



## Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 07:34 PM EST

PDB ID : 7RU9  
EMDB ID : EMD-24700  
Title : Metazoan pre-targeting GET complex (cBUGG-in)  
Authors : Keszei, A.F.A.; Yip, M.C.J.; Shao, S.  
Deposited on : 2021-08-16  
Resolution : 3.30 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>.

---

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

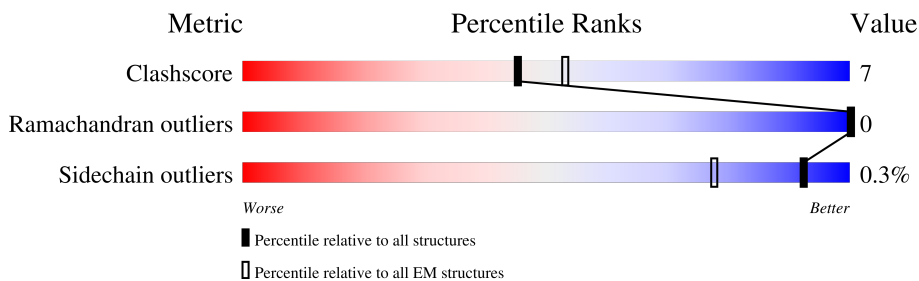
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	343	13% (Poor fit) 74% (0 outliers) 15% (1 outlier) 11% (2+ outliers)
1	B	343	13% (Poor fit) 75% (0 outliers) 15% (1 outlier) 11% (2+ outliers)
2	C	333	10% (Poor fit) 71% (0 outliers) 10% (1 outlier) 19% (2+ outliers)
2	F	333	10% (Poor fit) 72% (0 outliers) 10% (1 outlier) 19% (2+ outliers)
3	D	132	57% (Poor fit) 62% (0 outliers) 12% (1 outlier) 25% (2+ outliers)
3	G	132	58% (Poor fit) 60% (0 outliers) 14% (1 outlier) 25% (2+ outliers)
4	E	165	29% (Poor fit) 24% (0 outliers) 71% (1+ outliers)
4	H	165	29% (Poor fit) 23% (0 outliers) 5% (1 outlier) 71% (2+ outliers)

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11595 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 ATPase GET3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	306	2417	1540	400	458	19	0	0
1	B	306	2417	1540	400	458	19	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q6IQE5
A	0	HIS	-	expression tag	UNP Q6IQE5
A	68	ASN	ASP	engineered mutation	UNP Q6IQE5
B	-1	GLY	-	expression tag	UNP Q6IQE5
B	0	HIS	-	expression tag	UNP Q6IQE5
B	68	ASN	ASP	engineered mutation	UNP Q6IQE5

- Molecule 2 is a protein called Golgi to ER traffic protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	271	2175	1390	372	401	12	0	0
2	F	271	2175	1390	372	401	12	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q7L5D6
C	-4	PRO	-	expression tag	UNP Q7L5D6
C	-3	LEU	-	expression tag	UNP Q7L5D6
C	-2	GLY	-	expression tag	UNP Q7L5D6
C	-1	SER	-	expression tag	UNP Q7L5D6
C	0	THR	-	expression tag	UNP Q7L5D6
F	-5	GLY	-	expression tag	UNP Q7L5D6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	PRO	-	expression tag	UNP Q7L5D6
F	-3	LEU	-	expression tag	UNP Q7L5D6
F	-2	GLY	-	expression tag	UNP Q7L5D6
F	-1	SER	-	expression tag	UNP Q7L5D6
F	0	THR	-	expression tag	UNP Q7L5D6

- Molecule 3 is a protein called Large proline-rich protein BAG6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	99	Total	C	N	O	S	0	0
			781	487	144	149	1		
3	G	99	Total	C	N	O	S	0	0
			781	487	144	149	1		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1001	GLY	-	expression tag	UNP P46379
D	1002	PRO	-	expression tag	UNP P46379
D	1003	GLY	-	expression tag	UNP P46379
G	1001	GLY	-	expression tag	UNP P46379
G	1002	PRO	-	expression tag	UNP P46379
G	1003	GLY	-	expression tag	UNP P46379

- Molecule 4 is a protein called Ubiquitin-like protein 4A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	48	Total	C	N	O	0	0
			392	245	74	73		
4	H	48	Total	C	N	O	0	0
			392	245	74	73		

There are 16 discrepancies between the modelled and reference sequences:

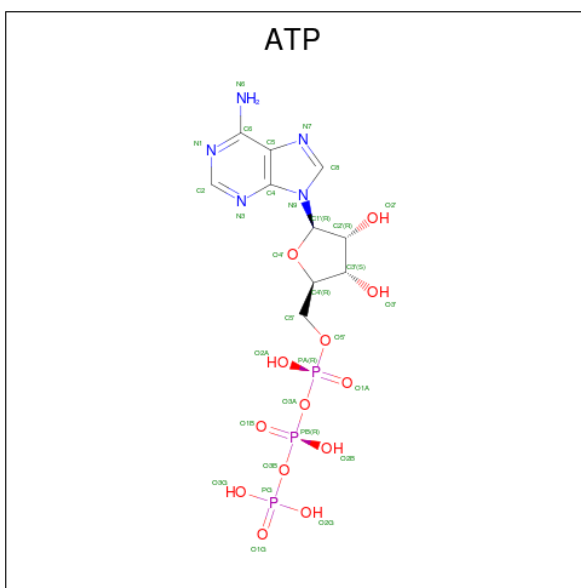
Chain	Residue	Modelled	Actual	Comment	Reference
E	158	GLY	-	expression tag	UNP P11441
E	159	SER	-	expression tag	UNP P11441
E	160	GLU	-	expression tag	UNP P11441
E	161	ASN	-	expression tag	UNP P11441
E	162	LEU	-	expression tag	UNP P11441
E	163	TYR	-	expression tag	UNP P11441
E	164	PHE	-	expression tag	UNP P11441

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	165	GLN	-	expression tag	UNP P11441
H	158	GLY	-	expression tag	UNP P11441
H	159	SER	-	expression tag	UNP P11441
H	160	GLU	-	expression tag	UNP P11441
H	161	ASN	-	expression tag	UNP P11441
H	162	LEU	-	expression tag	UNP P11441
H	163	TYR	-	expression tag	UNP P11441
H	164	PHE	-	expression tag	UNP P11441
H	165	GLN	-	expression tag	UNP P11441

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	

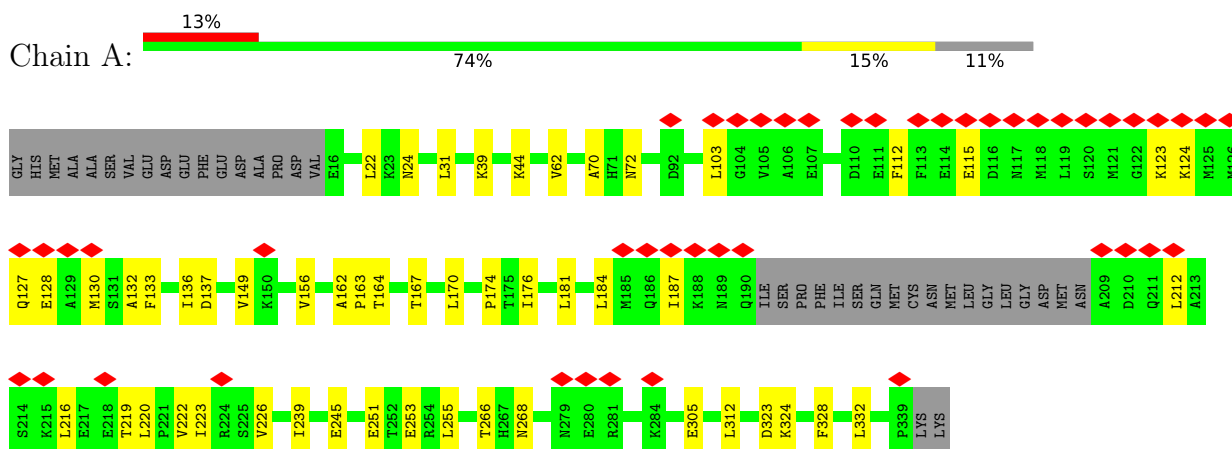
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
7	A	1	1	1	0

