



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 04:40 AM UTC

PDB ID : 9QVN / pdb_00009qvn
EMDB ID : EMD-53400
Title : Cryo-EM reconstruction of the NEDD1 anchor protein bound to the gamma-tubulin ring complex
Authors : Munoz-Hernandez, H.; Xu, Y.; Wieczorek, M.
Deposited on : 2025-04-11
Resolution : 4.70 Å(reported)
Based on initial model : .

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:

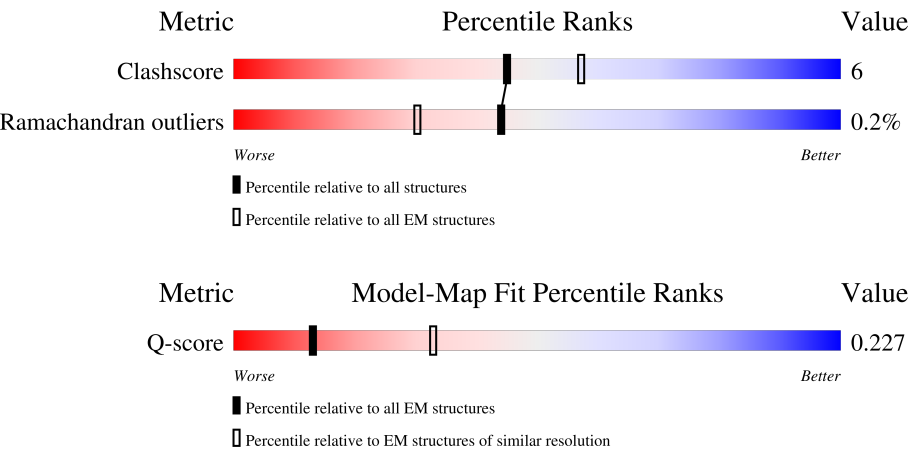
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	907	66% 5% 29%
1	D	907	68% . 28%
1	F	907	66% 6% 28%
1	H	907	67% 5% 28%
1	N	907	42% 66% . 31%

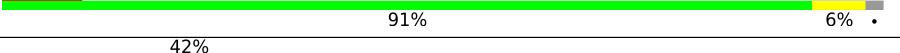
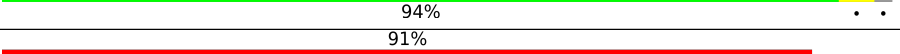
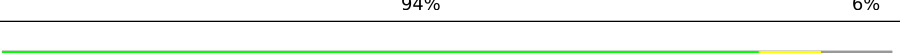
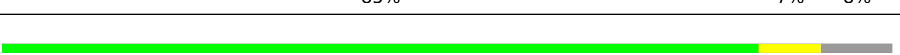
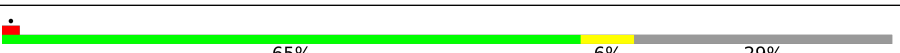
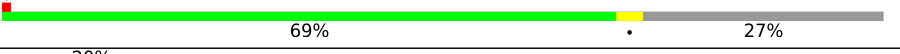
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Mol	Chain	Length	Quality of chain
1	r	907	
1	s	907	
1	t	907	
1	u	907	
1	v	907	
2	O	82	
2	P	82	
2	Q	82	
2	R	82	
2	S	82	
2	T	82	
2	U	82	
3	V	660	
3	W	660	
3	X	660	
3	Y	660	
4	Z	375	
5	a	457	
5	b	457	
5	c	457	
5	d	457	
5	e	457	
5	f	457	
5	g	457	
5	h	457	

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Mol	Chain	Length	Quality of chain
5	i	457	
5	j	457	
5	k	457	
5	l	457	
5	m	457	
5	n	457	
6	I	667	
6	K	667	
7	A	930	
7	C	930	
7	E	930	
7	G	930	
7	M	930	
8	L	1811	
9	J	1024	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 87756 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 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	D	657	Total	C	N	O	0	0
			3256	1942	657	657		
1	F	657	Total	C	N	O	0	0
			3256	1942	657	657		
1	H	656	Total	C	N	O	0	0
			3252	1940	656	656		
1	r	113	Total	C	N	O	0	0
			562	336	113	113		
1	s	115	Total	C	N	O	0	0
			572	342	115	115		
1	t	120	Total	C	N	O	0	0
			597	357	120	120		
1	u	120	Total	C	N	O	0	0
			597	357	120	120		
1	v	129	Total	C	N	O	0	0
			642	384	129	129		
1	B	644	Total	C	N	O	0	0
			3192	1904	644	644		
1	N	630	Total	C	N	O	0	0
			3123	1863	630	630		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	73	Total	C	N	O	0	0
			363	217	73	73		
2	R	66	Total	C	N	O	0	0
			328	196	66	66		
2	S	66	Total	C	N	O	0	0
			328	196	66	66		
2	T	82	Total	C	N	O	0	0
			406	242	82	82		
2	U	82	Total	C	N	O	0	0
			406	242	82	82		

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	82	Total	C	N	O	0	0
			406	242	82	82		
2	Q	66	Total	C	N	O	0	0
			328	196	66	66		

- Molecule 3 is a protein called Protein NEDD1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	W	79	Total	C	N	O	0	0
			394	236	79	79		
3	X	78	Total	C	N	O	0	0
			389	233	78	78		
3	V	77	Total	C	N	O	0	0
			384	230	77	77		
3	Y	78	Total	C	N	O	0	0
			389	233	78	78		

- Molecule 4 is a protein called Actin, cytoplasmic 1, N-terminally processed.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Z	375	Total	C	N	O	0	0
			1847	1097	375	375		

- Molecule 5 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	a	446	Total	C	N	O	0	0
			2204	1312	446	446		
5	b	452	Total	C	N	O	0	0
			2233	1329	452	452		
5	c	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	e	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	f	451	Total	C	N	O	0	0
			2228	1326	451	451		
5	g	450	Total	C	N	O	0	0
			2223	1323	450	450		
5	h	451	Total	C	N	O	0	0
			2228	1326	451	451		
5	i	448	Total	C	N	O	0	0
			2213	1317	448	448		

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Mol	Chain	Residues	Atoms				AltConf	Trace
5	j	449	Total	C	N	O	0	0
			2218	1320	449	449		
5	k	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	l	447	Total	C	N	O	0	0
			2208	1314	447	447		
5	m	448	Total	C	N	O	0	0
			2213	1317	448	448		
5	n	457	Total	C	N	O	0	0
			2258	1344	457	457		
5	d	451	Total	C	N	O	0	0
			2228	1326	451	451		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	452	GLU	-	expression tag	UNP P23258
a	453	ASN	-	expression tag	UNP P23258
a	454	LEU	-	expression tag	UNP P23258
a	455	TYR	-	expression tag	UNP P23258
a	456	PHE	-	expression tag	UNP P23258
a	457	GLN	-	expression tag	UNP P23258
b	452	GLU	-	expression tag	UNP P23258
b	453	ASN	-	expression tag	UNP P23258
b	454	LEU	-	expression tag	UNP P23258
b	455	TYR	-	expression tag	UNP P23258
b	456	PHE	-	expression tag	UNP P23258
b	457	GLN	-	expression tag	UNP P23258
c	452	GLU	-	expression tag	UNP P23258
c	453	ASN	-	expression tag	UNP P23258
c	454	LEU	-	expression tag	UNP P23258
c	455	TYR	-	expression tag	UNP P23258
c	456	PHE	-	expression tag	UNP P23258
c	457	GLN	-	expression tag	UNP P23258
e	452	GLU	-	expression tag	UNP P23258
e	453	ASN	-	expression tag	UNP P23258
e	454	LEU	-	expression tag	UNP P23258
e	455	TYR	-	expression tag	UNP P23258
e	456	PHE	-	expression tag	UNP P23258
e	457	GLN	-	expression tag	UNP P23258
f	452	GLU	-	expression tag	UNP P23258
f	453	ASN	-	expression tag	UNP P23258
f	454	LEU	-	expression tag	UNP P23258

