



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:01 AM UTC

PDB ID : 9G3Y / pdb_00009g3y
EMDB ID : EMD-51018
Title : Structure of the Native CMG-decorated gamma-Tubulin Ring Complex from Pig Brain
Authors : Munoz-Hernandez, H.; Wieczorek, M.
Deposited on : 2024-07-12
Resolution : 6.80 Å(reported)

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

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

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:

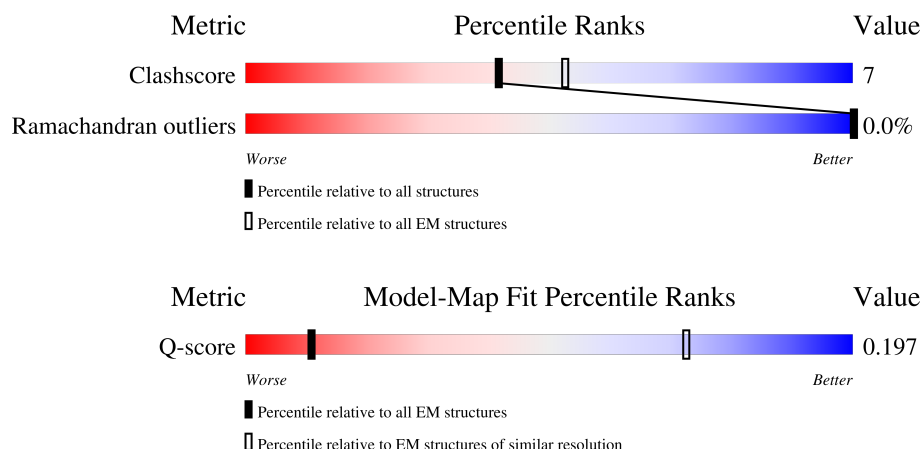
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 6.80 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.



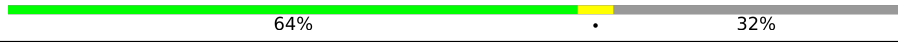
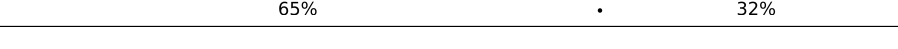
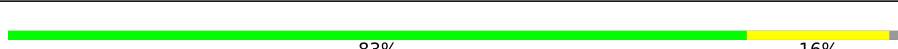
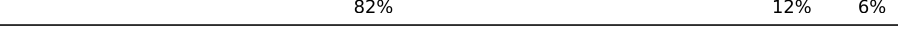
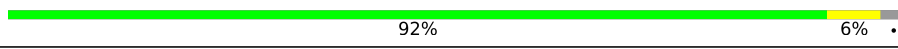
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	503 (6.30 - 7.30)

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	A	905	
1	C	905	
1	E	905	
1	G	905	
1	M	905	

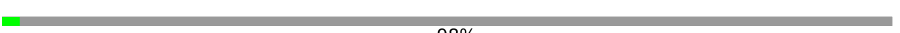
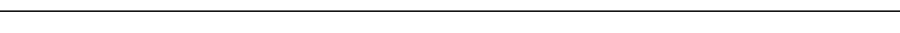
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Mol	Chain	Length	Quality of chain
2	B	910	
2	D	910	
2	F	910	
2	H	910	
2	N	910	
3	I	667	
3	K	667	
4	J	1061	
5	L	1715	
6	O	79	
6	P	79	
6	Q	79	
7	V	155	
7	W	155	
7	X	155	
7	Y	155	
8	a	451	
8	b	451	
8	c	451	
8	d	451	
8	e	451	
8	f	451	
8	g	451	
8	h	451	
8	i	451	

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Mol	Chain	Length	Quality of chain
8	j	451	 86% 11%
8	k	451	 85% 12%
8	l	451	 11% 85% 10% 5%
8	m	451	 52% 93% 5%
8	n	451	 92% 93% 5%
9	o	1663	 98%
9	p	1663	 98%
9	q	1663	 98%
9	r	1663	 98%
9	s	1663	 98%
9	t	1663	 98%
9	u	1663	 98%
9	v	1663	 98%
9	w	1663	 98%
9	x	1663	 98%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 118940 atoms, of which 36534 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	682	Total	C	H	N	O	0	0
			4887	2021	1502	682	682		
1	C	797	Total	C	H	N	O	0	0
			5721	2363	1764	797	797		
1	E	797	Total	C	H	N	O	0	0
			5721	2363	1764	797	797		
1	G	797	Total	C	H	N	O	0	0
			5721	2363	1764	797	797		
1	M	778	Total	C	H	N	O	0	0
			5575	2307	1712	778	778		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	617	Total	C	H	N	O	0	0
			4433	1826	1373	617	617		
2	D	617	Total	C	H	N	O	0	0
			4433	1826	1373	617	617		
2	F	617	Total	C	H	N	O	0	0
			4433	1826	1373	617	617		
2	H	735	Total	C	H	N	O	0	0
			5289	2176	1643	735	735		
2	N	720	Total	C	H	N	O	0	0
			5179	2133	1606	720	720		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	608	Total	C	H	N	O	0	0
			4325	1795	1314	608	608		
3	K	608	Total	C	H	N	O	0	0
			4325	1795	1314	608	608		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	629	Total	C	H	N	O	0	0
			4466	1867	1341	629	629		

- Molecule 5 is a protein called Tubulin gamma complex associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	790	Total	C	H	N	O	0	0
			5669	2320	1769	790	790		

- Molecule 6 is a protein called Mitotic spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	67	Total	C	H	N	O	0	0
			497	199	164	67	67		
6	Q	64	Total	C	H	N	O	0	0
			464	190	146	64	64		
6	O	67	Total	C	H	N	O	0	0
			497	199	164	67	67		

- Molecule 7 is a protein called Mitotic-spindle organizing protein 2A isoform X4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	45	Total	C	H	N	O	0	0
			336	132	114	45	45		
7	W	45	Total	C	H	N	O	0	0
			336	132	114	45	45		
7	X	45	Total	C	H	N	O	0	0
			336	132	114	45	45		
7	Y	51	Total	C	H	N	O	0	0
			379	150	127	51	51		

- Molecule 8 is a protein called Tubulin gamma chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	444	Total	C	H	N	O	0	0
			3161	1306	967	444	444		
8	b	442	Total	C	H	N	O	0	0
			3146	1299	963	442	442		
8	c	440	Total	C	H	N	O	0	0
			3129	1293	956	440	440		
8	d	426	Total	C	H	N	O	0	0
			3030	1252	926	426	426		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	432	Total	C	H	N	O	0	0
			3074	1270	940	432	432		
8	f	433	Total	C	H	N	O	0	0
			3081	1273	942	433	433		
8	g	433	Total	C	H	N	O	0	0
			3081	1273	942	433	433		
8	h	439	Total	C	H	N	O	0	0
			3122	1291	953	439	439		
8	i	438	Total	C	H	N	O	0	0
			3115	1288	951	438	438		
8	j	439	Total	C	H	N	O	0	0
			3122	1292	952	439	439		
8	k	438	Total	C	H	N	O	0	0
			3115	1288	951	438	438		
8	l	428	Total	C	H	N	O	0	0
			3044	1258	930	428	428		
8	m	444	Total	C	H	N	O	0	0
			3161	1306	967	444	444		
8	n	442	Total	C	H	N	O	0	0
			3146	1299	963	442	442		

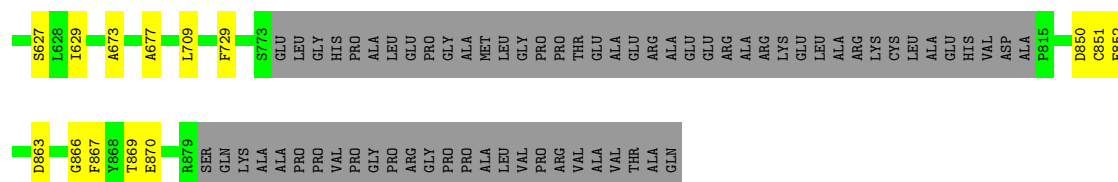
- Molecule 9 is a protein called CDK5 regulatory subunit-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	o	33	Total	C	H	N	O	0	0
			230	99	65	33	33		
9	q	33	Total	C	H	N	O	0	0
			230	99	65	33	33		
9	r	33	Total	C	H	N	O	0	0
			230	99	65	33	33		
9	s	36	Total	C	H	N	O	0	0
			251	108	71	36	36		
9	t	36	Total	C	H	N	O	0	0
			251	108	71	36	36		
9	v	36	Total	C	H	N	O	0	0
			251	108	71	36	36		
9	u	36	Total	C	H	N	O	0	0
			251	108	71	36	36		
9	w	33	Total	C	H	N	O	0	0
			230	99	65	33	33		
9	x	34	Total	C	H	N	O	0	0
			237	102	67	34	34		

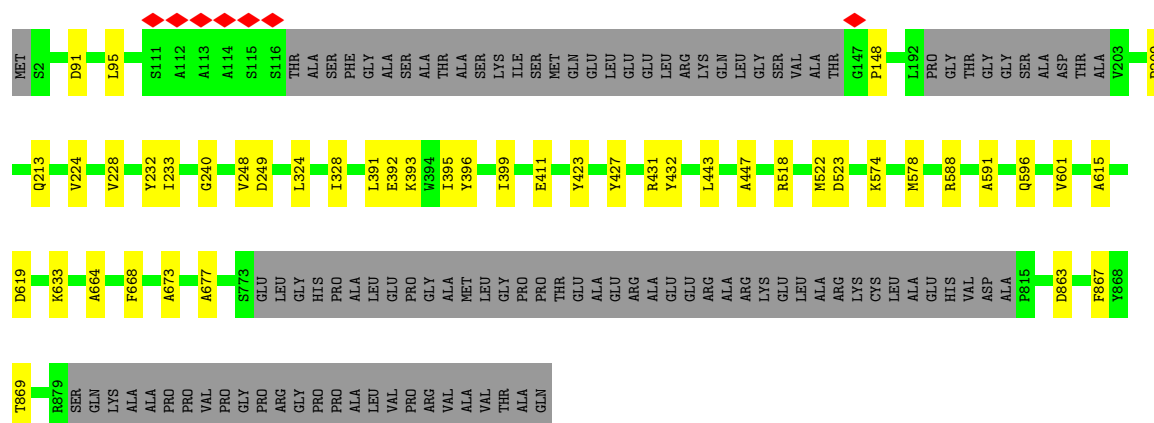
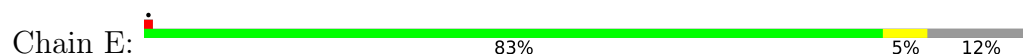
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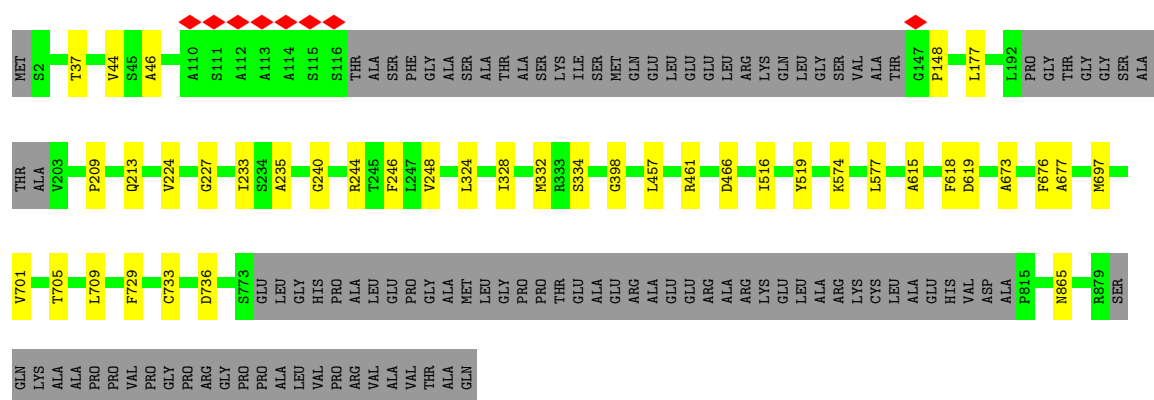
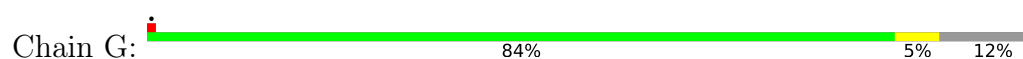
Mol	Chain	Residues	Atoms					AltConf	Trace
9	p	33	Total	C	H	N	O	0	0
			230	99	65	33	33		



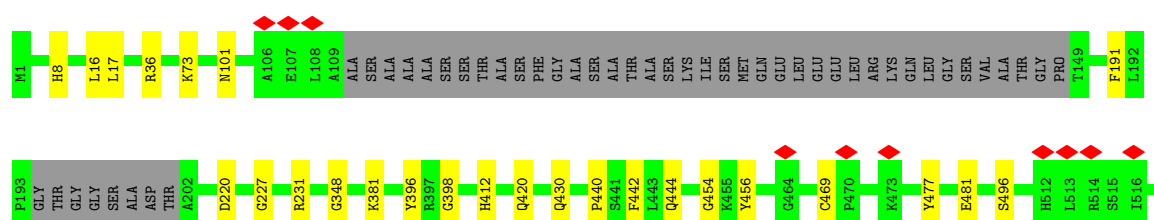
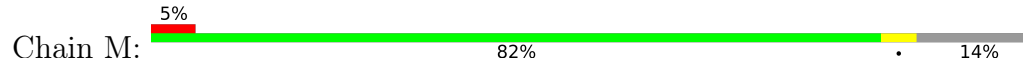
• Molecule 1: Gamma-tubulin complex component

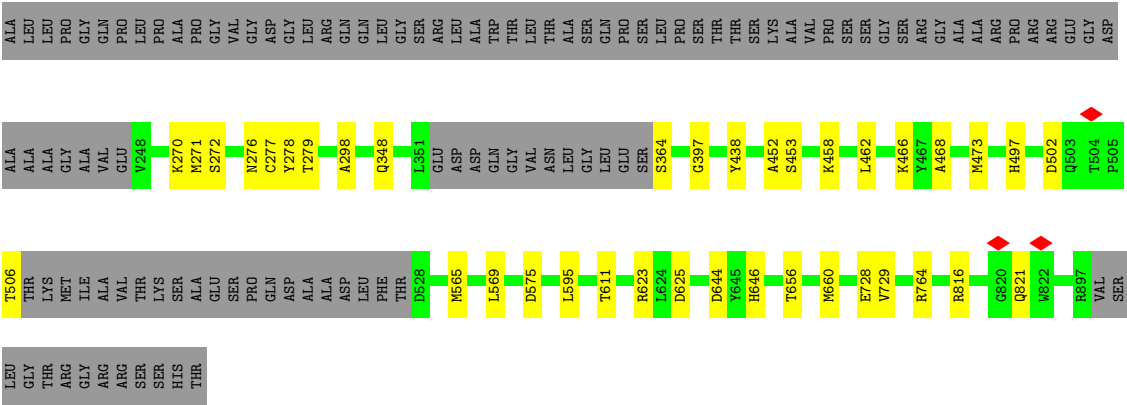


• Molecule 1: Gamma-tubulin complex component



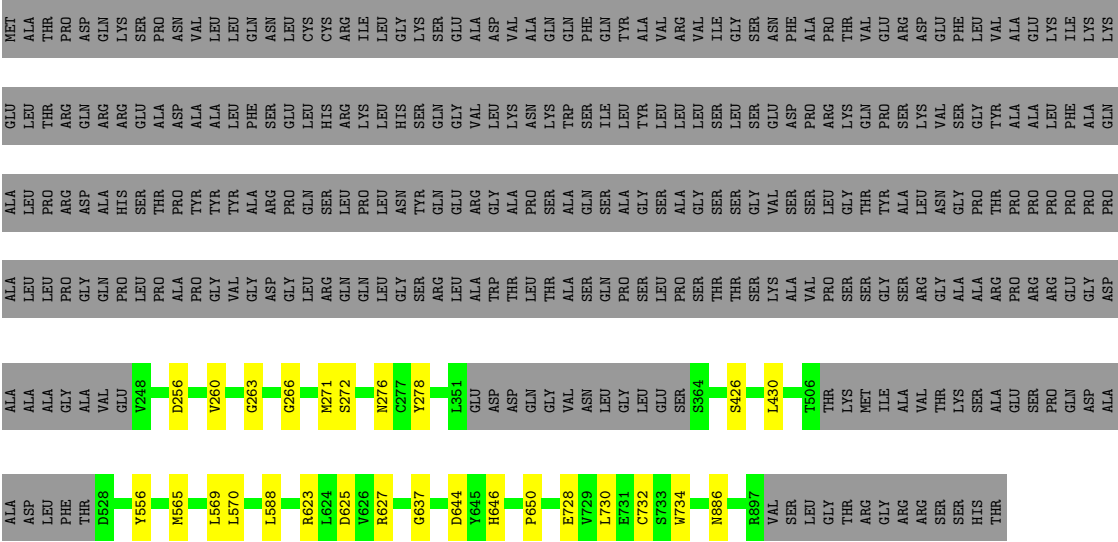
• Molecule 1: Gamma-tubulin complex component





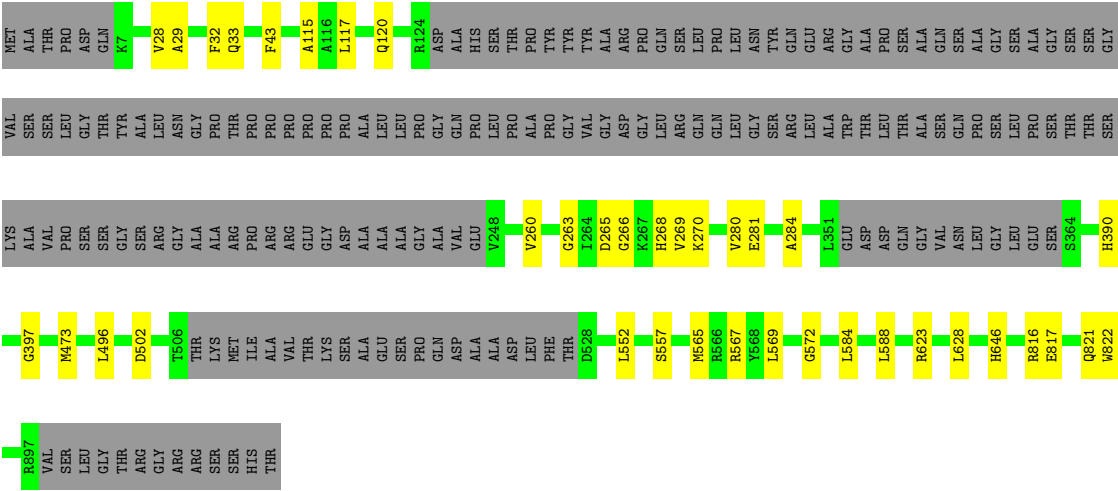
• Molecule 2: Gamma-tubulin complex component 3

