



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:30 AM UTC

PDB ID : 7QJ0 / pdb_00007qj0
EMDB ID : EMD-14005
Title : Structure of recombinant human gamma-Tubulin Ring Complex 6-spoked assembly intermediate (spokes 7-12)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 5.32 Å (reported)
Based on initial models : 6V6S, 6X0U, 6L81, 7AS4

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

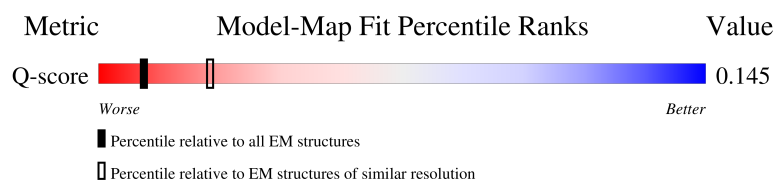
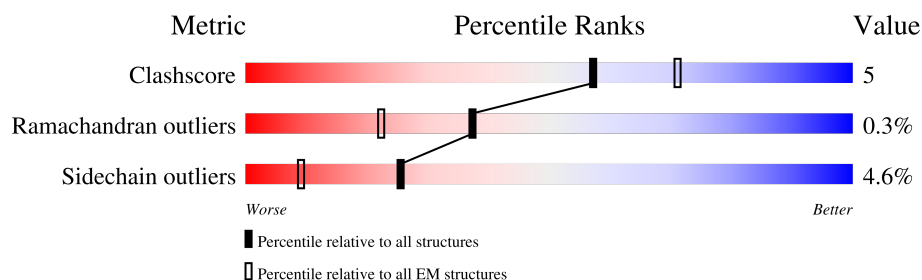
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 5.32 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	506 (4.82 - 5.82)

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 ≥ 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	82	39% 52% 21% 6% 21%
1	m	82	56% 17% 6% 21%
2	H	907	60% 6% 35%
2	a	907	7% 11% 87%

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Mol	Chain	Length	Quality of chain
3	J	1024	
3	I	1024	
4	G	902	
5	I	667	
5	K	667	
6	L	1819	
7	U	451	
7	V	451	
7	W	451	
7	X	451	
7	Y	451	
7	Z	451	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50927 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 Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
1	b	65	Total	C	N	O	S	0	0
			484	299	85	96	4		

- Molecule 2 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
2	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		

- Molecule 3 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	l	108	Total	C	N	O	S	0	0
			875	556	151	167	1		
3	J	534	Total	C	N	O	S	0	0
			4429	2893	737	776	23		

- Molecule 4 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	636	Total	C	N	O	S	0	0
			5186	3342	871	940	33		

- Molecule 5 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	521	Total	C	N	O	S	0	0
			4225	2737	720	750	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	562	Total	C	N	O	S	0	0
			4579	2964	781	816	18		

- Molecule 6 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	566	Total	C	N	O	S	0	0
			4587	3000	773	789	25		

- Molecule 7 is a protein called Tubulin gamma-1 chain.

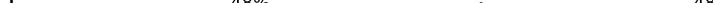
Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	V	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	W	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	X	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	Y	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	Z	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		

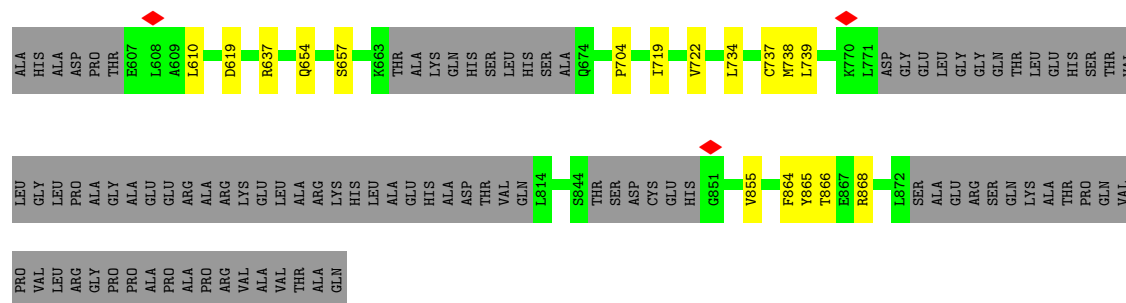
[illegible]

- Molecule 2: Gamma-tubulin complex component 3

Chain H:

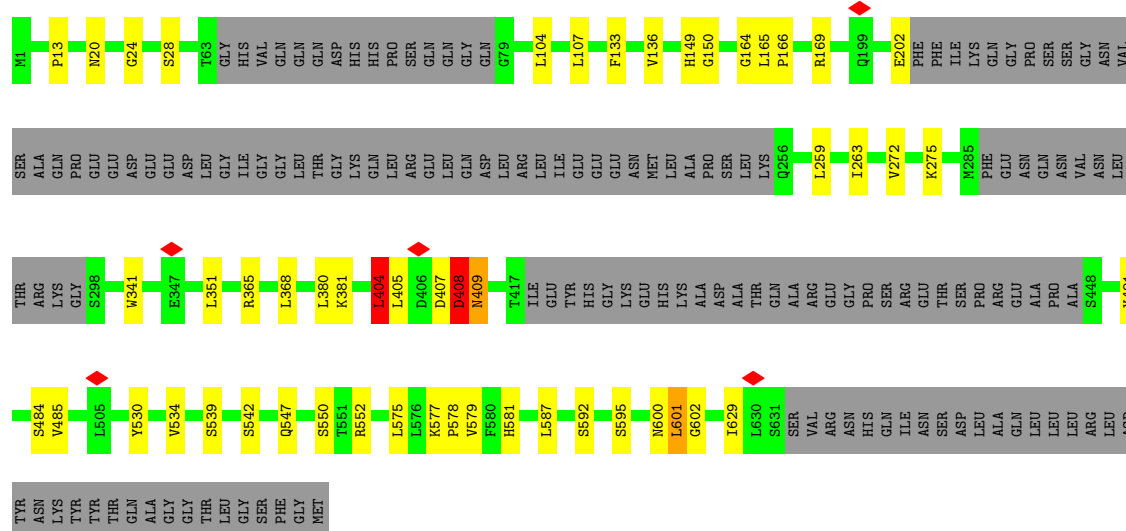
Met	D645	F447	GLY	LEU	ALA	GLU
	D645	V448	THR	PRO	LEU	ALA
	V651		MET	GLY	ILE	THR
	E655	V454	GLU	GLN	ARG	PRO
		K455	ASP	ASN	ASP	GLN
				GLN	ARG	GLN
		R467	E278	ASN	HIS	LYS
			GLY	ALA	SER	SER
			LYS	PRO	THR	ALA
		D478	ALA	GLY	PRO	ASN
Cys	K682		ASN	VAL	TYR	VAL
	C686	K482	LEU	GLY	ALA	LEU
	N687	V483	SER	ASP	TYR	LEU
		L494		CYS	ALA	GLN
	H702		R295	LEU	ARG	ASN
		G487	K286	ARG	PRO	LEU
			L287	GLN	THR	CYS
	H705			GLN	THR	CYS
		I490	A326	GLN	LEU	ARG
		Y720		LEU	LEU	ILE
Gln	F724	L493	GLY	GLY	PRO	LYS
			LEU	SER	LEU	ILE
	Q781		GLU	ARG	SER	GLY
		K505	ASP	LEU	TYR	ARG
	E784		ASP	ALA	GLN	SER
			GLN	TRP	ASP	GLY
		VAL	GLY	THR	ARG	VAL
		THR	VAL	LEU	SER	ALA
		LYS	ASN	THR	ALA	LYS
		SER	LEU	ALA	GLN	ALA
Thr	R811		GLN	ASN	LYS	GLN
		ARG	GLU	GLU	TRP	GLN
		ILE	GLU	PRO	GLN	SER
		GLY	LEU	SER	ILE	GLN
		GLN	SER	SER	LEU	TYR
		TRP	ASN	GLN	TYR	ALA
		GLY	ALA	ALA	LEU	VAL
		VAL	GLY	THR	ARG	VAL
		THR	THR	SER	ILE	VAL
		ALA	LEU	SER	GLY	GLY
Asn		ALA	PHE	LYS	SER	GLY
				GLY	SER	SER
		T524	W370	VAL	ILE	ASN
		GLU		PRO	SER	ASP
		GLU	D407	SER	SER	PHE
			D408	ALA	ILE	ALA
			P409	VAL	GLY	ARG
				SER	LEU	THR
			R412	ARG	CYS	VAL
				ASN	ALA	GLU
Arg		L592	V415	ASN	SER	ARG
			Y593	MET	LEU	GLU
		Q594	H417	THR	SER	ASP
			L418	ARG	GLY	PHE
		L597	L419	SER	PRO	LEU
			S420	ARG	ALA	VAL
		L601	L421	ARG	PRO	ALA
			V422	GLU	THR	GLU
		V623	V422	GLY	PRO	LYS
			W433	ASP	GLN	ILE
Lys		L626		THR	PHE	LYS
				GLY	ALA	CYS
				THR	LEU	LYS
				GLY	THR	ALA
				THR	LEU	VAL
				GLY	THR	ALA
				THR	LEU	VAL
				GLY	THR	ALA
				THR	LEU	VAL
				GLY	THR	ALA

Chain J: 



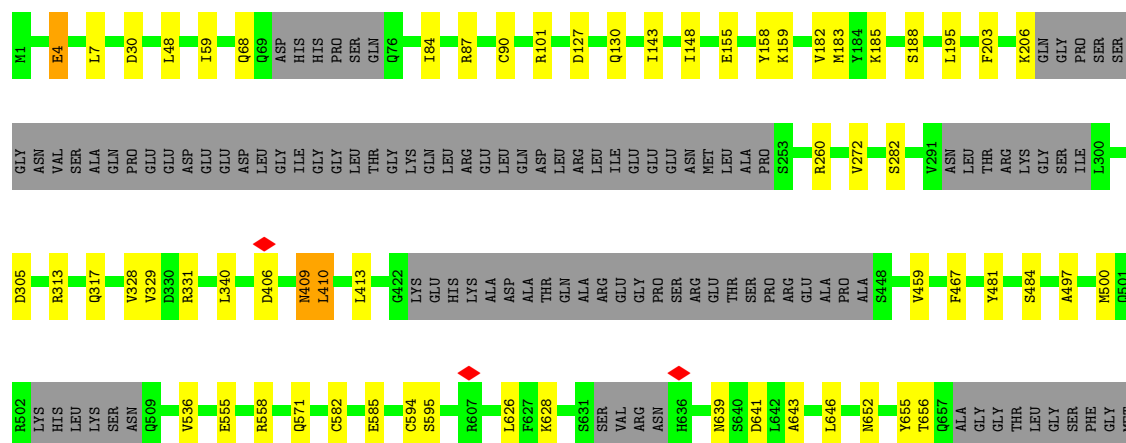
• Molecule 5: Gamma-tubulin complex component 4

Chain I: 70% 7% 22%



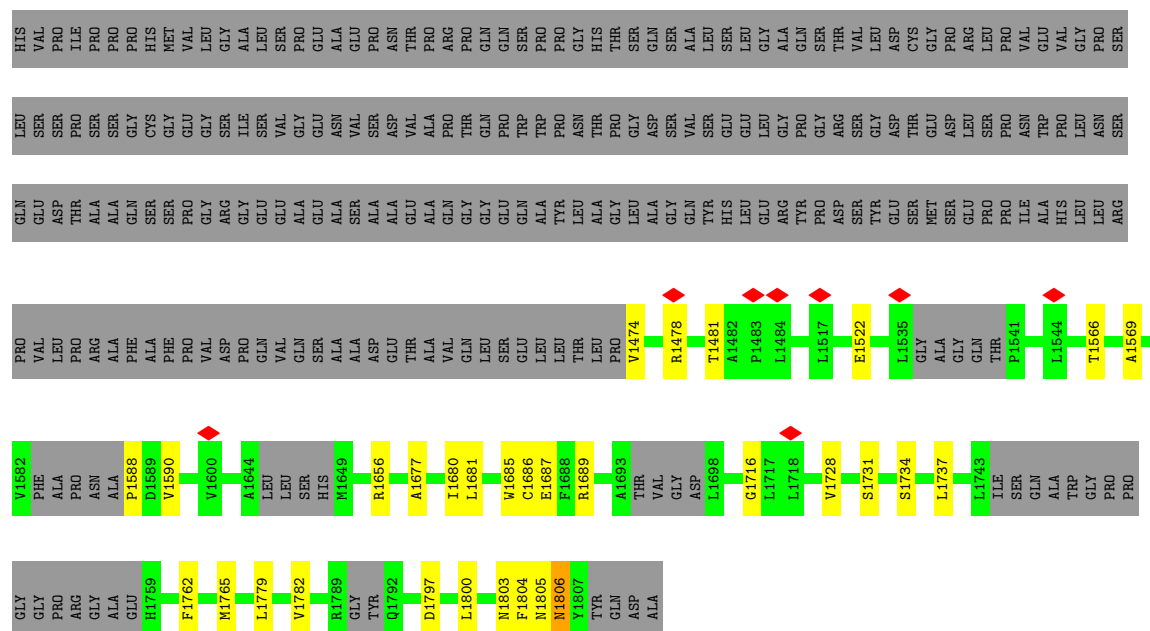
• Molecule 5: Gamma-tubulin complex component 4

