



## Full wwPDB EM Validation Report ⓘ

Jan 27, 2025 – 02:41 PM EST

PDB ID : 9BW5  
EMDB ID : EMD-44953  
Title : Human Vault Cage  
Authors : Lodwick, J.E.; Zhao, M.  
Deposited on : 2024-05-20  
Resolution : 3.30 Å(reported)  
Based on initial model : 4v60

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) : 2.40

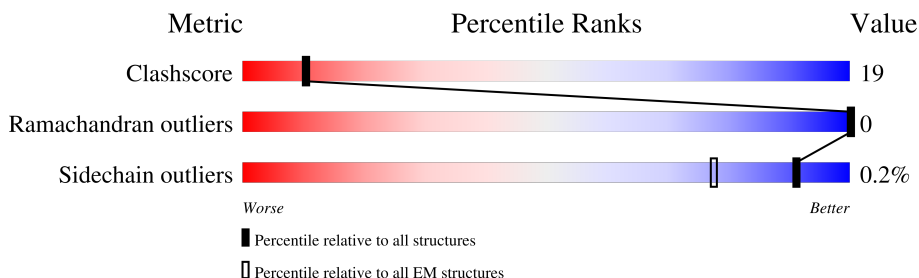
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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	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	893	
1	B	893	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12300 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.

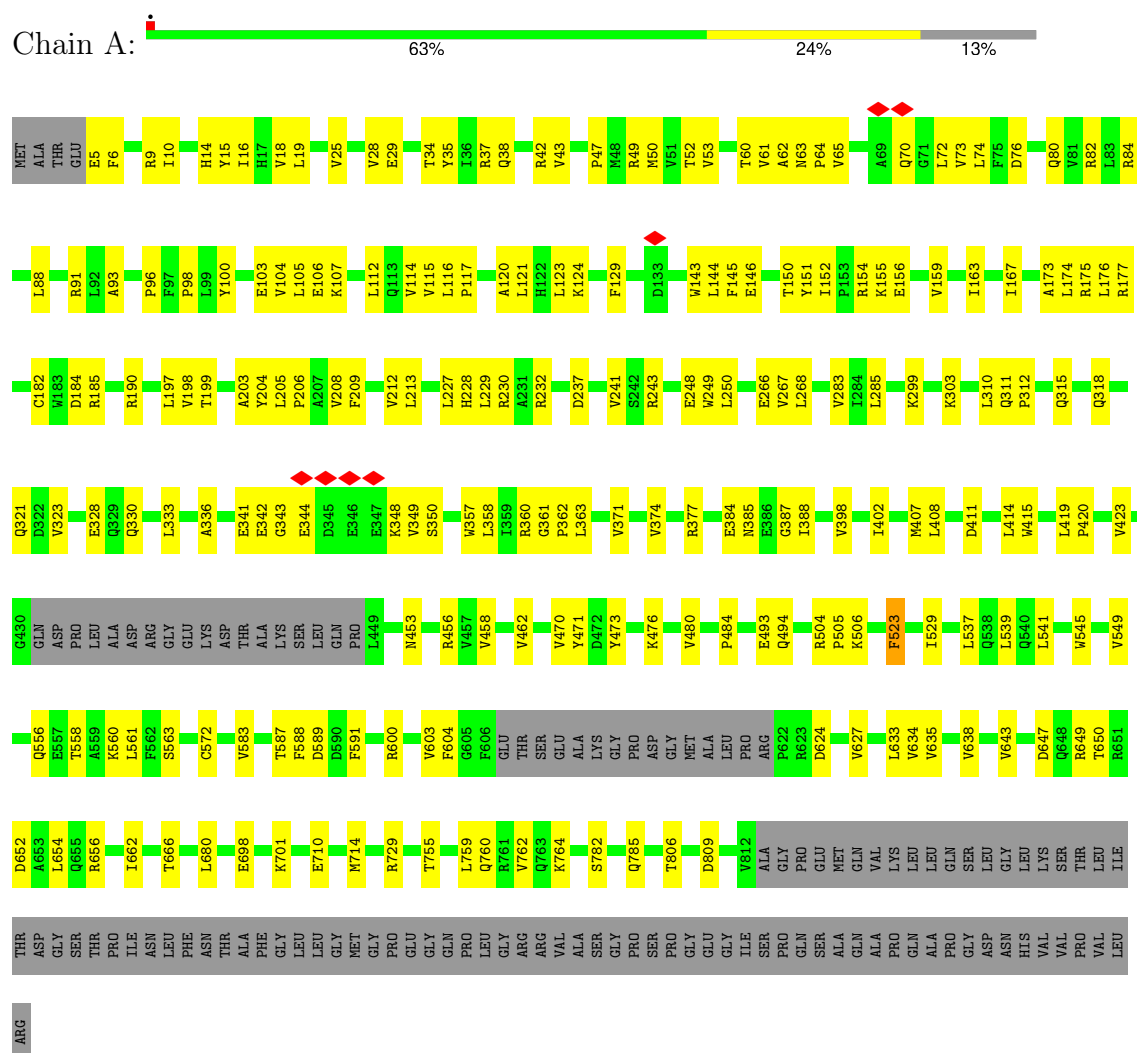
- Molecule 1 is a protein called Major vault protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	775	Total	C	N	O	S	0	0
			6150	3874	1099	1167	10		
1	B	775	Total	C	N	O	S	0	0
			6150	3874	1099	1167	10		

### 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: Major vault protein



#### • Molecule 1: Major vault protein



ASN	GLY	Q548	ASP	Q329	R91	MET
HIS	LEU	R649	PRO	Q330	R190	ALA
VAL	LYS	T650	LEU	Q333	LEU	THR
VAL	SER	R651	ALA	L333	V198	GLU
VAL	THR	D652	ASP	F557	T199	E5
LEU	LEU	A653	ARG	A336	L39	F6
ILE	ILE	A654	GLY	A203	Y100	R9
THR	THR	Q655	GLU	E341	ZY04	I10
ASP	ASP	R656	LYS	E342	L205	
			ASP	G343	P206	HI4
	GLY	I662	THR	E344	A207	L105
SER	THR		ALA	D345	V208	Y15
THR	THR	T666	LYS	E346	F209	I16
ILE	ILE		SER	E347	LEU	H17
ASN	ASN	L680	LEU	GLN	L112	H18
LEU	LEU	E698	GLN	K348	L213	L19
ASN	ASN	F588	PRO	V349	V114	V28
THR	THR	K701	L449	S350	V115	E29
ALA	ALA	D589	M453	S350	P117	
PHE	GLY	E710		W357	L227	T34
GLY	GLY		R456	L358	H228	Y35
LEU	LEU	W114	W457	T359	L229	T36
LEU	LEU		V458	R360	R230	T37
GLY	GLY	R729		G361	A231	Q38
MET	MET		V462	P362	R232	
	GLY	T755		L363		R42
PRO	PRO	F604	V470	L371	D237	V43
GLU	GLU	L759	Y471	V371	E130	
GLY	GLY	Q760	D472	V241	D131	P47
GLN	GLN	R761	Y473	S242	K132	M48
PRO	PRO	V762		R243	D133	R49
LEU	LEU	Q763	SER	R377		N50
GLY	GLY	K764	K476	E248	V143	V51
ARG	ARG	S782	V480	W249	L144	T52
	VAL	Q785	LYS	N385	F145	
ALA	ALA		P484	G387	E146	T60
SER	SER		I388	I266	V61	V61
GLY	GLY	K793	E493	V267	T150	A62
PRO	PRO	K794	Q494	L268	Y151	N63
SER	SER	T806	R504	V283	I152	V65
PRO	PRO		P505	L285	K155	
GLY	GLY		K506	L285	E156	
GLU	GLU	D809	ARG	K299	V159	A69
GLY	ILE	V812	L514	I402		Q70
ILE	ALA	R623	F523	M407	G71	L72
SER	GLY	D624	L408	L408	I163	W73
PRO	PRO					L74
GLN	GLN	V627	I629	D411	T167	F75
SER	SER					D76
ALA	ALA	L633	L537	Q315	A173	
GLN	GLN	V634	Q538	L174	L174	Q80
ALA	ALA	V635	L539	W415	R175	V81
PRO	PRO	LYS	Q540	Q318	L176	R82
GLN	GLN	V638	L541	Q321	R177	
ALA	ALA			D322	L83	L84
PRO	PRO		W545	V323	C182	
GLY	GLY	V643		V423	V183	R84
SER	SER		V549	G430	D184	
ASP	LEU	D647		GLN	R185	L88

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D39	Depositor
Number of particles used	98674	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed when movies were imported into cryoSPARC Live	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.136	Depositor
Minimum map value	-0.938	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.3	Depositor
Map size ( $\text{\AA}$ )	1075.2, 1075.2, 1075.2	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.344, 1.344, 1.344	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	A	0.46	0/6259	0.56	0/8488
1	B	0.46	0/6259	0.56	0/8488
All	All	0.46	0/12518	0.56	0/16976

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6150	0	6183	231	0
1	B	6150	0	6183	229	0
All	All	12300	0	12366	458	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 19.

