



## Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 04:49 AM EST

PDB ID : 6MZC  
EMDB ID : EMD-9298  
Title : Human TFIID BC core  
Authors : Patel, A.B.; Louder, R.K.; Greber, B.J.; Grunberg, S.; Luo, J.; Fang, J.; Liu, Y.; Ranish, J.; Hahn, S.; Nogales, E.  
Deposited on : 2018-11-05  
Resolution : 4.50 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.dev43  
MolProbity : 4.02b-467  
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) : 2.31.2

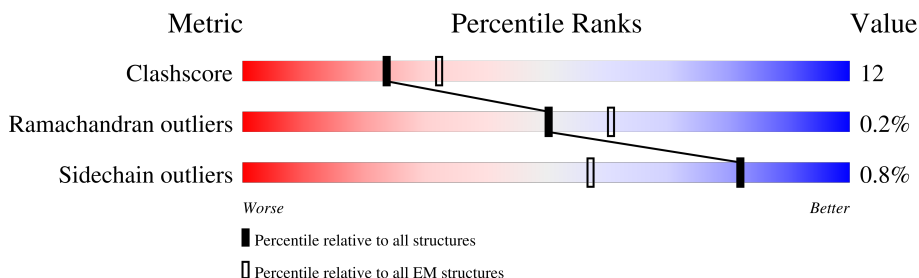
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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.



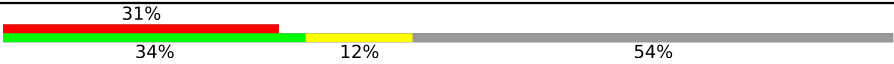
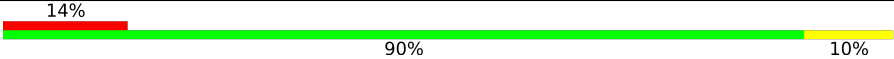
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	1199	<div> <div>21%</div> <div>52%</div> <div>27%</div> <div>19%</div> </div>
2	E	1085	<div> <div>8%</div> <div>91%</div> </div>
3	G	800	<div> <div>20%</div> <div>42%</div> <div>17%</div> <div>41%</div> </div>
4	H	677	<div> <div>6%</div> <div>26%</div> <div>12%</div> <div>62%</div> </div>
5	I	677	<div> <div>14%</div> <div>36%</div> <div>13%</div> <div>50%</div> </div>
6	K	310	<div> <div>19%</div> <div>52%</div> <div>14%</div> <div>35%</div> </div>
7	M	264	<div> <div>16%</div> <div>32%</div> <div>7%</div> <div>61%</div> </div>
8	O	218	<div> <div>23%</div> <div>28%</div> <div>10%</div> <div>62%</div> </div>

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Mol	Chain	Length	Quality of chain
9	R	161	
10	Z	238	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 21254 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 Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	968	Total	C	N	O	S	0	0
			7832	5031	1322	1421	58		

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	102	Total	C	N	O	0	0
			686	423	130	133		

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	473	Total	C	N	O	S	0	0
			3646	2314	638	679	15		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	257	Total	C	N	O	S	0	0
			1943	1230	347	355	11		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	339	Total	C	N	O	S	0	0
			2520	1585	445	474	16		

- Molecule 6 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	202	Total	C	N	O	S	0	0
			1449	906	260	278	5		

- Molecule 7 is a protein called Transcription initiation factor TFIID subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	104	Total	C	N	O	S	0	0
			732	456	129	142	5		

- Molecule 8 is a protein called Transcription initiation factor TFIID subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	82	Total	C	N	O	S	0	0
			645	413	102	126	4		

- Molecule 9 is a protein called Transcription initiation factor TFIID subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	74	Total	C	N	O	S	0	0
			611	381	107	120	3		

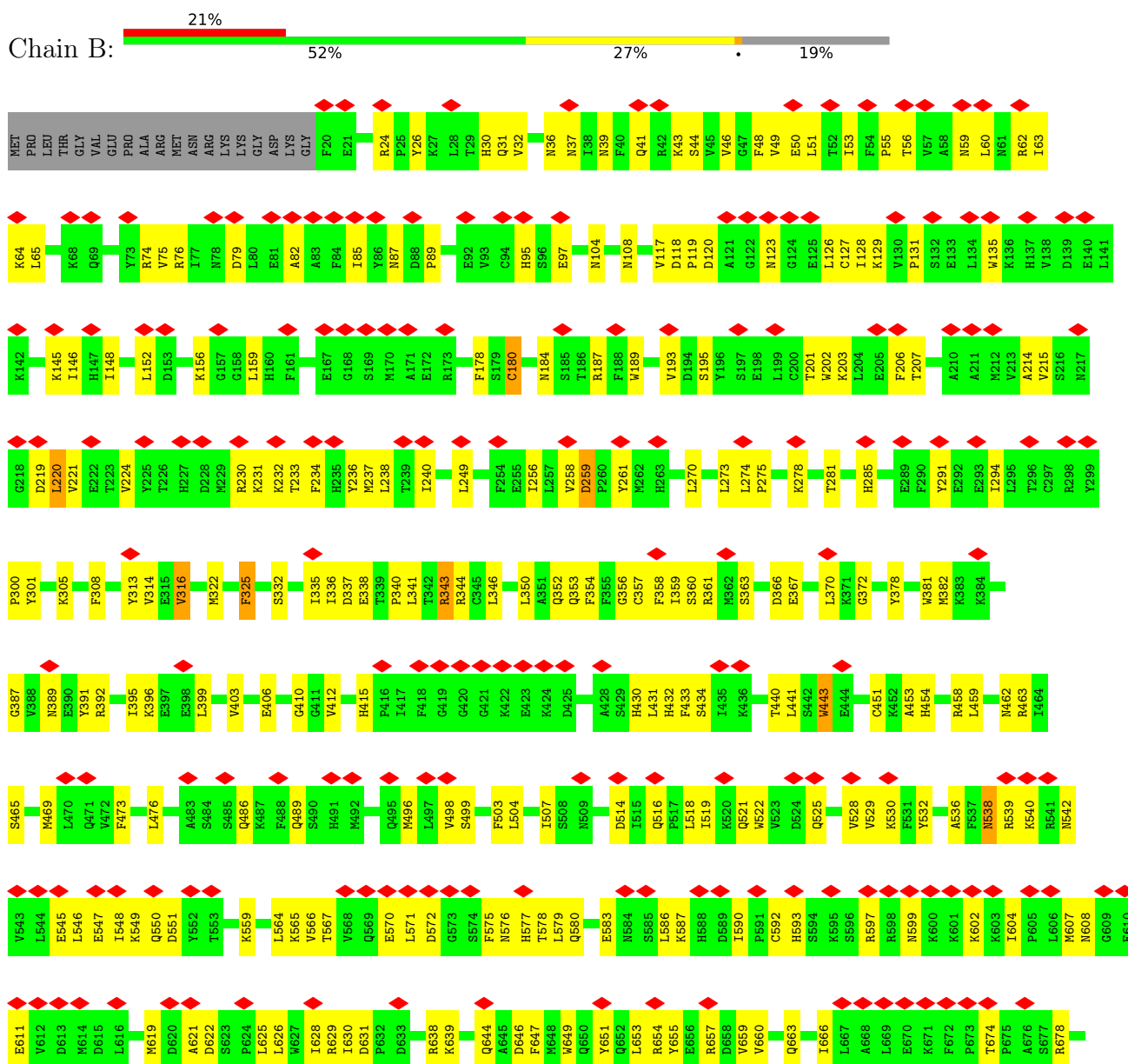
- Molecule 10 is a protein called poly(UNK).

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	238	Total	C	N	O	0	0
			1190	714	238	238		

### 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.

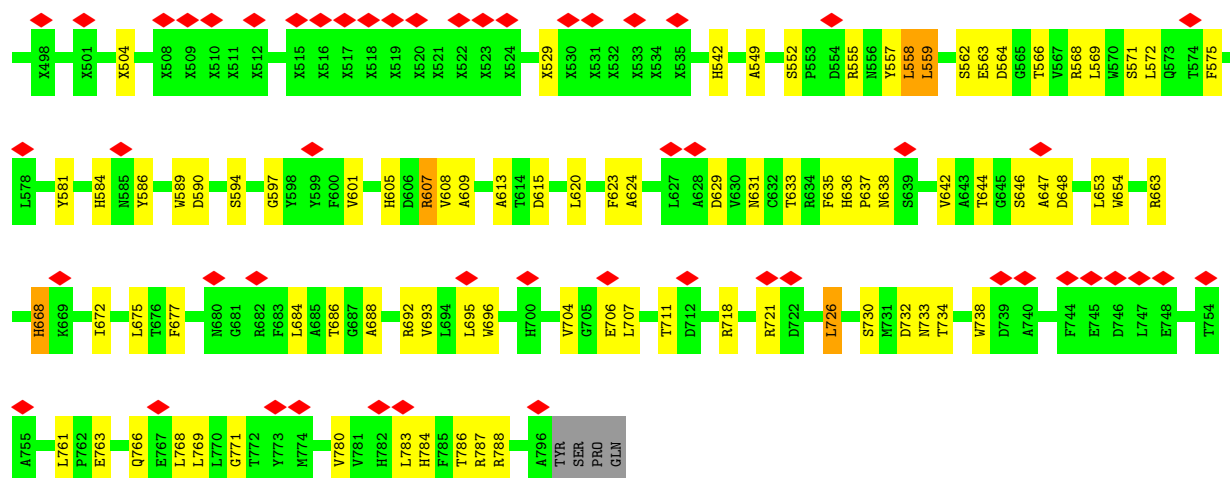
- Molecule 1: Transcription initiation factor TFIID subunit 2



