



## Full wwPDB EM Validation Report ⓘ

Sep 2, 2025 – 03:18 PM EDT

PDB ID : 9O2Z / pdb\_00009o2z  
EMDB ID : EMD-70053  
Title : Autoinhibited BRAF:(14-3-3)2:MEK complex from Insect cells  
Authors : Martinez Fiesco, J.A.; Zhang, P.  
Deposited on : 2025-04-04  
Resolution : 3.83 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.dev126  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
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) : 2.45.1

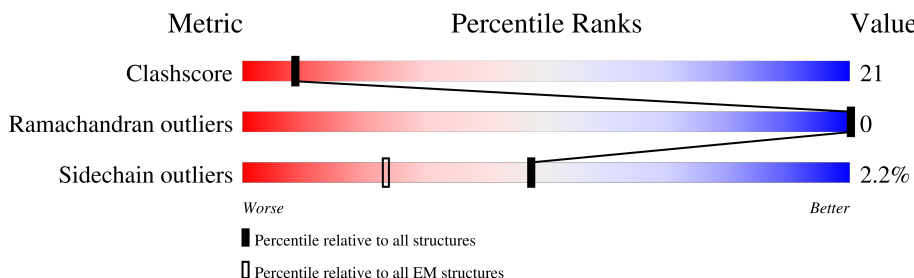
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.83 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	766	
2	B	393	
3	C	245	
3	D	245	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SEP	A	365	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9141 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 Serine/threonine-protein kinase B-raf.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	412	Total	C	N	O	P	S	0	0
			3311	2108	593	585	2	23		

- Molecule 2 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	293	Total	C	N	O	S	0	0
			2291	1465	390	421	15		

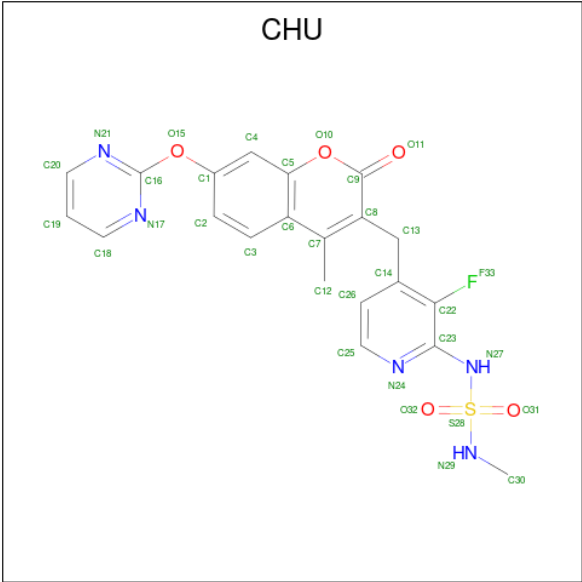
- Molecule 3 is a protein called 14-3-3 protein zeta/delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	220	Total	C	N	O	S	0	0
			1738	1095	290	344	9		
3	D	224	Total	C	N	O	S	0	0
			1766	1113	298	346	9		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

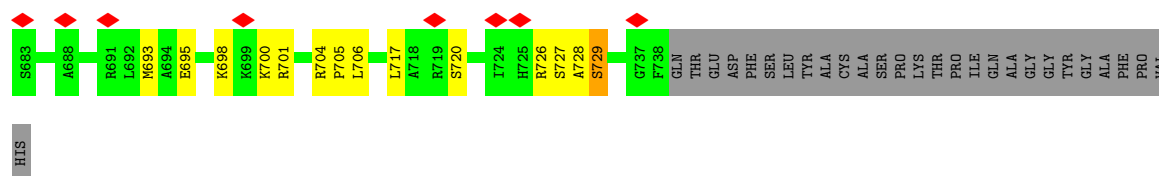
Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	

- Molecule 5 is N-(3-fluoro-4-{[4-methyl-2-oxo-7-(pyrimidin-2-yloxy)-2H-chromen-3-yl]methyl}pyridin-2-yl)-N'-methylsulfuric diamide (CCD ID: CHU) (formula: C<sub>21</sub>H<sub>18</sub>FN<sub>5</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



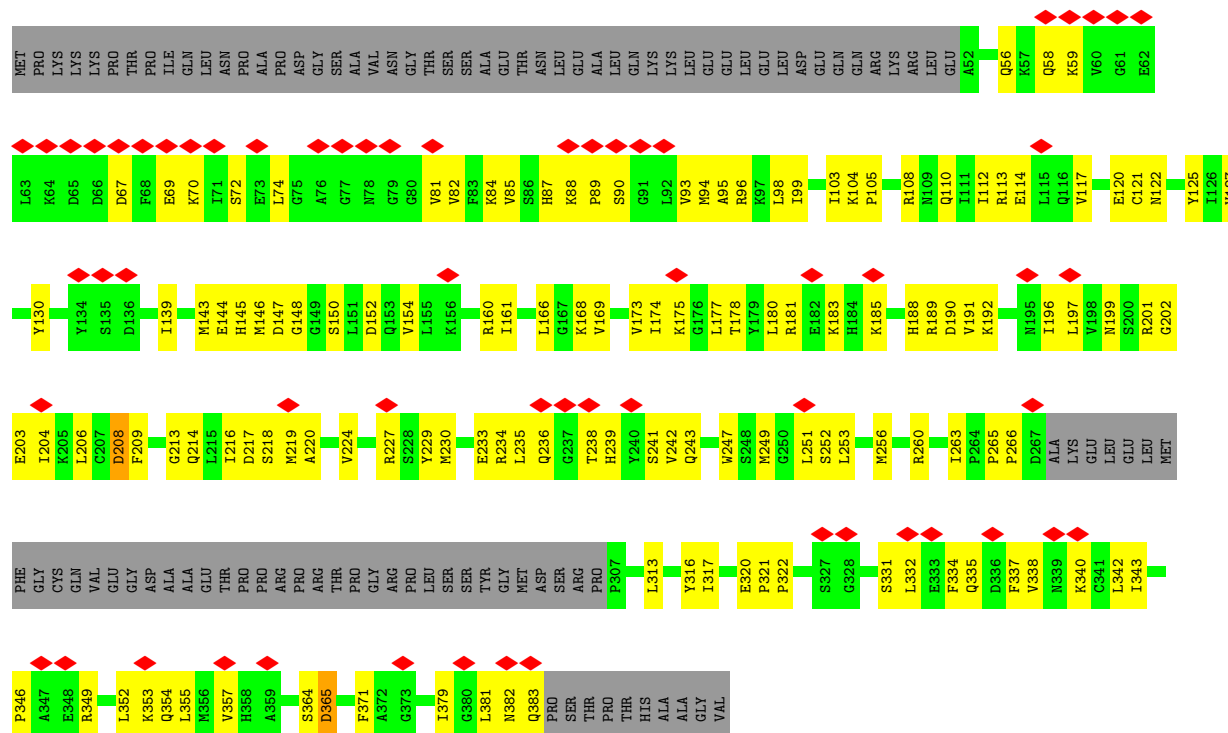
Mol	Chain	Residues	Atoms						AltConf
			Total	C	F	N	O	S	
5	B	1	33	21	1	5	5	1	0





• Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1

Chain B: 15% 40% 34% 25%



GLU	S156	Y52	MET
ALA	K157	R83	D2
GLY	K158	R84	K3
GLU	S159	K85	
GLY	M160	I86	V7
GLY	Q161	E87	
GLU	T162	L90	A10
ASN	T163	D91	
	H164	R92	Q14
	P165	D93	Q15
	I166	I93	A16
	R167	C94	E17
	L168	N95	R18
	G169	D96	
		V97	M22
	L172	L98	A23
	M173	S99	
	V176	L100	M26
	F177	L101	
	I181	L105	S37
	S190	I106	N38
		Q111	E39
	T194	A112	E40
	F195	E113	R41
	F196		M42
	T200	V116	L43
		F117	S45
	S207	Y118	V46
		L119	A47
	S210	K120	Y48
	Y211	M121	V51
	K212	D124	V52
	D213	Y125	R56
	S214	Y126	S57
	T215	R127	S58
	L216	Y128	M59
	T217	L129	R60
	M218	A130	V61
	Q219	A133	V62
	L220	ALA	S63
	L221	GLY	S64
	R222	ASP	I65
	D223	D137	E66
	M224	K138	Q67
	L225	K139	K68
	T226	G140	T69
		I141	GLU
	T229	V142	GLY
	S230		A72
	ASP	S145	K75
	THR		Q76
	GLN	E151	Q77
	GLY	A152	M78
	ASP	F153	A79
	GLU	E154	R80
	ALA	T155	E81

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.534	Depositor
Minimum map value	-0.381	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.079	Depositor
Map size (Å)	275.4, 275.4, 275.4	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CHU, SEP, ZN

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	0.20	0/3362	0.48	1/4528 (0.0%)
2	B	0.14	0/2338	0.42	0/3151
3	C	0.19	0/1761	0.51	0/2372
3	D	0.19	0/1788	0.53	0/2409
All	All	0.18	0/9249	0.48	1/12460 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	HIS	CB-CA-C	-8.44	94.06	110.10

There are no chirality outliers.

There are no planarity outliers.