Chain F: 65% 32%

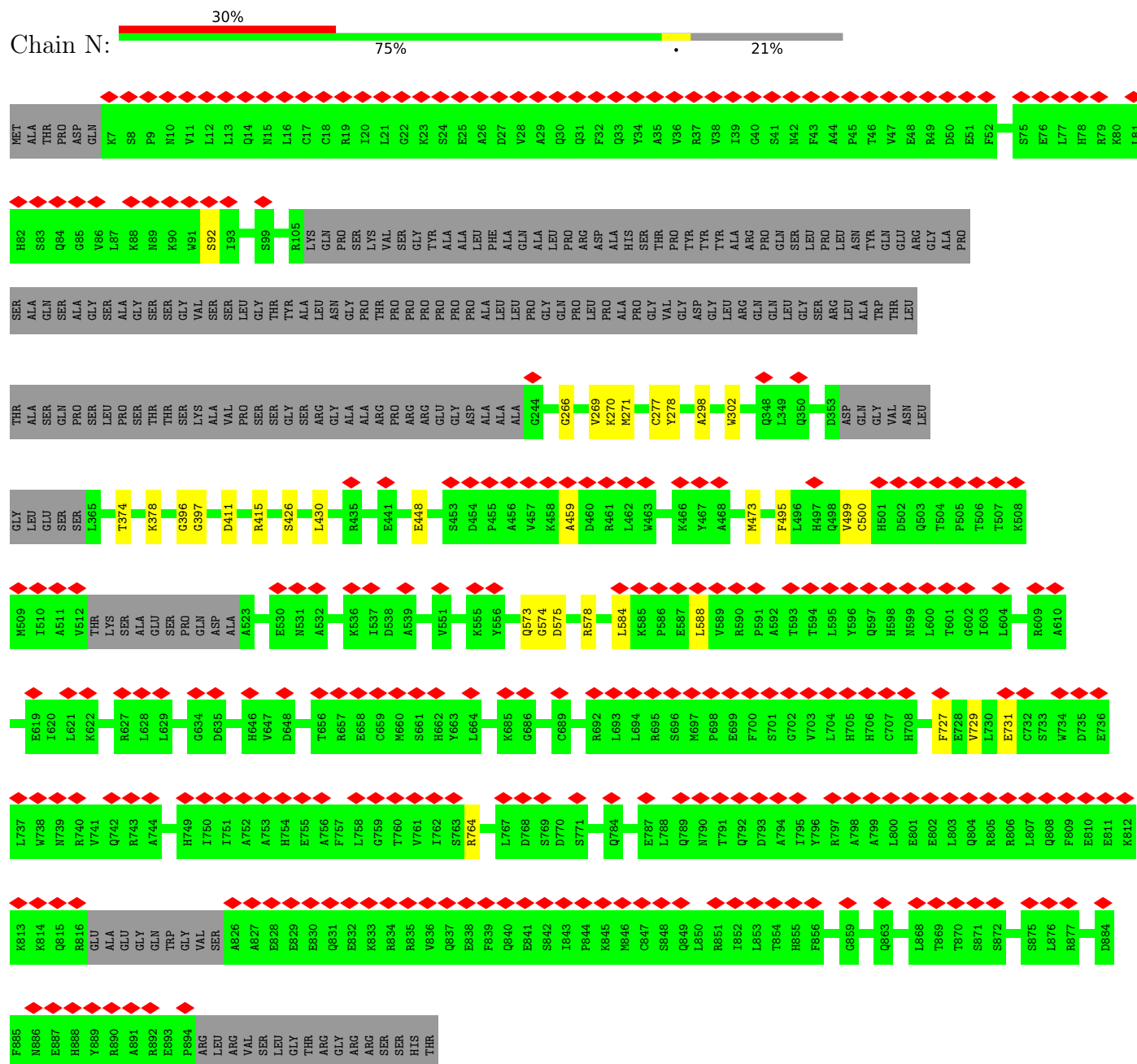


• Molecule 2: Gamma-tubulin complex component 3

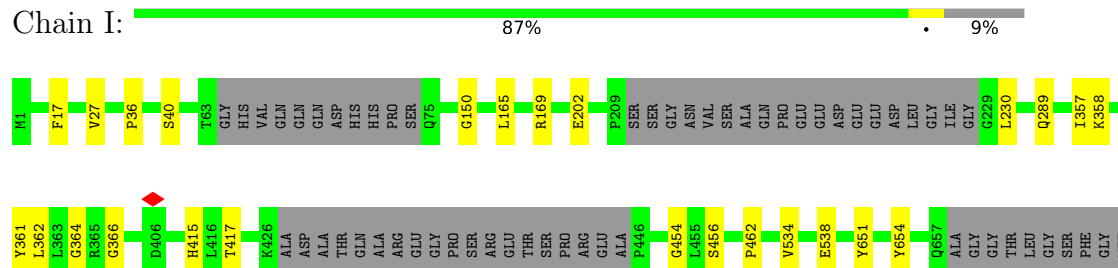
Chain H: 77% 19%



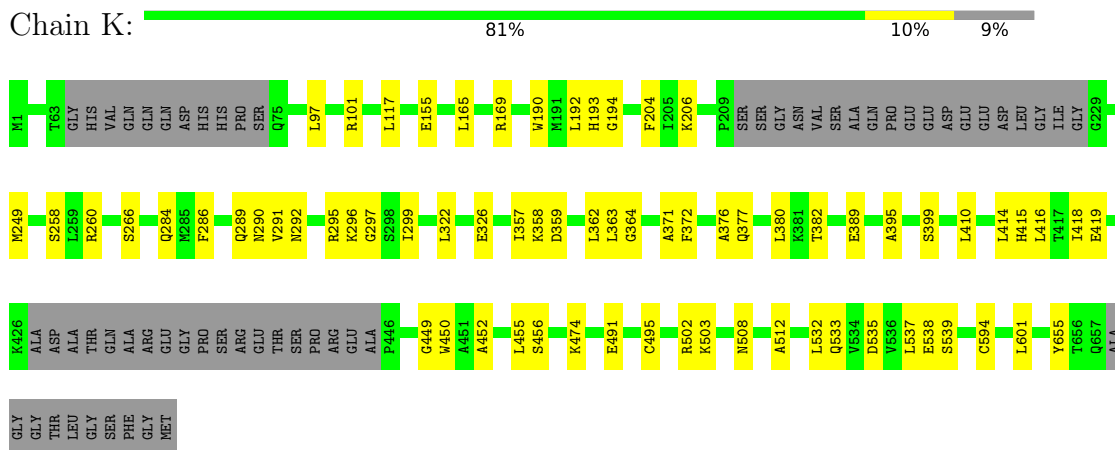
Chain N:



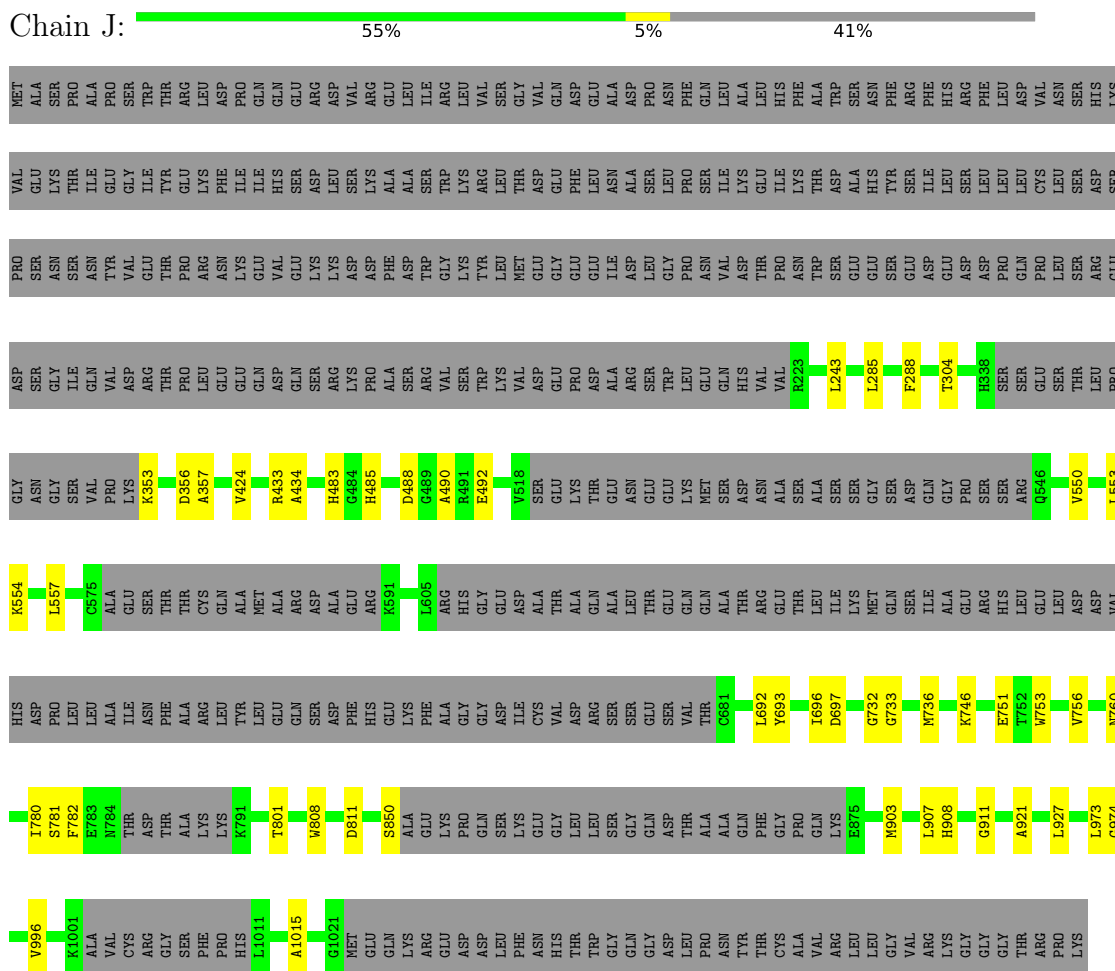
Chain I:



- Molecule 3: Gamma-tubulin complex component



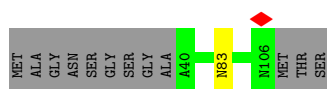
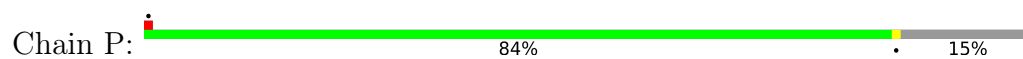
- Molecule 4: Gamma-tubulin complex component



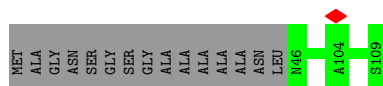
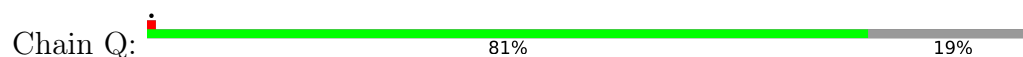
- Molecule 5: Tubulin gamma complex associated protein 6



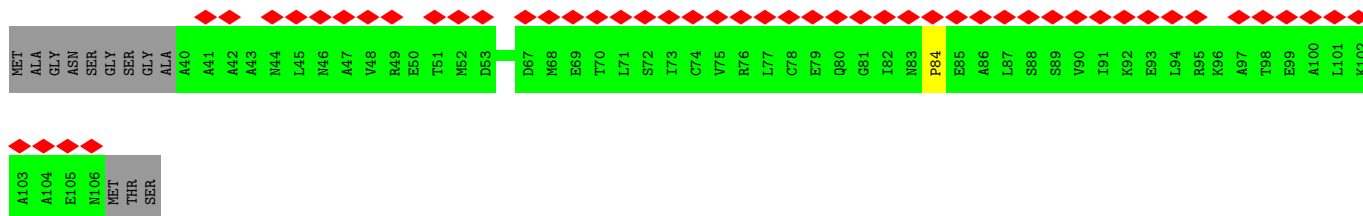
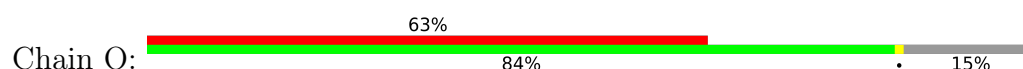




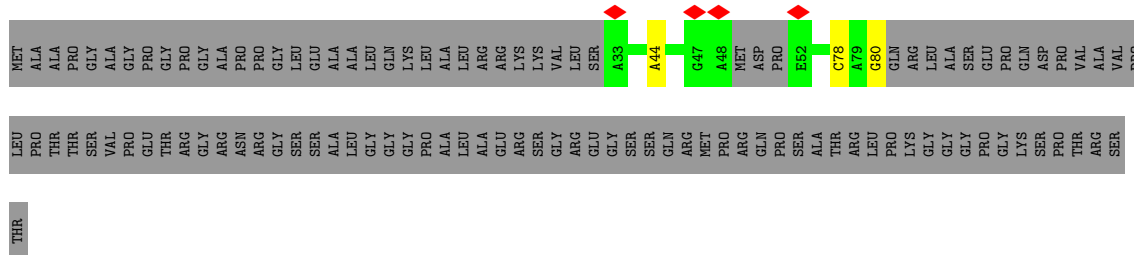
- Molecule 6: Mitotic spindle organizing protein 1



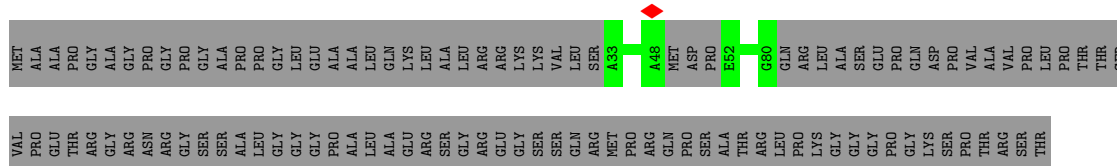
- Molecule 6: Mitotic spindle organizing protein 1



- Molecule 7: Mitotic-spindle organizing protein 2A isoform X4

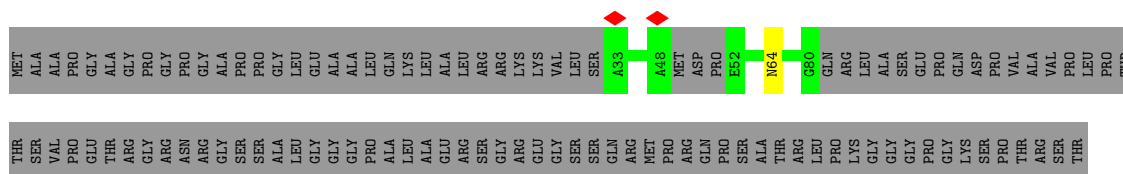


- Molecule 7: Mitotic-spindle organizing protein 2A isoform X4



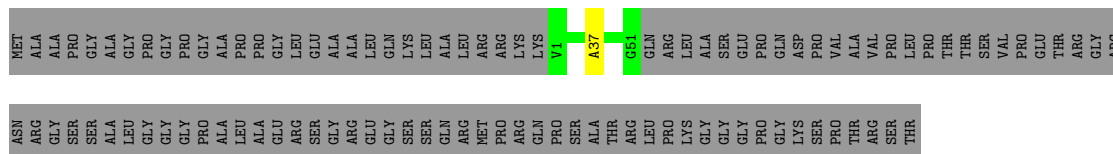
- Molecule 7: Mitotic-spindle organizing protein 2A isoform X4





• Molecule 7: Mitotic-spindle organizing protein 2A isoform X4

Chain Y: 32% . 67%



• Molecule 8: Tubulin gamma chain

Chain a: 83% . 16%



• Molecule 8: Tubulin gamma chain

Chain b: 84% . 14%



• Molecule 8: Tubulin gamma chain

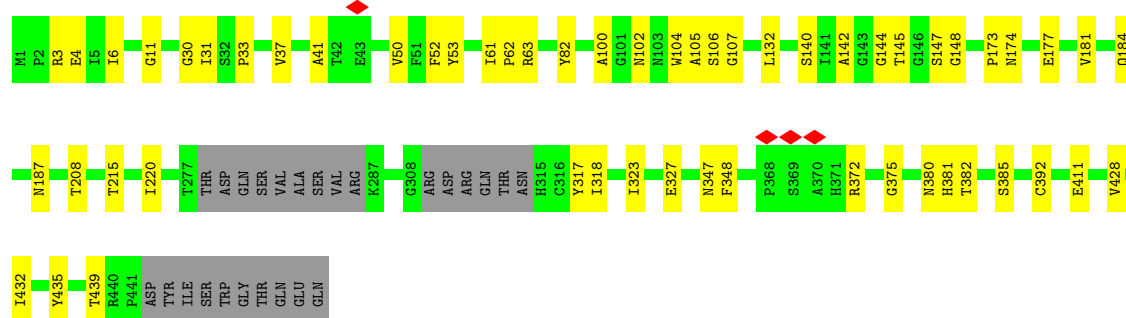
Chain c: 86% . 11%





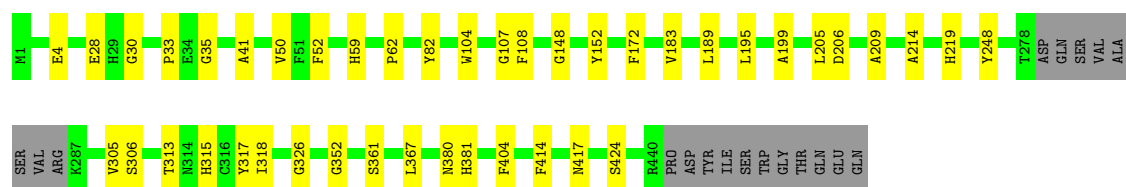
• Molecule 8: Tubulin gamma chain

Chain d: 82% 12% 6%



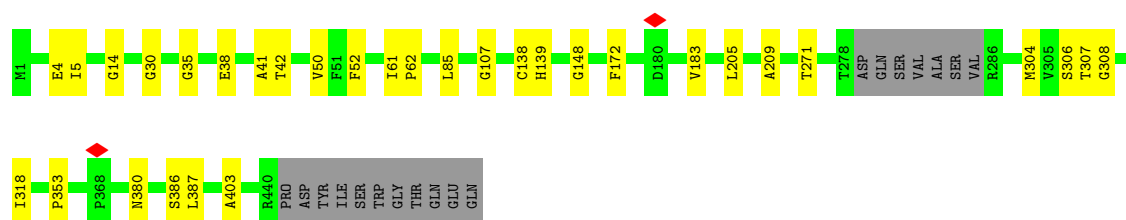
• Molecule 8: Tubulin gamma chain

Chain e: 86% 10% 4%



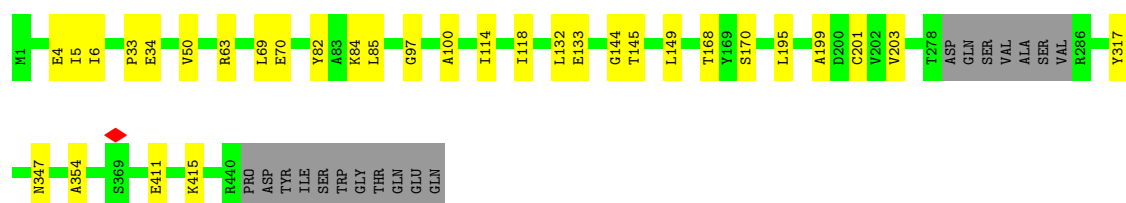
• Molecule 8: Tubulin gamma chain

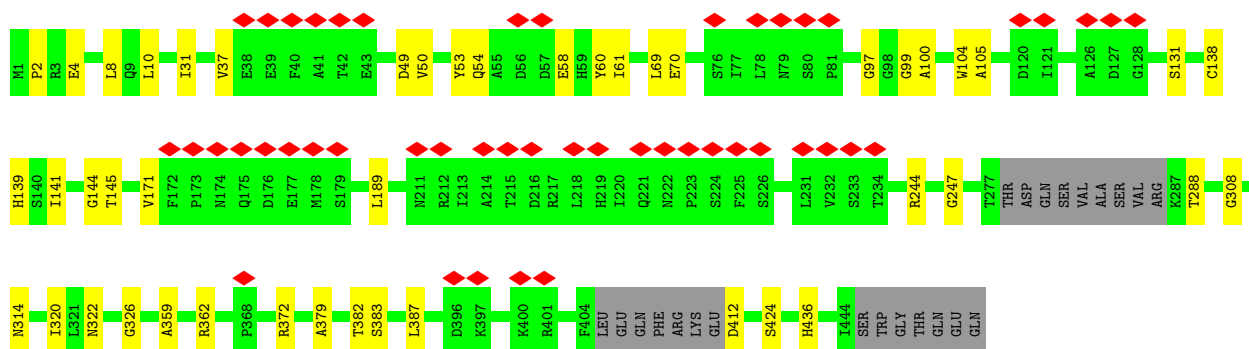
Chain f: 89% 7% 4%



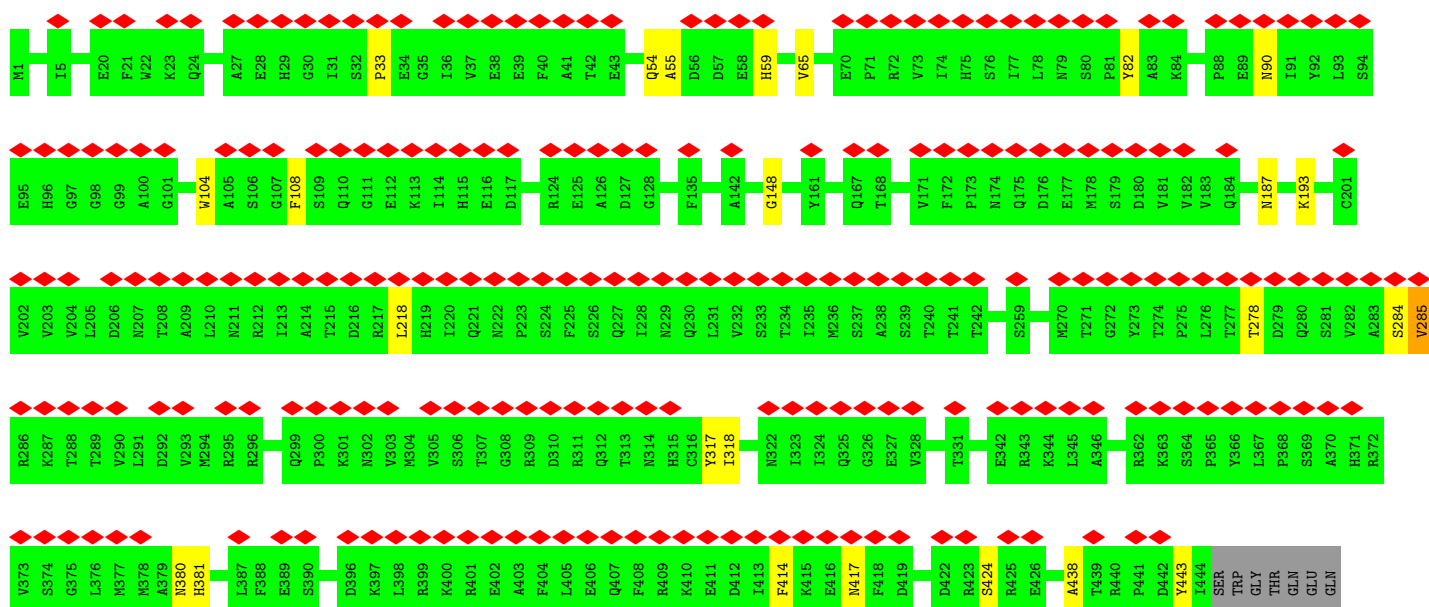
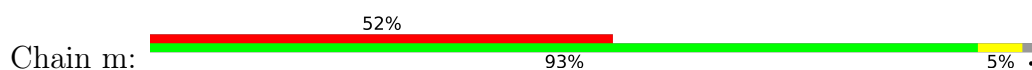
• Molecule 8: Tubulin gamma chain