Chain K: 75% 9% 16%

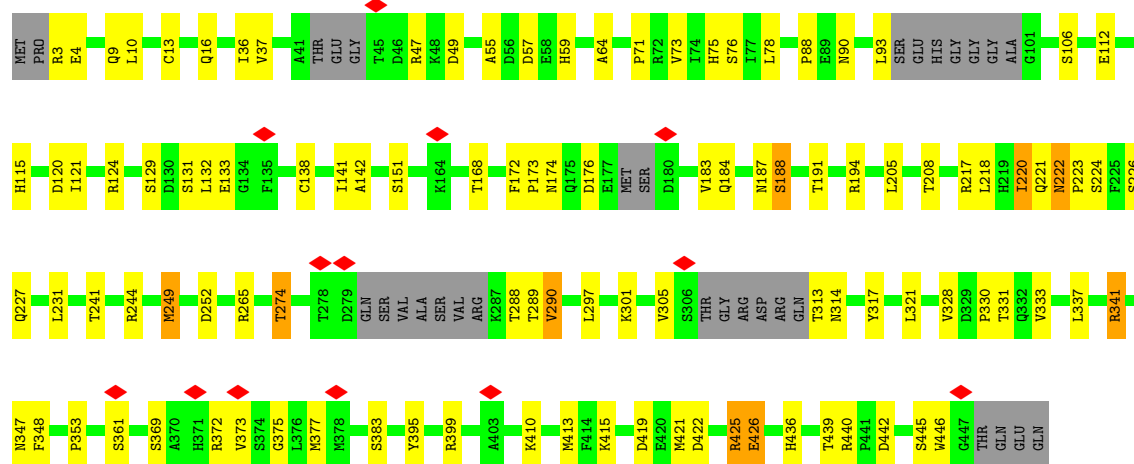


• Molecule 6: Gamma-tubulin complex component 6

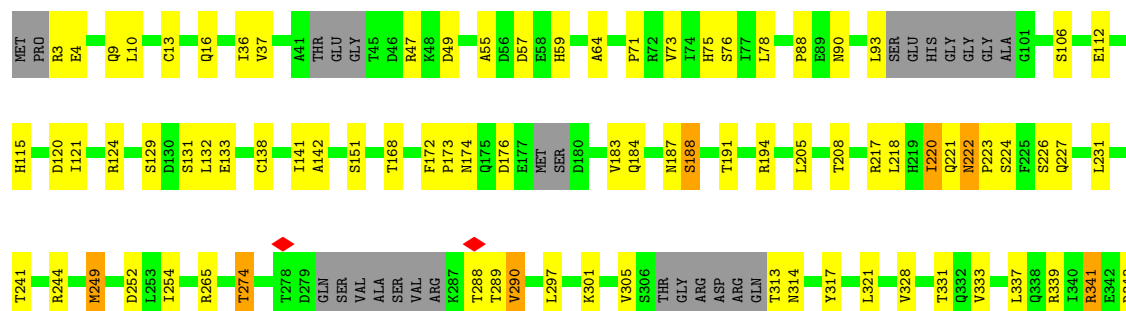


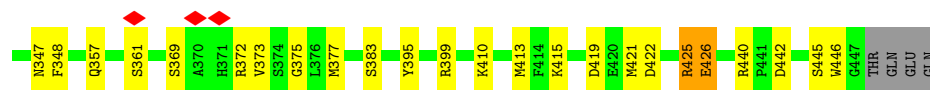


• Molecule 7: Tubulin gamma-1 chain



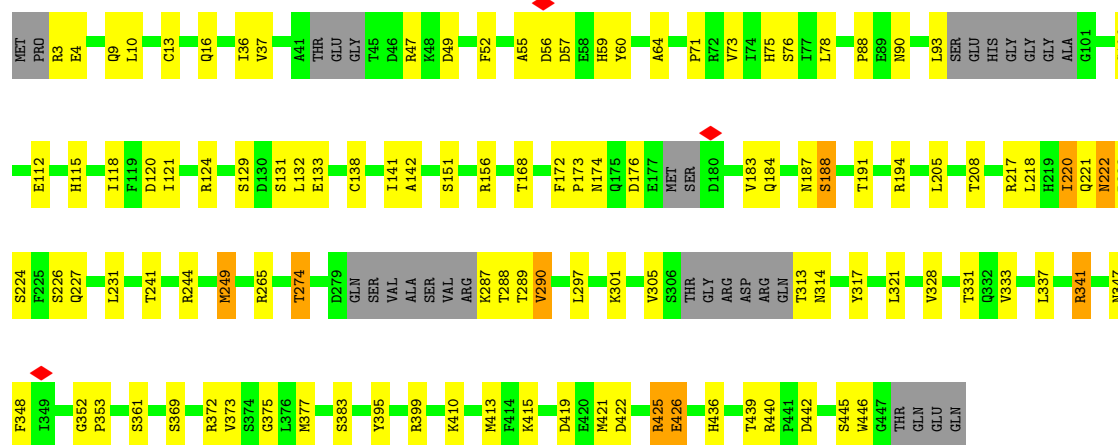
• Molecule 7: Tubulin gamma-1 chain





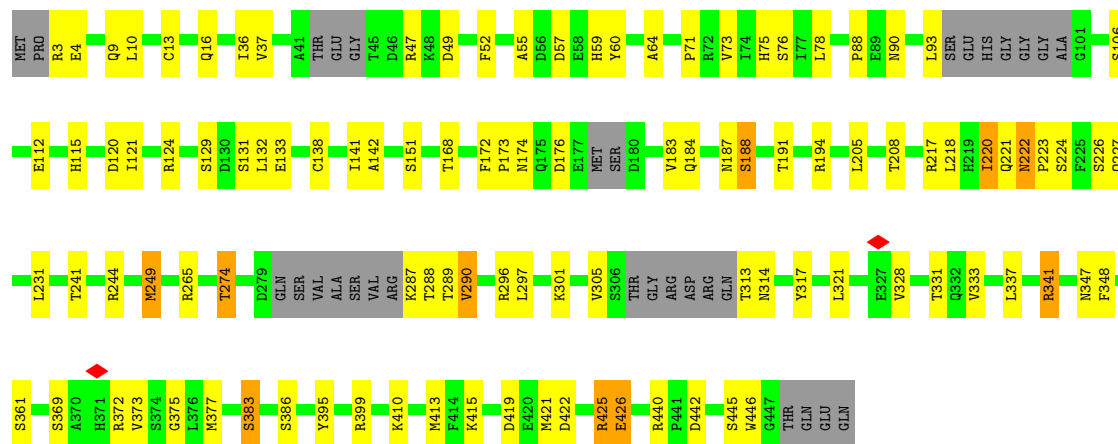
• Molecule 7: Tubulin gamma-1 chain

Chain W: 68% 23% 7%



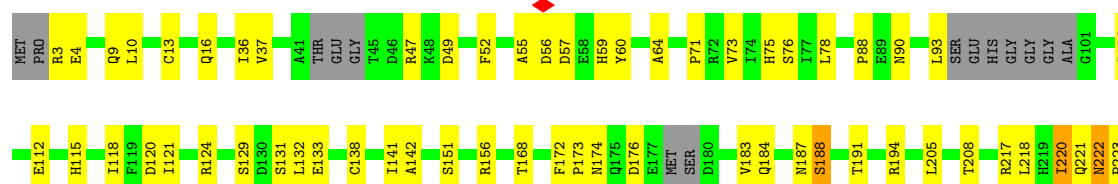
• Molecule 7: Tubulin gamma-1 chain

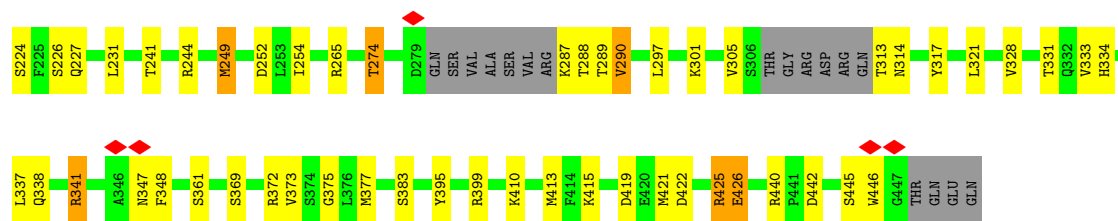
Chain X: 69% 22% 7%



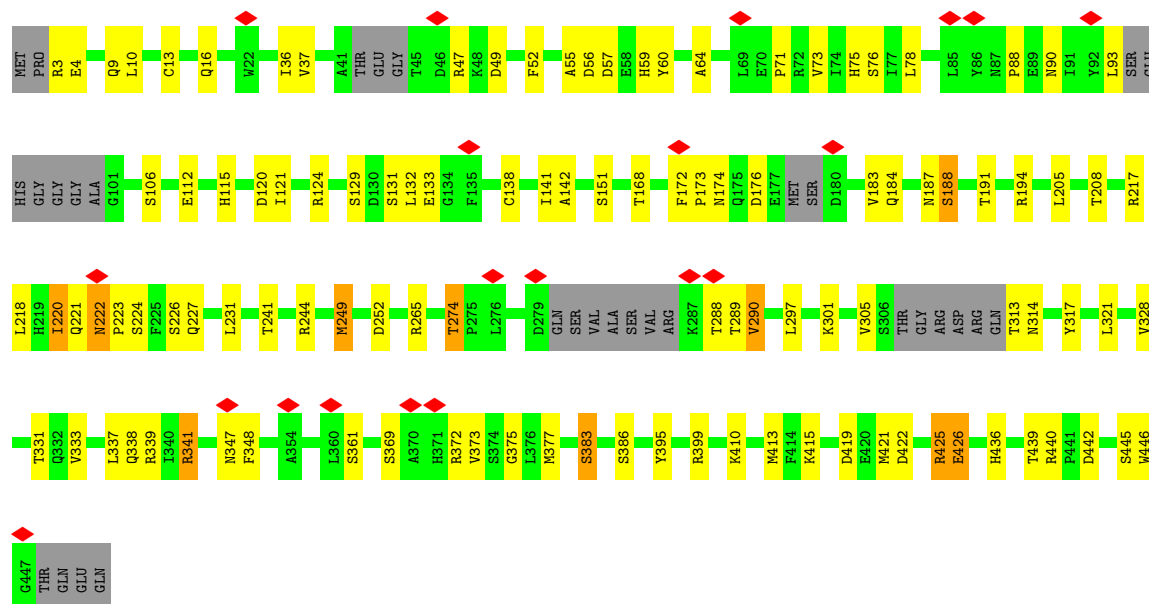
• Molecule 7: Tubulin gamma-1 chain

Chain Y: 68% 23% 7%





• Molecule 7: Tubulin gamma-1 chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	92149	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.255	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0468	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	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	0.32	0/484	0.77	0/653
1	m	0.32	0/484	0.77	0/653
2	H	0.34	0/5009	0.69	2/6761 (0.0%)
2	a	0.27	0/948	0.71	0/1277
3	J	0.34	0/4525	0.77	6/6119 (0.1%)
3	l	0.34	0/894	0.75	2/1209 (0.2%)
4	G	0.31	0/5295	0.71	5/7147 (0.1%)
5	I	0.34	0/4322	0.68	3/5853 (0.1%)
5	K	0.35	1/4683 (0.0%)	0.73	10/6338 (0.2%)
6	L	0.43	4/4697 (0.1%)	0.76	11/6348 (0.2%)
7	U	0.30	0/3441	0.65	1/4661 (0.0%)
7	V	0.30	0/3441	0.65	1/4661 (0.0%)
7	W	0.30	0/3441	0.65	1/4661 (0.0%)
7	X	0.30	0/3441	0.66	1/4661 (0.0%)
7	Y	0.30	0/3441	0.66	1/4661 (0.0%)
7	Z	0.30	0/3441	0.65	1/4661 (0.0%)
All	All	0.33	5/51987 (0.0%)	0.70	45/70324 (0.1%)

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
2	H	0	1
3	J	0	5
4	G	0	3
5	I	0	6
6	L	0	3
All	All	0	18

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	320	PHE	CE2-CZ	12.65	1.76	1.38
6	L	320	PHE	CG-CD1	7.05	1.53	1.38
6	L	320	PHE	N-CA	-6.46	1.38	1.46
5	K	4	GLU	CB-CG	6.00	1.70	1.52
6	L	320	PHE	CD1-CE1	5.50	1.55	1.38

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	4	GLU	CB-CG-CD	12.92	134.57	112.60
5	K	4	GLU	CA-CB-CG	9.38	132.85	114.10
3	l	121	PRO	CA-N-CD	-9.16	99.18	112.00
5	K	4	GLU	N-CA-CB	9.05	126.23	110.39
3	l	130	PRO	CA-N-CD	-8.99	99.41	112.00
3	J	237	HIS	CA-C-N	7.79	136.42	121.54
3	J	237	HIS	C-N-CA	7.79	136.42	121.54
5	K	409	ASN	CA-C-N	7.27	135.43	121.54
5	K	409	ASN	C-N-CA	7.27	135.43	121.54
4	G	580	HIS	CA-C-N	7.23	135.34	121.54
4	G	580	HIS	C-N-CA	7.23	135.34	121.54
5	I	404	LEU	CA-C-N	6.93	134.78	121.54
5	I	404	LEU	C-N-CA	6.93	134.78	121.54
6	L	320	PHE	CD1-CE1-CZ	-6.70	107.94	120.00
5	K	4	GLU	CB-CA-C	-6.47	96.97	110.17
6	L	1804	PHE	N-CA-C	-6.38	96.58	107.23
4	G	414	LEU	N-CA-C	-6.10	104.01	112.30
6	L	321	ASP	CA-CB-CG	-5.94	106.66	112.60
5	I	28	SER	N-CA-C	-5.92	105.63	114.64
6	L	320	PHE	N-CA-C	-5.71	104.52	112.45
3	J	256	LEU	CA-C-N	5.65	132.33	121.54
3	J	256	LEU	C-N-CA	5.65	132.33	121.54
6	L	1805	ASN	CA-C-N	5.42	131.90	121.54
6	L	1805	ASN	C-N-CA	5.42	131.90	121.54
4	G	264	LEU	N-CA-C	5.41	121.75	109.81
6	L	320	PHE	CB-CA-C	5.38	120.28	110.11
6	L	306	HIS	CA-C-N	5.30	131.67	121.54
6	L	306	HIS	C-N-CA	5.30	131.67	121.54
6	L	340	GLN	N-CA-C	5.22	117.01	110.91
5	K	68	GLN	CA-C-N	5.19	131.05	121.70
5	K	68	GLN	C-N-CA	5.19	131.05	121.70
2	H	724	PHE	CA-C-N	5.19	131.45	121.54
2	H	724	PHE	C-N-CA	5.19	131.45	121.54
3	J	714	TYR	N-CA-C	-5.17	107.99	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	203	PHE	CA-C-N	5.16	129.46	122.19
5	K	203	PHE	C-N-CA	5.16	129.46	122.19
6	L	320	PHE	CA-CB-CG	-5.14	108.66	113.80
3	J	238	LEU	N-CA-C	5.14	121.74	110.80
4	G	548	PRO	N-CA-C	5.11	116.94	110.70
7	U	249	MET	CB-CG-SD	5.06	127.89	112.70
7	W	249	MET	CB-CG-SD	5.05	127.86	112.70
7	Z	249	MET	CB-CG-SD	5.05	127.86	112.70
7	V	249	MET	CB-CG-SD	5.05	127.85	112.70
7	X	249	MET	CB-CG-SD	5.04	127.82	112.70
7	Y	249	MET	CB-CG-SD	5.04	127.82	112.70

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	240	GLY	Peptide
4	G	580	HIS	Peptide
4	G	581	ASP	Mainchain
2	H	454	VAL	Peptide
5	I	407	ASP	Peptide
5	I	408	ASP	Mainchain
5	I	409	ASN	Peptide
5	I	600	ASN	Peptide
5	I	601	LEU	Mainchain
5	I	602	GLY	Peptide
3	J	235	SER	Peptide
3	J	236	LEU	Mainchain
3	J	237	HIS	Peptide
3	J	257	TYR	Peptide
3	J	798	GLY	Peptide
6	L	1806	ASN	Peptide
6	L	306	HIS	Peptide
6	L	345	VAL	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	484	0	512	12	0
1	m	484	0	512	7	0
2	H	4907	0	4896	31	0
2	a	933	0	953	10	0
3	J	4429	0	4482	19	0
3	l	875	0	841	15	0
4	G	5186	0	5219	42	0
5	I	4225	0	4259	26	0
5	K	4579	0	4586	39	0
6	L	4587	0	4636	38	0
7	U	3373	0	3325	48	0
7	V	3373	0	3325	46	0
7	W	3373	0	3325	49	0
7	X	3373	0	3325	44	0
7	Y	3373	0	3325	51	0
7	Z	3373	0	3325	50	0
All	All	50927	0	50846	493	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 5.