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Chain	Residue	Modelled	Actual	Comment	Reference
f	455	TYR	-	expression tag	UNP P23258
f	456	PHE	-	expression tag	UNP P23258
f	457	GLN	-	expression tag	UNP P23258
g	452	GLU	-	expression tag	UNP P23258
g	453	ASN	-	expression tag	UNP P23258
g	454	LEU	-	expression tag	UNP P23258
g	455	TYR	-	expression tag	UNP P23258
g	456	PHE	-	expression tag	UNP P23258
g	457	GLN	-	expression tag	UNP P23258
h	452	GLU	-	expression tag	UNP P23258
h	453	ASN	-	expression tag	UNP P23258
h	454	LEU	-	expression tag	UNP P23258
h	455	TYR	-	expression tag	UNP P23258
h	456	PHE	-	expression tag	UNP P23258
h	457	GLN	-	expression tag	UNP P23258
i	452	GLU	-	expression tag	UNP P23258
i	453	ASN	-	expression tag	UNP P23258
i	454	LEU	-	expression tag	UNP P23258
i	455	TYR	-	expression tag	UNP P23258
i	456	PHE	-	expression tag	UNP P23258
i	457	GLN	-	expression tag	UNP P23258
j	452	GLU	-	expression tag	UNP P23258
j	453	ASN	-	expression tag	UNP P23258
j	454	LEU	-	expression tag	UNP P23258
j	455	TYR	-	expression tag	UNP P23258
j	456	PHE	-	expression tag	UNP P23258
j	457	GLN	-	expression tag	UNP P23258
k	452	GLU	-	expression tag	UNP P23258
k	453	ASN	-	expression tag	UNP P23258
k	454	LEU	-	expression tag	UNP P23258
k	455	TYR	-	expression tag	UNP P23258
k	456	PHE	-	expression tag	UNP P23258
k	457	GLN	-	expression tag	UNP P23258
l	452	GLU	-	expression tag	UNP P23258
l	453	ASN	-	expression tag	UNP P23258
l	454	LEU	-	expression tag	UNP P23258
l	455	TYR	-	expression tag	UNP P23258
l	456	PHE	-	expression tag	UNP P23258
l	457	GLN	-	expression tag	UNP P23258
m	452	GLU	-	expression tag	UNP P23258
m	453	ASN	-	expression tag	UNP P23258
m	454	LEU	-	expression tag	UNP P23258

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Chain	Residue	Modelled	Actual	Comment	Reference
m	455	TYR	-	expression tag	UNP P23258
m	456	PHE	-	expression tag	UNP P23258
m	457	GLN	-	expression tag	UNP P23258
n	452	GLU	-	expression tag	UNP P23258
n	453	ASN	-	expression tag	UNP P23258
n	454	LEU	-	expression tag	UNP P23258
n	455	TYR	-	expression tag	UNP P23258
n	456	PHE	-	expression tag	UNP P23258
n	457	GLN	-	expression tag	UNP P23258
d	452	GLU	-	expression tag	UNP P23258
d	453	ASN	-	expression tag	UNP P23258
d	454	LEU	-	expression tag	UNP P23258
d	455	TYR	-	expression tag	UNP P23258
d	456	PHE	-	expression tag	UNP P23258
d	457	GLN	-	expression tag	UNP P23258

- Molecule 6 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	614	Total	C	N	O	0	0
			3037	1809	614	614		
6	I	612	Total	C	N	O	0	0
			3027	1803	612	612		

- Molecule 7 is a protein called Isoform 3 of Gamma-tubulin complex component 2.

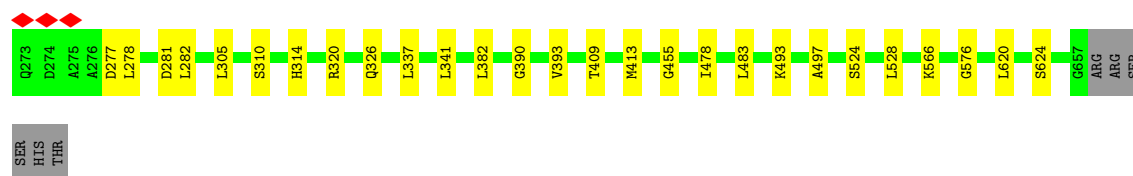
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	678	Total	C	N	O	0	0
			3367	2011	678	678		
7	M	665	Total	C	N	O	0	0
			3303	1973	665	665		
7	C	653	Total	C	N	O	0	0
			3244	1938	653	653		
7	A	657	Total	C	N	O	0	0
			3264	1950	657	657		
7	E	678	Total	C	N	O	0	0
			3367	2011	678	678		

- Molecule 8 is a protein called TUBGCP6 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	982	Total 4851	C 2887	N 982	O 982	0	0

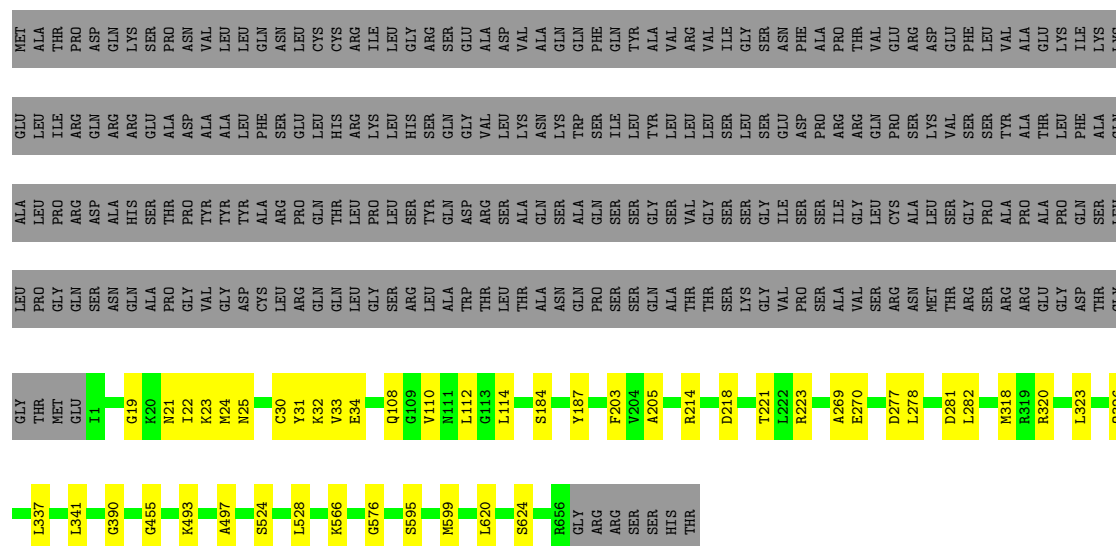
- Molecule 9 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	842	Total 4186	C 2502	N 842	O 842	0	0



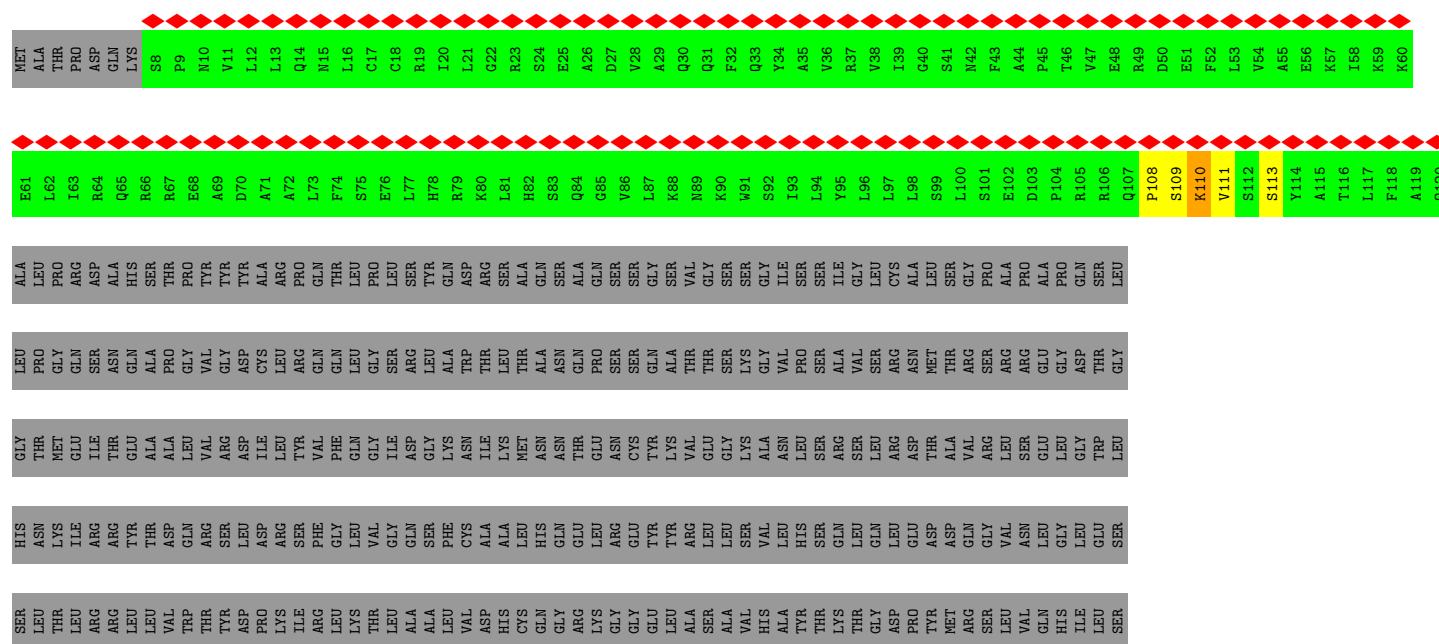
• Molecule 1: Gamma-tubulin complex component 3

