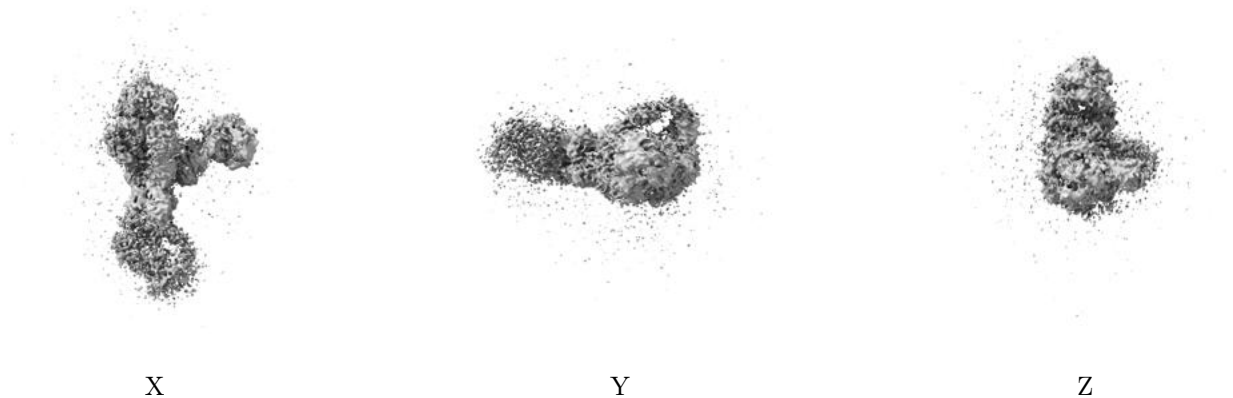


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

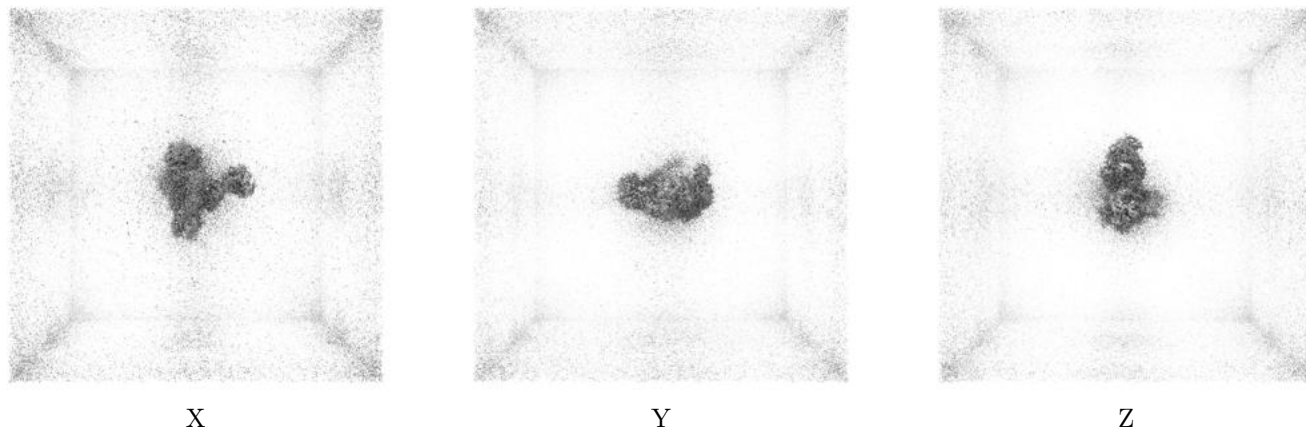
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

