Full wwPDB EM Validation Report

Jan 29, 2022 – 06:20 am GMT

PDB ID	:	7QJ1
EMDB ID	:	EMD-14006
Title	:	Structure of the recombinant human gamma-Tubulin Ring Complex 6-spoked assembly intermediate (spokes 7-12, homogeneous dataset)
Authors	:	Zupa, E.; Pfeffer, S.
Deposited on	:	2021-12-16
Resolution	:	7.00 Å(reported)
Based on initial models	:	7AS4, 6X0U, 6L81, 6V6S

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

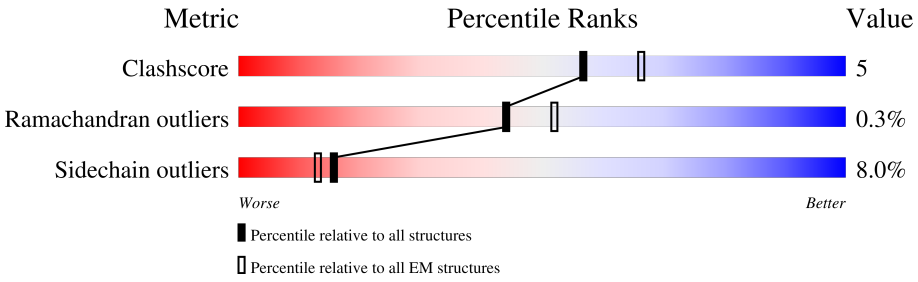
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	J	1024	46% 6% 48%
1	l	1024	10% 89%
2	b	82	39% 62% 13% • 21%
2	m	82	62% 13% • 21%
3	H	907	57% 9% 35%
3	a	907	7% 13% 87%
4	G	902	6% 61% 9% 29%
5	I	667	65% 12% 22%

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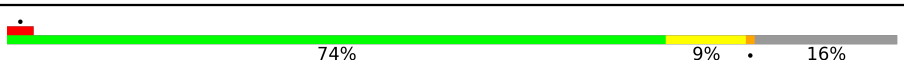
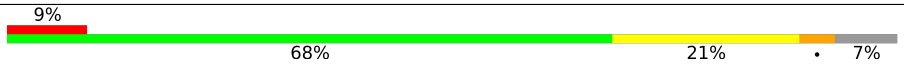
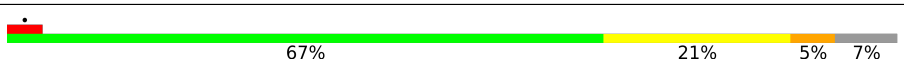
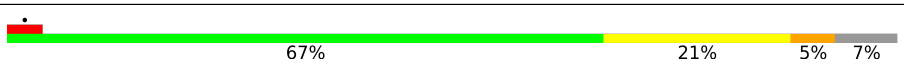
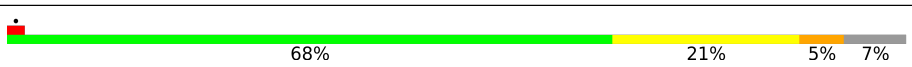
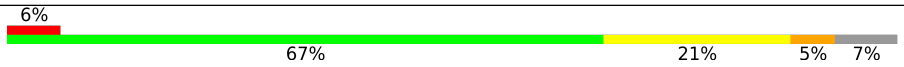
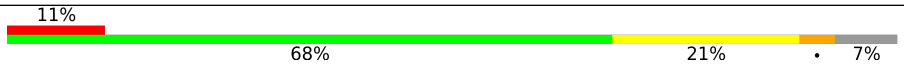
Mol	Chain	Length	Quality of chain
5	K	667	
6	L	1819	
7	U	451	
7	V	451	
7	W	451	
7	X	451	
7	Y	451	
7	Z	451	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 50899 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 Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	l	108	Total	C	N	O	S	0	0
			847	539	150	157	1		
1	J	534	Total	C	N	O	S	0	0
			4429	2893	737	776	23		

- Molecule 2 is a protein called Mitotic-spindle organizing protein 1.

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

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

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

- 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.

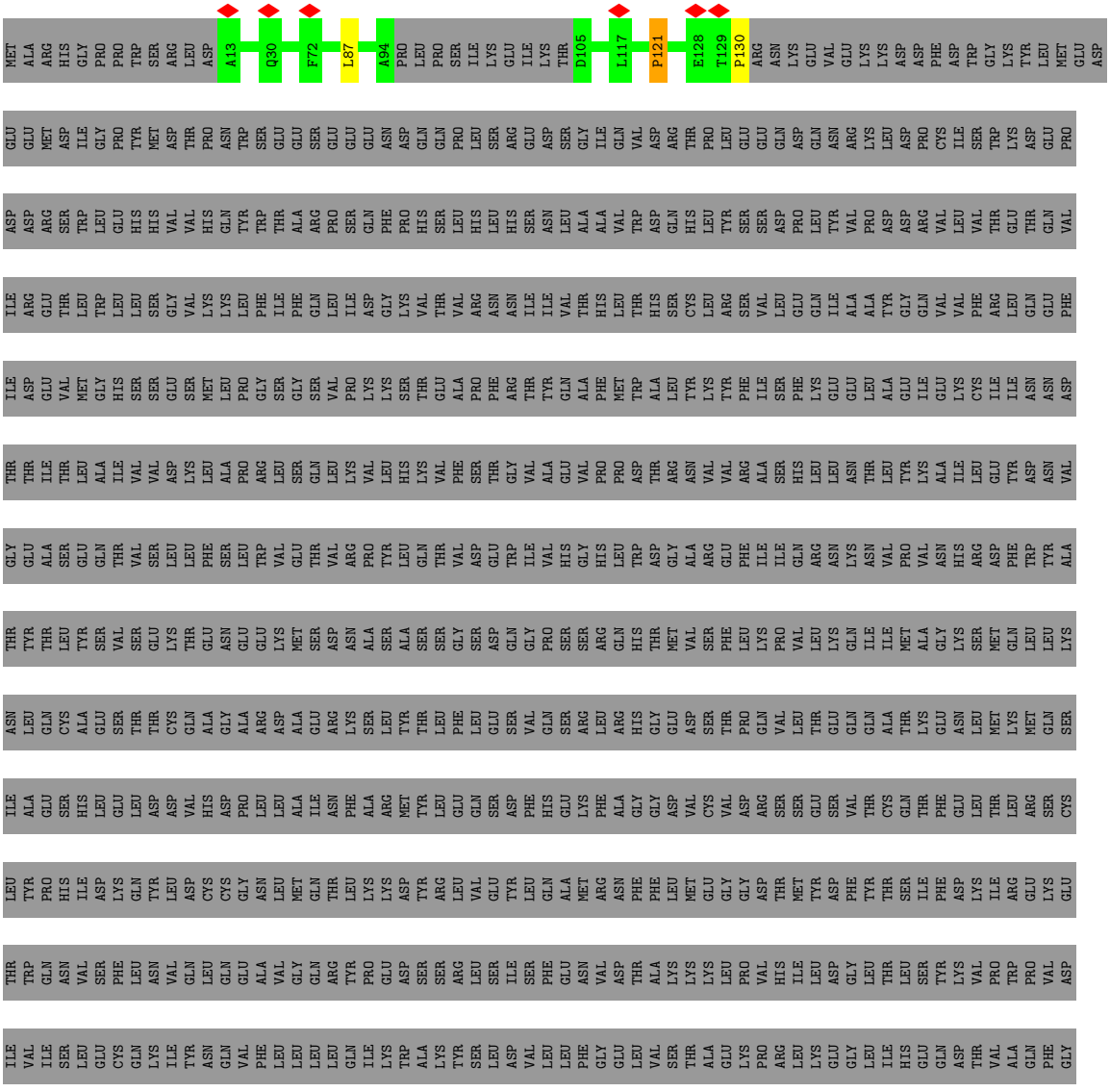
Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	V	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	W	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	X	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
7	Y	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15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

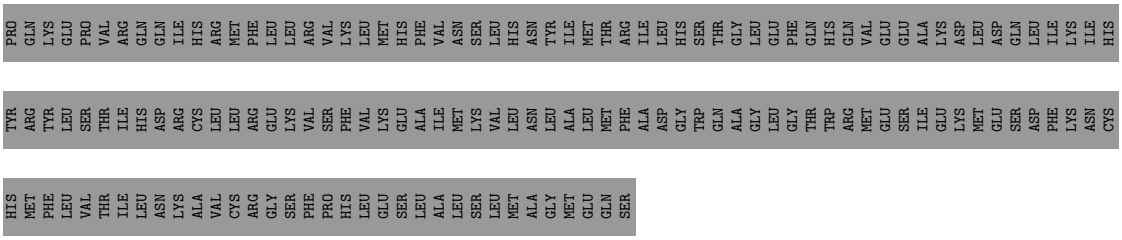
3 Residue-property plots (i)

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: Gamma-tubulin complex component 5

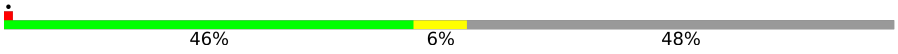
Chain l:

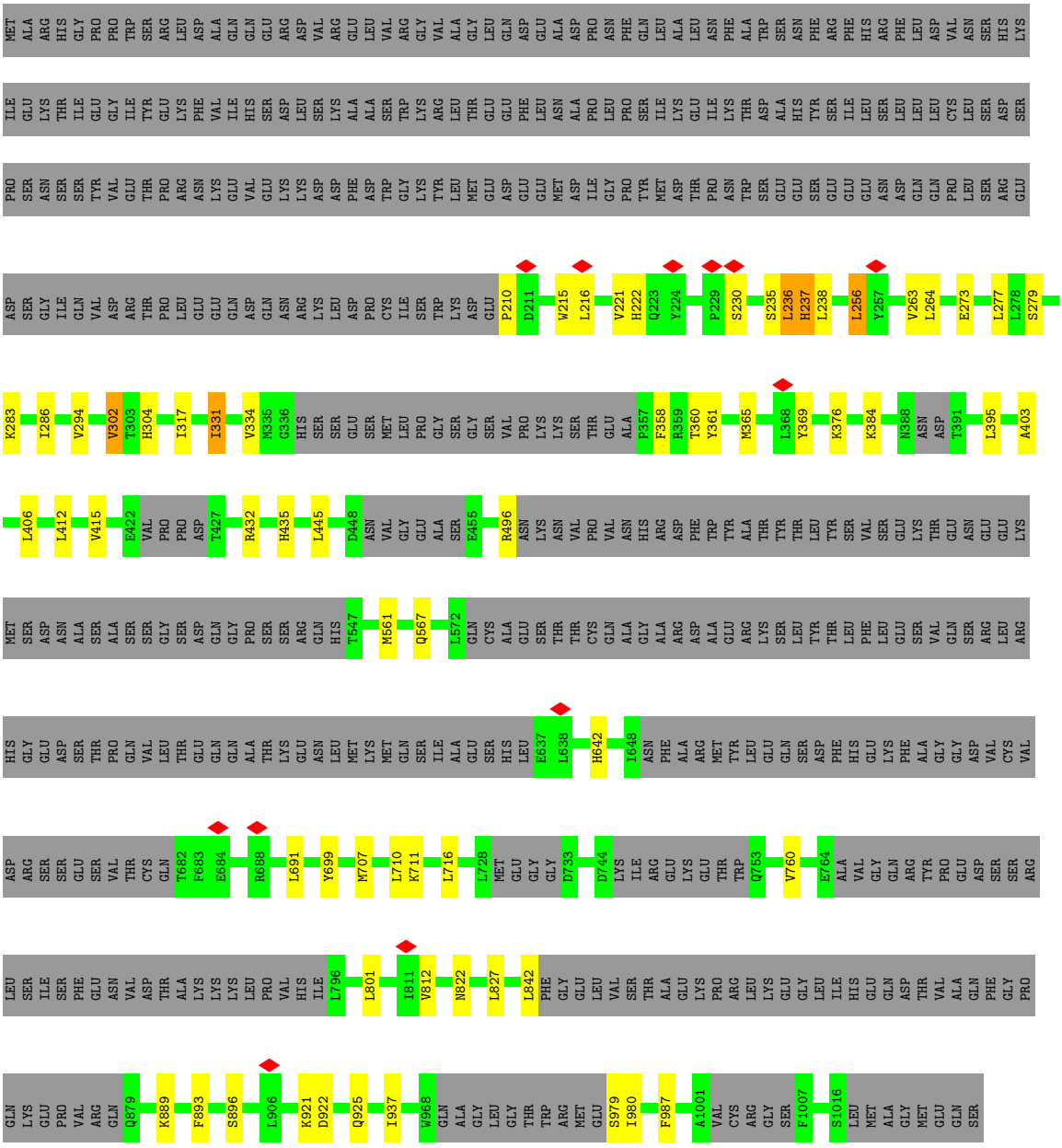




• Molecule 1: Gamma-tubulin complex component 5

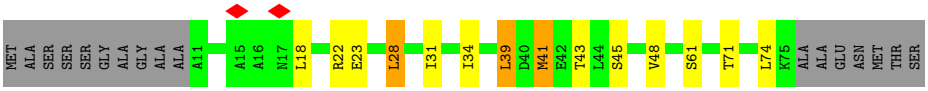
Chain J:





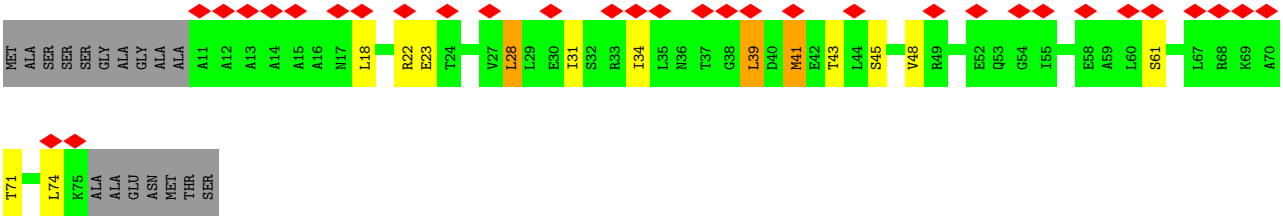
• Molecule 2: Mitotic-spindle organizing protein 1

Chain m:



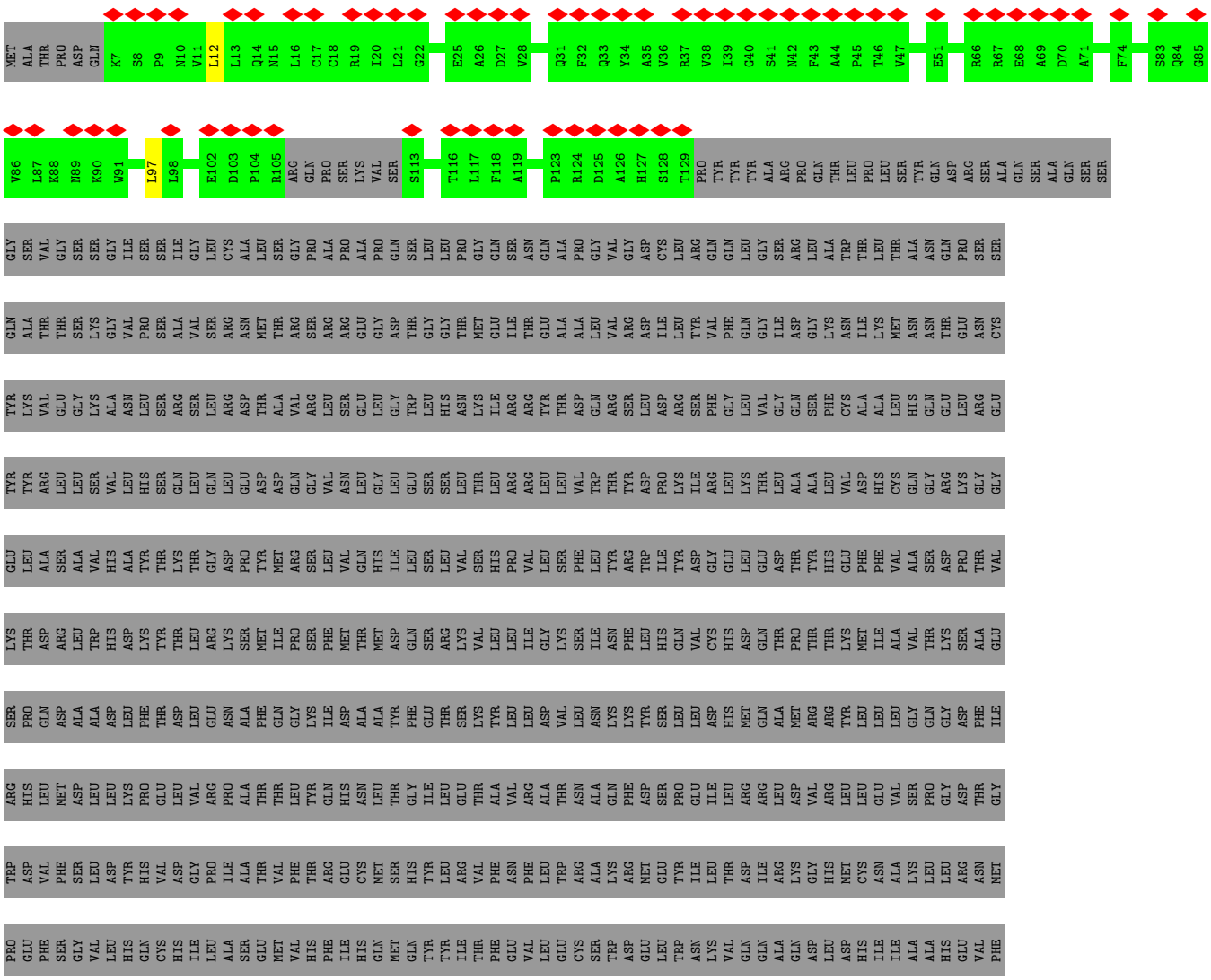
• Molecule 2: Mitotic-spindle organizing protein 1