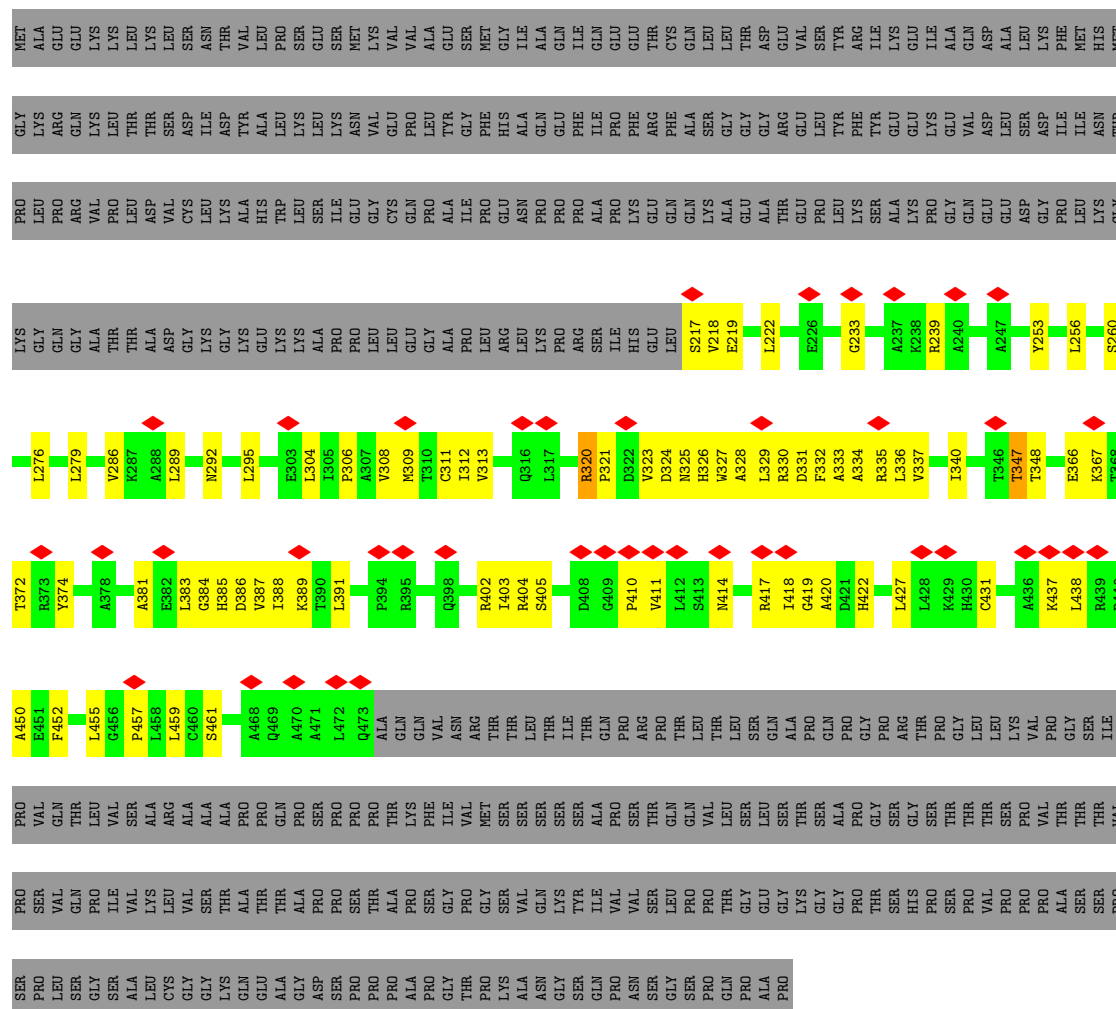




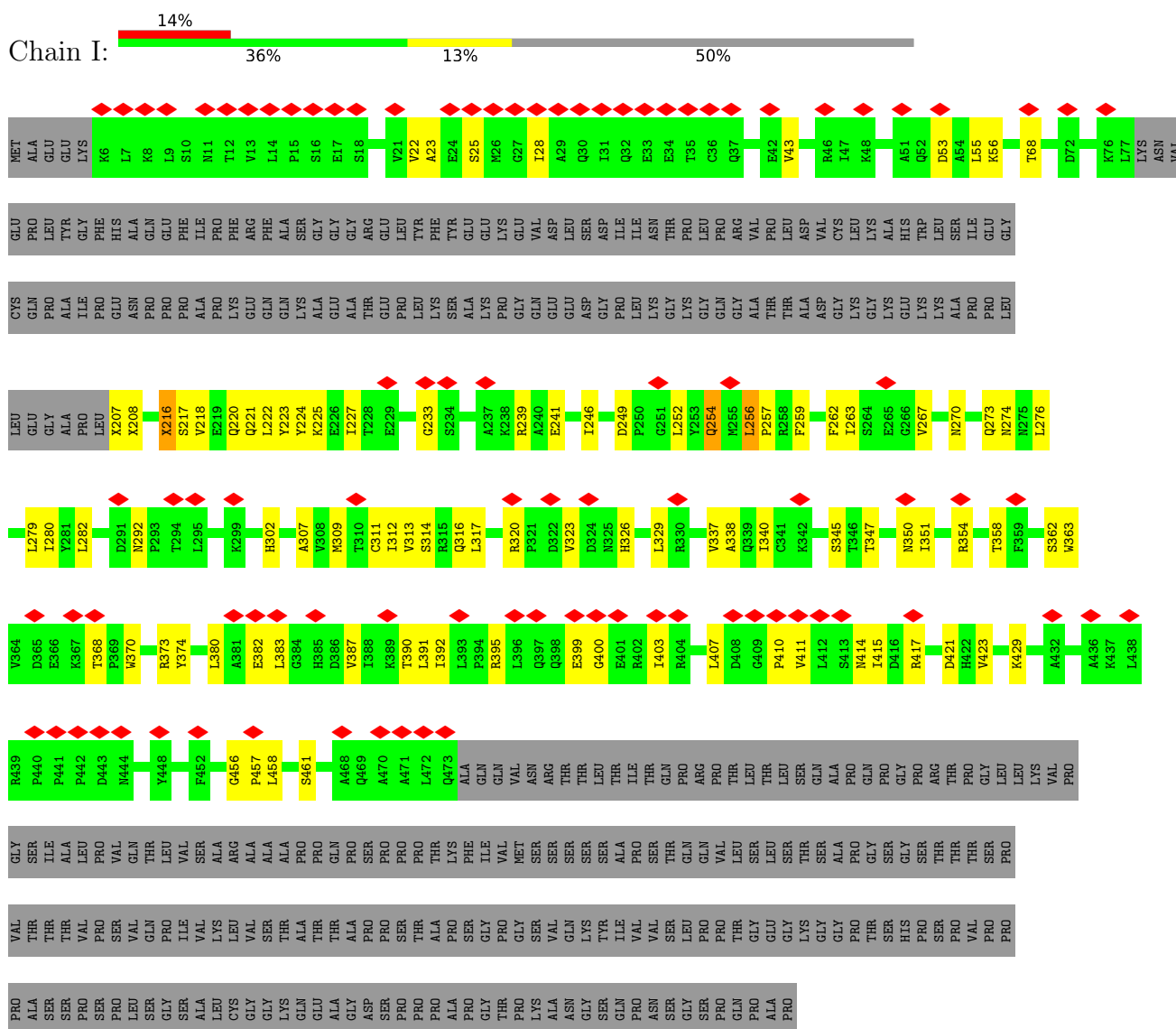




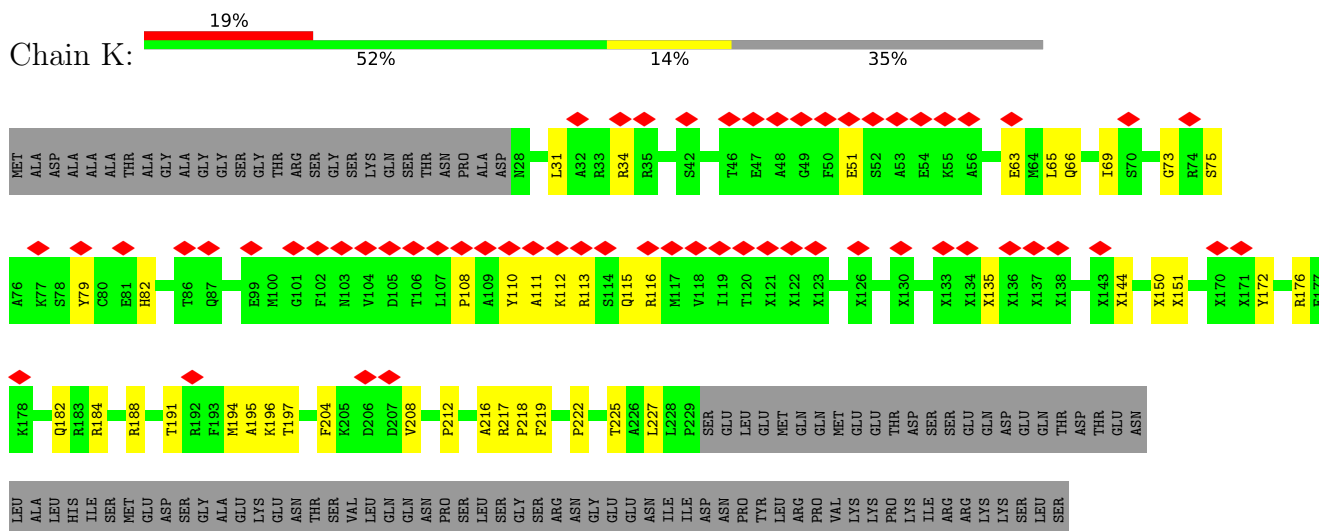
• Molecule 4: Transcription initiation factor TFIID subunit 6



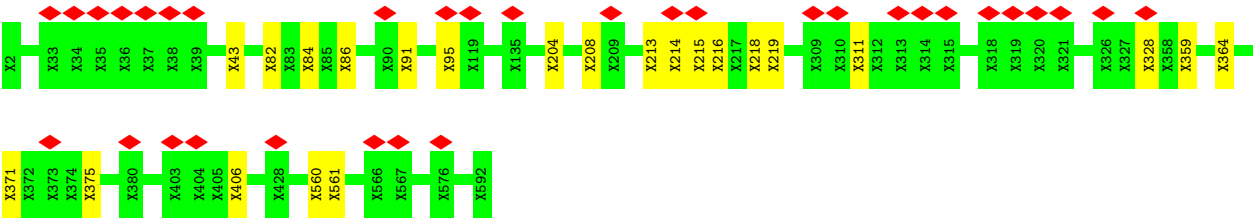
• Molecule 5: Transcription initiation factor TFIID subunit 6



- Molecule 6: Transcription initiation factor TFIID subunit 8







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	266328	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	380.16, 380.16, 380.16	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	B	0.57	2/8029 (0.0%)	0.74	3/10882 (0.0%)
2	E	0.31	0/692	0.50	0/945
3	G	0.52	0/3537	0.72	2/4802 (0.0%)
4	H	0.51	0/1978	0.71	0/2693
5	I	0.44	0/2506	0.64	0/3402
6	K	0.43	0/1212	0.59	0/1640
7	M	0.37	0/705	0.59	0/955
8	O	0.38	0/657	0.51	0/891
9	R	0.33	0/618	0.55	0/835
All	All	0.50	2/19934 (0.0%)	0.69	5/27045 (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
1	B	0	17
3	G	0	8
4	H	0	6
5	I	0	4
6	K	0	2
7	M	0	1
10	Z	0	1
All	All	0	39

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	443	TRP	CB-CG	-7.44	1.36	1.50
1	B	381	TRP	CB-CG	-5.07	1.41	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	LEU	CA-CB-CG	7.67	132.93	115.30
1	B	927	LEU	CA-CB-CG	-6.32	100.76	115.30
3	G	726	LEU	CB-CG-CD2	-6.05	100.72	111.00
3	G	607	ARG	CA-CB-CG	5.18	124.79	113.40
1	B	443	TRP	CA-CB-CG	-5.04	104.12	113.70

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	193	VAL	Peptide
1	B	259	ASP	Peptide
1	B	316	VAL	Peptide
1	B	325	PHE	Peptide
1	B	340	PRO	Peptide
1	B	415	HIS	Peptide
1	B	434	SER	Peptide
1	B	538	ASN	Peptide
1	B	540	LYS	Peptide
1	B	583	GLU	Peptide
1	B	674	THR	Peptide
1	B	737	LYS	Peptide
1	B	816	VAL	Peptide
1	B	820	ASP	Peptide
1	B	821	ASN	Peptide
1	B	822	LEU	Peptide
1	B	843	LEU	Peptide
3	G	275	TYR	Peptide
3	G	467	LEU	Peptide
3	G	479	THR	Peptide
3	G	489	PHE	Peptide
3	G	615	ASP	Peptide
3	G	668	HIS	Peptide
3	G	711	THR	Peptide
3	G	721	ARG	Peptide
4	H	313	VAL	Peptide
4	H	320	ARG	Peptide
4	H	347	THR	Peptide
4	H	348	THR	Peptide
4	H	384	GLY	Peptide
4	H	441	PRO	Peptide
5	I	216	UNK	Peptide
5	I	254	GLN	Peptide

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Mol	Chain	Res	Type	Group
5	I	256	LEU	Peptide
5	I	262	PHE	Peptide
6	K	144	UNK	Peptide
6	K	217	ARG	Peptide
7	M	28	ILE	Peptide
10	Z	364	UNK	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7832	0	7789	212	0
2	E	686	0	572	13	0
3	G	3646	0	3312	95	0
4	H	1943	0	1922	53	0
5	I	2520	0	2422	61	0
6	K	1449	0	1281	33	0
7	M	732	0	623	13	0
8	O	645	0	640	15	0
9	R	611	0	610	16	0
10	Z	1190	0	280	16	0
All	All	21254	0	19451	491	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 12.