Chain H: 67% 5% 28%



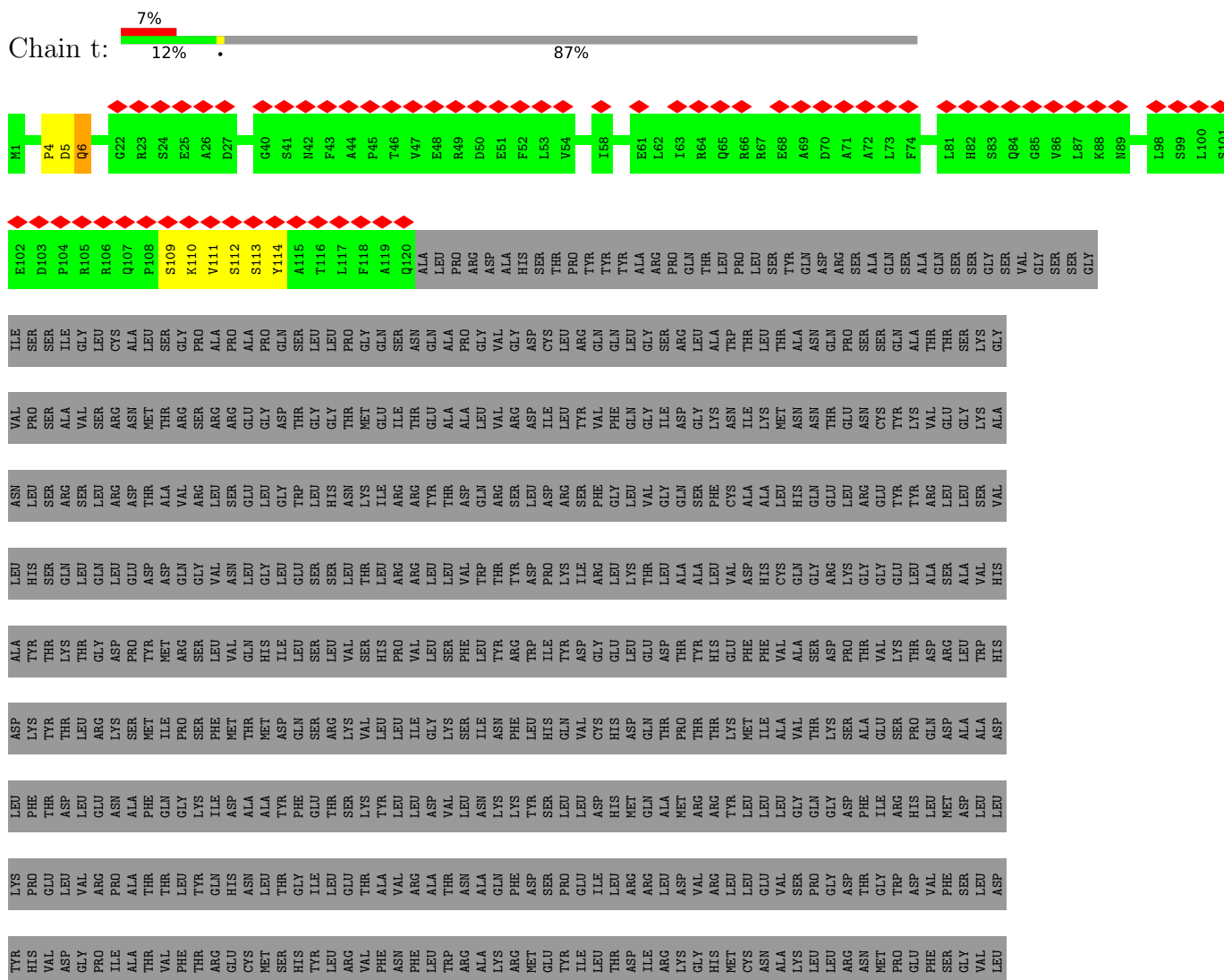
• Molecule 1: Gamma-tubulin complex component 3

Chain r: 12% 12% 88%

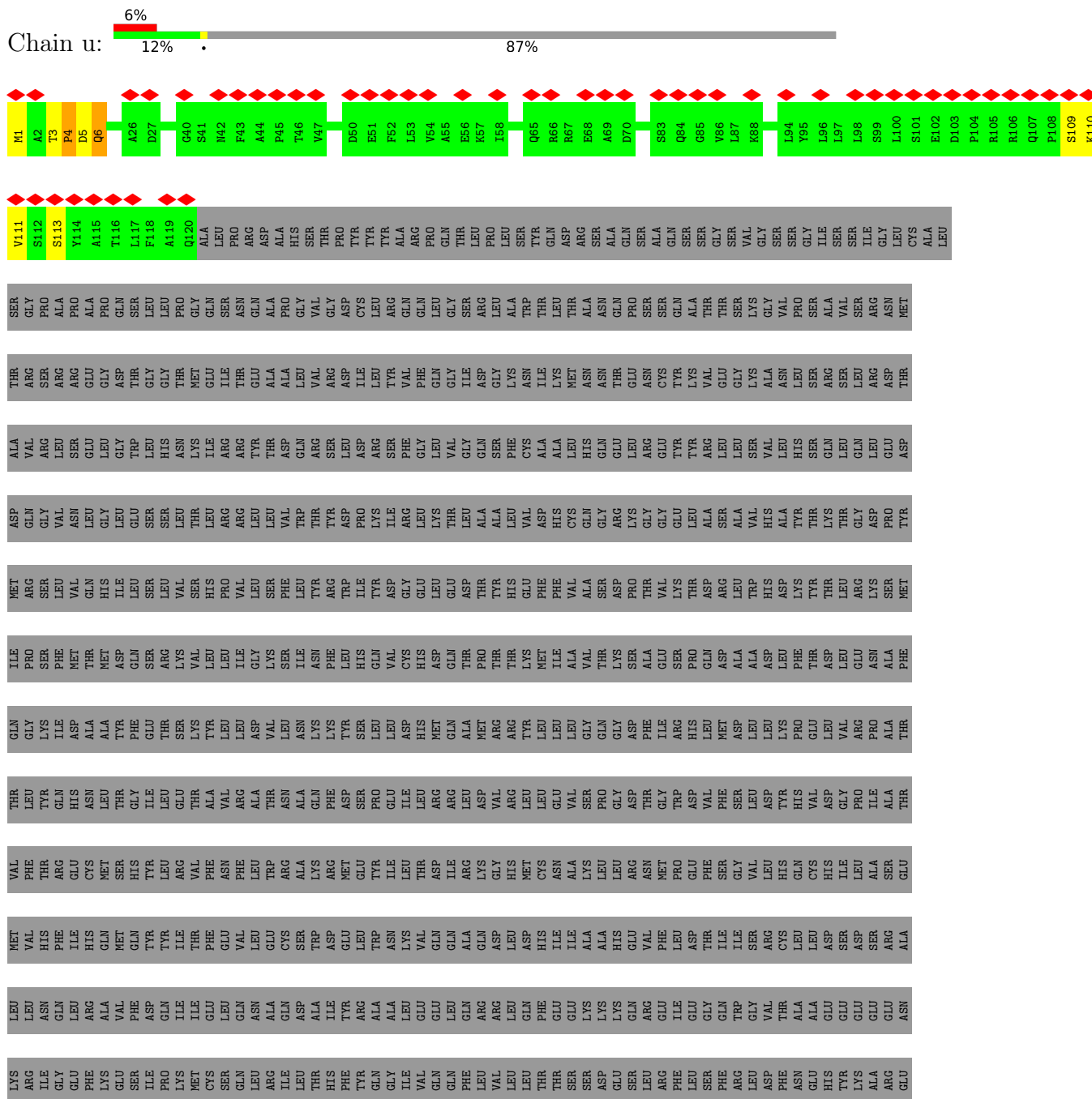


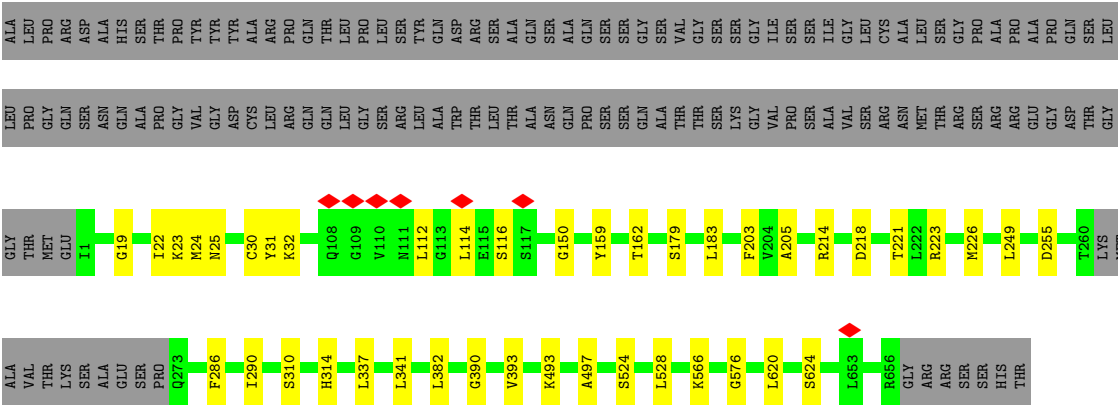
[illegible]