All (458) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:CYS:SG	1:A:209:PHE:CD1	2.26	1.28
1:B:182:CYS:SG	1:B:209:PHE:CD1	2.26	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:PHE:CE2	1:B:545:TRP:CD1	2.24	1.24
1:A:523:PHE:CE2	1:A:545:TRP:CD1	2.24	1.22
1:A:523:PHE:CD2	1:A:545:TRP:CD1	2.39	1.11
1:B:523:PHE:CD2	1:B:545:TRP:CD1	2.39	1.11
1:A:523:PHE:HE2	1:A:545:TRP:CG	1.71	1.09
1:B:182:CYS:SG	1:B:209:PHE:CE1	2.46	1.09
1:B:523:PHE:HE2	1:B:545:TRP:CG	1.71	1.08
1:A:523:PHE:CE2	1:A:545:TRP:CG	2.42	1.08
1:A:182:CYS:SG	1:A:209:PHE:CE1	2.46	1.07
1:A:333:LEU:HD13	1:A:377:ARG:HH12	1.13	1.06
1:A:333:LEU:CD1	1:A:377:ARG:HH12	1.68	1.06
1:B:523:PHE:CE2	1:B:545:TRP:CG	2.42	1.06
1:A:333:LEU:HB2	1:A:377:ARG:NH1	1.71	1.06
1:B:333:LEU:CD1	1:B:377:ARG:HH12	1.68	1.06
1:B:333:LEU:HD13	1:B:377:ARG:HH12	1.13	1.05
1:B:333:LEU:HB2	1:B:377:ARG:NH1	1.71	1.04
1:A:333:LEU:HD13	1:A:377:ARG:NH1	1.75	1.02
1:B:333:LEU:HD13	1:B:377:ARG:NH1	1.75	1.01
1:A:539:LEU:HB3	1:A:541:LEU:HD11	1.43	1.01
1:B:539:LEU:HB3	1:B:541:LEU:HD11	1.43	1.00
1:A:333:LEU:HD22	1:A:377:ARG:NH2	1.77	0.98
1:B:333:LEU:HD22	1:B:377:ARG:NH2	1.77	0.98
1:B:649:ARG:HG3	1:B:649:ARG:HH11	1.32	0.95
1:A:649:ARG:HG3	1:A:649:ARG:HH11	1.32	0.94
1:A:182:CYS:HG	1:A:209:PHE:HD1	1.20	0.90
1:A:303:LYS:NZ	1:A:323:VAL:CG2	2.35	0.90
1:B:303:LYS:NZ	1:B:323:VAL:CG2	2.35	0.89
1:A:358:LEU:HD13	1:A:377:ARG:HD2	1.55	0.89
1:A:14:HIS:CE1	1:A:49:ARG:HG2	2.07	0.89
1:B:303:LYS:HZ1	1:B:323:VAL:HG21	1.38	0.89
1:A:650:THR:O	1:A:654:LEU:HD23	1.73	0.88
1:A:303:LYS:HZ2	1:A:323:VAL:HG22	1.39	0.88
1:B:14:HIS:CE1	1:B:49:ARG:HG2	2.07	0.88
1:B:650:THR:O	1:B:654:LEU:HD23	1.72	0.88
1:B:182:CYS:HG	1:B:209:PHE:HD1	1.22	0.87
1:A:333:LEU:HD22	1:A:377:ARG:HH22	1.39	0.86
1:B:358:LEU:HD13	1:B:377:ARG:HD2	1.55	0.86
1:B:175:ARG:HB2	1:B:213:LEU:HB2	1.58	0.86
1:A:18:VAL:HG12	1:A:43:VAL:HG22	1.58	0.85
1:B:303:LYS:HZ1	1:B:323:VAL:CG2	1.88	0.85
1:B:18:VAL:HG12	1:B:43:VAL:HG22	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HB2	1:A:213:LEU:HB2	1.58	0.84
1:A:182:CYS:SG	1:A:209:PHE:HD1	1.98	0.84
1:B:348:LYS:HD3	1:B:348:LYS:H	1.42	0.83
1:A:348:LYS:H	1:A:348:LYS:HD3	1.42	0.83
1:B:343:GLY:HA2	1:B:348:LYS:HA	1.60	0.82
1:B:333:LEU:HD22	1:B:377:ARG:HH22	1.40	0.82
1:B:123:LEU:HB2	1:B:143:TRP:HB2	1.61	0.82
1:B:303:LYS:NZ	1:B:323:VAL:HG22	1.95	0.82
1:A:303:LYS:NZ	1:A:323:VAL:HG22	1.95	0.81
1:A:343:GLY:HA2	1:A:348:LYS:HA	1.60	0.81
1:A:123:LEU:HB2	1:A:143:TRP:HB2	1.61	0.80
1:B:303:LYS:HZ2	1:B:323:VAL:HG22	1.45	0.80
1:B:16:ILE:HG12	1:B:29:GLU:HB2	1.65	0.79
1:A:16:ILE:HG12	1:A:29:GLU:HB2	1.65	0.78
1:B:333:LEU:CB	1:B:377:ARG:NH1	2.47	0.78
1:B:182:CYS:SG	1:B:209:PHE:HD1	1.98	0.77
1:A:506:LYS:HD2	1:A:572:CYS:SG	2.25	0.77
1:A:333:LEU:CB	1:A:377:ARG:HH12	1.99	0.76
1:A:333:LEU:CB	1:A:377:ARG:NH1	2.47	0.76
1:B:506:LYS:HD2	1:B:572:CYS:SG	2.25	0.76
1:B:358:LEU:HD13	1:B:377:ARG:HH11	1.49	0.75
1:A:333:LEU:CD2	1:A:377:ARG:HH22	1.99	0.75
1:A:358:LEU:HD13	1:A:377:ARG:HH11	1.49	0.75
1:B:333:LEU:CB	1:B:377:ARG:HH12	1.99	0.74
1:B:333:LEU:CD2	1:B:377:ARG:HH22	1.99	0.74
1:A:303:LYS:HZ1	1:A:323:VAL:CG2	2.00	0.74
1:A:303:LYS:HZ1	1:A:323:VAL:HG21	1.53	0.73
1:B:627:VAL:HG22	1:B:634:VAL:HG13	1.70	0.73
1:A:333:LEU:HB2	1:A:377:ARG:HH12	1.54	0.73
1:A:627:VAL:HG22	1:A:634:VAL:HG13	1.70	0.73
1:B:333:LEU:HB2	1:B:377:ARG:HH12	1.54	0.73
1:B:384:GLU:O	1:B:385:ASN:CG	2.28	0.72
1:A:384:GLU:O	1:A:385:ASN:CG	2.28	0.71
1:A:174:LEU:HD11	1:A:212:VAL:HG13	1.73	0.71
1:A:336:ALA:HB2	1:A:357:TRP:HZ3	1.55	0.71
1:B:230:ARG:HB2	1:B:248:GLU:HG2	1.73	0.71
1:B:539:LEU:HB3	1:B:541:LEU:CD1	2.20	0.71
1:B:174:LEU:HD11	1:B:212:VAL:HG13	1.73	0.70
1:A:506:LYS:NZ	1:A:523:PHE:HB2	2.06	0.70
1:A:348:LYS:HD3	1:A:348:LYS:N	2.07	0.70
1:B:336:ALA:HB2	1:B:357:TRP:HZ3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LYS:HD3	1:B:348:LYS:N	2.07	0.70
1:B:506:LYS:NZ	1:B:523:PHE:HB2	2.06	0.70
1:A:348:LYS:H	1:A:348:LYS:CD	2.05	0.70
1:A:230:ARG:HB2	1:A:248:GLU:HG2	1.73	0.69
1:B:480:VAL:HG11	1:B:558:THR:HB	1.74	0.69
1:B:333:LEU:CG	1:B:377:ARG:HH12	2.05	0.69
1:B:523:PHE:CD2	1:B:545:TRP:NE1	2.61	0.69
1:A:121:LEU:HB2	1:A:145:PHE:HB3	1.75	0.69
1:A:333:LEU:CG	1:A:377:ARG:HH12	2.05	0.69
1:A:539:LEU:HB3	1:A:541:LEU:CD1	2.20	0.69
1:A:303:LYS:NZ	1:A:323:VAL:HG21	2.07	0.69
1:B:348:LYS:H	1:B:348:LYS:CD	2.05	0.69
1:B:121:LEU:HB2	1:B:145:PHE:HB3	1.75	0.69
1:A:182:CYS:HB2	1:A:209:PHE:CE1	2.28	0.68
1:B:182:CYS:HB2	1:B:209:PHE:CE1	2.28	0.68
1:B:61:VAL:HB	1:B:91:ARG:HH21	1.58	0.68
1:A:523:PHE:CD2	1:A:545:TRP:NE1	2.61	0.68
1:A:19:LEU:HD22	1:A:42:ARG:HH21	1.57	0.68
1:B:19:LEU:HD22	1:B:42:ARG:HH21	1.57	0.68
1:B:177:ARG:HB2	1:B:213:LEU:HD11	1.75	0.68
1:B:649:ARG:HG3	1:B:649:ARG:NH1	2.05	0.67
1:A:177:ARG:HB2	1:A:213:LEU:HD11	1.75	0.67
1:A:480:VAL:HG11	1:A:558:THR:HB	1.74	0.67
1:B:5:GLU:N	1:B:37:ARG:NH1	2.43	0.67
1:B:184:ASP:HB2	1:B:190:ARG:HE	1.60	0.67
1:A:61:VAL:HB	1:A:91:ARG:HH21	1.58	0.67
1:A:184:ASP:HB2	1:A:190:ARG:HE	1.60	0.67
1:B:182:CYS:CB	1:B:209:PHE:CE1	2.77	0.67
1:B:473:TYR:O	1:B:476:LYS:HD2	1.94	0.67
1:A:182:CYS:CB	1:A:209:PHE:CE1	2.77	0.67
1:A:473:TYR:O	1:A:476:LYS:HD2	1.94	0.67
1:B:182:CYS:CB	1:B:209:PHE:CD1	2.78	0.67
1:A:5:GLU:N	1:A:37:ARG:NH1	2.43	0.66
1:A:182:CYS:CB	1:A:209:PHE:CD1	2.78	0.66
1:A:14:HIS:NE2	1:A:49:ARG:HG2	2.11	0.65
1:A:303:LYS:HZ2	1:A:323:VAL:CG2	2.01	0.65
1:A:649:ARG:HG3	1:A:649:ARG:NH1	2.05	0.65
1:B:303:LYS:NZ	1:B:323:VAL:HG21	2.07	0.65
1:A:523:PHE:HD2	1:A:545:TRP:NE1	1.96	0.64
1:B:523:PHE:HD2	1:B:545:TRP:NE1	1.96	0.64
1:B:14:HIS:NE2	1:B:49:ARG:HG2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:CD1	1:A:377:ARG:HD2	2.28	0.64
1:B:112:LEU:HD21	1:B:152:ILE:HG22	1.80	0.64
1:A:9:ARG:HA	1:A:34:THR:HA	1.80	0.64
1:A:74:LEU:HB3	1:A:82:ARG:HD3	1.80	0.64
1:B:206:PRO:HB3	1:B:212:VAL:HG23	1.80	0.64
1:B:9:ARG:HA	1:B:34:THR:HA	1.80	0.63
1:B:358:LEU:CD1	1:B:377:ARG:HD2	2.28	0.63
1:A:112:LEU:HD21	1:A:152:ILE:HG22	1.80	0.63
1:B:74:LEU:HB3	1:B:82:ARG:HD3	1.80	0.63
1:A:174:LEU:HD21	1:A:212:VAL:HG22	1.82	0.62
1:A:206:PRO:HB3	1:A:212:VAL:HG23	1.80	0.62
1:B:174:LEU:HD21	1:B:212:VAL:HG22	1.82	0.61
1:B:419:LEU:HD11	1:B:458:VAL:HG11	1.82	0.61
1:A:419:LEU:HD11	1:A:458:VAL:HG11	1.82	0.61
1:A:333:LEU:HD13	1:A:377:ARG:CZ	2.31	0.60
1:B:755:THR:O	1:B:759:LEU:HG	2.02	0.60
1:B:115:VAL:HG21	1:B:121:LEU:HG	1.84	0.60
1:A:115:VAL:HG21	1:A:121:LEU:HG	1.84	0.59
1:B:333:LEU:HD13	1:B:377:ARG:CZ	2.31	0.59
1:A:303:LYS:HZ1	1:A:323:VAL:CG1	2.15	0.59
1:B:336:ALA:HB2	1:B:357:TRP:CZ3	2.36	0.59
1:B:129:PHE:CG	1:B:156:GLU:HG3	2.38	0.59
1:B:303:LYS:NZ	1:B:323:VAL:CG1	2.66	0.58
1:B:647:ASP:OD2	1:B:649:ARG:HB2	2.03	0.58
1:A:539:LEU:HG	1:A:643:VAL:HG22	1.84	0.58
1:A:647:ASP:OD2	1:A:649:ARG:HB2	2.03	0.58
1:A:303:LYS:NZ	1:A:323:VAL:CG1	2.66	0.58
1:A:336:ALA:HB2	1:A:357:TRP:CZ3	2.36	0.58
1:A:755:THR:O	1:A:759:LEU:HG	2.02	0.58