All (491) 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:566:VAL:O	1:B:577:HIS:HA	1.64	0.97
1:B:532:TYR:O	1:B:551:ASP:HB2	1.67	0.94
1:B:50:GLU:HA	1:B:146:ILE:O	1.70	0.92
3:G:309:ILE:O	3:G:341:ILE:HA	1.73	0.88
1:B:567:THR:O	1:B:629:ARG:HB3	1.73	0.87
1:B:350:LEU:O	1:B:353:GLN:HB3	1.77	0.84
4:H:329:LEU:O	4:H:332:PHE:HB3	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:350:ASN:O	5:I:354:ARG:HB2	1.82	0.79
1:B:538:ASN:HA	1:B:542:ASN:HD22	1.51	0.73
1:B:39:ASN:HB3	1:B:44:SER:H	1.52	0.73
1:B:835:ARG:HH22	6:K:184:ARG:HE	1.36	0.73
3:G:474:THR:O	3:G:486:ALA:HB3	1.89	0.72
5:I:392:ILE:HA	5:I:395:ARG:HB2	1.71	0.71
1:B:305:LYS:O	1:B:322:MET:HA	1.91	0.70
3:G:726:LEU:HB2	3:G:738:TRP:HB2	1.73	0.70
6:K:112:LYS:HA	6:K:116:ARG:HD2	1.74	0.70
1:B:564:LEU:H	1:B:580:GLN:HB2	1.57	0.69
3:G:475:ALA:HA	3:G:484:LEU:O	1.93	0.68
6:K:195:ALA:HB1	6:K:212:PRO:HG2	1.76	0.68
5:I:338:ALA:HB2	5:I:382:GLU:HB3	1.76	0.67
1:B:463:ARG:NH1	1:B:514:ASP:O	2.27	0.67
8:O:130:ILE:HG13	8:O:160:GLN:HE21	1.59	0.66
1:B:64:LYS:HA	1:B:126:LEU:O	1.96	0.66
4:H:330:ARG:O	4:H:333:ALA:HB3	1.95	0.66
4:H:333:ALA:O	4:H:336:LEU:HB2	1.94	0.66
4:H:325:ASN:O	4:H:328:ALA:HB3	1.95	0.66
5:I:323:VAL:HA	5:I:326:HIS:HD2	1.60	0.66
1:B:62:ARG:HG2	1:B:129:LYS:HG2	1.76	0.66
1:B:815:GLU:HA	1:B:819:LEU:HD12	1.79	0.65
1:B:835:ARG:HH21	6:K:188:ARG:HD2	1.61	0.65
1:B:354:PHE:O	1:B:357:CYS:HB2	1.97	0.65
4:H:323:VAL:O	4:H:327:TRP:N	2.29	0.65
1:B:359:ILE:HG23	1:B:498:VAL:HB	1.78	0.64
1:B:888:ILE:HD11	1:B:925:LYS:HG3	1.79	0.64
3:G:733:ASN:HB3	3:G:761:LEU:HB2	1.80	0.64
2:E:892:THR:H	9:R:109:SER:HB2	1.63	0.64
3:G:586:TYR:HB3	3:G:605:HIS:HB3	1.79	0.63
1:B:396:LYS:HD2	1:B:660:VAL:HA	1.80	0.63
1:B:630:ILE:O	1:B:638:ARG:NH1	2.31	0.63
6:K:108:PRO:O	6:K:111:ALA:HB3	1.99	0.63
1:B:118:ASP:O	1:B:123:ASN:ND2	2.32	0.63
1:B:32:VAL:HA	1:B:203:LYS:O	1.99	0.62
1:B:459:LEU:HD23	1:B:462:ASN:HD22	1.63	0.62
1:B:63:ILE:O	1:B:127:CYS:HA	2.00	0.62
1:B:646:ASP:HA	1:B:649:TRP:HD1	1.65	0.62
3:G:229:LEU:HB2	3:G:232:HIS:HD2	1.64	0.62
3:G:684:LEU:HB2	3:G:696:TRP:HB2	1.80	0.62
1:B:338:GLU:OE2	1:B:847:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:TYR:OH	1:B:654:ARG:NH2	2.33	0.62
7:M:57:TYR:OH	9:R:122:ARG:NH2	2.33	0.61
1:B:206:PHE:O	1:B:233:THR:HA	2.00	0.61
1:B:550:GLN:HB2	1:B:586:LEU:HB2	1.83	0.61
1:B:955:LYS:O	1:B:959:SER:N	2.31	0.61
3:G:464:TYR:HE1	6:K:151:UNK:HA	1.66	0.61
9:R:65:ASP:O	9:R:69:GLU:HB2	2.01	0.61
3:G:718:ARG:HG2	3:G:771:GLY:H	1.64	0.61
4:H:427:LEU:O	4:H:431:CYS:HB3	2.01	0.61
6:K:65:LEU:HD11	8:O:159:ALA:HB1	1.83	0.60
1:B:433:PHE:HB3	1:B:440:THR:HG21	1.84	0.60
1:B:911:LEU:HA	1:B:914:ILE:HD12	1.82	0.60
9:R:120:LEU:O	9:R:124:TRP:N	2.32	0.60
1:B:691:PHE:HD2	1:B:694:VAL:H	1.48	0.60
4:H:292:ASN:HD22	4:H:295:LEU:HG	1.67	0.60
1:B:41:GLN:O	1:B:43:LYS:NZ	2.35	0.60
6:K:31:LEU:HD11	6:K:34:ARG:HH21	1.67	0.59
5:I:55:LEU:HD13	7:M:28:ILE:HD12	1.84	0.59
1:B:24:ARG:NH1	1:B:120:ASP:OD1	2.33	0.59
3:G:787:ARG:NH2	10:Z:328:UNK:O	2.35	0.59
1:B:538:ASN:HD22	1:B:547:GLU:HB2	1.68	0.59
1:B:219:ASP:O	1:B:236:TYR:HA	2.02	0.59
1:B:352:GLN:O	1:B:356:GLY:N	2.35	0.59
4:H:233:GLY:O	4:H:239:ARG:NH1	2.35	0.59
7:M:77:CYS:SG	9:R:122:ARG:NH2	2.76	0.59
1:B:230:ARG:HG3	1:B:231:LYS:HG3	1.84	0.58
1:B:915:GLN:O	1:B:923:ARG:NH2	2.37	0.58
3:G:287:LYS:H	3:G:290:HIS:HD2	1.49	0.58
3:G:321:LEU:HD22	3:G:327:ASN:HD21	1.69	0.58
6:K:115:GLN:HE22	8:O:126:TYR:HB3	1.67	0.58
5:I:414:ASN:HA	5:I:417:ARG:HB2	1.85	0.58
3:G:472:GLY:HA3	3:G:783:LEU:HD13	1.85	0.58
10:Z:82:UNK:O	10:Z:86:UNK:N	2.37	0.58
1:B:917:ASP:OD1	1:B:923:ARG:NE	2.33	0.58
3:G:562:SER:OG	3:G:563:GLU:N	2.37	0.58
1:B:391:TYR:OH	1:B:458:ARG:NH1	2.33	0.58
1:B:608:ASN:O	1:B:657:ARG:NH2	2.37	0.58
1:B:341:LEU:O	1:B:344:ARG:HB3	2.04	0.57
3:G:552:SER:HB3	3:G:557:TYR:HB2	1.86	0.57
3:G:465:THR:HA	3:G:788:ARG:HG2	1.86	0.57
3:G:646:SER:OG	3:G:647:ALA:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:635:PHE:HA	3:G:642:VAL:HG12	1.85	0.57
6:K:73:GLY:HA3	8:O:142:ALA:HB1	1.86	0.57
1:B:550:GLN:HE22	1:B:580:GLN:HA	1.69	0.57
1:B:929:MET:HG2	1:B:932:LYS:HD2	1.87	0.57
3:G:278:ASP:O	3:G:282:LEU:HB2	2.04	0.57
4:H:324:ASP:O	4:H:327:TRP:HB2	2.04	0.57
1:B:184:ASN:OD1	1:B:195:SER:OG	2.23	0.57
1:B:599:ASN:HA	1:B:602:LYS:HB2	1.87	0.57
1:B:367:GLU:HG3	1:B:370:LEU:HD12	1.86	0.57
1:B:337:ASP:OD2	1:B:751:LYS:NZ	2.33	0.57
1:B:917:ASP:H	1:B:923:ARG:HH21	1.53	0.57
6:K:51:GLU:OE1	8:O:192:LYS:N	2.38	0.57
1:B:783:ASP:OD2	1:B:787:ASN:ND2	2.38	0.57
1:B:51:LEU:HB2	1:B:146:ILE:HB	1.86	0.56
3:G:564:ASP:HB2	3:G:566:THR:HG22	1.86	0.56
4:H:404:ARG:NH2	4:H:452:PHE:O	2.38	0.56
1:B:530:LYS:HE2	1:B:639:LYS:HD3	1.88	0.56
3:G:332:ILE:HA	3:G:336:HIS:HD2	1.71	0.56
3:G:476:VAL:HG22	3:G:768:LEU:HD22	1.87	0.56
5:I:363:TRP:NE1	5:I:399:GLU:OE2	2.38	0.56
6:K:75:SER:O	6:K:79:TYR:HB2	2.04	0.56
3:G:235:GLU:O	3:G:238:GLN:NE2	2.38	0.56
4:H:253:TYR:O	6:K:182:GLN:NE2	2.39	0.56
1:B:678:ARG:NH1	1:B:682:THR:OG1	2.39	0.56
4:H:306:PRO:HB3	10:Z:406:UNK:HA	1.86	0.56
1:B:631:ASP:O	1:B:638:ARG:NH1	2.38	0.56
6:K:191:THR:O	6:K:195:ALA:HB2	2.06	0.56
1:B:344:ARG:NH1	1:B:382:MET:SD	2.79	0.55
3:G:594:SER:HB2	3:G:597:GLY:H	1.71	0.55
1:B:946:ASN:ND2	1:B:986:CYS:SG	2.76	0.55
5:I:246:ILE:O	5:I:292:ASN:ND2	2.39	0.55
2:E:894:LEU:HA	9:R:111:LEU:H	1.71	0.55
3:G:613:ALA:HB2	3:G:620:LEU:HD11	1.89	0.55
6:K:196:LYS:HE2	6:K:208:VAL:HG12	1.87	0.55
8:O:139:LEU:HB3	8:O:144:PHE:HB3	1.88	0.55
1:B:597:ARG:NH1	1:B:621:ALA:O	2.37	0.55
1:B:806:VAL:HG13	1:B:864:ASN:HD21	1.70	0.55
1:B:820:ASP:HB2	1:B:822:LEU:HA	1.88	0.55
2:E:924:LYS:NZ	9:R:75:GLN:O	2.40	0.55
3:G:286:THR:HG22	3:G:287:LYS:HG3	1.87	0.55
5:I:337:VAL:HA	5:I:340:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:840:GLU:HG3	1:B:850:ILE:HB	1.87	0.55
2:E:873:LEU:HD23	9:R:58:LEU:HD13	1.87	0.55
5:I:233:GLY:O	5:I:239:ARG:NH1	2.37	0.55
10:Z:204:UNK:O	10:Z:208:UNK:N	2.40	0.54
4:H:217:SER:OG	4:H:218:VAL:N	2.41	0.54
6:K:172:TYR:OH	6:K:176:ARG:NH1	2.40	0.54
1:B:504:LEU:HA	1:B:507:ILE:HD12	1.89	0.54
1:B:536:ALA:H	1:B:548:ILE:HG12	1.72	0.54
1:B:32:VAL:HG22	1:B:203:LYS:HB3	1.87	0.54
3:G:609:ALA:HB3	3:G:623:PHE:HB2	1.88	0.54
5:I:345:SER:HB3	5:I:351:ILE:HB	1.90	0.54
5:I:208:UNK:HA	10:Z:560:UNK:HA	1.89	0.54
3:G:309:ILE:HD11	3:G:339:ILE:HG12	1.90	0.54
5:I:429:LYS:NZ	5:I:458:LEU:O	2.33	0.54
3:G:549:ALA:HA	3:G:559:LEU:O	2.07	0.54
2:E:940:VAL:O	2:E:944:LEU:N	2.40	0.53
1:B:82:ALA:HB3	1:B:128:ILE:HD11	1.88	0.53
3:G:240:PHE:HB3	3:G:271:GLN:HE22	1.73	0.53
5:I:224:TYR:HA	5:I:227:ILE:HD12	1.91	0.53
1:B:902:ARG:NH2	1:B:942:SER:O	2.42	0.53
3:G:468:ASN:HA	3:G:786:THR:HG23	1.91	0.53
1:B:406:GLU:OE2	1:B:412:VAL:N	2.42	0.53
1:B:663:GLN:HA	1:B:666:ILE:HB	1.91	0.53
1:B:761:ARG:NH2	1:B:804:ASN:O	2.41	0.53
3:G:653:LEU:HD12	3:G:663:ARG:HB2	1.90	0.53
1:B:206:PHE:HB2	1:B:234:PHE:HB2	1.91	0.53
5:I:368:THR:OG1	5:I:373:ARG:NE	2.42	0.53
9:R:106:ARG:HH22	9:R:112:GLU:HB2	1.74	0.53
1:B:392:ARG:HD3	1:B:395:ILE:HD12	1.91	0.52
1:B:486:GLN:OE1	1:B:489:GLN:NE2	2.41	0.52
3:G:692:ARG:NH2	3:G:706:GLU:OE1	2.41	0.52
5:I:276:LEU:HA	5:I:279:LEU:HD12	1.91	0.52
4:H:410:PRO:O	4:H:417:ARG:NH2	2.43	0.52
9:R:89:ASP:HA	9:R:92:ILE:HD12	1.91	0.52
3:G:300:PHE:HB3	3:G:301:ARG:HH11	1.75	0.52
1:B:859:ARG:HE	1:B:863:LYS:HE3	1.75	0.52
5:I:311:CYS:O	5:I:316:GLN:NE2	2.42	0.52
1:B:224:VAL:O	1:B:232:LYS:NZ	2.43	0.52
3:G:459:PRO:O	10:Z:359:UNK:N	2.43	0.52
6:K:110:TYR:HH	8:O:164:SER:HG	1.57	0.52
1:B:270:LEU:HB2	1:B:273:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:608:VAL:HG12	3:G:624:ALA:HB2	1.91	0.52
5:I:23:ALA:HB1	5:I:28:ILE:HD12	1.91	0.52
1:B:525:GLN:O	1:B:559:LYS:NZ	2.34	0.51
1:B:530:LYS:HG2	1:B:639:LYS:HB3	1.93	0.51
1:B:76:ARG:NH1	1:B:79:ASP:OD1	2.43	0.51
1:B:232:LYS:HE3	1:B:234:PHE:HE1	1.76	0.51
3:G:693:VAL:HB	3:G:707:LEU:HB2	1.93	0.51
4:H:256:LEU:HD22	4:H:295:LEU:HD22	1.92	0.51
10:Z:371:UNK:O	10:Z:375:UNK:N	2.44	0.51
1:B:353:GLN:O	1:B:357:CYS:N	2.44	0.51
4:H:328:ALA:O	4:H:331:ASP:HB2	2.10	0.51
1:B:392:ARG:HA	1:B:395:ILE:HD12	1.92	0.51
6:K:63:GLU:OE1	6:K:66:GLN:NE2	2.44	0.51
1:B:118:ASP:OD1	1:B:187:ARG:NH2	2.44	0.50
3:G:472:GLY:HA2	3:G:487:GLY:HA2	1.93	0.50
5:I:410:PRO:HG2	5:I:417:ARG:HE	1.76	0.50
1:B:366:ASP:HB3	1:B:499:SER:HB2	1.92	0.50
1:B:539:ARG:HG3	1:B:545:GLU:HA	1.92	0.50
1:B:565:LYS:HA	1:B:578:THR:O	2.12	0.50
6:K:66:GLN:HA	6:K:69:ILE:HD12	1.93	0.50
1:B:48:PHE:HA	1:B:148:ILE:O	2.11	0.50
1:B:688:GLU:H	1:B:695:ARG:HH12	1.60	0.50
5:I:207:UNK:O	10:Z:561:UNK:N	2.44	0.50
4:H:387:VAL:O	4:H:391:LEU:HB2	2.11	0.50
4:H:457:PRO:O	4:H:461:SER:N	2.42	0.50
5:I:223:TYR:OH	5:I:249:ASP:OD2	2.28	0.50
1:B:156:LYS:O	1:B:963:HIS:ND1	2.34	0.50
1:B:360:SER:OG	1:B:496:MET:O	2.26	0.50
5:I:43:VAL:HG21	7:M:47:VAL:HG22	1.92	0.50
5:I:410:PRO:O	5:I:417:ARG:NH2	2.44	0.50
10:Z:91:UNK:O	10:Z:95:UNK:N	2.45	0.50
1:B:24:ARG:HD3	1:B:120:ASP:HA	1.93	0.50
1:B:387:GLY:O	1:B:391:TYR:N	2.38	0.50
1:B:958:ASN:O	1:B:968:ARG:NH2	2.43	0.50
3:G:769:LEU:HD13	3:G:780:VAL:HG13	1.94	0.50
7:M:48:THR:HA	7:M:51:LEU:HD12	1.92	0.50
3:G:298:LEU:O	3:G:302:THR:OG1	2.28	0.50
5:I:217:SER:H	5:I:220:GLN:HG2	1.77	0.49
1:B:55:PRO:HB3	1:B:60:LEU:HD23	1.93	0.49
1:B:104:ASN:O	1:B:108:ASN:ND2	2.45	0.49
1:B:256:ILE:HD11	1:B:274:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:OG	1:B:152:LEU:O	2.23	0.49
3:G:244:PHE:HZ	3:G:264:PHE:HA	1.78	0.49
4:H:419:GLY:HA2	4:H:422:HIS:CE1	2.47	0.49
5:I:267:VAL:HG11	5:I:307:ALA:HB1	1.95	0.49
1:B:313:TYR:O	1:B:966:ARG:NH2	2.45	0.49
3:G:644:THR:HB	3:G:654:TRP:HE1	1.78	0.49
1:B:314:VAL:HG12	1:B:316:VAL:H	1.77	0.49
3:G:558:LEU:O	3:G:569:LEU:HA	2.13	0.49
1:B:215:VAL:HA	1:B:236:TYR:HE2	1.78	0.49
4:H:260:SER:HA	4:H:263:ILE:HD12	1.94	0.49
5:I:216:UNK:HA	5:I:220:GLN:HE21	1.78	0.49
9:R:106:ARG:NH1	9:R:112:GLU:OE1	2.41	0.49
1:B:451:CYS:HA	1:B:454:HIS:HD2	1.78	0.49
1:B:546:LEU:HB3	1:B:590:ILE:HB	1.93	0.49
1:B:727:PHE:HB3	1:B:736:VAL:HG11	1.94	0.49
3:G:601:VAL:HG11	3:G:642:VAL:HG11	1.95	0.49
1:B:220:LEU:HD23	1:B:236:TYR:HE1	1.78	0.49
1:B:570:GLU:OE1	1:B:593:HIS:ND1	2.38	0.49
1:B:291:TYR:HA	1:B:294:ILE:HD12	1.95	0.48
1:B:431:LEU:HD13	1:B:976:PHE:HB2	1.95	0.48
1:B:76:ARG:HD2	1:B:79:ASP:HA	1.95	0.48
4:H:371:THR:HG23	4:H:372:THR:HG23	1.95	0.48
5:I:270:ASN:HA	5:I:273:GLN:HB2	1.95	0.48
1:B:410:GLY:HA3	1:B:430:HIS:CD2	2.48	0.48
1:B:521:GLN:O	1:B:559:LYS:NZ	2.40	0.48
4:H:427:LEU:O	4:H:431:CYS:CB	2.61	0.48
7:M:96:ALA:O	7:M:100:ASN:CB	2.61	0.48
3:G:296:THR:O	3:G:300:PHE:HB3	2.13	0.48
4:H:337:VAL:HA	4:H:340:ILE:HD12	1.95	0.48
2:E:878:LEU:HD13	9:R:57:VAL:HG21	1.94	0.48
2:E:967:MET:O	2:E:971:LYS:N	2.44	0.48
5:I:374:TYR:HD1	5:I:423:VAL:HG13	1.79	0.48
1:B:26:TYR:HB2	1:B:53:ILE:HD11	1.96	0.48
4:H:336:LEU:O	4:H:340:ILE:N	2.47	0.48
9:R:81:GLU:HA	9:R:84:LEU:HD12	1.95	0.48
1:B:258:VAL:HG11	1:B:281:THR:HB	1.95	0.48
1:B:259:ASP:O	1:B:261:TYR:N	2.47	0.48
1:B:655:TYR:OH	10:Z:84:UNK:O	2.28	0.48
5:I:222:LEU:HD23	5:I:225:LYS:HD2	1.95	0.48
1:B:830:LEU:HD23	1:B:833:ILE:HD11	1.95	0.48
8:O:170:ALA:O	8:O:174:CYS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:894:LEU:HD22	2:E:899:VAL:HG21	1.95	0.48