- Molecule 1: Gamma-tubulin complex component 3

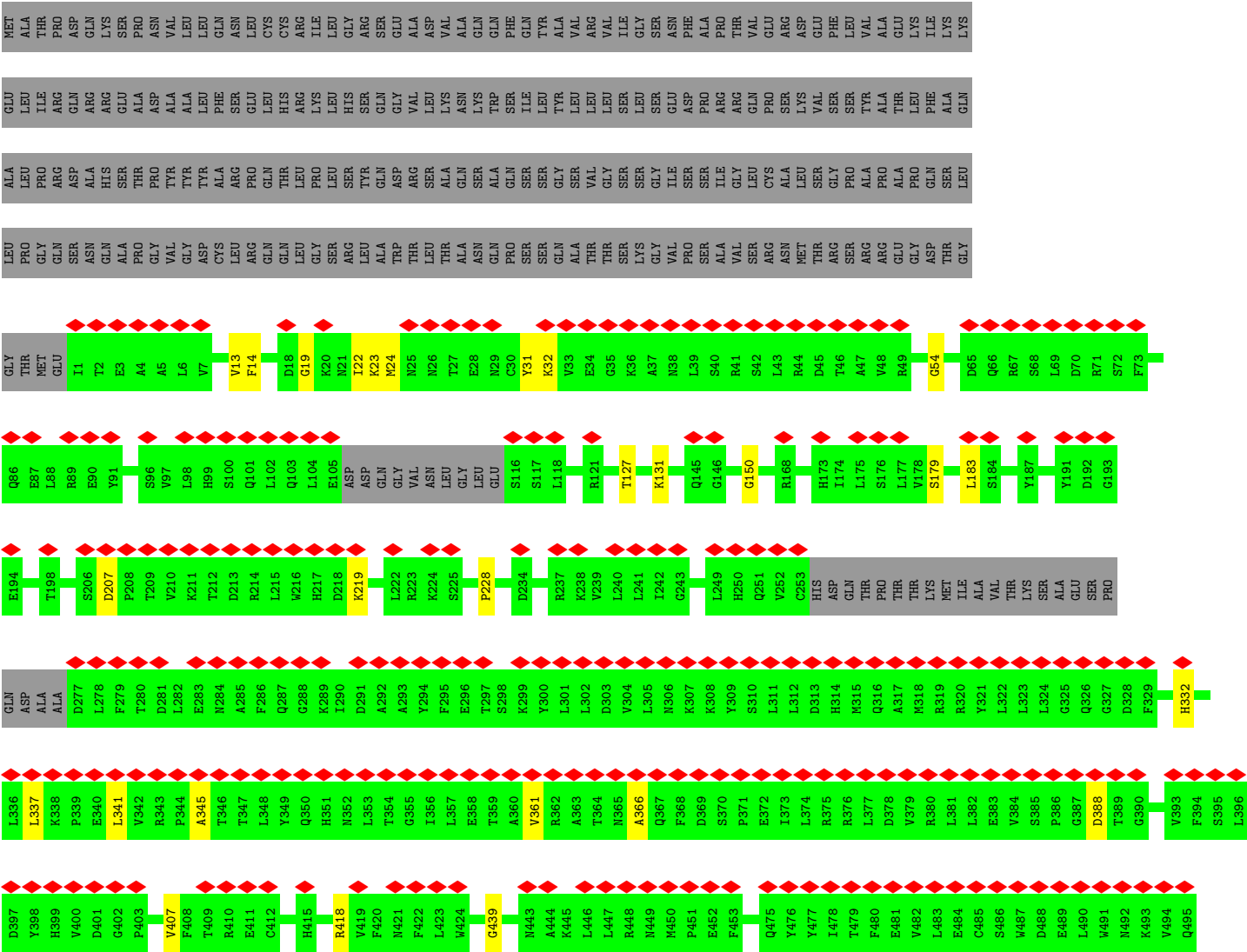


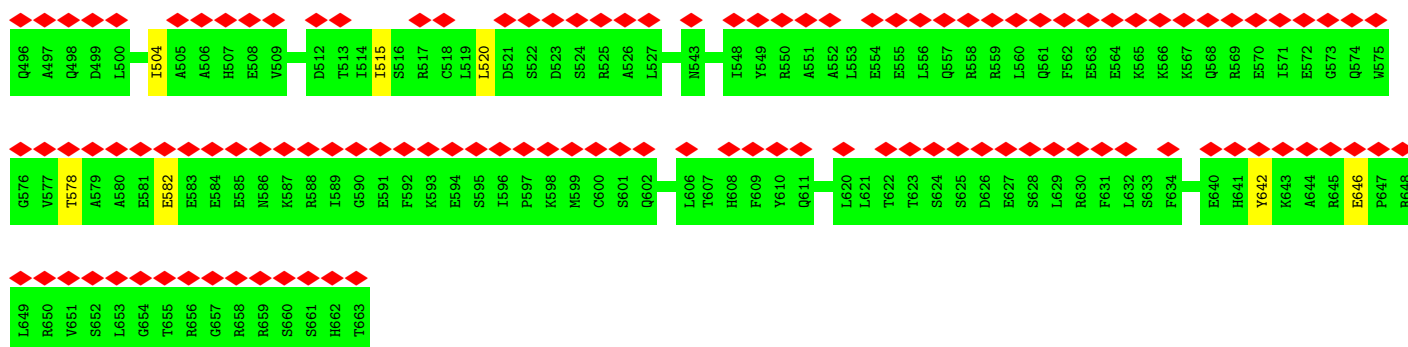
- Molecule 1: Gamma-tubulin complex component 3



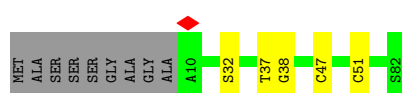
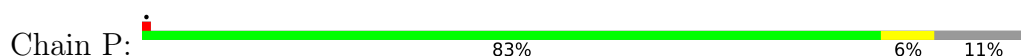


• Molecule 1: Gamma-tubulin complex component 3

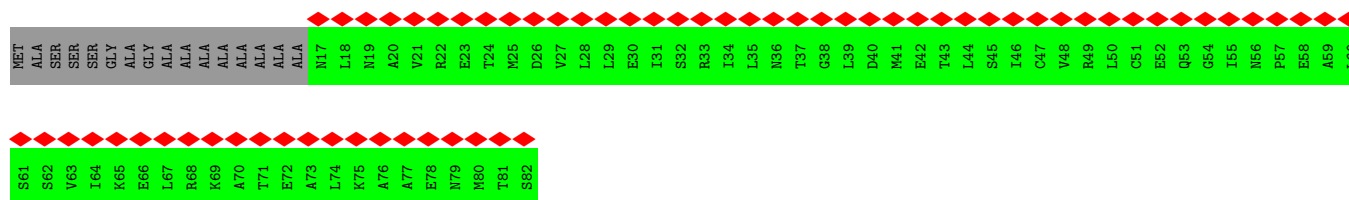
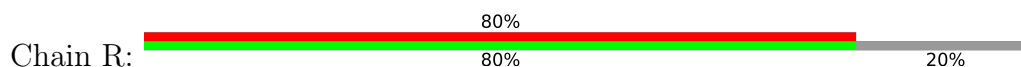




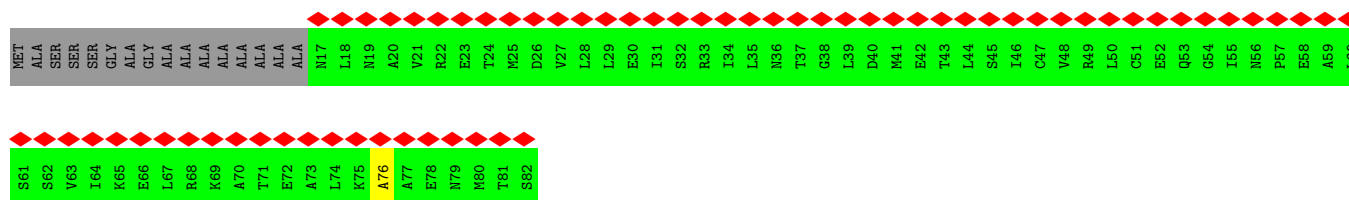
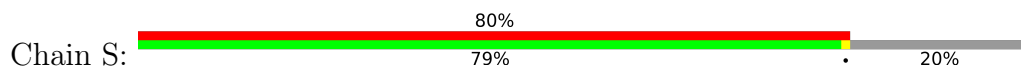
- Molecule 2: Mitotic-spindle organizing protein 1