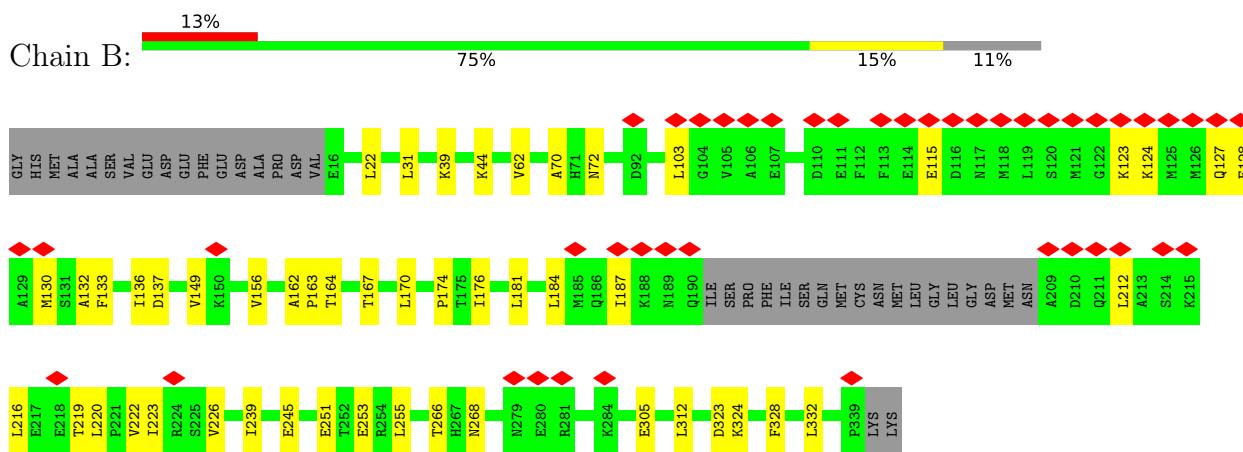
### 3 Residue-property plots

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

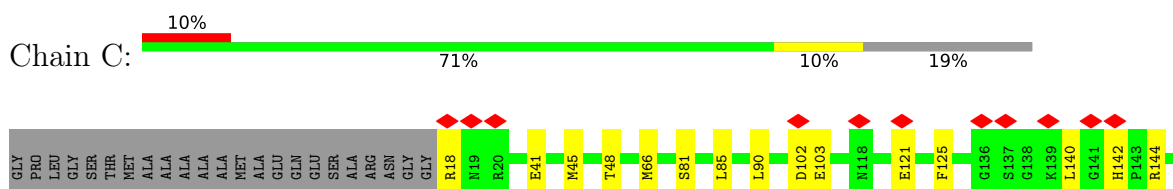
- Molecule 1: ATPase GET3

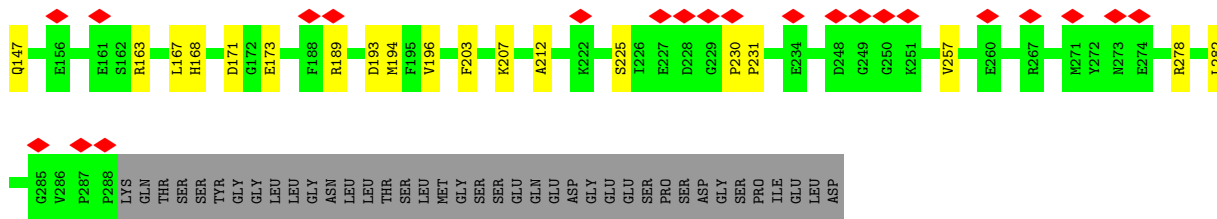


- Molecule 1: ATPase GET3

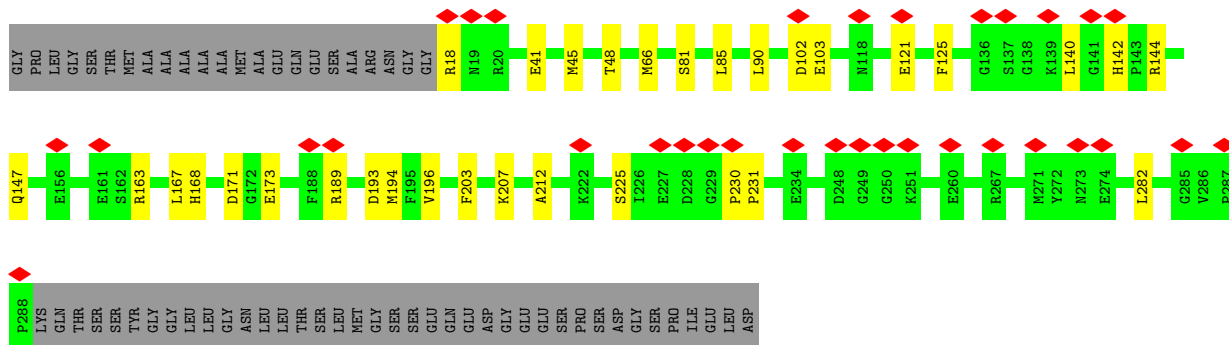


- Molecule 2: Golgi to ER traffic protein 4 homolog

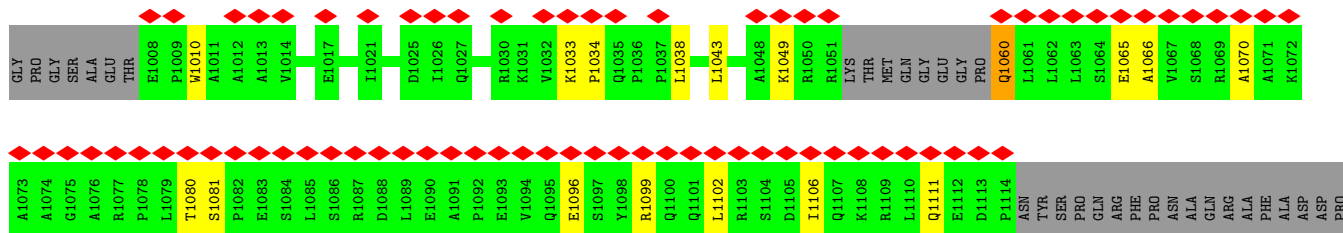




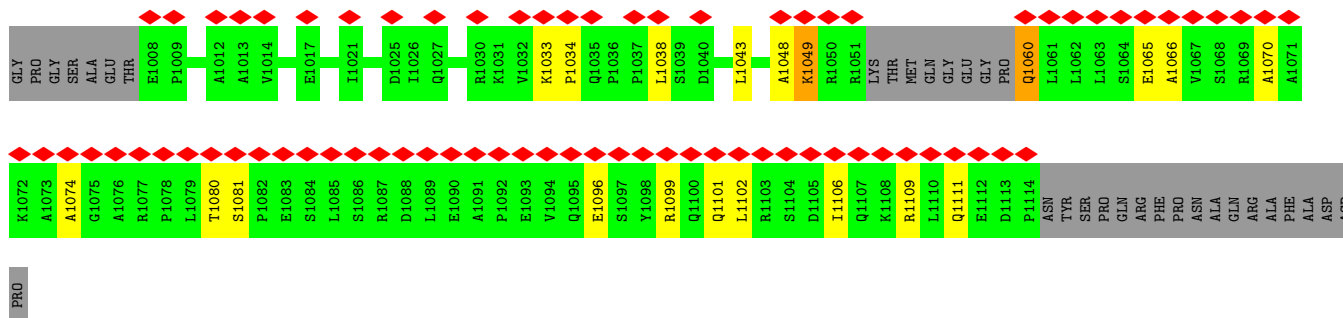
• Molecule 2: Golgi to ER traffic protein 4 homolog



• Molecule 3: Large proline-rich protein BAG6



• Molecule 3: Large proline-rich protein BAG6



• Molecule 4: Ubiquitin-like protein 4A





MET	GLN	LEU	THR	VAL	LYS	ALA	LEU	GLN	GLY	ARG	GLU	CYS	SER	LEU	GLN	VAL	PRO	GLU	ASP	LEU	GLU	VAL	SER	THR	LEU	LYS	GLN	ASN	VAL	PRO	VAL	ARG	GLN	ARG	GLN	ARG	LEU	PHE	LYS	GLY	LYS	ALA	LEU	ALA	ASP	GLY	LYS	ARG	LEU	SER	ASP	TYR	SER										
ILE	GLY	PRO	ASN	SER	LYS	LEU	ASN	LEU	VAL	VAL	LYS	PRO	LEU	GLU	VAL	VAL	LEU	LEU	GLU	GLU	GLY	GLY	ALA	SER	GLN	ARG	LEU	LYS	ALA	ALA	ASP	SER	PRO	PRO	PRO	P93	Q94	V95	W96	Q97	L98	I99	S100	K101	V102	L103	A104	R105	H106	F107	S108	A109	A110	D111	A112	S113	R114	V115	L116	E117	Q118	L119	Q120
R121	D122	Y123	E124	R125	S126	L127	S128	R129	L130	T131	L132	D133	D134	I135	E136	L137	L138	A139	S140	ARG	PHE	LEU	HIS	SER	PRO	GLU	VAL	THR	GLU	THR	GLU	THR	MET	GLU	LYS	GLY	PHE	SER	LYS	GLY	GLU	GLU	ASN	LEU	TYR	PHE	GLN																

• Molecule 4: Ubiquitin-like protein 4A



MET	GLN	LEU	THR	VAL	LYS	ALA	LEU	GLN	GLY	ARG	GLU	CYS	SER	LEU	GLN	VAL	PRO	GLU	ASP	LEU	GLU	VAL	SER	THR	LEU	LYS	ALA	ALA	ASP	SER	PRO	GLU	VAL	LYS	GLN	ARG	LEU	LYS	GLN	ALA	LEU	LEU	PHE	LYS	GLY	LYS	ALA	LEU	ALA	ASP	GLY	LYS	ARG	LEU	SER	ASP	TYR	SER				
ILE	GLY	PRO	ASN	SER	LYS	LEU	ASN	LEU	VAL	VAL	LYS	PRO	LEU	GLU	VAL	VAL	LEU	LEU	GLU	GLU	GLY	GLY	ALA	SER	GLN	ARG	LEU	LYS	ALA	ALA	ASP	SER	PRO	PRO	P93	Q94	V95	W96	Q97	L98	I99	S100	K101	V102	L103	A104	R105	H106	F107	S108	A109	A110	D111	A112	S113	R114	V115	L116	E117	Q118	L119	Q120
R121	D122	Y123	E124	R125	S126	L127	S128	R129	L130	T131	L132	D133	D134	I135	E136	L137	L138	A139	S140	ARG	PHE	LEU	HIS	SER	PRO	GLU	VAL	THR	GLU	THR	GLU	THR	MET	GLU	LYS	GLY	PHE	SER	LYS	GLY	GLU	GLU	ASN	LEU	TYR	PHE	GLN															

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	28439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	300.3, 300.3, 300.3	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: ZN, MG, ATP

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	0.28	0/2463	0.48	2/3327 (0.1%)
1	B	0.28	0/2463	0.48	2/3327 (0.1%)
2	C	0.27	0/2228	0.45	0/3010
2	F	0.27	0/2228	0.45	0/3010
3	D	0.26	0/797	0.60	1/1082 (0.1%)
3	G	0.26	0/797	0.60	1/1082 (0.1%)
4	E	0.23	0/397	0.53	0/535
4	H	0.23	0/397	0.53	0/535
All	All	0.27	0/11770	0.49	6/15908 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	E	0	1
4	H	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	LEU	CB-CG-CD2	6.24	121.61	111.00
1	A	184	LEU	CB-CG-CD2	6.22	121.58	111.00
3	D	1049	LYS	CA-CB-CG	5.08	124.58	113.40
3	G	1049	LYS	CA-CB-CG	5.08	124.57	113.40
1	A	184	LEU	CB-CG-CD1	5.05	119.59	111.00
1	B	184	LEU	CB-CG-CD1	5.03	119.55	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	121	ARG	Sidechain
4	H	121	ARG	Sidechain