1:B:15:TYR:CD2	1:B:50:MET:HG2	2.39	0.58
1:A:15:TYR:HD2	1:A:50:MET:HG2	1.68	0.58
1:A:38:GLN:N	1:A:38:GLN:OE1	2.37	0.58
1:B:470:VAL:HG11	1:B:493:GLU:OE1	2.04	0.58
1:B:38:GLN:N	1:B:38:GLN:OE1	2.37	0.58
1:B:229:LEU:HD23	1:B:267:VAL:HA	1.86	0.58
1:A:129:PHE:CG	1:A:156:GLU:HG3	2.38	0.58
1:A:15:TYR:CD2	1:A:50:MET:HG2	2.39	0.57
1:A:529:ILE:HD12	1:A:583:VAL:HG11	1.86	0.57
1:B:15:TYR:HD2	1:B:50:MET:HG2	1.68	0.57
1:B:529:ILE:HD12	1:B:583:VAL:HG11	1.86	0.57
1:A:65:VAL:O	1:A:84:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LEU:HG	1:B:643:VAL:HG22	1.84	0.57
1:A:144:LEU:HG	1:A:208:VAL:HG13	1.85	0.57
1:A:541:LEU:N	1:A:541:LEU:HD12	2.20	0.57
1:B:144:LEU:HG	1:B:208:VAL:HG13	1.86	0.57
1:A:470:VAL:HG11	1:A:493:GLU:OE1	2.04	0.56
1:A:229:LEU:HD23	1:A:267:VAL:HA	1.86	0.56
1:A:650:THR:O	1:A:654:LEU:CD2	2.52	0.56
1:B:18:VAL:HG11	1:B:35:TYR:CE2	2.40	0.56
1:B:537:LEU:HD11	1:B:591:PHE:CE2	2.39	0.56
1:B:698:GLU:HA	1:B:701:LYS:HZ3	1.70	0.56
1:A:537:LEU:HD11	1:A:591:PHE:CE2	2.40	0.56
1:B:70:GLN:HB2	1:B:72:LEU:HG	1.88	0.56
1:A:175:ARG:CB	1:A:213:LEU:HB2	2.35	0.56
1:B:318:GLN:HB2	1:B:321:GLN:HE21	1.71	0.56
1:B:541:LEU:HD12	1:B:541:LEU:N	2.20	0.56
1:B:65:VAL:O	1:B:84:ARG:NH2	2.38	0.56
1:A:18:VAL:HG11	1:A:35:TYR:CE2	2.40	0.56
1:A:60:THR:OG1	1:A:107:LYS:HB2	2.06	0.56
1:A:318:GLN:HB2	1:A:321:GLN:HE21	1.71	0.56
1:A:70:GLN:HB2	1:A:72:LEU:HG	1.88	0.55
1:B:182:CYS:HB2	1:B:209:PHE:CZ	2.42	0.55
1:B:14:HIS:NE2	1:B:49:ARG:CG	2.70	0.55
1:B:176:LEU:HD11	1:B:204:TYR:CE2	2.42	0.55
1:A:176:LEU:HD11	1:A:204:TYR:CE2	2.42	0.55
1:A:163:ILE:HD12	1:A:206:PRO:HG2	1.88	0.55
1:B:60:THR:OG1	1:B:107:LYS:HB2	2.06	0.55
1:B:62:ALA:N	1:B:104:VAL:O	2.35	0.54
1:B:163:ILE:HD12	1:B:206:PRO:HG2	1.88	0.54
1:A:14:HIS:NE2	1:A:49:ARG:CG	2.70	0.54
1:A:62:ALA:N	1:A:104:VAL:O	2.35	0.54
1:A:182:CYS:HB2	1:A:209:PHE:CZ	2.42	0.54
1:A:470:VAL:CG1	1:A:493:GLU:OE1	2.56	0.54
1:B:649:ARG:HH11	1:B:649:ARG:CG	2.13	0.54
1:A:398:VAL:HG11	1:A:415:TRP:CE3	2.43	0.53
1:B:650:THR:O	1:B:654:LEU:CD2	2.52	0.53
1:B:470:VAL:CG1	1:B:493:GLU:OE1	2.56	0.53
1:B:303:LYS:HZ3	1:B:323:VAL:HG13	1.72	0.53
1:B:398:VAL:HG11	1:B:415:TRP:CE3	2.43	0.53
1:A:243:ARG:HG2	1:A:249:TRP:CE3	2.44	0.53
1:B:243:ARG:HG2	1:B:249:TRP:CE3	2.44	0.53
1:B:185:ARG:HD2	1:B:204:TYR:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:HG21	1:A:100:TYR:CZ	2.45	0.52
1:B:76:ASP:N	1:B:80:GLN:O	2.42	0.52
1:B:358:LEU:HD13	1:B:377:ARG:NH1	2.23	0.52
1:A:185:ARG:HD2	1:A:204:TYR:HE1	1.74	0.52
1:A:539:LEU:HD21	1:A:591:PHE:HZ	1.74	0.52
1:A:649:ARG:HH11	1:A:649:ARG:CG	2.13	0.52
1:B:539:LEU:HD21	1:B:591:PHE:HZ	1.74	0.52
1:A:303:LYS:HZ1	1:A:323:VAL:HG11	1.73	0.52
1:B:73:VAL:HG21	1:B:100:TYR:CZ	2.45	0.52
1:B:420:PRO:O	1:B:423:VAL:HG12	2.10	0.52
1:B:229:LEU:HD21	1:B:267:VAL:HG22	1.92	0.52
1:A:420:PRO:O	1:A:423:VAL:HG12	2.10	0.51
1:A:76:ASP:N	1:A:80:GLN:O	2.42	0.51
1:A:358:LEU:HD13	1:A:377:ARG:NH1	2.23	0.51
1:B:360:ARG:HG2	1:B:361:GLY:N	2.25	0.51
1:A:523:PHE:CE2	1:A:545:TRP:CB	2.94	0.51
1:A:539:LEU:O	1:A:541:LEU:CD1	2.59	0.51
1:A:649:ARG:NH1	1:A:649:ARG:CG	2.73	0.51
1:B:250:LEU:HG	1:B:312:PRO:HD3	1.92	0.51
1:B:624:ASP:OD1	1:B:624:ASP:N	2.43	0.51
1:A:229:LEU:HD21	1:A:267:VAL:HG22	1.92	0.50
1:A:360:ARG:HG2	1:A:361:GLY:N	2.25	0.50
1:B:5:GLU:O	1:B:37:ARG:HD3	2.11	0.50
1:B:229:LEU:CD2	1:B:267:VAL:HG22	2.41	0.50
1:B:232:ARG:HE	1:B:266:GLU:HB2	1.76	0.50
1:B:523:PHE:CE2	1:B:545:TRP:CB	2.94	0.50
1:A:462:VAL:O	1:A:484:PRO:HA	2.11	0.50
1:B:62:ALA:HB3	1:B:104:VAL:HB	1.93	0.50
1:A:232:ARG:HE	1:A:266:GLU:HB2	1.76	0.50
1:B:167:ILE:HA	1:B:203:ALA:HA	1.93	0.50
1:A:5:GLU:O	1:A:37:ARG:HD3	2.11	0.50
1:B:539:LEU:O	1:B:541:LEU:CD1	2.59	0.50
1:A:250:LEU:HG	1:A:312:PRO:HD3	1.92	0.50
1:A:363:LEU:C	1:A:363:LEU:HD12	2.32	0.50
1:A:167:ILE:HA	1:A:203:ALA:HA	1.93	0.50
1:A:229:LEU:CD2	1:A:267:VAL:HG22	2.41	0.50
1:B:363:LEU:HD12	1:B:363:LEU:C	2.32	0.50
1:B:462:VAL:O	1:B:484:PRO:HA	2.11	0.50
1:B:388:ILE:HD12	1:B:414:LEU:HD21	1.95	0.49
1:B:649:ARG:NH1	1:B:649:ARG:CG	2.73	0.49
1:A:176:LEU:HD12	1:A:198:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:LEU:HD12	1:B:198:VAL:CG2	2.42	0.49
1:A:62:ALA:HB3	1:A:104:VAL:HB	1.93	0.49
1:A:243:ARG:HG2	1:A:249:TRP:CZ3	2.48	0.49
1:B:243:ARG:HG2	1:B:249:TRP:CZ3	2.48	0.49
1:A:388:ILE:HD12	1:A:414:LEU:HD21	1.94	0.49
1:B:652:ASP:O	1:B:656:ARG:HD2	2.13	0.49
1:A:624:ASP:OD1	1:A:624:ASP:N	2.43	0.49
1:A:504:ARG:HB2	1:A:505:PRO:HD3	1.94	0.49
1:A:652:ASP:O	1:A:656:ARG:HD2	2.13	0.49
1:A:523:PHE:CZ	1:A:545:TRP:HB3	2.48	0.49
1:B:504:ARG:HB2	1:B:505:PRO:HD3	1.94	0.48
1:B:5:GLU:C	1:B:37:ARG:HH11	2.17	0.48
1:B:114:VAL:HA	1:B:150:THR:HA	1.94	0.48
1:B:523:PHE:CZ	1:B:545:TRP:HB3	2.48	0.48
1:A:114:VAL:HA	1:A:150:THR:HA	1.94	0.48
1:A:5:GLU:C	1:A:37:ARG:HH11	2.17	0.48
1:B:328:GLU:HG2	1:B:362:PRO:HG3	1.96	0.48
1:A:227:LEU:O	1:A:250:LEU:HA	2.14	0.48
1:A:230:ARG:HB3	1:A:268:LEU:HD21	1.96	0.48
1:B:175:ARG:CB	1:B:213:LEU:HB2	2.35	0.48
1:B:37:ARG:O	1:B:37:ARG:HG2	2.14	0.48
1:B:182:CYS:HG	1:B:209:PHE:HE1	1.45	0.47
1:A:328:GLU:HG2	1:A:362:PRO:HG3	1.96	0.47
1:B:549:VAL:HG22	1:B:561:LEU:HD21	1.96	0.47
1:A:560:LYS:HA	1:A:563:SER:OG	2.15	0.47
1:B:560:LYS:HA	1:B:563:SER:OG	2.15	0.47
1:A:549:VAL:HG22	1:A:561:LEU:HD21	1.96	0.47
1:A:15:TYR:HE2	1:A:50:MET:HA	1.80	0.47
1:A:529:ILE:HD12	1:A:583:VAL:HG21	1.96	0.47
1:B:303:LYS:HZ1	1:B:323:VAL:CG1	2.26	0.47
1:A:539:LEU:O	1:A:541:LEU:HD12	2.15	0.47
1:A:710:GLU:O	1:A:714:MET:HG2	2.15	0.47
1:B:227:LEU:O	1:B:250:LEU:HA	2.14	0.47
1:A:28:VAL:HG21	1:A:98:PRO:HB2	1.97	0.46
1:B:15:TYR:O	1:B:47:PRO:HA	2.16	0.46
1:B:230:ARG:HB3	1:B:268:LEU:HD21	1.96	0.46
1:B:529:ILE:HD12	1:B:583:VAL:HG21	1.97	0.46
1:B:710:GLU:O	1:B:714:MET:HG2	2.15	0.46
1:B:342:GLU:OE2	1:B:344:GLU:HB2	2.15	0.46
1:B:537:LEU:HD11	1:B:591:PHE:HE2	1.81	0.46
1:B:88:LEU:HD11	1:B:106:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:OE2	1:A:344:GLU:HB2	2.15	0.46
1:B:539:LEU:O	1:B:541:LEU:HD12	2.15	0.46
1:A:37:ARG:O	1:A:37:ARG:HG2	2.15	0.46
1:A:537:LEU:HD11	1:A:591:PHE:HE2	1.81	0.46
1:A:714:MET:SD	1:A:714:MET:N	2.89	0.46
1:B:303:LYS:NZ	1:B:323:VAL:HG13	2.30	0.46
1:B:333:LEU:HD22	1:B:377:ARG:CZ	2.45	0.46
1:A:729:ARG:CZ	1:A:729:ARG:HB3	2.45	0.46
1:A:759:LEU:HA	1:A:762:VAL:HG22	1.98	0.46
1:B:15:TYR:HE2	1:B:50:MET:HA	1.80	0.46
1:B:28:VAL:HG21	1:B:98:PRO:HB2	1.97	0.46
1:A:303:LYS:HZ3	1:A:323:VAL:HG13	1.81	0.46
1:A:341:GLU:HA	1:A:350:SER:HA	1.97	0.46
1:B:173:ALA:HB2	1:B:199:THR:HG22	1.98	0.45
1:B:411:ASP:OD1	1:B:411:ASP:N	2.49	0.45
1:B:729:ARG:CZ	1:B:729:ARG:HB3	2.45	0.45
1:A:15:TYR:O	1:A:47:PRO:HA	2.16	0.45
1:A:146:GLU:OE1	1:A:205:LEU:HD22	2.16	0.45
1:A:760:GLN:O	1:A:764:LYS:HG3	2.16	0.45
1:B:341:GLU:HA	1:B:350:SER:HA	1.97	0.45
1:A:15:TYR:HD2	1:A:50:MET:CG	2.30	0.45
1:A:806:THR:HA	1:A:809:ASP:OD2	2.17	0.45
1:A:88:LEU:HD11	1:A:106:GLU:HG2	1.98	0.45