All (493) 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)
6:L:320:PHE:CZ	6:L:320:PHE:CE2	1.76	1.66
3:l:80:LYS:HE3	3:l:126:TYR:CE2	1.51	1.45
3:l:80:LYS:CE	3:l:126:TYR:CE2	2.26	1.17
3:l:124:SER:O	3:l:126:TYR:HD2	1.41	1.03
3:l:80:LYS:HE3	3:l:126:TYR:CD2	2.04	0.93
3:l:124:SER:O	3:l:126:TYR:CD2	2.22	0.92
3:l:80:LYS:CE	3:l:126:TYR:HE2	1.75	0.92
3:l:80:LYS:NZ	3:l:126:TYR:HE2	1.69	0.90
3:l:118:SER:O	3:l:119:ASP:OD1	1.95	0.85
7:W:56:ASP:HB2	7:X:296:ARG:HG2	1.61	0.82
3:l:80:LYS:HZ1	3:l:126:TYR:HE2	1.26	0.80
4:G:574:LYS:HB2	4:G:619:ASP:HB3	1.72	0.72
6:L:1677:ALA:HA	6:L:1681:LEU:HD12	1.73	0.70
3:J:884:PHE:O	3:J:887:ARG:HB3	1.93	0.69
7:U:13:CYS:HA	7:U:16:GLN:HE21	1.59	0.68
7:V:13:CYS:HA	7:V:16:GLN:HE21	1.59	0.67
7:X:13:CYS:HA	7:X:16:GLN:HE21	1.59	0.67
7:Y:13:CYS:HA	7:Y:16:GLN:HE21	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:364:LEU:H	2:H:367:LEU:H	1.43	0.67
7:W:13:CYS:HA	7:W:16:GLN:HE21	1.59	0.67
3:l:127:VAL:HG12	3:l:127:VAL:O	1.96	0.67
7:Z:13:CYS:HA	7:Z:16:GLN:HE21	1.59	0.66
7:U:121:ILE:HG23	7:U:124:ARG:HH21	1.62	0.65
7:V:121:ILE:HG23	7:V:124:ARG:HH21	1.62	0.65
7:Y:121:ILE:HG23	7:Y:124:ARG:HH21	1.62	0.65
6:L:1797:ASP:O	6:L:1800:LEU:HB3	1.97	0.64
7:X:121:ILE:HG23	7:X:124:ARG:HH21	1.62	0.64
2:H:409:PRO:HA	2:H:412:ARG:HE	1.62	0.64
7:W:121:ILE:HG23	7:W:124:ARG:HH21	1.62	0.64
7:X:55:ALA:HB3	7:X:59:HIS:HB2	1.81	0.63
7:V:55:ALA:HB3	7:V:59:HIS:HB2	1.81	0.63
7:Z:121:ILE:HG23	7:Z:124:ARG:HH21	1.62	0.63
7:Z:55:ALA:HB3	7:Z:59:HIS:HB2	1.81	0.62
5:K:4:GLU:HG2	6:L:320:PHE:CZ	2.34	0.62
7:W:55:ALA:HB3	7:W:59:HIS:HB2	1.81	0.62
1:m:33:ARG:HH12	3:l:127:VAL:H	1.45	0.62
5:K:272:VAL:HG23	5:K:329:VAL:HG11	1.81	0.62
7:U:55:ALA:HB3	7:U:59:HIS:HB2	1.81	0.62
3:J:394:THR:H	3:J:397:ILE:HD12	1.64	0.62
3:J:727:PHE:HE2	3:J:821:TYR:HB3	1.65	0.62
7:Y:55:ALA:HB3	7:Y:59:HIS:HB2	1.81	0.61
6:L:347:VAL:HG12	6:L:348:LYS:HG2	1.81	0.61
4:G:585:GLN:HE22	4:G:739:LEU:HD12	1.66	0.60
7:V:184:GLN:O	7:V:188:SER:OG	2.20	0.60
6:L:1800:LEU:HB2	7:Z:338:GLN:HE22	1.66	0.60
7:W:184:GLN:O	7:W:188:SER:OG	2.20	0.60
6:L:1522:GLU:OE2	7:Z:47:ARG:NH1	2.35	0.60
5:K:206:LYS:HA	5:K:260:ARG:HE	1.65	0.59
7:X:184:GLN:O	7:X:188:SER:OG	2.20	0.59
7:U:184:GLN:O	7:U:188:SER:OG	2.20	0.59
4:G:395:ILE:HD11	4:G:450:ILE:HG23	1.85	0.59
7:Y:184:GLN:O	7:Y:188:SER:OG	2.20	0.59
7:Z:184:GLN:O	7:Z:188:SER:OG	2.20	0.58
5:I:104:LEU:HA	5:I:107:LEU:HD12	1.84	0.57
5:K:646:LEU:HB3	7:Y:341:ARG:HE	1.68	0.57
2:a:100:LEU:HD12	1:b:65:LYS:HE3	1.86	0.57
4:G:448:ASP:OD2	4:G:448:ASP:N	2.36	0.57
5:K:48:LEU:HD21	5:K:130:GLN:HA	1.87	0.57
5:K:555:GLU:OE1	5:K:558:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:313:THR:OG1	7:U:314:ASN:N	2.38	0.57
7:W:313:THR:OG1	7:W:314:ASN:N	2.38	0.57
7:X:297:LEU:HD21	7:X:377:MET:HB3	1.87	0.57
7:X:313:THR:OG1	7:X:314:ASN:N	2.38	0.57
7:V:71:PRO:HG3	7:V:93:LEU:HD22	1.87	0.56
1:b:49:ARG:HH21	6:L:283:TRP:H	1.52	0.56
7:Y:297:LEU:HD21	7:Y:377:MET:HB3	1.87	0.56
7:Z:71:PRO:HG3	7:Z:93:LEU:HD22	1.87	0.56
7:Z:297:LEU:HD21	7:Z:377:MET:HB3	1.87	0.56
7:U:297:LEU:HD21	7:U:377:MET:HB3	1.87	0.56
7:U:71:PRO:HG3	7:U:93:LEU:HD22	1.87	0.56
7:W:71:PRO:HG3	7:W:93:LEU:HD22	1.87	0.56
5:K:497:ALA:HB2	7:Y:254:ILE:HD11	1.87	0.56
7:Y:71:PRO:HG3	7:Y:93:LEU:HD22	1.87	0.56
7:X:71:PRO:HG3	7:X:93:LEU:HD22	1.87	0.56
1:b:40:ASP:OD1	1:b:43:THR:OG1	2.24	0.55
5:I:575:LEU:O	5:I:577:LYS:NZ	2.39	0.55
5:K:410:LEU:HD13	5:K:413:LEU:HD12	1.87	0.55
7:V:297:LEU:HD21	7:V:377:MET:HB3	1.87	0.55
7:V:313:THR:OG1	7:V:314:ASN:N	2.38	0.55
7:Z:313:THR:OG1	7:Z:314:ASN:N	2.38	0.55
7:W:297:LEU:HD21	7:W:377:MET:HB3	1.87	0.54
4:G:864:PHE:CG	7:U:353:PRO:HB3	2.42	0.54
3:J:222:HIS:CD2	3:J:225:TRP:HE1	2.25	0.54
3:J:727:PHE:CE2	3:J:821:TYR:HB3	2.42	0.54
6:L:469:GLN:HA	6:L:517:HIS:HE1	1.72	0.54
7:Z:226:SER:OG	7:Z:227:GLN:NE2	2.41	0.54
2:H:702:HIS:O	2:H:705:HIS:HB2	2.08	0.54
1:m:40:ASP:OD1	1:m:43:THR:OG1	2.24	0.54
7:Y:425:ARG:NH2	7:Y:426:GLU:OE2	2.39	0.53
2:H:287:LEU:HB2	2:H:366:ARG:HH12	1.72	0.53
5:K:313:ARG:O	5:K:317:GLN:NE2	2.41	0.53
6:L:1566:THR:OG1	6:L:1569:ALA:N	2.37	0.53
6:L:1800:LEU:HD21	7:Z:337:LEU:HD23	1.90	0.53
7:V:226:SER:OG	7:V:227:GLN:NE2	2.41	0.53
7:W:425:ARG:NH2	7:W:426:GLU:OE2	2.40	0.53
2:a:9:PRO:HA	2:a:12:LEU:HD12	1.90	0.53
7:X:226:SER:OG	7:X:227:GLN:NE2	2.41	0.53
7:X:274:THR:HG1	7:X:375:GLY:H	1.55	0.53
3:J:387:ILE:O	6:L:307:ARG:NH2	2.41	0.53
7:U:184:GLN:HA	7:U:187:ASN:HD22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:592:SER:O	5:I:595:SER:OG	2.26	0.53
7:U:226:SER:OG	7:U:227:GLN:NE2	2.41	0.53
7:W:226:SER:OG	7:W:227:GLN:NE2	2.41	0.53
7:Y:226:SER:OG	7:Y:227:GLN:NE2	2.41	0.53
7:Z:184:GLN:HA	7:Z:187:ASN:HD22	1.74	0.53
7:X:425:ARG:NH2	7:X:426:GLU:OE2	2.39	0.53
7:Y:313:THR:OG1	7:Y:314:ASN:N	2.38	0.53
7:X:112:GLU:O	7:X:115:HIS:ND1	2.43	0.52
7:Y:274:THR:HG1	7:Y:375:GLY:H	1.55	0.52
7:U:112:GLU:O	7:U:115:HIS:ND1	2.43	0.52
7:U:274:THR:HG1	7:U:375:GLY:H	1.55	0.52
2:a:23:ARG:HB3	2:a:27:ASP:HB3	1.92	0.52
2:H:490:ILE:HA	2:H:493:LEU:HD12	1.91	0.52
7:W:112:GLU:O	7:W:115:HIS:ND1	2.43	0.52
7:X:184:GLN:HA	7:X:187:ASN:HD22	1.74	0.52
7:Y:112:GLU:O	7:Y:115:HIS:ND1	2.43	0.52
2:a:67:ARG:HH12	1:b:34:ILE:HB	1.74	0.52
5:K:571:GLN:HE22	5:K:641:ASP:HB2	1.75	0.52
7:W:184:GLN:HA	7:W:187:ASN:HD22	1.74	0.52
7:V:112:GLU:O	7:V:115:HIS:ND1	2.43	0.52
2:H:364:LEU:HD22	2:H:370:TRP:HE1	1.74	0.52
7:V:184:GLN:HA	7:V:187:ASN:HD22	1.74	0.52
7:Z:112:GLU:O	7:Z:115:HIS:ND1	2.43	0.52
7:Y:184:GLN:HA	7:Y:187:ASN:HD22	1.74	0.52
7:V:274:THR:HG1	7:V:375:GLY:H	1.58	0.52
7:Z:425:ARG:NH2	7:Z:426:GLU:OE2	2.40	0.52
4:G:351:LEU:O	4:G:354:SER:OG	2.27	0.51
7:V:4:GLU:O	7:V:133:GLU:N	2.42	0.51
7:U:4:GLU:O	7:U:133:GLU:N	2.42	0.51
4:G:218:VAL:HG12	4:G:321:LEU:HD13	1.92	0.51
6:L:390:PRO:HB2	6:L:393:ILE:HG12	1.91	0.51
7:V:415:LYS:HZ2	7:V:419:ASP:H	1.58	0.51
7:W:4:GLU:O	7:W:133:GLU:N	2.42	0.51
5:I:485:VAL:HG12	5:I:587:LEU:HD21	1.93	0.51
5:K:195:LEU:HD21	6:L:1474:VAL:HG21	1.93	0.51
4:G:201:THR:OG1	4:G:202:ALA:N	2.35	0.51
2:H:326:ALA:HB2	5:I:165:LEU:HD23	1.92	0.50
7:Z:172:PHE:N	7:Z:205:LEU:O	2.42	0.50
2:H:448:VAL:HG22	2:H:484:LEU:HD12	1.93	0.50
7:U:415:LYS:HZ2	7:U:419:ASP:H	1.59	0.50
6:L:1590:VAL:HG11	6:L:1734:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:289:THR:OG1	7:U:290:VAL:N	2.45	0.50
4:G:737:CYS:SG	4:G:738:MET:N	2.84	0.50
7:X:174:ASN:O	7:X:208:THR:OG1	2.30	0.50
2:H:478:ASP:O	2:H:482:LYS:NZ	2.45	0.50
7:W:172:PHE:N	7:W:205:LEU:O	2.42	0.50
7:Y:289:THR:OG1	7:Y:290:VAL:N	2.45	0.50
7:Z:337:LEU:O	7:Z:341:ARG:HB3	2.12	0.50
5:K:30:ASP:OD1	5:K:30:ASP:N	2.45	0.50
7:U:337:LEU:O	7:U:341:ARG:HB3	2.12	0.50
7:W:415:LYS:HZ2	7:W:419:ASP:H	1.58	0.50
7:V:289:THR:OG1	7:V:290:VAL:N	2.45	0.49
7:V:337:LEU:O	7:V:341:ARG:HB3	2.12	0.49
7:X:337:LEU:O	7:X:341:ARG:HB3	2.12	0.49
3:l:80:LYS:NZ	3:l:126:TYR:CE2	2.55	0.49
7:V:172:PHE:N	7:V:205:LEU:O	2.42	0.49
7:Z:415:LYS:HZ2	7:Z:419:ASP:H	1.59	0.49
4:G:864:PHE:CD1	7:U:353:PRO:HB3	2.48	0.49
5:K:84:ILE:HA	5:K:87:ARG:HE	1.78	0.49
7:W:289:THR:OG1	7:W:290:VAL:N	2.45	0.49
3:J:369:TYR:OH	5:K:127:ASP:O	2.30	0.49
5:K:143:ILE:HD13	5:K:148:ILE:HD12	1.94	0.49
7:V:425:ARG:NH2	7:V:426:GLU:OE2	2.39	0.49
7:W:337:LEU:O	7:W:341:ARG:HB3	2.12	0.49
7:X:172:PHE:N	7:X:205:LEU:O	2.42	0.49
3:l:127:VAL:O	3:l:127:VAL:CG1	2.61	0.49
7:W:47:ARG:HE	7:W:49:ASP:HB3	1.78	0.49
2:H:417:HIS:O	2:H:420:SER:OG	2.27	0.49
7:X:289:THR:OG1	7:X:290:VAL:N	2.45	0.49
7:X:415:LYS:HZ2	7:X:419:ASP:H	1.59	0.49
7:V:73:VAL:O	7:V:76:SER:OG	2.28	0.49