7:M:33:PRO:HA	7:M:36:ILE:HD12	1.96	0.48
8:O:128:PRO:HG3	8:O:153:ARG:HG2	1.95	0.47
4:H:324:ASP:HA	4:H:327:TRP:HD1	1.78	0.47
1:B:275:PRO:O	1:B:278:LYS:HB2	2.13	0.47
4:H:323:VAL:HA	4:H:326:HIS:HB2	1.94	0.47
4:H:332:PHE:O	4:H:335:ARG:HB3	2.14	0.47
1:B:403:VAL:HG22	1:B:528:VAL:HG11	1.96	0.47
1:B:607:MET:HG3	1:B:611:GLU:HB2	1.97	0.47
1:B:769:LYS:HA	1:B:772:LEU:HD12	1.95	0.47
4:H:370:TRP:O	4:H:374:TYR:CB	2.63	0.47
3:G:542:HIS:CD2	3:G:562:SER:HB2	2.50	0.47
4:H:455:LEU:O	4:H:459:LEU:N	2.43	0.47
7:M:28:ILE:O	7:M:31:TYR:OH	2.21	0.47
3:G:287:LYS:H	3:G:290:HIS:CD2	2.30	0.47
1:B:346:LEU:HD23	1:B:346:LEU:HA	1.76	0.47
1:B:389:ASN:HB3	1:B:659:VAL:HG21	1.97	0.47
1:B:565:LYS:HG2	1:B:579:LEU:HA	1.96	0.47
1:B:738:THR:HG22	1:B:739:ASN:HB2	1.97	0.47
1:B:820:ASP:HB2	1:B:822:LEU:HD23	1.96	0.47
3:G:786:THR:HG22	3:G:788:ARG:HG3	1.97	0.47
7:M:49:THR:OG1	7:M:78:ARG:NH1	2.40	0.47
1:B:37:ASN:HB2	1:B:46:VAL:HG22	1.97	0.47
1:B:89:PRO:HG2	1:B:117:VAL:HG22	1.96	0.47
1:B:529:VAL:HG22	1:B:559:LYS:HB3	1.96	0.47
2:E:879:GLN:HG3	2:E:894:LEU:HD21	1.96	0.47
8:O:119:PHE:HA	8:O:122:GLN:HG2	1.97	0.47
1:B:119:PRO:HA	1:B:123:ASN:HD22	1.80	0.47
1:B:459:LEU:HA	1:B:462:ASN:HD22	1.80	0.47
4:H:276:LEU:HA	4:H:279:LEU:HD12	1.97	0.47
3:G:636:HIS:HA	3:G:677:PHE:HD2	1.79	0.46
4:H:292:ASN:HB3	4:H:295:LEU:HB2	1.97	0.46
1:B:880:TYR:HD1	1:B:887:ARG:HH22	1.63	0.46
5:I:387:VAL:O	5:I:390:THR:OG1	2.28	0.46
1:B:473:PHE:HA	1:B:476:LEU:HD12	1.97	0.46
5:I:370:TRP:HA	5:I:373:ARG:HD3	1.97	0.46
1:B:961:THR:HB	1:B:968:ARG:HE	1.80	0.46
3:G:590:ASP:HB3	3:G:633:THR:HG22	1.97	0.46
3:G:631:ASN:ND2	3:G:672:ILE:O	2.49	0.46
4:H:381:ALA:HA	4:H:388:ILE:HD11	1.98	0.46
4:H:414:ASN:HA	4:H:417:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:684:LEU:O	3:G:695:LEU:HA	2.16	0.46
1:B:59:ASN:H	1:B:135:TRP:HE1	1.64	0.46
3:G:631:ASN:H	3:G:646:SER:HA	1.81	0.46
3:G:636:HIS:HD2	3:G:638:ASN:H	1.63	0.46
4:H:383:LEU:HB3	4:H:387:VAL:HG21	1.98	0.46
5:I:263:ILE:HG23	5:I:282:LEU:HD22	1.97	0.46
8:O:126:TYR:O	8:O:153:ARG:NE	2.45	0.46
1:B:221:VAL:HG11	1:B:237:MET:HB3	1.98	0.46
3:G:636:HIS:HA	3:G:677:PHE:CD2	2.51	0.46
5:I:326:HIS:HA	5:I:329:LEU:HD12	1.98	0.46
5:I:395:ARG:O	5:I:399:GLU:HB2	2.16	0.46
6:K:222:PRO:O	6:K:225:THR:OG1	2.33	0.46
7:M:47:VAL:HA	7:M:50:ILE:HD12	1.97	0.46
8:O:123:LEU:HA	8:O:126:TYR:HD2	1.81	0.46
1:B:539:ARG:HH11	1:B:592:CYS:HB3	1.80	0.46
1:B:300:PRO:HB2	1:B:358:PHE:HE2	1.81	0.45
4:H:370:TRP:O	4:H:374:TYR:HB2	2.16	0.45
6:K:219:PHE:HE2	6:K:222:PRO:HA	1.80	0.45
1:B:64:LYS:HD3	1:B:119:PRO:HB3	1.97	0.45
3:G:467:LEU:H	3:G:495:ARG:HH12	1.65	0.45
3:G:470:TYR:CD2	3:G:471:GLN:HG3	2.52	0.45
4:H:402:ARG:O	4:H:405:SER:OG	2.28	0.45
1:B:85:ILE:HD11	1:B:129:LYS:HE3	1.97	0.45
1:B:518:LEU:HD12	1:B:522:TRP:HD1	1.82	0.45
1:B:159:LEU:HD21	1:B:189:TRP:CD1	2.51	0.45
5:I:456:GLY:HA2	5:I:457:PRO:HA	1.78	0.45
1:B:908:GLN:HE21	1:B:912:ASN:HD21	1.63	0.45
3:G:783:LEU:HD21	3:G:787:ARG:HG3	1.98	0.45
1:B:26:TYR:N	1:B:56:THR:OG1	2.46	0.45
2:E:912:ASN:HB2	9:R:124:TRP:HH2	1.81	0.45
1:B:343:ARG:HA	1:B:346:LEU:HB2	1.99	0.45
1:B:880:TYR:HA	1:B:887:ARG:CZ	2.47	0.45
1:B:570:GLU:OE2	1:B:576:ASN:ND2	2.47	0.45
1:B:95:HIS:CE1	1:B:97:GLU:HB2	2.52	0.44
4:H:389:LYS:HG3	4:H:438:LEU:HD11	1.98	0.44
8:O:204:LEU:HB3	8:O:208:GLY:HA3	1.99	0.44
6:K:194:MET:HA	6:K:197:THR:HB	2.00	0.44
1:B:572:ASP:HA	1:B:607:MET:HA	1.99	0.44
2:E:910:LEU:HD23	2:E:913:LEU:HD12	2.00	0.44
3:G:668:HIS:HD2	3:G:688:ALA:HB3	1.81	0.44
1:B:848:HIS:CD2	1:B:886:ILE:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:251:LEU:HB3	3:G:260:ALA:HB2	1.98	0.44
3:G:254:ASN:HB3	3:G:256:HIS:HD2	1.82	0.44
5:I:55:LEU:HD23	5:I:55:LEU:HA	1.83	0.44
3:G:504:UNK:HA	3:G:529:UNK:HA	1.99	0.44
4:H:334:ALA:O	4:H:337:VAL:HB	2.17	0.44
7:M:22:ILE:O	7:M:26:MET:N	2.50	0.44
1:B:65:LEU:O	1:B:126:LEU:HB2	2.17	0.44
3:G:768:LEU:HB3	3:G:769:LEU:H	1.49	0.44
1:B:26:TYR:HA	1:B:55:PRO:HA	2.00	0.44
1:B:31:GLN:HB3	1:B:202:TRP:CD1	2.52	0.44
1:B:201:THR:OG1	1:B:238:LEU:O	2.26	0.44
3:G:638:ASN:HD22	10:Z:43:UNK:HA	1.83	0.44
5:I:68:THR:HG23	7:M:35:VAL:HG22	2.00	0.44
1:B:95:HIS:HE1	1:B:97:GLU:HB2	1.82	0.44
1:B:372:GLY:HA2	1:B:453:ALA:HB1	2.00	0.44
1:B:626:LEU:HD23	1:B:626:LEU:HA	1.84	0.44
3:G:236:LEU:HD22	3:G:239:LEU:HD11	2.00	0.44
3:G:542:HIS:CE1	3:G:568:ARG:HD2	2.53	0.44
5:I:457:PRO:O	5:I:461:SER:N	2.43	0.44
1:B:51:LEU:O	1:B:145:LYS:HA	2.18	0.43
1:B:332:SER:H	1:B:335:ILE:HD12	1.83	0.43
1:B:597:ARG:NH2	1:B:622:ASP:OD1	2.51	0.43
4:H:333:ALA:HA	4:H:336:LEU:HD12	1.98	0.43
5:I:417:ARG:O	5:I:421:ASP:HB2	2.18	0.43
1:B:214:ALA:HB1	1:B:249:LEU:HD11	1.98	0.43
1:B:628:ILE:H	1:B:644:GLN:NE2	2.16	0.43
3:G:479:THR:O	3:G:555:ARG:NH2	2.48	0.43
3:G:542:HIS:HD2	3:G:562:SER:HB2	1.83	0.43
1:B:862:GLN:NE2	1:B:870:ASP:H	2.16	0.43
1:B:891:LEU:HA	1:B:894:VAL:HG12	1.99	0.43
3:G:571:SER:HB2	3:G:575:PHE:N	2.33	0.43
3:G:648:ASP:N	3:G:648:ASP:OD1	2.50	0.43
1:B:36:ASN:OD1	1:B:207:THR:OG1	2.36	0.43
1:B:549:LYS:HG2	1:B:587:LYS:HG2	2.01	0.43
1:B:914:ILE:HD13	1:B:927:LEU:HD21	2.00	0.43
3:G:464:TYR:OH	6:K:150:UNK:O	2.25	0.43
1:B:835:ARG:NH2	6:K:184:ARG:HE	2.12	0.43
3:G:590:ASP:OD2	3:G:633:THR:N	2.40	0.43
3:G:732:ASP:N	3:G:732:ASP:OD1	2.49	0.43
5:I:22:VAL:O	5:I:25:SER:OG	2.28	0.43
2:E:892:THR:HG22	2:E:893:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:403:ILE:HG23	4:H:420:ALA:HB1	2.01	0.43
5:I:358:THR:O	5:I:362:SER:OG	2.30	0.43
1:B:308:PHE:HA	1:B:325:PHE:O	2.18	0.43
1:B:503:PHE:CE2	1:B:507:ILE:HD11	2.54	0.43
5:I:313:VAL:HG12	5:I:314:SER:HB3	2.00	0.43
10:Z:213:UNK:O	10:Z:216:UNK:CB	2.67	0.43
1:B:567:THR:HG23	1:B:577:HIS:HE1	1.83	0.43
1:B:611:GLU:OE2	1:B:657:ARG:NE	2.51	0.43
1:B:957:MET:HG2	1:B:971:ALA:HB1	2.01	0.43
1:B:975:TYR:O	1:B:980:GLY:HA2	2.19	0.43
3:G:566:THR:HA	3:G:581:TYR:O	2.18	0.43
1:B:180:CYS:HB3	1:B:313:TYR:HB2	2.01	0.43
1:B:443:TRP:CG	1:B:924:HIS:HE1	2.37	0.43
1:B:699:CYS:SG	1:B:753:MET:HG2	2.59	0.43
1:B:516:GLN:HA	1:B:519:ILE:HD12	1.99	0.42
3:G:594:SER:HB2	3:G:597:GLY:N	2.32	0.42
4:H:411:VAL:HA	4:H:417:ARG:HH21	1.84	0.42
1:B:706:ALA:HB3	1:B:760:LEU:HD22	2.01	0.42
4:H:385:HIS:HE1	4:H:437:LYS:HD2	1.84	0.42
4:H:418:ILE:O	4:H:422:HIS:ND1	2.38	0.42
1:B:30:HIS:ND1	1:B:201:THR:HG23	2.35	0.42
1:B:75:VAL:HG13	1:B:148:ILE:HG12	2.00	0.42
1:B:575:PHE:HB3	1:B:577:HIS:CE1	2.55	0.42
6:K:51:GLU:O	10:Z:311:UNK:N	2.51	0.42
1:B:363:SER:H	1:B:366:ASP:HB2	1.85	0.42
3:G:605:HIS:ND1	3:G:629:ASP:OD1	2.52	0.42
3:G:241:TYR:HD1	3:G:271:GLN:HG3	1.83	0.42
3:G:467:LEU:O	3:G:787:ARG:NE	2.41	0.42
4:H:308:VAL:O	4:H:311:CYS:HB2	2.19	0.42
4:H:320:ARG:O	4:H:323:VAL:HB	2.18	0.42
5:I:309:MET:HA	5:I:312:ILE:HD12	2.02	0.42
5:I:400:GLY:HA2	5:I:403:ILE:HD12	2.00	0.42
1:B:688:GLU:H	1:B:695:ARG:NH1	2.18	0.42
1:B:749:LEU:HD12	1:B:749:LEU:HA	1.87	0.42
3:G:730:SER:OG	3:G:734:THR:OG1	2.34	0.42
6:K:79:TYR:HA	6:K:82:HIS:HD2	1.85	0.42
10:Z:214:UNK:O	10:Z:218:UNK:N	2.52	0.42
1:B:87:ASN:HB3	1:B:89:PRO:HD3	2.02	0.42
1:B:261:TYR:HB2	1:B:285:HIS:CG	2.55	0.42
3:G:695:LEU:O	3:G:704:VAL:N	2.53	0.42
4:H:446:ASP:O	4:H:450:ALA:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:276:LEU:HB3	5:I:326:HIS:CE1	2.55	0.42
8:O:163:ILE:HD13	8:O:166:ILE:HD12	2.01	0.42
9:R:68:ARG:NH1	9:R:72:PRO:O	2.53	0.42
1:B:238:LEU:HD11	1:B:240:ILE:HB	2.01	0.42
1:B:571:LEU:HD23	1:B:626:LEU:HG	2.02	0.42
1:B:772:LEU:O	1:B:776:LEU:HG	2.20	0.42
3:G:623:PHE:HB3	3:G:654:TRP:CE2	2.55	0.42
3:G:730:SER:OG	3:G:732:ASP:OD1	2.37	0.42
1:B:51:LEU:HD21	1:B:65:LEU:HD21	2.01	0.42
1:B:867:VAL:HA	6:K:204:PHE:HE1	1.85	0.42
2:E:922:GLN:HA	2:E:925:ASN:HD22	1.85	0.42
4:H:369:PRO:O	4:H:372:THR:OG1	2.30	0.42
5:I:252:LEU:O	5:I:254:GLN:N	2.53	0.42
1:B:653:LEU:HA	1:B:653:LEU:HD23	1.83	0.41
9:R:65:ASP:O	9:R:69:GLU:CB	2.68	0.41
5:I:53:ASP:HA	5:I:56:LYS:HE3	2.01	0.41
5:I:403:ILE:O	5:I:407:LEU:N	2.37	0.41
1:B:838:ASN:HD22	6:K:191:THR:HG23	1.85	0.41
4:H:366:GLU:HG2	4:H:367:LYS:H	1.84	0.41
5:I:224:TYR:HE1	5:I:259:PHE:HD1	1.67	0.41
5:I:320:ARG:HD3	5:I:415:ILE:HD13	2.02	0.41
6:K:51:GLU:N	8:O:193:TYR:O	2.53	0.41
3:G:584:HIS:HB3	3:G:586:TYR:HB2	2.03	0.41
1:B:26:TYR:HB3	1:B:60:LEU:HD21	2.02	0.41
1:B:49:VAL:HG12	1:B:148:ILE:HB	2.01	0.41
1:B:926:ILE:O	1:B:930:LEU:HB2	2.20	0.41
3:G:286:THR:H	3:G:290:HIS:CD2	2.39	0.41
5:I:274:ASN:HD21	5:I:317:LEU:H	1.67	0.41
5:I:302:HIS:CD2	10:Z:213:UNK:HA	2.55	0.41
6:K:227:LEU:HA	6:K:227:LEU:HD12	1.84	0.41
1:B:178:PHE:HA	1:B:249:LEU:O	2.21	0.41
3:G:761:LEU:HD11	3:G:766:GLN:HE21	1.85	0.41
1:B:816:VAL:HB	1:B:817:ARG:HG3	2.02	0.41
1:B:882:HIS:CE1	6:K:216:ALA:HB1	2.56	0.41
4:H:286:VAL:HA	4:H:289:LEU:HD12	2.03	0.41
6:K:110:TYR:CD1	6:K:113:ARG:HD2	2.56	0.41
7:M:19:MET:HA	7:M:22:ILE:HD12	2.02	0.41
1:B:465:SER:O	1:B:469:MET:HG3	2.21	0.41
1:B:604:ILE:HG12	1:B:607:MET:HE3	2.02	0.41
1:B:619:MET:HG3	1:B:647:PHE:CE2	2.56	0.41
3:G:477:ASP:OD1	3:G:477:ASP:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:675:LEU:HG	3:G:686:THR:HG22	2.03	0.41
4:H:219:GLU:HA	4:H:222:LEU:HD12	2.03	0.41
4:H:304:LEU:O	4:H:308:VAL:N	2.41	0.41
5:I:411:VAL:O	5:I:417:ARG:NH2	2.53	0.41
1:B:31:GLN:HE21	1:B:49:VAL:HG21	1.86	0.41
1:B:432:HIS:NE2	1:B:441:LEU:HA	2.35	0.41
1:B:691:PHE:HE2	1:B:693:ARG:HB2	1.85	0.41
3:G:473:LEU:HD21	3:G:489:PHE:HE1	1.86	0.41
3:G:763:GLU:O	3:G:784:HIS:HB3	2.21	0.41
5:I:383:LEU:HB2	5:I:387:VAL:HG11	2.01	0.41
1:B:131:PRO:O	1:B:135:TRP:N	2.50	0.40
1:B:719:MET:HA	1:B:722:LEU:HG	2.02	0.40
5:I:218:VAL:HA	5:I:221:GLN:HG2	2.03	0.40
5:I:241:GLU:OE2	6:K:135:UNK:N	2.54	0.40
5:I:270:ASN:O	5:I:274:ASN:N	2.49	0.40
1:B:898:THR:HG21	1:B:907:LEU:HB2	2.03	0.40
4:H:386:ASP:HA	4:H:389:LYS:HB3	2.02	0.40
10:Z:215:UNK:O	10:Z:219:UNK:N	2.55	0.40
1:B:546:LEU:HD22	1:B:625:LEU:HD21	2.02	0.40
1:B:710:VAL:HG22	1:B:762:ASP:HA	2.04	0.40
1:B:761:ARG:HB3	1:B:766:LEU:HB3	2.03	0.40
5:I:252:LEU:HD12	5:I:252:LEU:HA	1.90	0.40
5:I:380:LEU:HD13	5:I:391:LEU:HD13	2.02	0.40
5:I:383:LEU:HB3	5:I:387:VAL:HG21	2.02	0.40
3:G:305:PHE:HD2	3:G:337:LEU:HD23	1.85	0.40
3:G:572:LEU:HD13	3:G:575:PHE:HE1	1.87	0.40
3:G:783:LEU:HA	3:G:783:LEU:HD23	1.77	0.40
5:I:280:ILE:HB	5:I:329:LEU:HD21	2.04	0.40
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.90	0.40
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.83	0.40
3:G:248:TYR:HE2	3:G:285:LEU:HD12	1.85	0.40
3:G:474:THR:O	3:G:486:ALA:CB	2.65	0.40
4:H:309:MET:HA	4:H:312:ILE:HD12	2.04	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	B	966/1199 (81%)	781 (81%)	183 (19%)	2 (0%)	47	81
2	E	100/1085 (9%)	94 (94%)	6 (6%)	0	100	100
3	G	429/800 (54%)	352 (82%)	77 (18%)	0	100	100
4	H	255/677 (38%)	228 (89%)	26 (10%)	1 (0%)	34	72
5	I	326/677 (48%)	292 (90%)	32 (10%)	2 (1%)	25	65
6	K	149/310 (48%)	133 (89%)	15 (10%)	1 (1%)	22	62
7	M	96/264 (36%)	89 (93%)	7 (7%)	0	100	100
8	O	78/218 (36%)	74 (95%)	4 (5%)	0	100	100
9	R	72/161 (45%)	68 (94%)	4 (6%)	0	100	100
All	All	2471/5391 (46%)	2111 (85%)	354 (14%)	6 (0%)	50	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	256	LEU
4	H	321	PRO
5	I	257	PRO
6	K	218	PRO
1	B	336	ILE
1	B	844	PRO