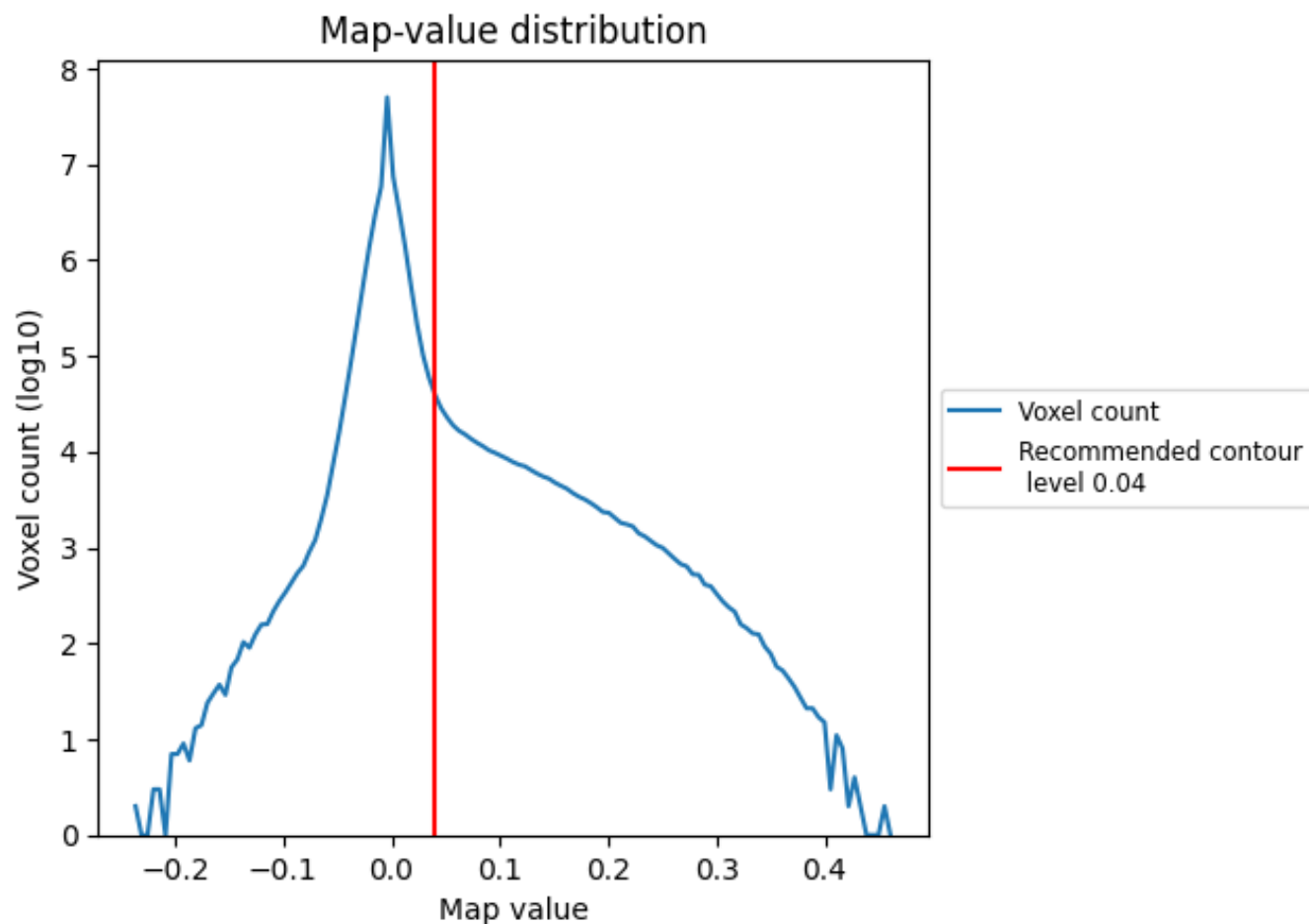
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