2:H:874:ARG:O	2:H:877:SER:OG	2.29	0.49
7:Y:337:LEU:O	7:Y:341:ARG:HB3	2.12	0.49
7:Z:4:GLU:O	7:Z:133:GLU:N	2.42	0.49
5:I:365:ARG:HG2	5:I:368:LEU:HG	1.94	0.49
6:L:506:TYR:O	6:L:509:ALA:HB3	2.13	0.49
7:V:47:ARG:HE	7:V:49:ASP:HB3	1.77	0.48
7:Z:174:ASN:O	7:Z:208:THR:OG1	2.30	0.48
5:K:406:ASP:OD2	7:Z:339:ARG:NH1	2.46	0.48
7:U:425:ARG:NH2	7:U:426:GLU:OE2	2.40	0.48
7:Z:289:THR:OG1	7:Z:290:VAL:N	2.45	0.48
4:G:864:PHE:HD1	4:G:865:TYR:HD1	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:447:PHE:O	2:H:467:ARG:N	2.41	0.48
7:U:151:SER:HB2	7:U:194:ARG:HG2	1.96	0.48
3:J:221:VAL:HG12	3:J:223:GLN:HG2	1.95	0.48
7:W:36:ILE:HG12	7:W:59:HIS:HE1	1.79	0.48
7:W:274:THR:HG1	7:W:375:GLY:H	1.56	0.48
2:H:781:GLN:HA	2:H:784:GLU:HG2	1.94	0.48
5:K:639:ASN:HB2	7:Y:334:HIS:NE2	2.28	0.48
7:W:151:SER:HB2	7:W:194:ARG:HG2	1.96	0.48
7:X:36:ILE:HG12	7:X:59:HIS:HE1	1.79	0.48
2:H:626:LEU:HB2	2:H:637:VAL:HG13	1.96	0.48
7:V:151:SER:HB2	7:V:194:ARG:HG2	1.96	0.48
7:X:151:SER:HB2	7:X:194:ARG:HG2	1.95	0.48
7:Z:47:ARG:HE	7:Z:49:ASP:HB3	1.78	0.48
5:K:594:CYS:SG	5:K:595:SER:N	2.86	0.48
7:U:47:ARG:HE	7:U:49:ASP:HB3	1.77	0.48
7:Y:36:ILE:HG12	7:Y:59:HIS:HE1	1.79	0.48
7:Y:47:ARG:HE	7:Y:49:ASP:HB3	1.78	0.48
4:G:542:PRO:HA	4:G:610:LEU:HD23	1.95	0.48
7:U:36:ILE:HG12	7:U:59:HIS:HE1	1.79	0.48
7:Y:151:SER:HB2	7:Y:194:ARG:HG2	1.95	0.48
6:L:428:VAL:HG12	6:L:531:PRO:HD2	1.94	0.47
7:X:47:ARG:HE	7:X:49:ASP:HB3	1.77	0.47
7:Y:75:HIS:HA	7:Y:78:LEU:HD12	1.96	0.47
7:Z:151:SER:HB2	7:Z:194:ARG:HG2	1.95	0.47
7:U:174:ASN:O	7:U:208:THR:OG1	2.29	0.47
7:X:75:HIS:HA	7:X:78:LEU:HD12	1.96	0.47
2:H:601:LEU:HD22	2:H:623:VAL:HG13	1.97	0.47
5:I:547:GLN:O	5:I:550:SER:OG	2.31	0.47
6:L:320:PHE:HD1	6:L:320:PHE:HA	1.53	0.47
7:V:75:HIS:HA	7:V:78:LEU:HD12	1.96	0.47
5:K:481:TYR:O	5:K:484:SER:OG	2.29	0.47
7:U:75:HIS:HA	7:U:78:LEU:HD12	1.96	0.47
7:Z:36:ILE:HG12	7:Z:59:HIS:HE1	1.79	0.47
7:V:174:ASN:O	7:V:208:THR:OG1	2.30	0.47
7:W:73:VAL:O	7:W:76:SER:OG	2.28	0.47
7:X:73:VAL:O	7:X:76:SER:OG	2.28	0.47
7:W:75:HIS:HA	7:W:78:LEU:HD12	1.96	0.47
7:X:141:ILE:HB	7:X:173:PRO:HD3	1.97	0.47
7:Y:4:GLU:O	7:Y:133:GLU:N	2.42	0.47
7:Z:73:VAL:O	7:Z:76:SER:OG	2.28	0.47
5:I:164:GLY:H	5:I:169:ARG:HE	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:166:PRO:HA	5:I:169:ARG:HD2	1.97	0.47
5:K:652:ASN:O	5:K:656:THR:N	2.35	0.47
7:X:4:GLU:O	7:X:133:GLU:N	2.42	0.47
7:U:172:PHE:N	7:U:205:LEU:O	2.42	0.47
4:G:277:ILE:O	4:G:281:SER:OG	2.28	0.47
2:H:594:GLN:HA	2:H:597:LEU:HD13	1.97	0.47
7:V:36:ILE:HG12	7:V:59:HIS:HE1	1.78	0.47
6:L:296:CYS:H	6:L:303:PRO:HG3	1.80	0.47
6:L:369:SER:OG	6:L:370:LEU:N	2.47	0.46
6:L:1686:CYS:SG	6:L:1687:GLU:N	2.88	0.46
7:W:141:ILE:HB	7:W:173:PRO:HD3	1.97	0.46
7:Z:187:ASN:O	7:Z:191:THR:OG1	2.31	0.46
4:G:287:GLN:HB3	2:H:407:GLY:HA3	1.97	0.46
4:G:654:GLN:O	4:G:657:SER:OG	2.33	0.46
5:K:4:GLU:HG2	6:L:320:PHE:HZ	1.78	0.46
5:K:4:GLU:HB3	5:K:7:LEU:HD22	1.95	0.46
7:Y:317:TYR:HD2	7:Y:348:PHE:HB3	1.80	0.46
2:H:535:ASP:OD1	2:H:535:ASP:N	2.46	0.46
7:Y:174:ASN:O	7:Y:208:THR:OG1	2.30	0.46
5:K:183:MET:HE3	5:K:183:MET:HB3	1.76	0.46
5:I:481:TYR:O	5:I:484:SER:OG	2.34	0.46
7:U:317:TYR:HD2	7:U:348:PHE:HB3	1.80	0.46
3:J:559:ILE:O	3:J:562:ALA:HB3	2.14	0.46
7:W:317:TYR:HD2	7:W:348:PHE:HB3	1.80	0.46
7:X:317:TYR:HD2	7:X:348:PHE:HB3	1.80	0.46
7:Z:75:HIS:HA	7:Z:78:LEU:HD12	1.96	0.46
4:G:392:GLU:HG2	4:G:396:TYR:HE2	1.81	0.46
5:I:579:VAL:HG12	5:I:629:ILE:HG12	1.98	0.46
7:Y:73:VAL:O	7:Y:76:SER:OG	2.28	0.46
4:G:497:LYS:HE3	4:G:497:LYS:HB3	1.77	0.46
2:H:655:GLU:O	2:H:658:SER:OG	2.28	0.46
5:K:328:VAL:HA	5:K:331:ARG:HE	1.81	0.46
6:L:318:ASP:OD1	6:L:318:ASP:N	2.41	0.46
7:V:141:ILE:HB	7:V:173:PRO:HD3	1.97	0.46
7:Z:317:TYR:HD2	7:Z:348:PHE:HB3	1.80	0.46
6:L:1685:TRP:CD1	6:L:1689:ARG:HH21	2.34	0.46
7:U:141:ILE:HB	7:U:173:PRO:HD3	1.97	0.46
7:V:317:TYR:HD2	7:V:348:PHE:HB3	1.80	0.46
2:a:20:ILE:HD11	1:b:64:ILE:HG12	1.98	0.45
3:l:121:PRO:HD2	3:l:121:PRO:O	2.15	0.45
4:G:567:ASP:OD2	4:G:567:ASP:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:222:HIS:HD2	3:J:225:TRP:HE1	1.61	0.45
5:I:164:GLY:HA2	5:I:169:ARG:HH21	1.81	0.45
7:Y:141:ILE:HB	7:Y:173:PRO:HD3	1.97	0.45
7:Z:141:ILE:HB	7:Z:173:PRO:HD3	1.97	0.45
7:Z:395:TYR:HE2	7:Z:425:ARG:HG3	1.82	0.45
3:l:38:GLN:HE21	3:l:42:ASN:HD21	1.64	0.45
5:I:20:ASN:H	5:I:24:GLY:HA2	1.82	0.45
7:V:252:ASP:OD1	7:V:252:ASP:N	2.48	0.45
7:X:142:ALA:HB3	7:X:173:PRO:HG3	1.99	0.45
5:I:149:HIS:CD2	5:I:202:GLU:HB3	2.52	0.45
7:U:73:VAL:O	7:U:76:SER:OG	2.28	0.45
7:U:142:ALA:HB3	7:U:173:PRO:HG3	1.99	0.45
7:Z:142:ALA:HB3	7:Z:173:PRO:HG3	1.99	0.45
5:K:643:ALA:HA	7:Y:338:GLN:HE22	1.82	0.45
7:Y:142:ALA:HB3	7:Y:173:PRO:HG3	1.99	0.45
5:I:272:VAL:HA	5:I:275:LYS:HD3	1.99	0.45
6:L:392:SER:O	6:L:395:SER:OG	2.21	0.45
1:m:44:LEU:O	1:m:48:VAL:HG12	2.17	0.45
1:b:49:ARG:HH22	6:L:282:LEU:HB3	1.82	0.45
7:Z:222:ASN:OD1	7:Z:222:ASN:N	2.50	0.45
4:G:557:LEU:HB3	7:V:343:ARG:HH11	1.83	0.44
7:U:222:ASN:OD1	7:U:222:ASN:N	2.50	0.44
7:U:436:HIS:O	7:U:439:THR:OG1	2.34	0.44
7:V:220:ILE:HB	7:V:223:PRO:HD2	1.99	0.44
4:G:257:ARG:HE	4:G:261:HIS:HE1	1.64	0.44
5:K:628:LYS:HA	5:K:628:LYS:HD2	1.73	0.44
6:L:1762:PHE:HA	6:L:1765:MET:HE3	1.98	0.44
7:V:395:TYR:HE2	7:V:425:ARG:HG3	1.82	0.44
7:W:174:ASN:O	7:W:208:THR:OG1	2.30	0.44
7:Y:415:LYS:HZ2	7:Y:419:ASP:H	1.63	0.44
5:K:305:ASP:OD1	5:K:305:ASP:N	2.50	0.44
6:L:319:ALA:HA	6:L:322:LYS:HE3	1.97	0.44
7:V:222:ASN:OD1	7:V:222:ASN:N	2.50	0.44
7:Y:395:TYR:HE2	7:Y:425:ARG:HG3	1.82	0.44
4:G:206:GLY:H	4:G:251:ASN:HD22	1.65	0.44
5:K:59:ILE:HG12	5:K:90:CYS:HB3	1.98	0.44
7:W:436:HIS:O	7:W:439:THR:OG1	2.34	0.44
7:Y:222:ASN:OD1	7:Y:222:ASN:N	2.50	0.44
2:a:51:GLU:HA	2:a:54:VAL:HG22	2.00	0.44
2:H:433:TRP:HE1	2:H:484:LEU:HA	1.83	0.44
5:I:341:TRP:CE2	5:I:552:ARG:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:9:GLN:HA	7:X:138:CYS:HB2	2.00	0.44
7:Y:172:PHE:N	7:Y:205:LEU:O	2.42	0.44
7:Z:220:ILE:HB	7:Z:223:PRO:HD2	2.00	0.44
5:I:530:TYR:O	5:I:534:VAL:HG23	2.18	0.44
7:U:88:PRO:HD2	7:U:90:ASN:HD22	1.83	0.44
7:X:395:TYR:HE2	7:X:425:ARG:HG3	1.82	0.44
3:J:222:HIS:HA	3:J:225:TRP:NE1	2.33	0.44
7:U:399:ARG:NH1	7:U:421:MET:SD	2.91	0.44
7:W:9:GLN:HA	7:W:138:CYS:HB2	2.00	0.44
7:W:142:ALA:HB3	7:W:173:PRO:HG3	1.99	0.44
7:X:88:PRO:HD2	7:X:90:ASN:HD22	1.83	0.44
2:a:31:GLN:HE21	1:b:66:GLU:HG2	1.82	0.44
1:b:44:LEU:O	1:b:48:VAL:HG12	2.17	0.44
5:I:578:PRO:HA	5:I:581:HIS:CD2	2.53	0.44
7:U:395:TYR:HE2	7:U:425:ARG:HG3	1.82	0.44
7:V:131:SER:OG	7:V:132:LEU:N	2.51	0.44
7:V:142:ALA:HB3	7:V:173:PRO:HG3	1.99	0.44
7:W:369:SER:H	7:W:372:ARG:NH2	2.16	0.44
7:Y:187:ASN:O	7:Y:191:THR:OG1	2.31	0.44
5:I:133:PHE:HA	5:I:136:VAL:HG22	2.00	0.44
5:I:539:SER:O	5:I:542:SER:OG	2.31	0.44
7:U:369:SER:H	7:U:372:ARG:NH2	2.16	0.44
7:W:395:TYR:HE2	7:W:425:ARG:HG3	1.82	0.44
7:X:220:ILE:HB	7:X:223:PRO:HD2	2.00	0.44
7:X:399:ARG:NH1	7:X:421:MET:SD	2.91	0.44
7:Y:131:SER:OG	7:Y:132:LEU:N	2.51	0.44
4:G:719:ILE:HA	4:G:722:VAL:HG22	1.99	0.43
7:V:369:SER:H	7:V:372:ARG:NH2	2.16	0.43
7:Y:220:ILE:HB	7:Y:223:PRO:HD2	1.99	0.43
7:Z:369:SER:H	7:Z:372:ARG:NH2	2.16	0.43
4:G:162:ARG:O	4:G:166:ASN:ND2	2.51	0.43
2:H:412:ARG:HA	2:H:415:VAL:HG12	1.99	0.43
7:U:9:GLN:HA	7:U:138:CYS:HB2	2.00	0.43
7:W:222:ASN:OD1	7:W:222:ASN:N	2.50	0.43
7:W:399:ARG:NH1	7:W:421:MET:SD	2.91	0.43
7:X:222:ASN:OD1	7:X:222:ASN:N	2.50	0.43
7:Y:399:ARG:NH1	7:Y:421:MET:SD	2.91	0.43
5:K:185:LYS:O	5:K:188:SER:OG	2.36	0.43
7:V:399:ARG:NH1	7:V:421:MET:SD	2.91	0.43
7:Z:274:THR:HG1	7:Z:375:GLY:H	1.60	0.43