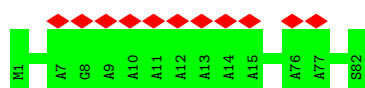
- Molecule 2: Mitotic-spindle organizing protein 1



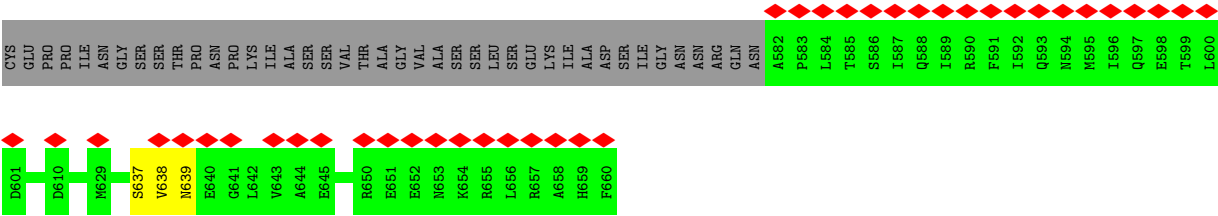
- Molecule 2: Mitotic-spindle organizing protein 1



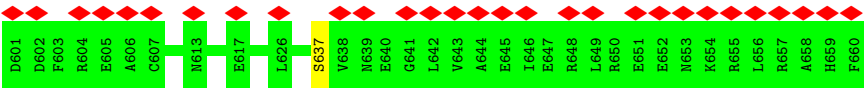
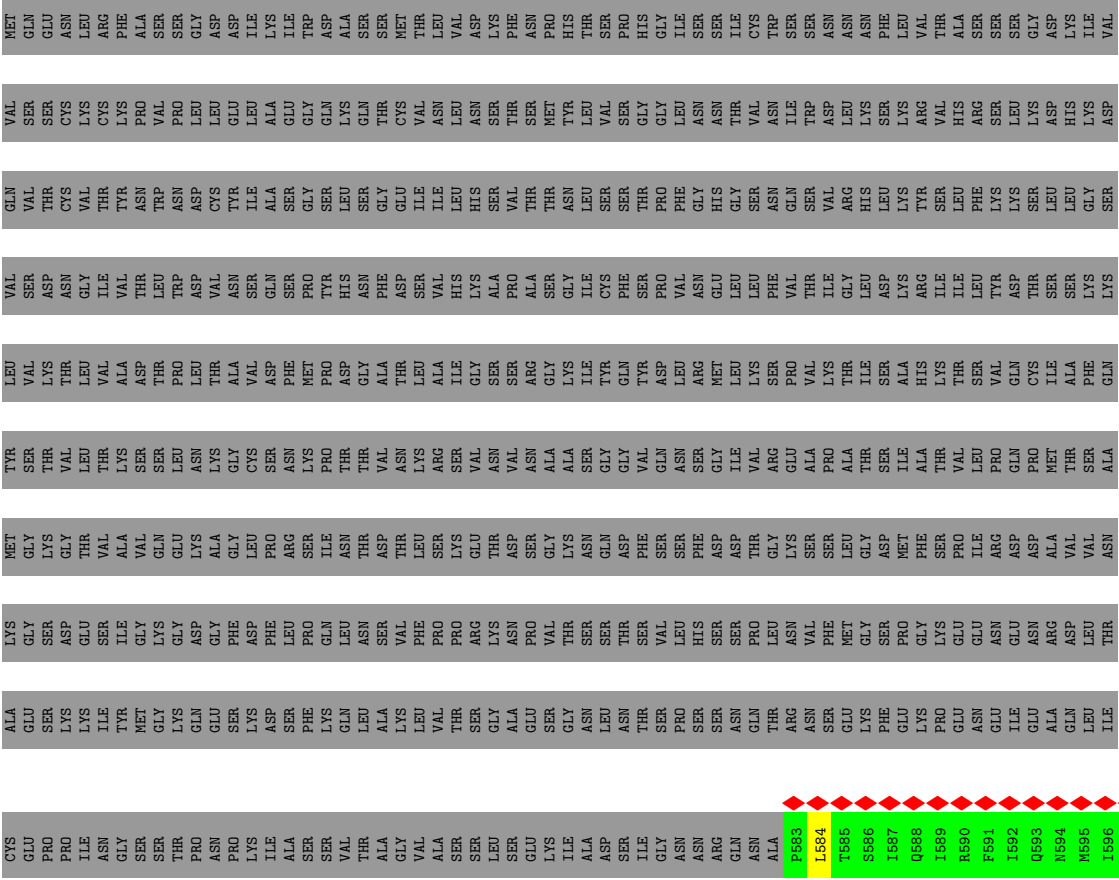
- Molecule 2: Mitotic-spindle organizing protein 1



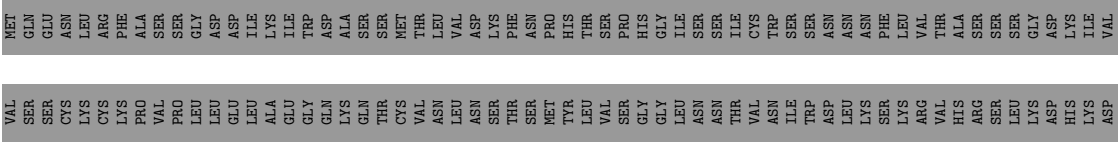
- Molecule 2: Mitotic-spindle organizing protein 1



• Molecule 3: Protein NEDD1



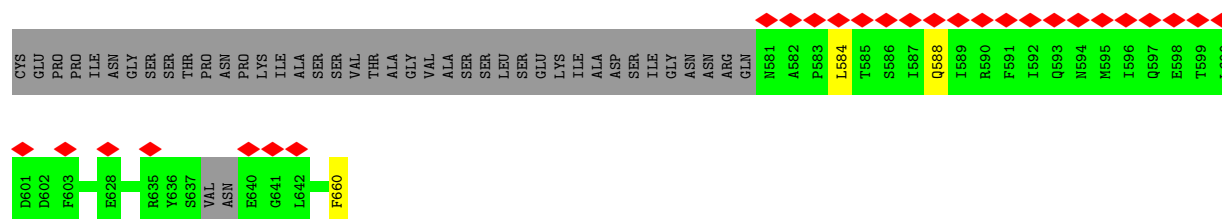
• Molecule 3: Protein NEDD1



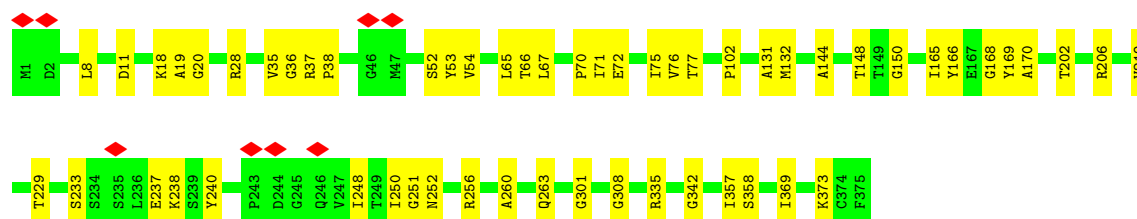
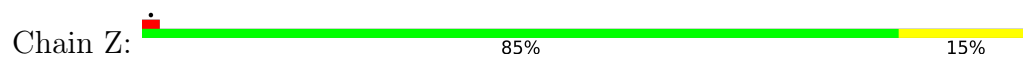
D601	D602	F603	R604	E605	A606	C607	H608	R609	D610	I611	V612	N613	L614	R635	Y636	S637	VAL	ASN	E640	F660
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Chain Y: 11% 88%

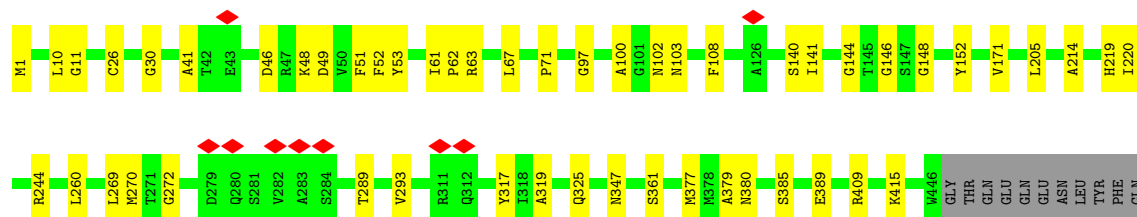
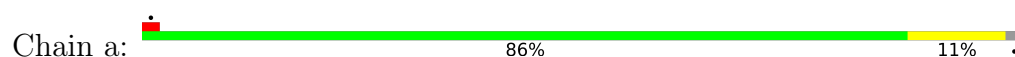