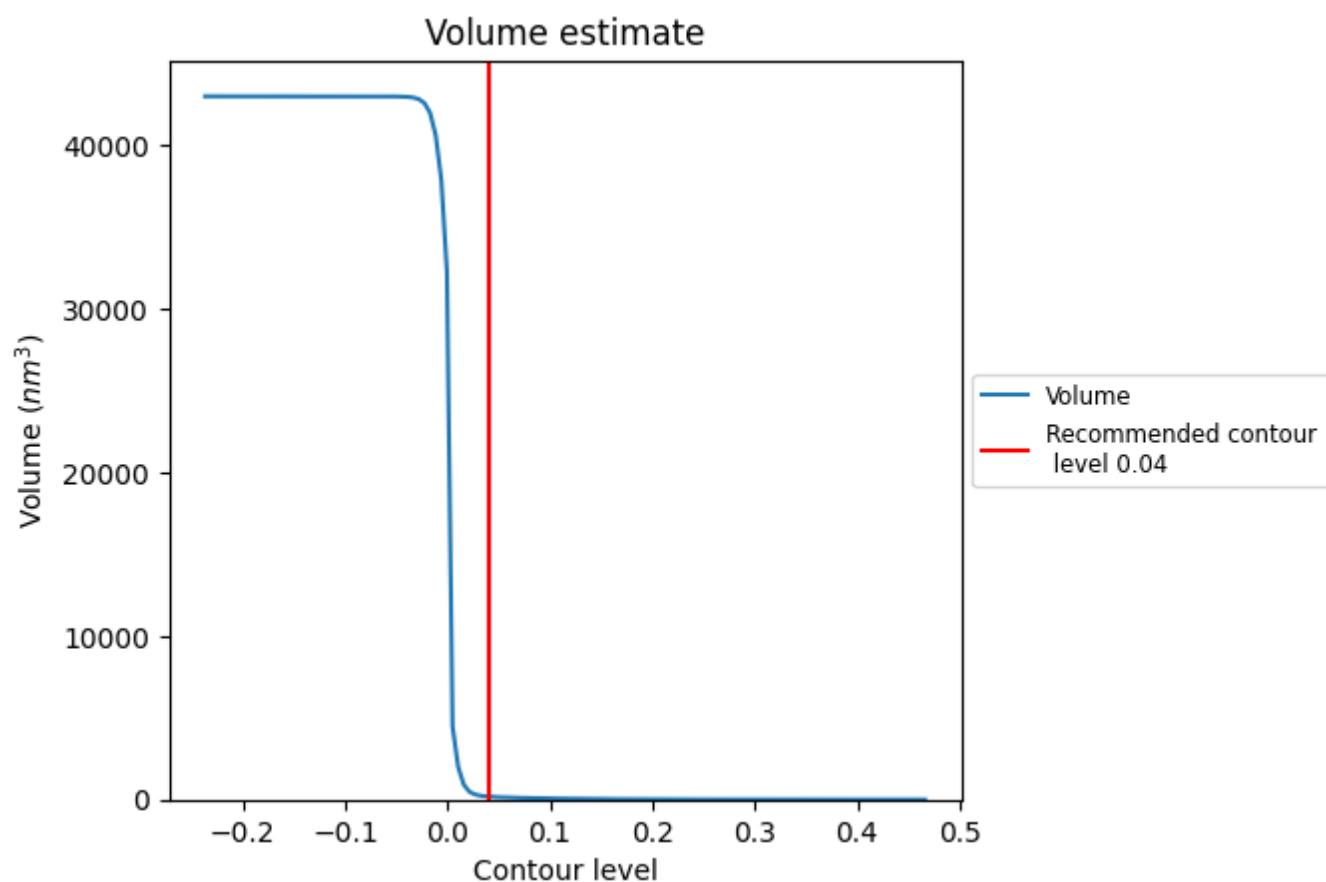
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