1:b:25:MET:HB3	1:b:41:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:652:ASN:HB3	5:K:655:TYR:HB3	2.00	0.43
6:L:1803:ASN:ND2	7:Z:341:ARG:HH21	2.15	0.43
7:U:252:ASP:OD1	7:U:252:ASP:N	2.48	0.43
1:m:25:MET:HB3	1:m:41:MET:HE1	2.00	0.43
6:L:297:TRP:HA	6:L:300:VAL:HG22	2.00	0.43
7:U:9:GLN:HE22	7:U:64:ALA:HB1	1.84	0.43
7:W:9:GLN:HE22	7:W:64:ALA:HB1	1.84	0.43
7:W:217:ARG:HG3	7:W:218:LEU:HG	2.01	0.43
7:W:220:ILE:HB	7:W:223:PRO:HD2	1.99	0.43
7:X:9:GLN:HE22	7:X:64:ALA:HB1	1.84	0.43
7:X:369:SER:H	7:X:372:ARG:NH2	2.16	0.43
7:Y:88:PRO:HD2	7:Y:90:ASN:HD22	1.83	0.43
7:Y:369:SER:H	7:Y:372:ARG:NH2	2.16	0.43
7:Z:88:PRO:HD2	7:Z:90:ASN:HD22	1.83	0.43
7:Z:131:SER:OG	7:Z:132:LEU:N	2.51	0.43
7:Z:399:ARG:NH1	7:Z:421:MET:SD	2.91	0.43
4:G:307:VAL:HA	4:G:310:LEU:HG	2.01	0.43
6:L:1728:VAL:O	6:L:1731:SER:OG	2.34	0.43
1:m:44:LEU:HA	1:m:47:CYS:HG	1.84	0.43
2:H:555:LEU:HD11	2:H:651:VAL:HG21	2.01	0.43
6:L:1656:ARG:H	6:L:1656:ARG:HG2	1.65	0.43
7:W:88:PRO:HD2	7:W:90:ASN:HD22	1.83	0.43
7:Y:9:GLN:HA	7:Y:138:CYS:HB2	2.00	0.43
7:U:131:SER:OG	7:U:132:LEU:N	2.51	0.43
7:V:9:GLN:HA	7:V:138:CYS:HB2	2.00	0.43
7:V:217:ARG:HG3	7:V:218:LEU:HG	2.01	0.43
4:G:305:ILE:O	4:G:308:SER:OG	2.29	0.43
2:H:482:LYS:HA	2:H:482:LYS:HD3	1.84	0.43
2:H:682:LYS:HB2	7:V:254:ILE:HD11	1.99	0.43
5:K:155:GLU:O	5:K:159:LYS:N	2.47	0.43
7:Z:217:ARG:HG3	7:Z:218:LEU:HG	2.01	0.43
4:G:259:LEU:HA	4:G:262:ARG:HE	1.84	0.43
2:H:887:LYS:HD3	2:H:887:LYS:HA	1.90	0.43
6:L:1779:LEU:HA	6:L:1782:VAL:HG12	2.01	0.43
7:U:217:ARG:HG3	7:U:218:LEU:HG	2.01	0.43
7:V:88:PRO:HD2	7:V:90:ASN:HD22	1.83	0.43
4:G:314:HIS:HB2	4:G:319:LEU:HD12	2.00	0.42
7:W:131:SER:OG	7:W:132:LEU:N	2.51	0.42
7:Z:9:GLN:HA	7:Z:138:CYS:HB2	2.00	0.42
7:Z:436:HIS:O	7:Z:439:THR:OG1	2.34	0.42
4:G:250:PRO:HA	4:G:257:ARG:HH12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:530:HIS:HA	7:U:3:ARG:HH22	1.84	0.42
4:G:457:LEU:HD22	4:G:467:VAL:HG11	2.00	0.42
4:G:704:PRO:HG3	7:U:330:PRO:HB2	2.00	0.42
7:U:220:ILE:HB	7:U:223:PRO:HD2	2.00	0.42
7:W:425:ARG:HH21	7:W:426:GLU:CD	2.27	0.42
3:J:290:ILE:HG13	3:J:291:ASP:H	1.85	0.42
7:V:9:GLN:HE22	7:V:64:ALA:HB1	1.84	0.42
7:X:131:SER:OG	7:X:132:LEU:N	2.51	0.42
7:X:217:ARG:HG3	7:X:218:LEU:HG	2.01	0.42
3:J:686:THR:O	3:J:689:SER:OG	2.35	0.42
3:J:709:THR:HA	3:J:712:LYS:HZ3	1.85	0.42
5:K:536:VAL:HG21	5:K:571:GLN:HG3	2.01	0.42
7:X:383:SER:O	7:X:386:SER:OG	2.35	0.42
7:Y:217:ARG:HG3	7:Y:218:LEU:HG	2.01	0.42
4:G:582:LEU:H	4:G:582:LEU:HG	1.69	0.42
4:G:865:TYR:HA	4:G:868:ARG:HG3	2.02	0.42
5:K:282:SER:HB3	5:K:340:LEU:HD11	2.01	0.42
5:K:585:GLU:OE1	5:K:585:GLU:N	2.52	0.42
7:W:187:ASN:O	7:W:191:THR:OG1	2.31	0.42
7:Z:3:ARG:HB2	7:Z:133:GLU:HB2	2.02	0.42
1:b:49:ARG:NH2	6:L:282:LEU:HB3	2.35	0.42
5:I:408:ASP:OD1	5:I:408:ASP:N	2.52	0.42
7:U:187:ASN:O	7:U:191:THR:OG1	2.31	0.42
7:X:3:ARG:HB2	7:X:133:GLU:HB2	2.02	0.42
5:K:582:CYS:SG	5:K:626:LEU:HB3	2.60	0.42
7:Y:241:THR:OG1	7:Y:244:ARG:NH2	2.53	0.42
7:Z:252:ASP:OD1	7:Z:252:ASP:N	2.48	0.42
2:a:77:LEU:HD22	1:b:27:VAL:HG13	2.02	0.42
7:Z:9:GLN:HE22	7:Z:64:ALA:HB1	1.84	0.42
5:I:351:LEU:HA	5:I:351:LEU:HD23	1.80	0.42
7:W:241:THR:OG1	7:W:244:ARG:NH2	2.53	0.41
7:Y:425:ARG:HH21	7:Y:426:GLU:CD	2.27	0.41
3:J:728:LEU:HD21	3:J:824:VAL:HG23	2.01	0.41
5:K:101:ARG:H	5:K:101:ARG:HG3	1.57	0.41
7:X:106:SER:HA	7:X:410:LYS:HE2	2.03	0.41
7:X:187:ASN:O	7:X:191:THR:OG1	2.31	0.41
7:Y:156:ARG:HA	7:Y:156:ARG:HD3	1.89	0.41
7:Y:287:LYS:HD2	7:Y:287:LYS:HA	1.88	0.41
5:I:259:LEU:HA	5:I:263:ILE:HD11	2.00	0.41
3:J:710:LEU:HG	3:J:716:LEU:HD21	2.02	0.41
7:Y:3:ARG:HB2	7:Y:133:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:106:SER:HA	7:Z:410:LYS:HE2	2.03	0.41
4:G:313:LEU:HD23	4:G:319:LEU:HD21	2.01	0.41
4:G:432:TYR:HB3	4:G:451:LEU:HD11	2.01	0.41
4:G:560:ARG:HB2	7:V:339:ARG:NH1	2.35	0.41
3:J:992:MET:HA	3:J:995:VAL:HG22	2.03	0.41
6:L:1478:ARG:HA	6:L:1481:THR:HG23	2.03	0.41
7:U:337:LEU:HD12	7:U:337:LEU:HA	1.95	0.41
7:U:425:ARG:HH21	7:U:426:GLU:CD	2.27	0.41
7:W:352:GLY:HA3	7:W:353:PRO:HD3	1.85	0.41
4:G:168:LYS:HG3	4:G:170:SER:H	1.85	0.41
4:G:637:ARG:HD2	4:G:734:LEU:HD21	2.03	0.41
2:H:419:LEU:HA	2:H:422:VAL:HG22	2.02	0.41
2:H:592:LEU:HD23	2:H:592:LEU:HA	1.86	0.41
7:U:3:ARG:HB2	7:U:133:GLU:HB2	2.02	0.41
7:V:106:SER:HA	7:V:410:LYS:HE2	2.03	0.41
7:V:187:ASN:O	7:V:191:THR:OG1	2.31	0.41
7:W:3:ARG:HB2	7:W:133:GLU:HB2	2.02	0.41
7:Z:241:THR:OG1	7:Z:244:ARG:NH2	2.53	0.41
4:G:381:LYS:HG2	4:G:476:ILE:HD12	2.03	0.41
3:J:902:MET:SD	3:J:903:THR:OG1	2.66	0.41
7:X:241:THR:OG1	7:X:244:ARG:NH2	2.53	0.41
2:H:686:CYS:SG	2:H:687:ASN:N	2.93	0.41
5:K:500:MET:HE3	5:K:500:MET:HB3	1.82	0.41
7:Y:9:GLN:HE22	7:Y:64:ALA:HB1	1.84	0.41
7:Y:56:ASP:OD1	7:Y:56:ASP:N	2.54	0.41
1:m:30:GLU:HA	1:m:33:ARG:HG2	2.02	0.41
4:G:864:PHE:O	4:G:866:THR:OG1	2.33	0.41
5:I:380:LEU:HD12	5:I:381:LYS:HG3	2.01	0.41
3:J:819:LYS:O	3:J:823:GLN:HG2	2.21	0.41
5:K:155:GLU:HA	5:K:158:TYR:HB3	2.03	0.41
6:L:1588:PRO:HB2	6:L:1737:LEU:HD23	2.03	0.41
7:V:3:ARG:HB2	7:V:133:GLU:HB2	2.02	0.41
7:W:52:PHE:HB3	7:W:60:TYR:HB3	2.03	0.41
7:Z:383:SER:O	7:Z:386:SER:OG	2.35	0.41
7:U:106:SER:HA	7:U:410:LYS:HE2	2.03	0.41
7:W:287:LYS:HD2	7:W:287:LYS:HA	1.88	0.41
7:W:337:LEU:HD12	7:W:337:LEU:HA	1.96	0.41
7:X:287:LYS:HA	7:X:287:LYS:HD2	1.88	0.41
2:a:113:SER:OG	2:a:114:TYR:N	2.54	0.40
2:a:122:LEU:HD23	2:a:122:LEU:HA	1.96	0.40
2:H:364:LEU:N	2:H:367:LEU:H	2.15	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:150:GLY:HA2	5:I:202:GLU:HA	2.03	0.40
6:L:295:ARG:HD2	6:L:303:PRO:HD2	2.03	0.40
7:W:106:SER:HA	7:W:410:LYS:HE2	2.03	0.40
7:Y:52:PHE:HB3	7:Y:60:TYR:HB3	2.03	0.40
4:G:446:MET:SD	4:G:446:MET:N	2.94	0.40
2:H:433:TRP:CE2	2:H:487:GLY:HA3	2.55	0.40
5:K:459:VAL:HG11	5:K:467:PHE:HB2	2.02	0.40
6:L:1680:ILE:HD11	6:L:1716:GLY:HA2	2.03	0.40
7:V:241:THR:OG1	7:V:244:ARG:NH2	2.53	0.40
1:m:59:ALA:O	1:m:62:SER:OG	2.27	0.40
7:V:425:ARG:HH21	7:V:426:GLU:CD	2.27	0.40
7:W:118:ILE:HA	7:W:121:ILE:HD12	2.04	0.40
7:W:156:ARG:HA	7:W:156:ARG:HD3	1.89	0.40
7:X:52:PHE:HB3	7:X:60:TYR:HB3	2.03	0.40
7:Z:52:PHE:HB3	7:Z:60:TYR:HB3	2.03	0.40
1:b:63:VAL:O	1:b:67:LEU:HD23	2.22	0.40
5:I:404:LEU:HA	5:I:404:LEU:HD12	1.77	0.40
7:U:241:THR:OG1	7:U:244:ARG:NH2	2.53	0.40
7:Y:106:SER:HA	7:Y:410:LYS:HE2	2.03	0.40
7:Y:252:ASP:OD1	7:Y:252:ASP:N	2.48	0.40
4:G:248:VAL:HG11	4:G:260:VAL:HG11	2.02	0.40
2:H:720:TYR:HE2	7:V:357:GLN:HB3	1.86	0.40
7:Y:118:ILE:HA	7:Y:121:ILE:HD12	2.04	0.40
7:Z:56:ASP:OD1	7:Z:56:ASP:N	2.54	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	b	63/82 (77%)	62 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	m	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
2	H	584/907 (64%)	566 (97%)	17 (3%)	1 (0%)	43	77
2	a	112/907 (12%)	108 (96%)	4 (4%)	0	100	100
3	J	506/1024 (49%)	474 (94%)	30 (6%)	2 (0%)	30	67
3	l	104/1024 (10%)	100 (96%)	2 (2%)	2 (2%)	6	30
4	G	624/902 (69%)	593 (95%)	29 (5%)	2 (0%)	36	71
5	I	511/667 (77%)	486 (95%)	19 (4%)	6 (1%)	10	42
5	K	548/667 (82%)	533 (97%)	13 (2%)	2 (0%)	30	67
6	L	540/1819 (30%)	507 (94%)	29 (5%)	4 (1%)	18	55
7	U	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
7	V	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
7	W	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
7	X	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
7	Y	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
7	Z	408/451 (90%)	387 (95%)	21 (5%)	0	100	100
All	All	6103/10787 (57%)	5813 (95%)	271 (4%)	19 (0%)	37	71