1:B:115:VAL:CG2	1:B:121:LEU:HG	2.47	0.45
1:B:357:TRP:HH2	1:B:371:VAL:HG22	1.82	0.45
1:B:806:THR:HA	1:B:809:ASP:OD2	2.17	0.45
1:A:115:VAL:CG2	1:A:121:LEU:HG	2.47	0.45
1:B:633:LEU:CD2	1:B:635:VAL:HG23	2.47	0.45
1:A:303:LYS:NZ	1:A:323:VAL:HG13	2.30	0.45
1:B:714:MET:SD	1:B:714:MET:N	2.89	0.45
1:B:759:LEU:HA	1:B:762:VAL:HG22	1.98	0.45
1:A:333:LEU:HD22	1:A:377:ARG:CZ	2.45	0.44
1:A:600:ARG:HD2	1:A:604:PHE:HD2	1.82	0.44
1:A:633:LEU:CD2	1:A:635:VAL:HG23	2.47	0.44
1:B:600:ARG:HD2	1:B:604:PHE:HD2	1.82	0.44
1:A:10:ILE:HG23	1:A:47:PRO:HB3	1.99	0.44
1:A:52:THR:HB	1:A:96:PRO:HG3	1.99	0.44
1:A:173:ALA:HB2	1:A:199:THR:HG22	1.98	0.44
1:B:52:THR:HB	1:B:96:PRO:HG3	1.99	0.44
1:B:760:GLN:O	1:B:764:LYS:HG3	2.16	0.44
1:A:311:GLN:HB3	1:A:312:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:HIS:NE2	1:A:312:PRO:HB3	2.33	0.44
1:A:357:TRP:HH2	1:A:371:VAL:HG22	1.82	0.44
1:A:698:GLU:HA	1:A:701:LYS:HZ3	1.82	0.44
1:B:15:TYR:HD2	1:B:50:MET:CG	2.30	0.44
1:B:146:GLU:OE1	1:B:205:LEU:HD22	2.16	0.44
1:B:228:HIS:NE2	1:B:312:PRO:HB3	2.33	0.44
1:B:64:PRO:HB2	1:B:84:ARG:NH2	2.33	0.44
1:B:333:LEU:O	1:B:374:VAL:HG22	2.18	0.44
1:B:473:TYR:HE1	1:B:494:GLN:HB2	1.83	0.44
1:B:654:LEU:HD13	1:B:654:LEU:HA	1.83	0.44
1:A:145:PHE:CE2	1:A:151:TYR:HB2	2.52	0.44
1:A:357:TRP:CH2	1:A:371:VAL:HG22	2.52	0.44
1:A:473:TYR:HE1	1:A:494:GLN:HB2	1.83	0.44
1:B:14:HIS:HE1	1:B:49:ARG:HH21	1.66	0.44
1:B:129:PHE:CD2	1:B:156:GLU:HG3	2.53	0.44
1:B:523:PHE:CE2	1:B:545:TRP:HB3	2.52	0.44
1:B:793:LYS:HE3	1:B:793:LYS:HB3	1.87	0.44
1:B:145:PHE:CE2	1:B:151:TYR:HB2	2.52	0.44
1:A:6:PHE:CZ	1:B:9:ARG:NH2	2.86	0.44
1:A:14:HIS:HE1	1:A:49:ARG:HH21	1.66	0.44
1:A:129:PHE:CD2	1:A:156:GLU:HG3	2.53	0.44
1:A:782:SER:HA	1:A:785:GLN:NE2	2.33	0.44
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.79	0.43
1:A:237:ASP:OD1	1:A:241:VAL:N	2.51	0.43
1:B:514:LEU:HD23	1:B:514:LEU:HA	1.87	0.43
1:B:553:LYS:HE3	1:B:553:LYS:HB2	1.75	0.43
1:A:120:ALA:HA	1:A:146:GLU:HA	2.00	0.43
1:A:603:VAL:HG21	1:A:638:VAL:HG21	1.99	0.43
1:B:28:VAL:HG13	1:B:28:VAL:O	2.18	0.43
1:B:115:VAL:HG12	1:B:116:LEU:O	2.18	0.43
1:B:357:TRP:CH2	1:B:371:VAL:HG22	2.52	0.43
1:A:333:LEU:O	1:A:374:VAL:HG22	2.18	0.43
1:A:782:SER:O	1:A:785:GLN:HG2	2.18	0.43
1:B:120:ALA:HA	1:B:146:GLU:HA	2.00	0.43
1:B:311:GLN:HB3	1:B:312:PRO:HD2	2.00	0.43
1:A:523:PHE:CE2	1:A:545:TRP:HB3	2.53	0.43
1:B:10:ILE:HG23	1:B:47:PRO:HB3	1.99	0.43
1:B:387:GLY:HA3	1:B:402:ILE:HA	2.01	0.43
1:A:115:VAL:HG12	1:A:116:LEU:O	2.18	0.43
1:A:333:LEU:HD13	1:A:377:ARG:NH2	2.34	0.43
1:A:662:ILE:O	1:A:666:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:LEU:C	1:B:541:LEU:HD12	2.39	0.43
1:A:64:PRO:HB2	1:A:84:ARG:NH2	2.33	0.43
1:A:123:LEU:HD23	1:A:159:VAL:HG23	2.01	0.43
1:A:471:TYR:OH	1:A:476:LYS:HG3	2.19	0.43
1:B:73:VAL:HG11	1:B:100:TYR:CD1	2.54	0.43
1:B:116:LEU:HB3	1:B:117:PRO:HD2	2.01	0.43
1:B:453:ASN:HB3	1:B:456:ARG:HG2	2.01	0.43
1:A:114:VAL:HG13	1:A:114:VAL:O	2.19	0.43
1:A:116:LEU:HB3	1:A:117:PRO:HD2	2.01	0.43
1:A:73:VAL:HG11	1:A:100:TYR:CE1	2.53	0.43
1:A:556:GLN:O	1:A:560:LYS:HG3	2.19	0.43
1:A:587:THR:OG1	1:A:588:PHE:N	2.52	0.43
1:B:237:ASP:OD1	1:B:241:VAL:N	2.51	0.43
1:B:556:GLN:O	1:B:560:LYS:HG3	2.19	0.43
1:B:662:ILE:O	1:B:666:THR:HG23	2.18	0.43
1:A:28:VAL:HG13	1:A:28:VAL:O	2.18	0.43
1:A:680:LEU:HD23	1:A:680:LEU:HA	1.73	0.42
1:B:471:TYR:OH	1:B:476:LYS:HG3	2.19	0.42
1:B:506:LYS:HZ2	1:B:523:PHE:HB2	1.82	0.42
1:B:782:SER:O	1:B:785:GLN:HG2	2.19	0.42
1:A:88:LEU:H	1:A:155:LYS:HD2	1.84	0.42
1:B:603:VAL:HG21	1:B:638:VAL:HG21	1.99	0.42
1:A:9:ARG:NH2	1:B:6:PHE:CZ	2.87	0.42
1:A:14:HIS:HB3	1:A:47:PRO:HB3	2.01	0.42
1:A:387:GLY:HA3	1:A:402:ILE:HA	2.01	0.42
1:A:539:LEU:C	1:A:541:LEU:HD12	2.39	0.42
1:B:73:VAL:HG11	1:B:100:TYR:CE1	2.53	0.42
1:B:589:ASP:OD1	1:B:589:ASP:N	2.53	0.42
1:B:680:LEU:HD23	1:B:680:LEU:HA	1.73	0.42
1:B:782:SER:HA	1:B:785:GLN:NE2	2.33	0.42
1:A:285:LEU:N	1:A:315:GLN:O	2.52	0.42
1:B:344:GLU:HB3	1:B:349:VAL:HG23	2.01	0.42
1:A:61:VAL:HG22	1:A:105:LEU:HD12	2.01	0.42
1:A:73:VAL:HG11	1:A:100:TYR:CD1	2.54	0.42
1:A:627:VAL:HG22	1:A:634:VAL:CG1	2.46	0.42
1:B:114:VAL:O	1:B:114:VAL:HG13	2.19	0.42
1:B:333:LEU:HD13	1:B:377:ARG:NH2	2.34	0.42
1:B:587:THR:OG1	1:B:588:PHE:N	2.52	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.86	0.42
1:B:344:GLU:HB3	1:B:349:VAL:CG2	2.50	0.42
1:A:18:VAL:HG11	1:A:35:TYR:HE2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:O	1:A:103:GLU:HG2	2.20	0.42
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.84	0.42
1:A:344:GLU:HB3	1:A:349:VAL:HG23	2.01	0.42
1:B:123:LEU:HD23	1:B:159:VAL:HG23	2.01	0.42
1:A:377:ARG:HB3	1:A:407:MET:SD	2.60	0.42
1:A:539:LEU:CB	1:A:541:LEU:HD11	2.31	0.42
1:B:377:ARG:HB3	1:B:407:MET:SD	2.60	0.42
1:B:61:VAL:HG22	1:B:105:LEU:HD12	2.01	0.41
1:B:627:VAL:HG22	1:B:634:VAL:CG1	2.45	0.41
1:A:453:ASN:HB3	1:A:456:ARG:HG2	2.01	0.41
1:B:539:LEU:CB	1:B:541:LEU:HD11	2.31	0.41
1:A:589:ASP:OD1	1:A:589:ASP:N	2.52	0.41
1:B:14:HIS:HB3	1:B:47:PRO:HB3	2.01	0.41
1:B:303:LYS:HZ3	1:B:323:VAL:CG1	2.32	0.41
1:B:18:VAL:HG11	1:B:35:TYR:HE2	1.83	0.41
1:A:283:VAL:HG11	1:A:299:LYS:HD3	2.01	0.41
1:A:344:GLU:HB3	1:A:349:VAL:CG2	2.50	0.41
1:B:63:ASN:O	1:B:103:GLU:HG2	2.20	0.41
1:A:175:ARG:HA	1:A:197:LEU:HD23	2.03	0.41
1:A:176:LEU:HD11	1:A:204:TYR:HE2	1.85	0.41
1:A:330:GLN:O	1:A:360:ARG:HG3	2.20	0.41
1:B:408:LEU:HD11	1:B:414:LEU:HG	2.03	0.41
1:A:506:LYS:HZ1	1:A:523:PHE:HB2	1.83	0.41
1:B:330:GLN:O	1:B:360:ARG:HG3	2.21	0.41
1:A:229:LEU:HD12	1:A:249:TRP:HE1	1.86	0.41
1:A:408:LEU:HD11	1:A:414:LEU:HG	2.03	0.41
1:B:65:VAL:HG13	1:B:103:GLU:OE2	2.21	0.41
1:B:283:VAL:HG11	1:B:299:LYS:HD3	2.01	0.41
1:B:285:LEU:N	1:B:315:GLN:O	2.52	0.41
1:A:9:ARG:HG2	1:A:34:THR:HB	2.03	0.41
1:B:88:LEU:H	1:B:155:LYS:HD2	1.84	0.41
1:A:154:ARG:NE	1:A:156:GLU:OE2	2.48	0.40
1:A:411:ASP:OD1	1:A:411:ASP:N	2.49	0.40
1:A:25:VAL:HG12	1:A:80:GLN:HG2	2.03	0.40
1:B:9:ARG:HG2	1:B:34:THR:HB	2.02	0.40
1:A:53:VAL:HB	1:A:93:ALA:HA	2.03	0.40
1:A:121:LEU:O	1:A:144:LEU:HA	2.22	0.40
1:A:384:GLU:O	1:A:385:ASN:OD1	2.39	0.40
1:B:18:VAL:HA	1:B:43:VAL:HA	2.04	0.40
1:B:75:PHE:HA	1:B:81:VAL:HA	2.04	0.40
1:B:794:LYS:HE2	1:B:794:LYS:HB3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:HG13	1:A:103:GLU:OE2	2.21	0.40
1:A:473:TYR:CE1	1:A:494:GLN:HB2	2.57	0.40
1:B:217:ASP:OD1	1:B:217:ASP:N	2.54	0.40
1:B:395:THR:HG21	1:B:397:LYS:HE2	2.04	0.40
1:B:591:PHE:O	1:B:595:SER:N	2.55	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	769/893 (86%)	712 (93%)	57 (7%)	0	100	100
1	B	769/893 (86%)	712 (93%)	57 (7%)	0	100	100
All	All	1538/1786 (86%)	1424 (93%)	114 (7%)	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	663/755 (88%)	662 (100%)	1 (0%)	92	95
1	B	663/755 (88%)	662 (100%)	1 (0%)	92	95
All	All	1326/1510 (88%)	1324 (100%)	2 (0%)	91	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	PHE
1	B	523	PHE