## 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	2417	0	2433	45	0
1	B	2417	0	2433	42	0
2	C	2175	0	2130	24	0
2	F	2175	0	2130	22	0
3	D	781	0	789	12	0
3	G	781	0	789	16	0
4	E	392	0	395	6	0
4	H	392	0	395	10	0
5	A	31	0	12	3	0
5	B	31	0	12	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
All	All	11595	0	11518	154	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (154) 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)
4:E:118:GLN:OE1	4:E:121:ARG:NH1	1.90	1.05
4:H:118:GLN:OE1	4:H:121:ARG:NH1	1.90	1.05
1:A:22:LEU:HD12	1:A:332:LEU:HD21	1.58	0.86
1:B:22:LEU:HD12	1:B:332:LEU:HD21	1.58	0.84
1:A:245:GLU:OE1	5:B:401:ATP:O3'	2.02	0.78
5:A:401:ATP:O3'	1:B:245:GLU:OE1	2.00	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:189:ARG:NH2	2:F:225:SER:OG	2.19	0.75
2:C:189:ARG:NH2	2:C:225:SER:OG	2.19	0.75
2:C:66:MET:CE	2:C:85:LEU:HD22	2.16	0.75
2:F:66:MET:CE	2:F:85:LEU:HD22	2.16	0.74
1:A:149:VAL:HG21	1:A:226:VAL:HG12	1.69	0.73
2:C:66:MET:HE1	2:C:85:LEU:HD22	1.71	0.73
1:B:149:VAL:HG21	1:B:226:VAL:HG12	1.69	0.72
1:A:305:GLU:OE1	2:F:18:ARG:NH1	2.24	0.70
2:F:66:MET:HE1	2:F:85:LEU:HD22	1.74	0.68
1:B:305:GLU:OE1	2:C:18:ARG:NH1	2.26	0.68
1:A:44:LYS:NZ	5:A:401:ATP:O3G	2.19	0.66
3:D:1102:LEU:O	3:D:1106:ILE:HD12	1.97	0.64
3:G:1102:LEU:O	3:G:1106:ILE:HD12	1.97	0.64
1:A:62:VAL:HG12	1:A:156:VAL:HG22	1.80	0.64
1:A:323:ASP:OD1	1:A:324:LYS:N	2.31	0.63
1:B:62:VAL:HG12	1:B:156:VAL:HG22	1.80	0.63
1:B:323:ASP:OD1	1:B:324:LYS:N	2.31	0.63
1:B:212:LEU:O	1:B:216:LEU:HD23	1.99	0.63
1:B:44:LYS:NZ	5:B:401:ATP:O3G	2.19	0.62
1:A:212:LEU:O	1:A:216:LEU:HD23	1.99	0.62
3:D:1080:THR:O	3:D:1081:SER:OG	2.17	0.62
1:A:132:ALA:HB1	1:B:176:ILE:HG21	1.82	0.61
2:F:102:ASP:OD1	2:F:103:GLU:N	2.33	0.61
2:C:102:ASP:OD1	2:C:103:GLU:N	2.33	0.61
1:A:176:ILE:HG21	1:B:132:ALA:HB1	1.82	0.60
1:A:312:LEU:HD23	1:A:328:PHE:CZ	2.38	0.59
1:B:312:LEU:HD23	1:B:328:PHE:CZ	2.37	0.58
3:G:1080:THR:O	3:G:1081:SER:OG	2.17	0.58
1:A:133:PHE:O	1:A:136:ILE:HG22	2.04	0.57
1:B:133:PHE:O	1:B:136:ILE:HG22	2.04	0.57
3:G:1074:ALA:O	4:H:114:ARG:NH2	2.38	0.57
1:B:123:LYS:O	1:B:127:GLN:HG2	2.07	0.55
3:D:1065:GLU:OE1	3:D:1065:GLU:N	2.39	0.55
1:A:123:LYS:O	1:A:127:GLN:HG2	2.07	0.54
2:F:163:ARG:CZ	2:F:167:LEU:HD11	2.37	0.54
2:C:121:GLU:N	2:C:121:GLU:OE1	2.40	0.54
2:F:121:GLU:OE1	2:F:121:GLU:N	2.40	0.54
1:A:22:LEU:CD1	1:A:332:LEU:HD21	2.35	0.54
2:C:163:ARG:CZ	2:C:167:LEU:HD11	2.37	0.54
3:G:1065:GLU:N	3:G:1065:GLU:OE1	2.39	0.53
1:B:22:LEU:CD1	1:B:332:LEU:HD21	2.35	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:111:ASP:O	4:E:115:VAL:HG23	2.09	0.53
3:D:1096:GLU:OE2	3:D:1099:ARG:NH1	2.41	0.53
4:H:111:ASP:O	4:H:115:VAL:HG23	2.09	0.53
1:A:132:ALA:HB1	1:B:176:ILE:HD13	1.91	0.52
3:G:1096:GLU:OE2	3:G:1099:ARG:NH1	2.41	0.52
1:A:130:MET:HG3	1:A:136:ILE:HD13	1.91	0.52
3:D:1060:GLN:HG2	3:D:1066:ALA:HB2	1.92	0.52
1:A:176:ILE:HD13	1:B:132:ALA:HB1	1.91	0.52
1:B:130:MET:HG3	1:B:136:ILE:HD13	1.91	0.52
3:G:1060:GLN:HG2	3:G:1066:ALA:HB2	1.92	0.51
2:F:163:ARG:NH2	2:F:167:LEU:HD11	2.26	0.51
1:B:162:ALA:O	1:B:167:THR:OG1	2.28	0.51
2:C:173:GLU:OE1	2:C:173:GLU:N	2.44	0.51
1:A:72:ASN:ND2	1:B:251:GLU:OE2	2.42	0.50
1:A:124:LYS:O	1:A:128:GLU:OE1	2.29	0.50
2:C:140:LEU:HD22	2:C:168:HIS:O	2.12	0.50
2:F:173:GLU:N	2:F:173:GLU:OE1	2.44	0.50
2:C:193:ASP:O	2:C:196:VAL:HG12	2.12	0.50
2:C:163:ARG:NH2	2:C:167:LEU:HD11	2.26	0.50
2:F:193:ASP:O	2:F:196:VAL:HG12	2.12	0.50
1:B:124:LYS:O	1:B:128:GLU:OE1	2.29	0.50
3:G:1101:GLN:OE1	4:H:123:TYR:OH	2.12	0.49
1:A:251:GLU:OE2	1:B:72:ASN:ND2	2.42	0.49
2:F:140:LEU:HD22	2:F:168:HIS:O	2.12	0.49
3:G:1070:ALA:O	4:H:118:GLN:HG2	2.13	0.48
1:A:162:ALA:O	1:A:167:THR:OG1	2.28	0.47
1:A:70:ALA:HB2	1:B:164:THR:OG1	2.14	0.47
2:C:193:ASP:OD1	2:C:194:MET:N	2.47	0.47
2:F:193:ASP:OD1	2:F:194:MET:N	2.47	0.47
1:A:266:THR:HG23	1:A:266:THR:O	2.14	0.47
1:A:115:GLU:N	1:A:115:GLU:OE1	2.44	0.47
1:A:162:ALA:HB1	1:A:163:PRO:HD2	1.97	0.47
1:B:115:GLU:N	1:B:115:GLU:OE1	2.44	0.47
1:B:266:THR:HG23	1:B:266:THR:O	2.14	0.47
3:G:1109:ARG:HG3	4:H:130:LEU:HD23	1.97	0.47
1:B:312:LEU:HD23	1:B:328:PHE:HZ	1.80	0.46
1:A:164:THR:OG1	1:B:70:ALA:HB2	2.15	0.46
2:F:167:LEU:HA	2:F:203:PHE:HE1	1.81	0.46
1:B:162:ALA:HB1	1:B:163:PRO:HD2	1.97	0.46
3:D:1070:ALA:O	4:E:118:GLN:HG2	2.14	0.46
1:B:136:ILE:HG23	1:B:137:ASP:N	2.31	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HG23	1:A:137:ASP:N	2.31	0.45
2:F:41:GLU:O	2:F:45:MET:HG3	2.17	0.45
2:C:207:LYS:NZ	2:C:282:LEU:O	2.50	0.45
2:F:207:LYS:NZ	2:F:282:LEU:O	2.50	0.45
3:G:1111:GLN:HA	3:G:1111:GLN:OE1	2.17	0.45
1:A:163:PRO:HG2	1:B:163:PRO:HG2	1.98	0.44
2:C:41:GLU:O	2:C:45:MET:HG3	2.17	0.44
2:C:167:LEU:HA	2:C:203:PHE:HE1	1.81	0.44
2:C:230:PRO:N	2:C:231:PRO:CD	2.80	0.44
3:G:1070:ALA:HA	4:H:118:GLN:HG2	1.98	0.44
1:B:162:ALA:HB1	1:B:163:PRO:CD	2.48	0.44
3:D:1111:GLN:HA	3:D:1111:GLN:OE1	2.17	0.44
3:G:1038:LEU:HB2	3:G:1043:LEU:HD21	2.00	0.44
3:D:1066:ALA:HB1	4:E:119:LEU:HD11	2.00	0.43
4:E:123:TYR:O	4:E:127:LEU:HG	2.19	0.43
1:A:312:LEU:HD23	1:A:328:PHE:HZ	1.80	0.43
3:G:1060:GLN:CG	3:G:1066:ALA:HB2	2.48	0.43
2:C:147:GLN:NE2	2:C:171:ASP:OD2	2.51	0.43
3:D:1060:GLN:CG	3:D:1066:ALA:HB2	2.48	0.43
1:A:31:LEU:O	1:A:156:VAL:HG12	2.19	0.43
1:B:124:LYS:O	1:B:127:GLN:N	2.51	0.43
2:F:147:GLN:NE2	2:F:171:ASP:OD2	2.51	0.43
2:F:230:PRO:N	2:F:231:PRO:CD	2.80	0.43
1:A:124:LYS:O	1:A:127:GLN:N	2.51	0.43
1:A:162:ALA:HB1	1:A:163:PRO:CD	2.48	0.42
1:B:223:ILE:O	1:B:226:VAL:HG22	2.19	0.42
4:H:123:TYR:O	4:H:127:LEU:HG	2.18	0.42
1:B:219:THR:O	1:B:222:VAL:HG12	2.19	0.42
1:A:239:ILE:HG23	1:A:268:ASN:OD1	2.19	0.42
1:B:31:LEU:O	1:B:156:VAL:HG12	2.19	0.42
1:A:219:THR:O	1:A:222:VAL:HG12	2.19	0.42
5:A:401:ATP:O3B	1:B:39:LYS:NZ	2.53	0.42
1:A:223:ILE:O	1:A:226:VAL:HG22	2.19	0.42
3:D:1038:LEU:HB2	3:D:1043:LEU:HD21	2.00	0.42
2:C:257:VAL:HG13	3:D:1010:TRP:HB2	2.01	0.42
1:A:170:LEU:O	1:A:174:PRO:HD3	2.20	0.42
1:A:253:GLU:HG2	2:F:48:THR:HG22	2.01	0.42
1:A:112:PHE:O	2:C:278:ARG:NH1	2.52	0.41
1:B:170:LEU:O	1:B:174:PRO:HD3	2.20	0.41
1:B:253:GLU:HG2	2:C:48:THR:HG22	2.02	0.41
2:F:90:LEU:HD11	2:F:125:PHE:CD1	2.55	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1074:ALA:HB2	4:H:118:GLN:HE21	1.84	0.41
1:B:239:ILE:HG23	1:B:268:ASN:OD1	2.19	0.41
4:E:130:LEU:HD12	4:E:134:ASP:HB2	2.01	0.41
1:B:103:LEU:HB3	1:B:127:GLN:OE1	2.20	0.41
2:C:203:PHE:HD2	2:C:212:ALA:HA	1.85	0.41
1:B:187:ILE:HG23	1:B:187:ILE:O	2.21	0.41
3:D:1033:LYS:HD2	3:D:1034:PRO:O	2.21	0.41
4:H:130:LEU:HD12	4:H:134:ASP:HB2	2.01	0.41
1:B:181:LEU:HD21	1:B:220:LEU:HA	2.03	0.41
1:A:39:LYS:NZ	5:B:401:ATP:O3B	2.54	0.41
1:A:181:LEU:HD21	1:A:220:LEU:HA	2.03	0.41
2:F:81:SER:O	2:F:85:LEU:HG	2.21	0.41
2:F:142:HIS:O	2:F:144:ARG:N	2.54	0.41
2:C:90:LEU:HD11	2:C:125:PHE:CD1	2.55	0.40
1:A:124:LYS:HE3	1:A:124:LYS:HB2	1.96	0.40
1:A:164:THR:CB	1:A:255:LEU:HD12	2.51	0.40
1:A:187:ILE:O	1:A:187:ILE:HG23	2.21	0.40
2:C:142:HIS:O	2:C:144:ARG:N	2.54	0.40
1:A:24:ASN:OD1	1:A:24:ASN:N	2.54	0.40
2:F:203:PHE:HD2	2:F:212:ALA:HA	1.85	0.40
1:A:103:LEU:HB3	1:A:127:GLN:OE1	2.20	0.40
1:B:164:THR:CB	1:B:255:LEU:HD12	2.51	0.40
2:C:81:SER:O	2:C:85:LEU:HG	2.21	0.40
3:G:1033:LYS:HD2	3:G:1034:PRO:O	2.21	0.40
3:G:1048:ALA:O	3:G:1049:LYS:HD3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	302/343 (88%)	292 (97%)	10 (3%)	0	100 100