### 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	3311	0	3326	129	0
2	B	2291	0	2321	104	0
3	C	1738	0	1690	71	0
3	D	1766	0	1725	92	0
4	A	2	0	0	0	0
5	B	33	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9141	0	9080	378	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 21.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:HIS:O	1:A:370:HIS:ND1	1.74	1.21
1:A:370:HIS:O	1:A:370:HIS:CG	2.23	0.91
2:B:99:ILE:HG12	2:B:219:MET:HE1	1.59	0.84
2:B:146:MET:HB3	2:B:199:ASN:HB3	1.65	0.78
1:A:695:GLU:HA	1:A:698:LYS:HD3	1.63	0.78
3:D:91:ARG:O	3:D:95:ASN:ND2	2.19	0.76
3:D:124:ASP:OD1	3:D:127:ARG:NH2	2.18	0.76
2:B:343:ILE:H	2:B:349:ARG:HH12	1.32	0.76
1:A:261:CYS:CB	1:A:264:CYS:SG	2.74	0.75
3:C:169:GLY:O	3:C:173:ASN:ND2	2.21	0.73
1:A:472:TYR:HB2	1:A:482:VAL:HB	1.71	0.73
1:A:646:LEU:HD23	1:A:693:MET:HB2	1.71	0.71
2:B:189:ARG:HH11	2:B:234:ARG:HH21	1.37	0.71
2:B:230:MET:HE1	2:B:234:ARG:NH1	2.06	0.71
3:C:37:SER:OG	3:C:40:GLU:OE1	2.07	0.71
2:B:173:VAL:HG23	2:B:206:LEU:HD11	1.73	0.71
1:A:550:MET:HA	1:A:553:LEU:HB3	1.73	0.71
2:B:230:MET:HE1	2:B:234:ARG:HH11	1.54	0.70
3:C:61:VAL:O	3:C:65:ILE:HD12	1.93	0.69
3:D:47:ALA:O	3:D:51:VAL:HG23	1.92	0.69
3:D:127:ARG:NH2	3:D:173:ASN:OD1	2.25	0.69
1:A:452:ILE:HD11	1:A:517:MET:HG3	1.73	0.68
1:A:187:MET:HE3	1:A:188:ARG:HH12	1.58	0.68
2:B:243:GLN:HB3	2:B:349:ARG:HG2	1.75	0.68
3:D:190:SER:O	3:D:194:THR:HG23	1.95	0.67
3:D:48:TYR:O	3:D:52:VAL:HG12	1.95	0.66
3:D:75:LYS:HG3	3:D:78:MET:HE2	1.78	0.66
3:C:124:ASP:OD1	3:C:127:ARG:NH2	2.18	0.66
1:A:662:ARG:HH12	2:B:224:VAL:HG23	1.60	0.66
1:A:462:ARG:NH2	1:A:464:GLY:O	2.29	0.65
2:B:104:LYS:HD3	2:B:105:PRO:HD2	1.79	0.65
1:A:626:ARG:HB3	1:A:628:GLN:HG3	1.77	0.65
2:B:105:PRO:HA	2:B:108:ARG:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LYS:NZ	2:B:364:SER:O	2.30	0.65
2:B:110:GLN:HA	2:B:113:ARG:HH12	1.61	0.64
1:A:487:VAL:O	1:A:524:GLN:NE2	2.29	0.63
3:C:48:TYR:O	3:C:52:VAL:HG23	1.99	0.63
3:D:97:VAL:O	3:D:101:LEU:HD12	1.97	0.63
3:D:116:VAL:HG21	3:D:156:SER:HB3	1.80	0.63
3:D:126:TYR:HB2	3:D:145:SER:HB3	1.80	0.63
2:B:70:LYS:HA	2:B:85:VAL:HG23	1.81	0.63
3:C:81:GLU:HA	3:C:84:GLU:HG3	1.81	0.62
3:C:125:TYR:O	3:C:129:LEU:HD12	1.99	0.62
3:C:137:ASP:O	3:C:141:ILE:HG12	2.00	0.62
3:D:38:ASN:HA	3:D:41:ARG:HH11	1.64	0.62
3:C:215:THR:OG1	3:C:219:GLN:NE2	2.32	0.62
2:B:166:LEU:HA	2:B:169:VAL:HG12	1.80	0.62
1:A:507:LYS:HA	1:A:507:LYS:HE2	1.81	0.62
2:B:74:LEU:HD12	2:B:82:VAL:HB	1.81	0.61
2:B:58:GLN:OE1	2:B:58:GLN:N	2.29	0.61
3:D:154:GLU:O	3:D:158:LYS:NZ	2.32	0.61
3:C:160:MET:HE1	3:C:167:ARG:HB2	1.82	0.61
3:C:6:LEU:HB3	3:C:29:VAL:HG22	1.83	0.61
2:B:196:ILE:HG23	2:B:206:LEU:HD12	1.83	0.60
1:A:726:ARG:HD3	3:D:60:ARG:NH1	2.17	0.60
3:C:122:LYS:HE2	3:C:126:TYR:HE2	1.67	0.60
2:B:337:PHE:HA	2:B:340:LYS:HE3	1.84	0.60
3:C:44:LEU:HD12	3:C:48:TYR:HE1	1.67	0.60
1:A:172:ARG:NH2	1:A:176:THR:O	2.35	0.60
3:D:164:HIS:CD2	3:D:166:ILE:HD12	2.37	0.60
2:B:230:MET:HB3	2:B:235:LEU:HD21	1.83	0.59
3:D:222:ARG:HA	3:D:225:LEU:HD12	1.83	0.59
1:A:182:LYS:HD3	1:A:192:PRO:HG3	1.84	0.59
1:A:472:TYR:N	1:A:482:VAL:O	2.36	0.59
2:B:147:ASP:N	2:B:147:ASP:OD2	2.36	0.59
1:A:646:LEU:HD12	1:A:649:LEU:HD12	1.85	0.59
3:D:119:LEU:HB3	3:D:152:ALA:HB2	1.84	0.59
3:D:213:ASP:O	3:D:217:ILE:HG12	2.02	0.59
3:C:59:TRP:NE1	3:C:87:GLU:OE2	2.35	0.58
2:B:177:LEU:HD11	2:B:352:LEU:HD21	1.85	0.58
3:D:221:LEU:HA	3:D:224:ASN:ND2	2.19	0.58
3:C:195:ALA:HA	3:C:198:GLU:OE1	2.04	0.58
3:D:101:LEU:HA	3:D:105:LEU:HB2	1.84	0.58
3:D:151:GLU:O	3:D:155:ILE:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:ASP:O	3:C:217:ILE:HG13	2.04	0.58
1:A:549:GLU:OE2	1:A:549:GLU:N	2.35	0.58
3:D:26:MET:HE2	3:D:26:MET:HA	1.86	0.58
1:A:178:ARG:O	1:A:182:LYS:HB2	2.04	0.58
1:A:247:PHE:HZ	3:C:216:LEU:HD11	1.70	0.57
3:D:130:ALA:HB1	3:D:142:VAL:HG12	1.86	0.57
3:D:90:LEU:HA	3:D:93:ILE:HG22	1.86	0.57
3:C:124:ASP:OD1	3:C:149:TYR:OH	2.23	0.57
3:C:178:TYR:HA	3:C:182:LEU:HB2	1.86	0.56
1:A:620:MET:HG3	1:A:624:VAL:HB	1.86	0.56
1:A:361:ASP:OD1	1:A:361:ASP:N	2.37	0.56
1:A:582:ILE:HG23	1:A:592:ILE:HG13	1.87	0.56
1:A:617:ILE:HA	1:A:620:MET:CE	2.35	0.56
2:B:189:ARG:HH11	2:B:234:ARG:NH2	2.02	0.56
2:B:334:PHE:O	2:B:338:VAL:HG23	2.05	0.56
1:A:255:LEU:HD11	1:A:269:HIS:HB2	1.87	0.56
1:A:370:HIS:ND1	1:A:370:HIS:C	2.58	0.56
3:D:38:ASN:OD1	3:D:38:ASN:N	2.39	0.56
3:C:58:SER:O	3:C:62:VAL:HG13	2.06	0.55
2:B:121:CYS:SG	2:B:183:LYS:NZ	2.79	0.55
1:A:185:LEU:O	1:A:190:LEU:N	2.27	0.55
1:A:495:LEU:O	1:A:499:LYS:HG2	2.06	0.55
1:A:576:ASP:O	1:A:581:ASN:ND2	2.39	0.55
2:B:146:MET:SD	2:B:197:LEU:HB3	2.46	0.55
1:A:617:ILE:HD11	1:A:662:ARG:NH1	2.22	0.55
2:B:332:LEU:HA	2:B:335:GLN:HG2	1.88	0.55
3:C:177:PHE:HD2	3:C:181:ILE:HD13	1.72	0.55
3:D:63:SER:O	3:D:67:GLN:HG2	2.07	0.55
3:D:125:TYR:HA	3:D:128:TYR:CD2	2.42	0.55
2:B:114:GLU:O	2:B:117:VAL:HG12	2.07	0.55
2:B:313:LEU:O	2:B:317:ILE:HG13	2.06	0.55
1:A:217:LEU:HD11	1:A:222:LEU:HD11	1.88	0.54
1:A:365:SEP:OG	1:A:366:ALA:N	2.30	0.54
3:C:217:ILE:O	3:C:221:LEU:HG	2.08	0.54
2:B:110:GLN:HA	2:B:113:ARG:NH1	2.23	0.54
3:C:74:LYS:O	3:C:77:GLN:NE2	2.39	0.54
3:C:83:ARG:HA	3:C:86:ILE:HD12	1.88	0.54
3:D:58:SER:O	3:D:62:VAL:HG23	2.07	0.54
2:B:150:SER:OG	2:B:152:ASP:OD1	2.25	0.54
3:C:43:LEU:HA	3:C:46:VAL:HG12	1.90	0.54
2:B:189:ARG:NH1	2:B:234:ARG:HH21	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:61:VAL:O	3:D:65:ILE:HG12	2.07	0.54
2:B:127:VAL:HG13	2:B:144:GLU:HB2	1.90	0.54
3:D:226:THR:O	3:D:229:THR:OG1	2.24	0.54
1:A:636:GLN:OE1	1:A:636:GLN:N	2.40	0.54
3:D:162:PRO:HA	3:D:167:ARG:NE	2.23	0.54
3:D:164:HIS:HD2	3:D:166:ILE:HD12	1.70	0.54
3:C:162:PRO:HA	3:C:167:ARG:HE	1.74	0.53
3:C:37:SER:OG	3:C:39:GLU:OE1	2.25	0.53
3:D:221:LEU:HA	3:D:224:ASN:HD22	1.74	0.53
1:A:172:ARG:HE	1:A:175:VAL:HB	1.73	0.53
1:A:186:MET:HE3	1:A:186:MET:HA	1.90	0.53
3:C:162:PRO:HA	3:C:167:ARG:NE	2.24	0.53
2:B:340:LYS:HA	2:B:343:ILE:HD11	1.91	0.53
2:B:352:LEU:HA	2:B:355:LEU:HD12	1.89	0.53
1:A:481:ALA:N	1:A:529:THR:O	2.34	0.52