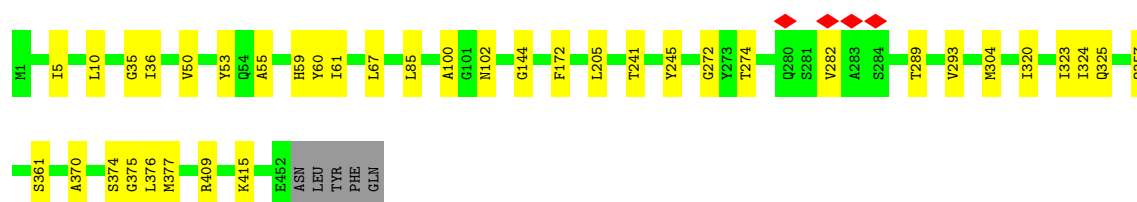
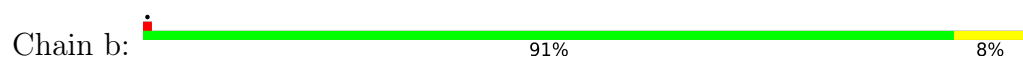
- Molecule 4: Actin, cytoplasmic 1, N-terminally processed



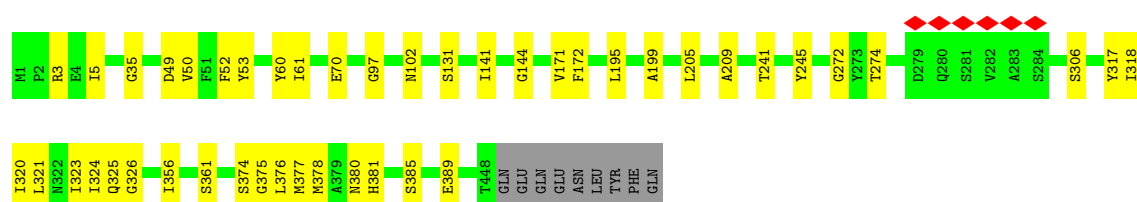
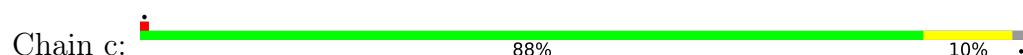
- Molecule 5: Tubulin gamma-1 chain



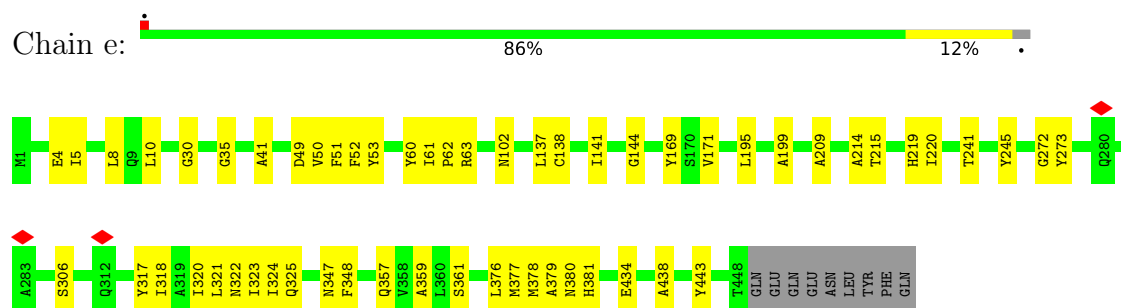
- Molecule 5: Tubulin gamma-1 chain



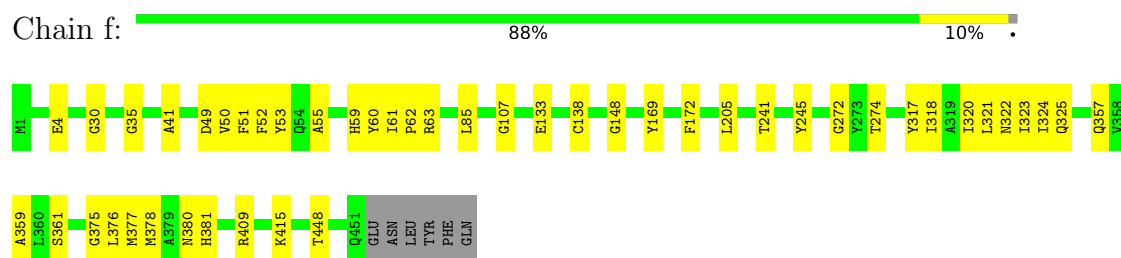
- Molecule 5: Tubulin gamma-1 chain



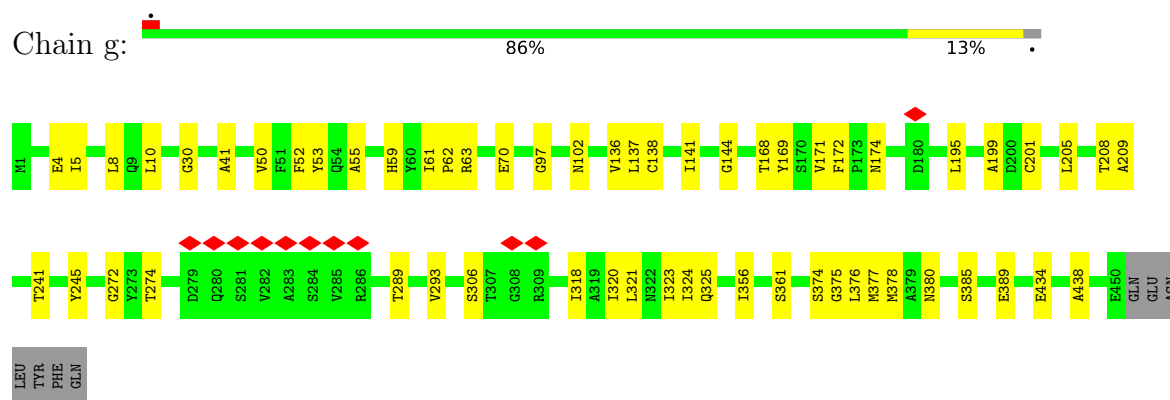
- Molecule 5: Tubulin gamma-1 chain



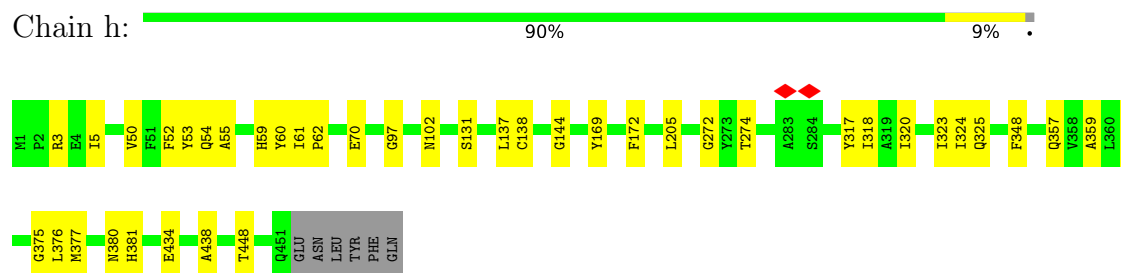
- Molecule 5: Tubulin gamma-1 chain



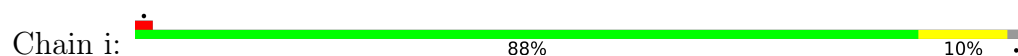
- Molecule 5: Tubulin gamma-1 chain

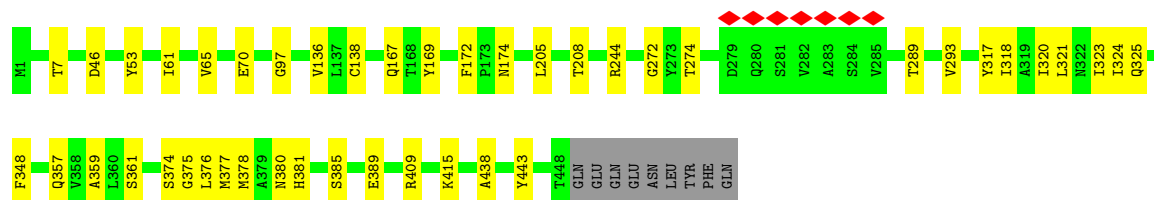


- Molecule 5: Tubulin gamma-1 chain

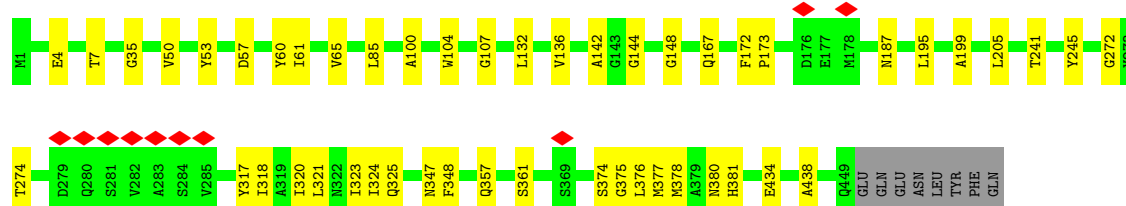
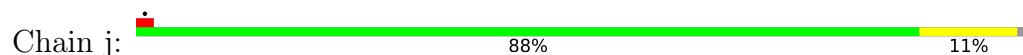