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	302/343 (88%)	292 (97%)	10 (3%)	0	100	100
2	C	269/333 (81%)	266 (99%)	3 (1%)	0	100	100
2	F	269/333 (81%)	266 (99%)	3 (1%)	0	100	100
3	D	95/132 (72%)	87 (92%)	8 (8%)	0	100	100
3	G	95/132 (72%)	87 (92%)	8 (8%)	0	100	100
4	E	46/165 (28%)	46 (100%)	0	0	100	100
4	H	46/165 (28%)	46 (100%)	0	0	100	100
All	All	1424/1946 (73%)	1382 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/305 (90%)	274 (100%)	0	100	100
1	B	274/305 (90%)	274 (100%)	0	100	100
2	C	236/281 (84%)	236 (100%)	0	100	100
2	F	236/281 (84%)	236 (100%)	0	100	100
3	D	85/110 (77%)	84 (99%)	1 (1%)	71	83
3	G	85/110 (77%)	84 (99%)	1 (1%)	71	83
4	E	42/148 (28%)	41 (98%)	1 (2%)	49	73
4	H	42/148 (28%)	41 (98%)	1 (2%)	49	73
All	All	1274/1688 (76%)	1270 (100%)	4 (0%)	92	96

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

Mol	Chain	Res	Type
3	D	1060	GLN
4	E	119	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	1060	GLN
4	H	119	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	142	HIS
2	F	142	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 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	$\# Z  > 2$
5	ATP	A	401	6	26,33,33	0.63	0	31,52,52	1.07	2 (6%)
5	ATP	B	401	6	26,33,33	0.62	0	31,52,52	1.07	2 (6%)

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	ATP	A	401	6	-	2/18/38/38	0/3/3/3
5	ATP	B	401	6	-	2/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	ATP	C5-C6-N6	2.27	123.81	120.35
5	A	401	ATP	C5-C6-N6	2.26	123.78	120.35
5	B	401	ATP	PB-O3B-PG	2.02	139.75	132.83
5	A	401	ATP	PB-O3B-PG	2.02	139.74	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	ATP	PA-O3A-PB-O2B
5	B	401	ATP	PA-O3A-PB-O2B
5	A	401	ATP	PA-O3A-PB-O1B
5	B	401	ATP	PA-O3A-PB-O1B

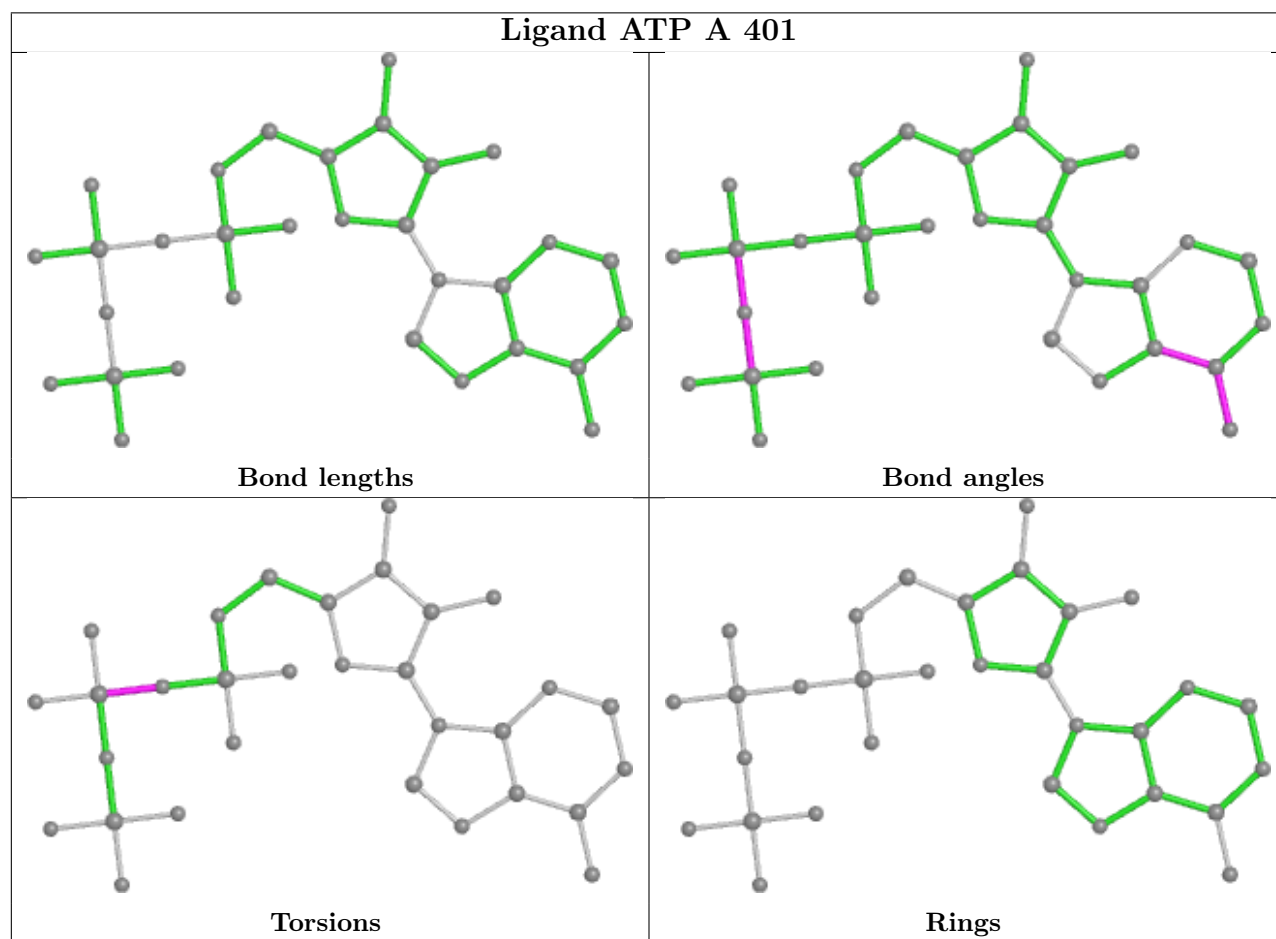
There are no ring outliers.