### 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	B	879/1083 (81%)	872 (99%)	7 (1%)	81	89
2	E	52/815 (6%)	52 (100%)	0	100	100
3	G	367/619 (59%)	362 (99%)	5 (1%)	67	81
4	H	200/574 (35%)	199 (100%)	1 (0%)	88	93
5	I	252/564 (45%)	251 (100%)	1 (0%)	91	94
6	K	132/223 (59%)	132 (100%)	0	100	100
7	M	61/229 (27%)	60 (98%)	1 (2%)	62	79
8	O	71/154 (46%)	71 (100%)	0	100	100
9	R	70/141 (50%)	69 (99%)	1 (1%)	67	81
All	All	2084/4402 (47%)	2068 (99%)	16 (1%)	82	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	74	ARG
1	B	180	CYS
1	B	301	TYR
1	B	343	ARG
1	B	361	ARG
1	B	378	TYR
1	B	961	THR
3	G	558	LEU
3	G	559	LEU
3	G	589	TRP
3	G	607	ARG
3	G	637	PRO
4	H	347	THR
5	I	347	THR
7	M	73	LEU
9	R	125	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	ASN
1	B	108	ASN
1	B	123	ASN
1	B	137	HIS
1	B	147	HIS

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Mol	Chain	Res	Type
1	B	160	HIS
1	B	430	HIS
1	B	437	HIS
1	B	454	HIS
1	B	462	ASN
1	B	486	GLN
1	B	489	GLN
1	B	509	ASN
1	B	538	ASN
1	B	542	ASN
1	B	550	GLN
1	B	644	GLN
1	B	740	ASN
1	B	838	ASN
1	B	864	ASN
1	B	908	GLN
1	B	912	ASN
1	B	924	HIS
2	E	925	ASN
3	G	232	HIS
3	G	246	HIS
3	G	256	HIS
3	G	290	HIS
3	G	327	ASN
3	G	336	HIS
3	G	542	HIS
3	G	636	HIS
3	G	638	ASN
3	G	784	HIS
4	H	274	ASN
4	H	343	HIS
4	H	385	HIS
5	I	220	GLN
5	I	244	GLN
5	I	326	HIS
5	I	385	HIS
5	I	397	GLN
6	K	82	HIS
8	O	122	GLN
8	O	160	GLN
8	O	168	ASN
9	R	125	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	Z	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	95:UNK	C	119:UNK	N	129.81
1	Z	52:UNK	C	81:UNK	N	116.40
1	Z	143:UNK	C	195:UNK	N	95.92
1	Z	223:UNK	C	309:UNK	N	54.56
1	Z	386:UNK	C	401:UNK	N	34.09
1	Z	328:UNK	C	358:UNK	N	33.32
1	Z	428:UNK	C	551:UNK	N	24.82
1	Z	571:UNK	C	573:UNK	N	4.23



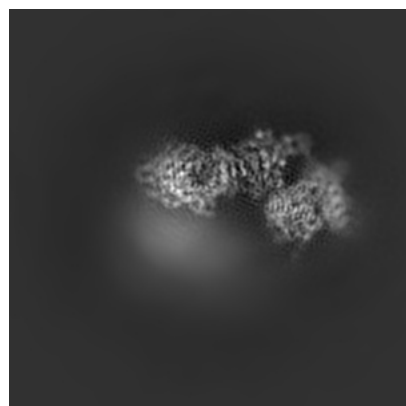
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9298. These allow visual inspection of the internal detail of the map and identification of artifacts.