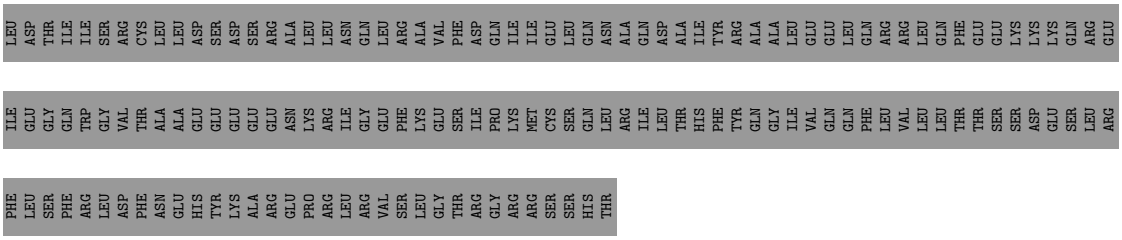
Chain b:



• Molecule 3: Gamma-tubulin complex component 3

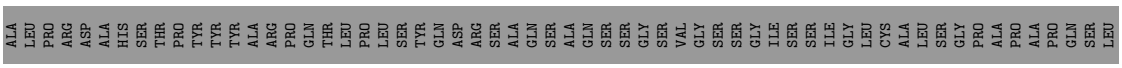
Chain a:

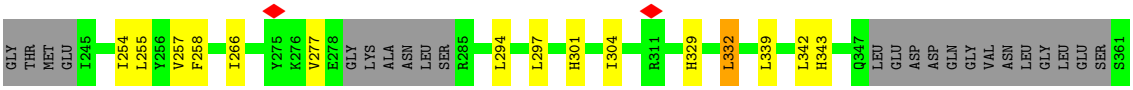


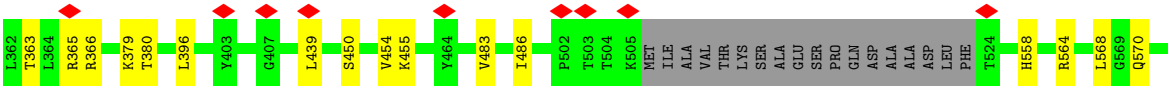


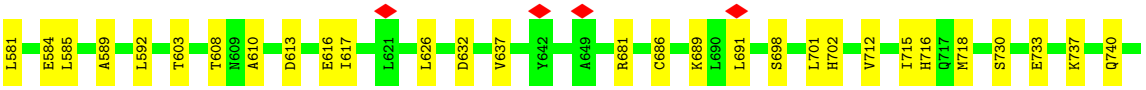
• Molecule 3: Gamma-tubulin complex component 3

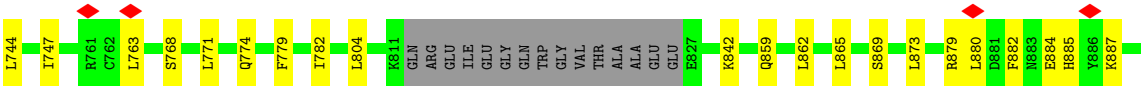
Chain H:

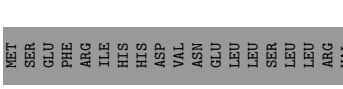






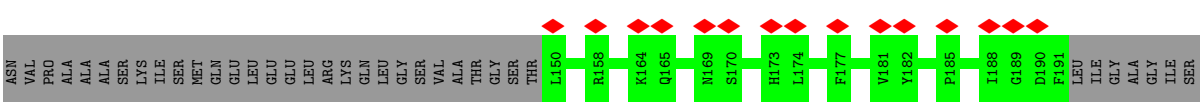


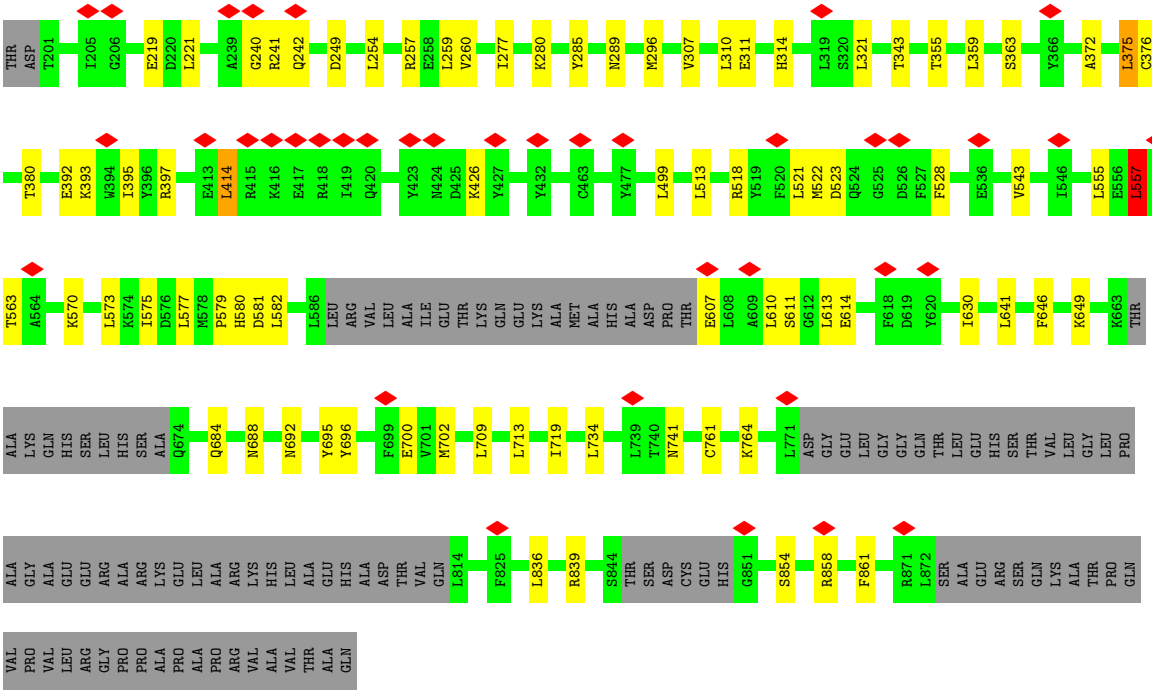




• Molecule 4: Gamma-tubulin complex component 2

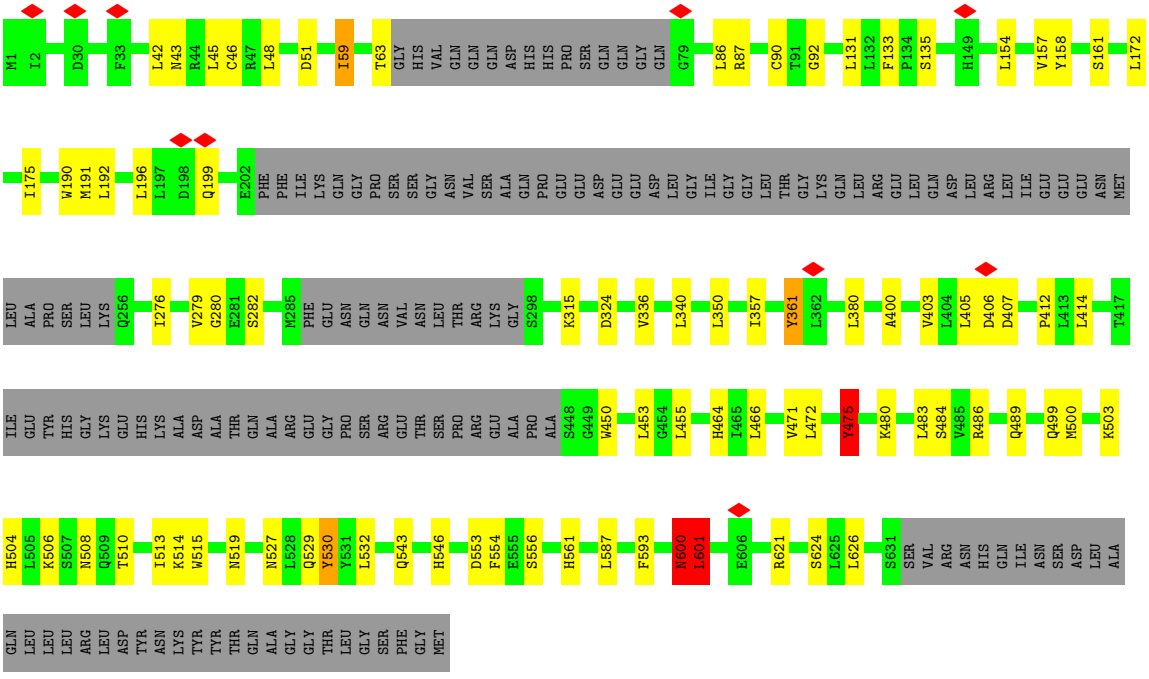
Chain G:





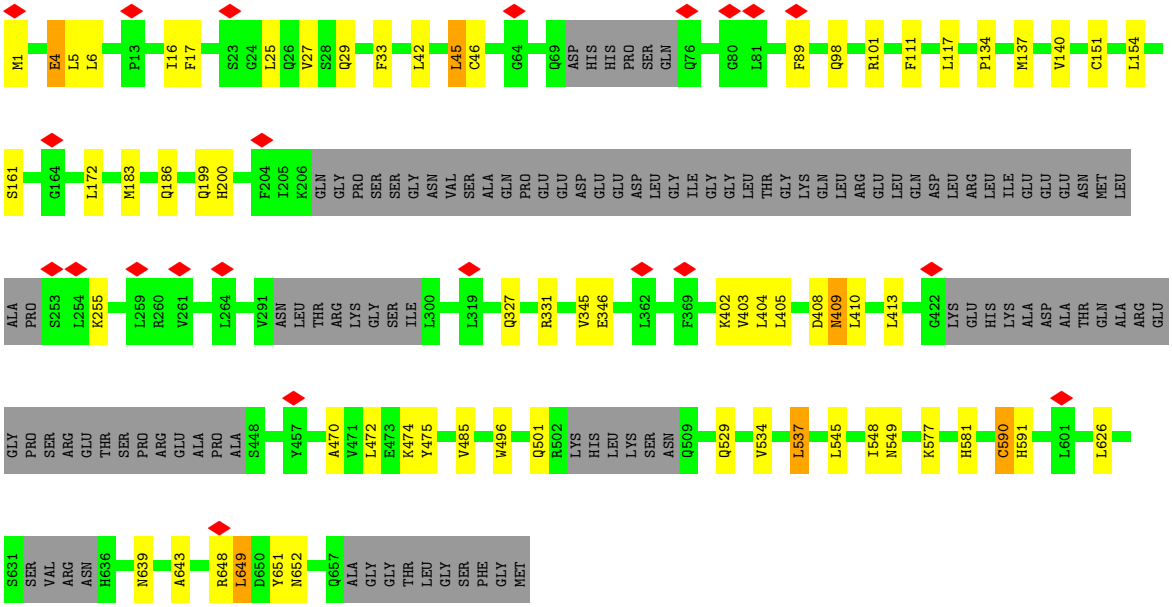
• Molecule 5: Gamma-tubulin complex component 4

Chain I:



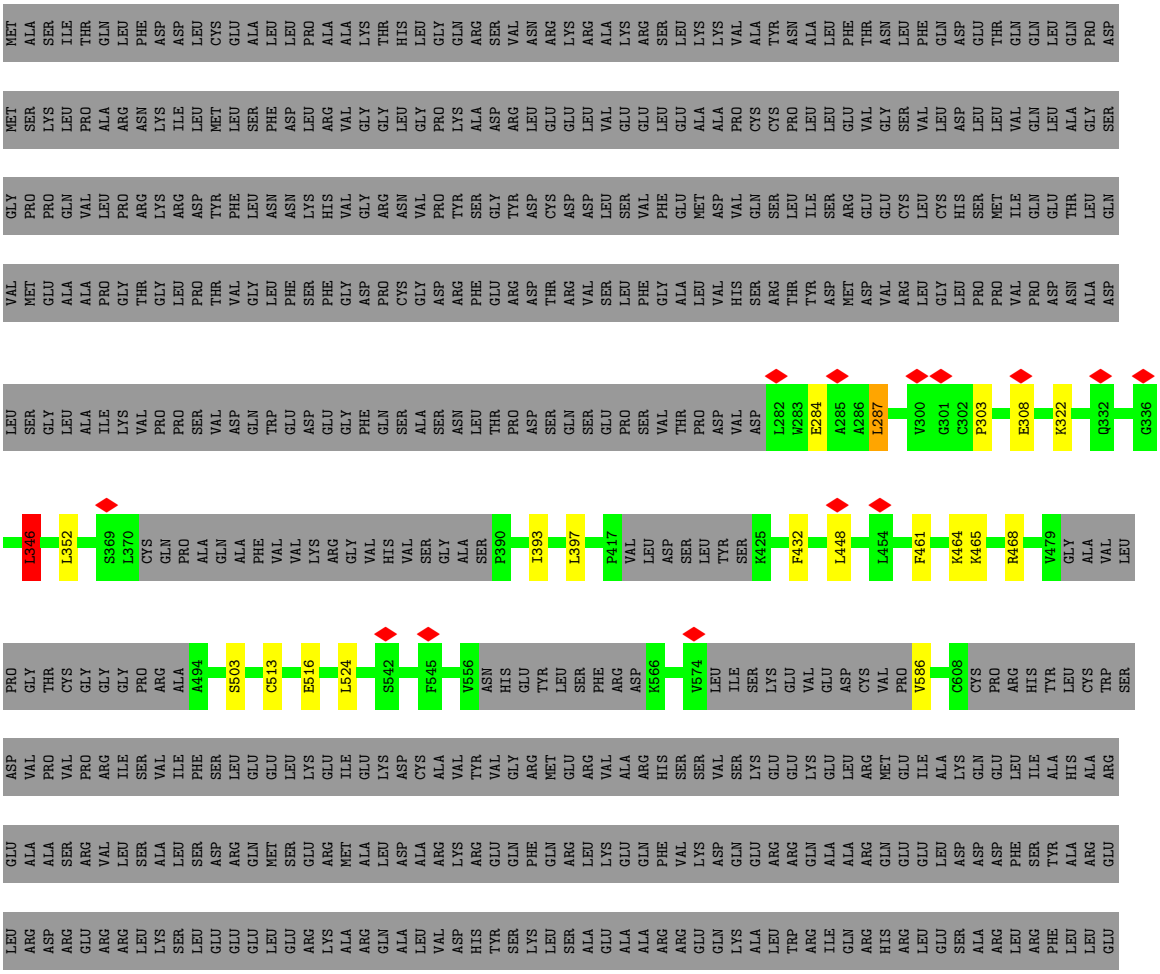
• Molecule 5: Gamma-tubulin complex component 4

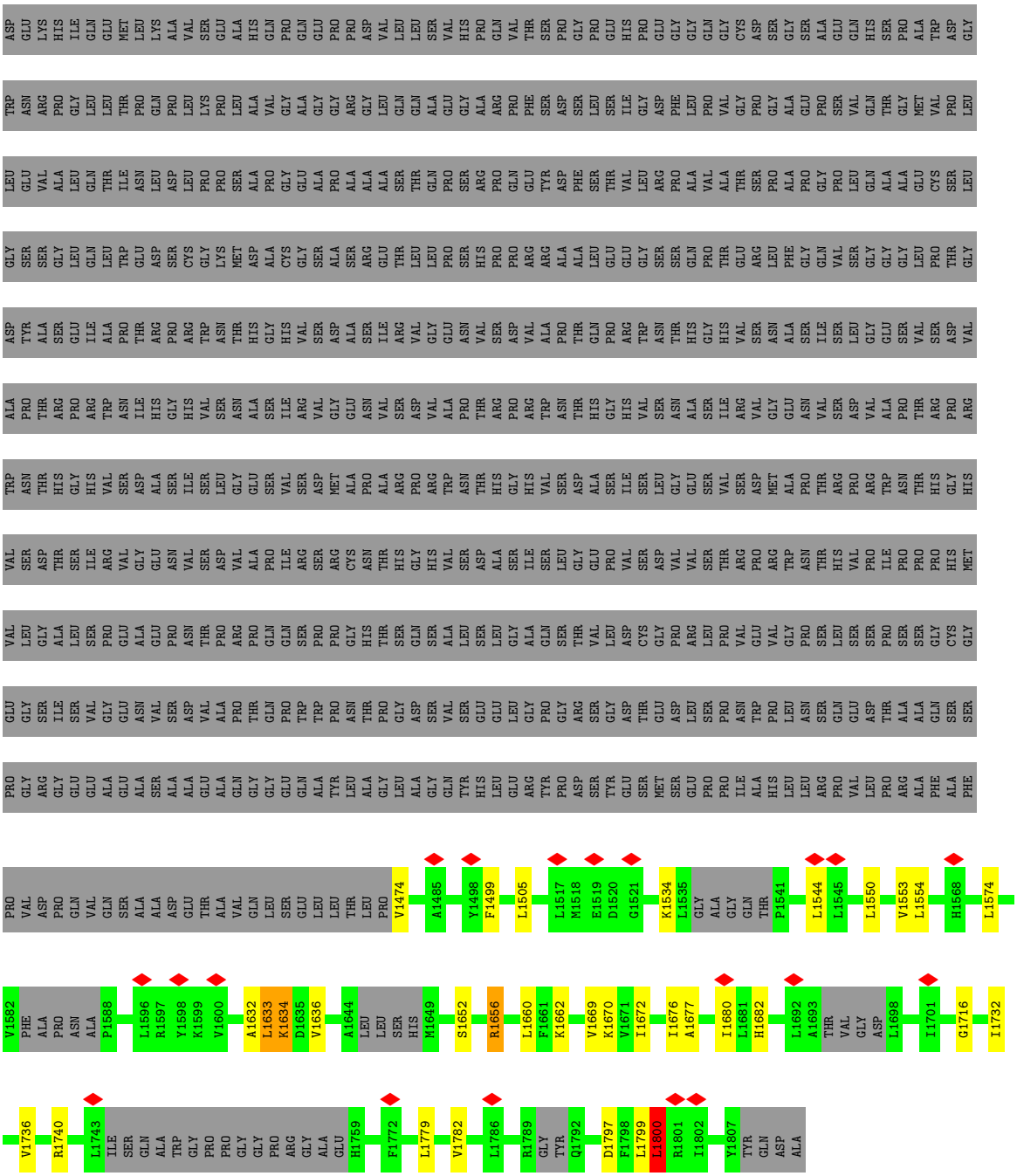
Chain K:



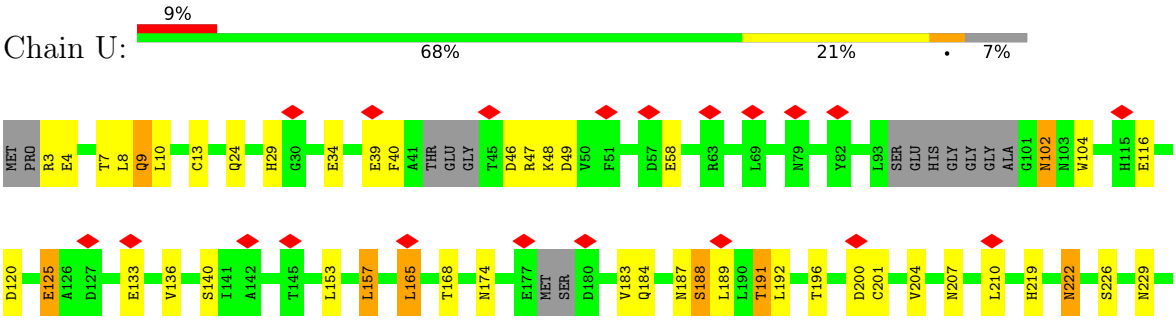
• Molecule 6: Gamma-tubulin complex component 6

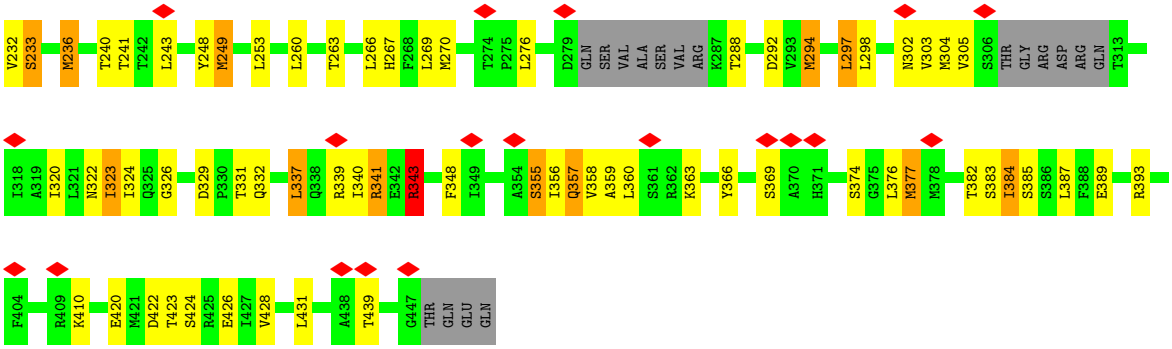
Chain L:





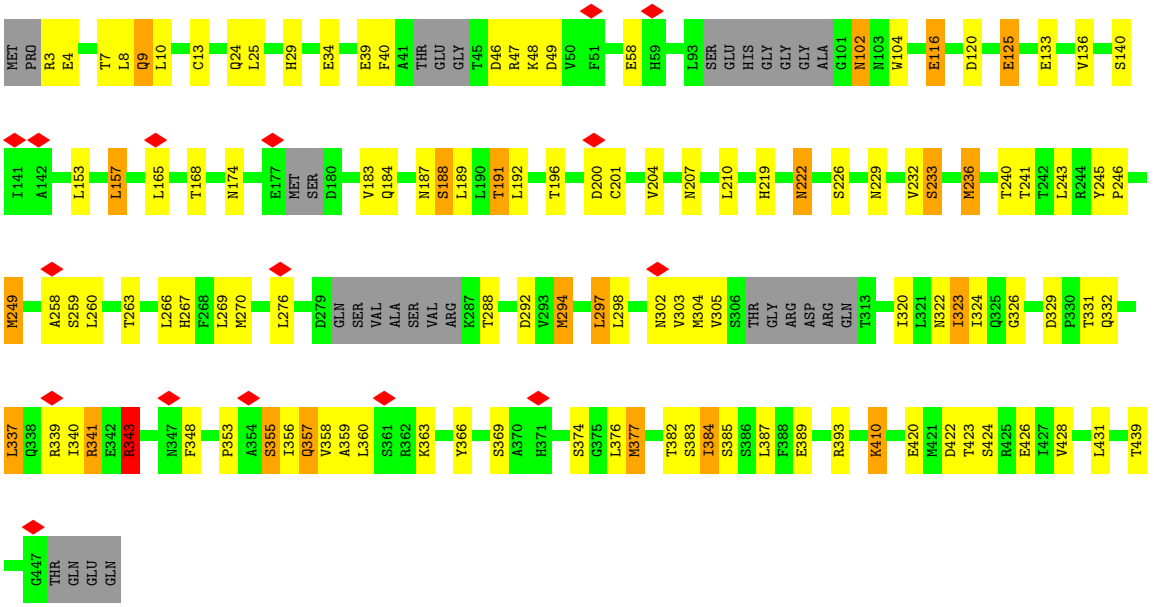
• Molecule 7: Tubulin gamma-1 chain





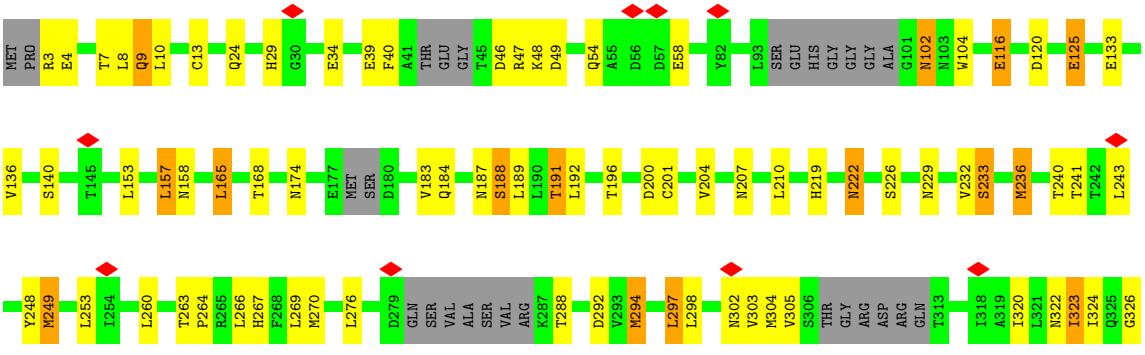
• Molecule 7: Tubulin gamma-1 chain

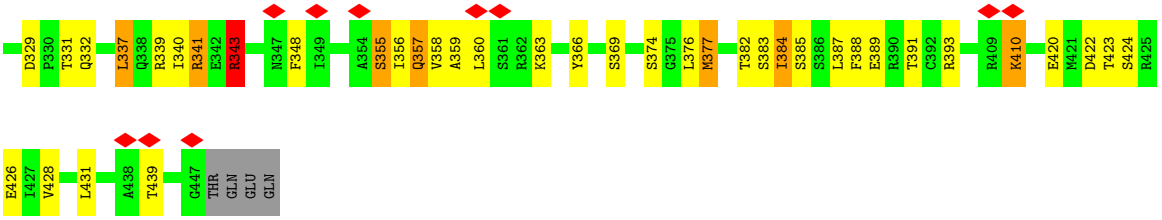
Chain V:



• Molecule 7: Tubulin gamma-1 chain

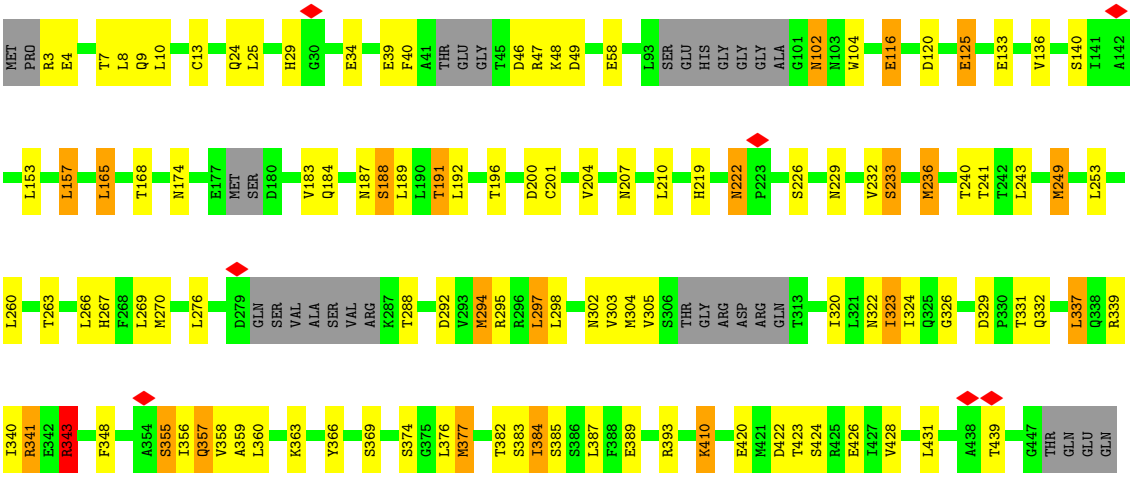
Chain W:





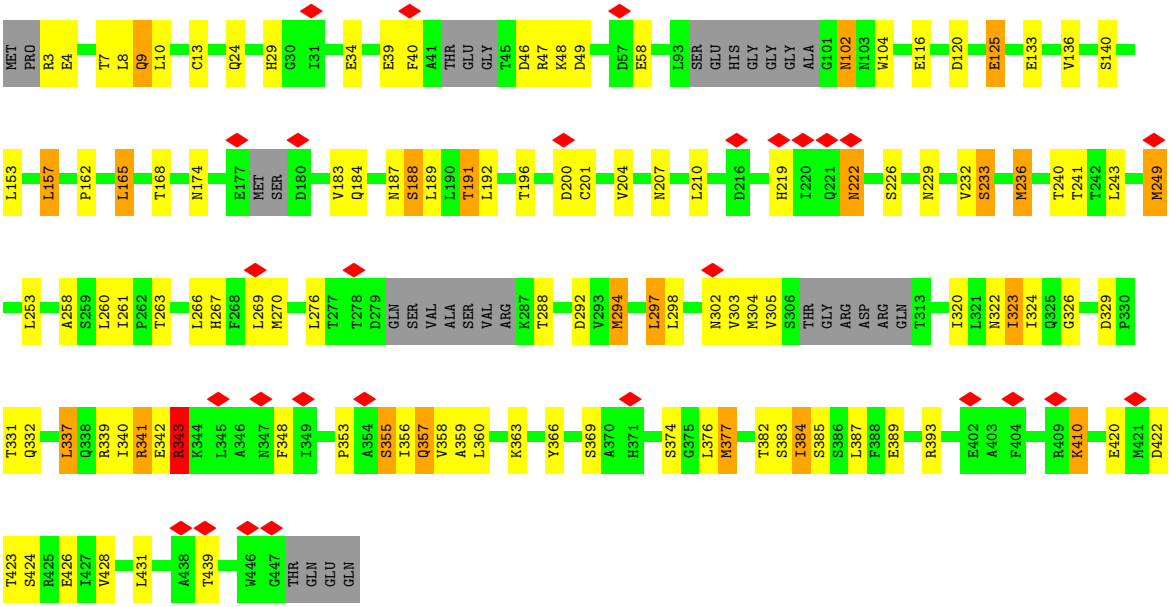
• Molecule 7: Tubulin gamma-1 chain

Chain X:



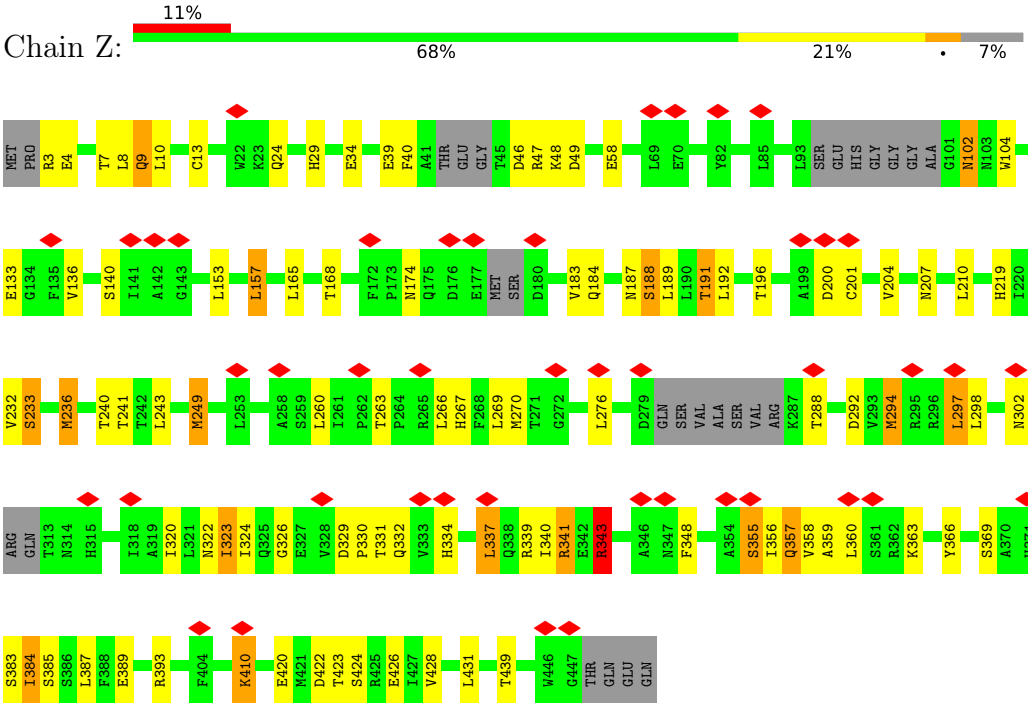
• Molecule 7: Tubulin gamma-1 chain

Chain Y:



• Molecule 7: Tubulin gamma-1 chain

Chain Z:


11%
68%
21%
7%
MET PRO R3 E4 T7 L8 Q9 L10 C13 W22 K23 Q24 H29 E34 E39 F40 A41 THR GLU GLY T45 D46 R47 K48 D49 E58 L69 E70 Y82 L85 L93 SER GLU HIS GLY GLY GLY ALA G101 N102 N103 W104 E116 D120 E125
E133 G134 F135 V136 S140 I141 A142 G143 L153 L157 L165 T168 F172 P173 N174 Q176 D176 E177 MET SER D180 V183 Q184 N187 S188 L189 L190 T191 L192 T196 A199 D200 C201 V204 N207 L210 H219 I220 Q221 N222 P223 S226 N229
V232 S233 M236 T240 T241 T242 L243 M249 L253 A258 S259 L260 I261 P262 T263 P264 R265 L266 H267 F268 L269 M270 T271 G272 L276 D279 GLN SER VAL ALA SER VAL ARG K287 T288 D292 V293 M294 R295 R296 L297 L298 N302 V303 M304 V305 S306 THR GLY ARG ASP
ARG GLN T313 N314 H315 I318 A319 I320 L321 N322 I323 I324 Q325 G326 E327 V328 D329 P330 T331 Q332 V333 H334 L337 Q338 R339 I340 R341 E342 R343 A346 N347 F348 A354 S355 I356 Q357 V358 A359 L360 S361 R362 K363 Y366 S369 A370 H371 R372 V373 S374 G375 L376 M377 T382
S383 I384 S385 S386 L387 F388 E389 R393 F404 K410 E420 M421 D422 T423 S424 R425 E426 T427 V428 L431 T439 W446 G447 THR GLN GLU GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59861	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 ($e^-/Å^2$)	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	0.338	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0571	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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	J	0.34	0/4525	0.70	6/6119 (0.1%)
1	l	0.34	0/863	0.66	3/1166 (0.3%)
2	b	0.42	0/484	0.98	4/653 (0.6%)
2	m	0.42	0/484	0.98	4/653 (0.6%)
3	H	0.35	0/5009	0.67	7/6761 (0.1%)
3	a	0.38	0/948	0.72	1/1277 (0.1%)
4	G	0.36	0/5295	0.71	5/7147 (0.1%)
5	I	0.42	3/4322 (0.1%)	0.67	5/5853 (0.1%)
5	K	0.36	0/4683	0.66	6/6338 (0.1%)
6	L	0.35	0/4697	0.65	7/6348 (0.1%)
7	U	0.33	0/3441	0.71	10/4661 (0.2%)
7	V	0.33	0/3441	0.71	10/4661 (0.2%)
7	W	0.33	0/3441	0.71	10/4661 (0.2%)
7	X	0.33	0/3441	0.71	10/4661 (0.2%)
7	Y	0.33	0/3441	0.71	10/4661 (0.2%)
7	Z	0.33	0/3441	0.71	10/4661 (0.2%)
All	All	0.35	3/51956 (0.0%)	0.70	108/70281 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	7
3	H	0	1
4	G	0	2
5	I	0	4
5	K	0	2
6	L	0	1
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	361	TYR	CB-CG	-7.70	1.40	1.51
5	I	530	TYR	CB-CG	-5.12	1.44	1.51
5	I	361	TYR	CD2-CE2	-5.05	1.31	1.39