Chain g: 89% 7% 4%

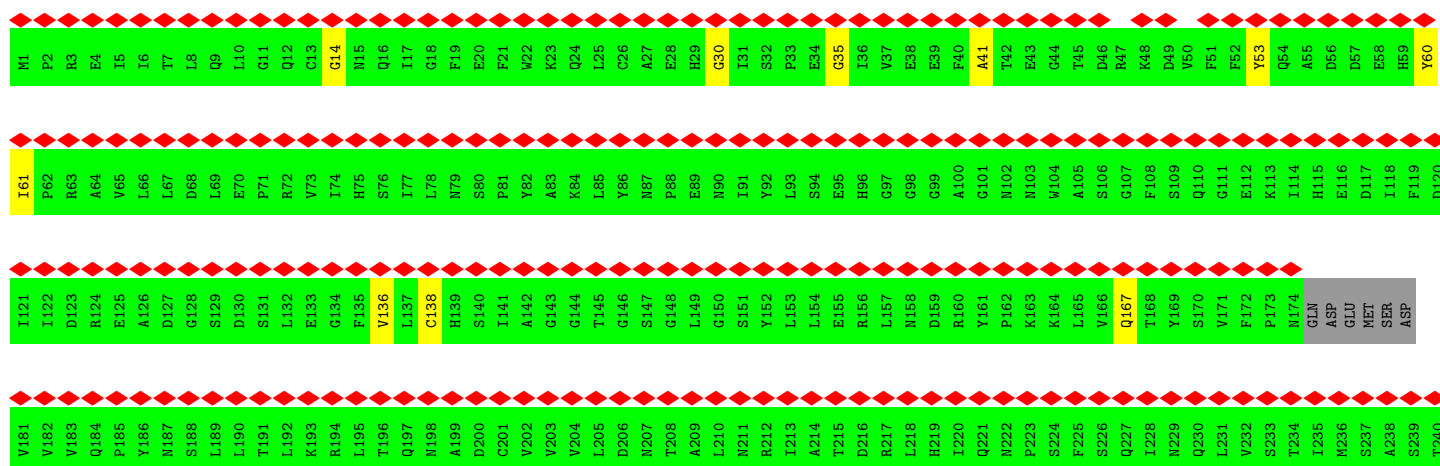
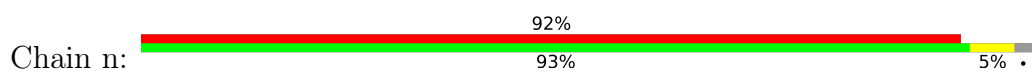


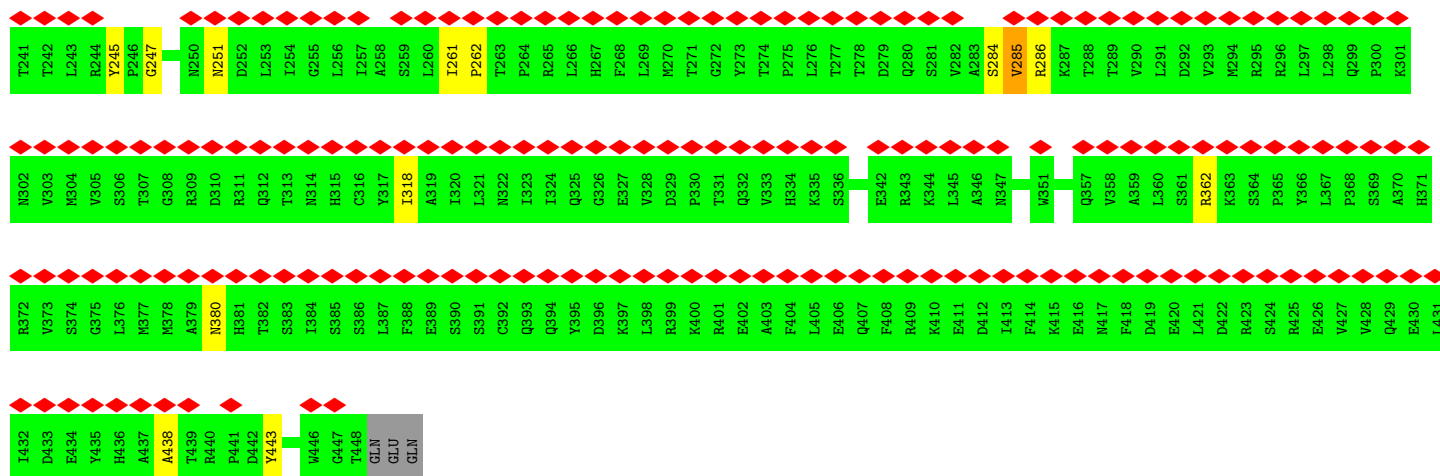


• Molecule 8: Tubulin gamma chain



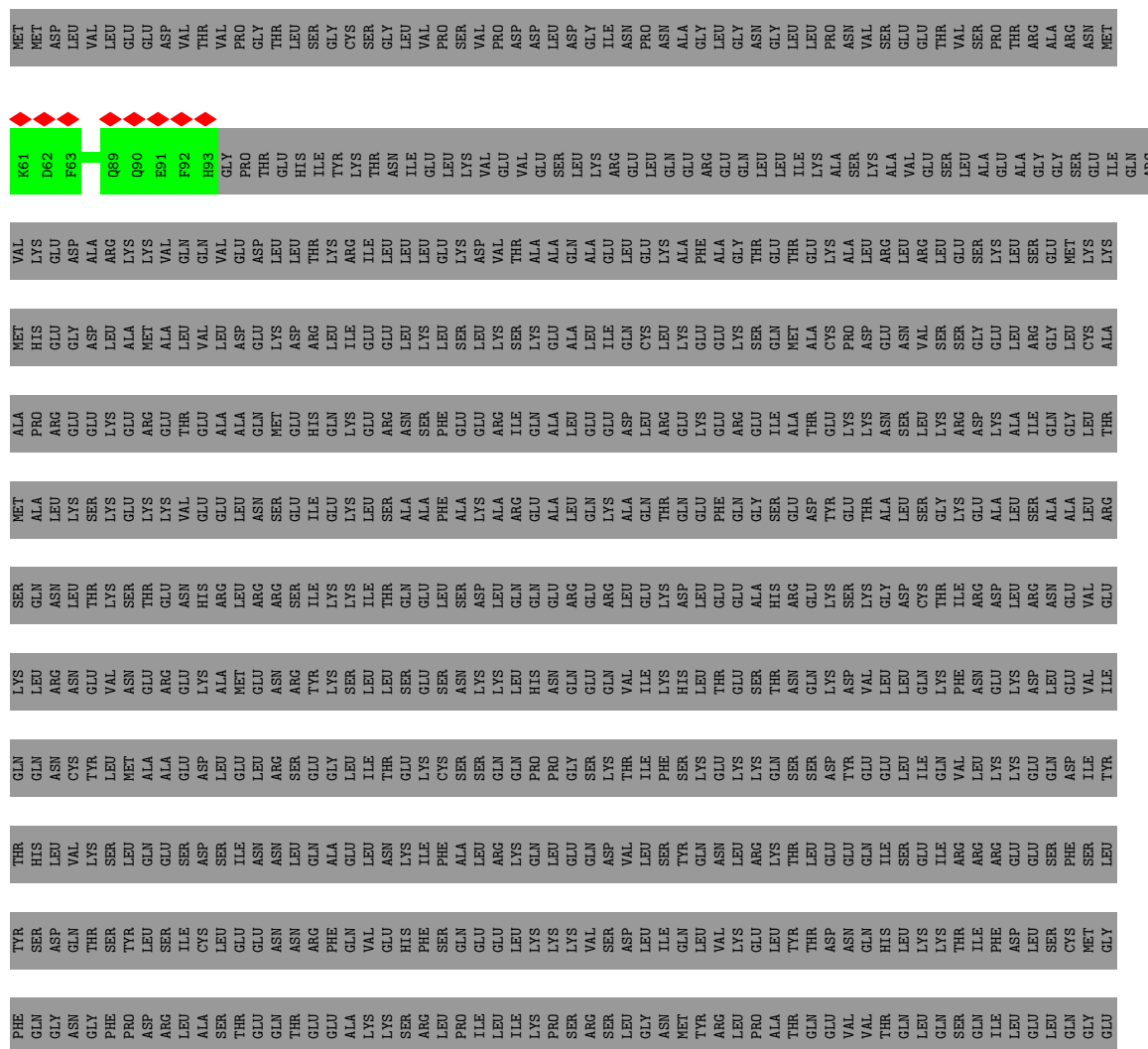
• Molecule 8: Tubulin gamma chain





• Molecule 9: CDK5 regulatory subunit-associated protein 2

Chain o: . 98%







[illegible]

- Molecule 9: CDK5 regulatory subunit-associated protein 2

Chain r: 98%

MET	ASP	THR	LYS	GLY	THR	THR	LYS	TTR	GLU	THR	SER	GLU	ASP	ALA	MET
ASP	THR	THR	SER	PHE	SER	THR	SER	LEU	VAL	LYS	LYS	GLU	ALA	ARG	MET
ASN	SER	PRO	LEU	PRO	LEU	THR	ASN	MET	ASN	THR	GLU	ASN	ARG	LYS	ASP
GLN	ASN	GLN	GLN	LEU	SER	THR	SER	GLU	ARG	GLU	VAL	VAL	ALA	VAL	LEU
LEU	ALA	ASP	ALA	ALA	ASP	CYS	LYS	ASP	LYS	HIS	GLU	GLU	VAL	GLN	LEU
GLU	LEU	SER	SER	SER	LEU	THR	LEU	LEU	ALA	GLU	GLU	ALA	VAL	GLN	GLU
THR	GLN	THR	THR	THR	GLU	GLU	GLU	GLU	ALA	ARG	GLU	ALA	VAL	GLN	GLU
GLY	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ALA	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
LEU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
THR	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
GLY	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	VAL	GLN	GLU
ASP	THR	GLU	GLU	GLU	GLU</										





[illegible]

- Molecule 9: CDK5 regulatory subunit-associated protein 2

Chain t: 98%

[illegible]





- Molecule 9: CDK5 regulatory subunit-associated protein 2

98%



[illegible]

- Molecule 9: CDK5 regulatory subunit-associated protein 2

Chain p: 98%

[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.715	Depositor
Minimum map value	-0.183	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.125	Depositor
Map size ($\text{\AA}$)	542.7199, 542.7199, 542.7199	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.413333, 1.413333, 1.413333	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/3382	0.51	0/4715
1	C	0.21	0/3953	0.48	0/5511
1	E	0.23	0/3953	0.52	0/5511
1	G	0.22	0/3953	0.48	0/5511
1	M	0.14	0/3857	0.39	0/5374
2	B	0.18	0/3057	0.45	0/4260
2	D	0.23	0/3057	0.52	0/4260
2	F	0.22	0/3057	0.46	0/4260
2	H	0.20	0/3642	0.45	0/5075
2	N	0.13	0/3568	0.33	0/4971
3	I	0.20	0/3007	0.45	0/4186
3	K	0.19	0/3007	0.41	0/4186
4	J	0.19	0/3117	0.41	0/4339
5	L	0.19	0/3891	0.43	0/5403
6	O	0.12	0/332	0.31	0/462
6	P	0.28	0/332	0.58	0/462
6	Q	0.14	0/317	0.34	0/441
7	V	0.17	0/220	0.46	0/303
7	W	0.20	0/220	0.54	0/303
7	X	0.22	0/220	0.47	0/303
7	Y	0.21	0/251	0.43	0/348
8	a	0.17	0/2193	0.46	0/3053
8	b	0.18	0/2181	0.50	0/3034
8	c	0.20	0/2171	0.51	0/3020
8	d	0.22	0/2101	0.56	0/2921
8	e	0.20	0/2132	0.48	0/2966
8	f	0.20	0/2137	0.49	0/2973
8	g	0.19	0/2137	0.47	0/2973
8	h	0.20	0/2167	0.49	0/3015
8	i	0.20	0/2162	0.47	0/3008
8	j	0.17	0/2168	0.44	0/3017
8	k	0.19	0/2162	0.44	0/3008
8	l	0.14	0/2111	0.40	0/2935
8	m	0.13	0/2193	0.37	0/3053

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	n	0.13	0/2181	0.37	0/3034
9	o	0.17	0/164	0.26	0/228
9	p	0.20	0/164	0.53	0/228
9	q	0.16	0/164	0.34	0/228
9	r	0.18	0/164	0.31	0/228
9	s	0.21	0/179	0.37	0/249
9	t	0.16	0/179	0.29	0/249
9	u	0.21	0/179	0.43	0/249
9	v	0.21	0/179	0.38	0/249
9	w	0.14	0/164	0.29	0/228
9	x	0.14	0/169	0.26	0/235
All	All	0.19	0/82294	0.45	0/114565

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	N	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	574	GLY	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	A	3385	1502	1502	59	0
1	C	3957	1764	1764	25	0
1	E	3957	1764	1764	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3957	1764	1764	25	0
1	M	3863	1712	1712	22	0
2	B	3060	1373	1373	38	0
2	D	3060	1373	1373	21	0
2	F	3060	1373	1373	15	0
2	H	3646	1643	1643	23	0
2	N	3573	1606	1606	19	0
3	I	3011	1314	1314	17	0
3	K	3011	1314	1314	44	0
4	J	3125	1341	1341	28	0
5	L	3900	1769	1769	38	0
6	O	333	164	164	1	0
6	P	333	164	164	1	0
6	Q	318	146	146	0	0
7	V	222	114	114	5	0
7	W	222	114	114	0	0
7	X	222	114	114	1	0
7	Y	252	127	129	1	0
8	a	2194	967	967	46	0
8	b	2183	963	963	41	0
8	c	2173	956	956	33	0
8	d	2104	926	926	33	0
8	e	2134	940	940	24	0
8	f	2139	942	942	18	0
8	g	2139	942	942	18	0
8	h	2169	953	953	13	0
8	i	2164	951	951	20	0
8	j	2170	952	952	32	0
8	k	2164	951	951	31	0
8	l	2114	930	930	29	0
8	m	2194	967	967	13	0
8	n	2183	963	963	15	0
9	o	165	65	65	0	0
9	p	165	65	65	0	0
9	q	165	65	65	1	0
9	r	165	65	65	1	0
9	s	180	71	71	0	0
9	t	180	71	71	1	0
9	u	180	71	71	0	0
9	v	180	71	71	0	0
9	w	165	65	65	1	0
9	x	170	67	67	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	82406	36534	36536	737	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 7.

