



## Full wwPDB EM Validation Report ⓘ

Oct 17, 2024 – 04:23 PM EDT

PDB ID : 7SZ5  
EMDB ID : EMD-25561  
Title : Cryo-EM structure of the extracellular module of the full-length EGFR bound to TGF- $\alpha$  "tips-separated" conformation  
Authors : Huang, Y.; Ognjenovic, J.; Karandur, D.; Miller, K.; Merk, A.; Subramaniam, S.; Kuriyan, J.  
Deposited on : 2021-11-25  
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

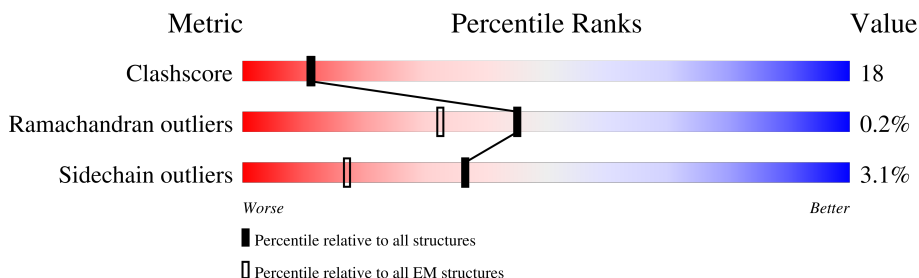
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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	1210	
1	B	1210	
2	C	50	
2	D	50	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9367 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	614	Total	C	N	O	S	0	0
			4723	2914	842	907	60		
1	B	500	Total	C	N	O	S	0	0
			3872	2401	686	743	42		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	ASN	ASP	conflict	UNP P00533
B	232	ASN	ASP	conflict	UNP P00533

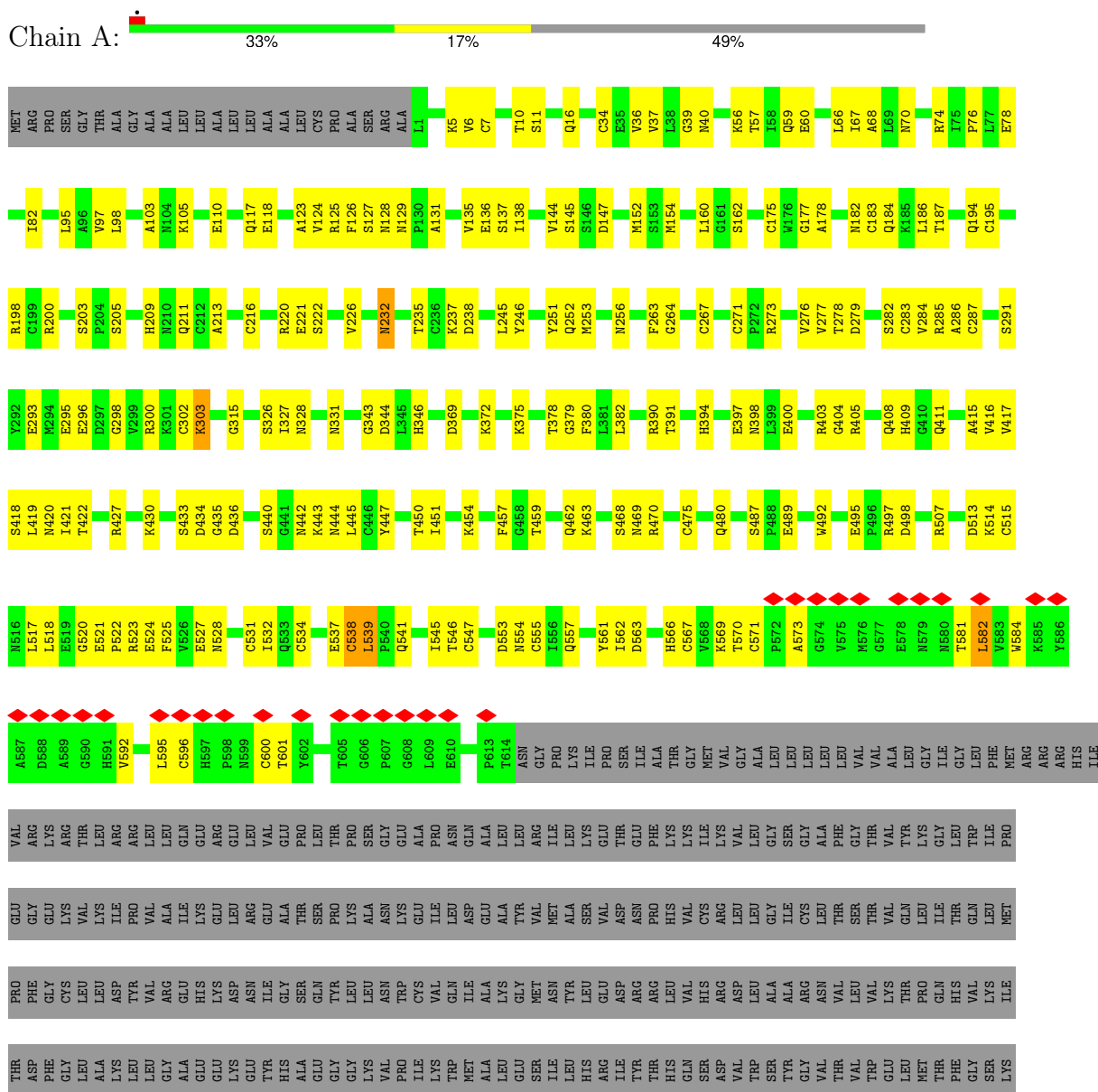
- Molecule 2 is a protein called Transforming growth factor alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	50	Total	C	N	O	S	0	0
			386	239	70	71	6		
2	D	50	Total	C	N	O	S	0	0
			386	239	70	71	6		

### 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.

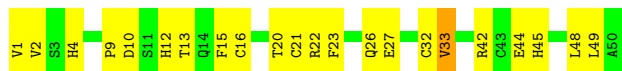
#### • Molecule 1: Epidermal growth factor receptor





GLU	TYR	PRO	ALA	TYR	ASP
LEU	THR	GLU	LEU	LEU	SER
ARG	TYR	LEU	THR	ILE	ARG
VAL	ARG	LEU	ASP	PRO	PRO
ALA	VAL	THR	SER	GLN	LYS
PRO	PRO	VAL	ILE	GLY	PHE
GLN	GLN	GLN	ASP	PHE	ARG
SER	SER	PRO	ASP	PHE	GLY
SER	THR	PRO	THR	SER	THR
GLU	THR	THR	THR	SER	THR
PHE	PHE	CYS	PHE	SER	ILE
GLY	GLY	VAL	LEU	PRO	GLU
ILE	ILE	ASN	PRO	SER	PHE
ALA	ALA	SER	VAL	THR	SER
		PHE	GLU	SER	LYS
		ASP	THR	ARG	GLY
		SER	TYR	THR	SER
		PRO	ASN	PRO	LYS
		ALA	GLN	LEU	PRO
		HIS	SER	GLN	ASP
		TRP	VAL	SER	GLY
		ALA	PRO	LEU	ILE
		GLN	LYS	SER	PRO
		LYS	ARG	ALA	ALA
		GLY	PRO	THR	SER
		SER	ALA	SER	GLU
		HIS	GLY	ASN	ILE
		GLN	SER	ASN	SER
		ILE	VAL	SER	SER
		SER	GLN	THR	ILE
		LEU	ASN	VAL	LEU
		ASP	PRO	ALA	GLU
		ASN	VAL	CYS	LYS
		PRO	TYR	ILE	GLY
		ASP	HIS	ASP	GLU
		TYR	ASN	ARG	ARG
		GLN	GLN	ASN	THR
		GLN	LEU	GLY	LEU
		ASP	LEU	LEU	GLN
		PHE	ASN	GLN	PRO
		PHE	PRO	SER	PRO
		PRO	ALA	CYS	ILE
		LYS	PRO	THR	CYS
		ALA	ARG	ILE	THR
		GLU	SER	LYS	ILE
		LYS	ASP	GLU	ASP
		PRO	PRO	ASP	VAL
		ASN	HIS	SER	TYR
		GLY	TYR	PHE	MET
		ILE	GLN	LEU	ILE
		PHE	ASP	GLN	MET
		LYS	PRO	ARG	VAL
		GLY	HIS	TYR	LYS
		SER	SER	SER	LYS
		THR	THR	ASP	TRP
		ALA	VAL	PRO	ILE
		GLU	VAL	ASP	ALA
		ASN	GLY	THR	GLU
		ALA	ASN	CTY	ALA

- Molecule 2: Transforming growth factor alpha



- Molecule 2: Transforming growth factor alpha



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102206	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 ( $e^-/\text{\AA}^2$ )	50	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	1.277	Depositor
Minimum map value	-0.509	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	431.75998, 431.75998, 431.75998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0794, 1.0794, 1.0794	Depositor

## 5 Model quality [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.39	0/4815	0.51	0/6514
1	B	0.39	0/3943	0.54	0/5327
2	C	0.50	0/397	0.56	0/538
2	D	0.44	0/397	0.51	0/538
All	All	0.40	0/9552	0.52	0/12917

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 [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	4723	0	4556	139	0
1	B	3872	0	3779	176	0
2	C	386	0	345	14	0
2	D	386	0	345	11	0
All	All	9367	0	9025	328	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 18.