1:A:575:ARG:HD3	1:A:633:TYR:HE2	1.74	0.52
1:A:244:THR:HG22	1:A:245:LEU:H	1.74	0.52
1:A:472:TYR:O	1:A:482:VAL:N	2.42	0.52
2:B:181:ARG:HH12	2:B:242:VAL:HG12	1.73	0.52
3:D:169:GLY:O	3:D:173:ASN:ND2	2.41	0.52
1:A:261:CYS:HB3	1:A:264:CYS:SG	2.45	0.52
1:A:485:LEU:HB3	1:A:600:VAL:HG11	1.92	0.52
1:A:538:TYR:N	1:A:579:SER:O	2.40	0.52
1:A:500:ASN:O	1:A:504:VAL:HG13	2.10	0.52
2:B:365:ASP:OD1	2:B:365:ASP:N	2.34	0.52
2:B:108:ARG:HH21	2:B:112:ILE:HD11	1.74	0.52
1:A:542:HIS:CE1	1:A:654:LEU:HD13	2.45	0.52
2:B:188:HIS:HD2	2:B:191:VAL:HG22	1.75	0.52
1:A:564:MET:HE3	1:A:577:LEU:HD22	1.91	0.52
2:B:233:GLU:HA	2:B:236:GLN:HE22	1.74	0.52
1:A:487:VAL:HG23	1:A:525:LEU:HD12	1.92	0.51
1:A:668:MET:SD	1:A:674:LEU:HB3	2.50	0.51
1:A:706:LEU:HD12	1:A:706:LEU:H	1.75	0.51
3:C:38:ASN:OD1	3:C:38:ASN:N	2.43	0.51
1:A:172:ARG:HH21	1:A:175:VAL:HG12	1.76	0.51
1:A:662:ARG:NH1	2:B:224:VAL:HA	2.25	0.51
3:C:87:GLU:HG2	3:C:132:VAL:HG21	1.92	0.51
2:B:343:ILE:H	2:B:349:ARG:NH1	2.05	0.51
3:C:98:LEU:HA	3:C:101:LEU:HD12	1.92	0.51
3:D:23:ALA:HB2	3:D:51:VAL:HG21	1.91	0.51
1:A:485:LEU:HD13	1:A:600:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:GLN:HE21	2:B:218:SER:HB2	1.75	0.51
3:D:160:MET:SD	3:D:167:ARG:NH2	2.84	0.51
1:A:506:ARG:CZ	1:A:516:PHE:HB3	2.41	0.51
2:B:95:ALA:HB2	2:B:145:HIS:HA	1.92	0.51
2:B:346:PRO:HA	2:B:349:ARG:HB3	1.93	0.51
2:B:353:LYS:O	2:B:357:VAL:HG13	2.10	0.51
3:D:172:LEU:O	3:D:176:VAL:HG23	2.10	0.51
1:A:552:LYS:NZ	1:A:587:ASP:O	2.40	0.50
3:D:121:MET:HG3	3:D:125:TYR:CE1	2.47	0.50
2:B:174:ILE:O	2:B:178:THR:OG1	2.24	0.50
3:D:101:LEU:HG	3:D:105:LEU:HD12	1.92	0.50
1:A:491:THR:OG1	1:A:493:GLN:OE1	2.28	0.50
3:D:42:ASN:OD1	3:D:42:ASN:N	2.44	0.50
3:C:18:ARG:NH2	3:D:82:TYR:OH	2.45	0.50
3:D:164:HIS:CG	3:D:165:PRO:HD2	2.47	0.50
3:C:128:TYR:HA	3:C:131:GLU:OE2	2.11	0.49
3:D:3:LYS:O	3:D:7:VAL:HG12	2.12	0.49
3:D:91:ARG:HG2	3:D:95:ASN:HD21	1.77	0.49
1:A:678:LEU:HD11	1:A:693:MET:HE1	1.95	0.49
2:B:125:TYR:HE1	2:B:175:LYS:HB2	1.77	0.49
3:C:82:TYR:O	3:C:86:ILE:HG13	2.12	0.49
3:D:84:GLU:HA	3:D:87:GLU:HB2	1.94	0.49
3:D:156:SER:HA	3:D:160:MET:HE1	1.94	0.49
1:A:564:MET:HE1	1:A:592:ILE:HG21	1.93	0.49
3:D:81:GLU:HA	3:D:84:GLU:OE1	2.13	0.49
3:C:91:ARG:O	3:C:95:ASN:ND2	2.37	0.49
3:D:161:GLN:OE1	3:D:163:THR:OG1	2.18	0.49
2:B:74:LEU:HD21	2:B:84:LYS:HB3	1.95	0.49
3:C:2:ASP:HB3	3:C:5:GLU:HG2	1.93	0.49
1:A:547:LYS:HE3	1:A:682:ARG:HH12	1.77	0.49
2:B:239:HIS:CE1	2:B:241:SER:HB2	2.48	0.49
3:C:26:MET:HE3	3:C:26:MET:HA	1.94	0.49
3:D:94:CYS:O	3:D:98:LEU:HG	2.13	0.49
3:D:111:GLN:OE1	3:D:113:GLU:HG3	2.13	0.49
1:A:187:MET:HG3	1:A:188:ARG:HH11	1.78	0.49
1:A:186:MET:HE2	3:D:219:GLN:HE21	1.78	0.48
3:D:111:GLN:OE1	3:D:112:ALA:N	2.46	0.48
1:A:460:GLY:H	1:A:472:TYR:HB3	1.78	0.48
2:B:260:ARG:HD2	2:B:266:PRO:HG3	1.95	0.48
2:B:379:ILE:HG23	2:B:381:LEU:H	1.78	0.48
1:A:252:ARG:NH1	1:A:705:PRO:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:LYS:O	1:A:704:ARG:NH2	2.46	0.48
3:C:25:CYS:O	3:C:29:VAL:HG23	2.13	0.48
3:D:42:ASN:O	3:D:46:VAL:HG12	2.13	0.48
2:B:147:ASP:OD1	2:B:201:ARG:NH1	2.47	0.48
2:B:227:ARG:NH2	2:B:229:TYR:OH	2.47	0.48
1:A:364:SER:OG	1:A:365:SEP:N	2.46	0.48
2:B:354:GLN:HA	2:B:357:VAL:HG22	1.96	0.48
1:A:186:MET:C	1:A:189:GLY:H	2.21	0.47
1:A:485:LEU:HD13	1:A:600:VAL:HG11	1.96	0.47
1:A:728:ALA:HB1	3:D:220:LEU:HD22	1.96	0.47
2:B:93:VAL:HG13	2:B:145:HIS:HB3	1.96	0.47
3:C:91:ARG:HG2	3:C:95:ASN:HD21	1.79	0.47
3:D:220:LEU:O	3:D:224:ASN:ND2	2.47	0.47
3:D:211:TYR:O	3:D:215:THR:HG23	2.14	0.47
1:A:617:ILE:HD11	1:A:662:ARG:HH11	1.78	0.47
3:D:98:LEU:HD12	3:D:99:SER:H	1.79	0.47
3:D:112:ALA:O	3:D:116:VAL:HG12	2.14	0.47
2:B:188:HIS:ND1	2:B:209:PHE:HB3	2.30	0.47
3:D:117:PHE:CZ	3:D:121:MET:HE1	2.50	0.47
1:A:471:VAL:HG22	1:A:483:LYS:HE3	1.96	0.47
1:A:547:LYS:HZ2	1:A:548:PHE:H	1.62	0.47
3:C:125:TYR:HD1	3:C:128:TYR:CD2	2.31	0.47
1:A:182:LYS:HA	1:A:185:LEU:HD12	1.96	0.47
1:A:717:LEU:HA	1:A:720:SER:HB3	1.96	0.47
3:D:76:GLN:O	3:D:80:ARG:HG3	2.15	0.47
3:D:221:LEU:O	3:D:225:LEU:HG	2.14	0.47
2:B:94:MET:HG3	2:B:130:TYR:CD2	2.50	0.46
2:B:148:GLY:H	2:B:199:ASN:HA	1.80	0.46
2:B:233:GLU:HA	2:B:236:GLN:NE2	2.30	0.46
3:D:207:SER:HG	3:D:210:SER:HG	1.53	0.46
1:A:668:MET:HE1	1:A:673:TYR:HB2	1.97	0.46
3:C:81:GLU:HA	3:C:84:GLU:CG	2.43	0.46
3:D:10:ALA:HA	3:D:22:MET:HG3	1.97	0.46
3:D:57:SER:O	3:D:61:VAL:HG23	2.15	0.46
3:D:101:LEU:O	3:D:106:ILE:HG13	2.14	0.46
1:A:519:TYR:HB2	1:A:526:ALA:O	2.15	0.46
3:D:26:MET:HG3	3:D:44:LEU:HA	1.98	0.46
1:A:487:VAL:HG22	1:A:600:VAL:HG13	1.98	0.46
1:A:571:SER:HA	1:A:635:PHE:HE1	1.81	0.46
1:A:602:SER:HB2	1:A:609:GLN:C	2.41	0.46
3:D:139:LYS:O	3:D:142:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:MET:O	1:A:485:LEU:HD23	2.15	0.46
1:A:728:ALA:HB3	3:D:224:ASN:OD1	2.15	0.46
3:C:57:SER:O	3:C:61:VAL:HG12	2.16	0.46
3:C:186:GLU:CD	3:C:186:GLU:H	2.23	0.46
3:D:91:ARG:HA	3:D:94:CYS:SG	2.56	0.46
1:A:539:HIS:HD2	1:A:543:ILE:HD12	1.81	0.46
1:A:729:SEP:O2P	3:D:127:ARG:NH1	2.38	0.46
1:A:187:MET:HE3	1:A:188:ARG:NH1	2.27	0.45
1:A:471:VAL:HG13	1:A:481:ALA:HB1	1.96	0.45
2:B:181:ARG:HE	2:B:352:LEU:HD12	1.81	0.45
2:B:213:GLY:HA2	2:B:216:ILE:HG13	1.98	0.45
3:C:65:ILE:HD12	3:C:65:ILE:H	1.81	0.45
2:B:87:HIS:CD2	2:B:90:SER:H	2.34	0.45
2:B:191:VAL:HG11	2:B:249:MET:HB3	1.99	0.45
3:D:98:LEU:HD12	3:D:99:SER:N	2.31	0.45
1:A:624:VAL:HG13	1:A:633:TYR:CE1	2.51	0.45
2:B:70:LYS:NZ	2:B:72:SER:O	2.50	0.45
2:B:253:LEU:HA	2:B:256:MET:HG2	1.99	0.45
1:A:365:SEP:O2P	3:C:49:LYS:NZ	2.36	0.45
1:A:555:ASP:OD1	1:A:558:ARG:NH2	2.42	0.45
3:D:90:LEU:HD12	3:D:91:ARG:N	2.31	0.45
2:B:247:TRP:HB2	2:B:349:ARG:HH21	1.82	0.45
1:A:526:ALA:C	1:A:527:ILE:HD13	2.41	0.44
1:A:618:LEU:HD12	1:A:618:LEU:H	1.82	0.44
3:D:37:SER:N	3:D:40:GLU:OE2	2.47	0.44
3:D:159:GLU:HG2	3:D:160:MET:H	1.82	0.44
1:A:602:SER:HA	1:A:611:GLU:HA	1.98	0.44
2:B:103:ILE:HG13	2:B:104:LYS:H	1.81	0.44
3:C:16:ALA:C	3:C:18:ARG:H	2.24	0.44
3:C:227:LEU:O	3:C:230:SER:OG	2.30	0.44