All (737) 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)
2:D:348:GLN:O	2:D:364:SER:N	1.96	0.97
2:H:584:LEU:O	2:H:588:LEU:N	2.09	0.85
2:D:656:THR:O	2:D:660:MET:N	2.10	0.85
8:e:318:ILE:N	8:e:380:ASN:O	2.10	0.85
1:C:203:VAL:N	1:C:231:ARG:O	2.10	0.85
8:i:317:TYR:N	8:i:347:ASN:O	2.09	0.84
5:L:463:PHE:O	5:L:467:GLY:N	2.12	0.83
8:k:411:GLU:O	8:k:415:LYS:N	2.11	0.82
2:D:623:ARG:O	2:D:646:HIS:N	2.12	0.82
1:G:324:LEU:O	1:G:328:ILE:N	2.13	0.82
8:d:318:ILE:N	8:d:380:ASN:O	2.12	0.82
8:h:317:TYR:N	8:h:347:ASN:O	2.14	0.81
8:g:317:TYR:N	8:g:347:ASN:O	2.12	0.81
1:C:673:ALA:O	1:C:677:ALA:N	2.14	0.80
8:k:114:ILE:O	8:k:118:ILE:N	2.15	0.80
8:b:327:GLU:N	8:b:372:ARG:O	2.15	0.79
1:E:209:PRO:O	1:E:213:GLN:N	2.15	0.78
3:K:117:LEU:N	5:L:314:GLU:O	2.16	0.78
8:a:274:THR:O	8:a:375:GLY:N	2.16	0.78
1:A:223:TYR:O	1:A:228:VAL:N	2.16	0.77
3:K:190:TRP:O	3:K:194:GLY:HA2	1.83	0.77
4:J:903:MET:O	4:J:908:HIS:N	2.14	0.77
8:d:317:TYR:N	8:d:347:ASN:O	2.17	0.76
1:M:539:LEU:O	1:M:613:LEU:N	2.18	0.76
8:l:2:PRO:O	8:l:131:SER:N	2.19	0.76
8:g:114:ILE:O	8:g:118:ILE:N	2.17	0.75
8:j:137:LEU:O	8:j:169:TYR:N	2.19	0.75
8:j:315:HIS:O	8:j:382:THR:N	2.20	0.75
2:B:574:GLY:N	8:b:247:GLY:O	2.20	0.75
8:k:30:GLY:HA3	8:k:41:ALA:HB1	1.68	0.74
1:C:384:SER:O	1:C:388:PHE:N	2.16	0.74
3:I:417:THR:N	3:I:454:GLY:O	2.20	0.73
8:b:30:GLY:O	8:b:38:GLU:N	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:243:LEU:N	4:J:304:THR:O	2.22	0.72
8:n:284:SER:O	8:n:286:ARG:N	2.21	0.72
2:F:565:MET:O	2:F:570:LEU:N	2.20	0.72
8:b:317:TYR:N	8:b:347:ASN:O	2.22	0.72
8:l:53:TYR:O	8:l:61:ILE:N	2.23	0.72
3:K:286:PHE:O	3:K:291:VAL:N	2.24	0.71
2:D:272:SER:O	2:D:276:ASN:N	2.24	0.71
1:E:232:TYR:O	1:E:249:ASP:N	2.25	0.70
5:L:536:ILE:O	5:L:541:TYR:N	2.24	0.70
8:l:8:LEU:O	8:l:138:CYS:N	2.24	0.70
4:J:732:GLY:O	4:J:736:MET:N	2.22	0.70
8:g:411:GLU:O	8:g:415:LYS:N	2.24	0.70
3:K:532:LEU:O	3:K:537:LEU:N	2.25	0.70
2:H:496:LEU:O	2:H:502:ASP:N	2.23	0.69
3:K:206:LYS:O	3:K:258:SER:N	2.25	0.69
8:c:411:GLU:O	8:c:415:LYS:N	2.25	0.69
1:A:450:VAL:O	1:A:454:GLY:N	2.26	0.68
8:a:318:ILE:N	8:a:380:ASN:O	2.21	0.68
1:C:223:TYR:O	1:C:228:VAL:N	2.24	0.68
2:N:374:THR:O	2:N:378:LYS:N	2.22	0.68
8:m:318:ILE:N	8:m:380:ASN:O	2.27	0.67
3:K:533:GLN:O	3:K:538:GLU:N	2.27	0.67
2:H:28:VAL:O	2:H:32:PHE:N	2.21	0.67
4:J:921:ALA:HB1	4:J:927:LEU:HA	1.77	0.67
4:J:693:TYR:O	4:J:697:ASP:CB	2.43	0.67
8:e:326:GLY:N	8:e:361:SER:O	2.28	0.67
3:K:415:HIS:N	3:K:456:SER:O	2.28	0.67
2:H:268:HIS:O	2:H:281:GLU:N	2.28	0.66
2:B:584:LEU:O	2:B:588:LEU:N	2.20	0.66
1:A:328:ILE:O	1:A:332:MET:N	2.20	0.66
2:B:656:THR:O	2:B:660:MET:N	2.26	0.66
3:K:97:LEU:O	3:K:101:ARG:N	2.25	0.66
8:d:327:GLU:N	8:d:372:ARG:O	2.25	0.65
8:h:195:LEU:HA	8:h:199:ALA:HB3	1.78	0.65
1:E:233:ILE:HA	1:E:248:VAL:HA	1.78	0.65
3:I:357:ILE:O	3:I:362:LEU:N	2.27	0.65
8:d:104:TRP:CB	8:d:187:ASN:HA	2.26	0.65
8:b:26:CYS:O	8:b:31:ILE:N	2.19	0.65
8:i:442:ASP:O	8:i:446:TRP:N	2.30	0.64
1:A:243:GLY:HA2	1:A:271:SER:CB	2.28	0.64
5:L:365:SER:O	5:L:369:SER:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:398:LEU:O	8:b:403:ALA:N	2.31	0.64
2:N:411:ASP:O	2:N:415:ARG:N	2.31	0.64
8:b:53:TYR:O	8:b:61:ILE:N	2.31	0.64
8:h:4:GLU:O	8:h:133:GLU:N	2.28	0.63
8:b:53:TYR:N	8:b:61:ILE:O	2.32	0.63
2:B:889:TYR:O	2:B:893:GLU:N	2.31	0.63
1:A:243:GLY:N	1:A:268:ALA:O	2.31	0.63
3:K:410:LEU:O	3:K:414:LEU:N	2.31	0.63
3:K:380:LEU:O	3:K:450:TRP:N	2.30	0.63
3:K:382:THR:O	3:K:449:GLY:N	2.27	0.63
8:a:30:GLY:HA3	8:a:41:ALA:HB2	1.80	0.63
8:j:141:ILE:N	8:j:171:VAL:O	2.25	0.63
8:d:107:GLY:HA3	8:d:148:GLY:HA3	1.81	0.62
8:a:195:LEU:HA	8:a:199:ALA:HB3	1.79	0.62
4:J:850:SER:O	4:J:973:LEU:N	2.32	0.62
2:F:623:ARG:O	2:F:646:HIS:N	2.26	0.62
1:A:243:GLY:HA3	1:A:268:ALA:HA	1.82	0.62
8:b:46:ASP:HA	8:b:245:TYR:HA	1.82	0.62
8:c:26:CYS:O	8:c:31:ILE:N	2.27	0.62
3:K:372:PHE:O	3:K:376:ALA:N	2.31	0.62
1:M:440:PRO:O	1:M:444:GLN:N	2.33	0.62
8:e:30:GLY:HA3	8:e:41:ALA:HB2	1.81	0.62
3:K:204:PHE:O	3:K:260:ARG:N	2.33	0.61
5:L:555:GLN:N	5:L:574:VAL:O	2.33	0.61
2:N:495:PHE:O	2:N:500:CYS:N	2.24	0.61
3:I:415:HIS:N	3:I:456:SER:O	2.33	0.61
3:K:503:LYS:O	8:k:198:ASN:HA	2.01	0.60
1:A:149:THR:C	1:A:240:GLY:HA2	2.26	0.60
2:F:886:ASN:CB	8:f:353:PRO:HA	2.31	0.60
8:f:209:ALA:HB2	8:f:306:SER:CB	2.31	0.60
3:I:417:THR:O	3:I:454:GLY:N	2.29	0.60
1:G:398:GLY:HA3	1:G:457:LEU:CB	2.31	0.60
8:c:52:PHE:HA	8:c:62:PRO:HA	1.83	0.60
1:E:148:PRO:O	1:E:240:GLY:N	2.34	0.60
8:k:189:LEU:CB	8:k:421:LEU:HA	2.31	0.60
1:A:618:PHE:O	1:A:639:GLN:HA	2.01	0.60
1:E:324:LEU:O	1:E:328:ILE:N	2.31	0.60
1:M:850:ASP:O	1:M:852:GLU:N	2.35	0.60
2:D:497:HIS:HA	2:D:502:ASP:O	2.02	0.59
1:E:392:GLU:O	1:E:396:TYR:N	2.35	0.59
2:H:623:ARG:O	2:H:646:HIS:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:655:TYR:H	8:k:353:PRO:N	2.00	0.59
8:g:168:THR:N	8:g:201:CYS:O	2.31	0.59
8:n:35:GLY:O	8:n:60:TYR:N	2.27	0.59
8:a:65:VAL:HA	8:a:90:ASN:O	2.02	0.59
5:L:543:GLY:O	5:L:616:CYS:N	2.35	0.58
5:L:591:VAL:O	5:L:595:VAL:N	2.35	0.58
3:K:357:ILE:O	3:K:362:LEU:N	2.33	0.58
8:m:55:ALA:N	8:m:59:HIS:O	2.37	0.58
8:c:4:GLU:HA	8:c:50:VAL:O	2.03	0.58
8:a:47:ARG:N	8:a:244:ARG:O	2.36	0.58
8:k:314:ASN:C	8:k:439:THR:HA	2.29	0.58
1:A:477:TYR:HA	1:A:484:TYR:CB	2.34	0.58
1:M:381:LYS:N	1:M:477:TYR:O	2.37	0.58
8:c:4:GLU:O	8:c:132:LEU:HA	2.03	0.58
8:d:317:TYR:HA	8:d:381:HIS:HA	1.85	0.58
1:C:328:ILE:O	1:C:332:MET:N	2.33	0.58
8:a:53:TYR:N	8:a:61:ILE:O	2.34	0.58
1:A:313:LEU:O	1:A:318:LEU:N	2.34	0.58
1:A:393:LYS:O	1:A:399:ILE:N	2.36	0.58
1:M:191:PHE:HA	1:M:227:GLY:HA2	1.84	0.58
2:N:266:GLY:N	2:N:269:VAL:O	2.36	0.58
8:i:104:TRP:CB	8:i:187:ASN:HA	2.34	0.58
8:j:308:GLY:HA3	8:j:390:SER:CB	2.32	0.57
8:l:53:TYR:N	8:l:61:ILE:O	2.37	0.57
4:J:756:VAL:HA	4:J:782:PHE:H	1.69	0.57
2:B:699:GLU:CB	2:B:840:GLN:HA	2.35	0.57
8:n:30:GLY:HA3	8:n:41:ALA:HB2	1.86	0.57
8:c:189:LEU:CB	8:c:395:TYR:CB	2.83	0.57
8:c:315:HIS:HA	8:c:382:THR:CB	2.34	0.57
8:h:104:TRP:O	8:h:148:GLY:HA3	2.05	0.57
1:A:384:SER:CB	1:A:477:TYR:H	2.18	0.57
2:H:269:VAL:HA	2:H:280:VAL:HA	1.86	0.57
2:F:426:SER:O	2:F:430:LEU:N	2.24	0.57
1:A:525:GLY:HA3	8:a:246:PRO:CB	2.35	0.57
2:N:278:TYR:CB	2:N:298:ALA:HB1	2.34	0.57
8:c:53:TYR:N	8:c:61:ILE:O	2.38	0.57
3:K:358:LYS:O	3:K:364:GLY:N	2.36	0.56
5:L:497:THR:O	5:L:501:LEU:N	2.37	0.56
1:A:596:GLN:HA	1:A:599:ALA:HB3	1.88	0.56
1:E:393:LYS:O	1:E:399:ILE:N	2.38	0.56
8:f:4:GLU:HA	8:f:50:VAL:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:k:325:GLN:N	8:k:374:SER:O	2.38	0.56
2:B:259:TYR:O	2:B:264:ILE:N	2.38	0.56
8:d:52:PHE:HA	8:d:62:PRO:HA	1.87	0.56
8:i:145:THR:O	8:i:149:LEU:CB	2.53	0.56
8:b:104:TRP:CB	8:b:187:ASN:HA	2.35	0.56
1:E:664:ALA:O	1:E:668:PHE:N	2.35	0.56
5:L:1363:ASP:O	5:L:1365:ASP:N	2.36	0.56
8:b:4:GLU:O	8:b:132:LEU:HA	2.05	0.56
2:B:435:ARG:O	2:B:440:GLY:N	2.39	0.56
4:J:781:SER:O	4:J:801:THR:N	2.28	0.56
1:M:73:LYS:HA	1:M:348:GLY:HA3	1.86	0.56
8:l:31:ILE:HA	8:l:37:VAL:HA	1.88	0.55
1:A:426:LYS:O	1:A:430:GLN:C	2.49	0.55
8:a:209:ALA:HB2	8:a:306:SER:CA	2.36	0.55
8:i:4:GLU:HA	8:i:50:VAL:O	2.06	0.55
2:N:573:GLN:C	8:n:247:GLY:HA3	2.32	0.55
8:k:35:GLY:HA3	8:k:60:TYR:H	1.72	0.55
3:I:415:HIS:O	3:I:456:SER:N	2.38	0.55
1:M:17:LEU:HA	1:M:101:ASN:CB	2.37	0.55
8:f:172:PHE:N	8:f:205:LEU:O	2.40	0.55
1:M:850:ASP:O	1:M:851:CYS:N	2.40	0.54
8:a:437:ALA:O	8:a:440:ARG:O	2.25	0.54
1:A:758:PHE:HA	1:A:828:PHE:CB	2.37	0.54
1:E:224:VAL:HA	1:E:228:VAL:O	2.07	0.54
3:K:415:HIS:O	3:K:456:SER:N	2.39	0.54
8:b:206:ASP:CB	8:b:306:SER:H	2.20	0.54
4:J:553:LEU:O	4:J:557:LEU:N	2.40	0.54
1:G:209:PRO:O	1:G:213:GLN:N	2.38	0.54
8:g:69:LEU:O	8:g:97:GLY:HA2	2.08	0.54
8:d:4:GLU:O	8:d:132:LEU:HA	2.08	0.54
1:A:186:ALA:HB1	2:B:295:VAL:C	2.33	0.54
5:L:539:TRP:HA	5:L:544:VAL:H	1.73	0.54
8:f:52:PHE:HA	8:f:62:PRO:HA	1.90	0.54
8:g:195:LEU:O	8:g:199:ALA:N	2.30	0.54
2:N:92:SER:O	6:O:84:PRO:CB	2.56	0.54
8:n:245:TYR:CB	8:n:362:ARG:H	2.21	0.53
1:A:328:ILE:HA	1:A:331:ALA:HB3	1.89	0.53
1:E:673:ALA:O	1:E:677:ALA:N	2.38	0.53
3:I:165:LEU:O	3:I:169:ARG:N	2.29	0.53
8:l:247:GLY:HA2	8:l:362:ARG:CB	2.38	0.53
2:H:552:LEU:O	2:H:557:SER:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:402:GLU:O	8:j:405:LEU:N	2.42	0.53
8:l:49:ASP:HA	8:l:53:TYR:HA	1.91	0.53
8:e:172:PHE:N	8:e:205:LEU:O	2.41	0.53
8:f:61:ILE:HA	8:f:85:LEU:O	2.09	0.53
4:J:760:ASN:N	4:J:780:ILE:O	2.42	0.53
8:l:314:ASN:H	8:l:436:HIS:HA	1.74	0.53
1:G:701:VAL:HA	1:G:736:ASP:CB	2.38	0.53
8:c:382:THR:CB	8:c:439:THR:CB	2.87	0.53
8:n:53:TYR:O	8:n:61:ILE:N	2.39	0.53
4:J:907:LEU:O	4:J:911:GLY:N	2.39	0.53
1:E:391:LEU:O	1:E:395:ILE:N	2.42	0.53
4:J:996:VAL:HA	4:J:1015:ALA:HA	1.89	0.53
8:j:171:VAL:HA	8:j:205:LEU:CB	2.39	0.53
8:k:105:ALA:HB2	8:k:411:GLU:CB	2.39	0.53
3:K:502:ARG:CB	3:K:601:LEU:O	2.57	0.52
1:G:44:VAL:O	1:G:46:ALA:N	2.41	0.52
8:f:38:GLU:O	8:f:42:THR:N	2.42	0.52
1:M:16:LEU:O	1:M:101:ASN:CB	2.57	0.52
1:C:66:LYS:CB	7:V:44:ALA:HB1	2.40	0.52
1:C:416:LYS:HA	1:C:427:TYR:CB	2.40	0.52
2:D:458:LYS:O	2:D:462:LEU:N	2.42	0.52
2:F:272:SER:O	2:F:276:ASN:N	2.43	0.52
8:b:318:ILE:N	8:b:380:ASN:O	2.42	0.52
4:J:550:VAL:O	4:J:554:LYS:N	2.30	0.52
8:a:271:THR:O	8:a:304:MET:N	2.42	0.52
8:d:100:ALA:HB3	8:d:145:THR:N	2.25	0.52
2:B:276:ASN:O	2:B:301:GLY:C	2.53	0.52
1:A:453:THR:CB	1:A:492:PHE:HA	2.39	0.52
4:J:850:SER:O	4:J:974:GLY:N	2.43	0.52
5:L:375:GLN:HA	5:L:482:ALA:HB3	1.91	0.52
8:f:5:ILE:N	8:f:50:VAL:O	2.37	0.52
1:A:396:TYR:O	1:A:468:THR:HA	2.09	0.51
2:N:271:MET:HA	2:N:278:TYR:HA	1.92	0.51
8:i:61:ILE:HA	8:i:85:LEU:O	2.09	0.51
5:L:417:PRO:N	5:L:433:THR:CB	2.74	0.51
8:c:107:GLY:HA3	8:c:144:GLY:O	2.09	0.51
2:B:394:ARG:CB	2:B:399:LEU:HA	2.41	0.51
1:M:396:TYR:O	1:M:469:CYS:N	2.43	0.51
8:c:141:ILE:N	8:c:171:VAL:O	2.43	0.51
8:j:144:GLY:O	8:j:149:LEU:N	2.40	0.51
1:C:176:VAL:HA	1:C:283:PHE:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:PRO:O	1:C:546:ILE:N	2.43	0.51
5:L:425:LYS:CB	5:L:498:GLY:HA2	2.40	0.51
1:A:175:PRO:CB	1:A:283:PHE:O	2.58	0.51
1:M:412:HIS:N	1:M:430:GLN:O	2.43	0.51
8:b:324:ILE:HA	8:b:374:SER:O	2.11	0.51
8:c:30:GLY:HA3	8:c:41:ALA:CB	2.41	0.51
8:i:70:GLU:HA	8:i:97:GLY:HA2	1.92	0.51
8:m:104:TRP:CB	8:m:187:ASN:HA	2.40	0.51
4:J:434:ALA:HB3	4:J:492:GLU:O	2.11	0.51
3:K:192:LEU:HA	3:K:299:ILE:CB	2.40	0.51
8:a:144:GLY:O	8:a:148:GLY:N	2.40	0.51
8:a:206:ASP:CB	8:a:306:SER:CB	2.89	0.51
2:D:272:SER:N	2:D:277:CYS:O	2.43	0.50
5:L:375:GLN:CB	5:L:483:LEU:O	2.59	0.50
8:k:139:HIS:N	8:k:169:TYR:O	2.44	0.50
8:l:308:GLY:N	8:l:383:SER:O	2.45	0.50
1:A:868:TYR:CB	8:a:354:ALA:HB3	2.41	0.50
4:J:285:LEU:N	4:J:288:PHE:O	2.43	0.50
1:M:442:PHE:CB	1:M:481:GLU:CB	2.90	0.50
2:N:426:SER:O	2:N:430:LEU:N	2.33	0.50
8:b:189:LEU:C	8:b:424:SER:CB	2.85	0.50
2:D:397:GLY:HA3	2:D:473:MET:HA	1.94	0.50
1:G:673:ALA:O	1:G:677:ALA:N	2.36	0.50
8:a:272:GLY:HA2	8:a:304:MET:H	1.77	0.50
8:b:260:LEU:O	8:b:380:ASN:CB	2.59	0.50
3:K:165:LEU:O	3:K:169:ARG:N	2.35	0.50
8:e:33:PRO:O	8:e:82:TYR:HA	2.10	0.50
4:J:733:GLY:HA3	8:j:247:GLY:N	2.26	0.50
5:L:321:ASP:N	5:L:387:GLY:HA2	2.26	0.50