All (328) 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:B:154:MET:HB3	1:B:156:PHE:CE1	1.11	1.63
1:B:154:MET:CB	1:B:156:PHE:HE1	1.02	1.63
1:B:154:MET:HB3	1:B:156:PHE:CD1	1.87	1.09
1:B:154:MET:CG	1:B:156:PHE:CE1	2.39	1.05
1:B:154:MET:CG	1:B:156:PHE:HE1	1.70	1.04
1:B:416:VAL:HG13	1:B:419:LEU:HD21	1.59	0.84
1:B:154:MET:CB	1:B:156:PHE:CE1	1.95	0.83
1:B:156:PHE:HD1	1:B:156:PHE:H	1.23	0.81
1:B:349:PRO:HD3	1:B:384:GLN:HB2	1.64	0.79
1:B:274:ASN:O	1:B:405:ARG:NH1	2.18	0.77
1:A:397:GLU:OE2	1:A:427:ARG:NH1	2.18	0.76
2:D:12:HIS:HB3	2:D:15:PHE:HB2	1.68	0.76
2:C:9:PRO:HD3	2:C:23:PHE:HB2	1.67	0.76
1:B:154:MET:CG	1:B:156:PHE:CZ	2.69	0.76
1:B:427:ARG:HE	1:B:498:ASP:HB3	1.49	0.76
1:A:252:GLN:HE22	1:B:286:ALA:H	1.34	0.75
1:A:403:ARG:O	1:A:433:SER:OG	2.03	0.75
1:A:520:GLY:O	1:A:523:ARG:NH2	2.19	0.75
1:B:379:GLY:HA2	1:B:405:ARG:H	1.52	0.72
1:B:48:ARG:NH2	1:B:106:THR:OG1	2.22	0.72
1:B:311:LYS:NZ	1:B:338:CYS:SG	2.59	0.72
1:B:154:MET:HG3	1:B:156:PHE:CZ	2.24	0.71
1:A:103:ALA:O	1:A:105:LYS:NZ	2.23	0.71
1:B:136:GLU:HA	1:B:156:PHE:CD2	2.26	0.70
1:A:427:ARG:NH2	1:A:498:ASP:OD1	2.23	0.69
1:A:523:ARG:NH1	1:A:541:GLN:OE1	2.25	0.69
1:B:177:GLY:HA3	1:B:182:ASN:ND2	2.08	0.69
1:B:378:THR:O	1:B:404:GLY:N	2.24	0.69
1:A:328:ASN:OD1	1:A:331:ASN:ND2	2.26	0.68
2:C:21:CYS:HA	2:C:32:CYS:HB2	1.76	0.68
1:B:186:LEU:HD12	1:B:189:ILE:HD11	1.75	0.68
1:B:385:ALA:HA	1:B:419:LEU:HB3	1.75	0.68
1:B:328:ASN:OD1	1:B:331:ASN:ND2	2.28	0.67
1:A:213:ALA:HB3	1:A:226:VAL:HG23	1.77	0.67
1:B:134:ASN:N	1:B:136:GLU:OE1	2.27	0.67
2:C:10:ASP:HA	2:C:13:THR:HB	1.76	0.66
1:B:279:ASP:OD1	1:B:280:HIS:ND1	2.28	0.66
1:A:378:THR:HA	1:A:403:ARG:HB2	1.78	0.66
2:C:15:PHE:O	2:C:42:ARG:NH2	2.28	0.66
1:B:386:TRP:HE3	1:B:387:PRO:HD2	1.61	0.66
1:B:154:MET:SD	1:B:156:PHE:CZ	2.89	0.66
1:A:286:ALA:O	1:B:252:GLN:NE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:SER:HG	1:A:468:SER:HG	1.43	0.65
1:B:376:GLU:OE1	1:B:403:ARG:NH2	2.28	0.65
1:B:78:GLU:OE1	1:B:114:ARG:NE	2.29	0.65
1:B:343:GLY:N	1:B:378:THR:OG1	2.30	0.65
1:B:154:MET:HG3	1:B:156:PHE:CE1	2.32	0.65
1:A:232:ASN:HB3	1:A:267:CYS:HB2	1.80	0.64
1:B:199:CYS:HA	1:B:208:CYS:H	1.63	0.64
1:B:232:ASN:HB3	1:B:267:CYS:HB2	1.79	0.64
1:A:118:GLU:OE2	1:A:198:ARG:NH1	2.29	0.64
1:A:175:CYS:HA	1:A:183:CYS:HA	1.80	0.64
1:B:27:LEU:HD21	1:B:43:ILE:HG22	1.79	0.64
1:A:211:GLN:NE2	1:A:238:ASP:OD2	2.31	0.64
1:A:563:ASP:HB3	1:A:566:HIS:HB2	1.80	0.63
1:B:154:MET:SD	1:B:156:PHE:CE1	2.91	0.63
1:A:131:ALA:HB2	1:A:160:LEU:HD21	1.79	0.63
1:A:427:ARG:HA	1:A:492:TRP:CD1	2.34	0.62
1:A:293:GLU:HA	1:A:302:CYS:HA	1.81	0.62
1:B:292:TYR:OH	1:B:303:LYS:NZ	2.23	0.62
1:B:293:GLU:OE2	1:B:300:ARG:NE	2.27	0.62
2:C:4:HIS:ND1	2:C:26:GLN:HG3	2.16	0.61
1:B:123:ALA:HB1	1:B:152:MET:HB3	1.83	0.61
1:A:409:HIS:O	1:A:411:GLN:NE2	2.34	0.60
1:A:435:GLY:N	1:A:462:GLN:HE22	1.99	0.60
1:B:363:LEU:HD21	1:B:368:LEU:HD11	1.83	0.60
1:B:136:GLU:HA	1:B:156:PHE:HD2	1.67	0.60
1:B:314:ASN:HB2	1:B:318:ILE:HD11	1.84	0.60
1:B:209:HIS:CD2	1:B:221:GLU:HA	2.37	0.60
1:B:435:GLY:O	1:B:462:GLN:NE2	2.35	0.59
1:A:187:THR:OG1	1:A:198:ARG:NH2	2.35	0.59
1:A:203:SER:OG	1:A:205:SER:OG	2.19	0.59
1:B:67:ILE:HG23	1:B:70:ASN:HD21	1.66	0.59
2:C:12:HIS:O	2:C:15:PHE:HB2	2.03	0.59
1:B:80:LEU:HD21	1:B:83:ILE:HG13	1.85	0.59
1:A:434:ASP:OD1	1:A:459:THR:OG1	2.20	0.58
1:B:453:TRP:HA	1:B:456:LEU:HD23	1.84	0.58
1:A:6:VAL:HG12	1:A:36:VAL:HB	1.85	0.58
1:A:390:ARG:HG3	1:A:394:HIS:CE1	2.37	0.58
1:B:47:GLN:HB2	1:B:50:TYR:HE2	1.67	0.58
1:A:7:CYS:HB2	1:A:37:VAL:HG12	1.85	0.58
1:B:339:THR:HA	1:B:374:VAL:HA	1.84	0.58
1:A:264:GLY:N	1:B:246:TYR:OH	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:HG13	1:A:419:LEU:HD12	1.86	0.58
1:A:475:CYS:O	1:A:480:GLN:N	2.35	0.58
1:A:495:GLU:OE1	1:A:497:ARG:NH1	2.37	0.57
1:B:400:GLU:HA	1:B:429:LEU:HA	1.85	0.57
1:A:447:TYR:O	1:A:450:THR:OG1	2.19	0.57
1:B:260:LYS:HB3	1:B:267:CYS:HB3	1.86	0.57
1:A:562:ILE:HD11	1:A:592:VAL:HG22	1.86	0.57
1:B:156:PHE:CD1	1:B:156:PHE:N	2.69	0.56
1:A:507:ARG:NH2	1:A:515:CYS:SG	2.75	0.56
1:B:446:CYS:HB3	1:B:470:ARG:HB2	1.86	0.56
2:C:27:GLU:O	2:C:27:GLU:HG3	2.05	0.56
1:B:193:GLN:OE1	1:B:193:GLN:HA	2.05	0.56
1:B:200:ARG:NH1	1:B:216:CYS:SG	2.77	0.56
1:A:513:ASP:OD1	1:A:514:LYS:N	2.39	0.56
1:B:136:GLU:OE1	1:B:136:GLU:N	2.39	0.56
1:B:470:ARG:HH12	1:B:478:THR:HG21	1.71	0.55
1:B:390:ARG:HG2	1:B:394:HIS:CE1	2.41	0.55
2:D:44:GLU:HB2	2:D:45:HIS:CD2	2.42	0.55
1:A:138:ILE:HG13	1:A:184:GLN:HG3	1.87	0.55
1:A:435:GLY:O	1:A:462:GLN:NE2	2.39	0.55
1:B:60:GLU:OE2	1:B:84:ARG:NE	2.33	0.55
1:B:229:LYS:HG3	1:B:230:PHE:HD1	1.72	0.55
1:A:524:GLU:HG3	1:A:531:CYS:SG	2.46	0.55
1:A:293:GLU:HB2	1:A:300:ARG:HH22	1.73	0.54
1:B:339:THR:HB	1:B:375:LYS:HG2	1.89	0.54
1:B:383:ILE:HB	1:B:416:VAL:HG22	1.89	0.54
1:B:382:LEU:HA	1:B:415:ALA:HB3	1.89	0.54
1:A:326:SER:OG	1:A:327:ILE:N	2.40	0.54
1:A:346:HIS:HE2	1:A:380:PHE:HZ	1.56	0.54
1:B:447:TYR:HE1	1:B:480:GLN:HB3	1.73	0.54
1:A:252:GLN:NE2	1:B:286:ALA:H	2.03	0.54
1:A:276:VAL:HG11	1:A:287:CYS:SG	2.48	0.54
1:B:380:PHE:HB2	1:B:413:SER:HA	1.89	0.54
2:D:7:ASP:OD1	2:D:8:CYS:N	2.40	0.53
1:A:518:LEU:HD21	1:A:545:ILE:HA	1.90	0.53
1:B:75:ILE:O	1:B:77:LEU:N	2.37	0.53
1:B:237:LYS:HG3	1:B:238:ASP:H	1.74	0.53
1:A:581:THR:HG21	1:A:601:THR:HG22	1.90	0.53
1:B:444:ASN:HA	1:B:470:ARG:HD2	1.90	0.53
1:A:541:GLN:OE1	1:A:546:THR:OG1	2.23	0.53
1:A:315:GLY:HA3	1:A:343:GLY:HA3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HD23	1:B:186:LEU:H	1.74	0.52
1:B:285:ARG:O	1:B:405:ARG:NE	2.35	0.52
1:B:427:ARG:CZ	1:B:497:ARG:HE	2.22	0.52
1:B:64:TYR:CD2	1:B:89:TYR:HB2	2.45	0.52
1:A:295:GLU:OE2	1:A:298:GLY:N	2.43	0.52
1:B:487:SER:N	1:B:499:CYS:SG	2.78	0.52
1:A:553:ASP:HA	1:A:566:HIS:HA	1.92	0.52
1:B:399:LEU:HD22	1:B:429:LEU:HD12	1.90	0.52
1:A:279:ASP:OD1	1:A:279:ASP:N	2.38	0.52
1:B:222:SER:OG	1:B:223:ASP:N	2.43	0.52
1:A:178:ALA:H	1:A:182:ASN:HD22	1.57	0.52
1:B:325:LEU:H	1:B:325:LEU:HD23	1.74	0.52
1:B:316:ILE:N	1:B:344:ASP:OD1	2.43	0.51
2:C:21:CYS:HA	2:C:32:CYS:CB	2.40	0.51
1:A:220:ARG:HG3	1:A:222:SER:H	1.75	0.51
1:B:29:ARG:HH22	2:D:50:ALA:HB2	1.76	0.51
1:A:291:SER:HB3	1:A:303:LYS:O	2.09	0.51
1:B:432:ILE:HB	1:B:457:PHE:HB3	1.93	0.51
1:A:178:ALA:O	1:A:182:ASN:ND2	2.43	0.51
1:A:440:SER:OG	1:A:468:SER:OG	2.20	0.50
1:B:154:MET:HG3	1:B:156:PHE:HZ	1.73	0.50
1:A:251:TYR:O	1:B:284:VAL:HG23	2.11	0.50
1:B:290:ASP:OD1	1:B:290:ASP:N	2.43	0.50
1:A:154:MET:SD	1:A:154:MET:N	2.84	0.50
1:B:28:GLN:O	1:B:32:ASN:HB2	2.11	0.50
1:A:391:THR:OG1	1:A:422:THR:OG1	2.15	0.50
1:B:379:GLY:O	1:B:404:GLY:HA2	2.12	0.50
1:B:483:HIS:CE1	1:B:496:PRO:HD3	2.47	0.50
2:C:44:GLU:HG2	2:C:45:HIS:N	2.27	0.49
1:A:245:LEU:HG	1:A:256:ASN:HB2	1.94	0.49
1:B:422:THR:O	1:B:445:LEU:HA	2.12	0.49
1:B:450:THR:HG22	1:B:490:GLY:HA2	1.94	0.49
1:B:145:SER:HB3	1:B:148:PHE:HD2	1.77	0.49
1:B:174:SER:OG	1:B:174:SER:O	2.29	0.49
1:B:213:ALA:HB2	1:B:228:ARG:HB2	1.94	0.49
1:B:379:GLY:HA2	1:B:405:ARG:N	2.24	0.49
1:A:539:LEU:HD23	1:A:557:GLN:HB3	1.93	0.49
1:B:414:LEU:HD23	1:B:437:VAL:HG23	1.94	0.49
1:B:117:GLN:HG3	1:B:214:ALA:HB1	1.94	0.49
1:A:411:GLN:O	1:A:436:ASP:N	2.38	0.49
1:B:397:GLU:OE2	1:B:427:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLN:NE2	1:B:225:LEU:HD12	2.27	0.48
1:B:338:CYS:O	1:B:339:THR:OG1	2.25	0.48