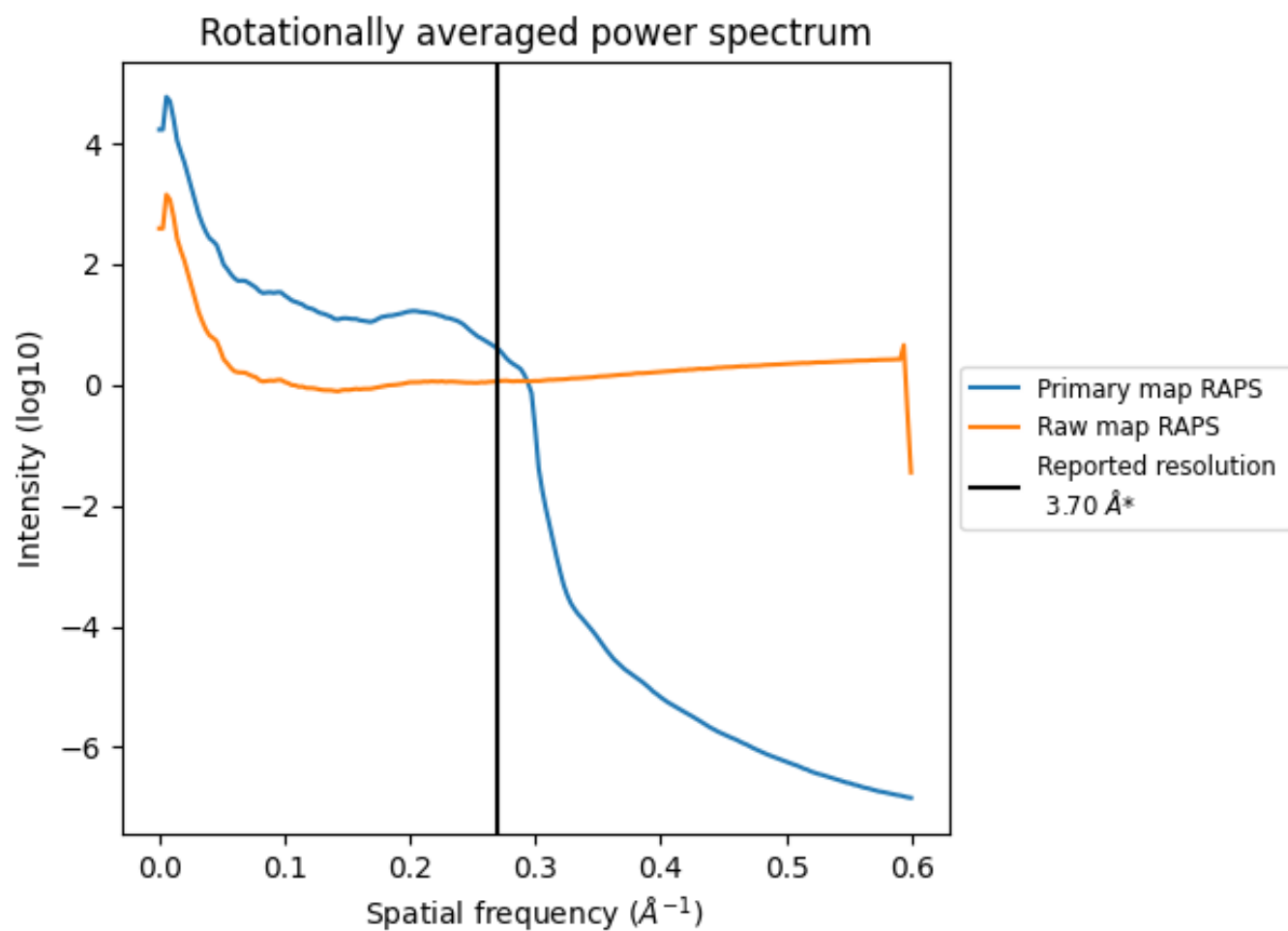
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 184 nm³; this corresponds to an approximate mass of 166 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 ⓘ