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	557	LEU	CB-CG-CD2	14.86	136.26	111.00
4	G	557	LEU	CB-CG-CD1	-12.97	88.95	111.00
7	X	343	ARG	NE-CZ-NH2	11.06	125.83	120.30
7	W	343	ARG	NE-CZ-NH2	11.06	125.83	120.30
7	V	343	ARG	NE-CZ-NH2	11.02	125.81	120.30
7	U	343	ARG	NE-CZ-NH2	11.00	125.80	120.30
7	Z	343	ARG	NE-CZ-NH2	10.99	125.80	120.30
7	Y	343	ARG	NE-CZ-NH2	10.97	125.78	120.30
3	H	691	LEU	CA-CB-CG	8.87	135.69	115.30
7	Y	157	LEU	CA-CB-CG	8.63	135.15	115.30
7	X	157	LEU	CA-CB-CG	8.61	135.10	115.30
7	Z	157	LEU	CA-CB-CG	8.61	135.10	115.30
7	W	157	LEU	CA-CB-CG	8.60	135.09	115.30
7	U	157	LEU	CA-CB-CG	8.60	135.08	115.30
7	V	157	LEU	CA-CB-CG	8.60	135.08	115.30
7	X	343	ARG	NE-CZ-NH1	-8.11	116.25	120.30
7	Y	343	ARG	NE-CZ-NH1	-8.07	116.27	120.30
7	V	343	ARG	NE-CZ-NH1	-8.02	116.29	120.30
7	W	343	ARG	NE-CZ-NH1	-7.99	116.31	120.30
7	U	343	ARG	NE-CZ-NH1	-7.95	116.32	120.30
7	Z	343	ARG	NE-CZ-NH1	-7.95	116.33	120.30
6	L	448	LEU	CA-CB-CG	7.89	133.44	115.30
4	G	557	LEU	CA-CB-CG	-7.88	97.19	115.30
1	l	121	PRO	N-CA-CB	7.36	112.13	103.30
3	H	585	LEU	CB-CG-CD1	-7.02	99.07	111.00
5	K	404	LEU	CA-CB-CG	6.99	131.38	115.30
2	b	18	LEU	CA-CB-CG	6.96	131.31	115.30
2	m	18	LEU	CA-CB-CG	6.95	131.29	115.30
6	L	1800	LEU	CB-CG-CD1	-6.93	99.21	111.00
3	H	396	LEU	CA-CB-CG	6.89	131.14	115.30
2	b	28	LEU	CA-CB-CG	6.88	131.11	115.30
2	m	28	LEU	CA-CB-CG	6.87	131.10	115.30
6	L	287	LEU	CA-CB-CG	6.38	129.98	115.30
5	K	537	LEU	CA-CB-CG	6.32	129.84	115.30
2	b	39	LEU	CB-CG-CD1	-6.31	100.27	111.00
2	m	39	LEU	CB-CG-CD1	-6.29	100.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	W	337	LEU	CA-CB-CG	6.23	129.62	115.30
7	Z	337	LEU	CA-CB-CG	6.22	129.62	115.30
7	U	337	LEU	CA-CB-CG	6.22	129.60	115.30
7	X	337	LEU	CA-CB-CG	6.22	129.60	115.30
7	V	337	LEU	CA-CB-CG	6.21	129.59	115.30
7	Y	337	LEU	CA-CB-CG	6.20	129.56	115.30
6	L	1799	LEU	CA-CB-CG	6.18	129.53	115.30
6	L	1800	LEU	CB-CG-CD2	6.10	121.37	111.00
5	K	45	LEU	CA-CB-CG	6.08	129.28	115.30
7	U	294	MET	CB-CG-SD	6.04	130.53	112.40
7	V	294	MET	CB-CG-SD	6.04	130.51	112.40
7	Z	294	MET	CB-CG-SD	6.03	130.50	112.40
7	W	294	MET	CB-CG-SD	6.03	130.49	112.40
7	X	294	MET	CB-CG-SD	6.02	130.47	112.40
7	Y	294	MET	CB-CG-SD	6.02	130.46	112.40
2	m	41	MET	CA-CB-CG	6.00	123.50	113.30
2	b	41	MET	CA-CB-CG	5.98	123.47	113.30
5	K	649	LEU	CA-CB-CG	5.95	128.99	115.30
3	H	804	LEU	CA-CB-CG	5.93	128.94	115.30
7	Y	125	GLU	CA-CB-CG	5.85	126.26	113.40
7	V	125	GLU	CA-CB-CG	5.84	126.26	113.40
7	X	125	GLU	CA-CB-CG	5.84	126.24	113.40
1	J	827	LEU	CA-CB-CG	5.84	128.73	115.30
7	W	125	GLU	CA-CB-CG	5.83	126.24	113.40
7	Z	125	GLU	CA-CB-CG	5.82	126.21	113.40
7	U	125	GLU	CA-CB-CG	5.82	126.20	113.40
6	L	1633	LEU	CA-CB-CG	5.80	128.65	115.30
4	G	836	LEU	CA-CB-CG	5.73	128.47	115.30
1	J	237	HIS	C-N-CA	5.67	135.89	121.70
7	U	343	ARG	CD-NE-CZ	5.64	131.50	123.60
7	Z	343	ARG	CD-NE-CZ	5.64	131.50	123.60
7	W	343	ARG	CD-NE-CZ	5.64	131.50	123.60
7	V	343	ARG	CD-NE-CZ	5.62	131.47	123.60
7	W	210	LEU	CA-CB-CG	5.62	128.23	115.30
7	U	210	LEU	CA-CB-CG	5.62	128.23	115.30
7	Y	343	ARG	CD-NE-CZ	5.62	131.47	123.60
7	Z	210	LEU	CA-CB-CG	5.62	128.23	115.30
7	Y	210	LEU	CA-CB-CG	5.62	128.22	115.30
7	X	210	LEU	CA-CB-CG	5.62	128.22	115.30
1	l	130	PRO	N-CA-CB	5.60	110.02	103.30
3	H	568	LEU	CA-CB-CG	5.60	128.18	115.30
7	X	343	ARG	CD-NE-CZ	5.59	131.43	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	210	LEU	CA-CB-CG	5.59	128.16	115.30
1	J	256	LEU	CA-CB-CG	5.57	128.12	115.30
3	a	97	LEU	CA-CB-CG	5.52	128.00	115.30
5	K	5	LEU	CA-CB-CG	5.46	127.85	115.30
5	K	626	LEU	CA-CB-CG	5.37	127.64	115.30
1	J	395	LEU	CA-CB-CG	5.35	127.60	115.30
7	V	189	LEU	CA-CB-CG	5.35	127.59	115.30
1	J	710	LEU	CA-CB-CG	5.34	127.59	115.30
7	U	189	LEU	CA-CB-CG	5.34	127.58	115.30
7	Y	189	LEU	CA-CB-CG	5.33	127.56	115.30
7	Z	189	LEU	CA-CB-CG	5.32	127.54	115.30
7	Y	294	MET	CA-CB-CG	5.32	122.34	113.30
7	X	189	LEU	CA-CB-CG	5.31	127.52	115.30
7	U	294	MET	CA-CB-CG	5.31	122.33	113.30
7	X	294	MET	CA-CB-CG	5.31	122.33	113.30
7	W	189	LEU	CA-CB-CG	5.30	127.50	115.30
7	V	294	MET	CA-CB-CG	5.30	122.31	113.30
7	W	294	MET	CA-CB-CG	5.30	122.31	113.30
7	Z	294	MET	CA-CB-CG	5.28	122.27	113.30
6	L	1799	LEU	CB-CG-CD2	-5.22	102.12	111.00
4	G	375	LEU	CA-CB-CG	5.16	127.17	115.30
5	I	626	LEU	CA-CB-CG	5.16	127.16	115.30
1	l	87	LEU	CA-CB-CG	5.12	127.09	115.30
5	I	600	ASN	C-N-CA	5.12	134.51	121.70
5	I	475	TYR	CB-CG-CD2	-5.09	117.94	121.00
5	I	86	LEU	CA-CB-CG	5.09	127.01	115.30
5	I	472	LEU	CA-CB-CG	5.09	127.01	115.30
1	J	264	LEU	CA-CB-CG	5.06	126.94	115.30
3	H	701	LEU	CA-CB-CG	5.04	126.90	115.30
3	H	332	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	240	GLY	Peptide
4	G	580	HIS	Peptide
3	H	454	VAL	Peptide
5	I	407	ASP	Peptide
5	I	503	LYS	Peptide
5	I	600	ASN	Peptide
5	I	601	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	J	210	PRO	Peptide
1	J	221	VAL	Peptide
1	J	235	SER	Peptide
1	J	236	LEU	Mainchain
1	J	237	HIS	Peptide
1	J	256	LEU	Peptide
1	J	263	VAL	Peptide
5	K	408	ASP	Peptide
5	K	409	ASN	Mainchain
6	L	346	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4429	0	4482	29	0
1	l	847	0	789	0	0
2	b	484	0	512	0	0
2	m	484	0	512	0	0
3	H	4907	0	4896	46	0
3	a	933	0	953	0	0
4	G	5186	0	5219	44	0
5	I	4225	0	4259	48	0
5	K	4579	0	4586	43	0
6	L	4587	0	4636	31	0
7	U	3373	0	3325	45	0
7	V	3373	0	3325	47	0
7	W	3373	0	3325	46	0
7	X	3373	0	3325	43	0
7	Y	3373	0	3325	47	0
7	Z	3373	0	3325	45	0
All	All	50899	0	50794	484	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 (484) 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)
5:I:527:ASN:O	5:I:530:TYR:HB3	1.70	0.91
5:K:4:GLU:OE1	5:K:17:PHE:CE1	2.27	0.87
6:L:284:GLU:HA	6:L:287:LEU:HG	1.64	0.79
5:K:4:GLU:OE1	5:K:17:PHE:HE1	1.70	0.74
5:K:4:GLU:CD	5:K:17:PHE:CE1	2.61	0.73
5:K:4:GLU:CD	5:K:17:PHE:HE1	1.92	0.72
5:I:412:PRO:HB3	5:I:455:LEU:HD11	1.76	0.66
7:W:54:GLN:O	7:X:295:ARG:NH2	2.25	0.65
5:K:4:GLU:OE1	5:K:17:PHE:CD1	2.49	0.65
7:V:329:ASP:HB2	7:V:332:GLN:HE21	1.62	0.65
7:X:329:ASP:HB2	7:X:332:GLN:HE21	1.62	0.65
7:Z:329:ASP:HB2	7:Z:332:GLN:HE21	1.62	0.64
3:H:564:ARG:HH21	3:H:570:GLN:HG2	1.64	0.63
7:U:329:ASP:HB2	7:U:332:GLN:HE21	1.62	0.63
7:Y:329:ASP:HB2	7:Y:332:GLN:HE21	1.62	0.63
7:W:329:ASP:HB2	7:W:332:GLN:HE21	1.62	0.63
4:G:280:LYS:HB3	4:G:289:ASN:HD21	1.64	0.63
7:U:263:THR:HB	7:U:266:LEU:HG	1.81	0.63
7:V:263:THR:HB	7:V:266:LEU:HG	1.81	0.62
6:L:513:CYS:HG	6:L:1474:VAL:N	1.97	0.62
7:U:382:THR:O	7:U:385:SER:OG	2.18	0.62
7:V:382:THR:O	7:V:385:SER:OG	2.17	0.62
7:W:183:VAL:HG13	7:W:187:ASN:HD21	1.65	0.62
7:X:183:VAL:HG13	7:X:187:ASN:HD21	1.65	0.62
3:H:768:SER:O	3:H:771:LEU:HB2	1.99	0.62
7:W:382:THR:O	7:W:385:SER:OG	2.18	0.62
7:Y:263:THR:HB	7:Y:266:LEU:HG	1.81	0.62
4:G:741:ASN:HD22	4:G:839:ARG:HH21	1.48	0.62
7:W:323:ILE:HG13	7:W:359:ALA:HB3	1.81	0.62
7:X:263:THR:HB	7:X:266:LEU:HG	1.81	0.62
7:W:263:THR:HB	7:W:266:LEU:HG	1.81	0.62
7:Y:183:VAL:HG13	7:Y:187:ASN:HD21	1.65	0.62
7:Z:263:THR:HB	7:Z:266:LEU:HG	1.81	0.62
5:K:590:CYS:SG	5:K:591:HIS:N	2.72	0.62
7:V:183:VAL:HG13	7:V:187:ASN:HD21	1.65	0.62
7:Z:183:VAL:HG13	7:Z:187:ASN:HD21	1.65	0.62
7:U:323:ILE:HG13	7:U:359:ALA:HB3	1.81	0.62
7:X:201:CYS:HA	7:X:267:HIS:HB2	1.82	0.62
3:H:363:THR:HB	3:H:366:ARG:HE	1.63	0.61
7:Y:201:CYS:HA	7:Y:267:HIS:HB2	1.82	0.61
7:V:276:LEU:HD21	7:V:302:ASN:HA	1.82	0.61
7:Z:323:ILE:HG13	7:Z:359:ALA:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:276:LEU:HD21	7:X:302:ASN:HA	1.82	0.61
7:Y:382:THR:O	7:Y:385:SER:OG	2.18	0.61
7:Z:276:LEU:HD21	7:Z:302:ASN:HA	1.82	0.61
7:V:201:CYS:HA	7:V:267:HIS:HB2	1.82	0.61
7:V:323:ILE:HG13	7:V:359:ALA:HB3	1.81	0.61
7:W:276:LEU:HD21	7:W:302:ASN:HA	1.83	0.61
7:X:323:ILE:HG13	7:X:359:ALA:HB3	1.81	0.61
7:Z:196:THR:HG21	7:Z:431:LEU:HD11	1.83	0.61
7:Z:382:THR:O	7:Z:385:SER:OG	2.17	0.61
7:Y:276:LEU:HD21	7:Y:302:ASN:HA	1.82	0.61
7:U:183:VAL:HG13	7:U:187:ASN:HD21	1.65	0.60
7:Y:323:ILE:HG13	7:Y:359:ALA:HB3	1.81	0.60
4:G:254:LEU:HA	4:G:257:ARG:HD3	1.83	0.60
7:Y:196:THR:HG21	7:Y:431:LEU:HD11	1.83	0.60
5:I:530:TYR:OH	7:W:248:TYR:O	2.20	0.60
1:J:642:HIS:HD2	1:J:691:LEU:HD13	1.66	0.60
5:K:639:ASN:O	5:K:643:ALA:HB2	2.02	0.60
7:X:196:THR:HG21	7:X:431:LEU:HD11	1.83	0.60
7:U:276:LEU:HD21	7:U:302:ASN:HA	1.83	0.59
5:I:500:MET:O	5:I:504:HIS:ND1	2.32	0.59
7:V:355:SER:OG	7:V:356:ILE:N	2.35	0.59
3:H:862:LEU:HA	3:H:865:LEU:HD12	1.85	0.59
7:U:201:CYS:HA	7:U:267:HIS:HB2	1.82	0.59
7:X:382:THR:O	7:X:385:SER:OG	2.17	0.59
5:I:157:VAL:HB	5:I:172:LEU:HD21	1.84	0.59
7:Y:355:SER:OG	7:Y:356:ILE:N	2.35	0.59
5:I:361:TYR:CE2	5:I:475:TYR:HB3	2.38	0.59
6:L:468:ARG:NH1	6:L:516:GLU:OE2	2.33	0.59
6:L:1800:LEU:HD11	7:Z:341:ARG:HD3	1.84	0.59
7:W:196:THR:HG21	7:W:431:LEU:HD11	1.83	0.59
7:W:201:CYS:HA	7:W:267:HIS:HB2	1.82	0.59
4:G:249:ASP:O	4:G:257:ARG:NH1	2.34	0.59
7:V:187:ASN:O	7:V:191:THR:OG1	2.21	0.59
7:Z:201:CYS:HA	7:Z:267:HIS:HB2	1.82	0.59
7:W:187:ASN:O	7:W:191:THR:OG1	2.21	0.59
7:U:187:ASN:O	7:U:191:THR:OG1	2.21	0.59
7:Z:187:ASN:O	7:Z:191:THR:OG1	2.21	0.59
7:U:196:THR:HG21	7:U:431:LEU:HD11	1.83	0.58
7:V:196:THR:HG21	7:V:431:LEU:HD11	1.83	0.58
7:X:355:SER:OG	7:X:356:ILE:N	2.35	0.58
7:V:249:MET:SD	7:V:249:MET:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:249:MET:SD	7:U:249:MET:N	2.77	0.58