1:A:521:GLU:HB2	1:A:522:PRO:HD3	1.96	0.48
1:B:408:GLN:N	1:B:412:PHE:O	2.40	0.48
1:B:194:GLN:HG3	1:B:204:PRO:CB	2.43	0.48
1:B:99:SER:OG	2:D:26:GLN:NE2	2.46	0.48
1:A:436:ASP:OD1	1:A:463:LYS:N	2.45	0.48
1:A:451:ILE:HG13	1:A:492:TRP:CZ3	2.49	0.48
1:A:82:ILE:HG21	1:A:226:VAL:HG21	1.96	0.48
1:B:109:LYS:HA	1:B:131:ALA:O	2.14	0.48
1:B:194:GLN:HG3	1:B:204:PRO:HB2	1.96	0.48
1:A:378:THR:O	1:A:404:GLY:N	2.47	0.48
1:A:398:ASN:OD1	1:A:398:ASN:N	2.40	0.48
1:B:279:ASP:OD1	1:B:280:HIS:N	2.38	0.48
1:B:401:ILE:HA	1:B:431:GLU:HB3	1.96	0.48
1:A:527:GLU:HG2	1:A:528:ASN:ND2	2.29	0.48
2:C:21:CYS:SG	2:C:22:ARG:N	2.87	0.48
1:B:337:ASN:ND2	1:B:373:THR:OG1	2.29	0.48
1:A:561:TYR:HD2	1:A:571:CYS:SG	2.37	0.47
1:B:81:GLN:HE22	1:B:225:LEU:HD12	1.79	0.47
1:B:483:HIS:HB3	1:B:486:CYS:HB2	1.94	0.47
1:A:595:LEU:HG	1:A:596:CYS:H	1.78	0.47
2:D:47:ASP:OD1	2:D:47:ASP:N	2.46	0.47
1:A:95:LEU:HB3	1:A:124:VAL:HG22	1.96	0.47
1:B:337:ASN:O	1:B:339:THR:HG23	2.14	0.47
1:B:483:HIS:ND1	1:B:494:PRO:O	2.42	0.47
1:A:128:ASN:N	1:A:128:ASN:OD1	2.44	0.47
1:B:12:ASN:HD22	1:B:17:LEU:HD21	1.80	0.47
1:B:42:GLU:OE2	1:B:64:TYR:OH	2.30	0.47
1:B:141:ARG:HH12	1:B:189:ILE:HG21	1.79	0.47
1:B:181:GLU:HG2	1:B:182:ASN:N	2.29	0.47
1:A:160:LEU:O	1:A:162:SER:N	2.45	0.47
1:A:76:PRO:O	1:A:78:GLU:N	2.48	0.46
1:B:353:ARG:HH12	2:D:14:GLN:HE22	1.62	0.46
1:A:178:ALA:N	1:A:182:ASN:HD22	2.13	0.46
1:B:19:THR:HG23	1:B:21:GLU:H	1.80	0.46
1:A:57:THR:O	1:A:59:GLN:HG3	2.15	0.46
1:A:418:SER:O	1:A:418:SER:OG	2.31	0.46
1:B:393:LEU:HD12	1:B:424:LEU:HB2	1.98	0.46
1:B:346:HIS:HD2	1:B:382:LEU:HD23	1.81	0.46
1:A:5:LYS:HG3	1:A:34:CYS:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PHE:HB2	1:A:283:CYS:SG	2.55	0.46
1:A:495:GLU:HB3	1:A:497:ARG:NH1	2.30	0.46
1:B:46:VAL:O	1:B:46:VAL:HG23	2.16	0.46
1:A:16:GLN:HB3	2:C:33:VAL:HB	1.98	0.45
1:A:76:PRO:O	1:A:78:GLU:HG2	2.17	0.45
1:A:420:ASN:HB2	1:A:443:LYS:HE3	1.97	0.45
1:B:457:PHE:CE1	1:B:462:GLN:HB2	2.51	0.45
1:A:125:ARG:HG2	1:A:126:PHE:N	2.30	0.45
1:A:271:CYS:SG	1:A:277:VAL:HG22	2.56	0.45
2:C:20:THR:O	2:C:32:CYS:HB2	2.16	0.45
1:A:375:LYS:HD3	1:A:400:GLU:HG3	1.98	0.45
1:B:317:GLY:H	1:B:321:PHE:HB3	1.82	0.45
1:A:285:ARG:O	1:A:405:ARG:NH1	2.49	0.45
1:B:224:CYS:HB2	1:B:236:CYS:SG	2.57	0.45
1:A:547:CYS:HB2	1:A:554:ASN:HB2	1.98	0.45
1:B:328:ASN:H	1:B:331:ASN:HD21	1.64	0.45
1:B:75:ILE:O	1:B:112:PRO:HD2	2.16	0.44
1:B:345:LEU:HD23	1:B:381:LEU:HD13	1.98	0.44
1:B:78:GLU:OE2	1:B:112:PRO:HB2	2.17	0.44
1:A:369:ASP:OD1	1:A:372:LYS:NZ	2.37	0.44
2:D:6:ASN:OD1	2:D:23:PHE:HB3	2.17	0.44
1:A:524:GLU:HA	1:A:534:CYS:H	1.83	0.44
1:B:271:CYS:SG	1:B:277:VAL:HG12	2.57	0.44
1:A:235:THR:HG22	1:A:237:LYS:HG2	2.00	0.44
1:A:344:ASP:OD1	1:A:344:ASP:N	2.50	0.44
1:B:175:CYS:HB3	1:B:183:CYS:SG	2.57	0.44
1:B:486:CYS:SG	1:B:487:SER:N	2.91	0.44
1:A:444:ASN:HA	1:A:470:ARG:HB2	1.99	0.44
1:B:341:ILE:HB	1:B:377:ILE:HG12	1.99	0.44
1:A:177:GLY:H	1:A:182:ASN:HB3	1.83	0.44
1:B:47:GLN:HB2	1:B:50:TYR:CE2	2.49	0.44
1:B:373:THR:HG22	1:B:398:ASN:OD1	2.18	0.44
1:A:523:ARG:NH1	1:A:541:GLN:H	2.16	0.44
1:B:51:ASP:OD1	1:B:51:ASP:N	2.38	0.44
1:B:100:ASN:O	1:B:107:GLY:HA2	2.18	0.44
1:B:135:VAL:HG12	1:B:135:VAL:O	2.18	0.44
1:B:229:LYS:HG3	1:B:230:PHE:CD1	2.50	0.44
1:B:427:ARG:NE	1:B:498:ASP:HB3	2.24	0.44
1:B:437:VAL:O	1:B:464:THR:OG1	2.16	0.44
1:B:147:ASP:OD1	1:B:147:ASP:N	2.48	0.43
1:B:194:GLN:CG	1:B:204:PRO:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASN:HD21	1:B:237:LYS:HB2	1.84	0.43
1:A:417:VAL:HG21	2:C:48:LEU:HD22	1.99	0.43
1:A:487:SER:O	1:A:489:GLU:N	2.48	0.43
1:A:563:ASP:H	1:A:567:CYS:HA	1.82	0.43
1:B:38:LEU:HD23	1:B:38:LEU:HA	1.83	0.43
1:B:74:ARG:HB3	1:B:110:GLU:HG3	2.00	0.43
1:B:377:ILE:HB	1:B:402:ILE:HD13	1.98	0.43
1:B:474:SER:OG	1:B:475:CYS:N	2.51	0.43
1:B:12:ASN:N	1:B:12:ASN:OD1	2.50	0.43
1:B:175:CYS:HB2	1:B:182:ASN:O	2.19	0.43
1:A:200:ARG:NH1	1:A:216:CYS:SG	2.92	0.43
1:A:422:THR:O	1:A:445:LEU:HA	2.19	0.43
1:B:386:TRP:CZ2	1:B:393:LEU:HD23	2.53	0.43
1:A:10:THR:O	1:A:40:ASN:HB2	2.19	0.43
1:A:39:GLY:O	1:A:40:ASN:ND2	2.52	0.43
1:B:41:LEU:HB3	1:B:65:VAL:HG22	1.99	0.43
1:A:11:SER:O	1:A:11:SER:OG	2.22	0.43
1:A:573:ALA:HA	1:A:584:TRP:CD1	2.54	0.43
1:A:582:LEU:H	1:A:582:LEU:HG	1.49	0.43
1:B:370:ILE:HD12	1:B:370:ILE:H	1.84	0.43
1:B:386:TRP:CE3	1:B:387:PRO:HD2	2.47	0.43
1:A:125:ARG:NH1	1:A:127:SER:HB2	2.34	0.43
1:A:152:MET:SD	1:A:154:MET:HE1	2.59	0.43
1:A:209:HIS:CE1	1:A:221:GLU:HB3	2.55	0.42
1:B:472:GLU:O	1:B:476:LYS:HB2	2.19	0.42
1:A:74:ARG:HD2	1:A:110:GLU:OE2	2.19	0.42
1:B:127:SER:OG	1:B:128:ASN:N	2.51	0.42
1:B:407:LYS:HE3	1:B:435:GLY:HA2	2.00	0.42
1:A:56:LYS:NZ	1:A:78:GLU:OE2	2.43	0.42
1:A:278:THR:HG22	1:A:282:SER:O	2.19	0.42
1:A:284:VAL:HG12	1:A:286:ALA:H	1.85	0.42
1:B:134:ASN:OD1	1:B:177:GLY:N	2.52	0.42
1:A:382:LEU:HD12	1:A:415:ALA:HB3	2.00	0.42
1:B:320:GLU:OE1	1:B:320:GLU:N	2.39	0.42
1:A:135:VAL:C	1:A:137:SER:H	2.23	0.42
1:B:138:ILE:HG21	1:B:176:TRP:CZ2	2.54	0.42
1:B:175:CYS:HA	1:B:183:CYS:HA	2.01	0.42
1:A:538:CYS:HB3	1:A:555:CYS:HB3	1.81	0.42
1:B:339:THR:HA	1:B:375:LYS:H	1.84	0.42
1:A:343:GLY:O	1:A:379:GLY:N	2.51	0.42
1:B:352:PHE:CZ	1:B:387:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ILE:HG12	1:A:346:HIS:O	2.20	0.42
1:A:442:ASN:O	1:A:469:ASN:HA	2.19	0.41
1:A:561:TYR:CG	1:A:570:THR:HA	2.55	0.41
1:B:97:VAL:O	1:B:129:ASN:ND2	2.53	0.41
1:B:311:LYS:HE3	1:B:336:LYS:HB3	2.01	0.41
1:A:454:LYS:HD2	1:A:454:LYS:HA	1.81	0.41
1:B:27:LEU:HD12	1:B:27:LEU:HA	1.84	0.41
1:B:47:GLN:OE1	1:B:71:THR:OG1	2.38	0.41
1:B:386:TRP:NE1	1:B:393:LEU:HD23	2.35	0.41
1:A:98:LEU:HD12	1:A:98:LEU:O	2.20	0.41
1:A:129:ASN:OD1	1:A:129:ASN:N	2.54	0.41
1:A:421:ILE:HG13	1:A:445:LEU:HD12	2.03	0.41
1:B:158:ASN:OD1	1:B:159:HIS:N	2.53	0.41
1:B:187:THR:HB	1:B:199:CYS:O	2.20	0.41
1:B:291:SER:HG	1:B:292:TYR:H	1.68	0.41
1:A:457:PHE:HB3	1:A:462:GLN:HG3	2.01	0.41
1:A:525:PHE:CE1	1:A:532:ILE:HB	2.56	0.41
1:B:329:ALA:HB2	1:B:363:LEU:HB2	2.03	0.41
1:B:419:LEU:H	1:B:442:ASN:HD22	1.68	0.41
1:A:282:SER:OG	1:B:253:MET:SD	2.76	0.41
1:A:59:GLN:O	1:A:60:GLU:HG3	2.20	0.41
1:B:134:ASN:ND2	1:B:177:GLY:O	2.51	0.41
2:D:23:PHE:HD1	2:D:30:PRO:HB3	1.86	0.41
1:A:117:GLN:NE2	1:A:187:THR:OG1	2.54	0.41
1:A:123:ALA:HB1	1:A:152:MET:HB3	2.03	0.41
1:A:246:TYR:HD1	1:A:253:MET:HE2	1.86	0.41
1:B:41:LEU:HD23	1:B:65:VAL:HG13	2.03	0.41
1:B:200:ARG:HH12	1:B:219:PRO:HD3	1.85	0.41
1:A:562:ILE:HG13	1:A:592:VAL:HG13	2.02	0.41
1:A:66:LEU:HD11	1:A:68:ALA:HB2	2.03	0.40
1:B:214:ALA:HB3	1:B:225:LEU:CB	2.51	0.40
2:D:9:PRO:C	2:D:11:SER:H	2.25	0.40
1:A:186:LEU:HD23	1:A:186:LEU:HA	1.94	0.40
1:B:387:PRO:O	1:B:389:ASN:N	2.50	0.40
1:A:408:GLN:HE22	2:C:45:HIS:CD2	2.40	0.40
1:A:295:GLU:OE2	1:A:296:GLU:N	2.53	0.40
1:A:400:GLU:O	1:A:430:LYS:N	2.50	0.40
1:A:67:ILE:HB	1:A:97:VAL:HG22	2.03	0.40
1:A:445:LEU:H	1:A:470:ARG:HB3	1.86	0.40
2:D:29:LYS:HD2	2:D:29:LYS:HA	1.91	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	612/1210 (51%)	502 (82%)	109 (18%)	1 (0%)	44	73
1	B	498/1210 (41%)	420 (84%)	77 (16%)	1 (0%)	44	73
2	C	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
2	D	48/50 (96%)	38 (79%)	10 (21%)	0	100	100
All	All	1206/2520 (48%)	1001 (83%)	203 (17%)	2 (0%)	45	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	441	GLY
1	A	145	SER