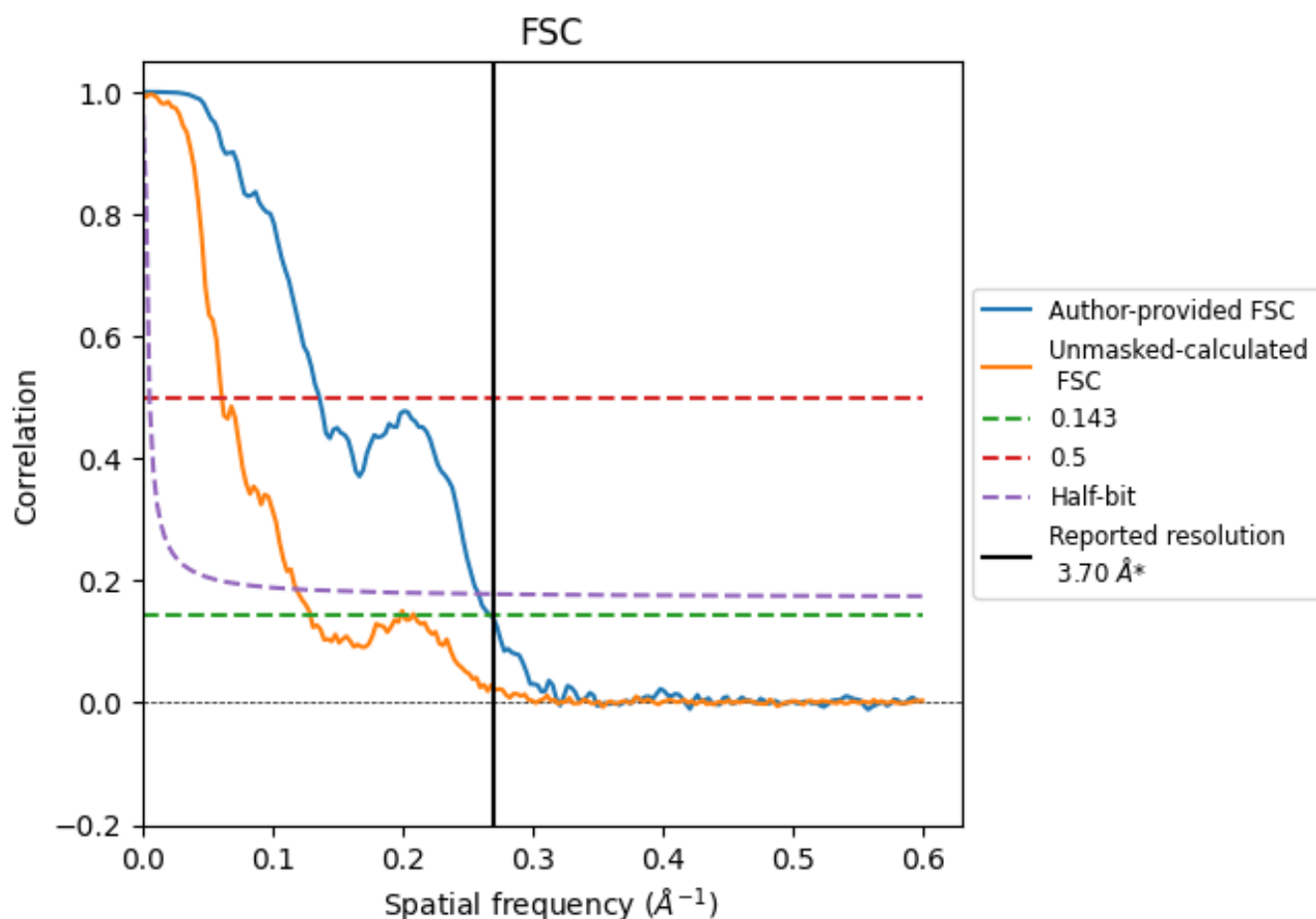


*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

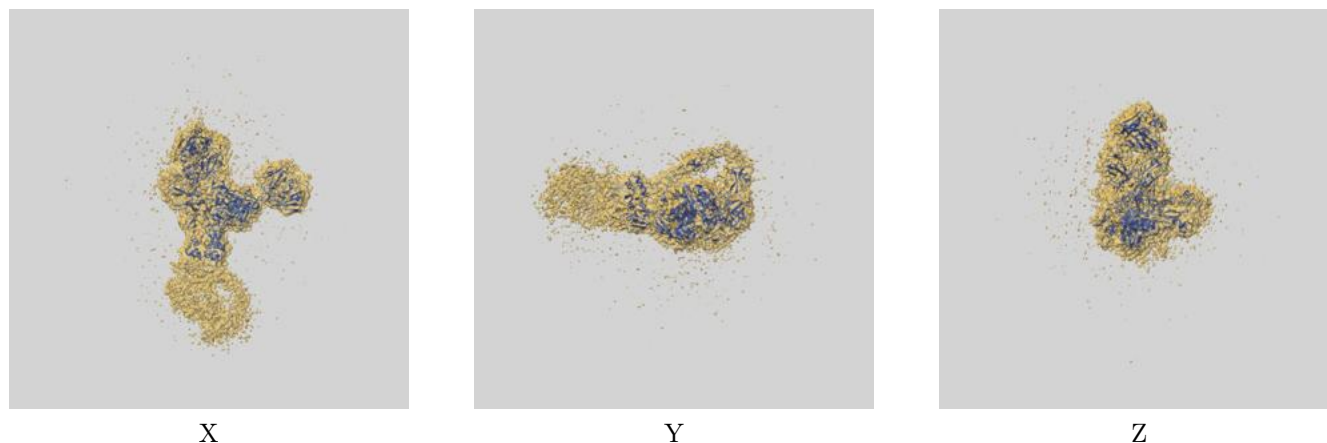
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	7.35	3.87
Unmasked-calculated*	7.74	16.34	8.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.74 