8:g:6:ILE:HA	8:g:63:ARG:O	2.12	0.50
8:m:54:GLN:O	8:n:285:VAL:N	2.44	0.50
1:A:768:SER:O	1:A:773:SER:N	2.44	0.50
1:E:411:GLU:HA	1:E:432:TYR:HA	1.94	0.50
1:M:420:GLN:HA	1:M:630:ILE:O	2.12	0.50
8:b:442:ASP:O	8:b:446:TRP:N	2.44	0.50
8:h:151:SER:HA	8:h:194:ARG:CB	2.42	0.50
1:E:91:ASP:O	1:E:95:LEU:N	2.36	0.50
3:K:376:ALA:HA	3:K:395:ALA:HB1	1.94	0.50
5:L:1385:VAL:O	5:L:1389:LEU:N	2.38	0.50
8:d:105:ALA:C	8:d:411:GLU:CB	2.85	0.50
8:h:316:CYS:O	8:h:381:HIS:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:586:PRO:O	2:B:590:ARG:N	2.44	0.49
8:d:11:GLY:HA2	8:d:145:THR:CB	2.42	0.49
2:B:737:LEU:CB	2:B:757:PHE:CB	2.89	0.49
1:G:235:ALA:HA	1:G:246:PHE:HA	1.94	0.49
8:b:102:ASN:HA	8:b:144:GLY:N	2.28	0.49
8:e:35:GLY:O	8:e:59:HIS:HA	2.12	0.49
4:J:353:LYS:N	4:J:356:ASP:O	2.45	0.49
1:A:220:ASP:CB	1:A:233:ILE:O	2.60	0.49
4:J:424:VAL:CB	4:J:433:ARG:HA	2.42	0.49
3:K:491:GLU:C	3:K:594:CYS:CB	2.85	0.49
2:N:396:GLY:HA3	2:N:448:GLU:CB	2.41	0.49
8:g:5:ILE:N	8:g:50:VAL:O	2.46	0.49
8:j:206:ASP:CB	8:j:306:SER:H	2.25	0.49
8:l:69:LEU:HA	8:l:99:GLY:HA3	1.95	0.49
8:i:36:ILE:HA	8:i:59:HIS:HA	1.93	0.49
3:K:508:ASN:O	3:K:512:ALA:N	2.46	0.49
8:a:190:LEU:HA	8:a:424:SER:CB	2.43	0.49
8:c:182:VAL:CB	8:c:403:ALA:HB1	2.42	0.49
8:f:318:ILE:N	8:f:380:ASN:O	2.45	0.49
8:j:61:ILE:HA	8:j:86:TYR:HA	1.94	0.49
1:A:392:GLU:O	1:A:397:ARG:N	2.31	0.49
1:A:461:ARG:O	1:A:464:GLY:N	2.45	0.49
2:H:115:ALA:O	2:H:120:GLN:N	2.45	0.49
3:K:389:GLU:CB	3:K:418:ILE:H	2.25	0.49
8:b:413:ILE:O	8:b:420:GLU:CB	2.60	0.49
8:c:209:ALA:HB2	8:c:306:SER:N	2.27	0.49
8:i:30:GLY:O	8:i:38:GLU:N	2.26	0.49
8:k:438:ALA:HA	8:k:443:TYR:CB	2.43	0.49
1:A:327:TYR:O	1:A:331:ALA:N	2.42	0.49
2:B:397:GLY:HA3	2:B:474:ILE:C	2.38	0.49
8:b:414:PHE:HA	8:b:417:ASN:O	2.13	0.49
8:a:35:GLY:O	8:a:59:HIS:HA	2.13	0.49
8:j:61:ILE:HA	8:j:85:LEU:O	2.13	0.49
1:C:97:TYR:CB	7:V:78:CYS:O	2.61	0.48
1:A:230:GLY:O	2:B:289:SER:CB	2.61	0.48
1:A:410:GLU:O	1:A:412:HIS:N	2.43	0.48
3:K:290:ASN:O	3:K:296:LYS:N	2.47	0.48
5:L:435:GLY:HA2	5:L:1361:GLN:N	2.28	0.48
1:C:863:ASP:HA	1:C:869:THR:CB	2.44	0.48
2:D:575:ASP:CB	2:D:611:THR:CB	2.91	0.48
2:H:266:GLY:N	2:H:269:VAL:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:30:GLY:HA3	8:f:41:ALA:HB2	1.94	0.48
8:l:322:ASN:N	8:l:359:ALA:HB3	2.28	0.48
5:L:368:PHE:C	5:L:377:PHE:HA	2.39	0.48
8:b:151:SER:HA	8:b:194:ARG:CB	2.43	0.48
8:c:139:HIS:CB	8:c:146:GLY:HA2	2.44	0.48
8:f:35:GLY:HA3	8:f:85:LEU:HA	1.94	0.48
4:J:357:ALA:HB3	4:J:490:ALA:HB2	1.95	0.48
3:K:419:GLU:O	3:K:452:ALA:HB1	2.13	0.48
1:A:186:ALA:O	2:B:295:VAL:O	2.31	0.48
2:F:728:GLU:O	2:F:732:CYS:CB	2.62	0.48
8:d:323:ILE:O	8:d:375:GLY:HA2	2.14	0.48
8:g:4:GLU:O	8:g:133:GLU:N	2.43	0.48
1:A:192:LEU:H	1:A:228:VAL:HA	1.79	0.48
1:M:456:TYR:CB	1:M:496:SER:HA	2.43	0.48
1:A:172:GLN:HA	1:A:402:ASP:CB	2.43	0.48
8:a:290:VAL:CB	8:a:336:SER:CB	2.92	0.48
8:j:100:ALA:HB1	8:j:107:GLY:HA2	1.96	0.48
2:B:423:SER:HA	2:B:528:ASP:N	2.28	0.48
1:C:13:LEU:O	1:C:17:LEU:CB	2.62	0.48
1:G:224:VAL:O	1:G:227:GLY:N	2.36	0.48
2:N:270:LYS:O	2:N:278:TYR:HA	2.14	0.47
8:a:209:ALA:HB2	8:a:306:SER:CB	2.43	0.47
2:B:497:HIS:HA	2:B:502:ASP:O	2.14	0.47
5:L:364:VAL:HA	5:L:368:PHE:O	2.13	0.47
8:a:104:TRP:CB	8:a:187:ASN:HA	2.44	0.47
8:k:53:TYR:N	8:k:61:ILE:O	2.47	0.47
2:D:565:MET:O	2:D:569:LEU:N	2.46	0.47
2:F:627:ARG:CB	2:F:644:ASP:CB	2.92	0.47
4:J:483:HIS:C	4:J:485:HIS:H	2.22	0.47
8:c:189:LEU:C	8:c:424:SER:CB	2.87	0.47
8:k:291:LEU:HA	8:k:336:SER:HA	1.96	0.47
1:A:220:ASP:HA	1:A:230:GLY:HA3	1.97	0.47
1:A:233:ILE:HA	1:A:248:VAL:HA	1.96	0.47
1:A:461:ARG:HA	1:A:466:ASP:N	2.28	0.47
2:B:699:GLU:CB	2:B:843:ILE:CB	2.93	0.47
2:N:575:ASP:HA	8:n:251:ASN:CB	2.45	0.47
8:d:3:ARG:O	8:d:50:VAL:O	2.32	0.47
8:f:308:GLY:O	8:f:386:SER:CB	2.62	0.47
8:l:37:VAL:CB	8:l:58:GLU:O	2.62	0.47
4:J:733:GLY:HA3	8:j:247:GLY:H	1.79	0.47
3:K:193:HIS:O	3:K:284:GLN:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:584:LEU:O	2:N:588:LEU:N	2.47	0.47
8:c:438:ALA:HA	8:c:443:TYR:CB	2.44	0.47
9:w:70:LEU:CB	9:x:70:LEU:CB	2.92	0.47
2:B:497:HIS:O	2:B:501:HIS:HA	2.15	0.47
2:D:816:ARG:O	2:D:821:GLN:N	2.45	0.47
1:G:328:ILE:O	1:G:332:MET:N	2.45	0.47
4:J:357:ALA:HB2	4:J:488:ASP:HA	1.95	0.47
8:a:217:ARG:O	8:a:277:THR:HA	2.14	0.47
8:e:28:GLU:HA	8:e:367:LEU:CB	2.45	0.47
8:l:141:ILE:N	8:l:171:VAL:O	2.47	0.47
8:h:46:ASP:HA	8:h:244:ARG:O	2.14	0.47
2:F:556:TYR:CB	2:F:650:PRO:CB	2.93	0.47
2:H:623:ARG:HA	2:H:646:HIS:O	2.15	0.47
8:c:48:LYS:O	8:c:52:PHE:O	2.33	0.47
8:m:193:LYS:CB	8:m:424:SER:HA	2.44	0.47
1:A:460:VAL:O	1:A:465:HIS:N	2.48	0.47
8:b:298:LEU:CB	8:b:345:LEU:CB	2.93	0.47
8:c:217:ARG:O	8:c:277:THR:HA	2.14	0.47
8:j:65:VAL:HA	8:j:90:ASN:O	2.15	0.47
1:A:391:LEU:O	1:A:392:GLU:C	2.58	0.46
3:K:155:GLU:HA	3:K:266:SER:H	1.81	0.46
8:i:438:ALA:HA	8:i:443:TYR:CB	2.45	0.46
8:m:284:SER:O	8:m:285:VAL:C	2.57	0.46
2:N:277:CYS:HA	2:N:302:TRP:CB	2.44	0.46
8:b:185:PRO:CB	8:b:394:GLN:O	2.63	0.46
8:d:31:ILE:HA	8:d:37:VAL:HA	1.96	0.46
8:d:100:ALA:HB2	8:d:107:GLY:HA2	1.95	0.46
8:e:195:LEU:O	8:e:199:ALA:N	2.45	0.46
2:H:29:ALA:O	2:H:33:GLN:N	2.46	0.46
8:e:206:ASP:CB	8:e:306:SER:H	2.27	0.46
8:f:14:GLY:HA3	8:f:138:CYS:O	2.16	0.46
8:j:145:THR:HA	8:j:149:LEU:CB	2.46	0.46
1:C:867:PHE:CB	8:c:350:PRO:HA	2.45	0.46
4:J:746:LYS:HA	4:J:751:GLU:CB	2.46	0.46
8:b:409:ARG:HA	8:b:414:PHE:C	2.40	0.46
3:I:366:GLY:HA3	8:i:248:TYR:O	2.16	0.46
8:d:53:TYR:N	8:d:61:ILE:O	2.44	0.46
3:I:289:GLN:CB	3:I:462:PRO:HA	2.46	0.46
8:a:284:SER:O	8:a:285:VAL:C	2.59	0.46
8:a:316:CYS:O	8:a:381:HIS:HA	2.16	0.46
8:k:437:ALA:HB1	8:k:442:ASP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:PHE:CB	1:A:484:TYR:CB	2.94	0.46
1:C:19:VAL:CB	7:V:80:GLY:HA2	2.45	0.46
1:G:148:PRO:O	1:G:240:GLY:N	2.33	0.46
4:J:753:TRP:O	4:J:782:PHE:CB	2.64	0.46
8:d:106:SER:N	8:d:411:GLU:CB	2.79	0.46
8:m:438:ALA:HA	8:m:443:TYR:CB	2.45	0.46
8:n:284:SER:O	8:n:285:VAL:C	2.58	0.46
1:C:627:SER:C	1:C:629:ILE:H	2.24	0.46
2:H:816:ARG:O	2:H:821:GLN:N	2.49	0.46
1:M:8:HIS:HA	9:x:78:LYS:O	2.16	0.46
8:j:104:TRP:H	8:j:187:ASN:CB	2.28	0.46
8:m:33:PRO:O	8:m:82:TYR:HA	2.16	0.46
2:B:716:HIS:CB	2:B:885:PHE:CB	2.94	0.46
4:J:808:TRP:HA	4:J:811:ASP:H	1.81	0.46
1:M:220:ASP:CB	1:M:231:ARG:H	2.28	0.46
8:b:100:ALA:HB3	8:b:145:THR:N	2.31	0.46
8:i:316:CYS:O	8:i:381:HIS:HA	2.15	0.46
2:B:453:SER:HA	2:B:467:TYR:HA	1.97	0.45
1:E:423:TYR:HA	1:E:633:LYS:N	2.30	0.45
1:G:516:ILE:HA	1:G:519:TYR:O	2.16	0.45
5:L:610:PRO:O	5:L:616:CYS:N	2.49	0.45
8:a:145:THR:O	8:a:149:LEU:CB	2.64	0.45
1:C:578:MET:N	1:C:615:ALA:O	2.31	0.45
1:C:588:ARG:CB	1:C:601:VAL:HA	2.46	0.45
3:K:535:ASP:HA	3:K:539:SER:CB	2.47	0.45
8:l:322:ASN:H	8:l:359:ALA:HB3	1.81	0.45
1:A:242:GLN:O	1:A:272:THR:N	2.50	0.45
1:A:393:LYS:O	1:A:398:GLY:N	2.48	0.45
8:b:308:GLY:O	8:b:386:SER:CB	2.65	0.45
8:d:102:ASN:HA	8:d:144:GLY:N	2.31	0.45
8:e:107:GLY:HA3	8:e:148:GLY:HA3	1.97	0.45
1:C:850:ASP:O	1:C:852:GLU:N	2.49	0.45
1:G:461:ARG:HA	1:G:466:ASP:CB	2.47	0.45
5:L:1443:GLY:HA3	5:L:1488:PHE:CB	2.46	0.45
8:h:183:VAL:CB	8:h:404:PHE:CB	2.95	0.45
8:m:317:TYR:HA	8:m:381:HIS:HA	1.99	0.45
8:k:189:LEU:O	8:k:424:SER:CB	2.65	0.45
1:C:709:LEU:CB	1:C:729:PHE:CB	2.95	0.45
1:E:578:MET:N	1:E:615:ALA:O	2.50	0.45
1:G:705:THR:CB	1:G:733:CYS:N	2.80	0.45
8:a:115:HIS:O	8:a:119:PHE:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:274:THR:O	8:a:375:GLY:CA	2.65	0.45
8:j:273:TYR:HA	8:j:376:LEU:HA	1.98	0.45
8:l:70:GLU:HA	8:l:97:GLY:O	2.17	0.45
1:A:397:ARG:HA	1:A:468:THR:CA	2.47	0.45
1:A:578:MET:C	1:A:580:HIS:H	2.25	0.45
5:L:376:ALA:HB1	5:L:405:THR:CA	2.47	0.45
5:L:384:HIS:HA	5:L:390:PRO:HA	1.98	0.45
8:f:14:GLY:HA3	8:f:139:HIS:HA	1.99	0.45
8:i:291:LEU:N	8:i:336:SER:CB	2.79	0.45
2:H:260:VAL:O	2:H:263:GLY:N	2.37	0.45
2:H:397:GLY:HA3	2:H:473:MET:C	2.41	0.45
3:K:322:LEU:O	3:K:326:GLU:CB	2.64	0.45
3:K:416:LEU:HA	3:K:455:LEU:HA	1.98	0.45
8:a:151:SER:HA	8:a:194:ARG:CB	2.47	0.45
8:b:190:LEU:HA	8:b:424:SER:CB	2.47	0.45
8:k:6:ILE:HA	8:k:63:ARG:O	2.17	0.45
2:D:729:VAL:HA	2:D:764:ARG:CB	2.47	0.45
8:a:140:SER:H	8:a:146:GLY:HA3	1.81	0.45
8:a:209:ALA:HB2	8:a:306:SER:N	2.32	0.45
8:c:52:PHE:CB	8:c:62:PRO:HA	2.47	0.45
8:d:30:GLY:HA3	8:d:41:ALA:HB2	1.98	0.45
1:A:185:PRO:O	1:A:186:ALA:HB3	2.17	0.45
2:B:567:ARG:HA	2:B:572:GLY:HA3	1.99	0.45
2:B:884:ASP:CB	8:b:355:SER:CA	2.95	0.45
8:a:14:GLY:HA3	8:a:139:HIS:HA	1.99	0.45
8:d:317:TYR:O	8:d:348:PHE:HA	2.17	0.45
8:j:279:ASP:O	8:j:370:ALA:HB1	2.17	0.45
1:A:392:GLU:O	1:A:397:ARG:CB	2.65	0.44
1:G:577:LEU:HA	1:G:615:ALA:O	2.17	0.44
2:N:727:PHE:HA	2:N:731:GLU:CB	2.47	0.44
8:i:437:ALA:HB1	8:i:446:TRP:CB	2.47	0.44
8:m:65:VAL:HA	8:m:90:ASN:O	2.16	0.44
3:I:150:GLY:HA2	3:I:202:GLU:HA	1.98	0.44
5:L:529:CYS:O	5:L:533:THR:N	2.47	0.44
8:c:316:CYS:O	8:c:381:HIS:HA	2.17	0.44
1:G:233:ILE:HA	1:G:248:VAL:HA	1.99	0.44
5:L:376:ALA:HB1	5:L:405:THR:CB	2.47	0.44
8:d:100:ALA:CB	8:d:107:GLY:HA2	2.48	0.44
8:j:316:CYS:O	8:j:380:ASN:O	2.35	0.44
8:d:33:PRO:O	8:d:82:TYR:HA	2.16	0.44
2:D:270:LYS:O	2:D:279:THR:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:260:VAL:O	2:F:263:GLY:N	2.42	0.44
1:G:37:THR:O	7:X:64:ASN:CB	2.66	0.44
1:G:235:ALA:HB1	1:G:244:ARG:CB	2.48	0.44
8:n:438:ALA:HA	8:n:443:TYR:CB	2.47	0.44
2:B:565:MET:O	2:B:570:LEU:N	2.51	0.44
1:E:518:ARG:O	1:E:522:MET:O	2.35	0.44
3:K:249:MET:CB	3:K:474:LYS:HA	2.47	0.44
1:M:381:LYS:HA	1:M:477:TYR:N	2.33	0.44
8:d:140:SER:O	8:d:147:SER:N	2.50	0.44
8:h:321:LEU:O	8:h:377:MET:HA	2.17	0.44
8:k:41:ALA:HA	8:k:366:TYR:HA	2.00	0.44
2:B:608:VAL:O	2:B:614:GLN:N	2.50	0.44
2:D:728:GLU:C	2:D:764:ARG:CB	2.90	0.44
8:a:46:ASP:HA	8:a:244:ARG:O	2.18	0.44
8:b:65:VAL:HA	8:b:90:ASN:O	2.17	0.44
8:b:140:SER:H	8:b:146:GLY:HA3	1.83	0.44
8:j:313:THR:CB	8:j:436:HIS:HA	2.48	0.44
1:A:337:ILE:HA	1:A:372:ALA:HB2	2.00	0.44
8:b:409:ARG:HA	8:b:414:PHE:O	2.18	0.44
8:c:31:ILE:HA	8:c:37:VAL:HA	2.00	0.44
8:c:35:GLY:O	8:c:59:HIS:CB	2.66	0.44
8:f:271:THR:O	8:f:304:MET:CB	2.65	0.44
1:A:475:VAL:CB	1:A:488:ILE:H	2.31	0.44
1:E:588:ARG:CB	1:E:601:VAL:HA	2.48	0.44
8:a:104:TRP:O	8:a:148:GLY:HA3	2.18	0.44
8:d:174:ASN:O	8:d:177:GLU:O	2.36	0.44
8:l:4:GLU:HA	8:l:50:VAL:HA	1.98	0.44
8:m:108:PHE:N	8:m:148:GLY:HA3	2.32	0.44
1:A:283:PHE:O	1:A:285:TYR:N	2.51	0.43
1:A:581:ASP:HA	1:A:614:GLU:O	2.18	0.43
1:C:866:GLY:HA2	1:C:870:GLU:H	1.82	0.43
8:b:183:VAL:N	8:b:404:PHE:CB	2.81	0.43
8:l:105:ALA:HB1	8:l:412:ASP:N	2.32	0.43
2:B:687:HIS:CB	2:B:711:ALA:HB3	2.47	0.43
3:I:534:VAL:O	3:I:538:GLU:N	2.50	0.43
5:L:490:GLU:O	5:L:492:ARG:N	2.51	0.43
8:b:145:THR:O	8:b:149:LEU:CB	2.67	0.43
8:e:189:LEU:O	8:e:424:SER:CB	2.66	0.43
8:g:70:GLU:HA	8:g:97:GLY:HA2	1.99	0.43
8:l:50:VAL:CB	8:l:244:ARG:HA	2.49	0.43
1:C:10:VAL:CB	1:C:29:ILE:CB	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:GLY:O	7:V:80:GLY:C	2.62	0.43
1:G:334:SER:CB	2:H:117:LEU:HA	2.48	0.43
5:L:438:ARG:CB	5:L:1360:VAL:HA	2.47	0.43
8:e:214:ALA:O	8:e:219:HIS:N	2.52	0.43
8:h:7:THR:O	8:h:64:ALA:HA	2.19	0.43
8:i:4:GLU:N	8:i:132:LEU:HA	2.33	0.43