### 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	536/1053 (51%)	520 (97%)	16 (3%)	36	63
1	B	439/1053 (42%)	428 (98%)	11 (2%)	42	66
2	C	43/43 (100%)	38 (88%)	5 (12%)	4	23
2	D	43/43 (100%)	42 (98%)	1 (2%)	45	68
All	All	1061/2192 (48%)	1028 (97%)	33 (3%)	37	62

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	136	GLU
1	A	144	VAL
1	A	147	ASP
1	A	194	GLN
1	A	195	CYS
1	A	232	ASN
1	A	273	ARG
1	A	303	LYS
1	A	517	LEU
1	A	537	GLU
1	A	538	CYS
1	A	539	LEU
1	A	569	LYS
1	A	582	LEU
1	A	600	CYS
2	C	1	VAL
2	C	2	VAL
2	C	16	CYS
2	C	33	VAL
2	C	49	LEU
1	B	38	LEU
1	B	108	LEU
1	B	109	LYS
1	B	156	PHE
1	B	193	GLN
1	B	194	GLN
1	B	207	CYS
1	B	232	ASN
1	B	419	LEU
1	B	420	ASN
1	B	431	GLU
2	D	1	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	40	ASN
1	A	117	GLN
1	A	182	ASN
1	A	252	GLN
1	A	408	GLN