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

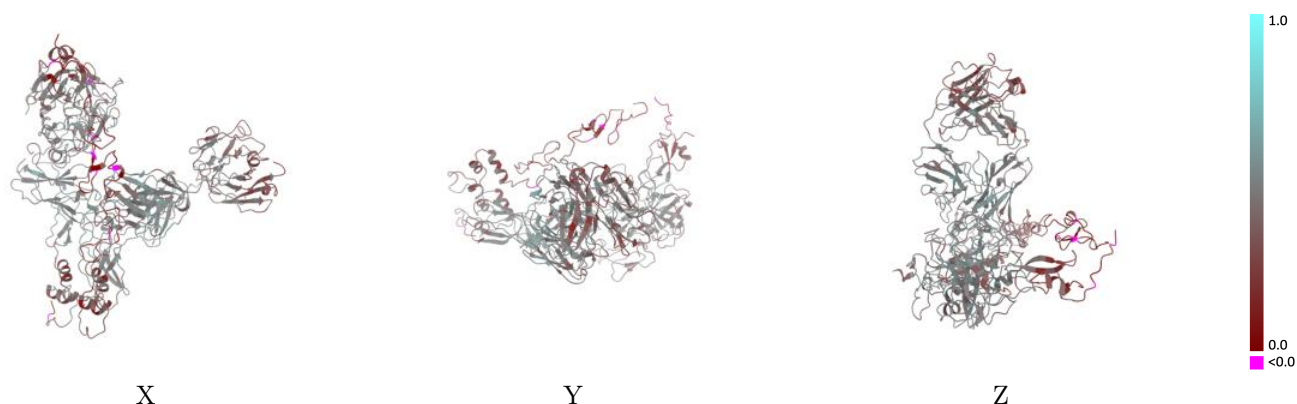
This section contains information regarding the fit between EMDB map EMD-71090 and PDB model 9P0X. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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](#)