8:n:136:VAL:HA	8:n:167:GLN:O	2.18	0.43
8:g:33:PRO:O	8:g:82:TYR:HA	2.18	0.43
8:l:189:LEU:O	8:l:424:SER:CB	2.67	0.43
8:n:318:ILE:N	8:n:380:ASN:O	2.42	0.43
1:A:581:ASP:H	1:A:584:THR:CB	2.32	0.43
2:H:268:HIS:CB	2:H:284:ALA:HB2	2.48	0.43
3:K:359:ASP:O	3:K:363:LEU:HA	2.19	0.43
2:N:729:VAL:CB	2:N:764:ARG:CB	2.97	0.43
8:a:6:ILE:HA	8:a:63:ARG:O	2.18	0.43
8:b:4:GLU:HA	8:b:50:VAL:O	2.17	0.43
8:m:414:PHE:HA	8:m:417:ASN:O	2.18	0.43
9:q:70:LEU:CB	9:r:70:LEU:CB	2.97	0.43
2:B:374:THR:O	2:B:378:LYS:N	2.36	0.43
2:D:452:ALA:O	2:D:468:ALA:O	2.36	0.43
2:D:453:SER:HA	2:D:466:LYS:O	2.18	0.43
3:K:289:GLN:HA	3:K:292:ASN:CB	2.49	0.43
5:L:343:GLN:O	5:L:344:PRO:C	2.61	0.43
8:d:6:ILE:HA	8:d:63:ARG:O	2.18	0.43
1:C:10:VAL:O	1:C:25:ALA:HB3	2.19	0.43
8:a:182:VAL:CB	8:a:403:ALA:HB1	2.48	0.43
8:a:193:LYS:CB	8:a:424:SER:HA	2.48	0.43
8:c:46:ASP:CB	8:c:244:ARG:HA	2.49	0.43
8:d:392:CYS:CB	8:d:428:VAL:CB	2.96	0.43
8:g:4:GLU:CB	8:g:132:LEU:HA	2.49	0.43
8:k:8:LEU:O	8:k:137:LEU:HA	2.18	0.43
8:k:206:ASP:O	8:k:306:SER:N	2.37	0.43
8:k:314:ASN:O	8:k:348:PHE:O	2.37	0.43
1:E:863:ASP:CB	1:E:869:THR:CB	2.97	0.43
2:H:43:PHE:O	6:P:83:ASN:N	2.51	0.43
3:K:495:CYS:CB	3:K:594:CYS:HA	2.48	0.43
5:L:406:HIS:HA	5:L:487:GLY:O	2.19	0.43
5:L:536:ILE:C	5:L:541:TYR:H	2.26	0.43
8:a:107:GLY:HA3	8:a:144:GLY:O	2.19	0.43
8:e:52:PHE:HA	8:e:62:PRO:HA	2.01	0.43
8:f:107:GLY:HA3	8:f:148:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:313:THR:O	8:j:382:THR:CB	2.67	0.43
2:B:710:LEU:CB	2:B:853:LEU:C	2.92	0.43
3:I:357:ILE:O	3:I:361:TYR:N	2.52	0.43
3:I:358:LYS:O	3:I:364:GLY:N	2.50	0.43
3:K:372:PHE:CB	3:K:376:ALA:HB3	2.49	0.43
1:M:398:GLY:HA2	1:M:454:GLY:O	2.18	0.43
8:i:33:PRO:O	8:i:82:TYR:HA	2.19	0.43
2:B:694:LEU:CB	2:B:799:ALA:HA	2.48	0.43
1:G:709:LEU:CB	1:G:729:PHE:CB	2.97	0.43
4:J:357:ALA:H	4:J:490:ALA:HA	1.84	0.43
8:e:4:GLU:HA	8:e:50:VAL:O	2.18	0.43
2:B:692:ARG:HA	2:B:695:ARG:CB	2.49	0.42
3:K:291:VAL:CB	3:K:297:GLY:H	2.32	0.42
2:N:578:ARG:CB	8:n:251:ASN:N	2.82	0.42
8:a:438:ALA:HA	8:a:443:TYR:CB	2.49	0.42
8:j:206:ASP:CB	8:j:306:SER:CB	2.97	0.42
8:k:100:ALA:HB3	8:k:144:GLY:O	2.18	0.42
8:n:261:ILE:O	8:n:262:PRO:C	2.62	0.42
1:G:177:LEU:HA	2:H:390:HIS:CB	2.49	0.42
3:I:651:TYR:CB	8:i:354:ALA:HB3	2.49	0.42
3:I:654:TYR:CB	8:i:352:GLY:C	2.92	0.42
5:L:500:ARG:N	5:L:582:ALA:HA	2.33	0.42
8:a:34:GLU:HA	8:a:84:LYS:CB	2.49	0.42
8:e:209:ALA:HB3	8:e:305:VAL:C	2.44	0.42
2:D:438:TYR:HA	2:D:506:THR:HA	2.02	0.42
1:E:392:GLU:HA	1:E:396:TYR:H	1.84	0.42
3:K:533:GLN:HA	3:K:537:LEU:CB	2.50	0.42
8:b:31:ILE:HA	8:b:37:VAL:HA	1.99	0.42
8:b:49:ASP:HA	8:b:52:PHE:O	2.19	0.42
8:c:218:LEU:HA	8:c:277:THR:HA	2.01	0.42
8:f:183:VAL:CB	8:f:403:ALA:O	2.67	0.42
8:g:170:SER:O	8:g:203:VAL:O	2.37	0.42
8:l:314:ASN:O	8:l:382:THR:CB	2.68	0.42
8:m:218:LEU:HA	8:m:278:THR:CB	2.49	0.42
1:A:380:THR:C	1:A:477:TYR:O	2.62	0.42
1:A:450:VAL:HA	1:A:453:THR:CB	2.49	0.42
1:E:427:TYR:O	1:E:431:ARG:CB	2.68	0.42
1:G:697:MET:HA	1:G:701:VAL:CB	2.50	0.42
5:L:339:LEU:O	5:L:341:ALA:N	2.52	0.42
8:g:145:THR:O	8:g:149:LEU:CB	2.68	0.42
8:e:317:TYR:HA	8:e:381:HIS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:100:ALA:HB3	8:h:145:THR:N	2.35	0.42
8:k:9:GLN:CB	8:k:15:ASN:HA	2.50	0.42
1:E:574:LYS:N	1:E:619:ASP:O	2.52	0.42
8:b:398:LEU:HA	8:b:403:ALA:HB3	2.01	0.42
8:c:69:LEU:HA	8:c:94:SER:CB	2.50	0.42
1:A:242:GLN:C	1:A:268:ALA:O	2.63	0.42
1:C:388:PHE:CB	1:C:475:VAL:CB	2.98	0.42
3:K:291:VAL:HA	3:K:295:ARG:O	2.20	0.42
5:L:344:PRO:HA	5:L:382:GLY:O	2.19	0.42
1:M:587:LEU:HA	1:M:742:PRO:CB	2.50	0.42
8:e:108:PHE:HA	8:e:152:TYR:CB	2.49	0.42
8:k:6:ILE:O	8:k:136:VAL:N	2.38	0.42
1:G:673:ALA:HB1	1:G:676:PHE:CB	2.49	0.42
2:H:817:GLU:HA	2:H:822:TRP:HA	2.01	0.42
8:d:215:THR:HA	8:d:220:ILE:O	2.20	0.42
8:d:385:SER:CB	8:d:435:TYR:CB	2.97	0.42
8:l:104:TRP:N	8:l:144:GLY:HA3	2.34	0.42
2:D:271:MET:HA	2:D:278:TYR:HA	2.02	0.42
8:d:385:SER:CB	8:d:432:ILE:O	2.68	0.42
8:e:209:ALA:HB2	8:e:306:SER:CA	2.50	0.42
8:j:137:LEU:H	8:j:168:THR:HA	1.84	0.42
8:j:437:ALA:HB1	8:j:442:ASP:O	2.20	0.42
8:k:288:THR:O	8:k:373:VAL:CB	2.68	0.42
2:B:295:VAL:O	2:B:298:ALA:N	2.39	0.41
2:D:278:TYR:O	2:D:298:ALA:HB1	2.20	0.41
5:L:368:PHE:O	5:L:377:PHE:HA	2.19	0.41
5:L:409:ARG:O	5:L:479:VAL:CB	2.68	0.41
8:d:142:ALA:HB2	8:d:173:PRO:CB	2.50	0.41
8:d:382:THR:CB	8:d:439:THR:CB	2.98	0.41
8:h:4:GLU:CB	8:h:50:VAL:O	2.68	0.41
8:l:10:LEU:O	8:l:139:HIS:HA	2.20	0.41
8:l:320:ILE:HA	8:l:379:ALA:HA	2.01	0.41
3:I:36:PRO:O	3:I:40:SER:N	2.53	0.41
3:K:371:ALA:HB1	3:K:399:SER:O	2.20	0.41
8:a:52:PHE:HA	8:a:62:PRO:HA	2.02	0.41
8:e:414:PHE:HA	8:e:417:ASN:O	2.20	0.41
8:j:34:GLU:HA	8:j:81:PRO:O	2.21	0.41
8:k:100:ALA:HB3	8:k:144:GLY:C	2.45	0.41
2:B:276:ASN:O	2:B:302:TRP:N	2.52	0.41
2:B:625:ASP:O	2:B:644:ASP:N	2.37	0.41
1:C:66:LYS:CB	7:V:44:ALA:CB	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:692:LEU:HA	4:J:696:ILE:CB	2.51	0.41
3:K:286:PHE:HA	3:K:290:ASN:CB	2.51	0.41
2:N:397:GLY:H	2:N:473:MET:HA	1.85	0.41
8:a:35:GLY:CA	8:a:85:LEU:HA	2.50	0.41
8:c:206:ASP:CB	8:c:306:SER:CB	2.98	0.41
8:k:389:GLU:CB	8:k:432:ILE:CB	2.98	0.41
2:H:565:MET:HA	2:H:569:LEU:CB	2.50	0.41
1:M:712:ASN:CB	1:M:725:HIS:CB	2.98	0.41
8:a:189:LEU:C	8:a:424:SER:CB	2.94	0.41
8:b:189:LEU:CB	8:b:395:TYR:CB	2.98	0.41
8:c:46:ASP:HA	8:c:244:ARG:HA	2.02	0.41
8:e:313:THR:O	8:e:315:HIS:N	2.50	0.41
8:j:107:GLY:C	8:j:149:LEU:N	2.79	0.41
1:A:238:LEU:N	1:A:244:ARG:HA	2.35	0.41
1:E:591:ALA:HB1	1:E:596:GLN:CB	2.51	0.41
2:F:565:MET:HA	2:F:569:LEU:CB	2.51	0.41
3:I:17:PHE:HA	3:I:27:VAL:HA	2.02	0.41
1:M:36:ARG:HA	7:Y:37:ALA:H	1.85	0.41
8:a:102:ASN:HA	8:a:144:GLY:N	2.34	0.41
8:c:193:LYS:CB	8:c:424:SER:HA	2.50	0.41
8:d:174:ASN:HA	8:d:208:THR:N	2.36	0.41
8:d:181:VAL:O	8:d:184:GLN:CB	2.69	0.41
8:j:411:GLU:O	8:j:415:LYS:CB	2.69	0.41
2:F:625:ASP:O	2:F:644:ASP:O	2.39	0.41
5:L:1369:VAL:O	5:L:1373:GLU:CB	2.68	0.41
1:M:623:THR:C	1:M:627:SER:H	2.29	0.41
8:h:102:ASN:HA	8:h:144:GLY:N	2.35	0.41
2:B:458:LYS:O	2:B:459:ALA:C	2.62	0.41
2:F:271:MET:HA	2:F:278:TYR:HA	2.02	0.41
1:G:865:ASN:CB	8:g:354:ALA:H	2.33	0.41
8:b:217:ARG:CB	8:b:276:LEU:O	2.68	0.41
8:c:209:ALA:HB1	8:c:304:MET:C	2.46	0.41
1:A:184:ARG:CB	2:B:302:TRP:CB	2.99	0.41
2:B:295:VAL:O	2:B:297:LEU:N	2.54	0.41
2:B:436:TRP:HA	2:B:441:GLU:N	2.36	0.41
2:D:625:ASP:O	2:D:644:ASP:O	2.38	0.41
1:E:523:ASP:H	8:e:248:TYR:HA	1.85	0.41
2:H:265:ASP:CB	2:H:270:LYS:HA	2.51	0.41
8:a:315:HIS:HA	8:a:382:THR:CB	2.51	0.41
8:c:414:PHE:HA	8:c:417:ASN:O	2.20	0.41
8:e:104:TRP:HA	8:e:148:GLY:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:307:THR:HA	8:f:387:LEU:CB	2.50	0.41
8:g:34:GLU:HA	8:g:84:LYS:CB	2.51	0.41
1:A:673:ALA:O	1:A:674:LYS:C	2.62	0.41
1:A:868:TYR:CB	8:a:354:ALA:H	2.34	0.41
1:E:443:LEU:O	1:E:447:ALA:N	2.54	0.41
1:E:867:PHE:CB	8:e:352:GLY:N	2.84	0.41
2:F:256:ASP:CB	2:F:266:GLY:HA3	2.50	0.41
1:G:574:LYS:O	1:G:619:ASP:N	2.45	0.41
3:K:372:PHE:O	3:K:377:GLN:N	2.54	0.41
8:e:183:VAL:CB	8:e:404:PHE:CB	2.99	0.41
8:g:100:ALA:HB3	8:g:144:GLY:C	2.46	0.41
8:i:217:ARG:O	8:i:277:THR:HA	2.21	0.41
8:i:409:ARG:HA	8:i:415:LYS:HA	2.03	0.41
8:j:10:LEU:O	8:j:139:HIS:HA	2.21	0.41
8:k:104:TRP:CB	8:k:187:ASN:CB	2.99	0.41
8:l:54:GLN:HA	8:l:60:TYR:HA	2.02	0.41
8:l:288:THR:H	8:l:372:ARG:CB	2.34	0.41
1:A:453:THR:CB	1:A:492:PHE:CA	2.98	0.41
2:B:885:PHE:HA	8:b:352:GLY:HA3	2.03	0.41
2:H:628:LEU:H	3:I:230:LEU:CB	2.34	0.41
5:L:541:TYR:O	5:L:613:TYR:HA	2.20	0.41
8:j:9:GLN:O	8:j:67:LEU:C	2.64	0.41
8:j:215:THR:HA	8:j:219:HIS:HA	2.02	0.41
8:j:402:GLU:O	8:j:403:ALA:C	2.64	0.41
8:k:382:THR:O	8:k:435:TYR:CB	2.69	0.41
8:l:100:ALA:HB3	8:l:145:THR:CB	2.50	0.41
8:l:308:GLY:H	8:l:387:LEU:CB	2.33	0.41
2:D:595:LEU:O	9:t:58:ARG:N	2.54	0.40
2:F:588:LEU:HA	2:F:637:GLY:C	2.46	0.40
8:l:314:ASN:H	8:l:436:HIS:CB	2.33	0.40
1:A:465:HIS:O	1:A:467:VAL:N	2.54	0.40
1:G:574:LYS:O	1:G:618:PHE:HA	2.21	0.40
5:L:1582:ALA:HB1	5:L:1587:HIS:HA	2.02	0.40
8:b:324:ILE:O	8:b:361:SER:O	2.40	0.40
8:g:33:PRO:O	8:g:85:LEU:N	2.55	0.40
1:A:515:SER:O	1:A:569:PHE:CB	2.69	0.40
2:N:459:ALA:HB1	2:N:499:VAL:HA	2.04	0.40
8:j:147:SER:HA	8:j:191:THR:CB	2.51	0.40
8:k:318:ILE:CB	8:k:349:ILE:CB	2.99	0.40
2:F:730:LEU:O	2:F:734:TRP:CB	2.69	0.40
3:K:190:TRP:O	3:K:194:GLY:CA	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:14:GLY:HA3	8:a:138:CYS:O	2.22	0.40
8:a:136:VAL:HA	8:a:167:GLN:O	2.22	0.40
8:c:189:LEU:O	8:c:424:SER:CB	2.69	0.40
8:k:33:PRO:O	8:k:85:LEU:N	2.54	0.40
8:l:326:GLY:H	8:l:362:ARG:HA	1.86	0.40
8:n:14:GLY:HA3	8:n:138:CYS:O	2.22	0.40
2:H:567:ARG:HA	2:H:572:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	676/905 (75%)	625 (92%)	51 (8%)	0	100	100
1	C	789/905 (87%)	749 (95%)	38 (5%)	2 (0%)	36	72
1	E	789/905 (87%)	763 (97%)	26 (3%)	0	100	100
1	G	789/905 (87%)	764 (97%)	25 (3%)	0	100	100
1	M	766/905 (85%)	751 (98%)	15 (2%)	0	100	100
2	B	611/910 (67%)	585 (96%)	26 (4%)	0	100	100
2	D	611/910 (67%)	590 (97%)	21 (3%)	0	100	100
2	F	611/910 (67%)	597 (98%)	14 (2%)	0	100	100
2	H	727/910 (80%)	702 (97%)	25 (3%)	0	100	100
2	N	710/910 (78%)	698 (98%)	12 (2%)	0	100	100
3	I	600/667 (90%)	577 (96%)	23 (4%)	0	100	100
3	K	600/667 (90%)	568 (95%)	32 (5%)	0	100	100
4	J	613/1061 (58%)	578 (94%)	35 (6%)	0	100	100
5	L	772/1715 (45%)	697 (90%)	74 (10%)	1 (0%)	48	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	O	65/79 (82%)	65 (100%)	0	0	100	100
6	P	65/79 (82%)	64 (98%)	1 (2%)	0	100	100
6	Q	62/79 (78%)	62 (100%)	0	0	100	100
7	V	41/155 (26%)	39 (95%)	2 (5%)	0	100	100
7	W	41/155 (26%)	41 (100%)	0	0	100	100
7	X	41/155 (26%)	40 (98%)	1 (2%)	0	100	100
7	Y	49/155 (32%)	48 (98%)	1 (2%)	0	100	100
8	a	442/451 (98%)	429 (97%)	13 (3%)	0	100	100
8	b	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
8	c	436/451 (97%)	426 (98%)	10 (2%)	0	100	100
8	d	420/451 (93%)	410 (98%)	10 (2%)	0	100	100
8	e	428/451 (95%)	418 (98%)	10 (2%)	0	100	100
8	f	429/451 (95%)	422 (98%)	7 (2%)	0	100	100
8	g	429/451 (95%)	424 (99%)	5 (1%)	0	100	100
8	h	435/451 (96%)	426 (98%)	9 (2%)	0	100	100
8	i	434/451 (96%)	426 (98%)	8 (2%)	0	100	100
8	j	435/451 (96%)	400 (92%)	34 (8%)	1 (0%)	43	78
8	k	434/451 (96%)	392 (90%)	42 (10%)	0	100	100
8	l	422/451 (94%)	394 (93%)	28 (7%)	0	100	100
8	m	442/451 (98%)	435 (98%)	6 (1%)	1 (0%)	43	78
8	n	438/451 (97%)	425 (97%)	12 (3%)	1 (0%)	43	78
9	o	31/1663 (2%)	30 (97%)	1 (3%)	0	100	100
9	p	31/1663 (2%)	31 (100%)	0	0	100	100
9	q	31/1663 (2%)	31 (100%)	0	0	100	100
9	r	31/1663 (2%)	31 (100%)	0	0	100	100
9	s	34/1663 (2%)	34 (100%)	0	0	100	100
9	t	34/1663 (2%)	34 (100%)	0	0	100	100
9	u	34/1663 (2%)	34 (100%)	0	0	100	100
9	v	34/1663 (2%)	34 (100%)	0	0	100	100
9	w	31/1663 (2%)	31 (100%)	0	0	100	100
9	x	32/1663 (2%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	16413/36986 (44%)	15781 (96%)	626 (4%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	n	285	VAL
1	C	522	MET
1	C	851	CYS
5	L	340	GLN
8	j	285	VAL
8	m	285	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	850:ASP	C	851:CYS	N	2.92