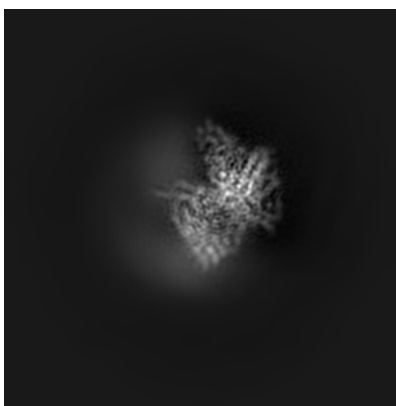
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

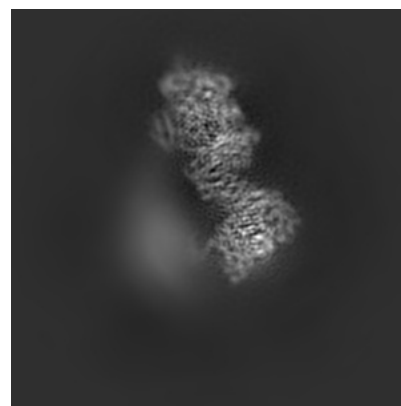
#### 6.1.1 Primary map



X

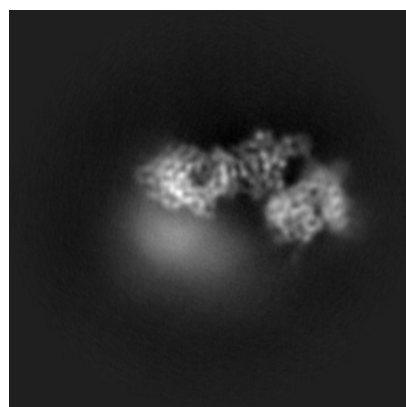


Y

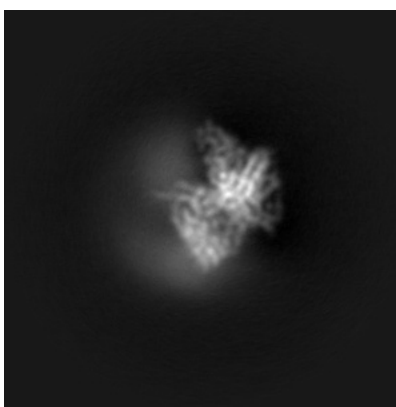


Z

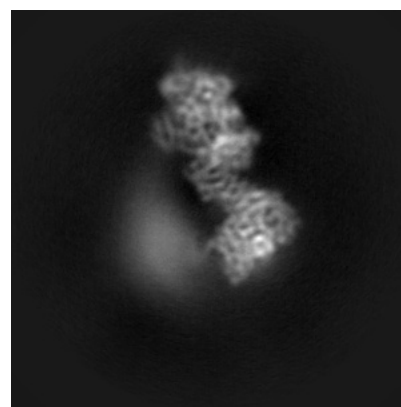
#### 6.1.2 Raw map



X



Y

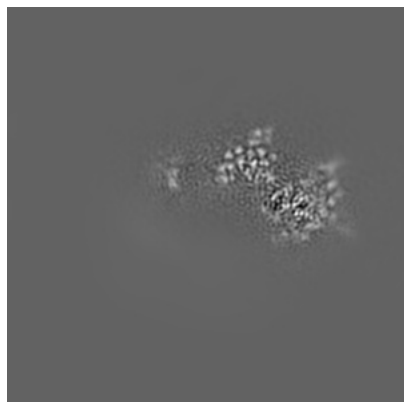


Z

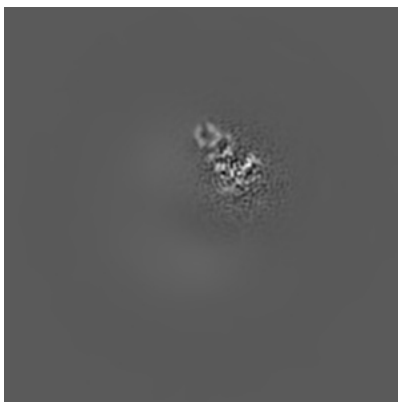
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

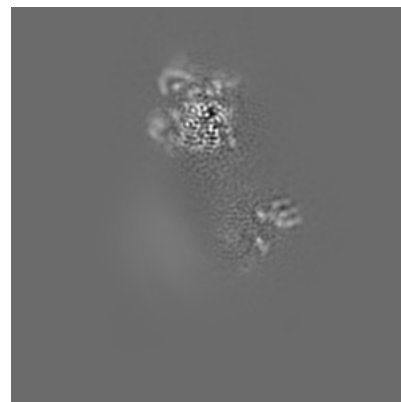
### 6.2.1 Primary map



X Index: 144

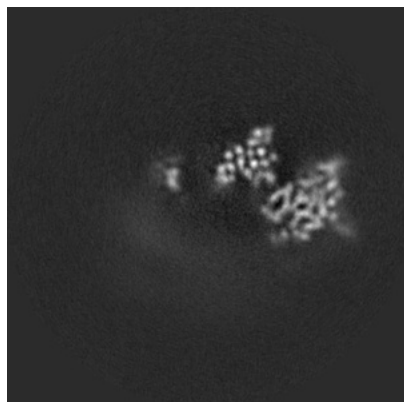


Y Index: 144

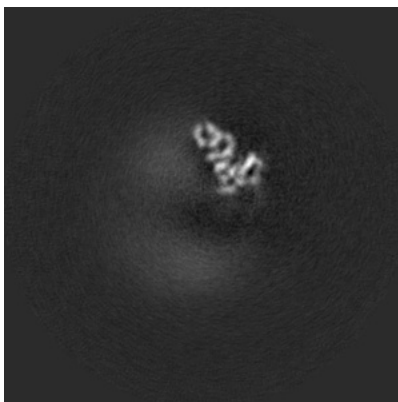


Z Index: 144

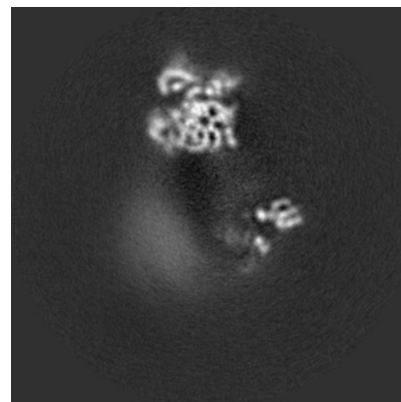
### 6.2.2 Raw map



X Index: 144



Y Index: 144

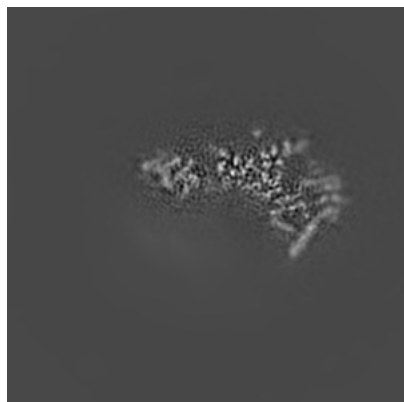


Z Index: 144

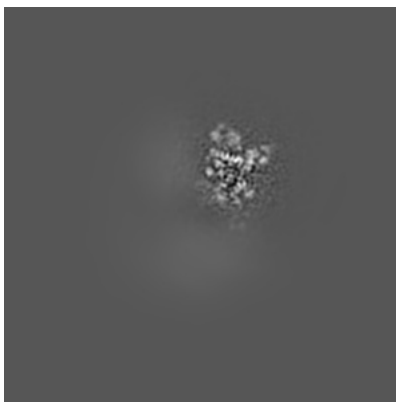
The images above show central slices of the map in three orthogonal directions.

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

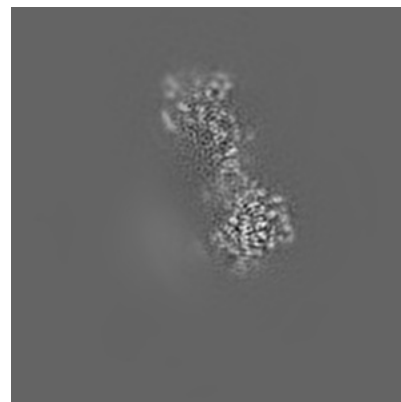
### 6.3.1 Primary map



X Index: 154

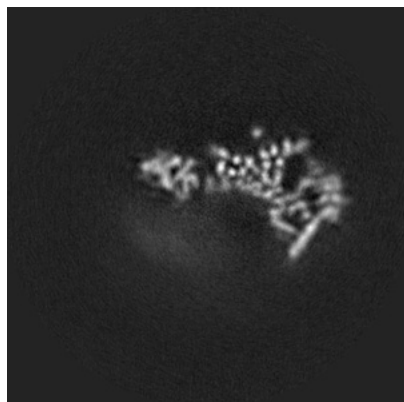


Y Index: 123

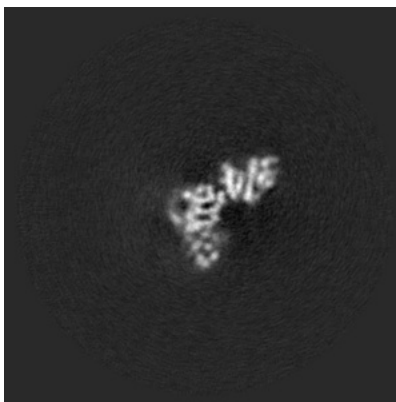


Z Index: 157

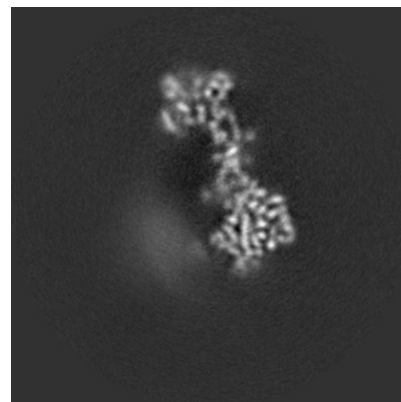
### 6.3.2 Raw map



X Index: 154



Y Index: 195

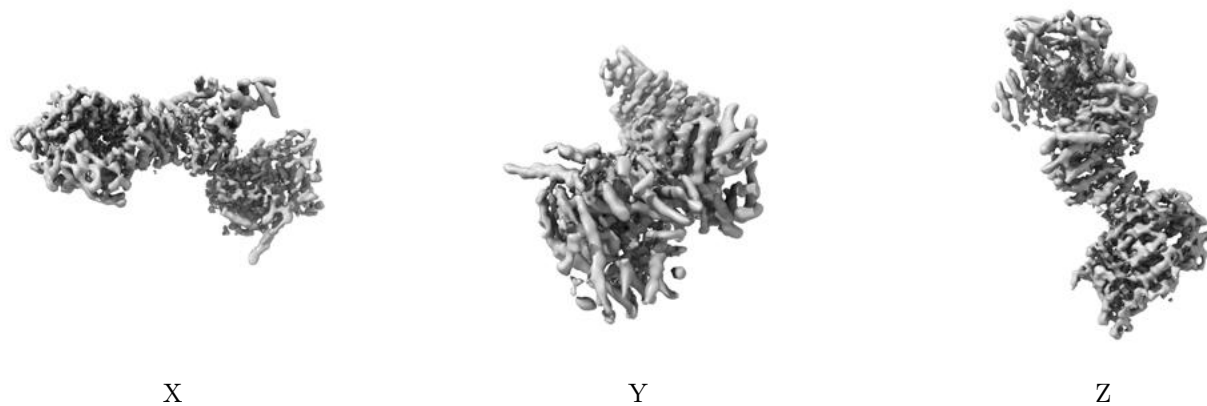


Z Index: 157

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

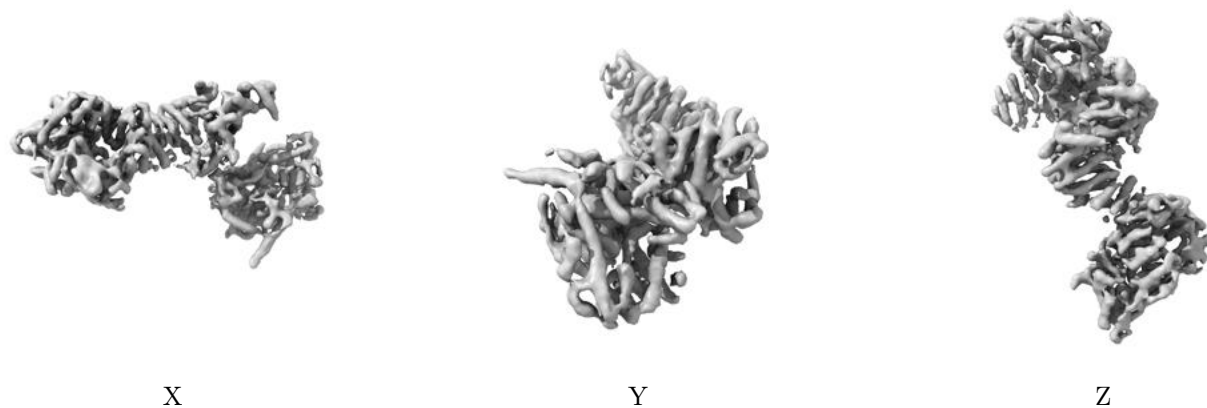
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. 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.