3:D:95:ASN:HA	3:D:98:LEU:HG	1.99	0.44
3:D:16:ALA:C	3:D:18:ARG:H	2.26	0.44
3:D:196:PHE:O	3:D:200:ILE:HG12	2.17	0.44
2:B:265:PRO:HD3	2:B:316:TYR:CE1	2.52	0.44
2:B:340:LYS:NZ	2:B:355:LEU:HD23	2.32	0.44
3:C:155:ILE:HG23	3:C:159:GLU:HG3	2.00	0.44
1:A:472:TYR:HE1	1:A:484:MET:HG3	1.83	0.44
2:B:160:ARG:C	2:B:161:ILE:HD13	2.43	0.44
3:C:115:LYS:HG3	3:C:119:LEU:HD12	1.99	0.44
3:D:141:ILE:HD12	3:D:141:ILE:H	1.82	0.44
3:D:177:PHE:HD2	3:D:181:ILE:HD13	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:VAL:O	3:C:11:LYS:HG2	2.18	0.44
1:A:726:ARG:HD3	3:D:60:ARG:HH12	1.81	0.44
3:C:85:LYS:HA	3:C:88:THR:OG1	2.17	0.44
1:A:636:GLN:HG2	1:A:701:ARG:O	2.18	0.43
3:D:133:ALA:HB1	3:D:138:LYS:HG3	2.00	0.43
1:A:660:ASN:HA	2:B:217:ASP:OD1	2.17	0.43
3:C:52:VAL:HG13	3:C:90:LEU:CD1	2.48	0.43
3:C:119:LEU:HB2	3:C:152:ALA:HB2	2.00	0.43
3:C:127:ARG:HG2	3:C:131:GLU:OE1	2.18	0.43
1:A:662:ARG:NE	2:B:220:ALA:O	2.45	0.43
2:B:94:MET:C	2:B:145:HIS:HB2	2.43	0.43
2:B:190:ASP:CG	2:B:190:ASP:O	2.61	0.43
3:D:86:ILE:HD12	3:D:86:ILE:HA	1.90	0.43
1:A:698:LYS:HD2	1:A:698:LYS:N	2.33	0.43
2:B:69:GLU:HG2	2:B:88:LYS:HZ2	1.84	0.43
2:B:96:ARG:HE	2:B:98:LEU:HD21	1.84	0.43
1:A:572:ILE:O	1:A:572:ILE:HG13	2.18	0.43
2:B:87:HIS:HD2	2:B:90:SER:H	1.66	0.43
1:A:365:SEP:O1P	3:C:56:ARG:NH2	2.52	0.43
1:A:651:THR:HG22	1:A:681:VAL:HA	2.01	0.43
3:C:178:TYR:HB2	3:C:188:ALA:HB2	2.01	0.43
3:C:226:THR:O	3:C:229:THR:OG1	2.34	0.43
1:A:620:MET:HE3	1:A:625:ILE:HD11	2.00	0.43
1:A:729:SEP:HA	3:D:172:LEU:HD21	2.01	0.43
3:D:37:SER:OG	3:D:39:GLU:OE2	2.24	0.43
2:B:342:LEU:HD23	2:B:342:LEU:HA	1.81	0.43
3:C:39:GLU:HG2	3:C:40:GLU:N	2.33	0.43
3:C:211:TYR:O	3:C:215:THR:HG22	2.19	0.43
1:A:647:TYR:OH	1:A:677:ASP:O	2.24	0.43
2:B:192:LYS:HG2	2:B:229:TYR:CE2	2.53	0.43
2:B:247:TRP:CH2	2:B:322:PRO:HB3	2.54	0.43
2:B:352:LEU:HD23	2:B:355:LEU:HD12	2.00	0.43
3:C:197:ASP:HA	3:C:200:ILE:HG22	2.00	0.43
1:A:625:ILE:HG13	1:A:669:VAL:HG23	2.01	0.42
3:D:159:GLU:HG2	3:D:160:MET:HE3	2.01	0.42
1:A:726:ARG:HG3	1:A:727:SER:O	2.19	0.42
2:B:56:GLN:HB2	2:B:59:LYS:NZ	2.34	0.42
2:B:208:ASP:H	5:B:401:CHU:C18	2.32	0.42
3:D:80:ARG:O	3:D:83:ARG:HG2	2.19	0.42
1:A:197:VAL:HG23	1:A:208:ILE:HG23	2.01	0.42
1:A:618:LEU:O	1:A:644:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:93:ILE:HA	3:D:96:ASP:OD2	2.18	0.42
3:D:105:LEU:HD13	3:D:118:TYR:CE1	2.53	0.42
1:A:498:PHE:O	1:A:502:VAL:HG22	2.19	0.42
3:C:91:ARG:HG2	3:C:95:ASN:ND2	2.35	0.42
1:A:574:HIS:HA	1:A:595:PHE:CD2	2.55	0.42
2:B:340:LYS:O	2:B:349:ARG:NH1	2.53	0.42
3:D:14:GLU:OE1	3:D:14:GLU:HA	2.19	0.42
2:B:199:ASN:ND2	2:B:203:GLU:OE2	2.50	0.42
3:C:3:LYS:O	3:C:7:VAL:HG13	2.19	0.42
3:C:224:ASN:O	3:C:227:LEU:HD12	2.19	0.42
1:A:465:SER:OG	1:A:466:GLY:N	2.53	0.42
3:C:2:ASP:OD2	3:C:3:LYS:N	2.53	0.42
3:C:166:ILE:HD12	3:C:166:ILE:H	1.84	0.42
1:A:484:MET:C	1:A:485:LEU:HD23	2.44	0.42
2:B:263:ILE:HD12	2:B:263:ILE:H	1.84	0.42
1:A:172:ARG:NE	1:A:175:VAL:HB	2.34	0.42
1:A:491:THR:HG23	1:A:494:GLN:H	1.85	0.42
1:A:646:LEU:HB3	1:A:693:MET:HG3	2.02	0.42
2:B:122:ASN:OD1	2:B:122:ASN:N	2.53	0.42
2:B:229:TYR:HA	2:B:251:LEU:HD23	2.02	0.42
2:B:99:ILE:HG22	2:B:139:ILE:HB	2.01	0.42
2:B:185:LYS:HA	2:B:185:LYS:HD3	1.89	0.42
3:C:101:LEU:HD23	3:C:105:LEU:HD12	2.02	0.42
1:A:189:GLY:HA3	3:D:222:ARG:NH1	2.35	0.41
1:A:495:LEU:HG	1:A:499:LYS:HE2	2.02	0.41
1:A:499:LYS:HD3	1:A:519:TYR:OH	2.20	0.41
3:C:172:LEU:O	3:C:176:VAL:HG12	2.19	0.41
3:D:80:ARG:HA	3:D:83:ARG:HG2	2.02	0.41
2:B:202:GLY:HA2	2:B:371:PHE:HD2	1.85	0.41
1:A:483:LYS:NZ	1:A:529:THR:OG1	2.44	0.41
2:B:87:HIS:CD2	2:B:89:PRO:HD2	2.55	0.41
2:B:238:THR:HG22	2:B:239:HIS:H	1.86	0.41
1:A:236:ASN:HD21	1:A:262:GLN:HB2	1.85	0.41
1:A:551:ILE:HD13	1:A:551:ILE:HA	1.91	0.41
2:B:331:SER:O	2:B:335:GLN:NE2	2.52	0.41
3:D:77:GLN:HG3	3:D:81:GLU:OE1	2.21	0.41
1:A:362:ARG:HE	3:C:60:ARG:HD3	1.84	0.41
2:B:117:VAL:O	2:B:120:GLU:HG2	2.20	0.41
2:B:316:TYR:HA	2:B:320:GLU:CD	2.46	0.41
1:A:642:PHE:HA	1:A:645:VAL:HG12	2.02	0.41
1:A:451:GLU:HG2	1:A:519:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:SER:HA	1:A:583:PHE:HA	2.02	0.41
1:A:542:HIS:NE2	1:A:654:LEU:HD13	2.36	0.41
1:A:668:MET:SD	1:A:674:LEU:N	2.94	0.41
1:A:729:SEP:O3P	3:D:56:ARG:NH2	2.51	0.41
2:B:252:SER:O	2:B:256:MET:HG2	2.19	0.41
1:A:216:TRP:CZ3	1:A:217:LEU:HD13	2.55	0.41
2:B:320:GLU:HB2	2:B:321:PRO:HD2	2.02	0.41
3:C:160:MET:CE	3:C:167:ARG:HB2	2.49	0.41
1:A:269:HIS:ND1	1:A:270:GLN:N	2.69	0.40
3:C:116:VAL:HG23	3:C:152:ALA:HB1	2.03	0.40
2:B:169:VAL:HG23	2:B:204:ILE:HD13	2.03	0.40
2:B:208:ASP:H	5:B:401:CHU:H11	1.86	0.40
2:B:88:LYS:HE2	2:B:88:LYS:HB2	1.85	0.40
2:B:95:ALA:HB3	2:B:143:MET:HB2	2.04	0.40
2:B:382:ASN:O	2:B:383:GLN:HG3	2.22	0.40
3:C:224:ASN:OD1	3:C:227:LEU:HD11	2.22	0.40
1:A:512:ASN:HD22	1:A:563:GLY:N	2.20	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	400/766 (52%)	380 (95%)	20 (5%)	0	100	100
2	B	289/393 (74%)	277 (96%)	12 (4%)	0	100	100
3	C	214/245 (87%)	209 (98%)	5 (2%)	0	100	100
3	D	218/245 (89%)	207 (95%)	11 (5%)	0	100	100
All	All	1121/1649 (68%)	1073 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	361/656 (55%)	354 (98%)	7 (2%)	52	70
2	B	254/338 (75%)	248 (98%)	6 (2%)	44	63
3	C	181/209 (87%)	175 (97%)	6 (3%)	33	56
3	D	184/209 (88%)	181 (98%)	3 (2%)	58	73
All	All	980/1412 (69%)	958 (98%)	22 (2%)	47	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	MET
1	A	449	ASP
1	A	450	TRP
1	A	548	PHE
1	A	570	LYS
1	A	594	ASP
1	A	665	ILE
2	B	67	ASP
2	B	81	VAL
2	B	154	VAL
2	B	180	LEU
2	B	208	ASP
2	B	365	ASP
3	C	38	ASN
3	C	58	SER
3	C	83	ARG
3	C	132	VAL
3	C	198	GLU
3	C	216	LEU
3	D	78	MET
3	D	84	GLU
3	D	121	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
1	A	725	HIS
2	B	87	HIS
2	B	164	GLN
2	B	195	ASN
3	C	4	ASN
3	C	144	GLN
3	C	161	GLN
3	C	219	GLN
3	D	32	GLN
3	D	164	HIS
3	D	219	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	SEP	A	365	1	8,9,10	1.60	1 (12%)	7,12,14	1.36	1 (14%)
1	SEP	A	729	1	8,9,10	1.58	1 (12%)	7,12,14	1.43	1 (14%)