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	241	ARG
4	G	581	ASP
5	I	408	ASP
5	I	601	LEU
3	J	236	LEU
3	J	238	LEU
2	H	455	LYS
5	I	405	LEU
6	L	307	ARG
6	L	1806	ASN
5	I	409	ASN
3	l	120	SER
5	I	404	LEU
5	K	409	ASN
6	L	309	GLU
5	K	410	LEU
5	I	13	PRO

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Mol	Chain	Res	Type
6	L	310	PRO
3	l	129	THR

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	53/62 (86%)	40 (76%)	13 (24%)	1	4
1	m	53/62 (86%)	40 (76%)	13 (24%)	1	4
2	H	539/798 (68%)	539 (100%)	0	100	100
2	a	101/798 (13%)	100 (99%)	1 (1%)	68	76
3	J	498/933 (53%)	497 (100%)	1 (0%)	87	85
3	l	96/933 (10%)	96 (100%)	0	100	100
4	G	572/791 (72%)	569 (100%)	3 (0%)	81	82
5	I	472/594 (80%)	472 (100%)	0	100	100
5	K	509/594 (86%)	508 (100%)	1 (0%)	87	85
6	L	501/1546 (32%)	501 (100%)	0	100	100
7	U	376/400 (94%)	338 (90%)	38 (10%)	7	23
7	V	376/400 (94%)	338 (90%)	38 (10%)	7	23
7	W	376/400 (94%)	338 (90%)	38 (10%)	7	23
7	X	376/400 (94%)	338 (90%)	38 (10%)	7	23
7	Y	376/400 (94%)	338 (90%)	38 (10%)	7	23
7	Z	376/400 (94%)	338 (90%)	38 (10%)	7	23
All	All	5650/9511 (59%)	5390 (95%)	260 (5%)	25	45

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	m	21	VAL
1	m	25	MET

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Mol	Chain	Res	Type
1	m	30	GLU
1	m	31	ILE
1	m	34	ILE
1	m	37	THR
1	m	39	LEU
1	m	43	THR
1	m	45	SER
1	m	47	CYS
1	m	48	VAL
1	m	60	LEU
1	m	67	LEU
2	a	39	ILE
1	b	21	VAL
1	b	25	MET
1	b	30	GLU
1	b	31	ILE
1	b	34	ILE
1	b	37	THR
1	b	39	LEU
1	b	43	THR
1	b	45	SER
1	b	47	CYS
1	b	48	VAL
1	b	60	LEU
1	b	67	LEU
4	G	328	ILE
4	G	557	LEU
4	G	855	VAL
3	J	809	VAL
5	K	182	VAL
7	U	10	LEU
7	U	37	VAL
7	U	57	ASP
7	U	120	ASP
7	U	129	SER
7	U	168	THR
7	U	176	ASP
7	U	183	VAL
7	U	188	SER
7	U	220	ILE
7	U	221	GLN
7	U	222	ASN

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Mol	Chain	Res	Type
7	U	224	SER
7	U	231	LEU
7	U	249	MET
7	U	265	ARG
7	U	274	THR
7	U	288	THR
7	U	290	VAL
7	U	301	LYS
7	U	305	VAL
7	U	321	LEU
7	U	328	VAL
7	U	331	THR
7	U	333	VAL
7	U	341	ARG
7	U	347	ASN
7	U	361	SER
7	U	373	VAL
7	U	383	SER
7	U	413	MET
7	U	422	ASP
7	U	425	ARG
7	U	426	GLU
7	U	440	ARG
7	U	442	ASP
7	U	445	SER
7	U	446	TRP
7	V	10	LEU
7	V	37	VAL
7	V	57	ASP
7	V	120	ASP
7	V	129	SER
7	V	168	THR
7	V	176	ASP
7	V	183	VAL
7	V	188	SER
7	V	220	ILE
7	V	221	GLN
7	V	222	ASN
7	V	224	SER
7	V	231	LEU
7	V	249	MET
7	V	265	ARG

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Mol	Chain	Res	Type
7	V	274	THR
7	V	288	THR
7	V	290	VAL
7	V	301	LYS
7	V	305	VAL
7	V	321	LEU
7	V	328	VAL
7	V	331	THR
7	V	333	VAL
7	V	341	ARG
7	V	347	ASN
7	V	361	SER
7	V	373	VAL
7	V	383	SER
7	V	413	MET
7	V	422	ASP
7	V	425	ARG
7	V	426	GLU
7	V	440	ARG
7	V	442	ASP
7	V	445	SER
7	V	446	TRP
7	W	10	LEU
7	W	37	VAL
7	W	57	ASP
7	W	120	ASP
7	W	129	SER
7	W	168	THR
7	W	176	ASP
7	W	183	VAL
7	W	188	SER
7	W	220	ILE
7	W	221	GLN
7	W	222	ASN
7	W	224	SER
7	W	231	LEU
7	W	249	MET
7	W	265	ARG
7	W	274	THR
7	W	288	THR
7	W	290	VAL
7	W	301	LYS

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Mol	Chain	Res	Type
7	W	305	VAL
7	W	321	LEU
7	W	328	VAL
7	W	331	THR
7	W	333	VAL
7	W	341	ARG
7	W	347	ASN
7	W	361	SER
7	W	373	VAL
7	W	383	SER
7	W	413	MET
7	W	422	ASP
7	W	425	ARG
7	W	426	GLU
7	W	440	ARG
7	W	442	ASP
7	W	445	SER
7	W	446	TRP
7	X	10	LEU
7	X	37	VAL
7	X	57	ASP
7	X	120	ASP
7	X	129	SER
7	X	168	THR
7	X	176	ASP
7	X	183	VAL
7	X	188	SER
7	X	220	ILE
7	X	221	GLN
7	X	222	ASN
7	X	224	SER
7	X	231	LEU
7	X	249	MET
7	X	265	ARG
7	X	274	THR
7	X	288	THR
7	X	290	VAL
7	X	301	LYS
7	X	305	VAL
7	X	321	LEU
7	X	328	VAL
7	X	331	THR

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Mol	Chain	Res	Type
7	X	333	VAL
7	X	341	ARG
7	X	347	ASN
7	X	361	SER
7	X	373	VAL
7	X	383	SER
7	X	413	MET
7	X	422	ASP
7	X	425	ARG
7	X	426	GLU
7	X	440	ARG
7	X	442	ASP
7	X	445	SER
7	X	446	TRP
7	Y	10	LEU
7	Y	37	VAL
7	Y	57	ASP
7	Y	120	ASP
7	Y	129	SER
7	Y	168	THR
7	Y	176	ASP
7	Y	183	VAL
7	Y	188	SER
7	Y	220	ILE
7	Y	221	GLN
7	Y	222	ASN
7	Y	224	SER
7	Y	231	LEU
7	Y	249	MET
7	Y	265	ARG
7	Y	274	THR
7	Y	288	THR
7	Y	290	VAL
7	Y	301	LYS
7	Y	305	VAL
7	Y	321	LEU
7	Y	328	VAL
7	Y	331	THR
7	Y	333	VAL
7	Y	341	ARG
7	Y	347	ASN
7	Y	361	SER

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Mol	Chain	Res	Type
7	Y	373	VAL
7	Y	383	SER
7	Y	413	MET
7	Y	422	ASP
7	Y	425	ARG
7	Y	426	GLU
7	Y	440	ARG
7	Y	442	ASP
7	Y	445	SER
7	Y	446	TRP
7	Z	10	LEU
7	Z	37	VAL
7	Z	57	ASP
7	Z	120	ASP
7	Z	129	SER
7	Z	168	THR
7	Z	176	ASP
7	Z	183	VAL
7	Z	188	SER
7	Z	220	ILE
7	Z	221	GLN
7	Z	222	ASN
7	Z	224	SER
7	Z	231	LEU
7	Z	249	MET
7	Z	265	ARG
7	Z	274	THR
7	Z	288	THR
7	Z	290	VAL
7	Z	301	LYS
7	Z	305	VAL
7	Z	321	LEU
7	Z	328	VAL
7	Z	331	THR
7	Z	333	VAL
7	Z	341	ARG
7	Z	347	ASN
7	Z	361	SER
7	Z	373	VAL
7	Z	383	SER
7	Z	413	MET
7	Z	422	ASP

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Mol	Chain	Res	Type
7	Z	425	ARG
7	Z	426	GLU
7	Z	440	ARG
7	Z	442	ASP
7	Z	445	SER
7	Z	446	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
2	a	14	GLN
2	a	42	ASN
2	a	78	HIS
2	a	84	GLN
1	b	56	ASN
3	l	38	GLN
3	l	107	HIS
4	G	165	GLN
4	G	166	ASN
4	G	172	GLN
4	G	213	GLN
4	G	309	GLN
4	G	314	HIS
4	G	316	GLN
4	G	373	GLN
4	G	401	HIS
4	G	487	GLN
4	G	580	HIS
4	G	585	GLN
4	G	644	HIS
4	G	662	ASN
4	G	691	GLN
4	G	725	HIS
4	G	741	ASN
2	H	273	ASN
2	H	343	HIS
2	H	345	GLN
2	H	347	GLN
2	H	387	HIS
2	H	461	HIS
2	H	531	GLN
2	H	558	HIS

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Mol	Chain	Res	Type
2	H	576	HIS
2	H	687	ASN
2	H	693	ASN
2	H	702	HIS
2	H	705	HIS
2	H	739	GLN
2	H	781	GLN
2	H	786	GLN
2	H	830	ASN
2	H	860	GLN
5	I	29	GLN
5	I	109	GLN
5	I	121	HIS
5	I	128	GLN
5	I	149	HIS
5	I	284	GLN
5	I	303	GLN
5	I	317	GLN
5	I	509	GLN
5	I	519	ASN
5	I	527	ASN
5	I	540	GLN
5	I	543	GLN
5	I	549	ASN
5	I	581	HIS
5	I	600	ASN
5	I	622	GLN
3	J	219	HIS
3	J	222	HIS
3	J	248	GLN
3	J	249	HIS
3	J	269	GLN
3	J	288	GLN
3	J	304	HIS
3	J	408	GLN
3	J	474	GLN
3	J	818	GLN
3	J	822	ASN
3	J	830	GLN
3	J	898	HIS
3	J	915	HIS
3	J	916	GLN

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Mol	Chain	Res	Type
3	J	938	HIS
3	J	989	ASN
5	K	29	GLN
5	K	67	GLN
5	K	78	GLN
5	K	109	GLN
5	K	128	GLN
5	K	200	HIS
5	K	256	GLN
5	K	303	GLN
5	K	316	GLN
5	K	390	HIS
5	K	489	GLN
5	K	533	GLN
5	K	571	GLN
6	L	327	HIS
6	L	430	GLN
6	L	517	HIS
6	L	603	ASN
6	L	1492	ASN
6	L	1525	GLN
6	L	1551	ASN
6	L	1625	GLN
6	L	1654	GLN
6	L	1657	GLN
6	L	1666	GLN
6	L	1679	GLN
6	L	1702	GLN
6	L	1705	HIS
6	L	1742	GLN
6	L	1767	GLN
6	L	1770	ASN
6	L	1803	ASN
6	L	1805	ASN
7	U	15	ASN
7	U	16	GLN
7	U	59	HIS
7	U	102	ASN
7	U	103	ASN
7	U	139	HIS
7	U	187	ASN
7	U	227	GLN

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Mol	Chain	Res	Type
7	U	229	ASN
7	U	357	GLN
7	V	15	ASN
7	V	16	GLN
7	V	59	HIS
7	V	103	ASN
7	V	139	HIS
7	V	187	ASN
7	V	227	GLN
7	V	229	ASN
7	V	357	GLN
7	W	15	ASN
7	W	16	GLN
7	W	59	HIS
7	W	102	ASN
7	W	103	ASN
7	W	139	HIS
7	W	187	ASN
7	W	227	GLN
7	W	229	ASN
7	W	357	GLN
7	X	15	ASN
7	X	16	GLN
7	X	59	HIS
7	X	103	ASN
7	X	139	HIS
7	X	187	ASN
7	X	227	GLN
7	X	229	ASN
7	X	357	GLN
7	Y	15	ASN
7	Y	16	GLN
7	Y	59	HIS
7	Y	102	ASN
7	Y	103	ASN
7	Y	139	HIS
7	Y	187	ASN
7	Y	219	HIS
7	Y	227	GLN
7	Y	229	ASN
7	Y	357	GLN
7	Z	15	ASN

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Mol	Chain	Res	Type
7	Z	16	GLN
7	Z	59	HIS
7	Z	102	ASN
7	Z	103	ASN
7	Z	139	HIS
7	Z	187	ASN
7	Z	219	HIS
7	Z	227	GLN
7	Z	229	ASN
7	Z	338	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.