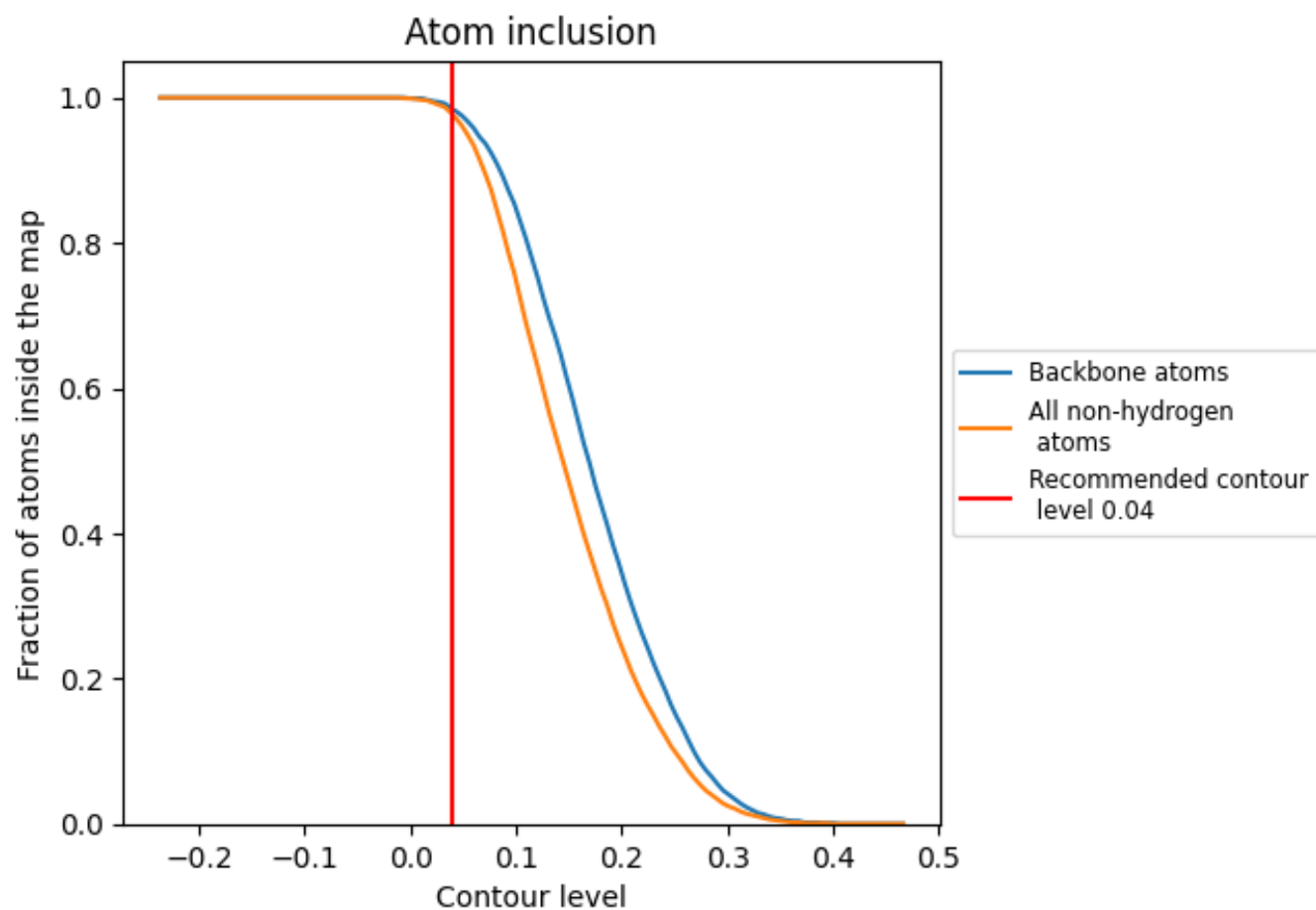
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9770</div>	<div><div></div>0.4250</div>
H	<div><div></div>0.9910</div>	<div><div></div>0.4530</div>
K	<div><div></div>0.9300</div>	<div><div></div>0.2910</div>
L	<div><div></div>0.9920</div>	<div><div></div>0.4330</div>
S	<div><div></div>0.9920</div>	<div><div></div>0.4620</div>
T	<div><div></div>0.9830</div>	<div><div></div>0.4960</div>
V	<div><div></div>0.9820</div>	<div><div></div>0.4240</div>
X	<div><div></div>0.9140</div>	<div><div></div>0.2590</div>

1.0

0.0

<0.0