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Mol	Chain	Res	Type
1	A	462	GLN
1	A	528	ASN
1	A	557	GLN
1	B	23	HIS
1	B	40	ASN
1	B	81	GLN
1	B	151	ASN
1	B	232	ASN
1	B	331	ASN
1	B	346	HIS
1	B	442	ASN
2	D	14	GLN
2	D	18	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 oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

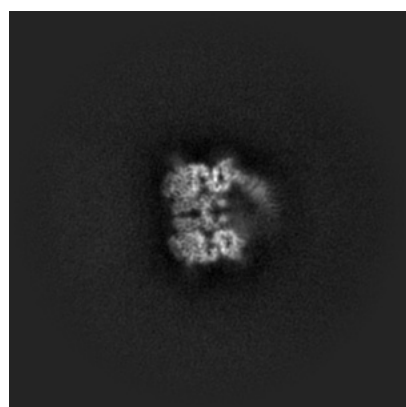
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25561. These allow visual inspection of the internal detail of the map and identification of artifacts.

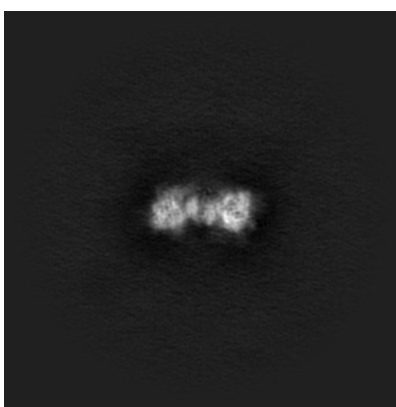
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

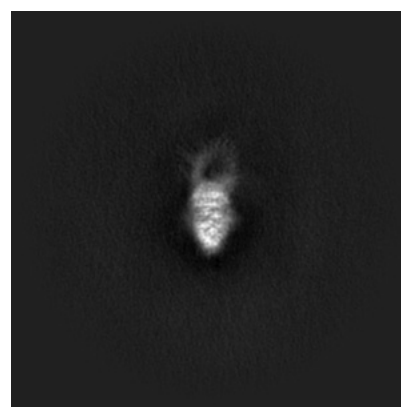
#### 6.1.1 Primary map



X



Y

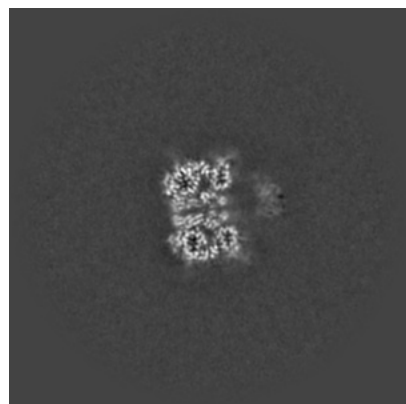


Z

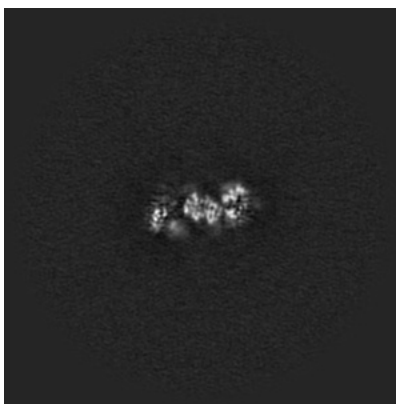
The images above show the map projected in three orthogonal directions.