7:X:249:MET:SD	7:X:249:MET:N	2.77	0.58
5:I:471:VAL:HG21	5:I:561:HIS:HE1	1.69	0.57
7:Y:249:MET:SD	7:Y:249:MET:N	2.77	0.57
7:Y:102:ASN:OD1	7:Y:102:ASN:N	2.37	0.57
7:Y:187:ASN:O	7:Y:191:THR:OG1	2.21	0.57
1:J:331:ILE:HD11	1:J:369:TYR:HB2	1.86	0.57
7:W:249:MET:SD	7:W:249:MET:N	2.77	0.57
7:W:355:SER:OG	7:W:356:ILE:N	2.35	0.57
7:W:102:ASN:OD1	7:W:102:ASN:N	2.37	0.57
4:G:518:ARG:HA	4:G:523:ASP:HB3	1.86	0.57
3:H:558:HIS:HE1	3:H:616:GLU:HG3	1.68	0.57
7:Z:249:MET:SD	7:Z:249:MET:N	2.77	0.57
7:U:3:ARG:HB2	7:U:133:GLU:HB2	1.87	0.57
7:X:187:ASN:O	7:X:191:THR:OG1	2.21	0.57
1:J:922:ASP:HB3	1:J:925:GLN:HG2	1.86	0.57
7:U:102:ASN:N	7:U:102:ASN:OD1	2.37	0.57
7:V:102:ASN:OD1	7:V:102:ASN:N	2.37	0.57
7:X:326:GLY:HA2	7:X:363:LYS:HB2	1.87	0.57
7:V:3:ARG:HB2	7:V:133:GLU:HB2	1.87	0.57
7:V:339:ARG:HD2	7:V:343:ARG:HH12	1.70	0.57
4:G:555:LEU:HD21	4:G:573:LEU:HD22	1.87	0.56
6:L:1677:ALA:O	6:L:1682:HIS:ND1	2.38	0.56
7:U:355:SER:OG	7:U:356:ILE:N	2.35	0.56
7:Y:339:ARG:HD2	7:Y:343:ARG:HH12	1.70	0.56
7:W:326:GLY:HA2	7:W:363:LYS:HB2	1.87	0.56
7:Y:3:ARG:HB2	7:Y:133:GLU:HB2	1.87	0.56
7:Z:102:ASN:N	7:Z:102:ASN:OD1	2.37	0.56
5:K:161:SER:HB3	5:K:172:LEU:HD22	1.88	0.56
4:G:557:LEU:O	4:G:560:ARG:N	2.39	0.56
1:J:279:SER:HB2	1:J:376:LYS:HE3	1.88	0.56
7:Z:339:ARG:HD2	7:Z:343:ARG:HH12	1.70	0.56
7:Z:355:SER:OG	7:Z:356:ILE:N	2.35	0.56
5:I:357:ILE:O	5:I:361:TYR:CB	2.53	0.56
1:J:273:GLU:HG2	1:J:286:ILE:HD13	1.87	0.56
7:V:326:GLY:HA2	7:V:363:LYS:HB2	1.87	0.56
7:X:102:ASN:OD1	7:X:102:ASN:N	2.37	0.56
4:G:696:TYR:O	4:G:700:GLU:HB3	2.06	0.56
7:Z:326:GLY:HA2	7:Z:363:LYS:HB2	1.87	0.56
5:K:27:VAL:HG13	5:K:29:GLN:HB2	1.88	0.56
6:L:1499:PHE:HB3	6:L:1505:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:3:ARG:HB2	7:X:133:GLU:HB2	1.87	0.56
3:H:608:THR:HG23	3:H:610:ALA:H	1.71	0.56
6:L:461:PHE:HA	6:L:464:LYS:HD2	1.88	0.56
6:L:1534:LYS:HD3	6:L:1544:LEU:HB2	1.87	0.56
7:W:339:ARG:HD2	7:W:343:ARG:HH12	1.70	0.56
7:Y:326:GLY:HA2	7:Y:363:LYS:HB2	1.87	0.55
5:I:529:GLN:O	5:I:532:LEU:HB3	2.06	0.55
1:J:412:LEU:HA	1:J:415:VAL:HG22	1.87	0.55
7:X:339:ARG:HD2	7:X:343:ARG:HH12	1.70	0.55
7:U:326:GLY:HA2	7:U:363:LYS:HB2	1.87	0.55
7:Z:3:ARG:HB2	7:Z:133:GLU:HB2	1.87	0.55
4:G:372:ALA:HA	4:G:375:LEU:HD12	1.88	0.55
5:K:1:MET:HA	5:K:4:GLU:HG2	1.89	0.55
7:U:339:ARG:HD2	7:U:343:ARG:HH12	1.70	0.54
7:W:3:ARG:HB2	7:W:133:GLU:HB2	1.87	0.54
5:I:506:LYS:HB3	5:I:508:ASN:HD22	1.73	0.54
5:I:515:TRP:HE1	5:I:519:ASN:H	1.56	0.54
7:X:324:ILE:HG22	7:X:360:LEU:HA	1.90	0.54
3:H:737:LYS:HA	3:H:740:GLN:HE21	1.72	0.54
6:L:1652:SER:O	6:L:1656:ARG:NE	2.40	0.54
3:H:885:HIS:HB2	7:V:353:PRO:HB3	1.89	0.54
7:U:324:ILE:HG22	7:U:360:LEU:HA	1.90	0.54
4:G:646:PHE:HA	4:G:649:LYS:HD2	1.90	0.54
5:I:161:SER:HB3	5:I:172:LEU:HD22	1.89	0.54
7:V:339:ARG:HB3	7:V:343:ARG:HH22	1.73	0.54
7:Y:324:ILE:HG22	7:Y:360:LEU:HA	1.90	0.54
5:I:279:VAL:HG13	5:I:336:VAL:HG21	1.91	0.53
7:W:324:ILE:HG22	7:W:360:LEU:HA	1.90	0.53
7:W:339:ARG:HB3	7:W:343:ARG:HH22	1.73	0.53
7:Z:324:ILE:HG22	7:Z:360:LEU:HA	1.90	0.53
7:Z:339:ARG:HB3	7:Z:343:ARG:HH22	1.74	0.53
7:W:322:ASN:ND2	7:W:357:GLN:O	2.42	0.53
5:K:648:ARG:NH2	7:Y:353:PRO:O	2.41	0.53
7:U:322:ASN:ND2	7:U:357:GLN:O	2.42	0.53
7:Y:184:GLN:O	7:Y:188:SER:OG	2.27	0.53
7:V:184:GLN:O	7:V:188:SER:OG	2.27	0.53
7:W:184:GLN:O	7:W:188:SER:OG	2.27	0.53
7:V:322:ASN:ND2	7:V:357:GLN:O	2.42	0.53
3:H:869:SER:H	3:H:873:LEU:HD12	1.74	0.53
7:X:184:GLN:O	7:X:188:SER:OG	2.27	0.53
4:G:559:LEU:HD21	4:G:570:LYS:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:339:ARG:HB3	7:X:343:ARG:HH22	1.74	0.52
5:I:486:ARG:HA	5:I:489:GLN:HE21	1.74	0.52
7:V:324:ILE:HG22	7:V:360:LEU:HA	1.90	0.52
7:Y:322:ASN:ND2	7:Y:357:GLN:O	2.42	0.52
4:G:311:GLU:OE2	3:H:365:ARG:NH2	2.43	0.52
7:Y:40:PHE:HB2	7:Y:366:TYR:HE1	1.75	0.52
7:Z:322:ASN:ND2	7:Z:357:GLN:O	2.42	0.52
7:X:40:PHE:HB2	7:X:366:TYR:HE1	1.75	0.52
7:X:322:ASN:ND2	7:X:357:GLN:O	2.42	0.52
7:Y:320:ILE:HB	7:Y:356:ILE:HG13	1.92	0.52
4:G:692:ASN:OD1	7:U:357:GLN:NE2	2.42	0.52
1:J:277:LEU:HD11	1:J:294:VAL:HG21	1.90	0.52
7:Y:339:ARG:HB3	7:Y:343:ARG:HH22	1.74	0.52
4:G:392:GLU:HA	4:G:395:ILE:HG12	1.91	0.51
7:U:339:ARG:HB3	7:U:343:ARG:HH22	1.74	0.51
3:H:439:LEU:HD23	3:H:450:SER:HB2	1.92	0.51
7:X:320:ILE:HB	7:X:356:ILE:HG13	1.92	0.51
7:V:320:ILE:HB	7:V:356:ILE:HG13	1.92	0.51
3:H:483:VAL:HA	3:H:486:ILE:HD12	1.91	0.51
1:J:801:LEU:O	1:J:822:ASN:ND2	2.44	0.51
5:K:183:MET:HG2	5:K:186:GLN:HE21	1.76	0.51
7:U:184:GLN:O	7:U:188:SER:OG	2.27	0.51
7:W:40:PHE:HB2	7:W:366:TYR:HE1	1.75	0.51
7:Z:320:ILE:HB	7:Z:356:ILE:HG13	1.92	0.51
7:Z:184:GLN:O	7:Z:188:SER:OG	2.27	0.51
3:H:254:ILE:HA	3:H:257:VAL:HG22	1.93	0.51
5:K:496:TRP:HZ2	7:Y:261:ILE:HD12	1.76	0.51
5:K:545:LEU:O	5:K:549:ASN:ND2	2.45	0.50
7:U:320:ILE:HB	7:U:356:ILE:HG13	1.92	0.50
7:Z:40:PHE:HB2	7:Z:366:TYR:HE1	1.75	0.50
5:K:42:LEU:HA	5:K:45:LEU:HG	1.93	0.50
5:K:485:VAL:HB	5:K:529:GLN:HE22	1.76	0.50
7:V:40:PHE:HB2	7:V:366:TYR:HE1	1.75	0.50
5:I:154:LEU:O	5:I:158:TYR:HB3	2.11	0.50
4:G:242:GLN:HE21	4:G:343:THR:HG23	1.76	0.50
1:J:216:LEU:HD11	5:K:33:PHE:HB3	1.94	0.50
5:K:410:LEU:HD23	5:K:413:LEU:HD12	1.93	0.50
7:W:320:ILE:HB	7:W:356:ILE:HG13	1.92	0.50
3:H:255:LEU:HD11	3:H:343:HIS:HA	1.93	0.50
5:I:191:MET:HE1	5:I:276:ILE:HA	1.94	0.50
3:H:715:ILE:HA	3:H:718:MET:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:607:GLU:N	4:G:610:LEU:O	2.44	0.50
3:H:768:SER:HA	3:H:771:LEU:HD23	1.94	0.50
7:U:40:PHE:HB2	7:U:366:TYR:HE1	1.75	0.50
5:I:499:GLN:HG3	7:W:264:PRO:HB3	1.94	0.50
1:J:334:VAL:HG21	1:J:365:MET:HG2	1.94	0.50
5:I:51:ASP:HB2	5:I:133:PHE:HD1	1.78	0.49
6:L:1676:ILE:HG23	6:L:1680:ILE:HD12	1.94	0.49
4:G:641:LEU:HD21	4:G:734:LEU:HA	1.95	0.49
3:H:842:LYS:O	3:H:842:LYS:NZ	2.42	0.49
5:I:361:TYR:HE2	5:I:475:TYR:HB3	1.76	0.49
4:G:307:VAL:HA	4:G:310:LEU:HG	1.94	0.49
3:H:779:PHE:HA	3:H:782:ILE:HD12	1.95	0.49
3:H:862:LEU:HD21	3:H:880:LEU:HB2	1.95	0.49
5:I:357:ILE:O	5:I:361:TYR:HB3	2.13	0.49
1:J:707:MET:SD	1:J:711:LYS:NZ	2.86	0.49
5:I:191:MET:HB2	5:I:192:LEU:HD12	1.95	0.48
1:J:760:VAL:HG21	7:Y:342:GLU:HG3	1.94	0.48
4:G:523:ASP:OD1	7:U:248:TYR:OH	2.32	0.48
3:H:716:HIS:CE1	7:V:259:SER:HB3	2.49	0.48
3:H:882:PHE:HD1	7:V:355:SER:HG	1.61	0.48
7:V:240:THR:HA	7:V:243:LEU:HD12	1.96	0.48
7:X:240:THR:HA	7:X:243:LEU:HD12	1.96	0.48
3:H:681:ARG:HG2	7:V:258:ALA:HA	1.94	0.48
1:J:302:VAL:HG23	1:J:304:HIS:H	1.78	0.48
7:W:388:PHE:O	7:W:391:THR:OG1	2.27	0.48
4:G:613:LEU:HD12	4:G:614:GLU:HG2	1.95	0.48
5:K:501:GLN:HE21	7:Y:162:PRO:HB2	1.77	0.48
6:L:1633:LEU:HB2	6:L:1662:LYS:HE2	1.95	0.48
3:H:879:ARG:HA	3:H:882:PHE:CZ	2.49	0.48
5:K:4:GLU:OE2	5:K:16:ILE:HB	2.13	0.47
7:Y:240:THR:HA	7:Y:243:LEU:HD12	1.96	0.47
7:Z:240:THR:HA	7:Z:243:LEU:HD12	1.96	0.47
5:K:17:PHE:HE2	5:K:42:LEU:HD21	1.79	0.47
5:K:651:TYR:CE1	7:Y:355:SER:HA	2.49	0.47
6:L:503:SER:HG	6:L:586:VAL:N	2.12	0.47
3:H:329:HIS:CE1	5:I:131:LEU:HD11	2.50	0.47
7:Z:222:ASN:OD1	7:Z:222:ASN:N	2.48	0.47
4:G:761:CYS:HA	4:G:764:LYS:HE2	1.97	0.47
3:H:884:GLU:HB3	3:H:887:LYS:HB3	1.97	0.47
7:V:343:ARG:HA	7:V:343:ARG:HD3	1.46	0.47
7:U:389:GLU:O	7:U:393:ARG:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:222:ASN:OD1	7:X:222:ASN:N	2.48	0.47
5:I:380:LEU:HG	5:I:450:TRP:HE1	1.80	0.47
5:I:601:LEU:HD23	5:I:601:LEU:HA	1.82	0.47
1:J:215:TRP:HB3	6:L:322:LYS:HE3	1.97	0.47
5:K:151:CYS:HA	5:K:154:LEU:HD13	1.96	0.47
7:Y:222:ASN:N	7:Y:222:ASN:OD1	2.48	0.47
7:W:389:GLU:O	7:W:393:ARG:N	2.48	0.47
7:X:389:GLU:O	7:X:393:ARG:N	2.48	0.47
4:G:684:GLN:O	4:G:688:ASN:ND2	2.48	0.46
3:H:716:HIS:HE1	7:V:259:SER:HB3	1.80	0.46
5:I:43:ASN:O	5:I:46:CYS:HB3	2.15	0.46
7:Z:324:ILE:HD12	7:Z:324:ILE:HA	1.80	0.46
3:H:859:GLN:HE21	3:H:859:GLN:HB2	1.57	0.46
5:K:577:LYS:O	5:K:581:HIS:HB2	2.15	0.46
7:U:222:ASN:OD1	7:U:222:ASN:N	2.48	0.46
7:U:240:THR:HA	7:U:243:LEU:HD12	1.96	0.46
7:V:222:ASN:OD1	7:V:222:ASN:N	2.48	0.46
7:V:389:GLU:O	7:V:393:ARG:N	2.48	0.46
7:Y:104:TRP:HE1	7:Y:191:THR:HG23	1.81	0.46
5:I:92:GLY:HA3	5:I:175:ILE:HG12	1.97	0.46
7:V:104:TRP:HE1	7:V:191:THR:HG23	1.81	0.46
7:X:384:ILE:O	7:X:387:LEU:HB2	2.16	0.46
3:H:712:VAL:O	3:H:716:HIS:HB2	2.15	0.46
5:K:199:GLN:O	5:K:200:HIS:ND1	2.48	0.46
7:W:104:TRP:HE1	7:W:191:THR:HG23	1.81	0.46
7:W:240:THR:HA	7:W:243:LEU:HD12	1.96	0.46
5:I:63:THR:HG22	5:I:87:ARG:HG2	1.97	0.46
5:I:357:ILE:O	5:I:361:TYR:HB2	2.15	0.46
7:V:384:ILE:O	7:V:387:LEU:HB2	2.16	0.46
7:W:174:ASN:H	7:W:207:ASN:HD21	1.64	0.46
7:X:174:ASN:H	7:X:207:ASN:HD21	1.64	0.46
7:Y:384:ILE:O	7:Y:387:LEU:HB2	2.16	0.46
5:I:59:ILE:HD13	5:I:90:CYS:HB2	1.97	0.46
7:V:174:ASN:H	7:V:207:ASN:HD21	1.64	0.46
1:J:496:ARG:HH11	1:J:567:GLN:HG2	1.81	0.46
1:J:979:SER:HB2	1:J:980:ILE:HD12	1.98	0.46
7:U:104:TRP:HE1	7:U:191:THR:HG23	1.81	0.46
7:W:222:ASN:N	7:W:222:ASN:OD1	2.48	0.46
7:X:104:TRP:HE1	7:X:191:THR:HG23	1.80	0.46
7:V:29:HIS:HB3	7:V:48:LYS:HD3	1.98	0.46
7:W:29:HIS:HB3	7:W:48:LYS:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:384:ILE:O	7:U:387:LEU:HB2	2.16	0.46
4:G:221:LEU:HD11	4:G:260:VAL:HG22	1.97	0.45
5:K:472:LEU:HD13	5:K:475:TYR:HD2	1.81	0.45
7:U:324:ILE:HD12	7:U:324:ILE:HA	1.80	0.45
7:U:29:HIS:HB3	7:U:48:LYS:HD3	1.98	0.45
7:Y:343:ARG:HA	7:Y:343:ARG:HD3	1.46	0.45