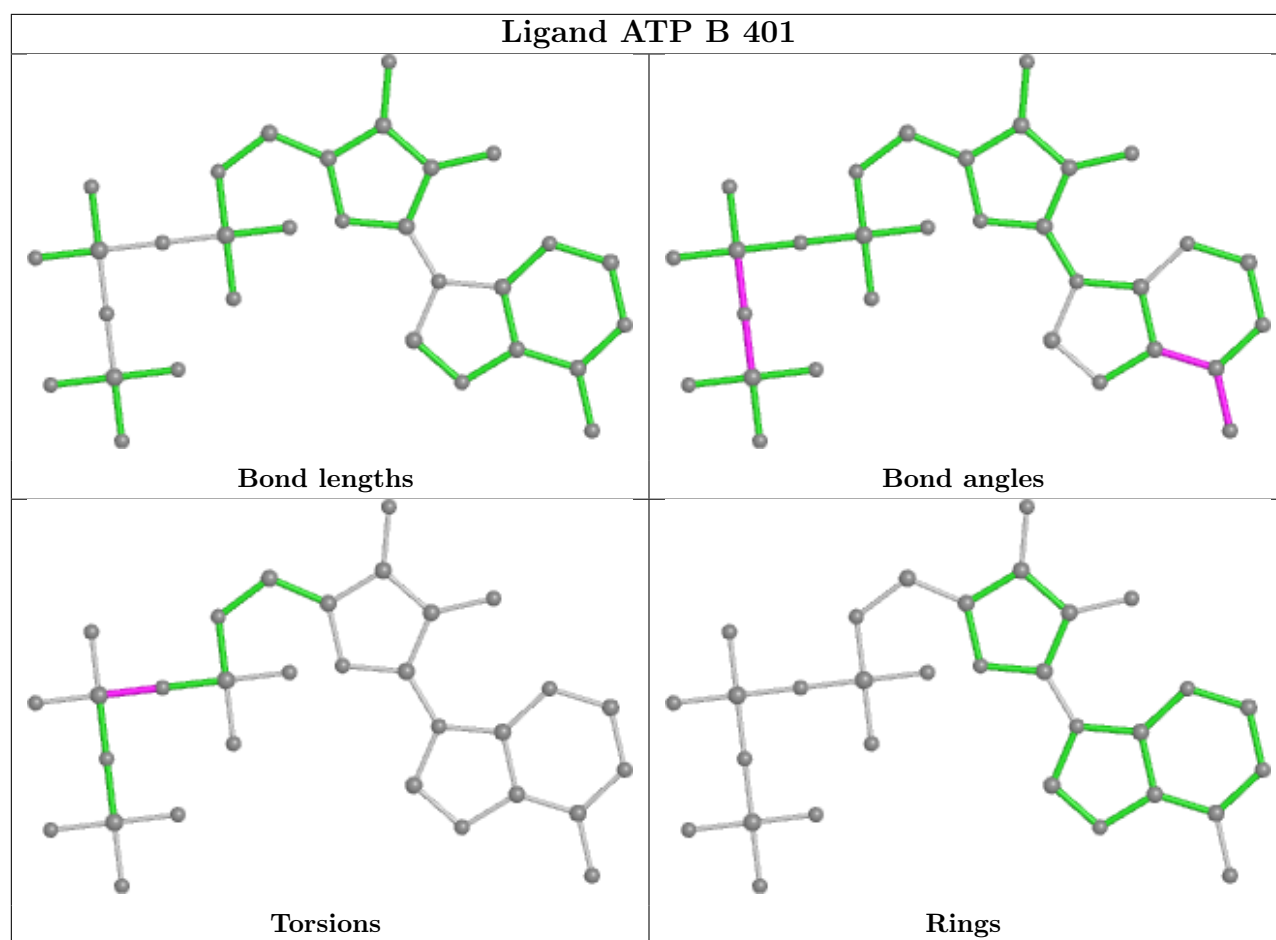
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	ATP	3	0
5	B	401	ATP	3	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.

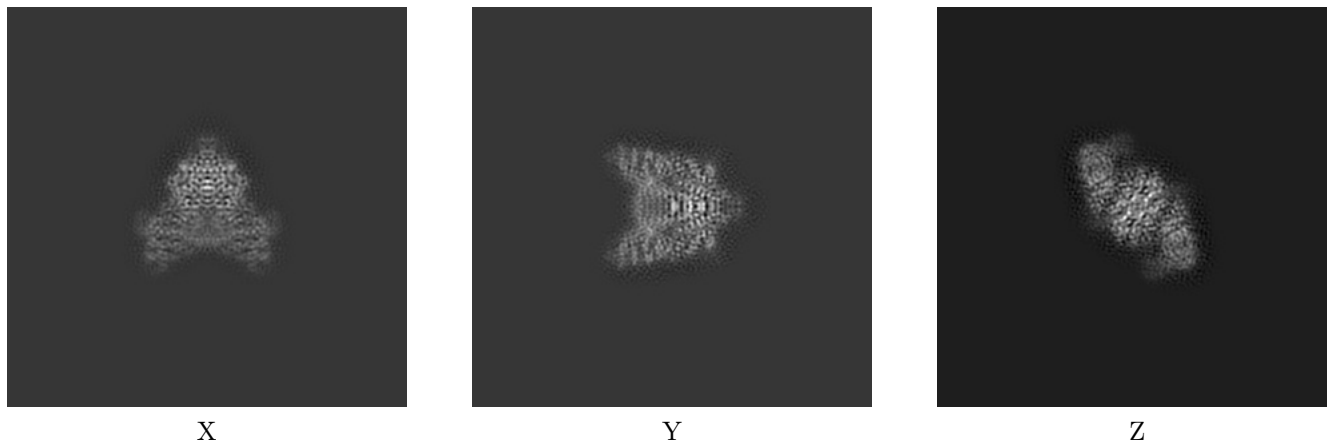
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24700. These allow visual inspection of the internal detail of the map and identification of artifacts.

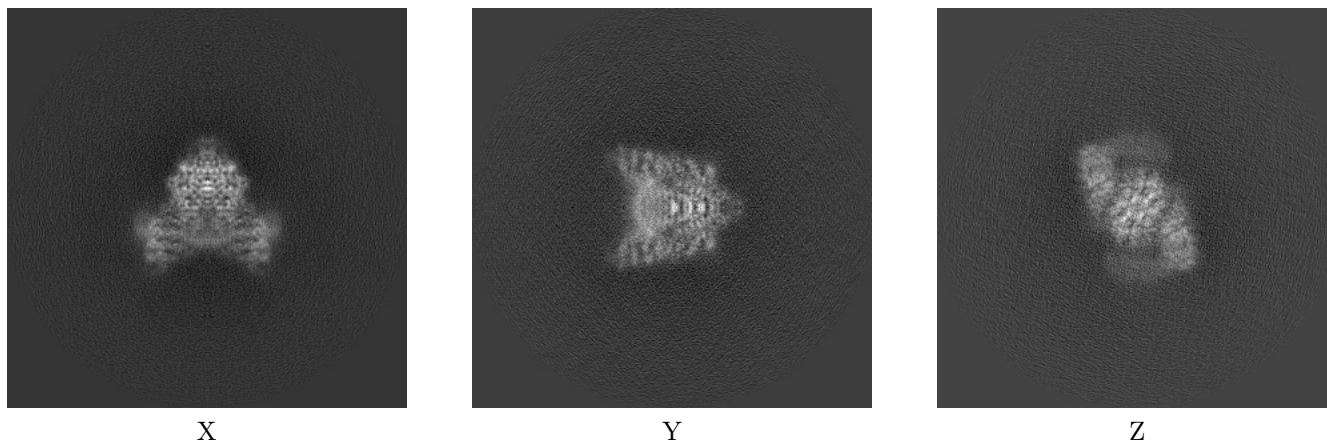
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



#### 6.1.2 Raw map



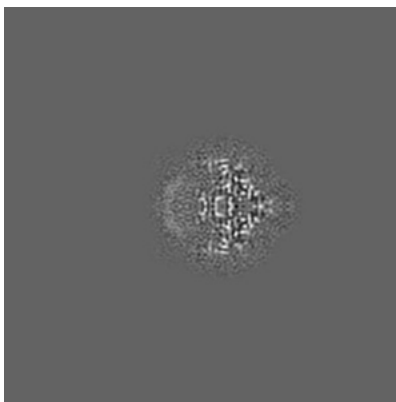
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

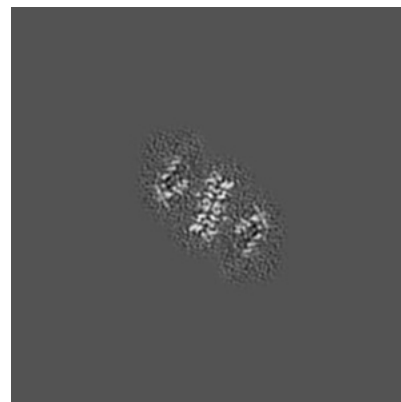
### 6.2.1 Primary map



X Index: 182

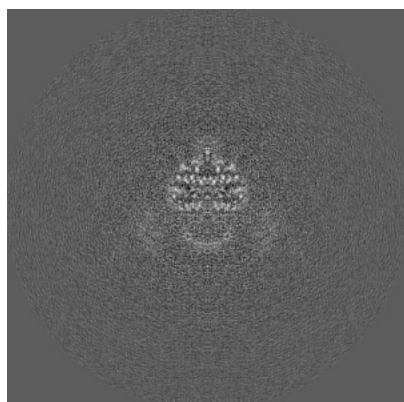


Y Index: 182

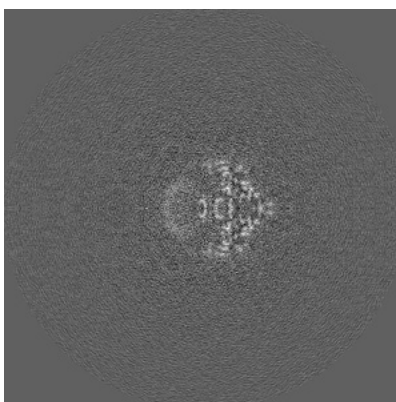


Z Index: 182

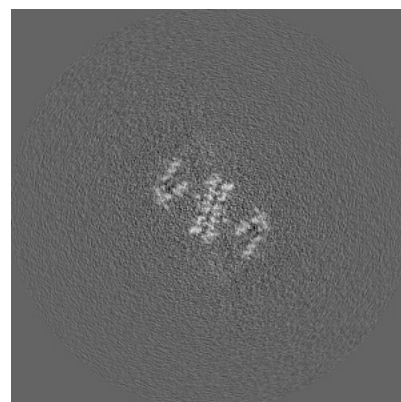
### 6.2.2 Raw map



X Index: 182



Y Index: 182

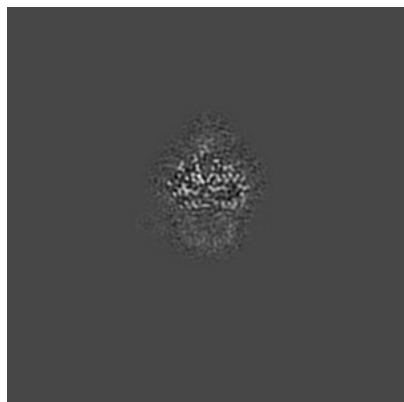


Z Index: 182

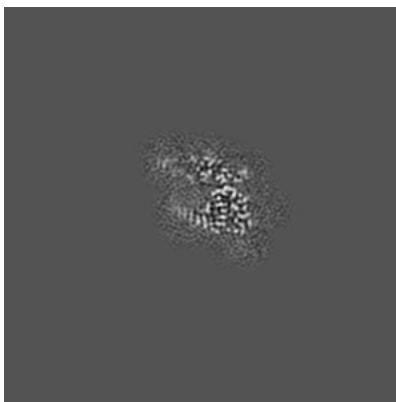
The images above show central slices of the map in three orthogonal directions.