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

#### 6.2.1 Primary map



X Index: 200



Y Index: 200

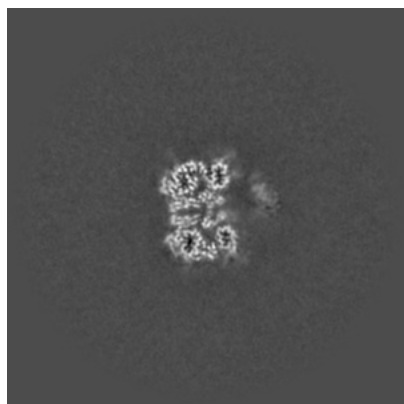


Z Index: 200

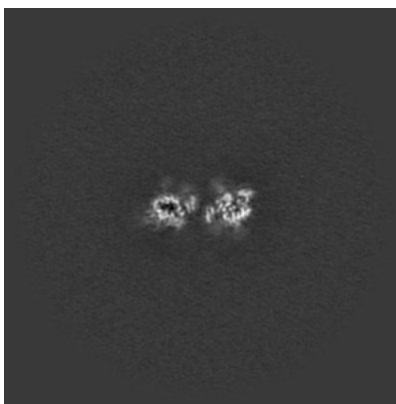
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 198



Y Index: 184

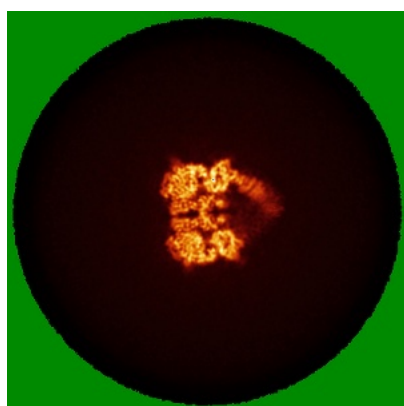


Z Index: 221

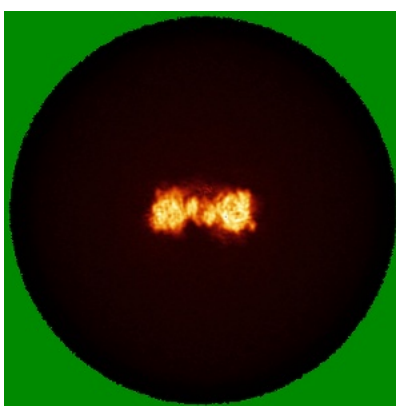
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X



Y

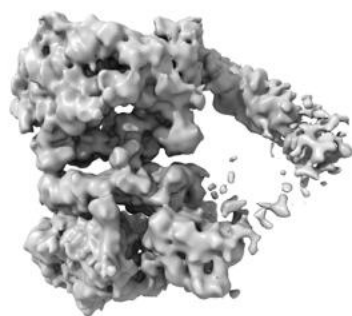


Z

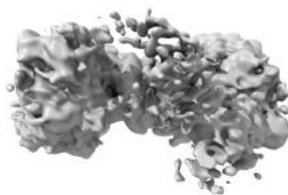
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

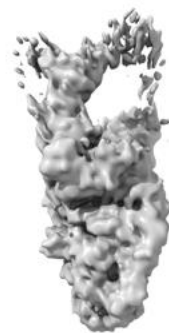
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

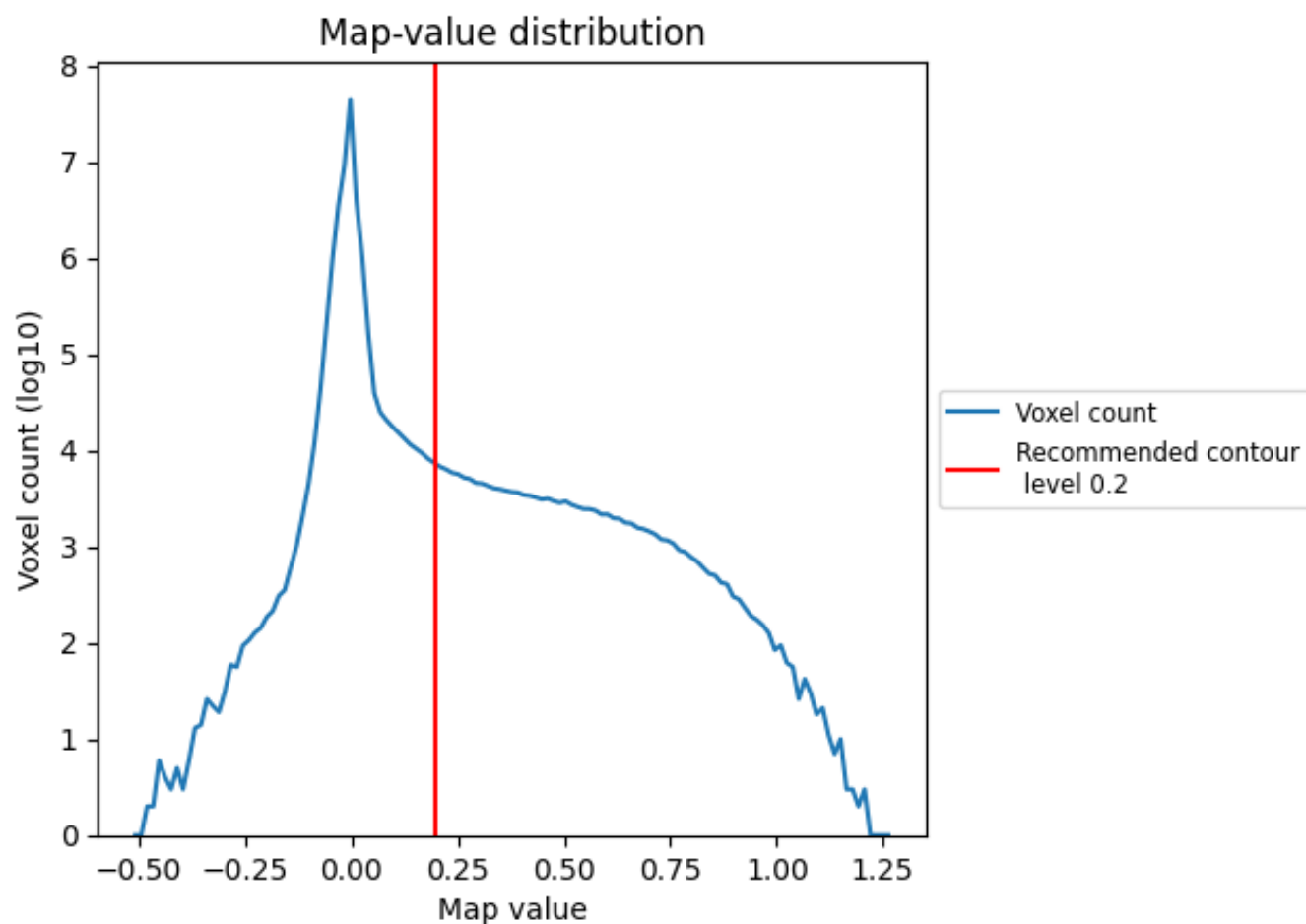
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