7:Z:104:TRP:HE1	7:Z:191:THR:HG23	1.81	0.45
7:Z:174:ASN:H	7:Z:207:ASN:HD21	1.64	0.45
6:L:1554:LEU:HD13	6:L:1574:LEU:HD22	1.98	0.45
7:V:337:LEU:HB2	7:V:341:ARG:NH1	2.32	0.45
7:W:297:LEU:HD11	7:W:377:MET:HB3	1.99	0.45
7:W:384:ILE:O	7:W:387:LEU:HB2	2.16	0.45
7:X:297:LEU:HD11	7:X:377:MET:HB3	1.99	0.45
7:X:337:LEU:HB2	7:X:341:ARG:NH1	2.32	0.45
4:G:555:LEU:HD22	4:G:575:ILE:HG13	1.98	0.45
6:L:1800:LEU:HD21	7:Z:341:ARG:NE	2.31	0.45
7:W:229:ASN:O	7:W:233:SER:OG	2.34	0.45
7:W:337:LEU:HB2	7:W:341:ARG:NH1	2.32	0.45
7:Z:389:GLU:O	7:Z:393:ARG:N	2.48	0.45
1:J:561:MET:HG3	1:J:699:TYR:CZ	2.51	0.45
6:L:1800:LEU:HD21	7:Z:341:ARG:CZ	2.46	0.45
7:X:29:HIS:HB3	7:X:48:LYS:HD3	1.98	0.45
7:Z:384:ILE:O	7:Z:387:LEU:HB2	2.16	0.45
4:G:695:TYR:CE1	7:U:249:MET:HG3	2.52	0.45
3:H:589:ALA:N	3:H:632:ASP:OD2	2.50	0.45
5:I:406:ASP:OD1	5:I:406:ASP:N	2.43	0.45
7:V:428:VAL:HA	7:V:431:LEU:HB2	1.99	0.45
7:W:232:VAL:O	7:W:236:MET:HG2	2.17	0.45
7:U:229:ASN:O	7:U:233:SER:OG	2.34	0.45
7:U:337:LEU:HB2	7:U:341:ARG:NH1	2.32	0.45
7:V:229:ASN:O	7:V:233:SER:OG	2.34	0.45
7:V:232:VAL:O	7:V:236:MET:HG2	2.17	0.45
7:W:343:ARG:HA	7:W:343:ARG:HD3	1.46	0.45
7:Y:337:LEU:HB2	7:Y:341:ARG:NH1	2.32	0.45
7:Z:29:HIS:HB3	7:Z:48:LYS:HD3	1.98	0.45
4:G:521:LEU:HD23	4:G:702:MET:HB3	1.98	0.45
7:U:428:VAL:HA	7:U:431:LEU:HB2	1.99	0.45
7:X:229:ASN:O	7:X:233:SER:OG	2.34	0.45
3:H:339:LEU:HA	3:H:342:LEU:HD12	1.99	0.45
7:Y:389:GLU:O	7:Y:393:ARG:N	2.48	0.45
5:I:543:GLN:O	5:I:546:HIS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:337:LEU:HB2	7:Z:341:ARG:NH1	2.32	0.44
5:K:534:VAL:HA	5:K:537:LEU:HG	1.99	0.44
6:L:1732:ILE:O	6:L:1736:VAL:HG23	2.16	0.44
7:U:232:VAL:O	7:U:236:MET:HG2	2.17	0.44
3:H:589:ALA:HA	3:H:592:LEU:HD13	1.98	0.44
5:I:45:LEU:HD12	5:I:48:LEU:HD13	2.00	0.44
5:I:480:LYS:HA	5:I:483:LEU:HD12	1.99	0.44
7:W:341:ARG:HH11	7:W:341:ARG:HD2	1.63	0.44
7:Y:229:ASN:O	7:Y:233:SER:OG	2.34	0.44
7:Y:232:VAL:O	7:Y:236:MET:HG2	2.17	0.44
7:Z:232:VAL:O	7:Z:236:MET:HG2	2.17	0.44
7:Z:343:ARG:HA	7:Z:343:ARG:HD3	1.46	0.44
3:H:763:LEU:HD21	3:H:771:LEU:HB3	1.99	0.44
5:K:6:LEU:HD21	5:K:111:PHE:HE2	1.81	0.44
5:K:183:MET:HG2	5:K:186:GLN:NE2	2.32	0.44
7:U:174:ASN:H	7:U:207:ASN:HD21	1.64	0.44
7:Y:174:ASN:H	7:Y:207:ASN:HD21	1.64	0.44
7:Z:297:LEU:HD11	7:Z:377:MET:HB3	1.99	0.44
7:W:410:LYS:H	7:W:410:LYS:HG2	1.62	0.44
7:X:232:VAL:O	7:X:236:MET:HG2	2.17	0.44
7:Y:29:HIS:HB3	7:Y:48:LYS:HD3	1.98	0.44
3:H:329:HIS:HA	3:H:332:LEU:HG	2.00	0.44
4:G:858:ARG:NH1	7:U:357:GLN:OE1	2.51	0.44
7:U:343:ARG:HA	7:U:343:ARG:HD3	1.46	0.44
7:X:324:ILE:HD12	7:X:324:ILE:HA	1.80	0.44
7:Z:229:ASN:O	7:Z:233:SER:OG	2.34	0.44
4:G:285:TYR:HB3	4:G:289:ASN:HD22	1.83	0.44
3:H:301:HIS:HA	3:H:304:ILE:HG12	1.99	0.44
5:I:42:LEU:O	5:I:46:CYS:N	2.50	0.44
7:W:339:ARG:HB3	7:W:343:ARG:NH2	2.33	0.44
7:Y:297:LEU:HD11	7:Y:377:MET:HB3	1.99	0.44
7:Y:339:ARG:HB3	7:Y:343:ARG:NH2	2.33	0.44
1:J:432:ARG:HA	1:J:435:HIS:CD2	2.52	0.44
6:L:393:ILE:O	6:L:397:LEU:N	2.50	0.44
7:U:297:LEU:HD11	7:U:377:MET:HB3	1.99	0.44
7:V:297:LEU:HD11	7:V:377:MET:HB3	1.99	0.44
7:X:25:LEU:HD13	7:X:25:LEU:HA	1.82	0.44
6:L:1797:ASP:HA	7:Z:334:HIS:CE1	2.52	0.43
7:W:428:VAL:HA	7:W:431:LEU:HB2	1.99	0.43
7:Z:339:ARG:HB3	7:Z:343:ARG:NH2	2.33	0.43
4:G:499:LEU:HB3	4:G:719:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:621:ARG:O	5:I:624:SER:OG	2.31	0.43
6:L:1634:LYS:HE3	6:L:1634:LYS:HB3	1.74	0.43
6:L:1632:ALA:HB1	6:L:1740:ARG:HG3	2.01	0.43
7:X:343:ARG:HA	7:X:343:ARG:HD3	1.46	0.43
3:H:744:LEU:HA	3:H:747:ILE:HG12	2.00	0.43
3:H:887:LYS:HA	3:H:887:LYS:HD3	1.75	0.43
7:Y:428:VAL:HA	7:Y:431:LEU:HB2	1.99	0.43
7:Z:428:VAL:HA	7:Z:431:LEU:HB2	1.99	0.43
5:K:345:VAL:HG23	5:K:346:GLU:HG3	2.01	0.43
3:H:266:ILE:HD13	3:H:277:VAL:HA	2.00	0.43
3:H:698:SER:O	3:H:702:HIS:HB3	2.19	0.43
5:I:190:TRP:CE2	5:I:280:GLY:HA3	2.54	0.43
6:L:1779:LEU:HA	6:L:1782:VAL:HG12	2.00	0.43
7:X:428:VAL:HA	7:X:431:LEU:HB2	1.99	0.43
7:Z:410:LYS:H	7:Z:410:LYS:HG2	1.62	0.43
5:K:98:GLN:HA	5:K:101:ARG:HD2	2.00	0.43
1:J:358:PHE:HD2	1:J:361:TYR:H	1.66	0.43
6:L:1550:LEU:HA	6:L:1553:VAL:HB	2.01	0.43
7:X:116:GLU:H	7:X:116:GLU:HG2	1.49	0.43
5:I:466:LEU:HD12	5:I:554:PHE:HE1	1.84	0.43
1:J:921:LYS:H	1:J:925:GLN:HE21	1.67	0.43
7:U:339:ARG:HB3	7:U:343:ARG:NH2	2.33	0.43
7:X:339:ARG:HB3	7:X:343:ARG:NH2	2.33	0.43
5:I:510:THR:HG23	5:I:513:ILE:HB	2.01	0.42
7:Y:47:ARG:HE	7:Y:49:ASP:HB2	1.84	0.42
5:I:414:LEU:HD22	5:I:453:LEU:HD11	2.00	0.42
5:K:327:GLN:HB3	5:K:331:ARG:HH21	1.84	0.42
7:W:47:ARG:HE	7:W:49:ASP:HB2	1.84	0.42
7:X:410:LYS:H	7:X:410:LYS:HG2	1.63	0.42
4:G:219:GLU:HB2	4:G:314:HIS:HE1	1.83	0.42
6:L:1662:LYS:O	6:L:1662:LYS:NZ	2.37	0.42
7:U:47:ARG:HE	7:U:49:ASP:HB2	1.84	0.42
6:L:1670:LYS:HA	6:L:1670:LYS:HD3	1.94	0.42
7:V:339:ARG:HB3	7:V:343:ARG:NH2	2.33	0.42
4:G:513:LEU:HD23	4:G:630:ILE:HD11	2.01	0.42
4:G:543:VAL:HG12	4:G:611:SER:HB3	2.01	0.42
5:I:553:ASP:O	5:I:556:SER:OG	2.35	0.42
1:J:716:LEU:HD22	1:J:812:VAL:HG11	2.02	0.42
5:K:25:LEU:HB2	5:K:46:CYS:HB2	2.01	0.42
5:K:470:ALA:O	5:K:474:LYS:HG2	2.19	0.42
4:G:861:PHE:CE1	7:U:341:ARG:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:277:ILE:HD12	4:G:277:ILE:HA	1.88	0.42
4:G:393:LYS:HG2	4:G:397:ARG:HH11	1.85	0.42
4:G:522:MET:HG3	4:G:528:PHE:CD2	2.55	0.42
3:H:581:LEU:HD12	3:H:584:GLU:HB2	2.02	0.42
3:H:686:CYS:HA	3:H:689:LYS:NZ	2.35	0.42
5:I:131:LEU:O	5:I:135:SER:OG	2.30	0.42
5:I:196:LEU:HD23	5:I:196:LEU:HA	1.96	0.42
6:L:1660:LEU:HA	6:L:1660:LEU:HD13	1.78	0.42
7:X:47:ARG:HE	7:X:49:ASP:HB2	1.84	0.42
7:Z:47:ARG:HE	7:Z:49:ASP:HB2	1.84	0.42
4:G:577:LEU:HD12	4:G:579:PRO:HD3	2.01	0.41
4:G:709:LEU:HG	4:G:713:LEU:HD23	2.01	0.41
3:H:613:ASP:HB3	3:H:617:ILE:HD11	2.02	0.41
1:J:842:LEU:HD23	1:J:842:LEU:HA	1.85	0.41
5:K:89:PHE:HE2	5:K:140:VAL:HG12	1.85	0.41
7:X:428:VAL:HA	7:X:431:LEU:HD12	2.02	0.41
7:Y:324:ILE:HD12	7:Y:324:ILE:HA	1.80	0.41
5:K:134:PRO:HA	5:K:137:MET:HE2	2.02	0.41
3:H:365:ARG:NH2	3:H:366:ARG:HH22	2.18	0.41
7:V:47:ARG:HE	7:V:49:ASP:HB2	1.84	0.41
5:K:403:VAL:HG23	5:K:405:LEU:H	1.85	0.41
6:L:352:LEU:HD21	6:L:397:LEU:HD13	2.01	0.41
6:L:1680:ILE:HD11	6:L:1716:GLY:HA2	2.02	0.41
4:G:296:MET:HB2	4:G:296:MET:HE2	1.65	0.41
4:G:363:SER:HA	4:G:376:CYS:SG	2.60	0.41
5:I:199:GLN:NE2	1:J:445:LEU:O	2.53	0.41
7:V:25:LEU:HA	7:V:25:LEU:HD13	1.82	0.41
7:Z:428:VAL:HA	7:Z:431:LEU:HD12	2.02	0.41
5:K:111:PHE:HD1	5:K:117:LEU:HD12	1.86	0.41
5:K:545:LEU:HA	5:K:548:ILE:HG12	2.03	0.41
5:K:639:ASN:O	5:K:643:ALA:CB	2.68	0.41
6:L:1682:HIS:HB3	7:Z:330:PRO:CB	2.51	0.41
1:J:384:LYS:HA	1:J:384:LYS:HD2	1.88	0.41
5:K:496:TRP:CE2	7:Y:258:ALA:HA	2.55	0.41
4:G:359:LEU:HG	4:G:380:THR:HB	2.03	0.41
5:I:350:LEU:HD13	5:I:464:HIS:CE1	2.56	0.41
1:J:889:LYS:HE2	1:J:987:PHE:CD2	2.55	0.41
7:U:9:GLN:OE1	7:U:9:GLN:N	2.54	0.41
7:U:165:LEU:HD13	7:U:253:LEU:HG	2.03	0.41
4:G:414:LEU:HB2	4:G:426:LYS:HD3	2.03	0.41
4:G:610:LEU:HD13	4:G:613:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:258:PHE:HD1	3:H:297:LEU:HD22	1.86	0.41
1:J:893:PHE:O	1:J:896:SER:OG	2.32	0.41
7:W:165:LEU:HD13	7:W:253:LEU:HG	2.03	0.41
7:Y:165:LEU:HD13	7:Y:253:LEU:HG	2.03	0.41
3:H:254:ILE:HD11	3:H:294:LEU:HB2	2.03	0.40
3:H:730:SER:HA	3:H:733:GLU:HG3	2.03	0.40
1:J:403:ALA:HA	1:J:406:LEU:HG	2.02	0.40
5:K:255:LYS:HD2	5:K:255:LYS:HA	1.81	0.40
6:L:432:PHE:HE2	6:L:524:LEU:HD13	1.86	0.40
7:V:9:GLN:N	7:V:9:GLN:OE1	2.54	0.40
7:X:165:LEU:HD13	7:X:253:LEU:HG	2.03	0.40
7:Y:428:VAL:HA	7:Y:431:LEU:HD12	2.02	0.40
7:Z:9:GLN:OE1	7:Z:9:GLN:N	2.54	0.40
5:K:649:LEU:HD12	5:K:652:ASN:HA	2.03	0.40
6:L:1669:VAL:HA	6:L:1672:ILE:HG22	2.02	0.40
7:V:428:VAL:HA	7:V:431:LEU:HD12	2.02	0.40
4:G:259:LEU:HB3	4:G:321:LEU:HD21	2.02	0.40
3:H:626:LEU:HB2	3:H:637:VAL:HG13	2.03	0.40
5:I:282:SER:HB3	5:I:340:LEU:HD21	2.04	0.40
7:U:428:VAL:HA	7:U:431:LEU:HD12	2.02	0.40
7:V:116:GLU:H	7:V:116:GLU:HG2	1.49	0.40
7:V:245:TYR:HA	7:V:246:PRO:HD3	1.92	0.40
7:W:9:GLN:N	7:W:9:GLN:OE1	2.54	0.40
7:W:116:GLU:H	7:W:116:GLU:HG2	1.49	0.40
7:Y:410:LYS:H	7:Y:410:LYS:HG2	1.63	0.40
5:I:504:HIS:CE1	7:W:158:ASN:HD21	2.40	0.40
1:J:283:LYS:HA	1:J:283:LYS:HD2	1.89	0.40
1:J:937:ILE:HD12	1:J:937:ILE:HA	1.91	0.40
7:Y:9:GLN:N	7:Y:9:GLN:OE1	2.54	0.40
5:I:400:ALA:HB1	5:I:405:LEU:HD22	2.04	0.40
5:I:484:SER:HB2	5:I:587:LEU:HD11	2.02	0.40
7:V:410:LYS:H	7:V:410:LYS:HG2	1.63	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	J	506/1024 (49%)	469 (93%)	34 (7%)	3 (1%)	25	66
1	l	104/1024 (10%)	98 (94%)	5 (5%)	1 (1%)	15	54
2	b	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	m	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
3	H	584/907 (64%)	572 (98%)	11 (2%)	1 (0%)	47	81
3	a	112/907 (12%)	108 (96%)	4 (4%)	0	100	100
4	G	624/902 (69%)	597 (96%)	22 (4%)	5 (1%)	19	60
5	I	511/667 (77%)	489 (96%)	20 (4%)	2 (0%)	34	72
5	K	548/667 (82%)	530 (97%)	17 (3%)	1 (0%)	47	81
6	L	540/1819 (30%)	509 (94%)	27 (5%)	4 (1%)	22	63
7	U	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	V	408/451 (90%)	391 (96%)	17 (4%)	0	100	100
7	W	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	X	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	Y	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
7	Z	408/451 (90%)	392 (96%)	16 (4%)	0	100	100
All	All	6103/10787 (57%)	5845 (96%)	241 (4%)	17 (0%)	44	77