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

Mol	Chain	Res	Type
1	A	254	GLN
1	B	254	GLN

### 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.

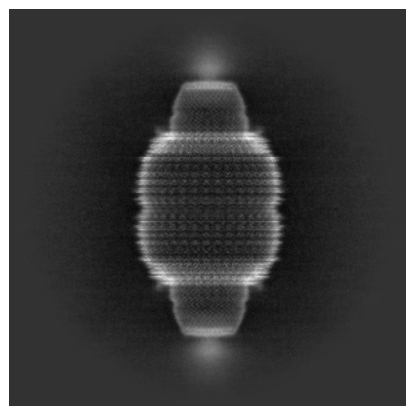
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44953. These allow visual inspection of the internal detail of the map and identification of artifacts.

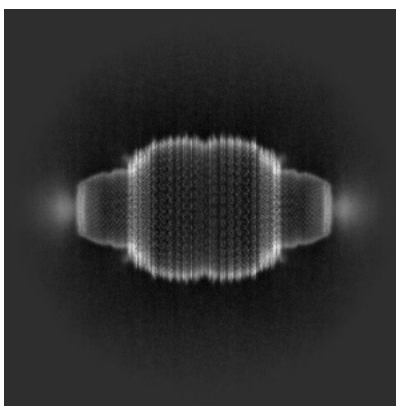
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

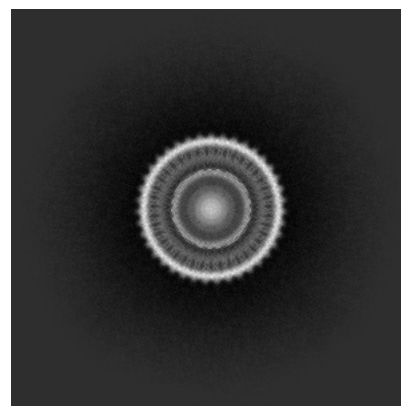
#### 6.1.1 Primary map



X

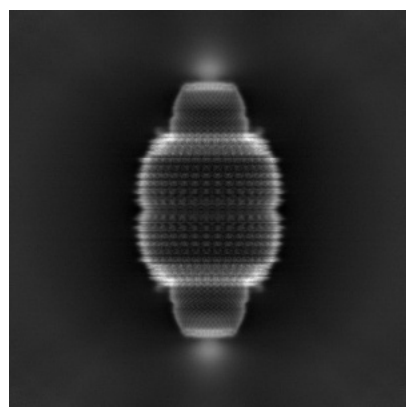


Y

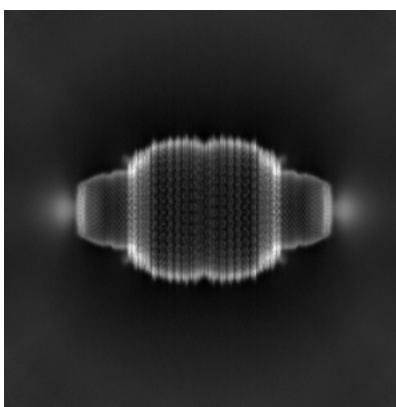


Z

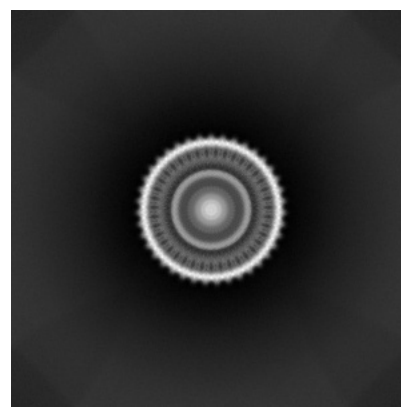
#### 6.1.2 Raw map



X



Y

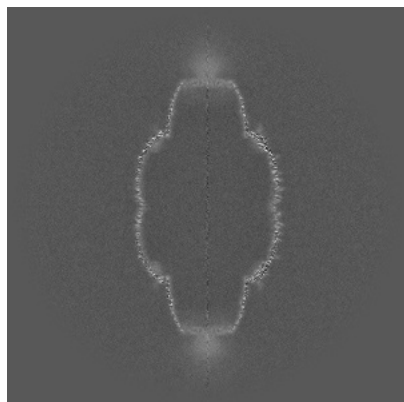


Z

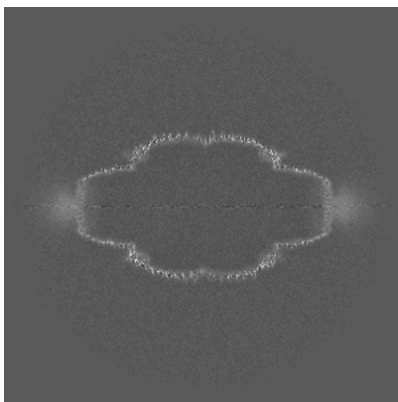
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