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	SEP	A	365	1	-	4/6/8/10	-
1	SEP	A	729	1	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	365	SEP	P-O1P	3.48	1.61	1.50
1	A	729	SEP	P-O1P	3.46	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	SEP	OG-CB-CA	3.15	111.21	108.14
1	A	365	SEP	OG-CB-CA	2.96	111.03	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	365	SEP	C-CA-CB-OG
1	A	365	SEP	CB-OG-P-O2P
1	A	365	SEP	CB-OG-P-O3P
1	A	365	SEP	N-CA-CB-OG
1	A	729	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	365	SEP	4	0
1	A	729	SEP	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
5	CHU	B	401	-	35,36,36	0.85	1 (2%)	45,52,52	0.99	4 (8%)

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
5	CHU	B	401	-	-	1/15/16/16	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	CHU	O10-C5	-2.22	1.35	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	CHU	C22-C23-N24	3.08	121.57	119.50
5	B	401	CHU	C20-N21-C16	2.45	116.08	114.46
5	B	401	CHU	F33-C22-C14	2.40	121.25	118.00
5	B	401	CHU	C12-C7-C6	-2.22	115.95	118.49

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	401	CHU	C30-N29-S28-O31

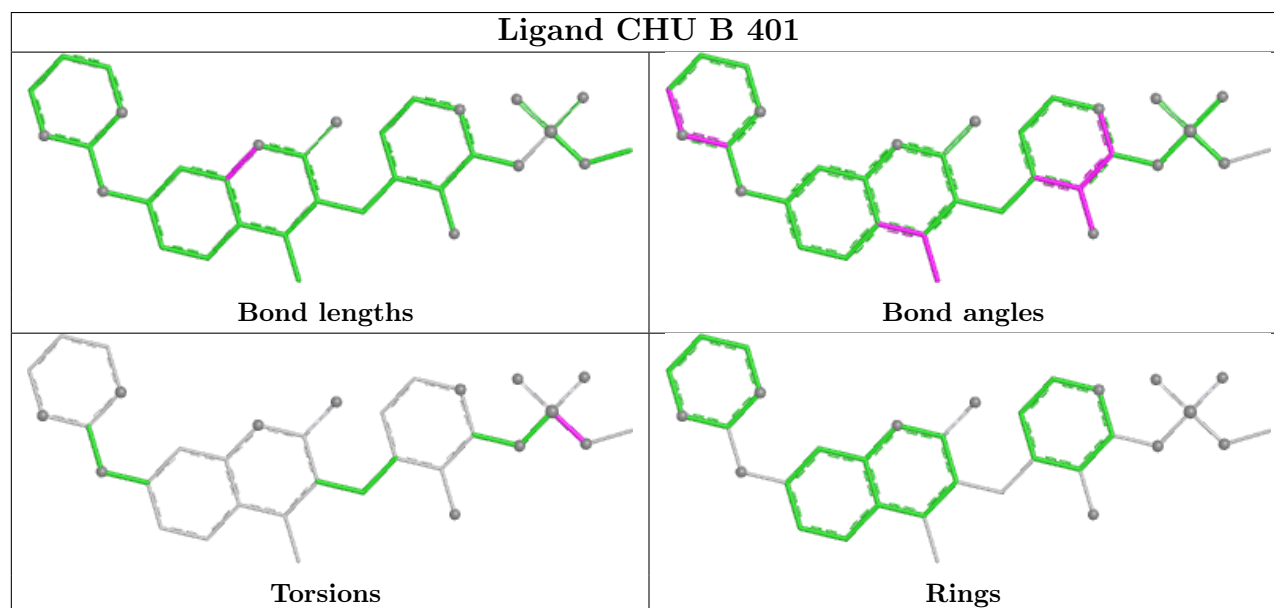
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	401	CHU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.



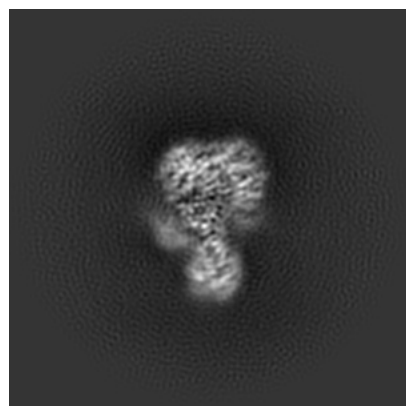
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70053. These allow visual inspection of the internal detail of the map and identification of artifacts.

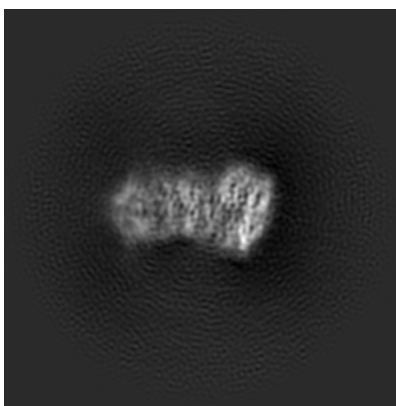
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

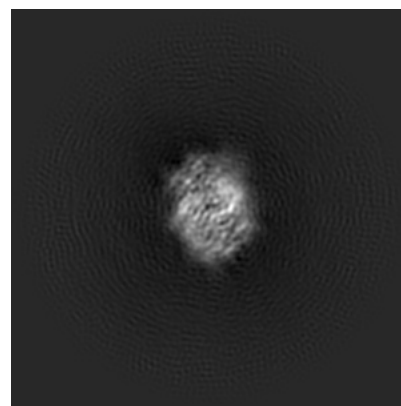
#### 6.1.1 Primary map



X

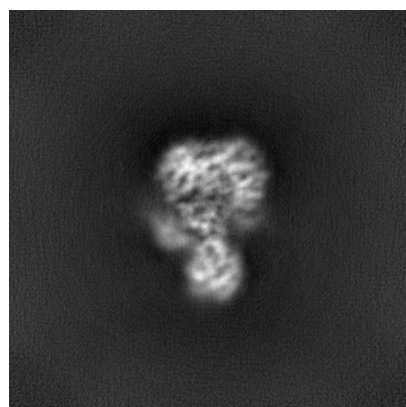


Y

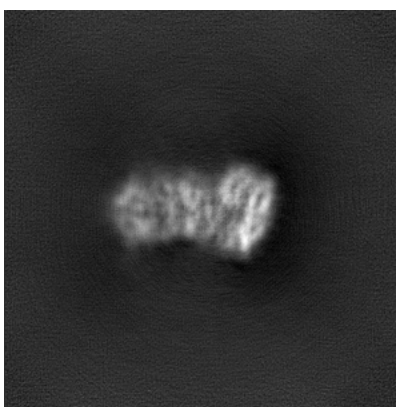


Z

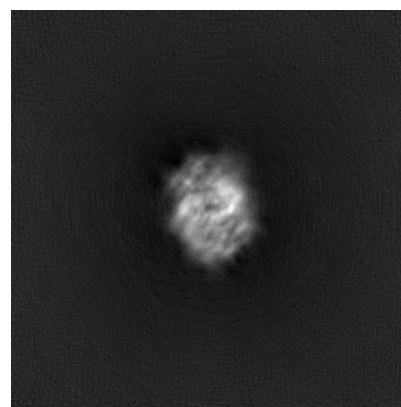
#### 6.1.2 Raw map



X



Y

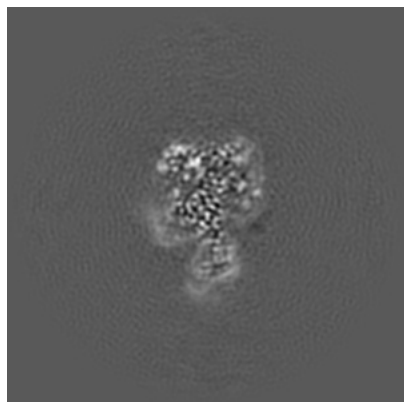


Z

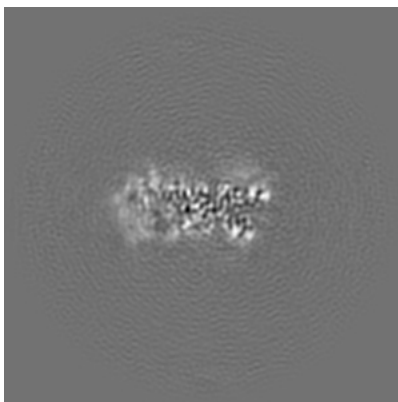
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

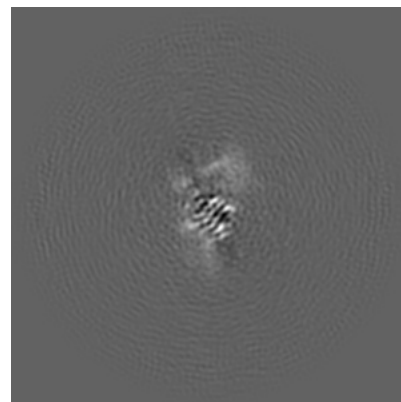
### 6.2.1 Primary map



X Index: 170

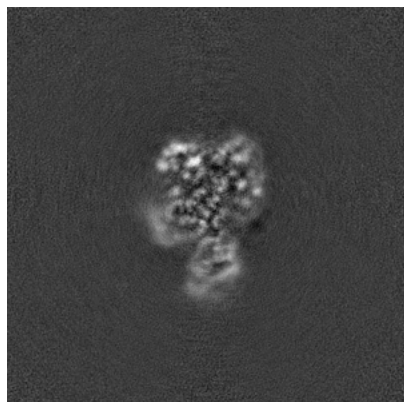


Y Index: 170

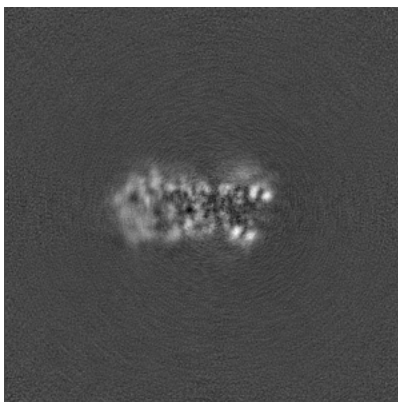


Z Index: 170

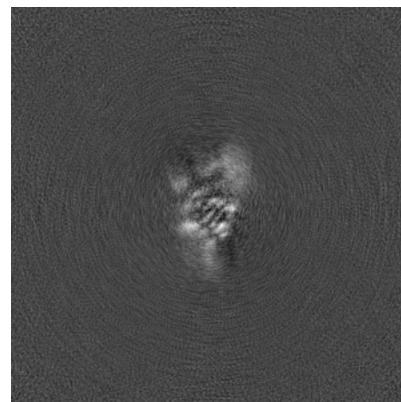
### 6.2.2 Raw map



X Index: 170



Y Index: 170

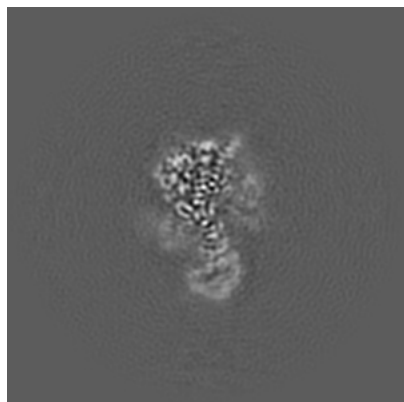


Z Index: 170

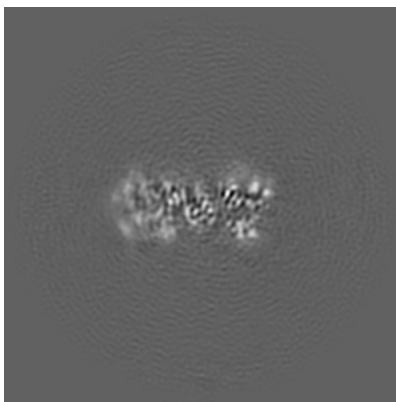
The images above show central slices of the map in three orthogonal directions.