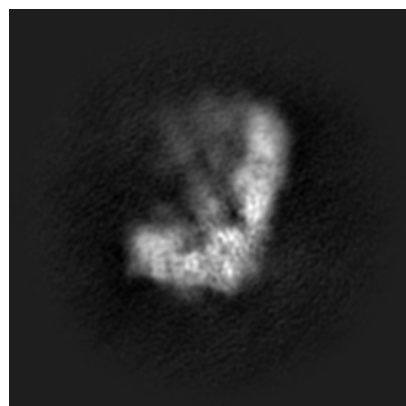
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51018. These allow visual inspection of the internal detail of the map and identification of artifacts.

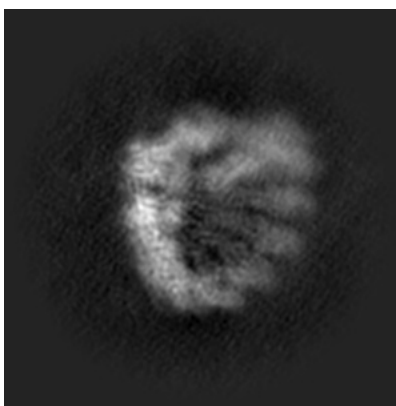
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

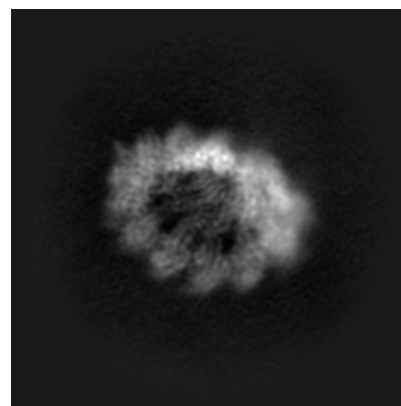
6.1.1 Primary map



X

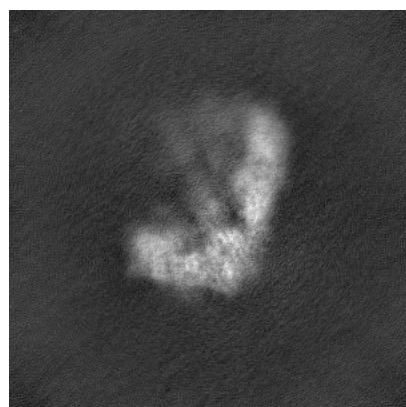


Y

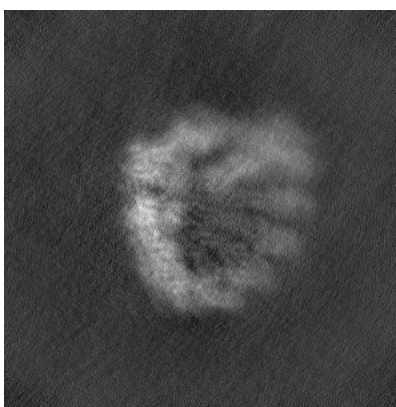


Z

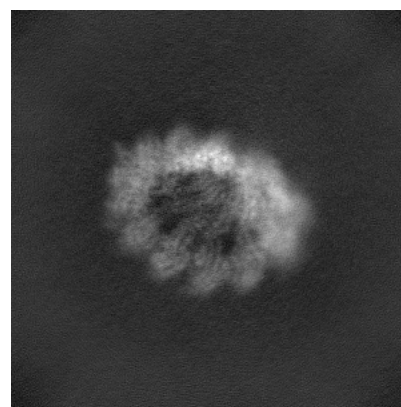
6.1.2 Raw map



X



Y

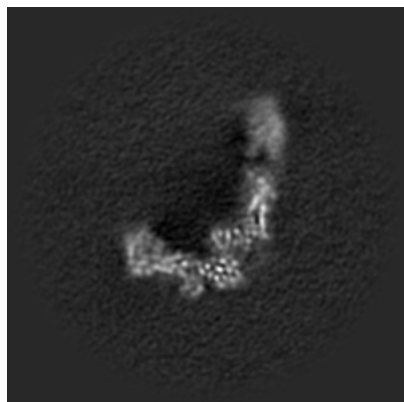


Z

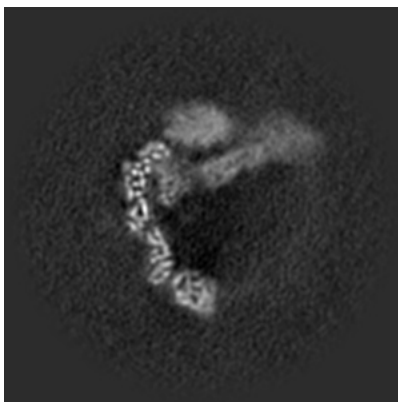
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

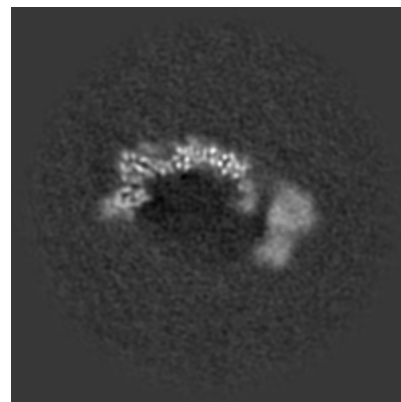
6.2.1 Primary map



X Index: 192

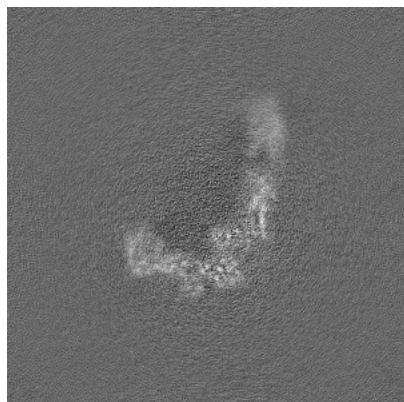


Y Index: 192



Z Index: 192

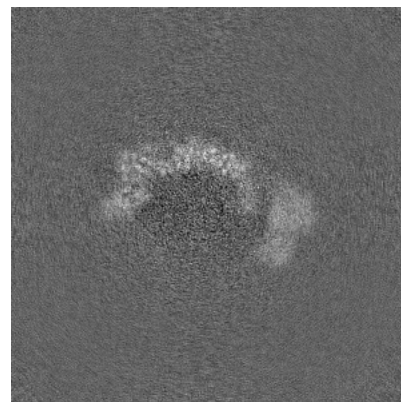
6.2.2 Raw map



X Index: 192



Y Index: 192

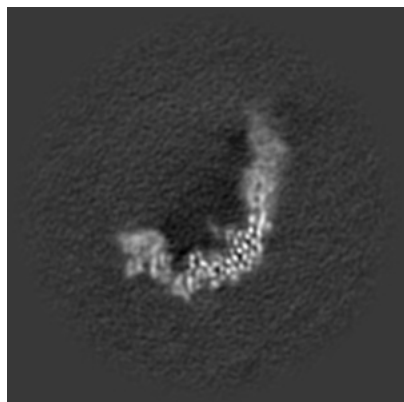


Z Index: 192

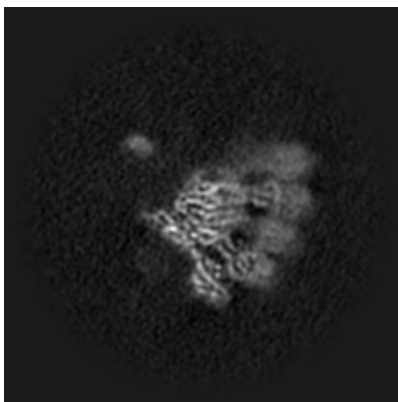
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

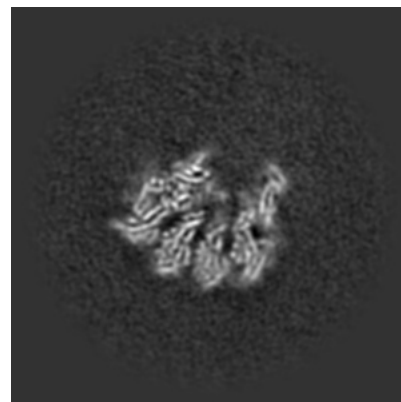
6.3.1 Primary map



X Index: 180



Y Index: 238

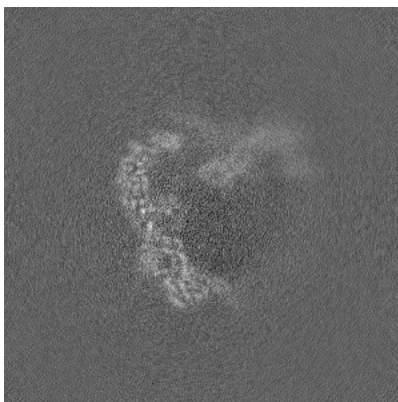


Z Index: 145

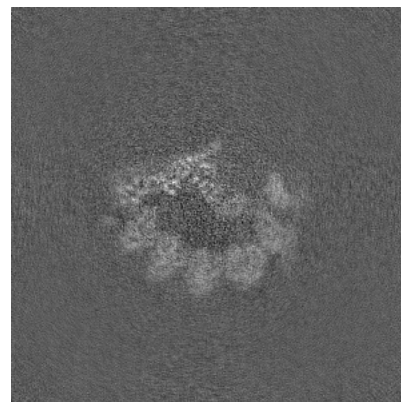
6.3.2 Raw map



X Index: 185



Y Index: 209

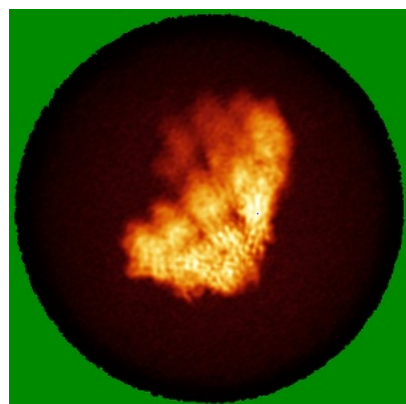


Z Index: 161

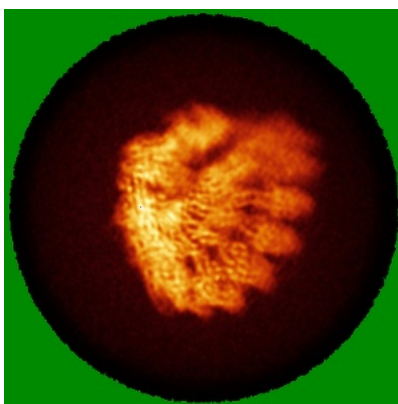
The images above show the largest variance slices of the map in three orthogonal directions.

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

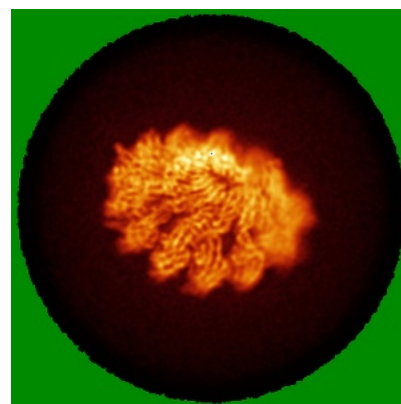
6.4.1 Primary map



X

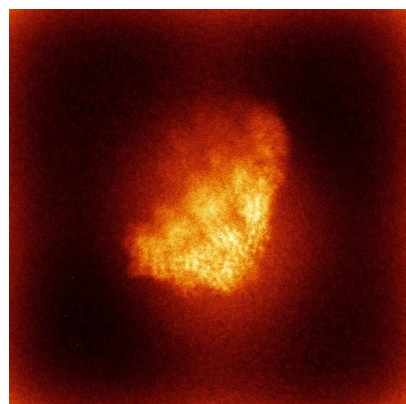


Y

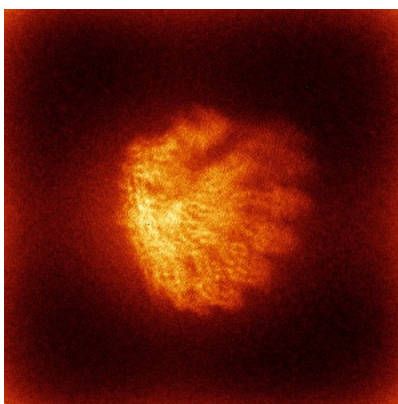


Z

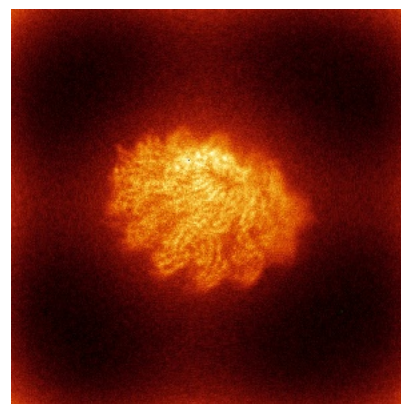
6.4.2 Raw map



X



Y



Z

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

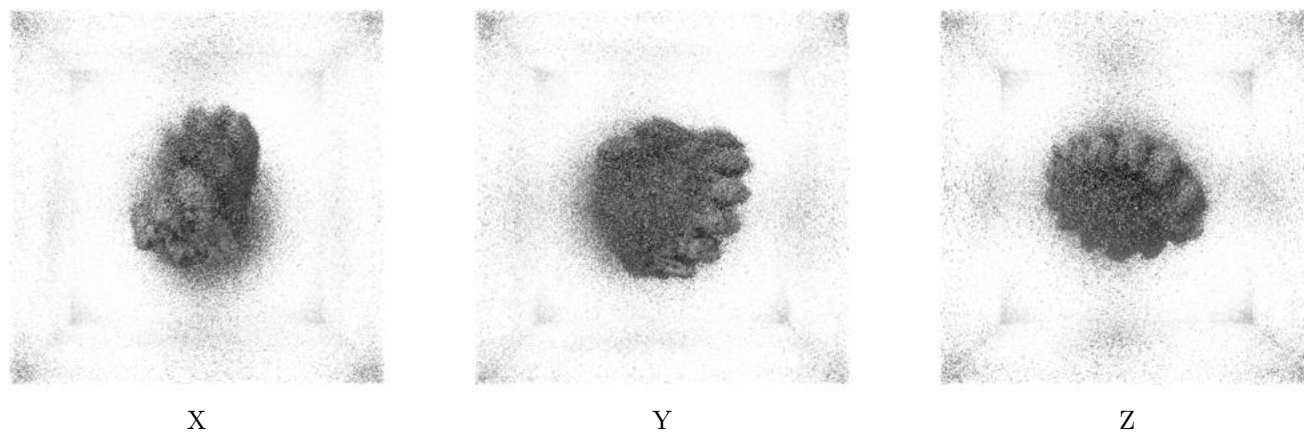
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

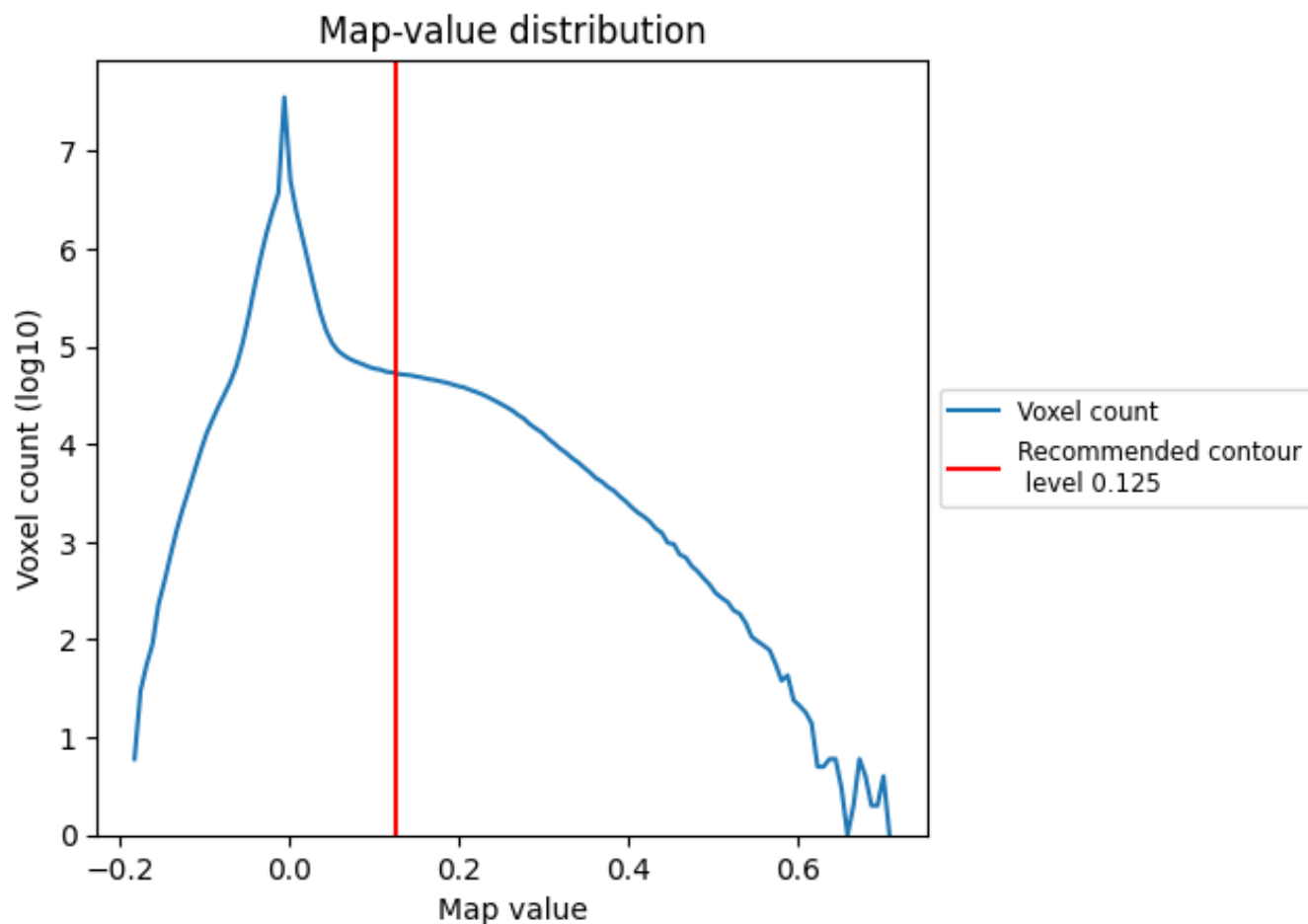
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

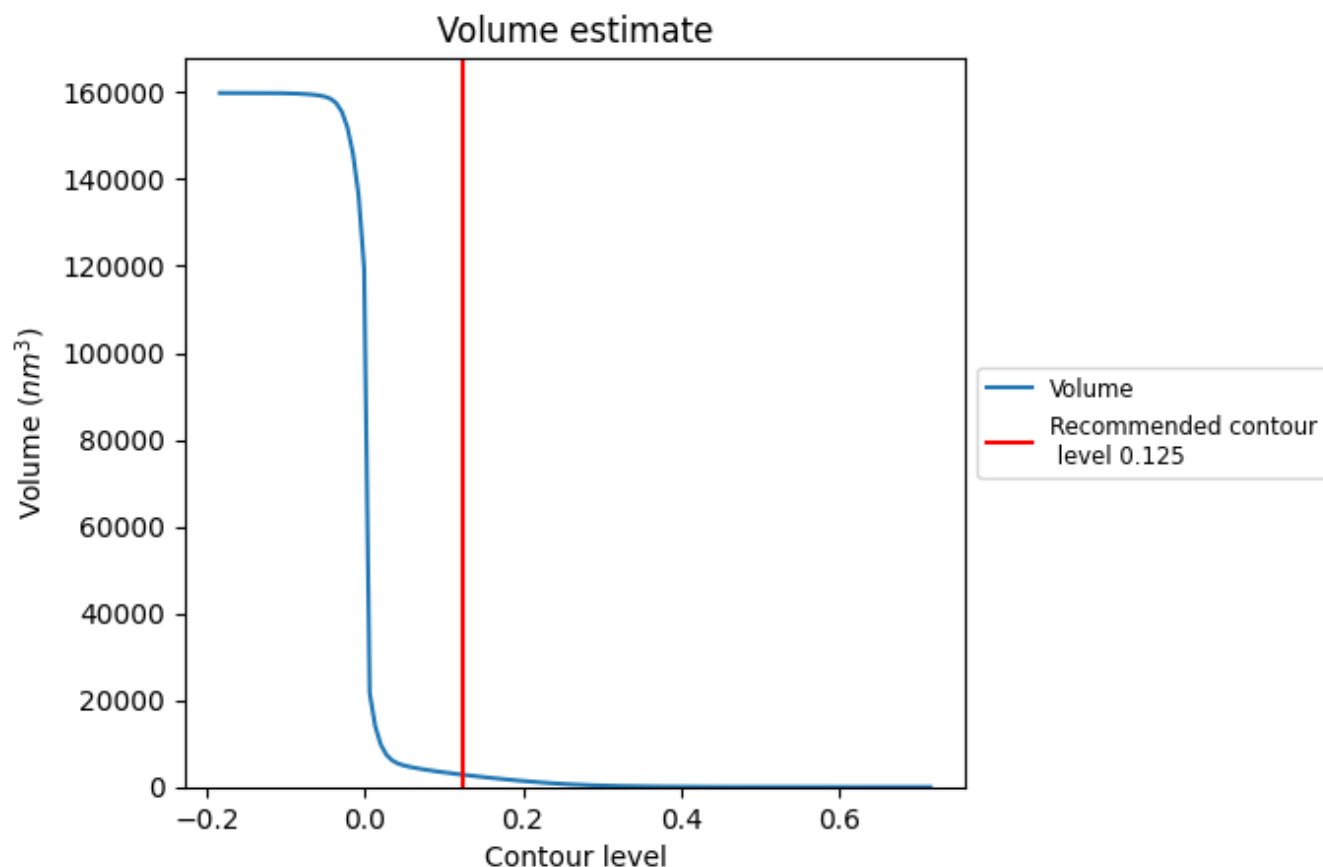
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