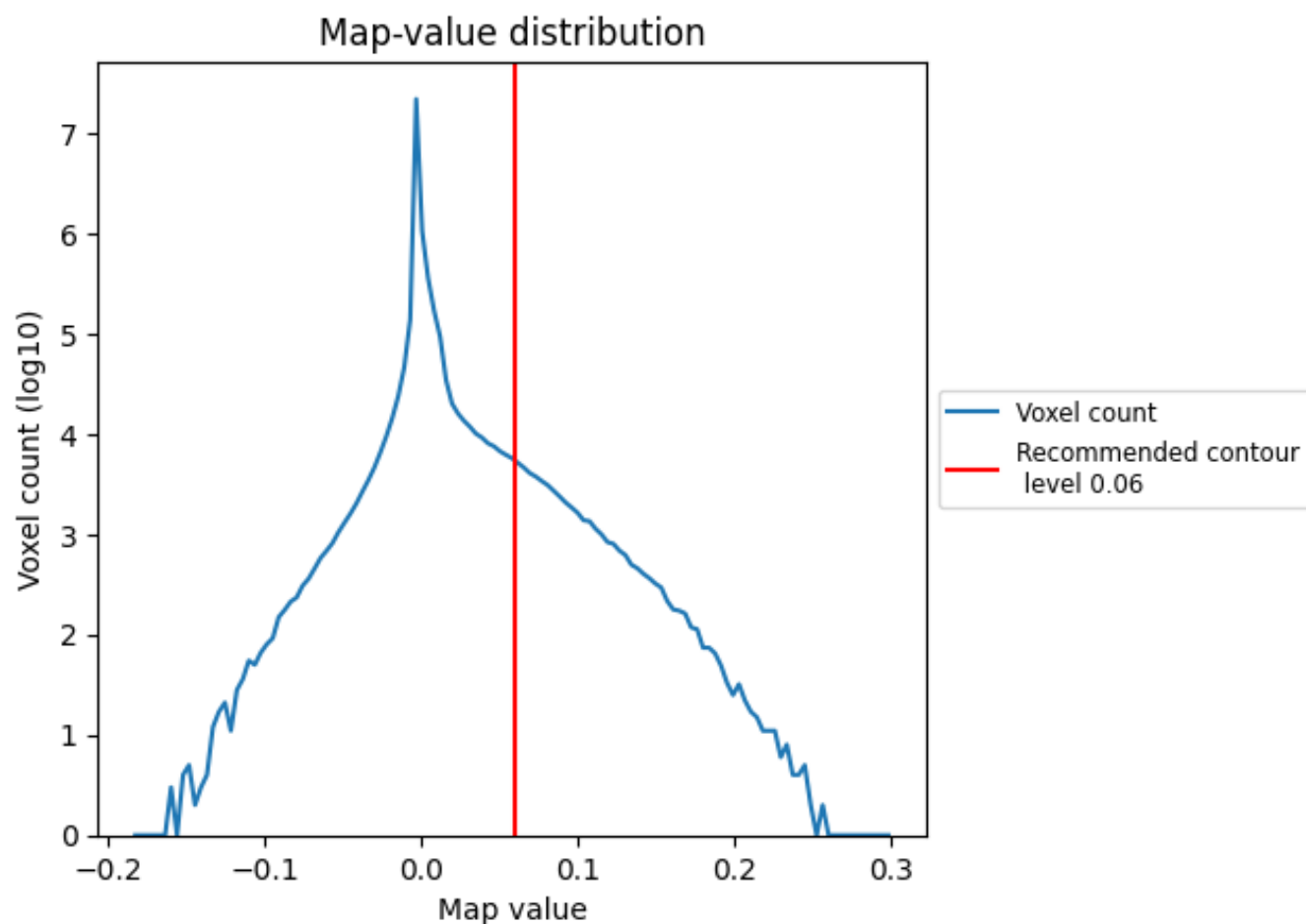
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

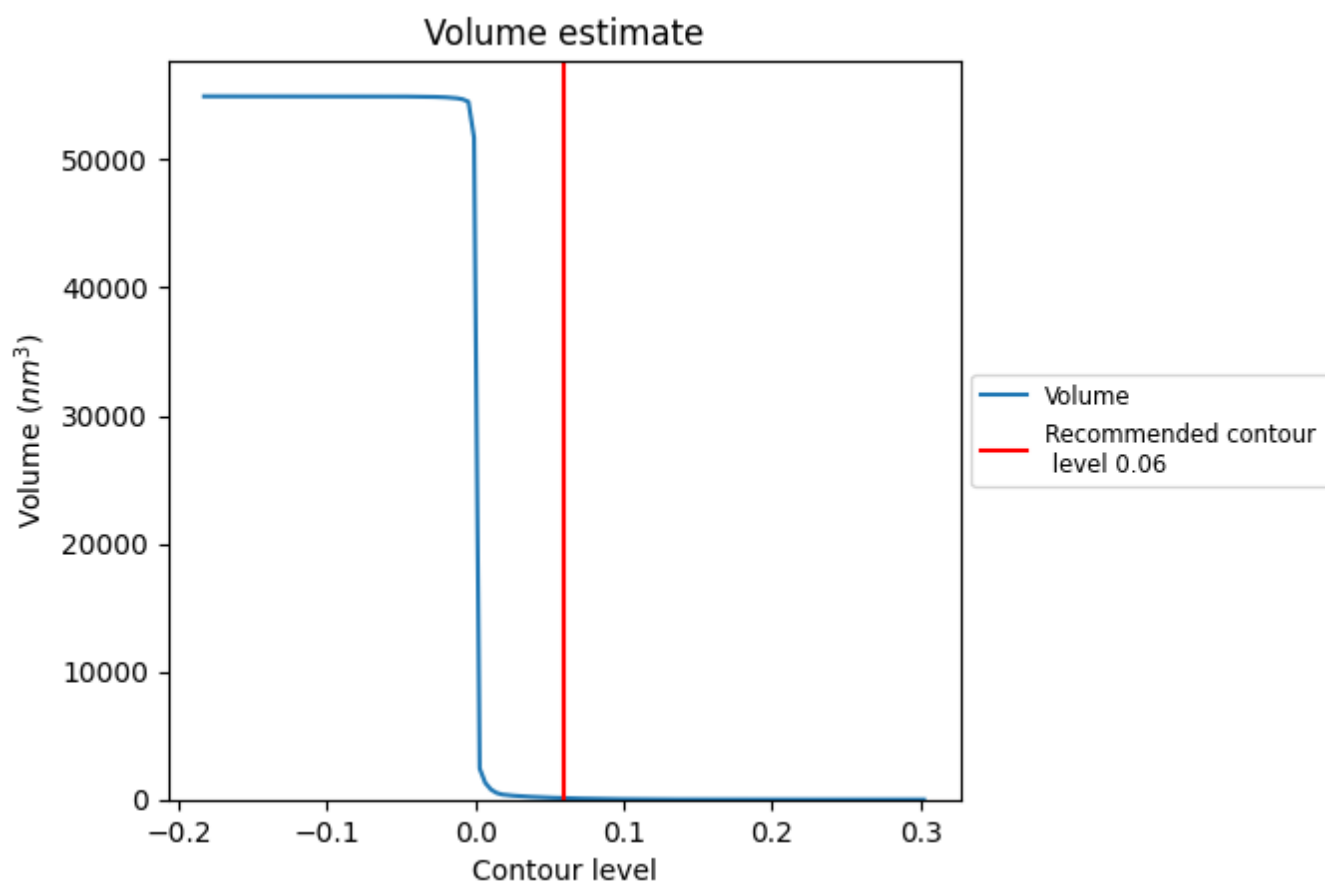
This section contains the results of statistical analysis of the map.

### 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.

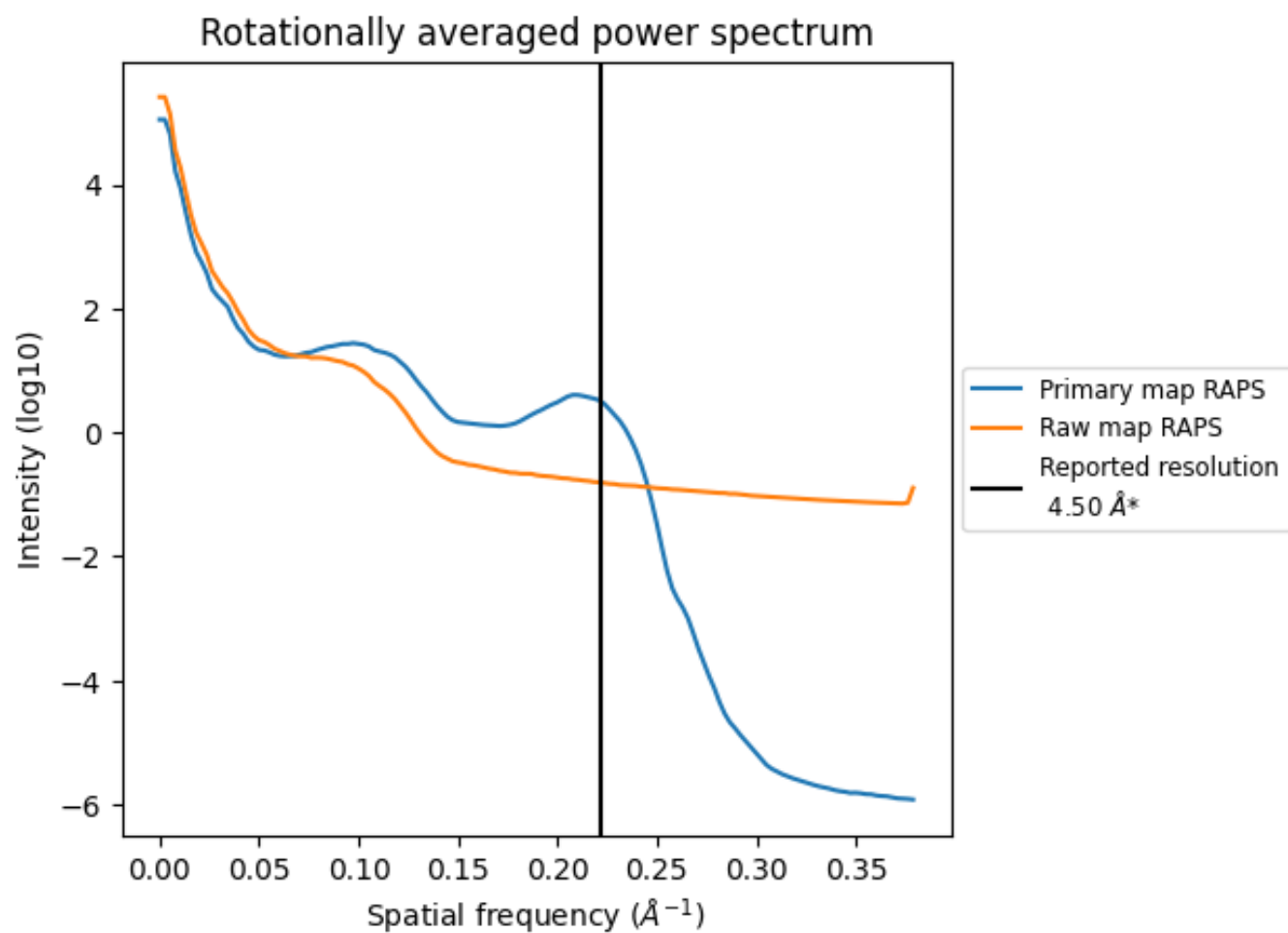
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 112 nm<sup>3</sup>; this corresponds to an approximate mass of 101 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 ⓘ