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

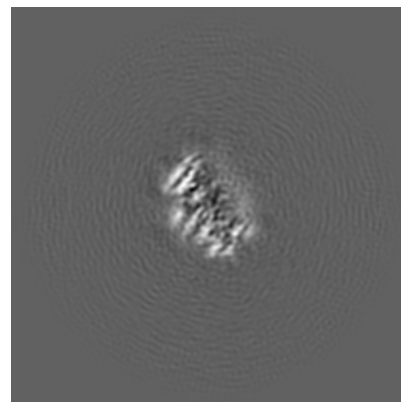
### 6.3.1 Primary map



X Index: 179

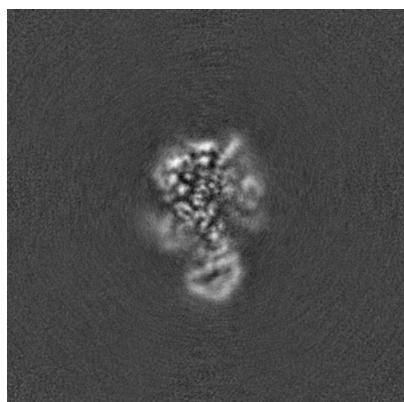


Y Index: 175

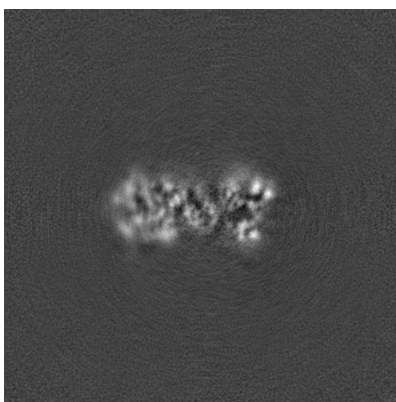


Z Index: 203

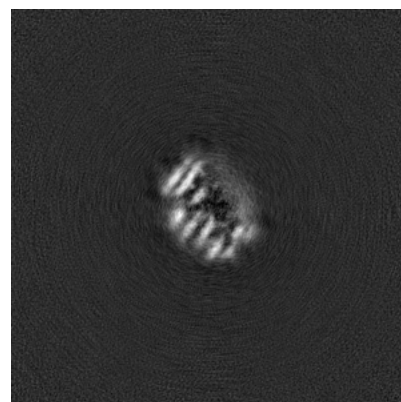
### 6.3.2 Raw map



X Index: 178



Y Index: 176

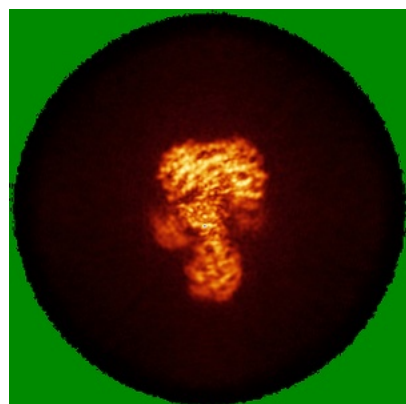


Z Index: 205

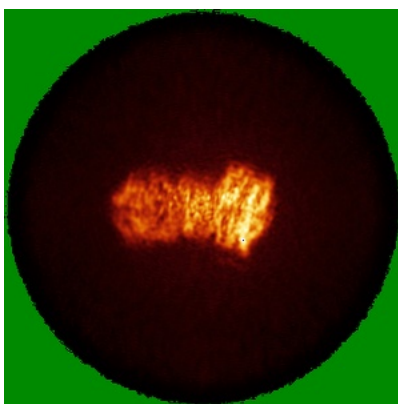
The images above show the largest variance slices of the map in three orthogonal directions.

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

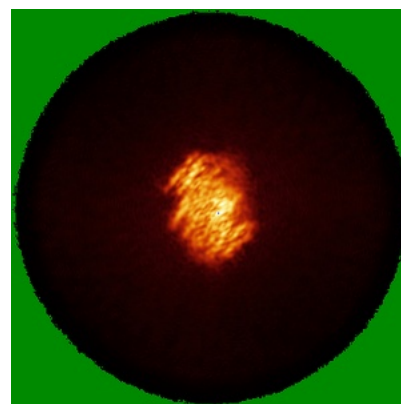
### 6.4.1 Primary map



X

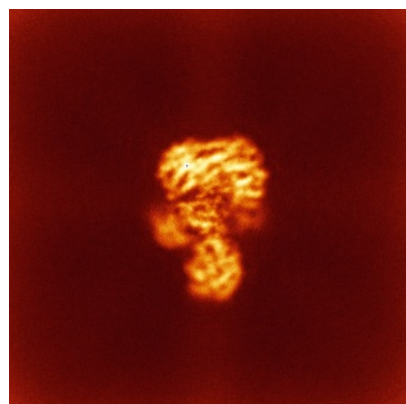


Y

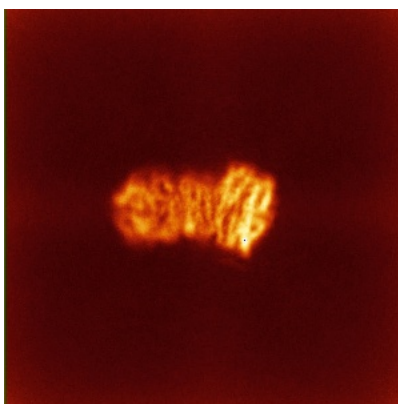


Z

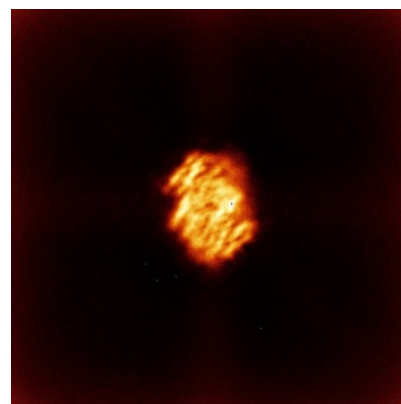
### 6.4.2 Raw map



X



Y

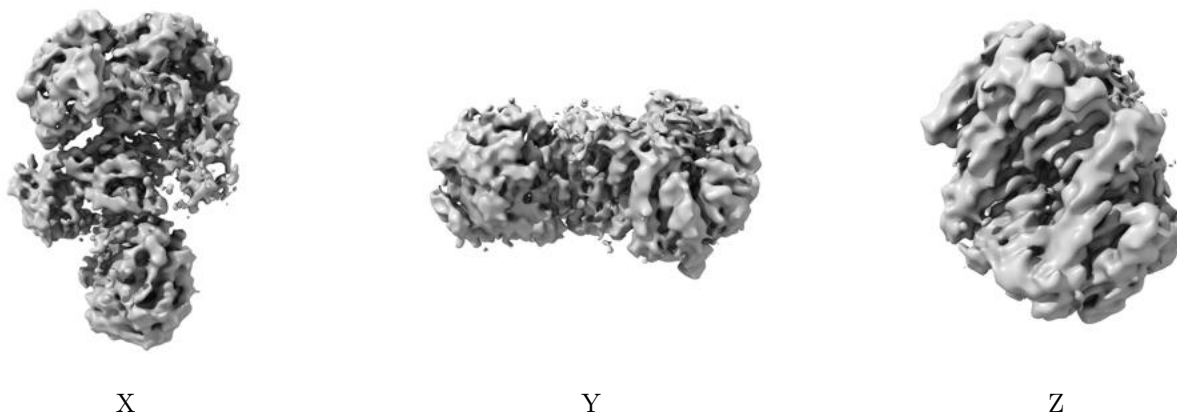


Z

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.

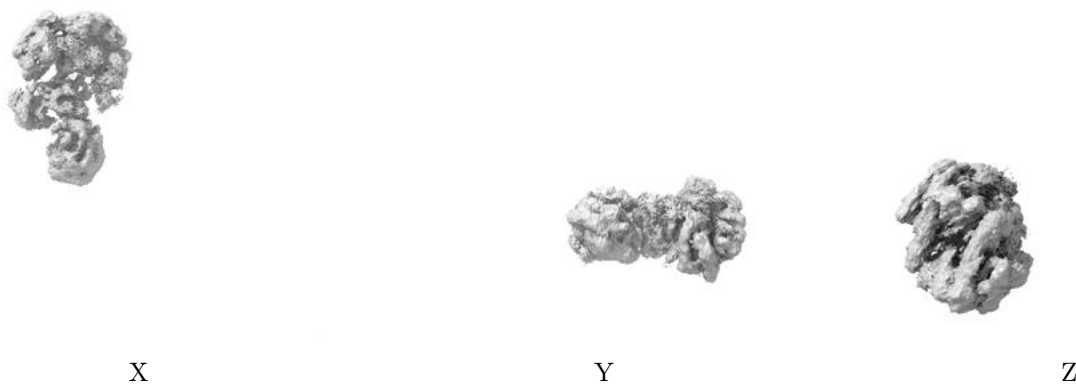
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.079. 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.

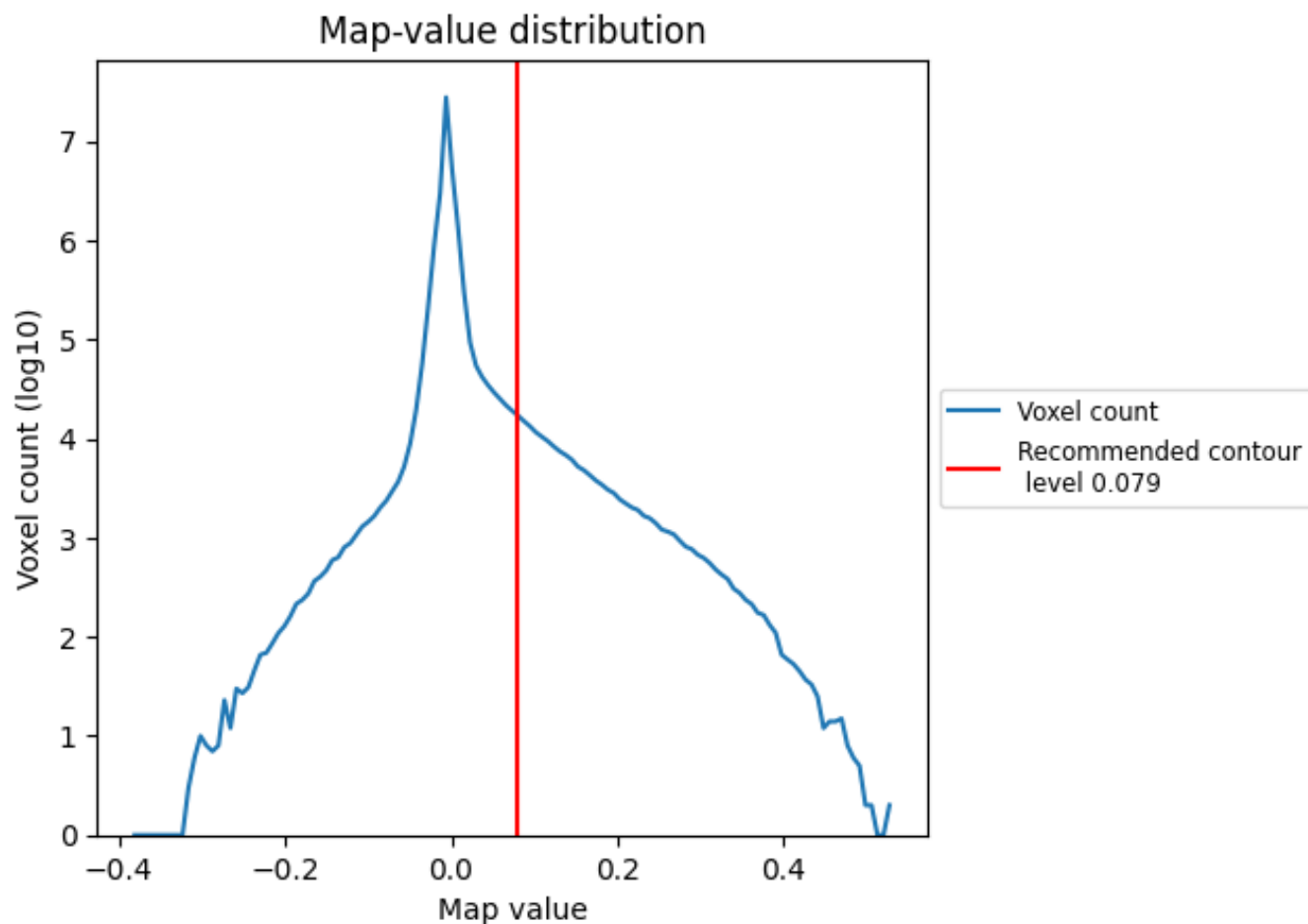
## 6.6 Mask visualisation [i](#)

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.