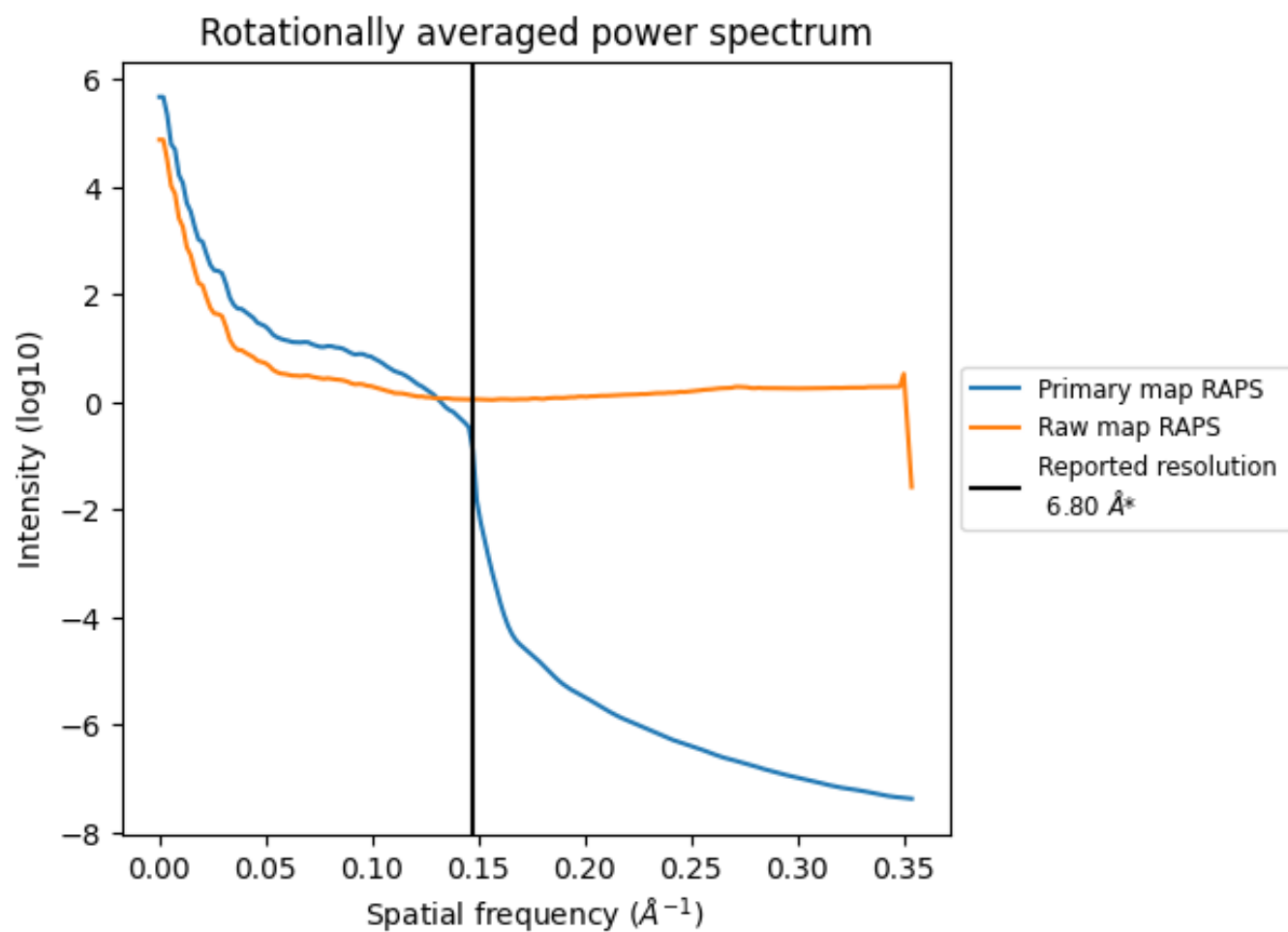
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2794 nm^3 ; this corresponds to an approximate mass of 2524 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 ⓘ

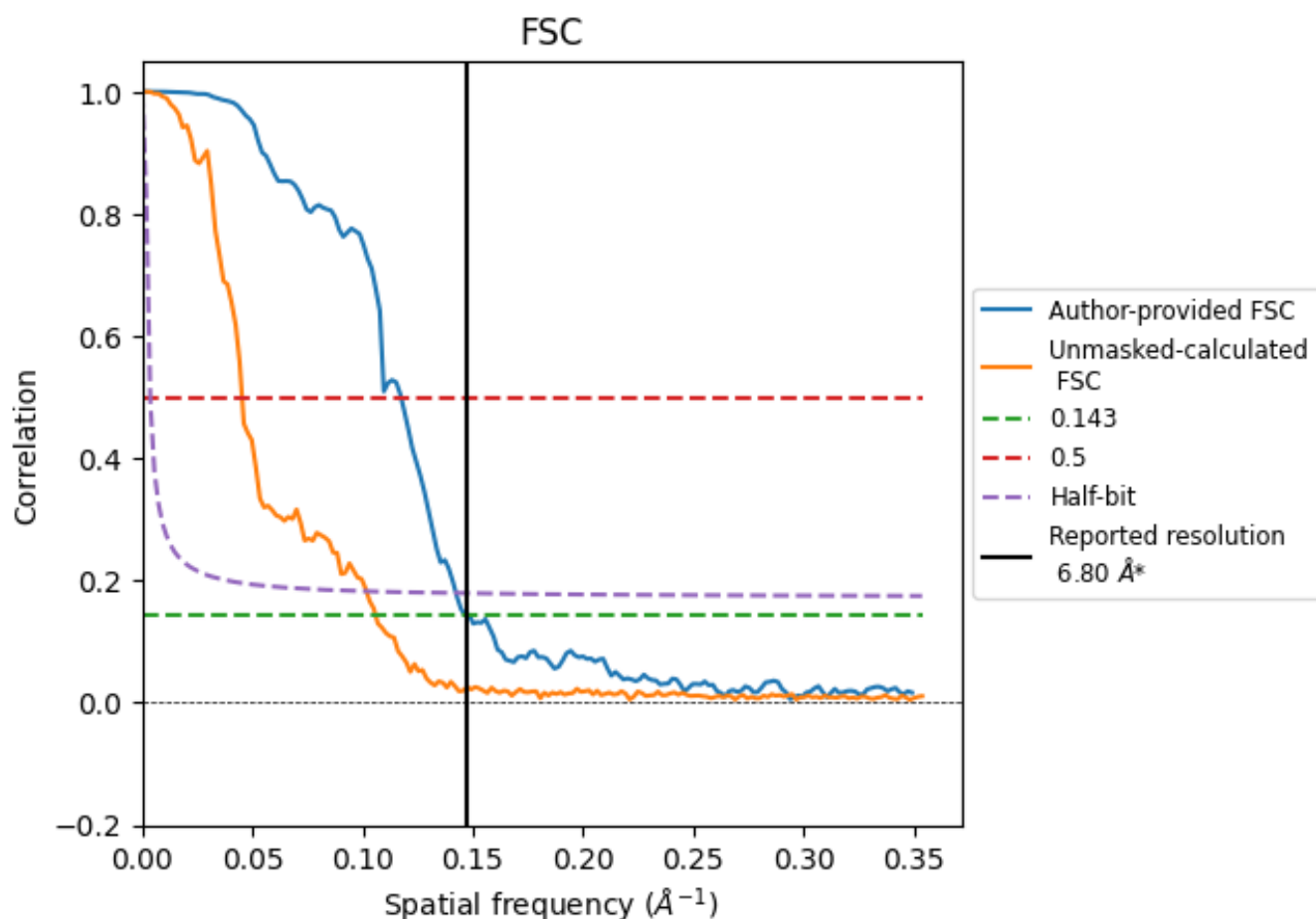


*Reported resolution corresponds to spatial frequency of 0.147 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.147 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

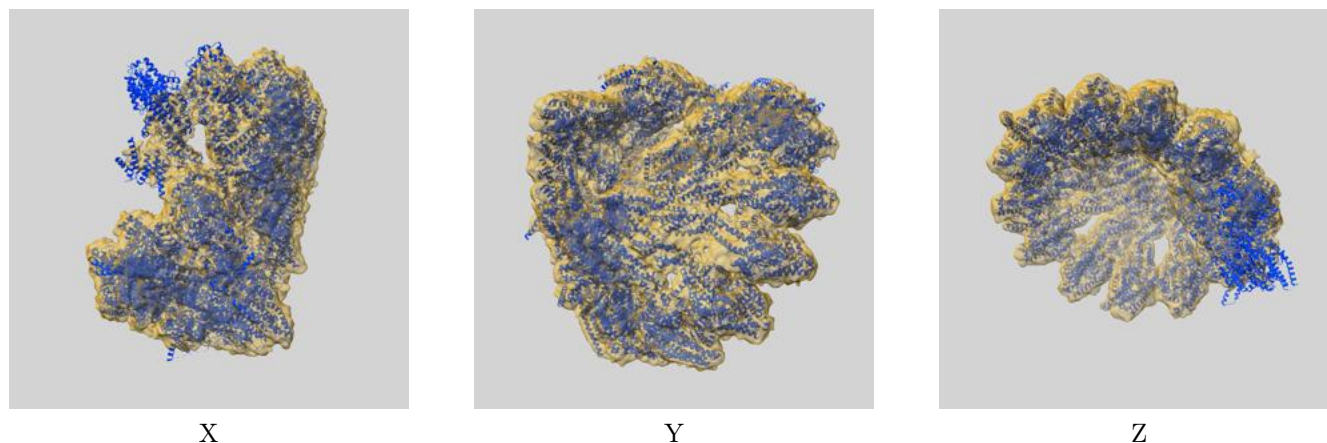
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.83	8.52	7.03
Unmasked-calculated*	9.44	22.08	9.83

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.44 differs from the reported value 6.8 by more than 10 %

9 Map-model fit [i](#)

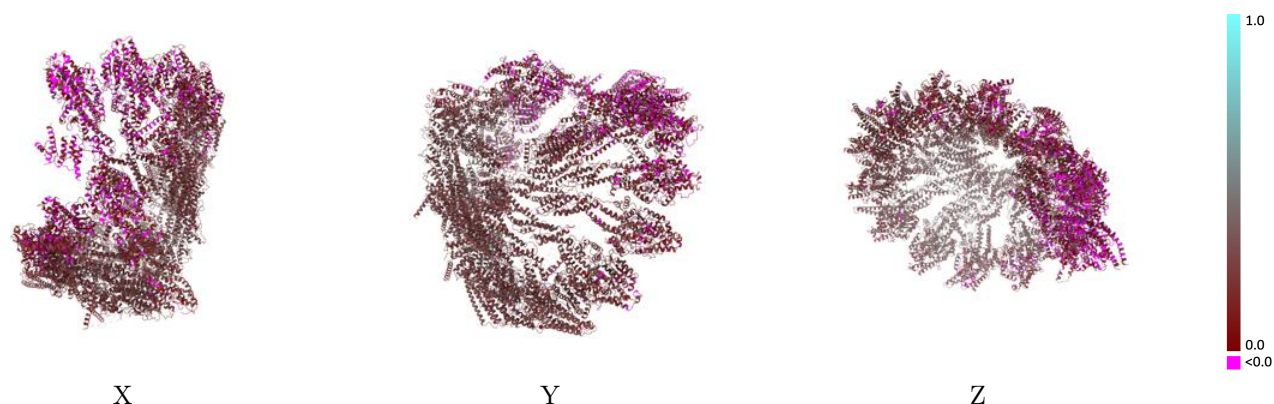
This section contains information regarding the fit between EMDB map EMD-51018 and PDB model 9G3Y. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



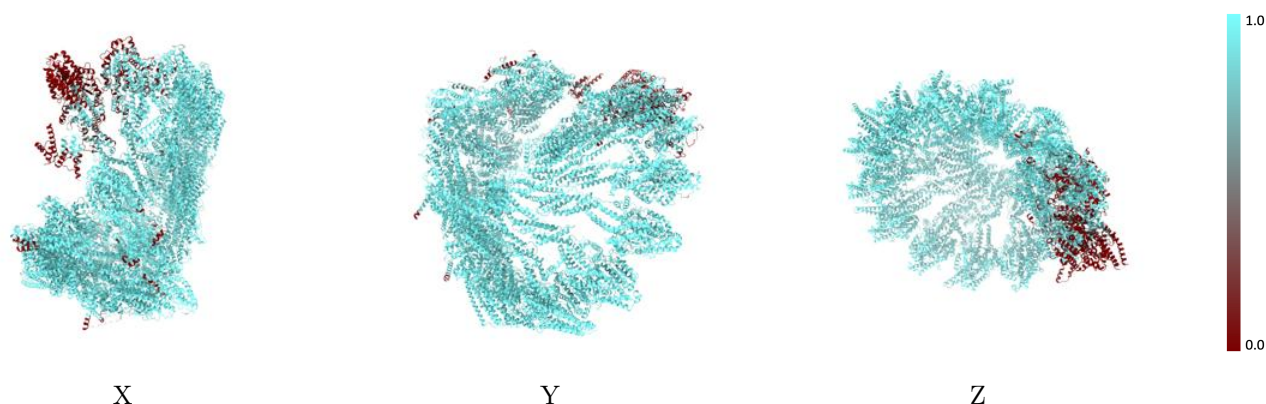
The images above show the 3D surface view of the map at the recommended contour level 0.125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



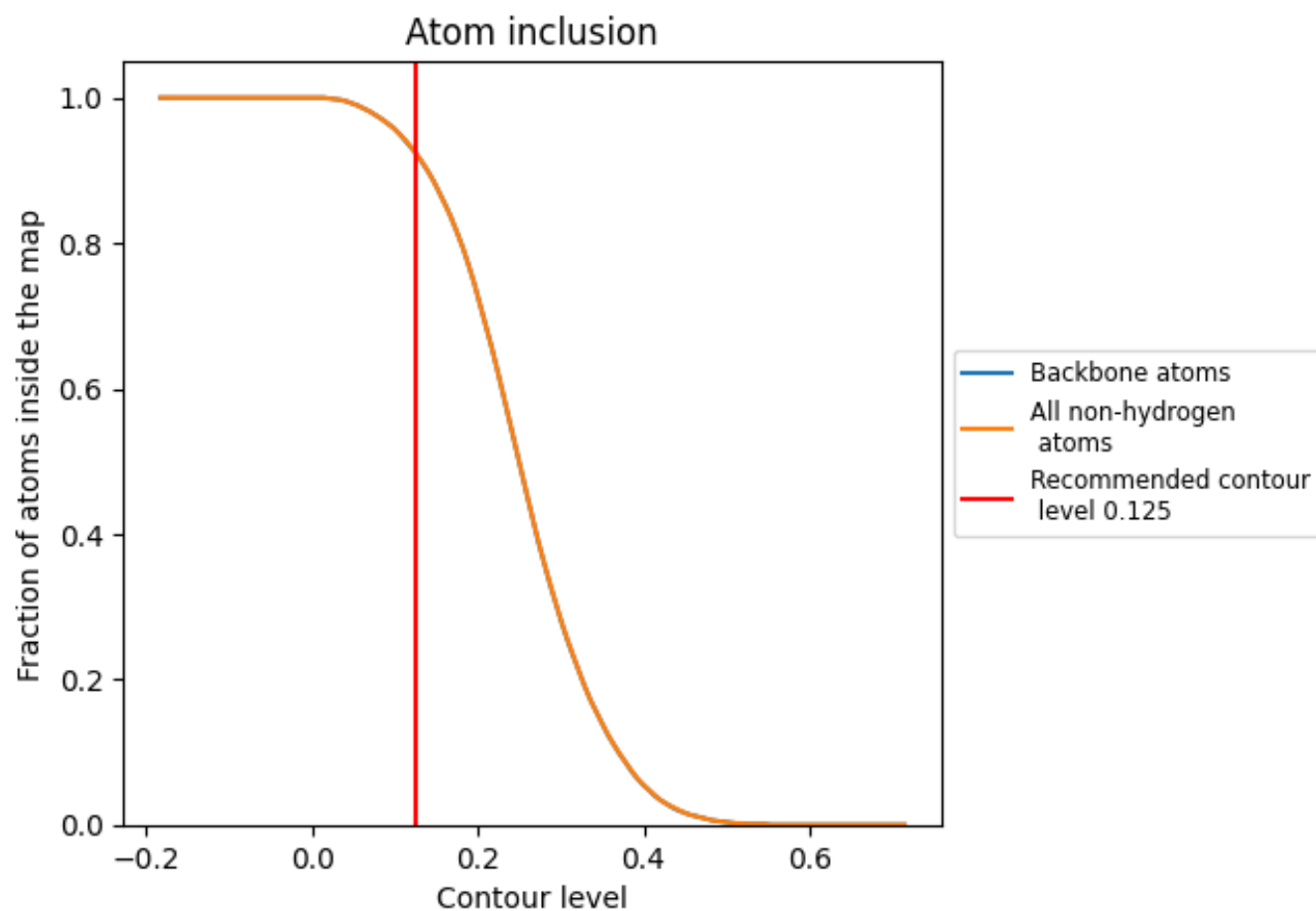
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.1970
A	 0.9470	 0.1740
B	 0.9380	 0.2180
C	 0.9820	 0.2490
D	 0.9930	 0.2630
E	 0.9910	 0.2730
F	 0.9980	 0.2760
G	 0.9900	 0.2760
H	 1.0000	 0.2790
I	 0.9980	 0.2650
J	 0.9990	 0.2310
K	 0.9980	 0.2200
L	 0.9970	 0.1970
M	 0.9410	 0.1400
N	 0.6140	 0.0890
O	 0.2670	 0.0270
P	 0.9760	 0.2810
Q	 0.9810	 0.2490
V	 0.8960	 0.2290
W	 0.9780	 0.2560
X	 0.9690	 0.2570
Y	 1.0000	 0.1690
a	 1.0000	 0.0820
b	 0.9950	 0.0760
c	 0.9890	 0.1420
d	 0.9870	 0.1650
e	 0.9990	 0.2370
f	 0.9930	 0.2360
g	 0.9930	 0.2530
h	 0.9950	 0.2500
i	 0.9960	 0.2090
j	 1.0000	 0.1710
k	 0.9840	 0.1300
l	 0.8760	 0.1070
m	 0.4770	 0.0490



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Chain	Atom inclusion	Q-score
n	 0.0730	 0.0360
o	 0.7460	 0.1430
p	 0.3580	 0.0780
q	 1.0000	 0.2470
r	 1.0000	 0.2200
s	 1.0000	 0.2540
t	 1.0000	 0.2640
u	 1.0000	 0.2530
v	 1.0000	 0.2650
w	 0.9820	 0.0260
x	 0.9940	 0.1150