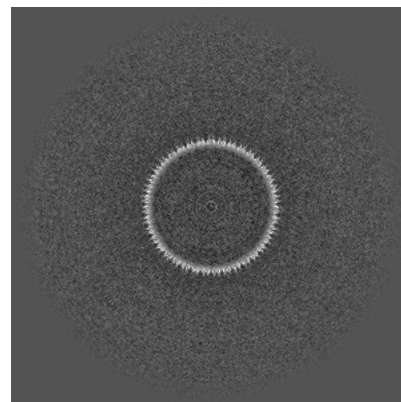
### 6.2.1 Primary map



X Index: 400

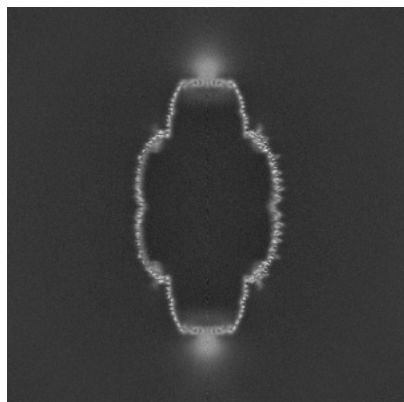


Y Index: 400

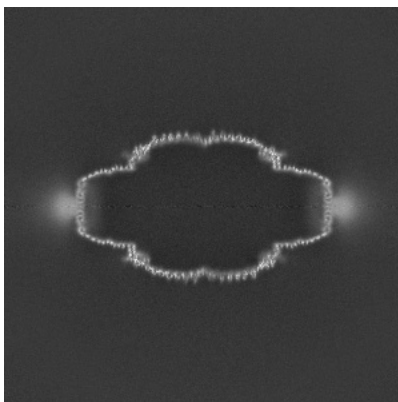


Z Index: 400

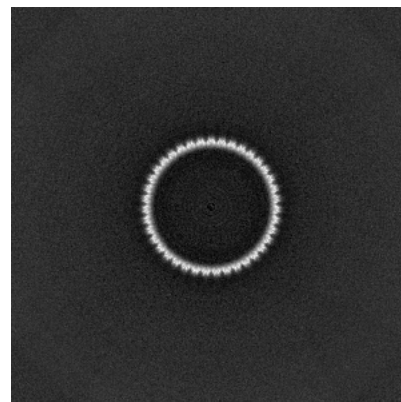
### 6.2.2 Raw map



X Index: 400



Y Index: 400



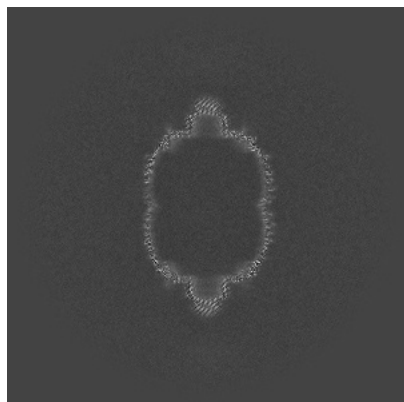
Z Index: 400

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

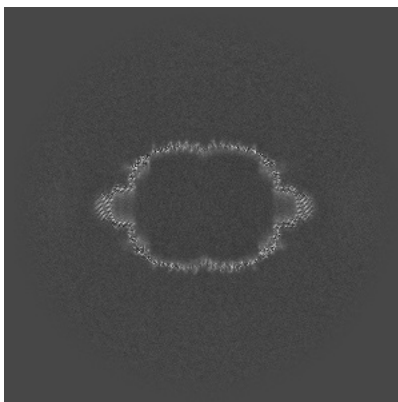


## 6.3 Largest variance slices [i](#)

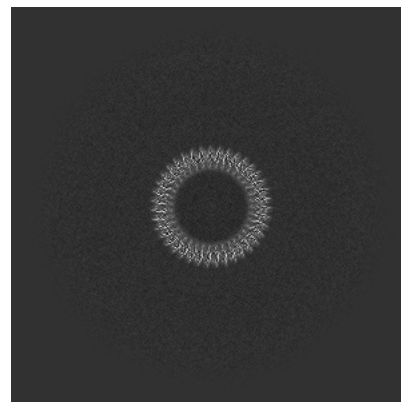
### 6.3.1 Primary map



X Index: 470

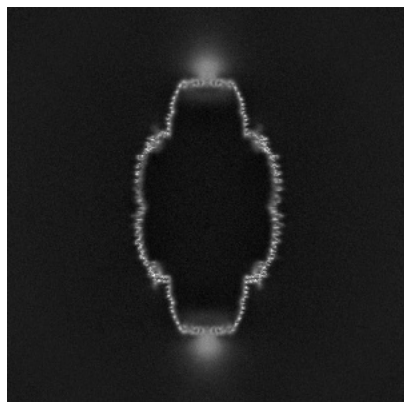


Y Index: 330

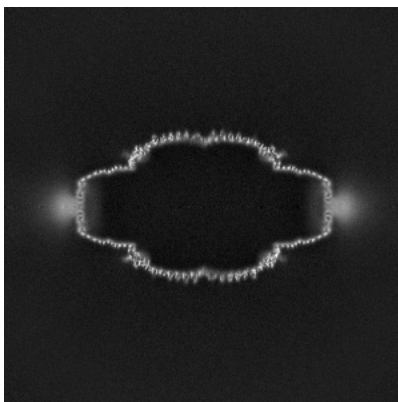


Z Index: 539

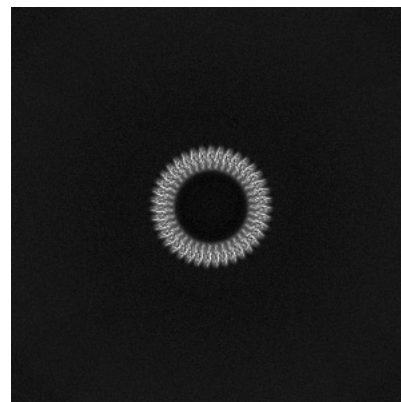
### 6.3.2 Raw map



X Index: 404



Y Index: 398

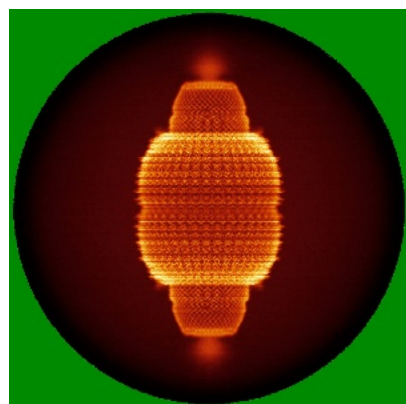


Z Index: 539

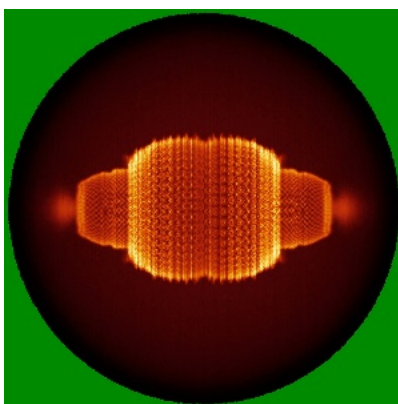
The images above show the largest variance slices of the map in three orthogonal directions.

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

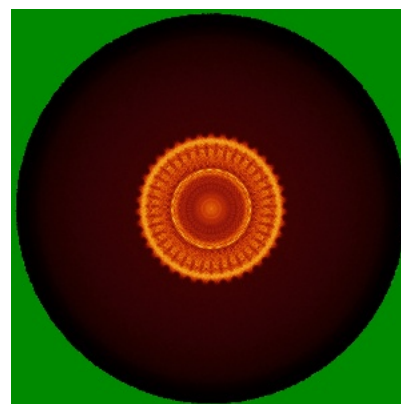
### 6.4.1 Primary map



X

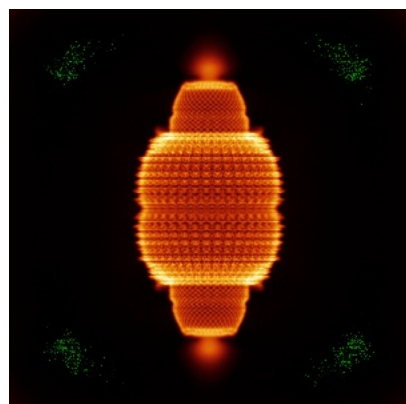


Y

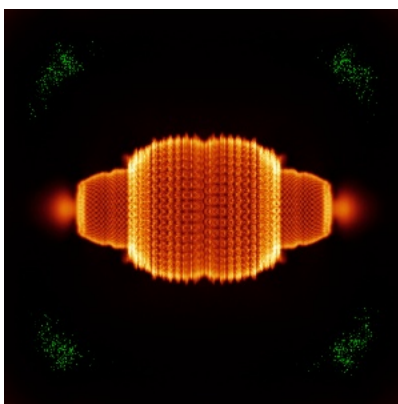


Z

### 6.4.2 Raw map



X



Y



Z

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



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

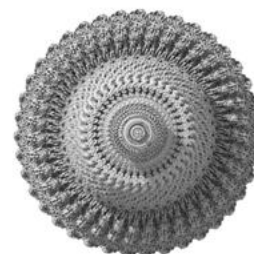
### 6.5.1 Primary map



X



Y



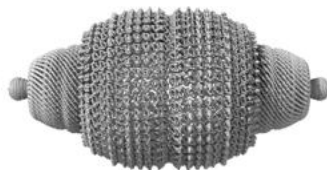
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