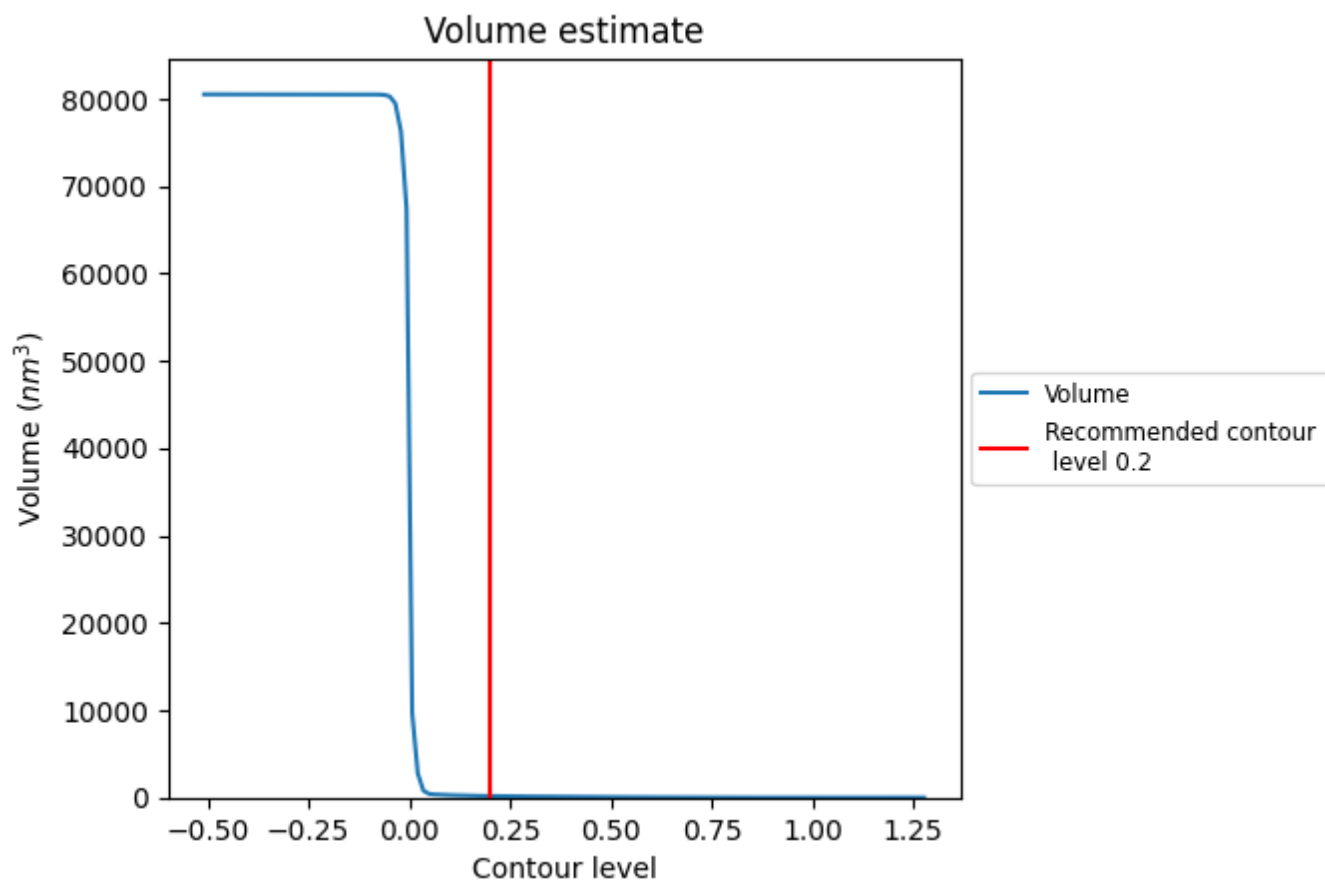
This section contains the results of statistical analysis of the map.

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



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

## 7.2 Volume estimate [i](#)

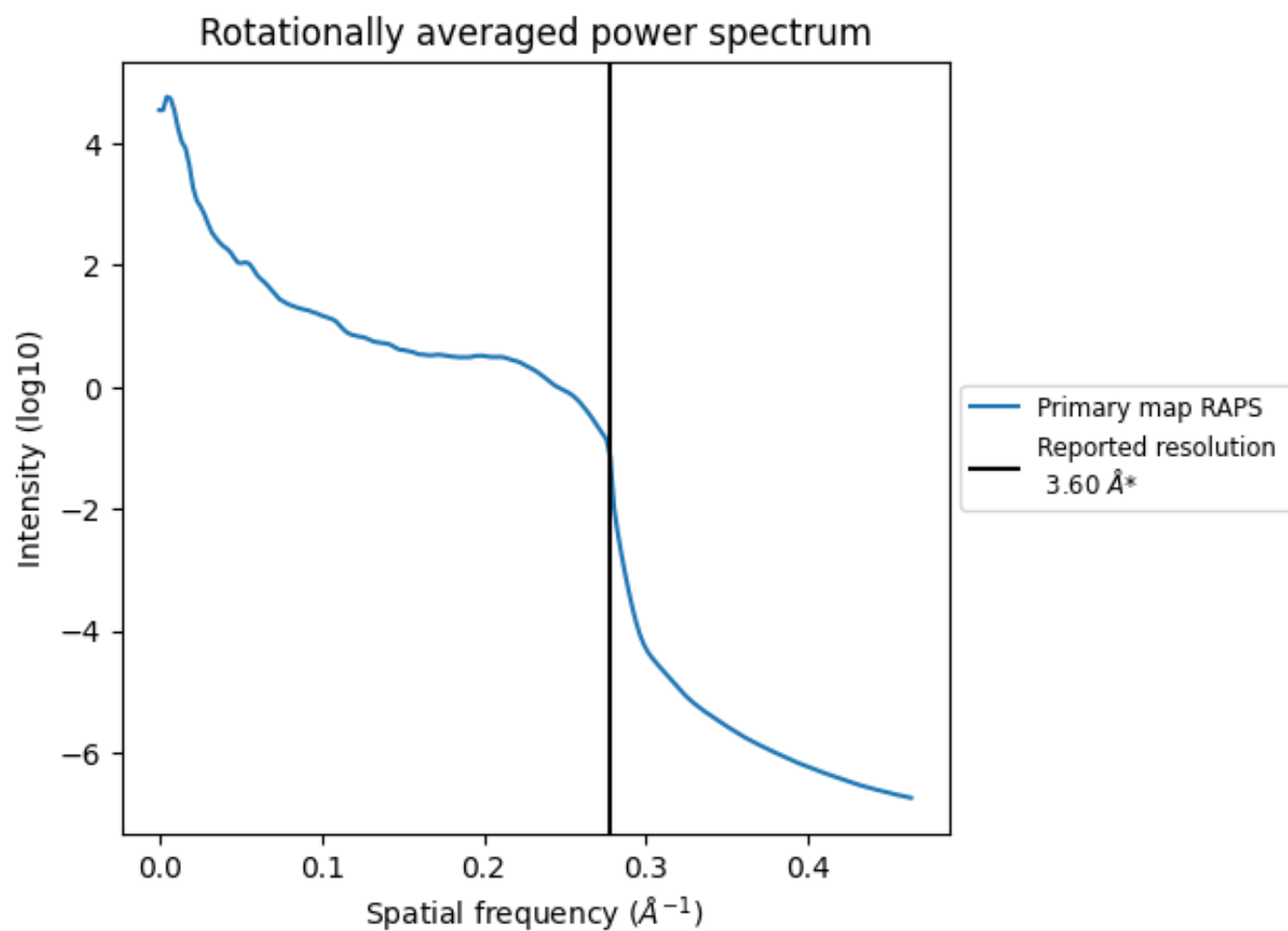


The volume at the recommended contour level is 174 nm<sup>3</sup>; this corresponds to an approximate mass of 157 kDa.

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 0.278 Å<sup>-1</sup>

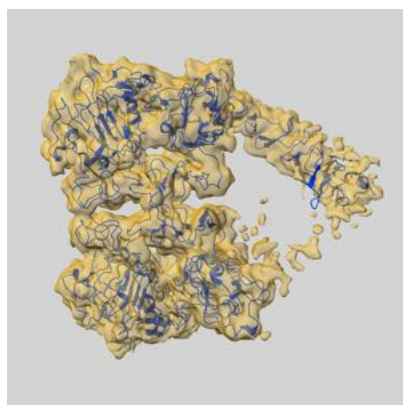
## 8 Fourier-Shell correlation

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

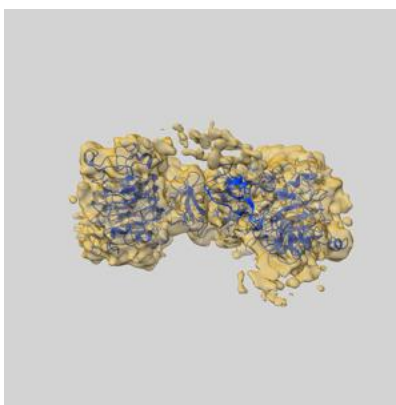
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25561 and PDB model 7SZ5. Per-residue inclusion information can be found in section [3](#) on page [4](#).