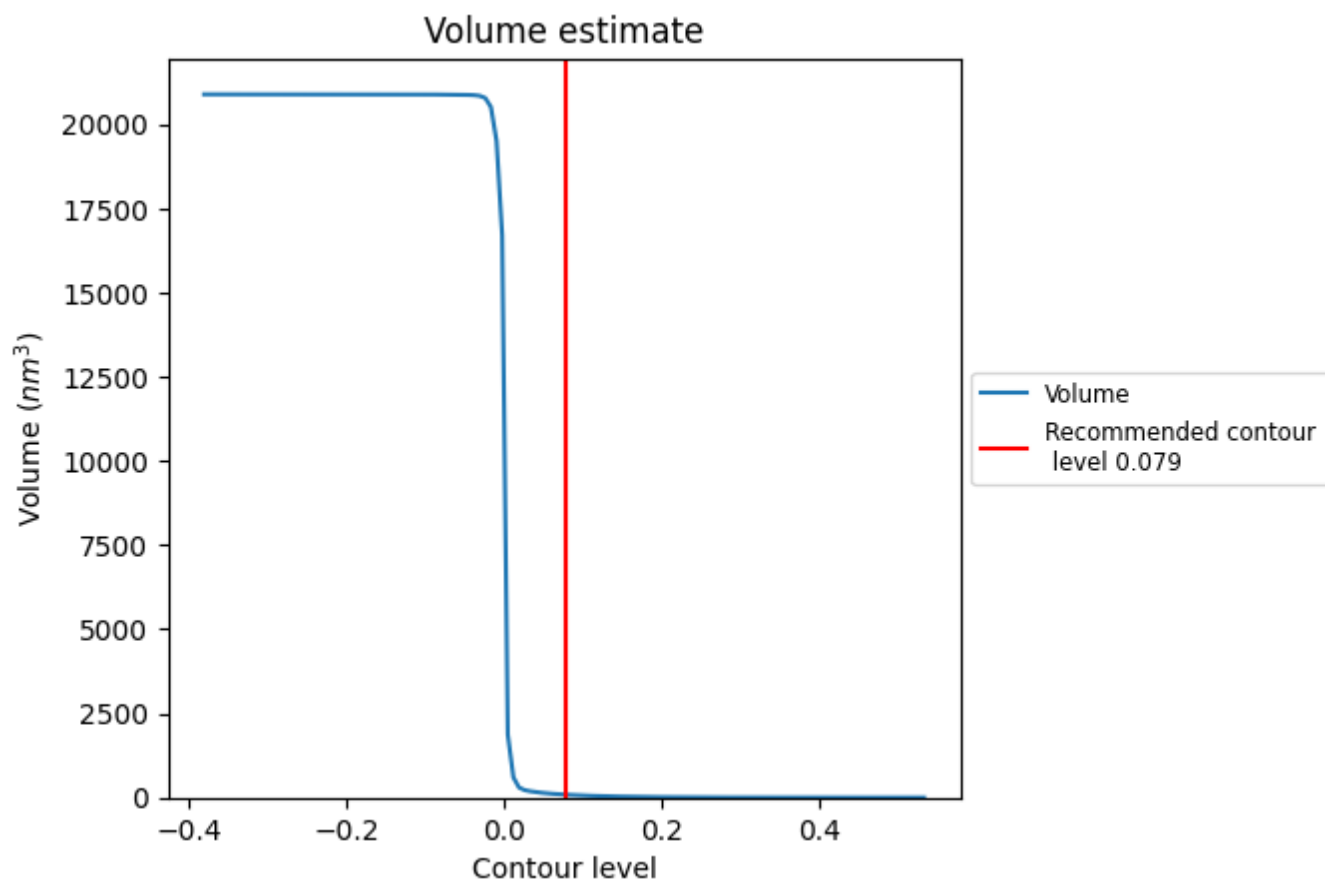
### 7.1 Map-value distribution [i](#)



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.



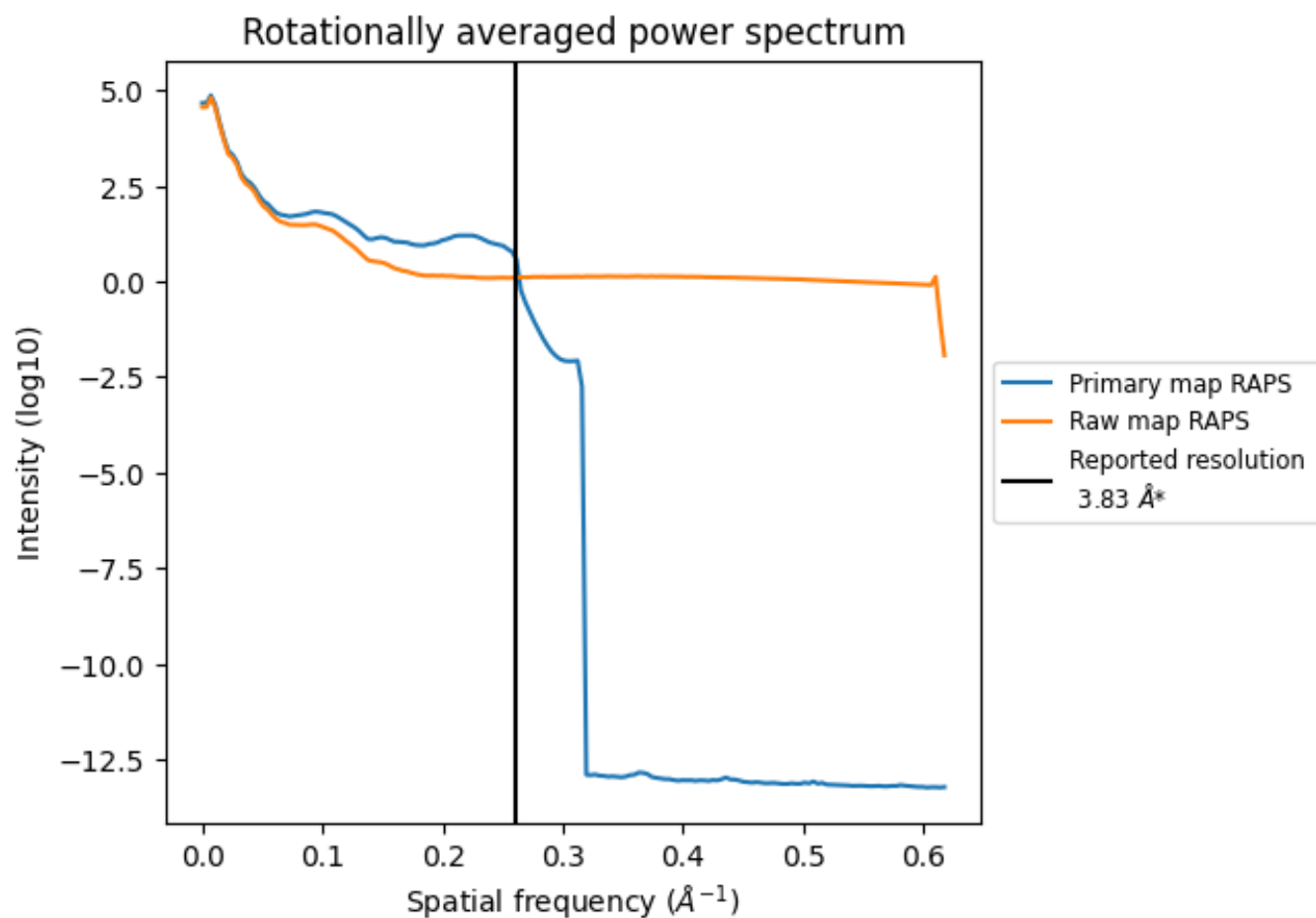
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm<sup>3</sup>; this corresponds to an approximate mass of 77 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 ⓘ



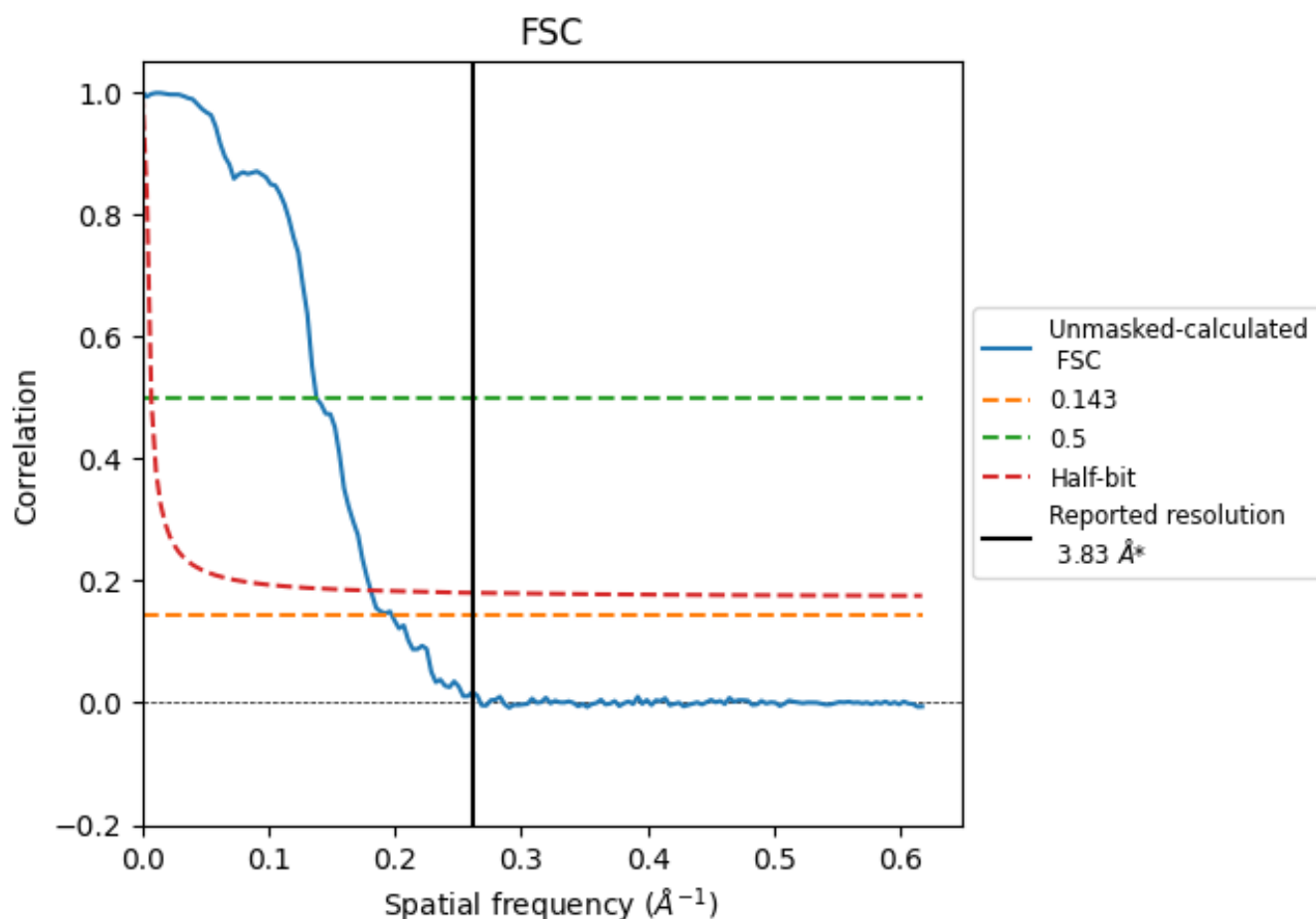
\*Reported resolution corresponds to spatial frequency of 0.261 Å<sup>-1</sup>