- Molecule 5: Tubulin gamma-1 chain

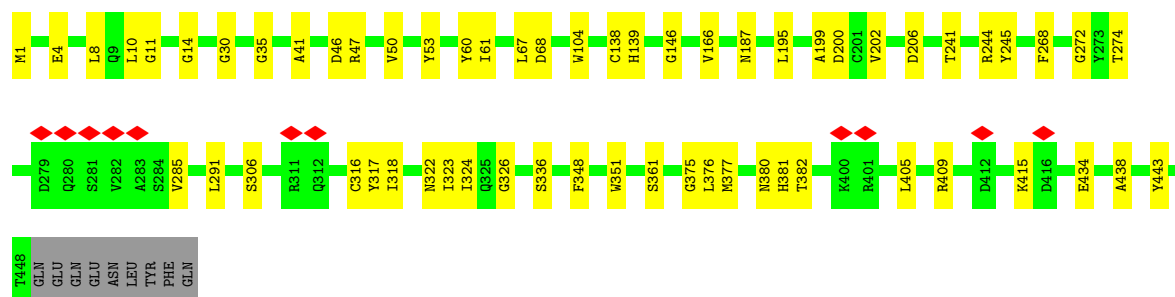
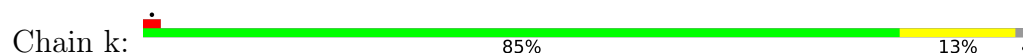




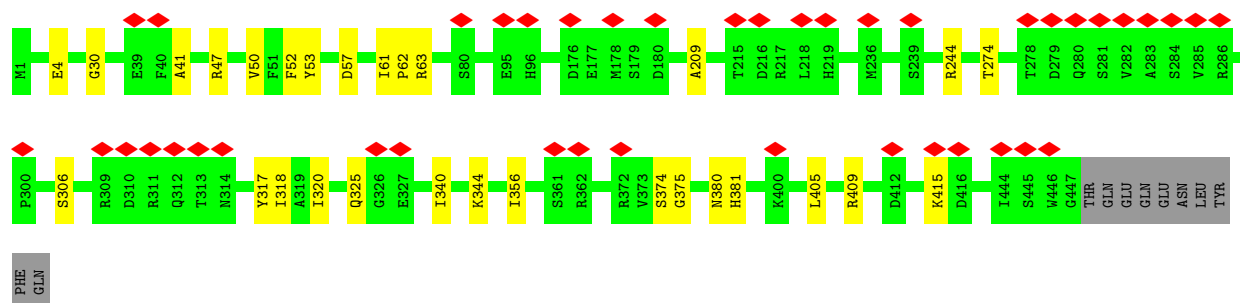
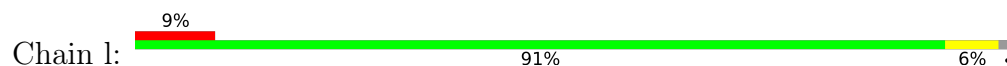
• Molecule 5: Tubulin gamma-1 chain



• Molecule 5: Tubulin gamma-1 chain

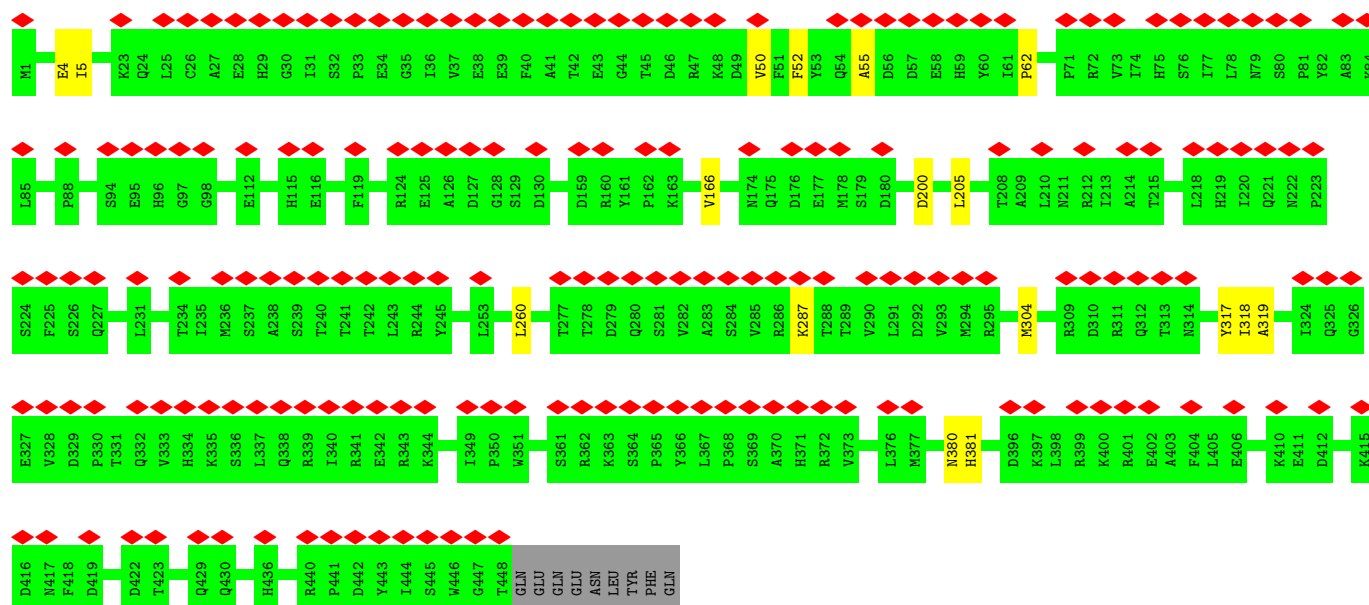


• Molecule 5: Tubulin gamma-1 chain

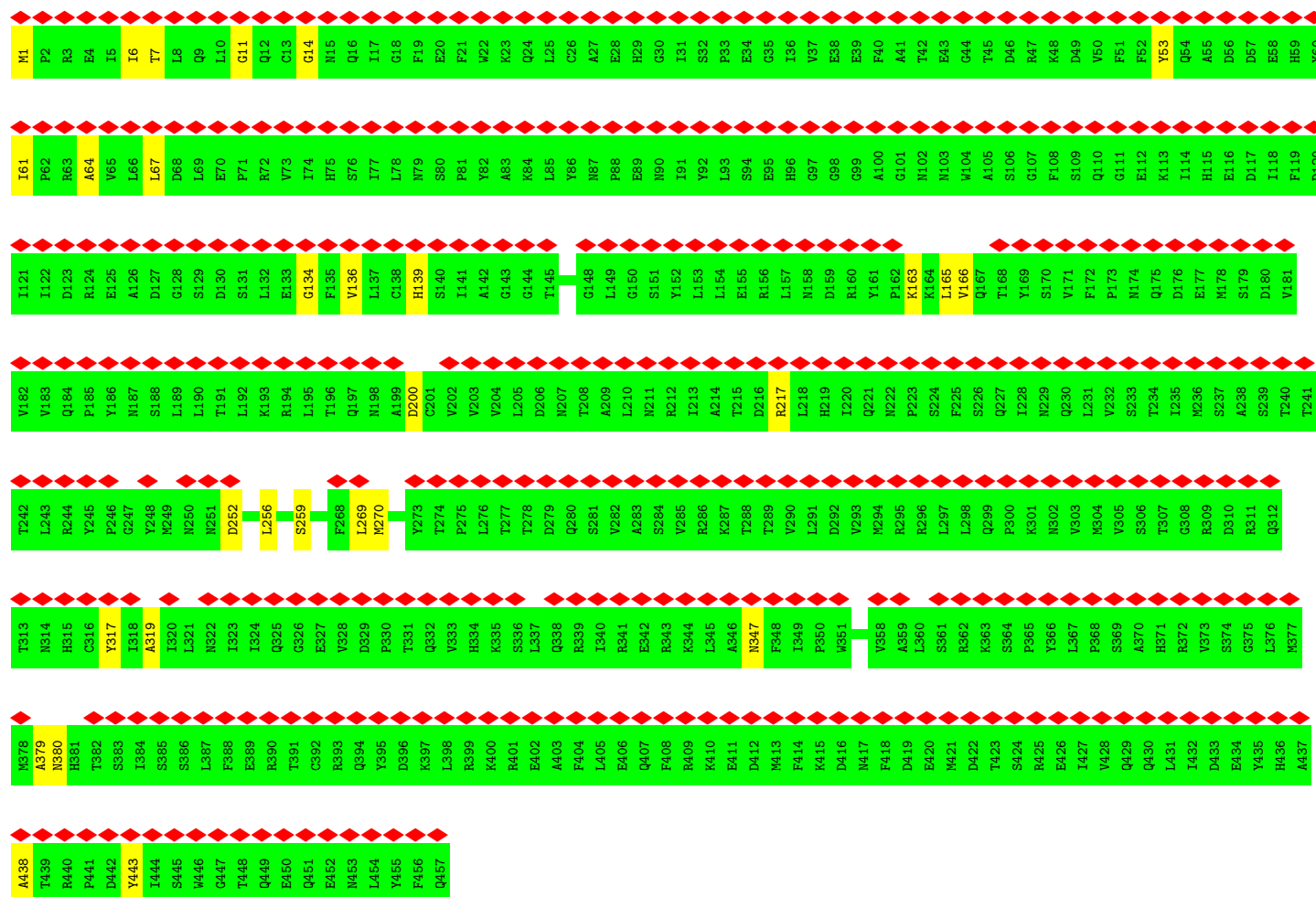
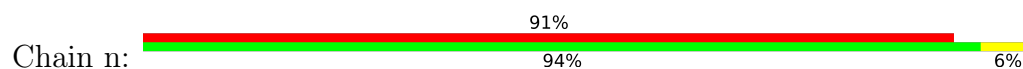