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

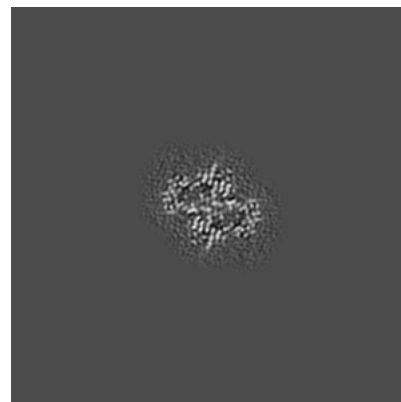
### 6.3.1 Primary map



X Index: 184

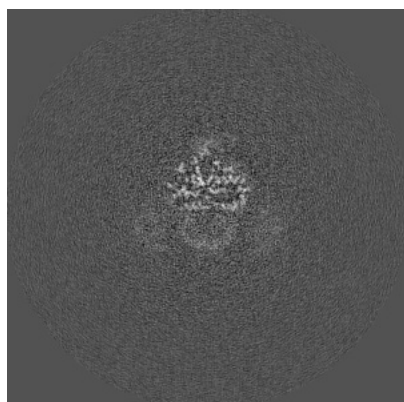


Y Index: 162

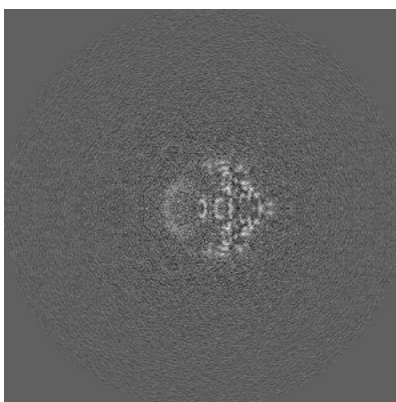


Z Index: 199

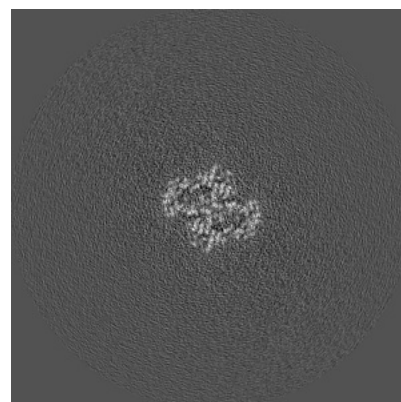
### 6.3.2 Raw map



X Index: 184



Y Index: 182



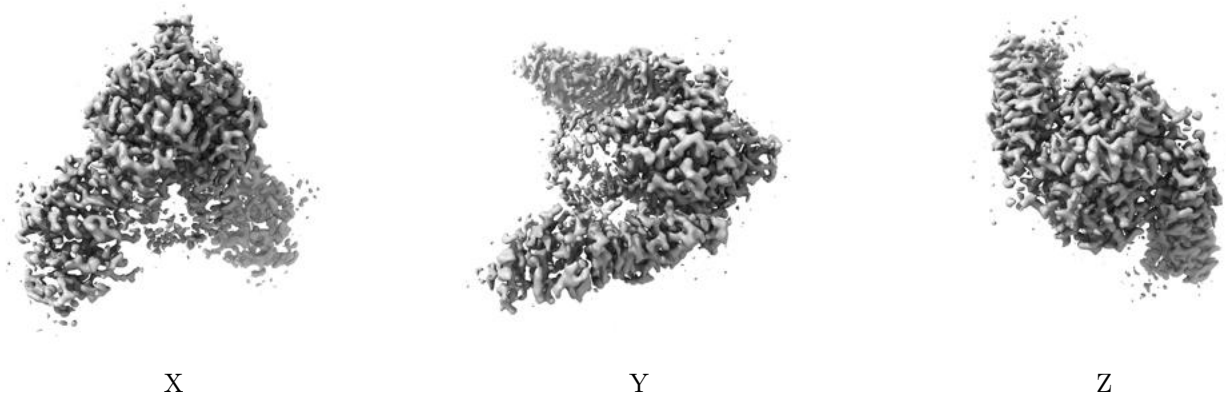
Z Index: 199

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



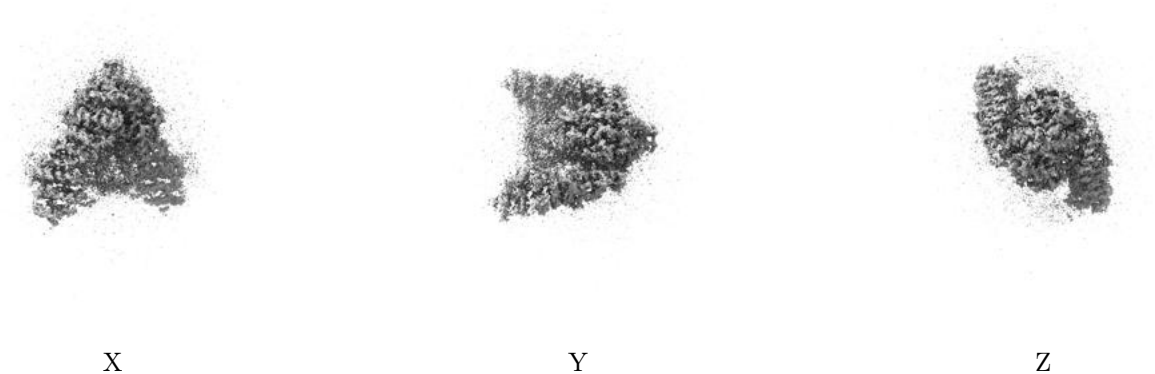
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

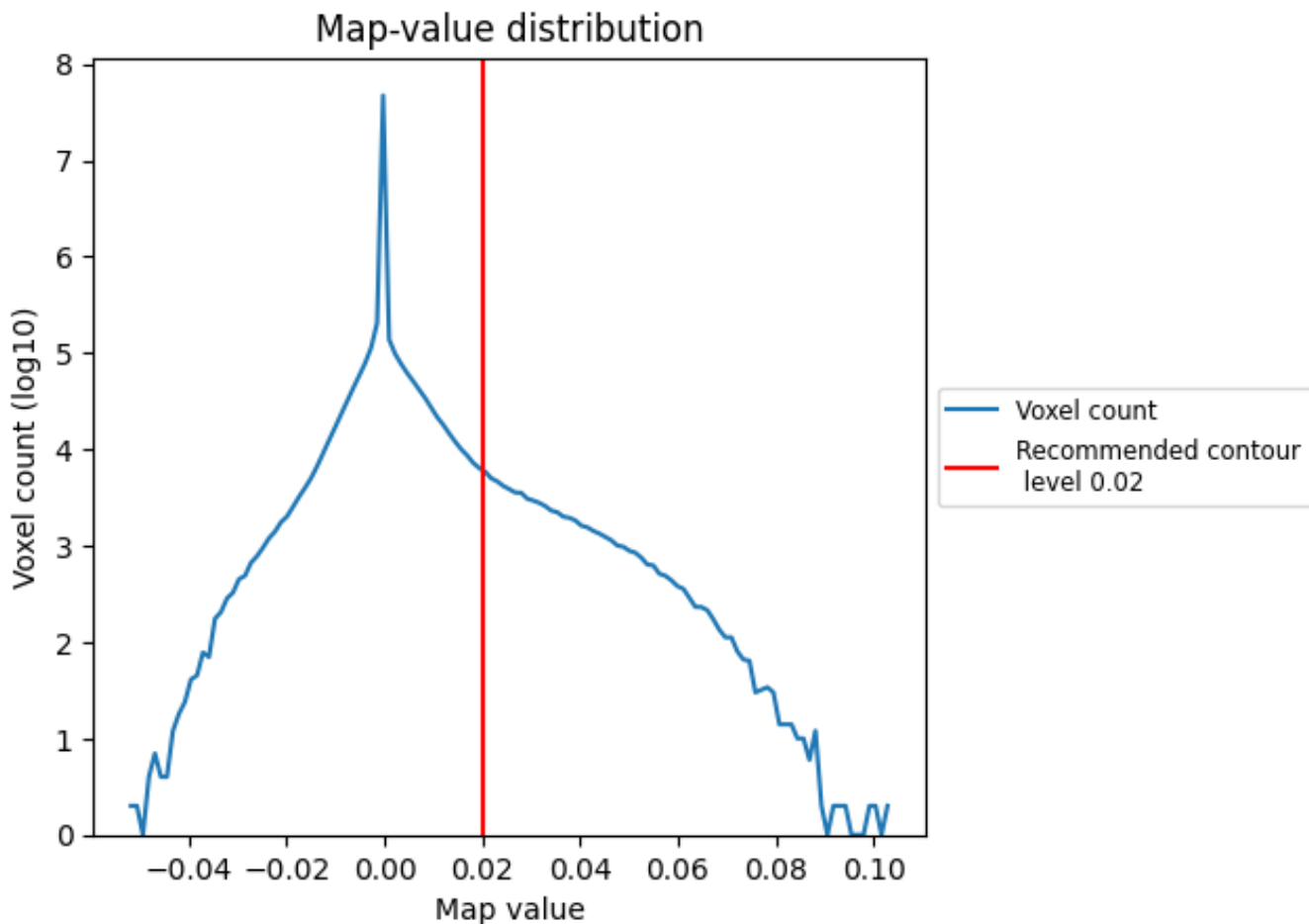
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