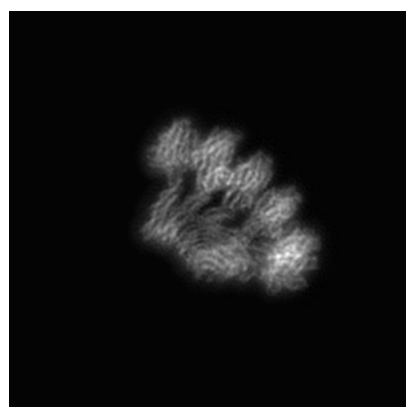
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14005. These allow visual inspection of the internal detail of the map and identification of artifacts.

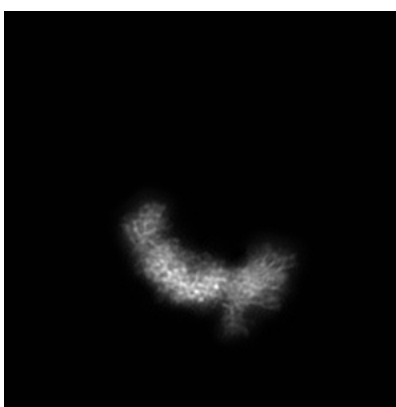
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

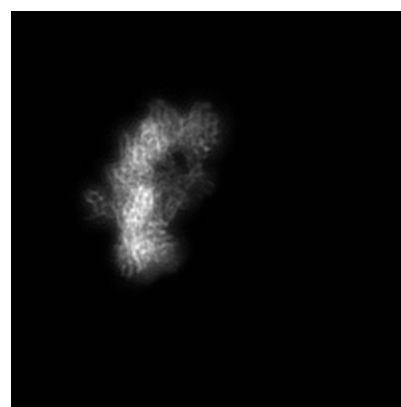
6.1.1 Primary map



X



Y

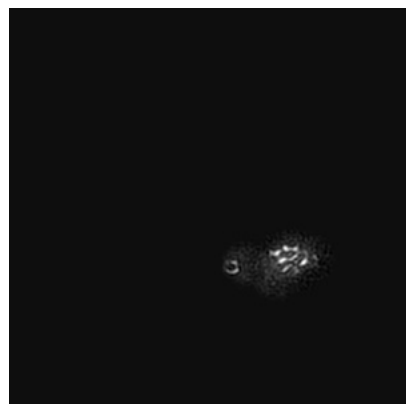


Z

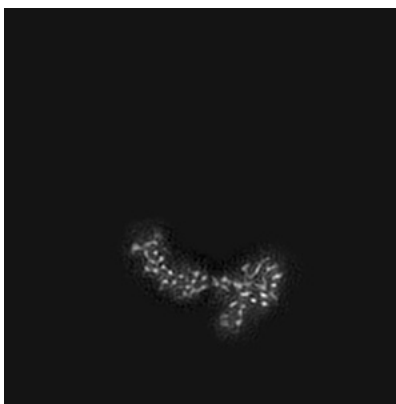
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

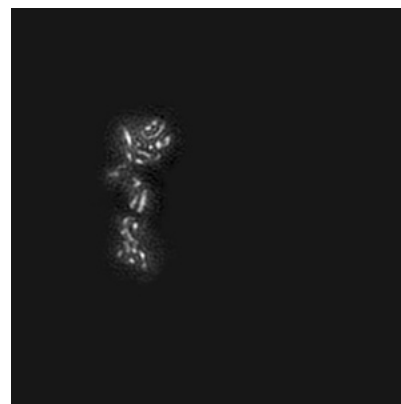
6.2.1 Primary map



X Index: 100



Y Index: 100

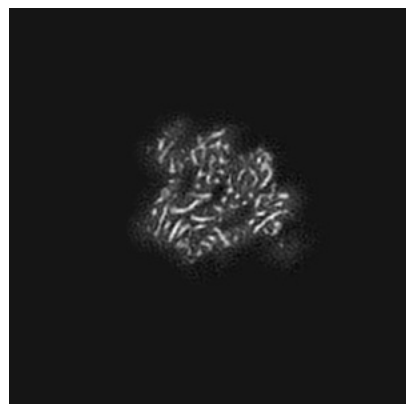


Z Index: 100

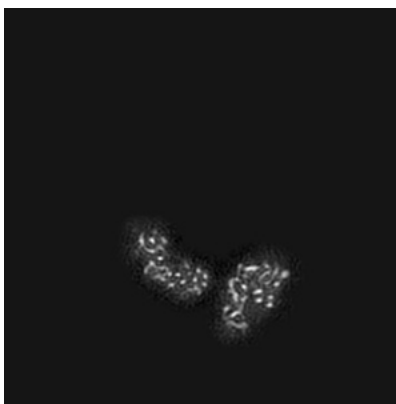
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

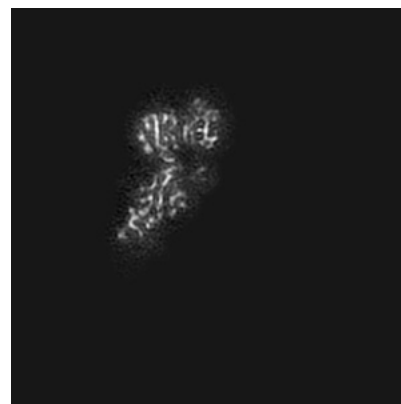
6.3.1 Primary map



X Index: 62



Y Index: 103

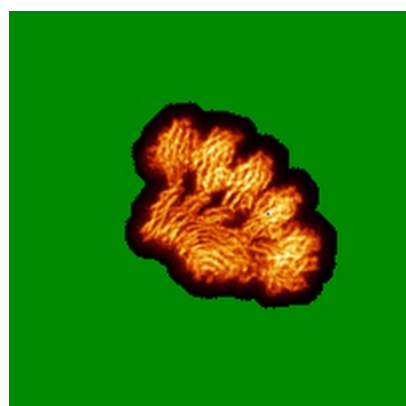


Z Index: 77

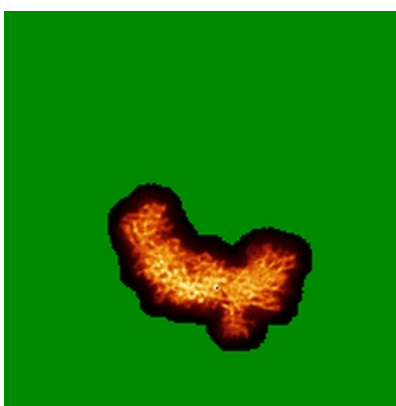
The images above show the largest variance slices of the map in three orthogonal directions.

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

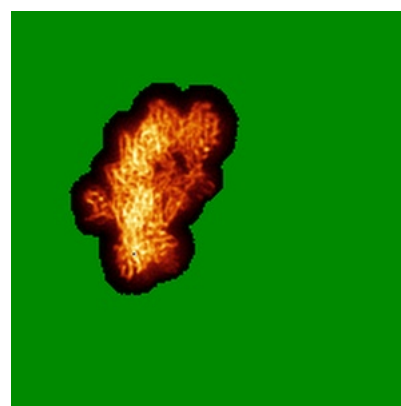
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

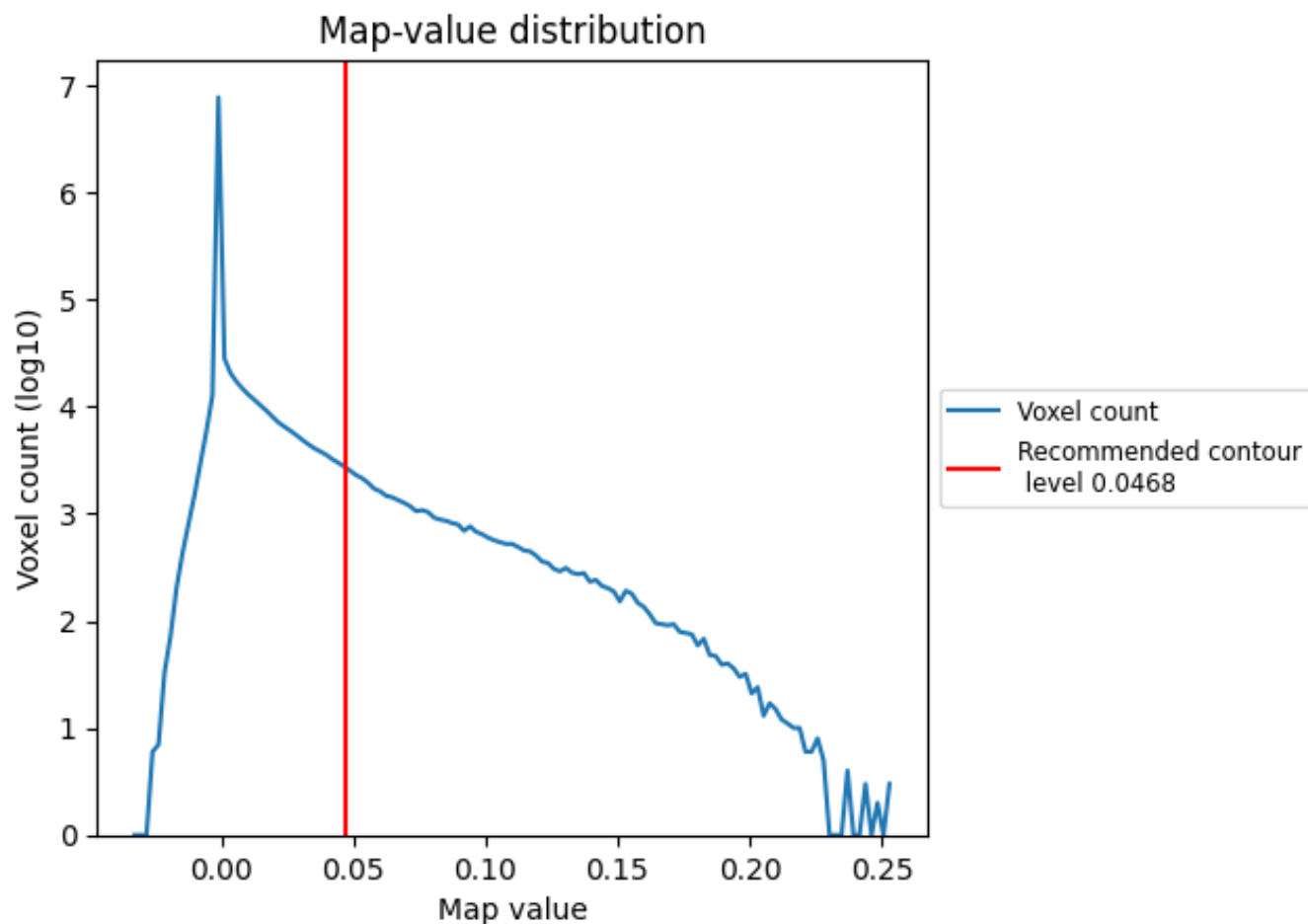
6.6 Mask visualisation

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

7 Map analysis [i](#)

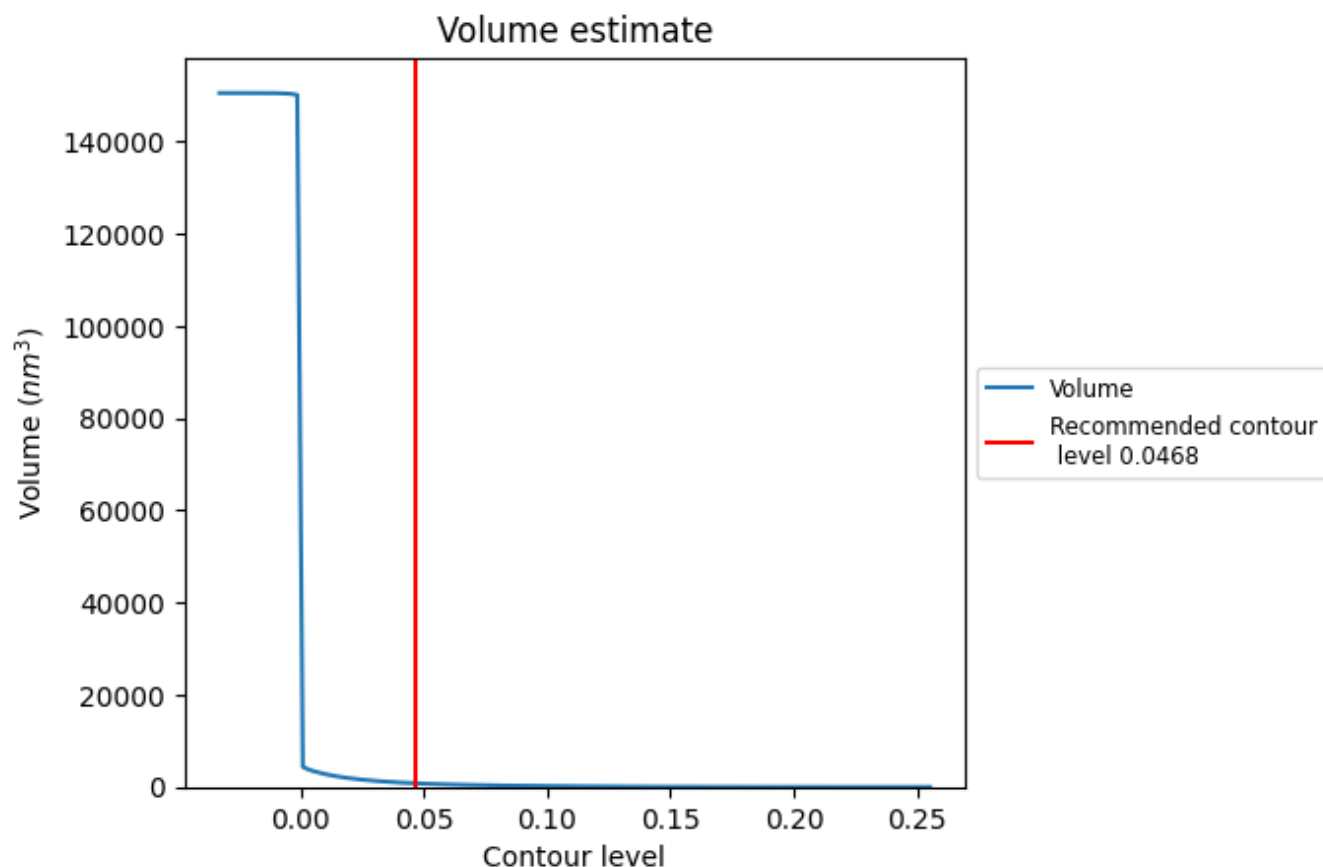
This section contains the results of statistical analysis of the map.