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	121	PRO
4	G	241	ARG
4	G	581	ASP
3	H	455	LYS
5	I	601	LEU
1	J	236	LEU
1	J	238	LEU
5	K	409	ASN
6	L	308	GLU
4	G	557	LEU
5	I	600	ASN
1	J	222	HIS

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Mol	Chain	Res	Type
6	L	1800	LEU
4	G	582	LEU
4	G	854	SER
6	L	346	LEU
6	L	303	PRO

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	J	498/933 (53%)	493 (99%)	5 (1%)	76 86
1	l	84/933 (9%)	84 (100%)	0	100 100
2	b	53/62 (86%)	40 (76%)	13 (24%)	0 3
2	m	53/62 (86%)	40 (76%)	13 (24%)	0 3
3	H	539/798 (68%)	535 (99%)	4 (1%)	84 90
3	a	101/798 (13%)	100 (99%)	1 (1%)	76 86
4	G	572/791 (72%)	568 (99%)	4 (1%)	84 90
5	I	472/594 (80%)	465 (98%)	7 (2%)	65 80
5	K	509/594 (86%)	506 (99%)	3 (1%)	86 92
6	L	501/1546 (32%)	496 (99%)	5 (1%)	76 86
7	U	376/400 (94%)	310 (82%)	66 (18%)	2 11
7	V	376/400 (94%)	310 (82%)	66 (18%)	2 11
7	W	376/400 (94%)	310 (82%)	66 (18%)	2 11
7	X	376/400 (94%)	310 (82%)	66 (18%)	2 11
7	Y	376/400 (94%)	310 (82%)	66 (18%)	2 11
7	Z	376/400 (94%)	310 (82%)	66 (18%)	2 11
All	All	5638/9511 (59%)	5187 (92%)	451 (8%)	16 35

All (451) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	m	22	ARG
2	m	23	GLU
2	m	28	LEU
2	m	31	ILE
2	m	34	ILE
2	m	39	LEU
2	m	41	MET
2	m	43	THR
2	m	45	SER
2	m	48	VAL
2	m	61	SER
2	m	71	THR
2	m	74	LEU
2	b	22	ARG
2	b	23	GLU
2	b	28	LEU
2	b	31	ILE
2	b	34	ILE
2	b	39	LEU
2	b	41	MET
2	b	43	THR
2	b	45	SER
2	b	48	VAL
2	b	61	SER
2	b	71	THR
2	b	74	LEU
3	a	12	LEU
4	G	355	THR
4	G	414	LEU
4	G	557	LEU
4	G	563	THR
3	H	379	LYS
3	H	380	THR
3	H	603	THR
3	H	774	GLN
5	I	59	ILE
5	I	315	LYS
5	I	324	ASP
5	I	403	VAL
5	I	475	TYR
5	I	514	LYS
5	I	593	PHE
1	J	230	SER

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Mol	Chain	Res	Type
1	J	302	VAL
1	J	317	ILE
1	J	331	ILE
1	J	360	THR
5	K	4	GLU
5	K	402	LYS
5	K	590	CYS
6	L	346	LEU
6	L	465	LYS
6	L	1634	LYS
6	L	1636	VAL
6	L	1656	ARG
7	U	4	GLU
7	U	7	THR
7	U	8	LEU
7	U	9	GLN
7	U	10	LEU
7	U	13	CYS
7	U	24	GLN
7	U	34	GLU
7	U	39	GLU
7	U	46	ASP
7	U	58	GLU
7	U	102	ASN
7	U	116	GLU
7	U	120	ASP
7	U	125	GLU
7	U	136	VAL
7	U	140	SER
7	U	153	LEU
7	U	157	LEU
7	U	165	LEU
7	U	168	THR
7	U	188	SER
7	U	191	THR
7	U	192	LEU
7	U	200	ASP
7	U	204	VAL
7	U	219	HIS
7	U	222	ASN
7	U	226	SER
7	U	233	SER

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Mol	Chain	Res	Type
7	U	236	MET
7	U	241	THR
7	U	249	MET
7	U	260	LEU
7	U	269	LEU
7	U	270	MET
7	U	288	THR
7	U	292	ASP
7	U	294	MET
7	U	297	LEU
7	U	298	LEU
7	U	303	VAL
7	U	304	MET
7	U	305	VAL
7	U	323	ILE
7	U	331	THR
7	U	340	ILE
7	U	341	ARG
7	U	343	ARG
7	U	348	PHE
7	U	355	SER
7	U	357	GLN
7	U	358	VAL
7	U	369	SER
7	U	374	SER
7	U	376	LEU
7	U	377	MET
7	U	383	SER
7	U	384	ILE
7	U	410	LYS
7	U	420	GLU
7	U	422	ASP
7	U	423	THR
7	U	424	SER
7	U	426	GLU
7	U	439	THR
7	V	4	GLU
7	V	7	THR
7	V	8	LEU
7	V	9	GLN
7	V	10	LEU
7	V	13	CYS

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Mol	Chain	Res	Type
7	V	24	GLN
7	V	34	GLU
7	V	39	GLU
7	V	46	ASP
7	V	58	GLU
7	V	102	ASN
7	V	116	GLU
7	V	120	ASP
7	V	125	GLU
7	V	136	VAL
7	V	140	SER
7	V	153	LEU
7	V	157	LEU
7	V	165	LEU
7	V	168	THR
7	V	188	SER
7	V	191	THR
7	V	192	LEU
7	V	200	ASP
7	V	204	VAL
7	V	219	HIS
7	V	222	ASN
7	V	226	SER
7	V	233	SER
7	V	236	MET
7	V	241	THR
7	V	249	MET
7	V	260	LEU
7	V	269	LEU
7	V	270	MET
7	V	288	THR
7	V	292	ASP
7	V	294	MET
7	V	297	LEU
7	V	298	LEU
7	V	303	VAL
7	V	304	MET
7	V	305	VAL
7	V	323	ILE
7	V	331	THR
7	V	340	ILE
7	V	341	ARG

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Mol	Chain	Res	Type
7	V	343	ARG
7	V	348	PHE
7	V	355	SER
7	V	357	GLN
7	V	358	VAL
7	V	369	SER
7	V	374	SER
7	V	376	LEU
7	V	377	MET
7	V	383	SER
7	V	384	ILE
7	V	410	LYS
7	V	420	GLU
7	V	422	ASP
7	V	423	THR
7	V	424	SER
7	V	426	GLU
7	V	439	THR
7	W	4	GLU
7	W	7	THR
7	W	8	LEU
7	W	9	GLN
7	W	10	LEU
7	W	13	CYS
7	W	24	GLN
7	W	34	GLU
7	W	39	GLU
7	W	46	ASP
7	W	58	GLU
7	W	102	ASN
7	W	116	GLU
7	W	120	ASP
7	W	125	GLU
7	W	136	VAL
7	W	140	SER
7	W	153	LEU
7	W	157	LEU
7	W	165	LEU
7	W	168	THR
7	W	188	SER
7	W	191	THR
7	W	192	LEU

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Mol	Chain	Res	Type
7	W	200	ASP
7	W	204	VAL
7	W	219	HIS
7	W	222	ASN
7	W	226	SER
7	W	233	SER
7	W	236	MET
7	W	241	THR
7	W	249	MET
7	W	260	LEU
7	W	269	LEU
7	W	270	MET
7	W	288	THR
7	W	292	ASP
7	W	294	MET
7	W	297	LEU
7	W	298	LEU
7	W	303	VAL
7	W	304	MET
7	W	305	VAL
7	W	323	ILE
7	W	331	THR
7	W	340	ILE
7	W	341	ARG
7	W	343	ARG
7	W	348	PHE
7	W	355	SER
7	W	357	GLN
7	W	358	VAL
7	W	369	SER
7	W	374	SER
7	W	376	LEU
7	W	377	MET
7	W	383	SER
7	W	384	ILE
7	W	410	LYS
7	W	420	GLU
7	W	422	ASP
7	W	423	THR
7	W	424	SER
7	W	426	GLU
7	W	439	THR

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Mol	Chain	Res	Type
7	X	4	GLU
7	X	7	THR
7	X	8	LEU
7	X	9	GLN
7	X	10	LEU
7	X	13	CYS
7	X	24	GLN
7	X	34	GLU
7	X	39	GLU
7	X	46	ASP
7	X	58	GLU
7	X	102	ASN
7	X	116	GLU
7	X	120	ASP
7	X	125	GLU
7	X	136	VAL
7	X	140	SER
7	X	153	LEU
7	X	157	LEU
7	X	165	LEU
7	X	168	THR
7	X	188	SER
7	X	191	THR
7	X	192	LEU
7	X	200	ASP
7	X	204	VAL
7	X	219	HIS
7	X	222	ASN
7	X	226	SER
7	X	233	SER
7	X	236	MET
7	X	241	THR
7	X	249	MET
7	X	260	LEU
7	X	269	LEU
7	X	270	MET
7	X	288	THR
7	X	292	ASP
7	X	294	MET
7	X	297	LEU
7	X	298	LEU
7	X	303	VAL

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Mol	Chain	Res	Type
7	X	304	MET
7	X	305	VAL
7	X	323	ILE
7	X	331	THR
7	X	340	ILE
7	X	341	ARG
7	X	343	ARG
7	X	348	PHE
7	X	355	SER
7	X	357	GLN
7	X	358	VAL
7	X	369	SER
7	X	374	SER
7	X	376	LEU
7	X	377	MET
7	X	383	SER
7	X	384	ILE
7	X	410	LYS
7	X	420	GLU
7	X	422	ASP
7	X	423	THR
7	X	424	SER
7	X	426	GLU
7	X	439	THR
7	Y	4	GLU
7	Y	7	THR
7	Y	8	LEU
7	Y	9	GLN
7	Y	10	LEU
7	Y	13	CYS
7	Y	24	GLN
7	Y	34	GLU
7	Y	39	GLU
7	Y	46	ASP
7	Y	58	GLU
7	Y	102	ASN
7	Y	116	GLU
7	Y	120	ASP
7	Y	125	GLU
7	Y	136	VAL
7	Y	140	SER
7	Y	153	LEU

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Mol	Chain	Res	Type
7	Y	157	LEU
7	Y	165	LEU
7	Y	168	THR
7	Y	188	SER
7	Y	191	THR
7	Y	192	LEU
7	Y	200	ASP
7	Y	204	VAL
7	Y	219	HIS
7	Y	222	ASN
7	Y	226	SER
7	Y	233	SER
7	Y	236	MET
7	Y	241	THR
7	Y	249	MET
7	Y	260	LEU
7	Y	269	LEU
7	Y	270	MET
7	Y	288	THR
7	Y	292	ASP
7	Y	294	MET
7	Y	297	LEU
7	Y	298	LEU
7	Y	303	VAL
7	Y	304	MET
7	Y	305	VAL
7	Y	323	ILE
7	Y	331	THR
7	Y	340	ILE
7	Y	341	ARG
7	Y	343	ARG
7	Y	348	PHE
7	Y	355	SER
7	Y	357	GLN
7	Y	358	VAL
7	Y	369	SER
7	Y	374	SER
7	Y	376	LEU
7	Y	377	MET
7	Y	383	SER
7	Y	384	ILE
7	Y	410	LYS

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Mol	Chain	Res	Type
7	Y	420	GLU
7	Y	422	ASP
7	Y	423	THR
7	Y	424	SER
7	Y	426	GLU
7	Y	439	THR
7	Z	4	GLU
7	Z	7	THR
7	Z	8	LEU
7	Z	9	GLN
7	Z	10	LEU
7	Z	13	CYS
7	Z	24	GLN
7	Z	34	GLU
7	Z	39	GLU
7	Z	46	ASP
7	Z	58	GLU
7	Z	102	ASN
7	Z	116	GLU
7	Z	120	ASP
7	Z	125	GLU
7	Z	136	VAL
7	Z	140	SER
7	Z	153	LEU
7	Z	157	LEU
7	Z	165	LEU
7	Z	168	THR
7	Z	188	SER
7	Z	191	THR
7	Z	192	LEU
7	Z	200	ASP
7	Z	204	VAL
7	Z	219	HIS
7	Z	222	ASN
7	Z	226	SER
7	Z	233	SER
7	Z	236	MET
7	Z	241	THR
7	Z	249	MET
7	Z	260	LEU
7	Z	269	LEU
7	Z	270	MET

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Mol	Chain	Res	Type
7	Z	288	THR
7	Z	292	ASP
7	Z	294	MET
7	Z	297	LEU
7	Z	298	LEU
7	Z	303	VAL
7	Z	304	MET
7	Z	305	VAL
7	Z	323	ILE
7	Z	331	THR
7	Z	340	ILE
7	Z	341	ARG
7	Z	343	ARG
7	Z	348	PHE
7	Z	355	SER
7	Z	357	GLN
7	Z	358	VAL
7	Z	369	SER
7	Z	374	SER
7	Z	376	LEU
7	Z	377	MET
7	Z	383	SER
7	Z	384	ILE
7	Z	410	LYS
7	Z	420	GLU
7	Z	422	ASP
7	Z	423	THR
7	Z	424	SER
7	Z	426	GLU
7	Z	439	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	l	38	GLN
1	l	42	ASN
2	m	17	ASN
2	b	17	ASN
2	b	36	ASN
2	b	56	ASN
3	a	84	GLN
3	a	127	HIS

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Mol	Chain	Res	Type
4	G	289	ASN
4	G	312	GLN
4	G	314	HIS
4	G	424	ASN
4	G	436	GLN
4	G	438	GLN
4	G	458	ASN
4	G	493	ASN
4	G	580	HIS
4	G	662	ASN
4	G	688	ASN
4	G	741	ASN
4	G	862	ASN
3	H	322	GLN
3	H	329	HIS
3	H	347	GLN
3	H	491	ASN
3	H	531	GLN
3	H	609	ASN
3	H	684	HIS
3	H	702	HIS
3	H	716	HIS
3	H	740	GLN
3	H	859	GLN
5	I	464	HIS
5	I	489	GLN
5	I	508	ASN
5	I	561	HIS
5	I	571	GLN
1	J	222	HIS
1	J	413	HIS
1	J	642	HIS
1	J	925	GLN
5	K	26	GLN
5	K	43	ASN
5	K	61	GLN
5	K	67	GLN
5	K	501	GLN
5	K	657	GLN
6	L	469	GLN
6	L	1492	ASN
6	L	1546	ASN

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Mol	Chain	Res	Type
6	L	1654	GLN
6	L	1673	GLN
6	L	1678	ASN
6	L	1679	GLN
7	U	16	GLN
7	U	24	GLN
7	U	158	ASN
7	U	187	ASN
7	U	197	GLN
7	U	229	ASN
7	U	322	ASN
7	V	16	GLN
7	V	24	GLN
7	V	187	ASN
7	V	197	GLN
7	V	229	ASN
7	V	322	ASN
7	W	16	GLN
7	W	187	ASN
7	W	197	GLN
7	W	229	ASN
7	W	322	ASN
7	X	16	GLN
7	X	24	GLN
7	X	158	ASN
7	X	187	ASN
7	X	197	GLN
7	X	229	ASN
7	X	322	ASN
7	Y	16	GLN
7	Y	158	ASN
7	Y	187	ASN
7	Y	197	GLN
7	Y	229	ASN
7	Y	322	ASN
7	Y	334	HIS
7	Z	16	GLN
7	Z	158	ASN
7	Z	187	ASN
7	Z	197	GLN
7	Z	229	ASN
7	Z	322	ASN

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Mol	Chain	Res	Type
7	Z	334	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

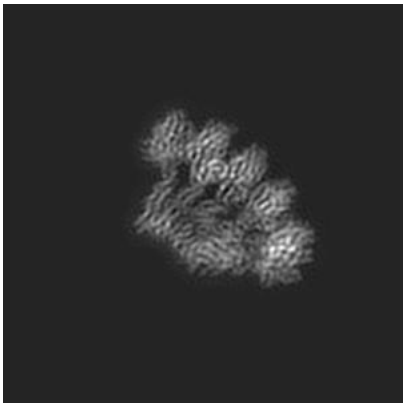
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14006. 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.