## 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 0.261  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

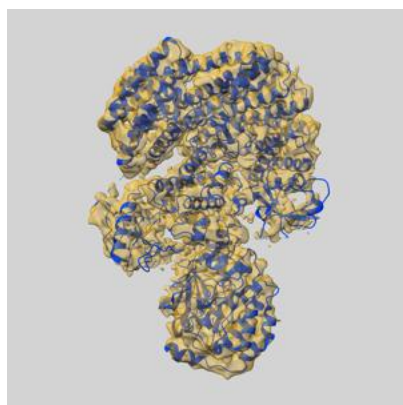
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.06	7.25	5.53

\*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 5.06 differs from the reported value 3.83 by more than 10 %

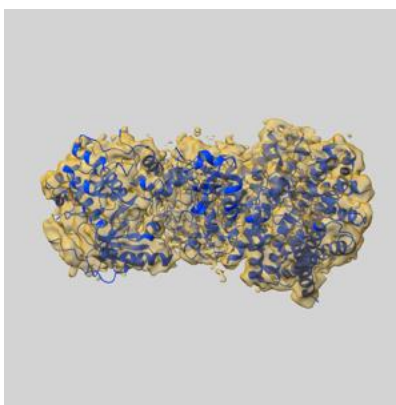
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70053 and PDB model 9O2Z. Per-residue inclusion information can be found in section [3](#) on page [5](#).

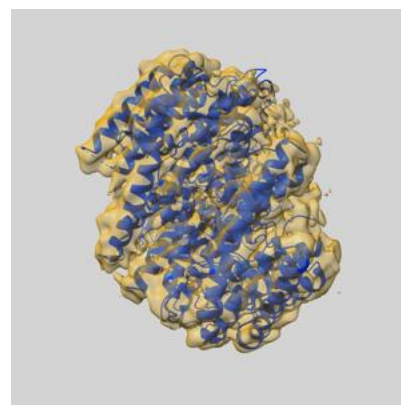
### 9.1 Map-model overlay [i](#)



X



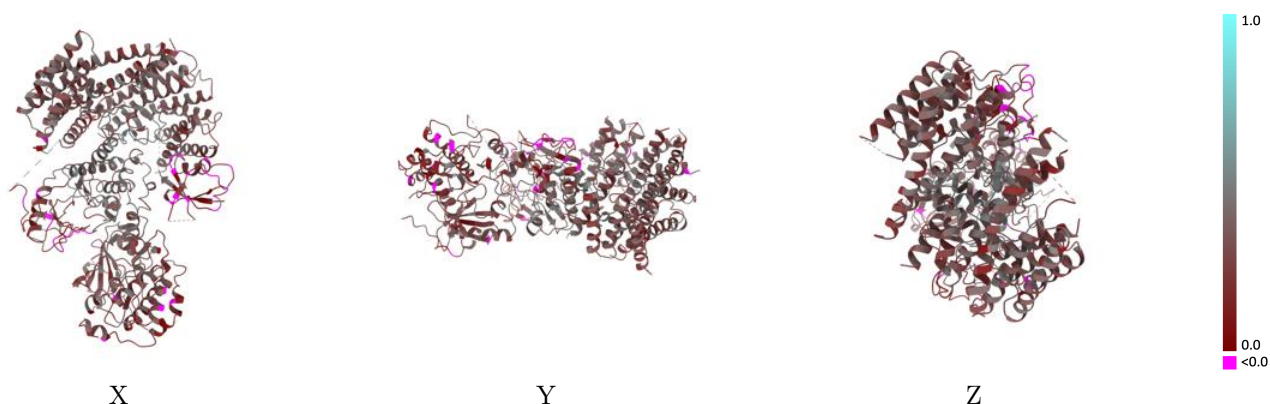
Y



Z

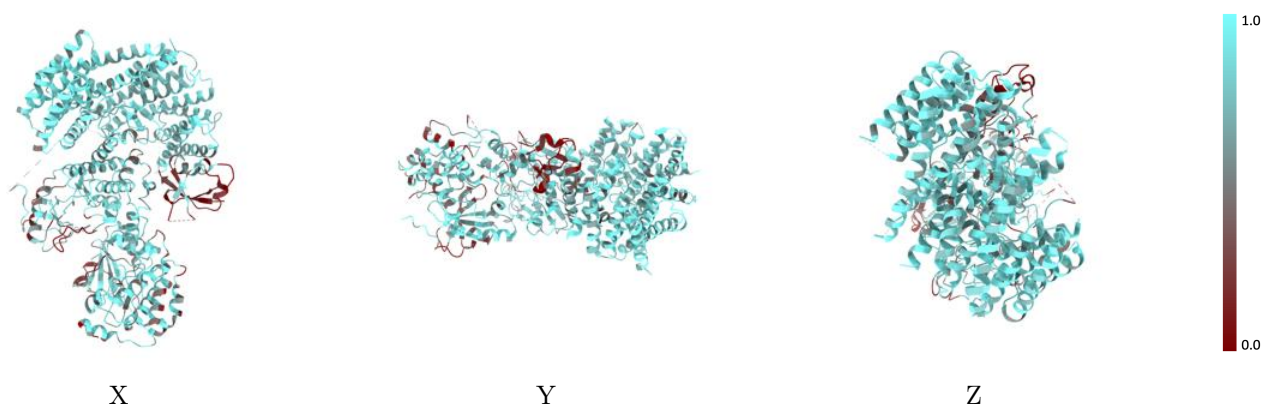
The images above show the 3D surface view of the map at the recommended contour level 0.079 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



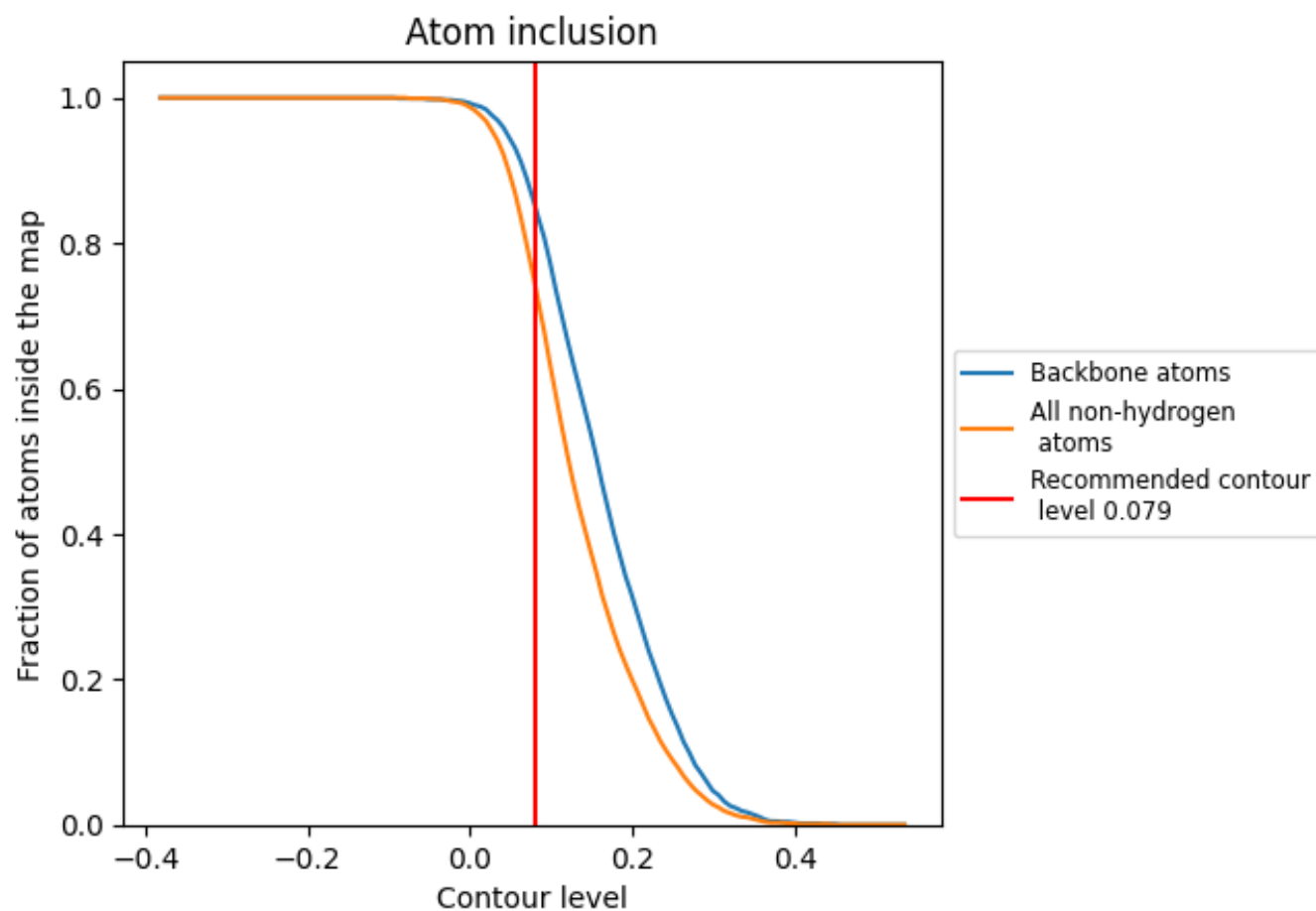
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.079).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 75% 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 (0.079) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7470	<div></div> 0.3060
A	<div></div> 0.6680	<div></div> 0.3090
B	<div></div> 0.7010	<div></div> 0.2690
C	<div></div> 0.8560	<div></div> 0.3300
D	<div></div> 0.8490	<div></div> 0.3250