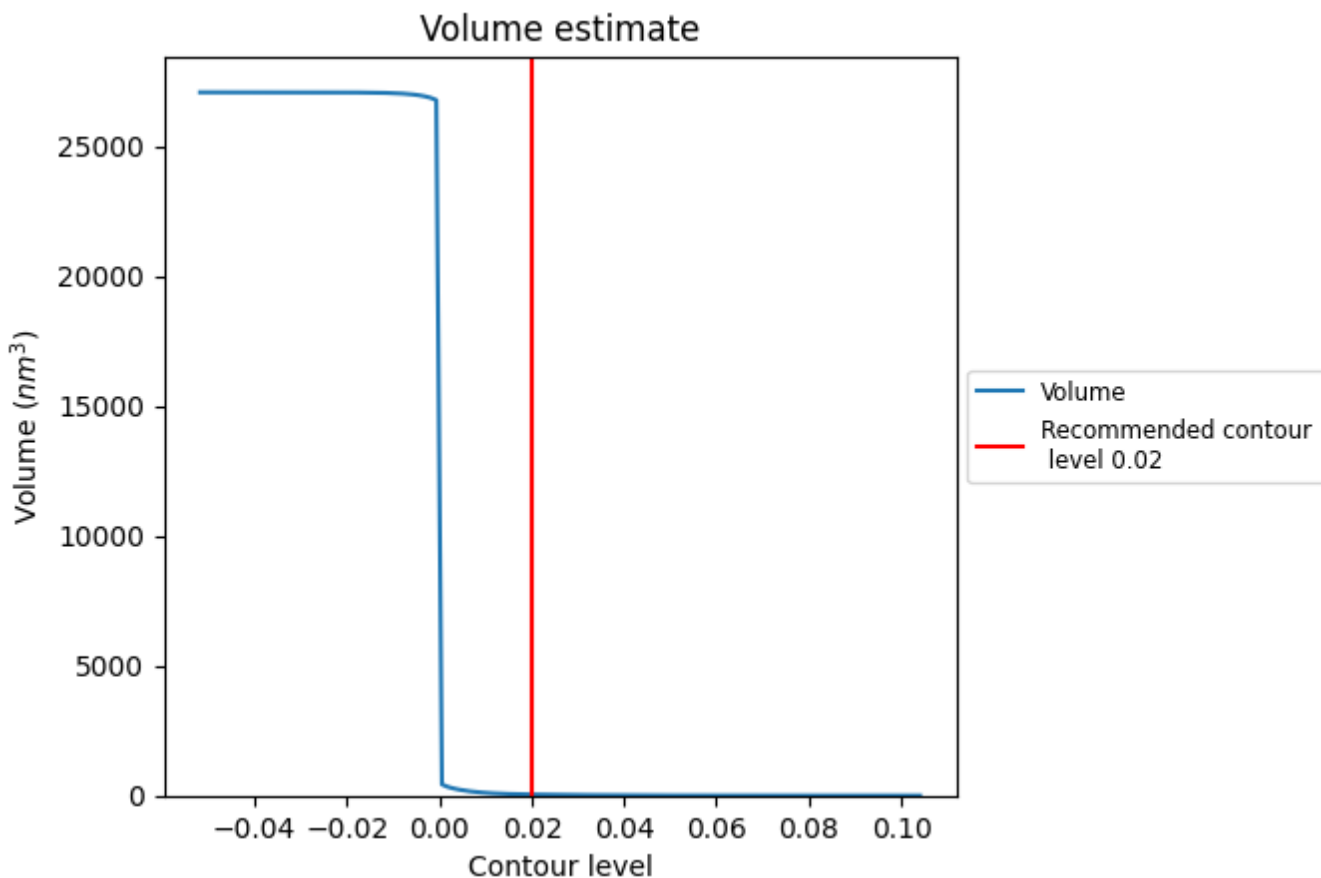
This section contains the results of statistical analysis of the map.

### 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.

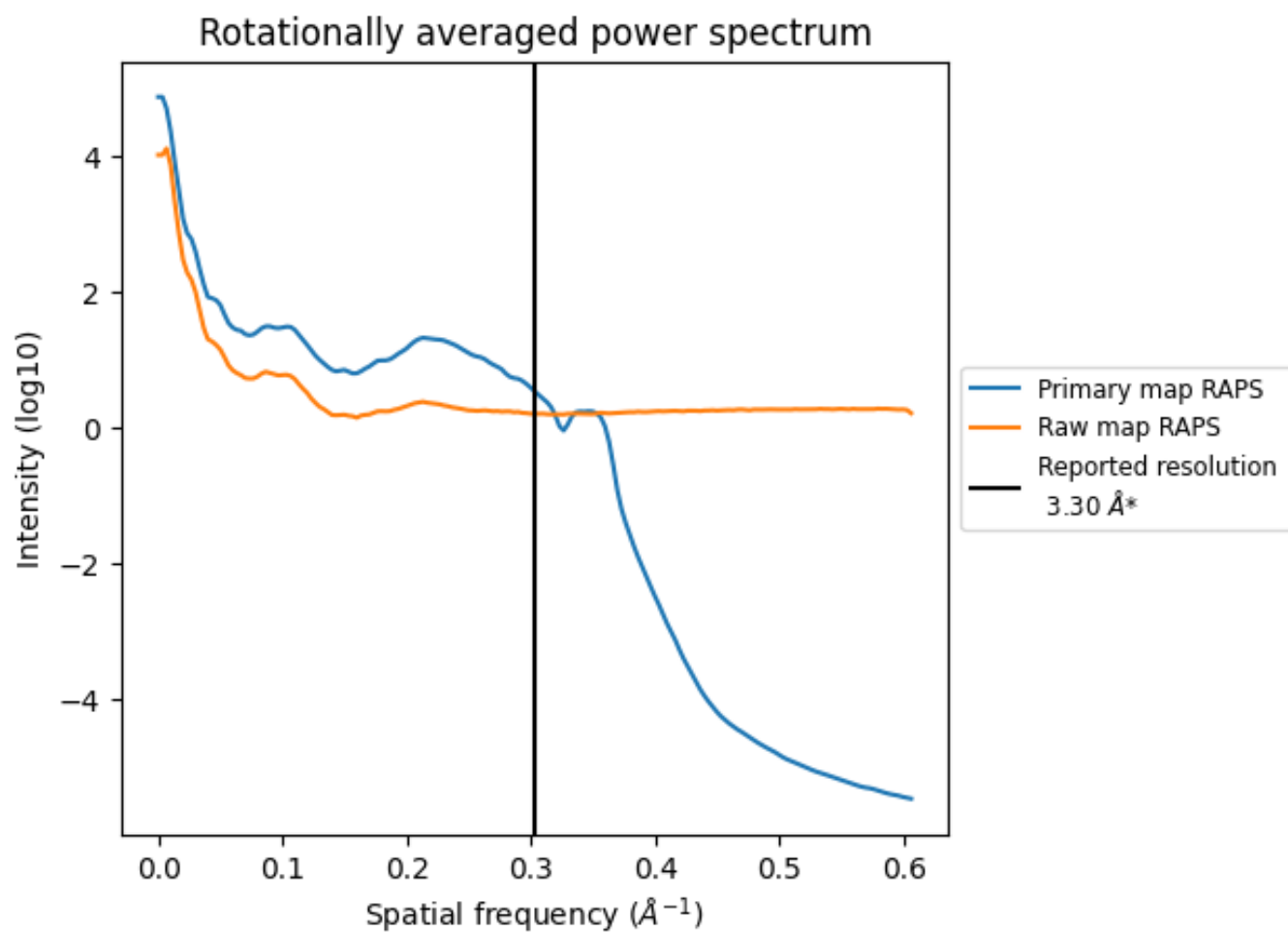
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 41  $\text{nm}^3$ ; this corresponds to an approximate mass of 37 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