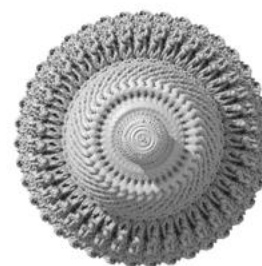
### 6.5.2 Raw map



X



Y



Z

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

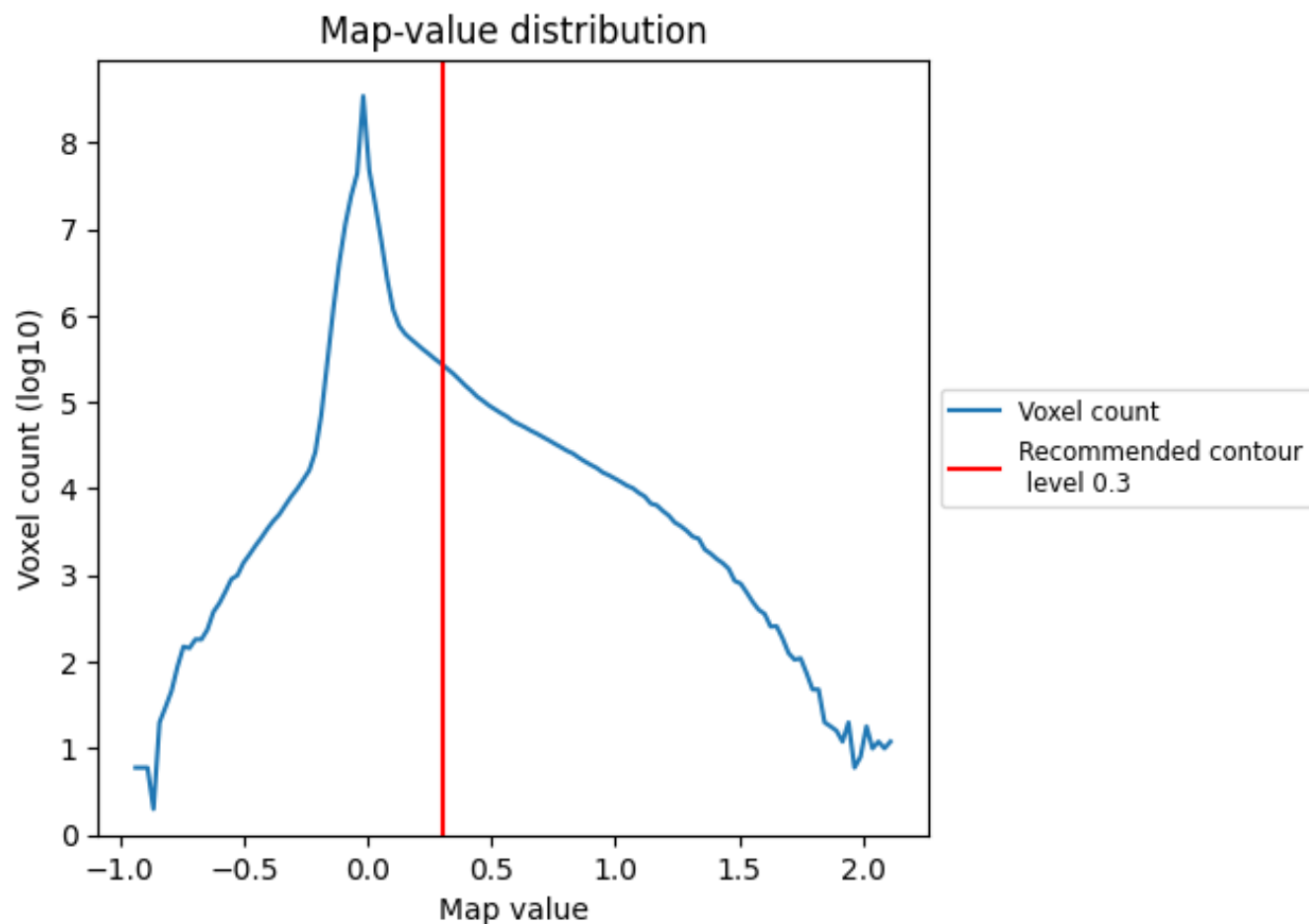
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

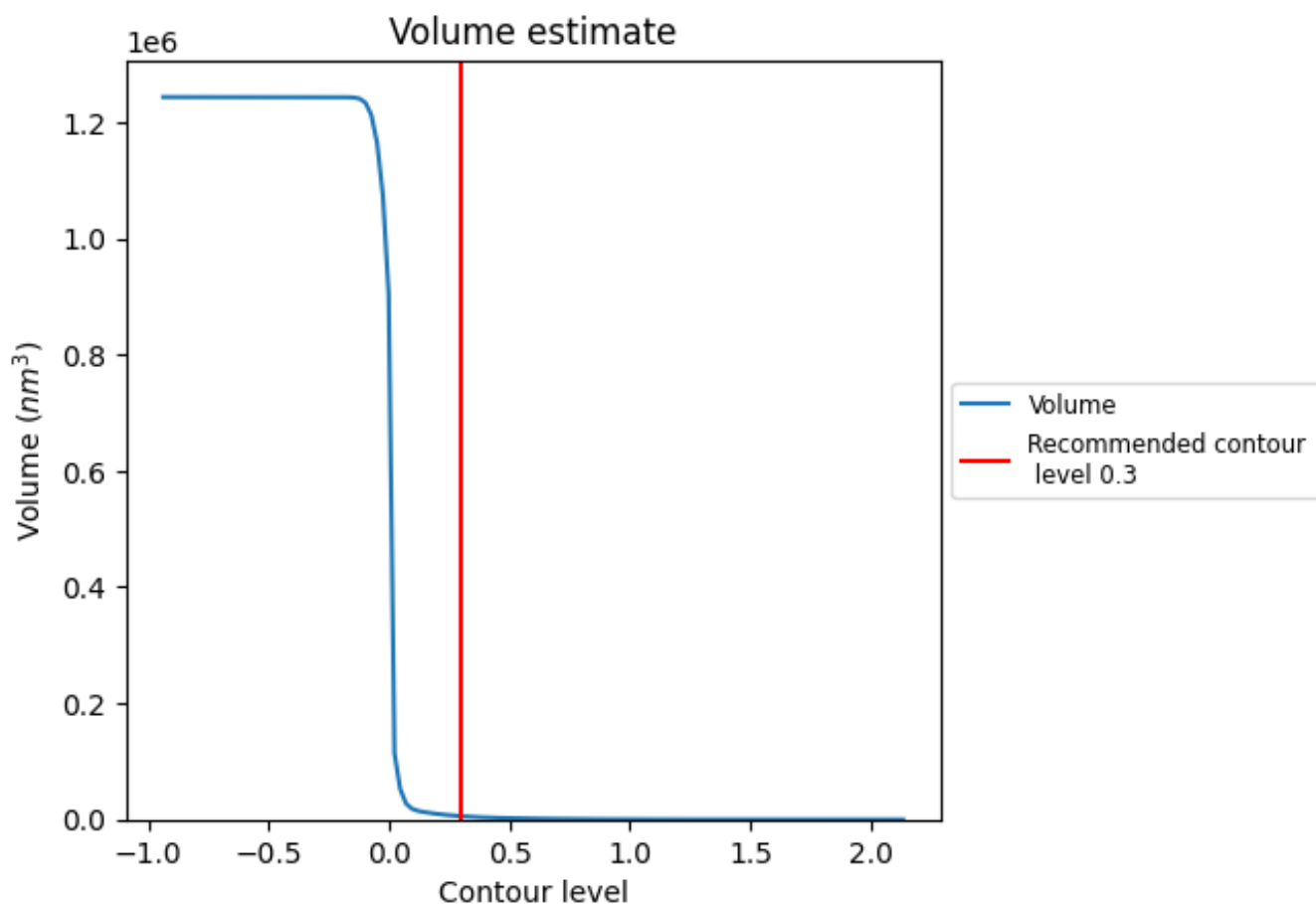
This section contains the results of statistical analysis of the map.

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



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

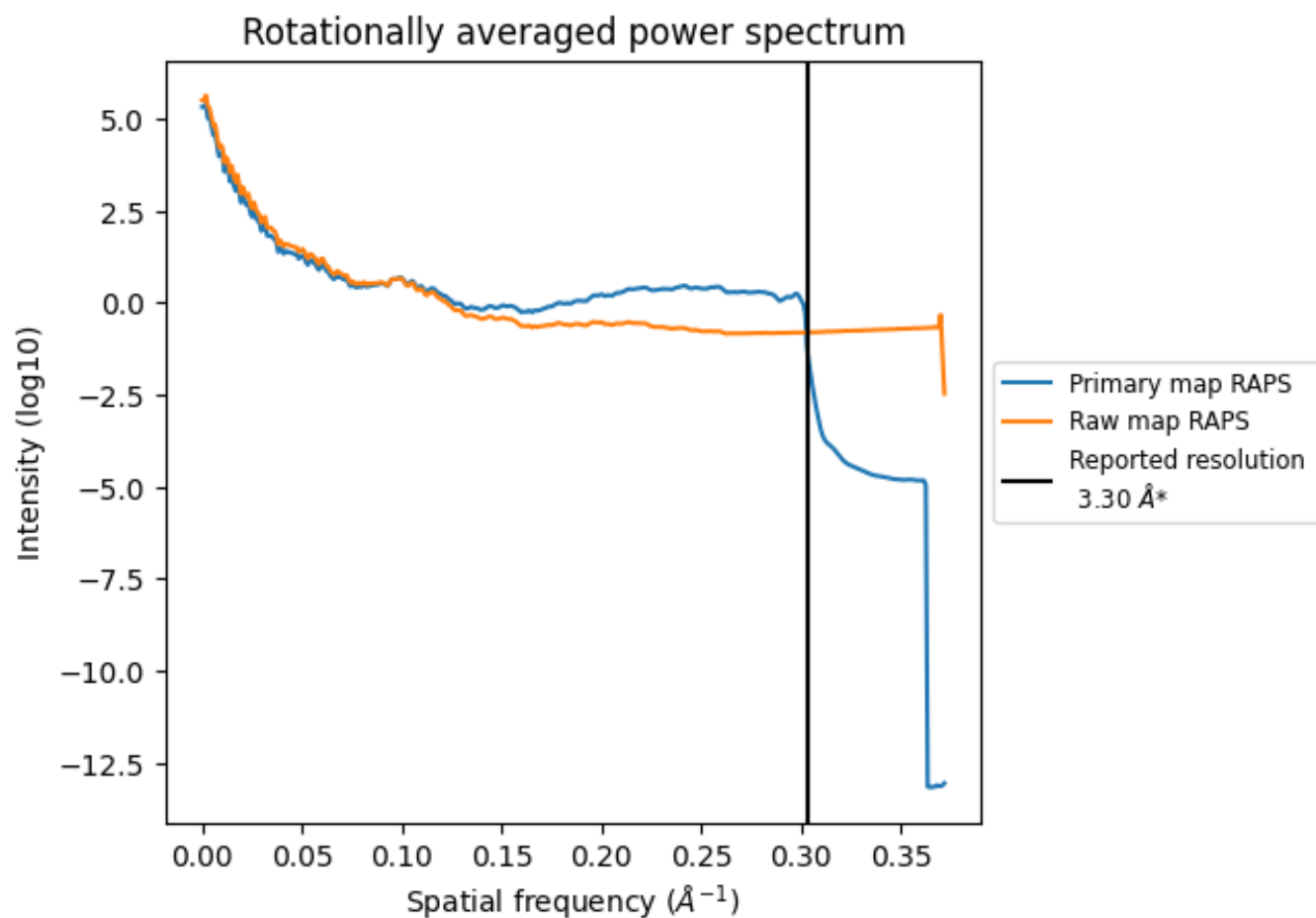
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5785 nm<sup>3</sup>; this corresponds to an approximate mass of 5225 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 ⓘ