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.

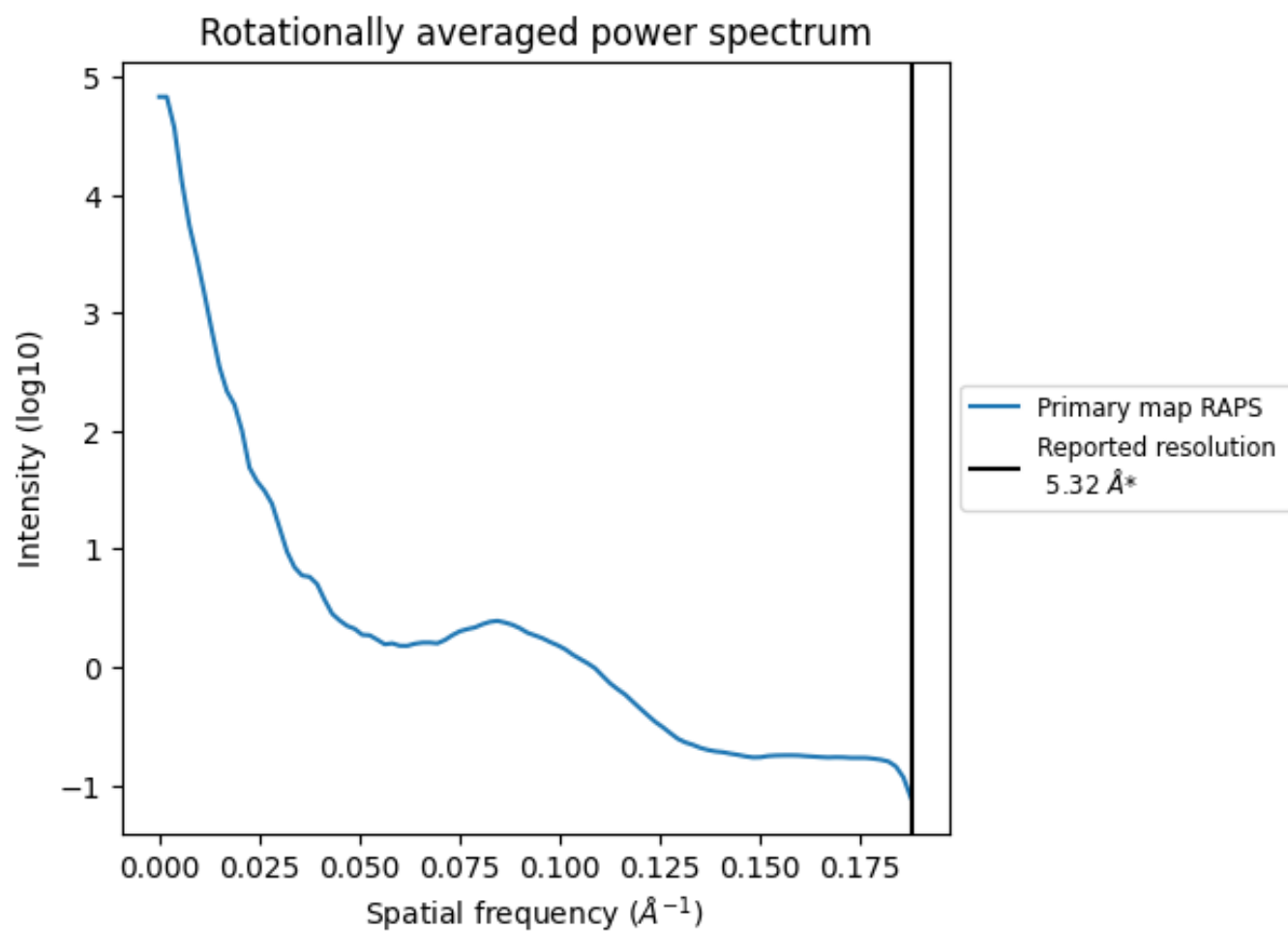
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 786 nm^3 ; this corresponds to an approximate mass of 710 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 0.188 Å⁻¹

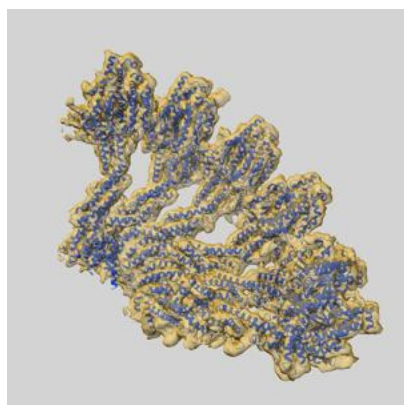
8 Fourier-Shell correlation ⓘ

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

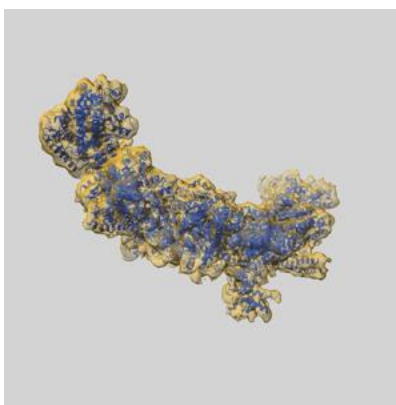
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14005 and PDB model 7QJ0. Per-residue inclusion information can be found in section [3](#) on page [6](#).

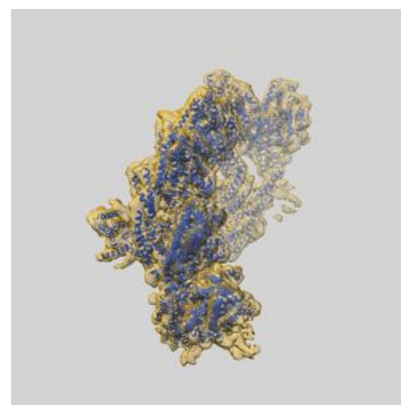
9.1 Map-model overlay [i](#)



X



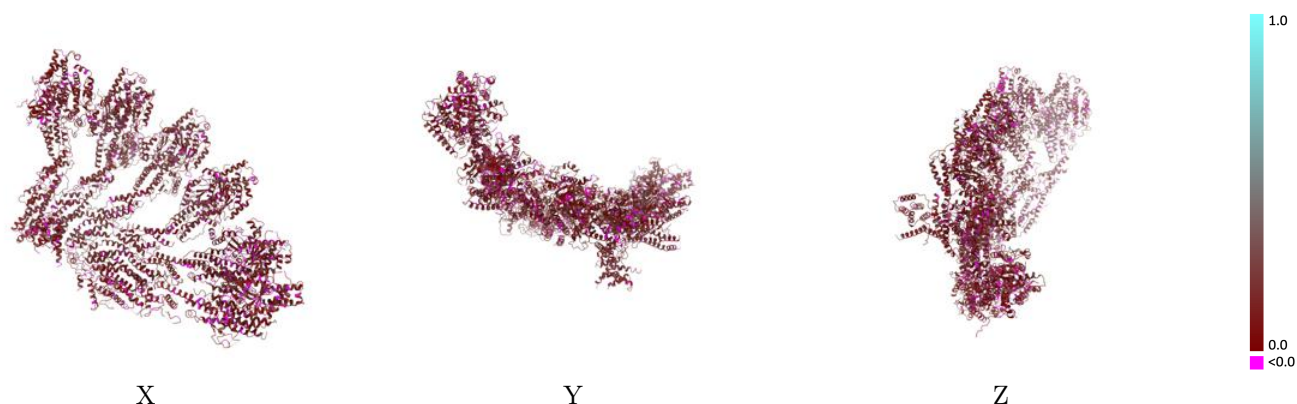
Y



Z

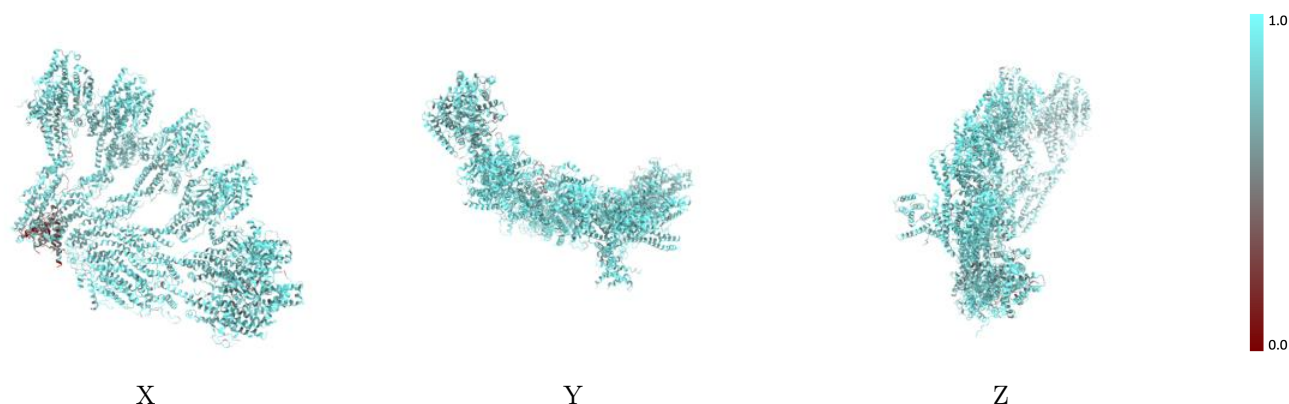
The images above show the 3D surface view of the map at the recommended contour level 0.0468 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



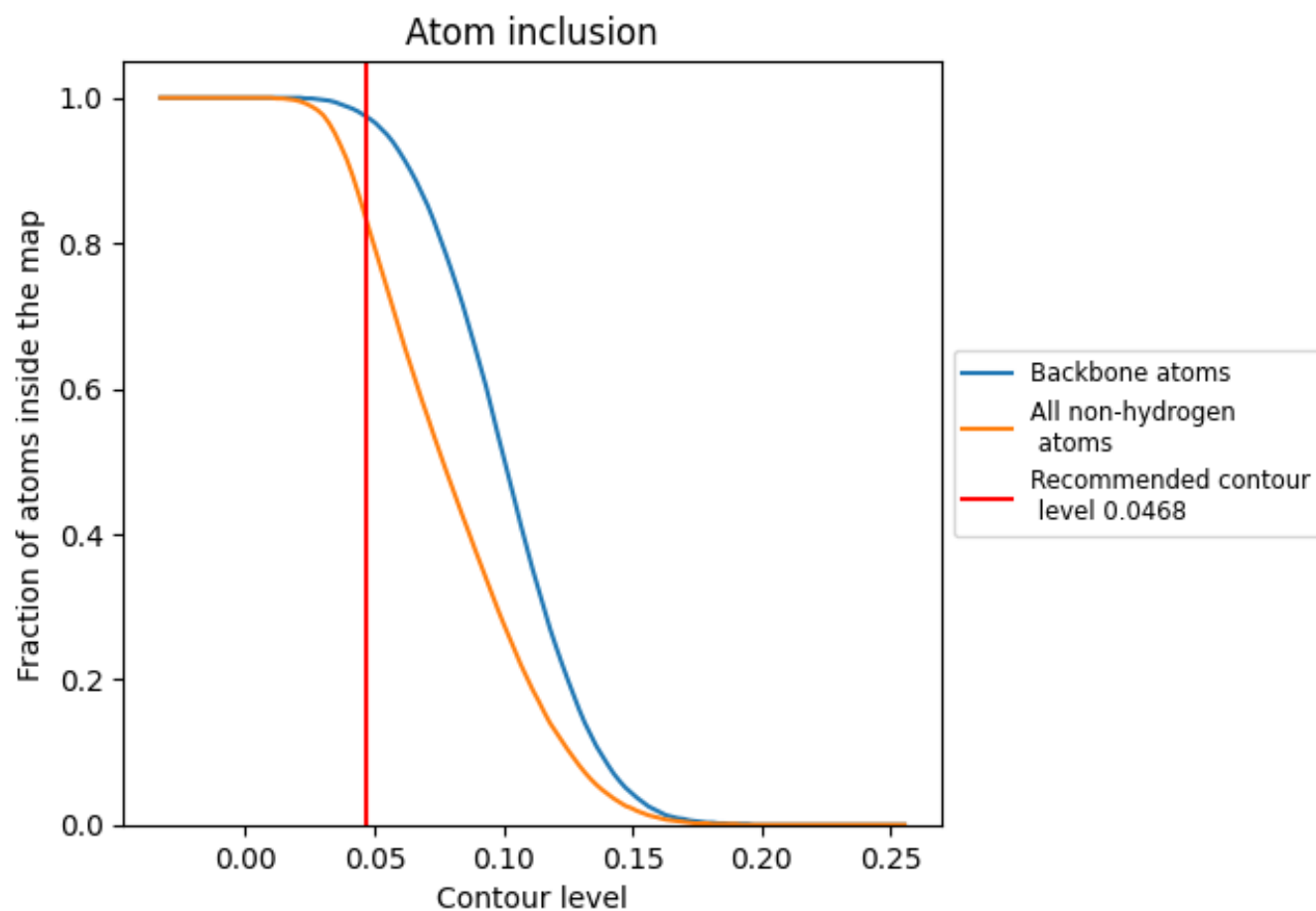
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0468).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 83% 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 (0.0468) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.1450
G	 0.7950	 0.1460
H	 0.8490	 0.1530
I	 0.8510	 0.1550
J	 0.8750	 0.1540
K	 0.8670	 0.1470
L	 0.8140	 0.1440
U	 0.8000	 0.1290
V	 0.8740	 0.1440
W	 0.8990	 0.1620
X	 0.8870	 0.1460
Y	 0.8800	 0.1210
Z	 0.7720	 0.1270
a	 0.3530	 0.1320
b	 0.4220	 0.1370
l	 0.8150	 0.1610
m	 0.8130	 0.1650