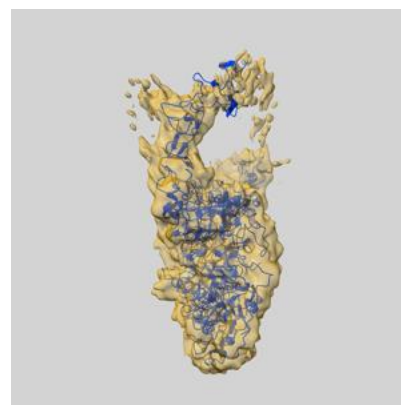
### 9.1 Map-model overlay [i](#)



X



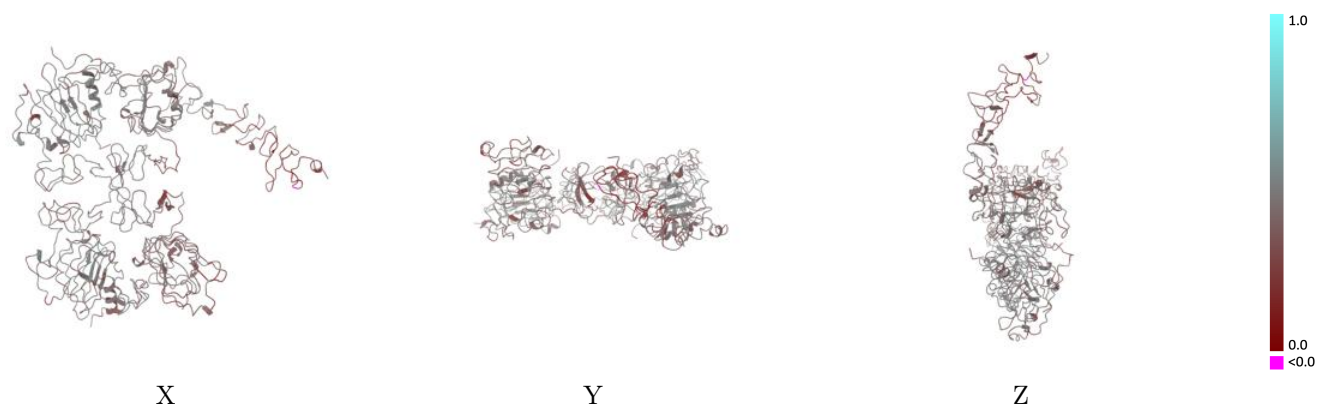
Y



Z

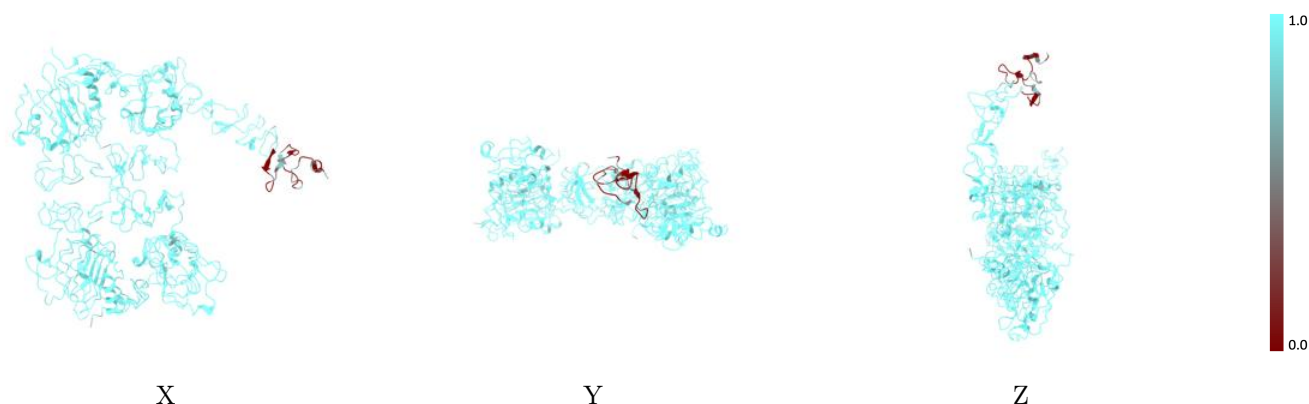
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



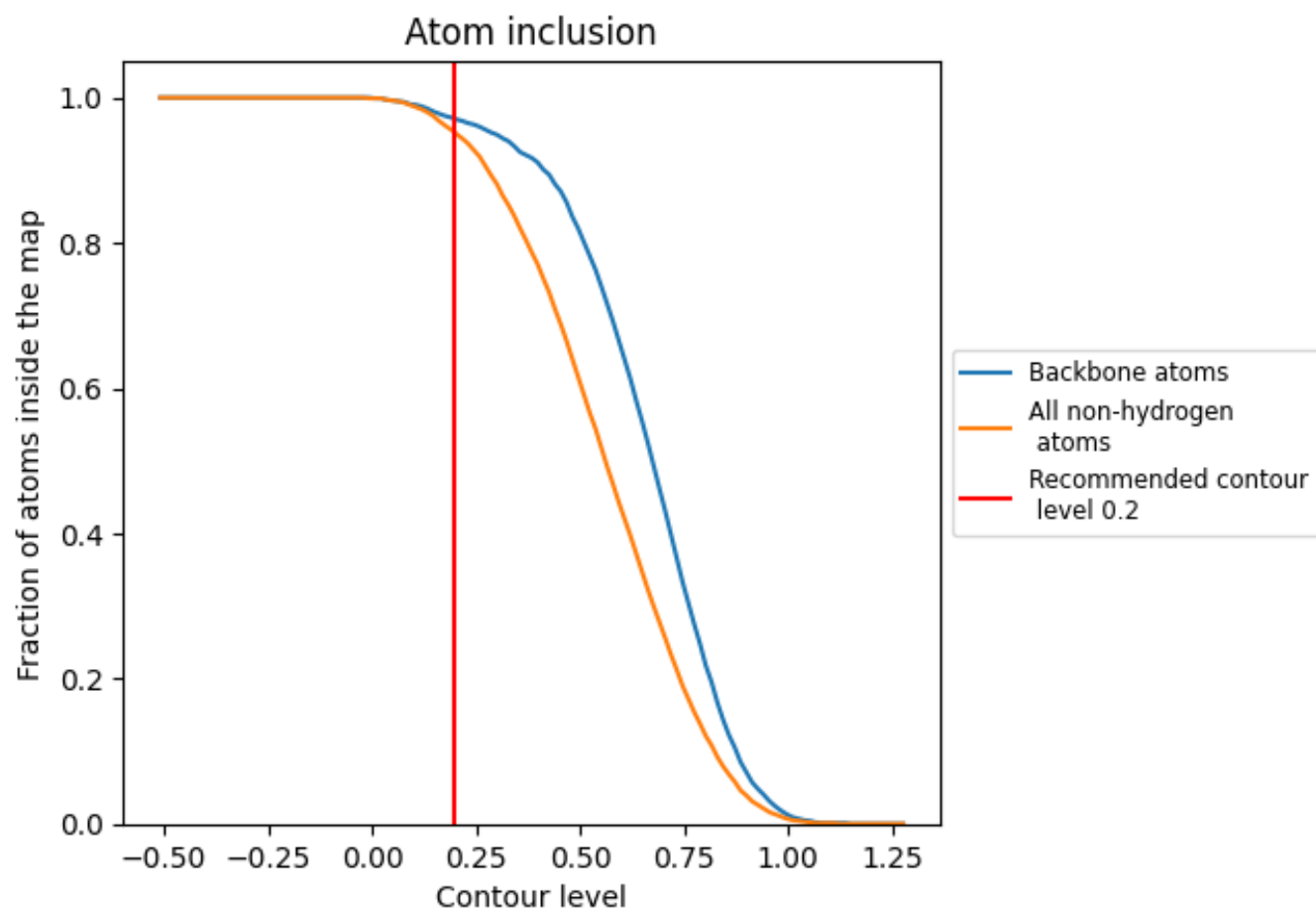
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9520	<div></div> 0.4100
A	<div></div> 0.9280	<div></div> 0.4100
B	<div></div> 0.9770	<div></div> 0.4080
C	<div></div> 1.0000	<div></div> 0.4370
D	<div></div> 0.9530	<div></div> 0.4110