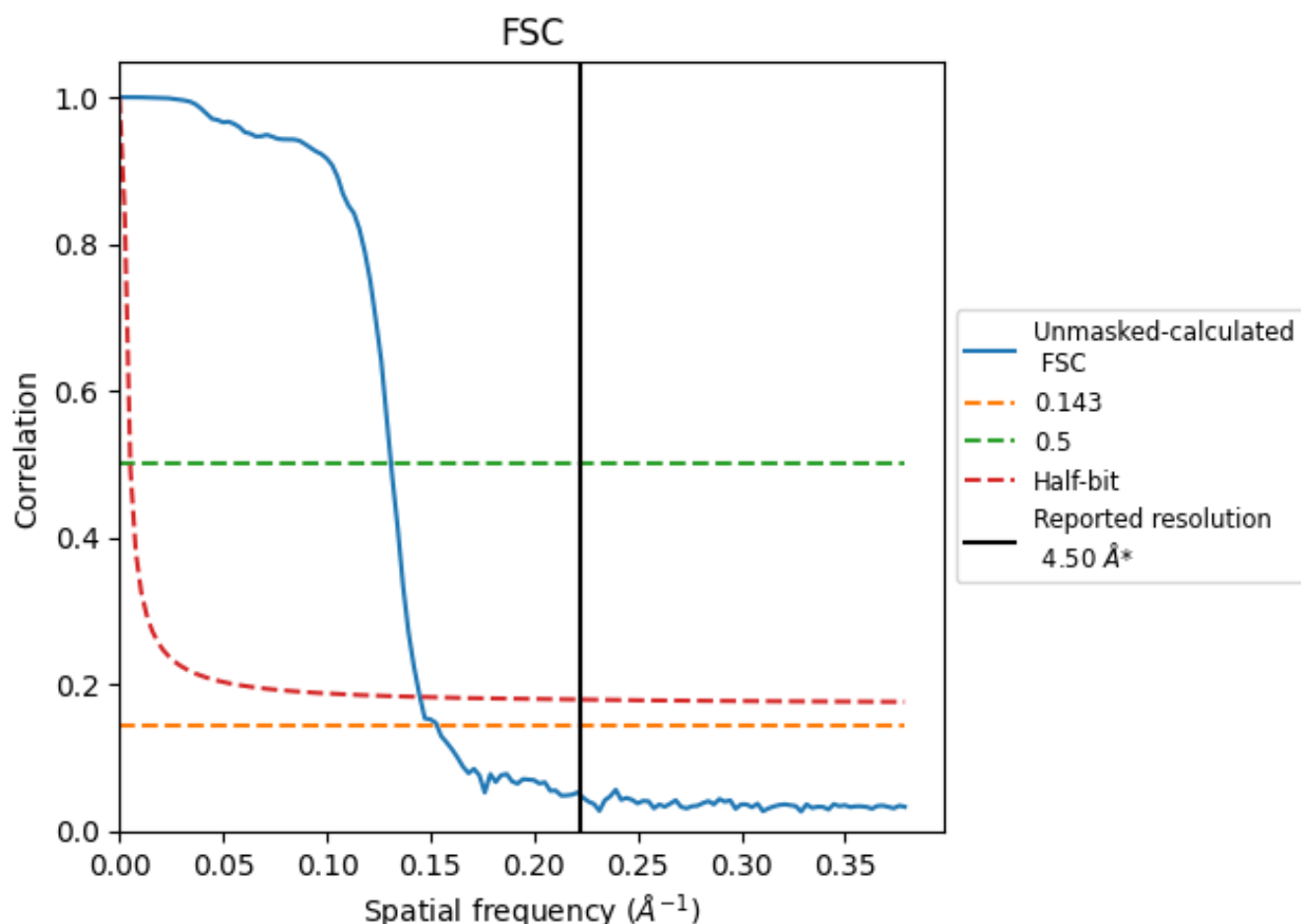


\*Reported resolution corresponds to spatial frequency of 0.222 Å<sup>-1</sup>

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



## 8.2 Resolution estimates [i](#)

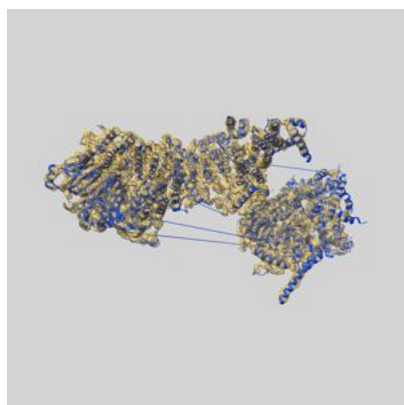
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.53	7.63	6.90

\*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 6.53 differs from the reported value 4.5 by more than 10 %

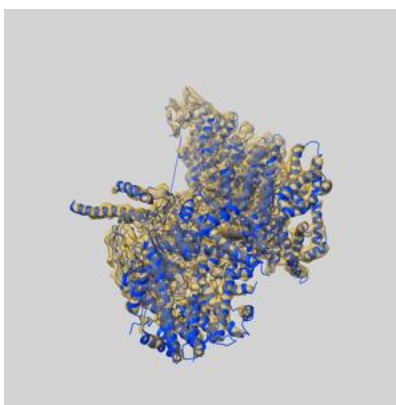
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9298 and PDB model 6MZC. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

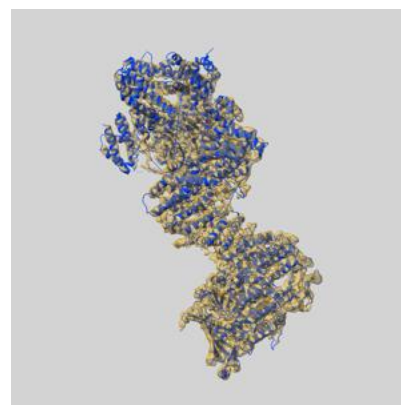
### 9.1 Map-model overlay [i](#)



X



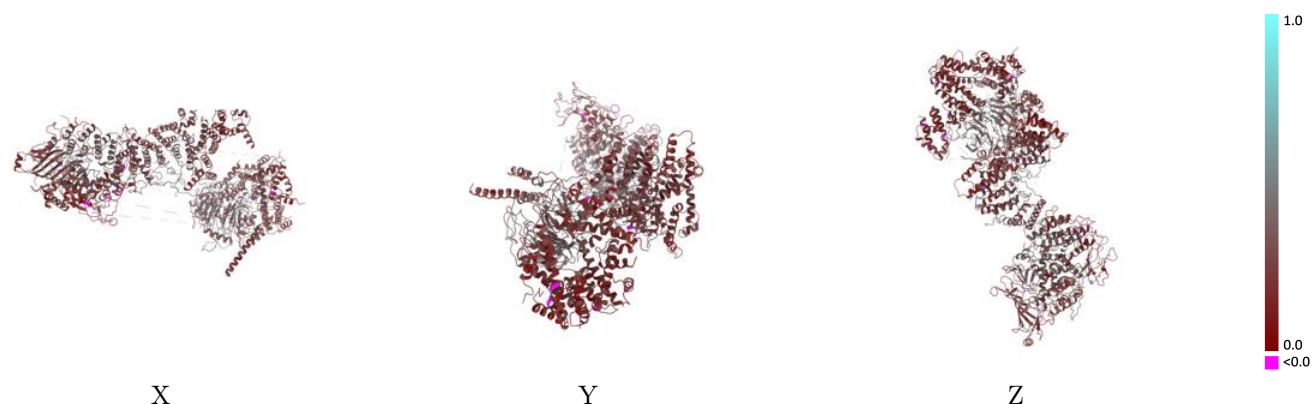
Y



Z

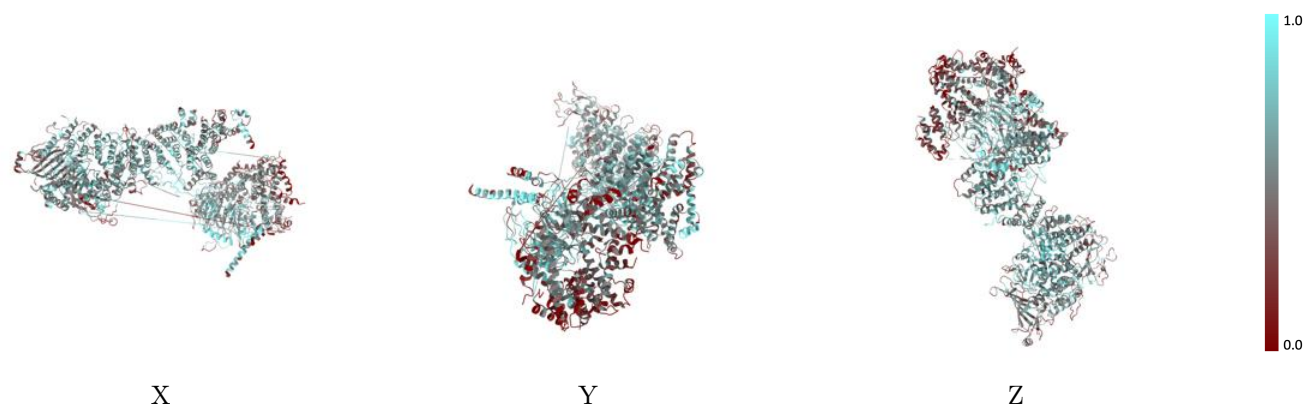
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



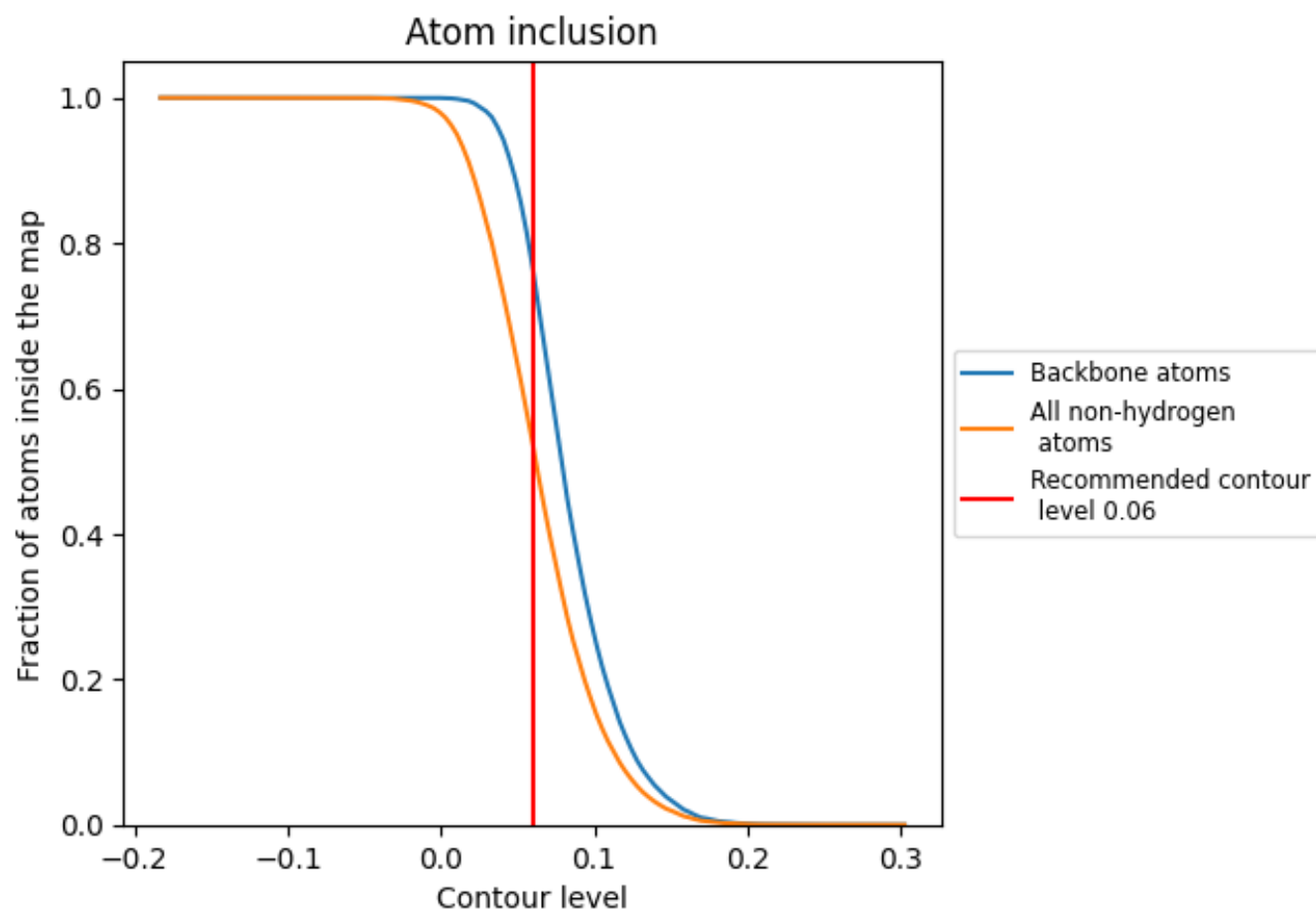
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 52% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5228	<div></div> 0.2960
B	<div></div> 0.5374	<div></div> 0.3010
E	<div></div> 0.4197	<div></div> 0.2300
G	<div></div> 0.5020	<div></div> 0.3130
H	<div></div> 0.5991	<div></div> 0.3000
I	<div></div> 0.5065	<div></div> 0.2590
K	<div></div> 0.5236	<div></div> 0.3090
M	<div></div> 0.4577	<div></div> 0.2550
O	<div></div> 0.3139	<div></div> 0.2420
R	<div></div> 0.2562	<div></div> 0.2050
Z	<div></div> 0.7471	<div></div> 0.3970

1.0

0.0

<0.0