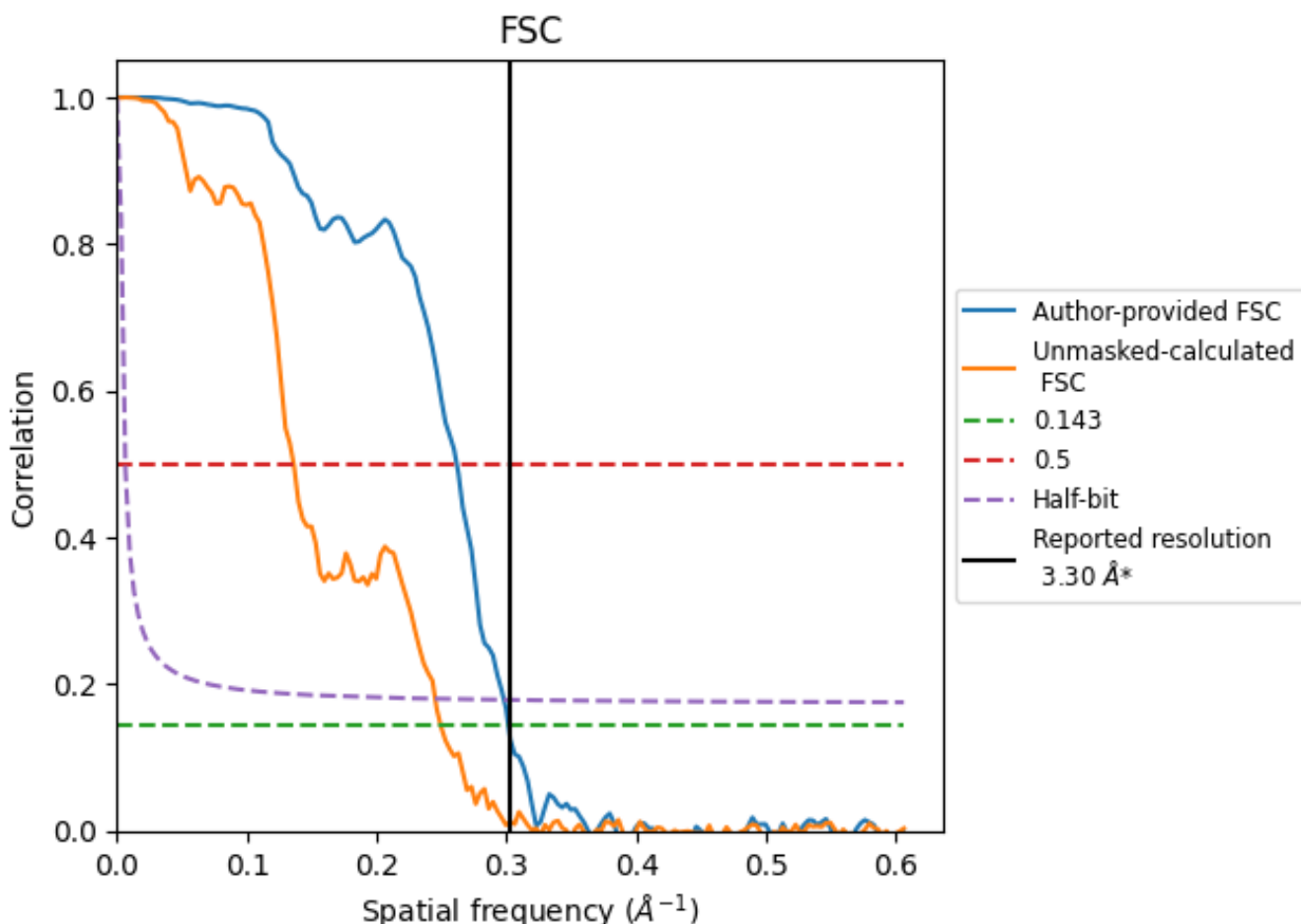


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

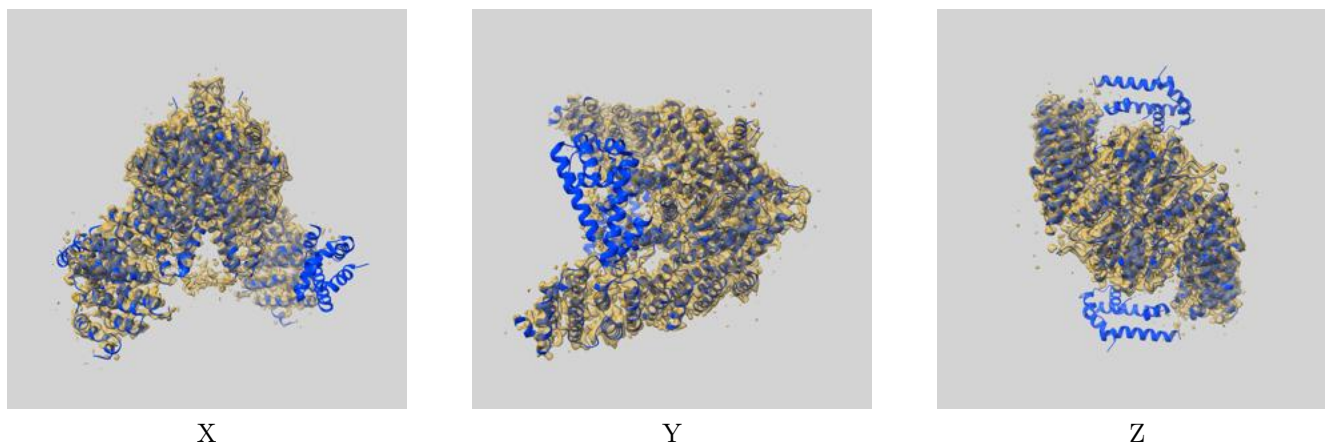
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.82	3.35
Unmasked-calculated*	4.01	7.34	4.08

\*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 4.01 differs from the reported value 3.3 by more than 10 %

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

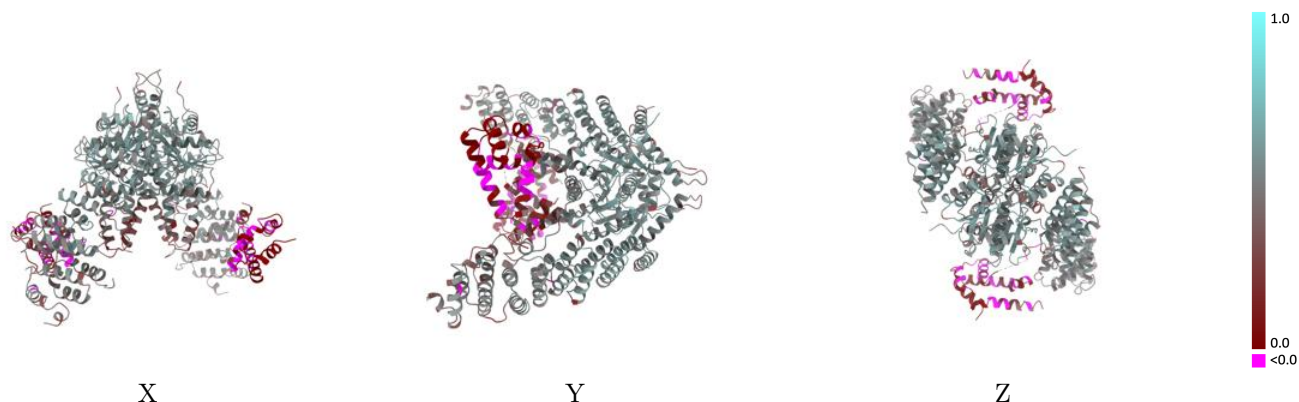
This section contains information regarding the fit between EMDB map EMD-24700 and PDB model 7RU9. Per-residue inclusion information can be found in section 3 on page 7.

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



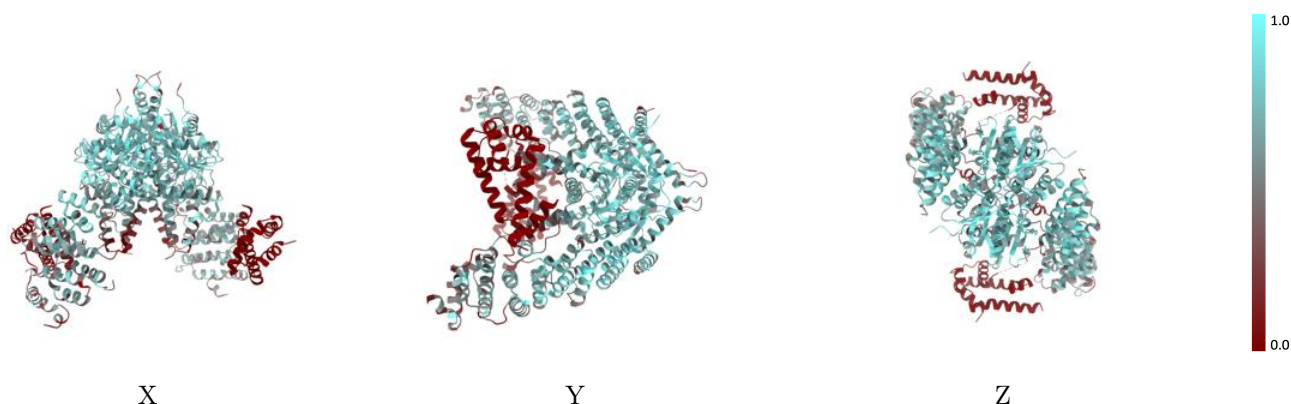
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

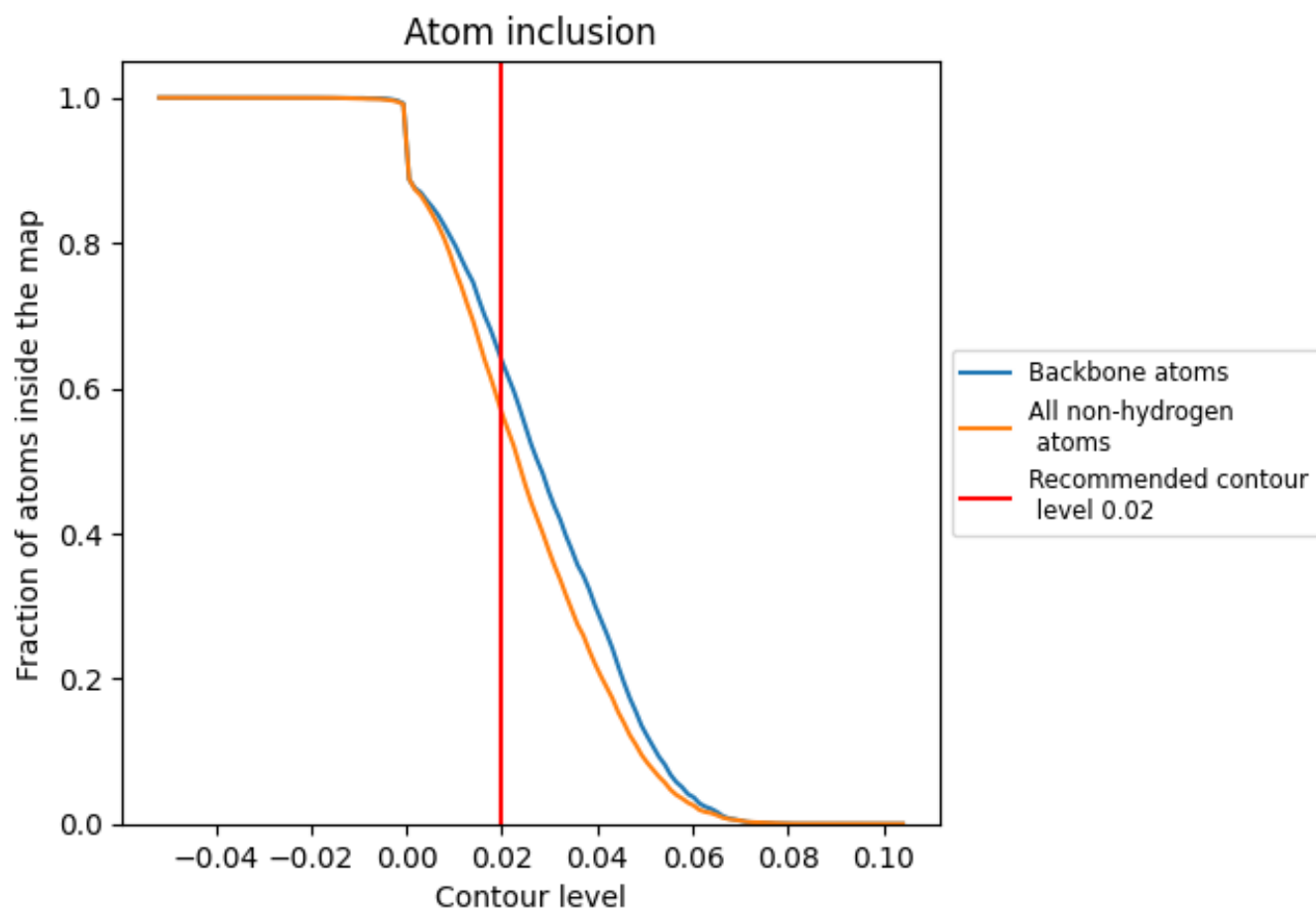
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.02).





















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 57% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5656	 0.4230
A	 0.6828	 0.5010
B	 0.6835	 0.4990
C	 0.6682	 0.4950
D	 0.1871	 0.1730
E	 0.0000	 0.0460
F	 0.6692	 0.4940
G	 0.1805	 0.1740
H	 0.0000	 0.0510