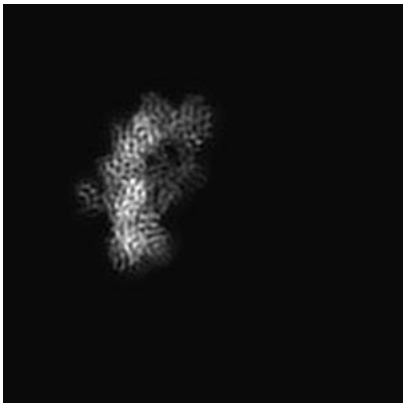
6.1 Orthogonal projections

6.1.1 Primary map



X

Y



Z

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

6.2 Central slices

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

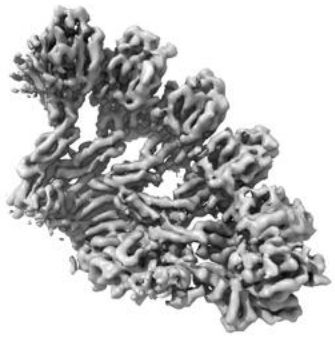
Y Index: 101

Z Index: 77

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

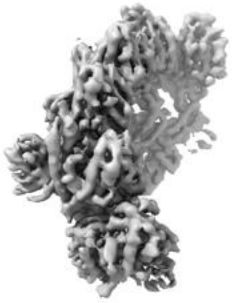
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0571. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

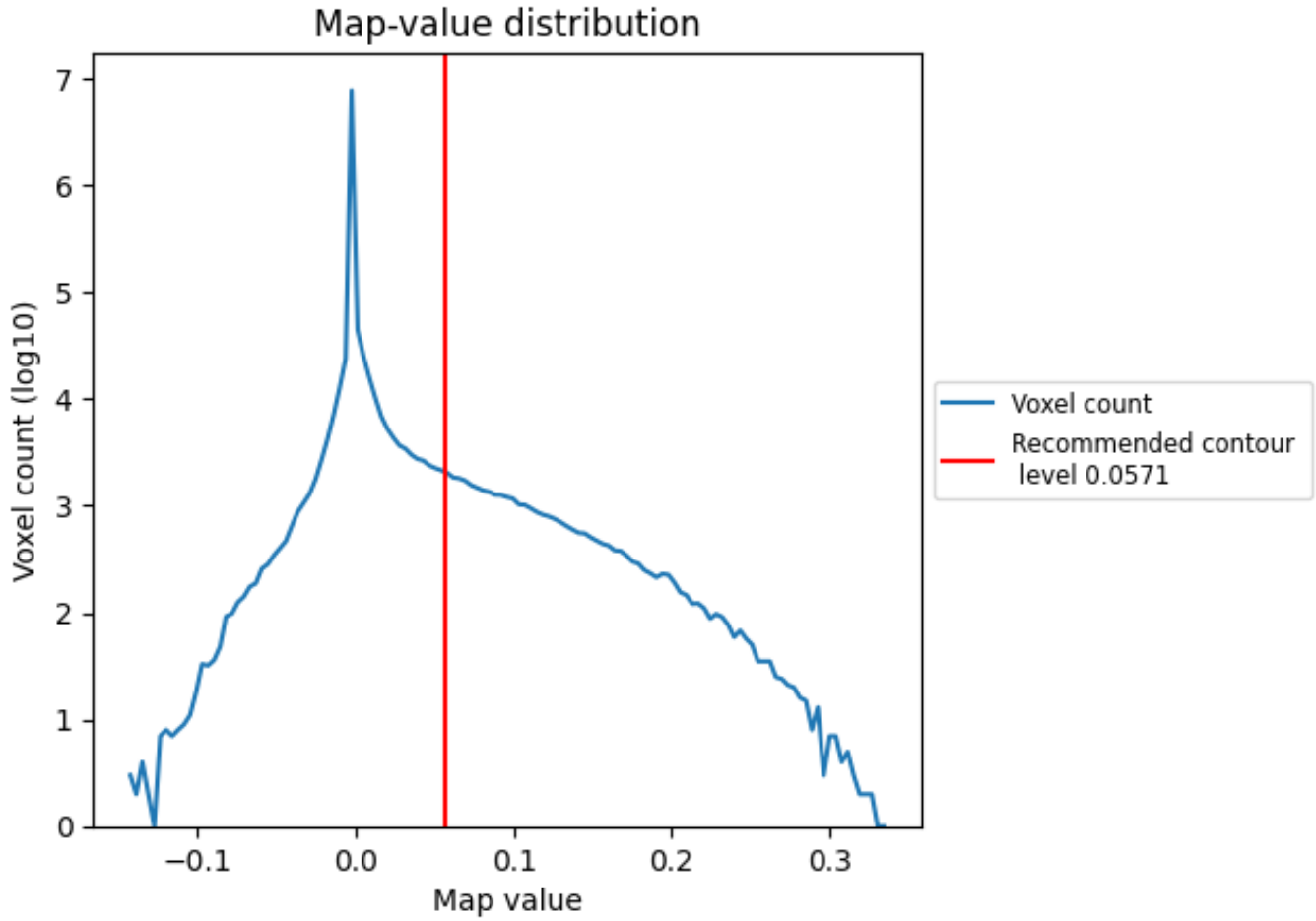
6.5 Mask visualisation (i)

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

7 Map analysis

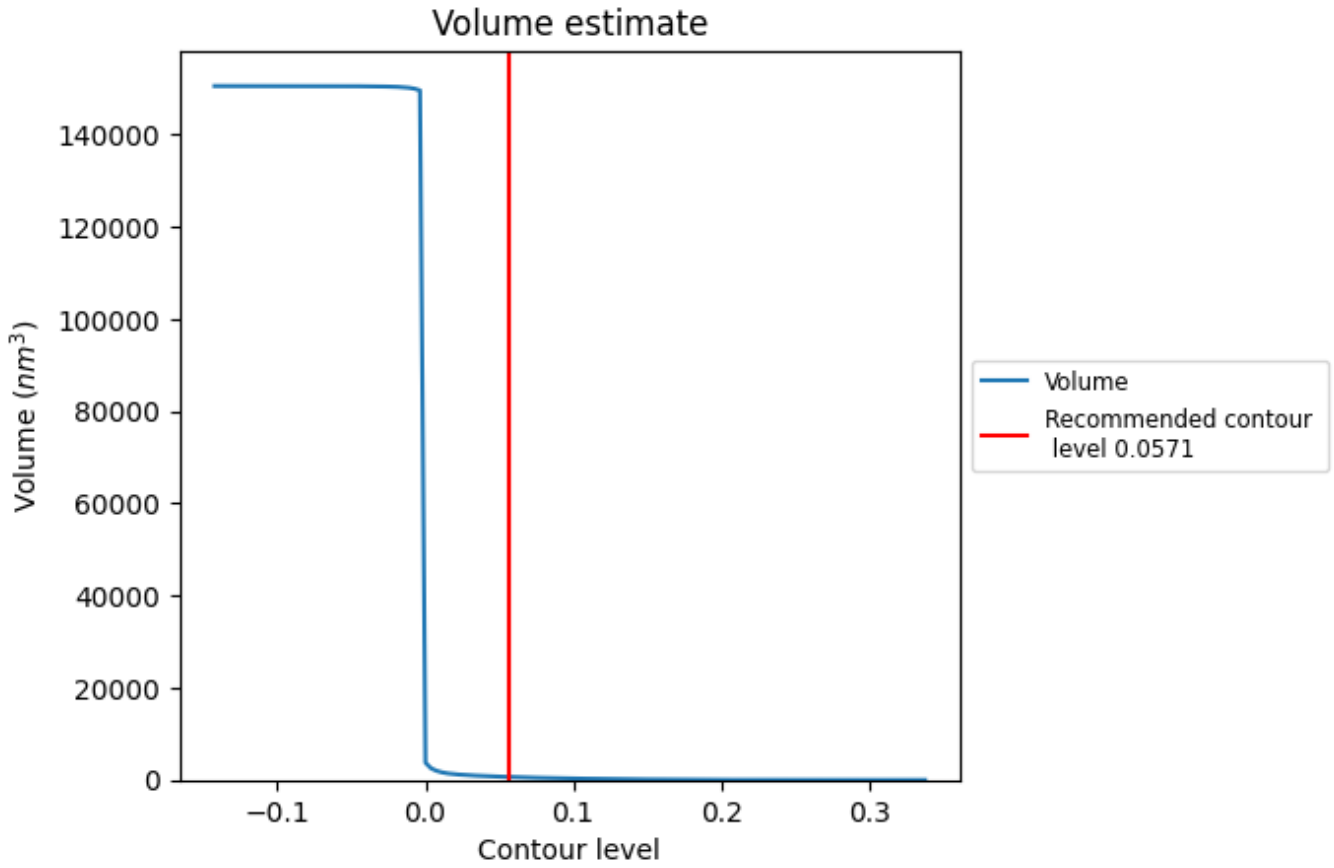
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

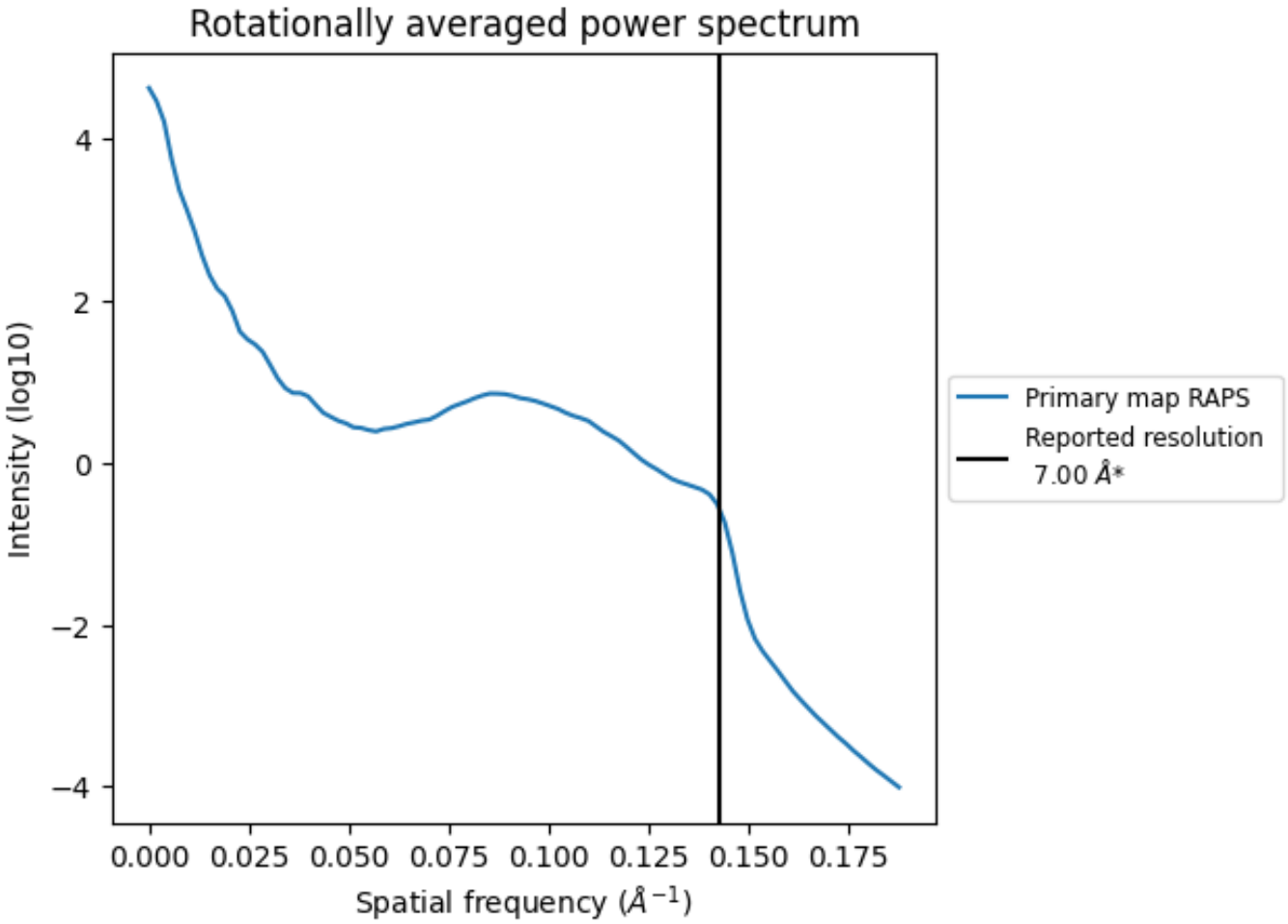
7.2 Volume estimate



The volume at the recommended contour level is 646 nm^3; this corresponds to an approximate mass of 584 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.143 Å^{-1}

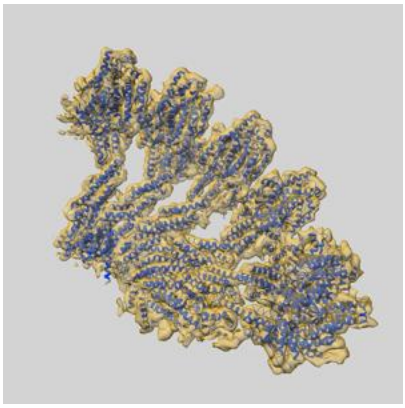
8 Fourier-Shell correlation

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

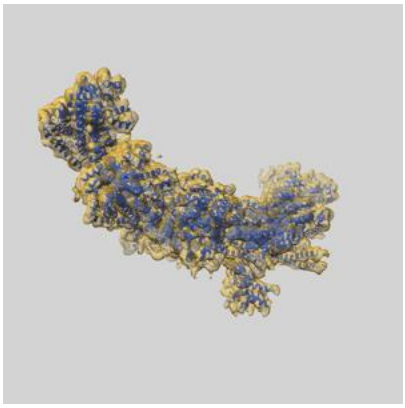
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14006 and PDB model 7QJ1. Per-residue inclusion information can be found in section 3 on page 6.

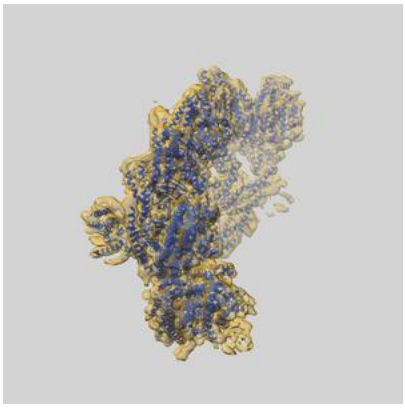
9.1 Map-model overlay



X



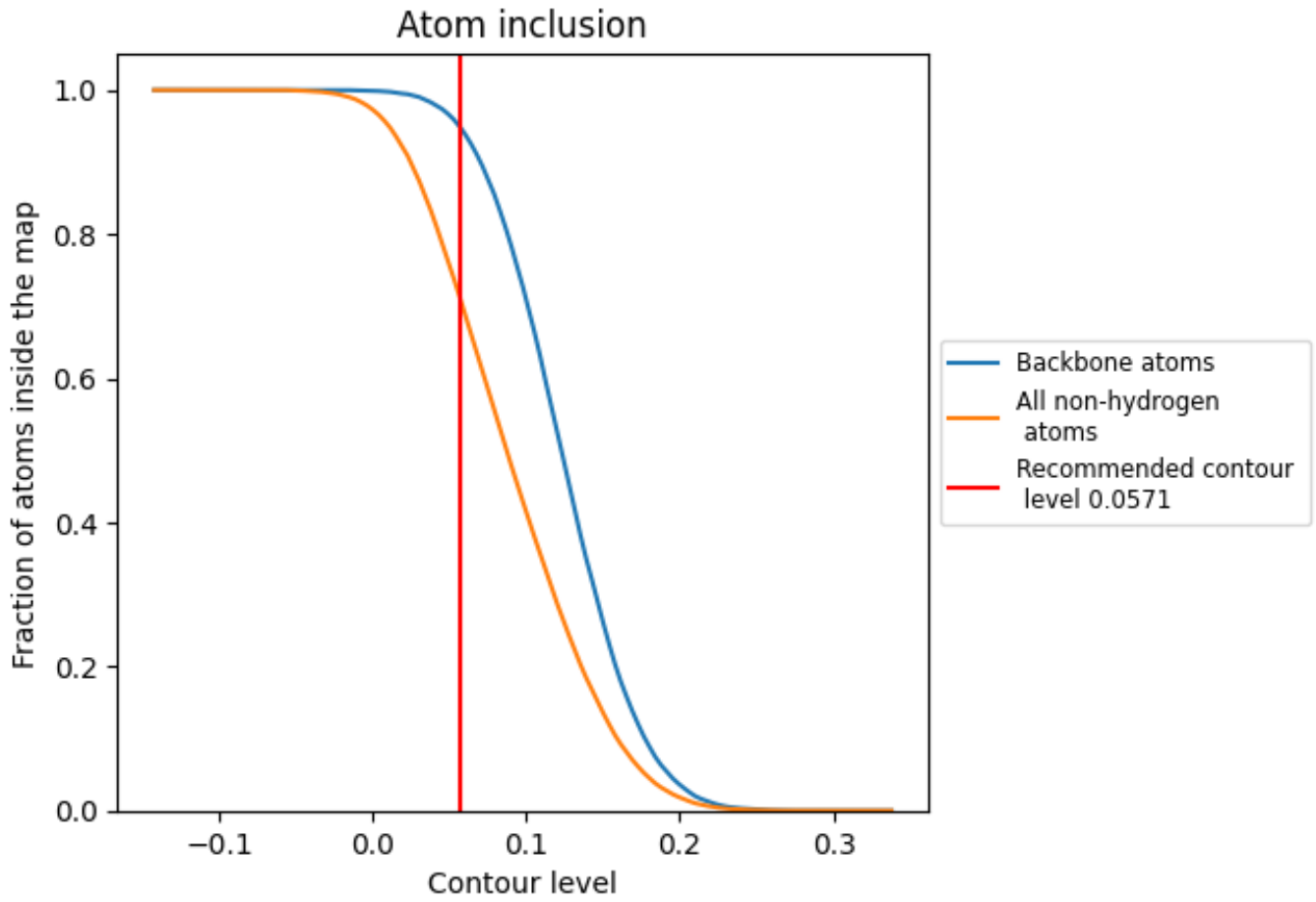
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0571 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 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.