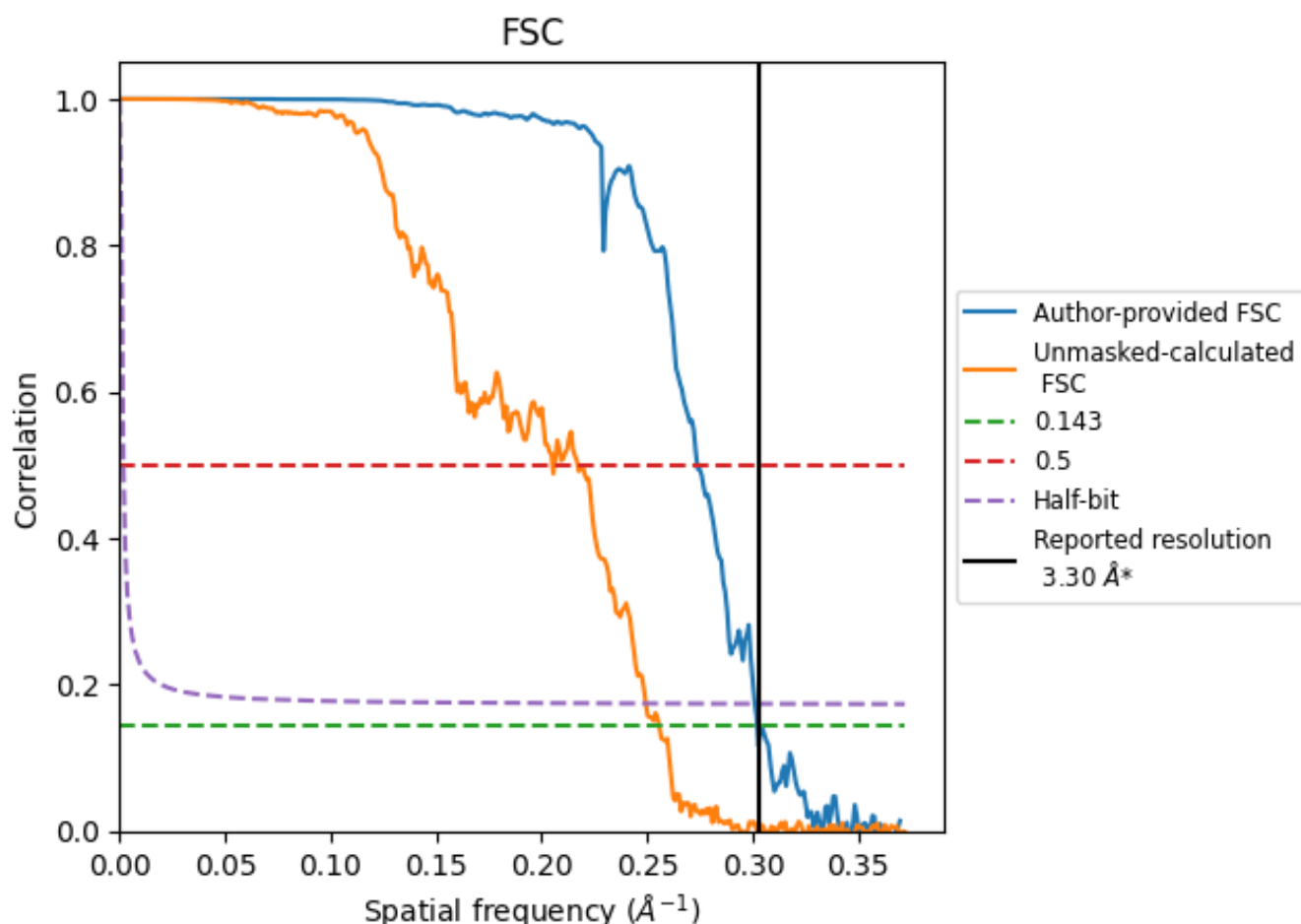


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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	3.31	3.65	3.32
Unmasked-calculated*	3.91	4.88	4.01

\*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 3.91 differs from the reported value 3.3 by more than 10 %

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

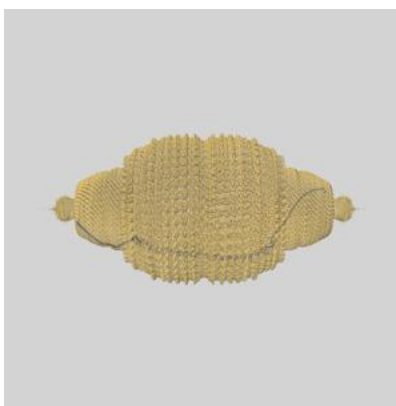
This section contains information regarding the fit between EMDB map EMD-44953 and PDB model 9BW5. Per-residue inclusion information can be found in section [3](#) on page [4](#).

### 9.1 Map-model overlays

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



X



Y

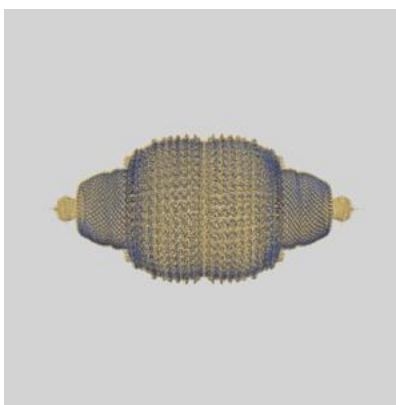


Z

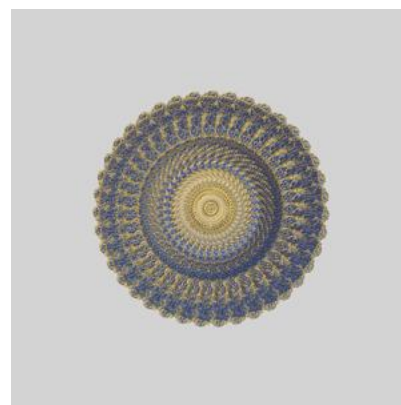
#### 9.1.2 Map-model assembly overlay [i](#)



X



Y



Z

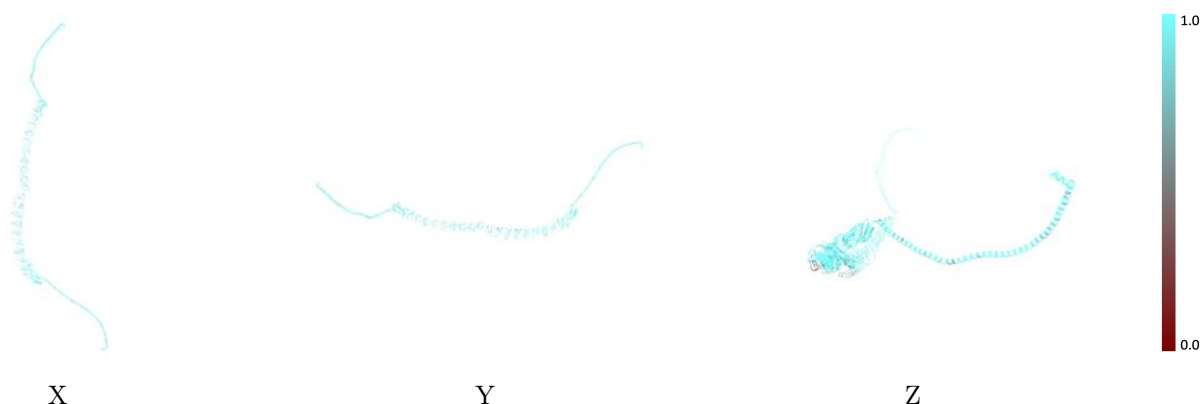
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

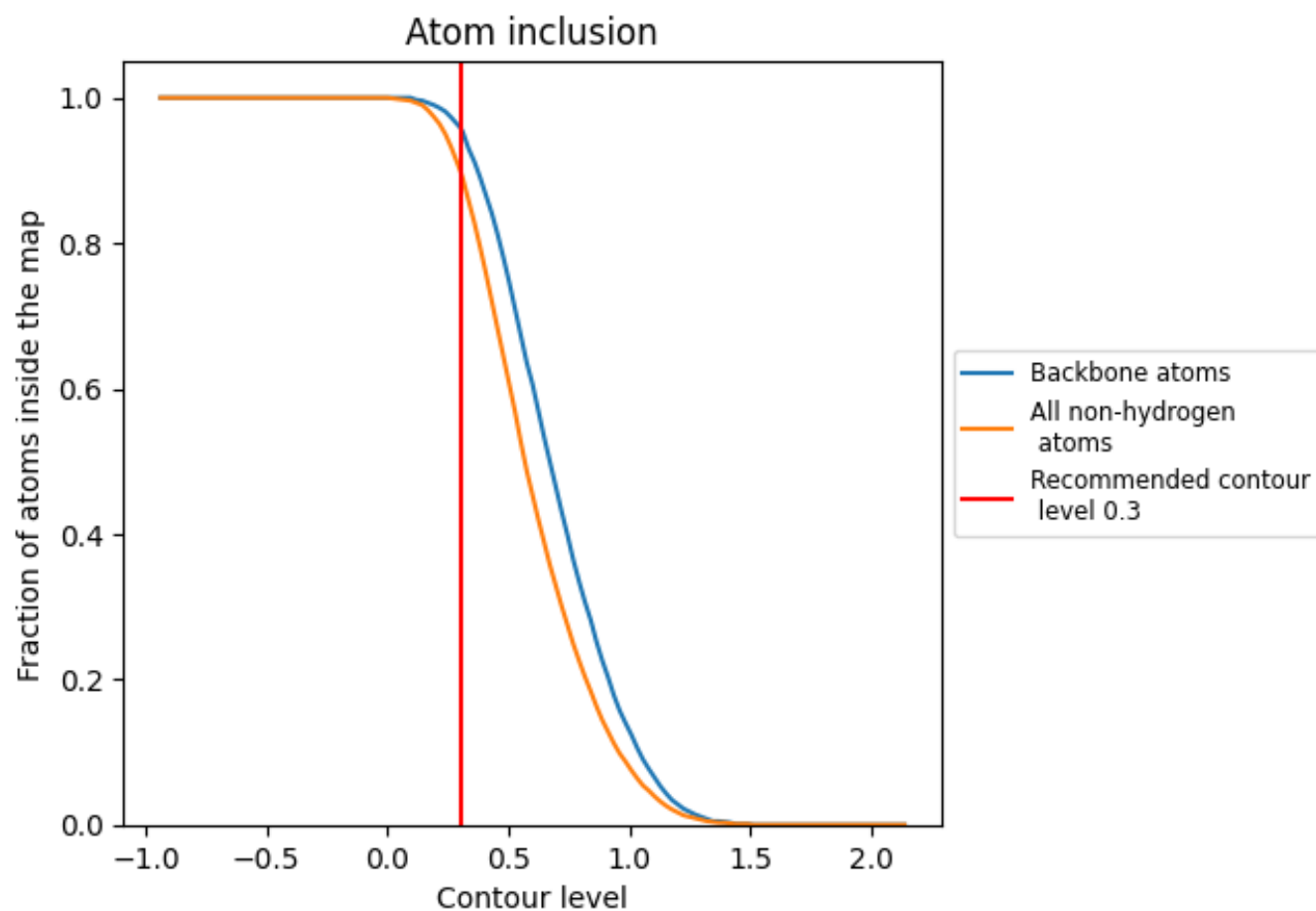
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.3).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9000	<div></div> 0.4600
A	<div></div> 0.9010	<div></div> 0.4600
B	<div></div> 0.8980	<div></div> 0.4590