• Molecule 5: Tubulin gamma-1 chain





• Molecule 5: Tubulin gamma-1 chain



Chain d:

85% 13%

Label	Color
N1	Green
P2	Green
R3	Green
E4	Green
I5	Green
L8	Green
Q9	Green
L10	Green
N15	Green
G30	Green
G35	Green
I36	Green
V37	Green
E38	Green
A41	Green
T42	Green
E43	Green
G44	Green
T45	Green
V50	Green
I318	Green
F51	Green
F52	Green
F53	Green
H59	Green
Y60	Green
I61	Green
P62	Green
V65	Green
L66	Green
L67	Green
A100	Green
G101	Green
N102	Green
G107	Green
S131	Green
C138	Green
I141	Green
G144	Green
G148	Green
V171	Green
F172	Green
L196	Green
A199	Green
L206	Green
A209	Green
T241	Green
Y245	Green
G272	Green
Y273	Green
T274	Green
D279	Green
Q280	Green
A283	Green
S284	Green
V285	Green
S306	Green
Y317	Green
I318	Green
A319	Green
I320	Green
L321	Green
N322	Green
I323	Green
I324	Green
Q325	Green
Q357	Green
V358	Green
A359	Green
L360	Green
S361	Green
S374	Green
G375	Green
L376	Green
M377	Green
M378	Green
A379	Green
N380	Green
H381	Green
E450	Green
GLN	Green
E452	Green
ASN	Green
LEU	Green
TYR	Green
PHE	Green
GLN	Green

Chain K: 85% 7% 8%

Residue	Position	Score	Category
M1	1	1.00	High
L5	5	1.00	High
L6	6	1.00	High
S10	10	1.00	High
N20	20	1.00	High
G24	24	1.00	High
S74	74	1.00	High
G79	79	1.00	High
V157	157	1.00	High
S161	161	1.00	High
H200	200	1.00	High
G212	212	1.00	High
ASN	213	0.99	High
VAL	214	0.98	High
SER	215	0.97	High
ALA	216	0.96	High
GLN	217	0.95	High
PRO	218	0.94	High
GLU	219	0.93	High
GLU	220	0.92	High
ASP	221	0.91	High
ASP	222	0.90	High
LEU	223	0.89	High
GLY	224	0.88	High
ILE	225	0.87	High
GLY	226	0.86	High
GLY	227	0.85	High
LEU	228	0.84	High
THR	229	0.83	High
GLY	230	0.82	High
LYS	231	0.81	High
GLN	232	0.80	High
LEU	233	0.79	High
ARG	234	0.78	High
GLU	235	0.77	High
LEU	236	0.76	High
GLN	237	0.75	High
ASP	238	0.74	High
LEU	239	0.73	High
ARG	240	0.72	High
ILE	241	0.71	High
GLU	242	0.70	High
PRO	243	0.69	High
GLU	244	0.68	High
ASN	245	0.67	High
H249	249	0.66	High
S253	253	0.65	High
Q256	256	0.64	High
P269	269	0.63	High
A273	273	0.62	High
T294	294	0.61	High
R295	295	0.60	High
K296	296	0.59	High
E338	338	0.58	High
L343	343	0.57	High
S348	348	0.56	High
K358	358	0.55	High
G364	364	0.54	High
A371	371	0.53	High
P383	383	0.52	High
P384	384	0.51	High
T385	385	0.50	High
T388	388	0.49	High
S399	399	0.48	High
A400	400	0.47	High
V403	403	0.46	High
L404	404	0.45	High
L405	405	0.44	High
T417	417	0.43	High
H421	421	0.42	High
Q422	422	0.41	High
K423	423	0.40	High
GLU	424	0.39	High
HIS	425	0.38	High
LYS	426	0.37	High
ALA	427	0.36	High
ASP	428	0.35	High
ALA	429	0.34	High
THR	430	0.33	High
GLN	431	0.32	High
ALA	432	0.31	High
ARG	433	0.30	High
GLU	434	0.29	High
PRO	435	0.28	High
SER	436	0.27	High
ARG	437	0.26	High
GLU	438	0.25	High
THR	439	0.24	High
S440	440	0.23	High
P441	441	0.22	High
P445	445	0.21	High
A446	446	0.20	High
S447	447	0.19	High
G448	448	0.18	High
Q532	532	0.17	High
E537	537	0.16	High
R551	551	0.15	High
D604	604	0.14	High
A608	608	0.13	High
M634	634	0.12	High
Y654	654	0.11	High
G659	659	0.10	High
G662	662	0.09	High
G665	665	0.08	High
M666	666	0.07	High

Chain I: 85% 7% 8%

Residue	Category
S440	Green
P441	Green
R442	Green
G448	Yellow
Q508	Green
Q532	Yellow
E537	Yellow
S622	Yellow
V632	Yellow
Q636	Yellow
K652	Yellow
Q656	Yellow
L661	Yellow
G665	Yellow
M666	Yellow
GLU	Grey
GLU	Grey
ASN	Grey
MET	Grey
LEU	Grey
A251	Green
P252	Yellow
S253	Yellow
Q256	Yellow
P257	Yellow
S258	Yellow
P269	Yellow
A273	Yellow
T294	Yellow
R295	Yellow
K296	Yellow
L343	Yellow
S348	Yellow
K358	Yellow
D359	Yellow
G364	Yellow
L380	Yellow
K381	Green
T382	Yellow
S399	Yellow
A400	Yellow
V403	Yellow
L404	Green
L405	Yellow
K423	Green
GLU	Grey
HIS	Grey
LYS	Grey
ALA	Grey
ASP	Grey
THR	Grey
GLN	Grey
GLN	Grey
LEU	Grey
ALA	Grey
ARG	Grey
GLU	Grey
GLY	Grey
PRO	Grey
SER	Grey
ARG	Grey
GLU	Grey
THR	Grey

Chain G:

Met Ser Asp Glu Phe Arg Tyr His His Asp Val Asn Glu Leu Leu Leu Leu Arg Val His His Gly Gly Asp Gly Ala Glu Val Tyr Tle Tle Asp Leu Leu Gln Asn Arg Thr Thr Tyr Val Val Ser His Ala Lys Lys Val Tle Ala Glu Phe Ser Arg Thr Pro

Glu Asp Phe Leu Lys Lys Tyr Asp Glu Leu Lys Ser Ser Lys Leu Asn Thr Arg Asp Pro Val Tyr Leu Ser Lys Thr Glu Thr Leu Gln Tyr Gln Thr Leu Asp Glu Lys Leu Ala Ala Arg Glu Ala Ala Val Gly Ser Ser Thr Thr Ser Tle

Asn Val Pro Ala Ala Ser Leu Lys Ile Ile Ser Glu Met Glu Glu Leu Leu Arg Lys Gln Tyr Glu S448 T149 L150 Q172 A179 E183 A186 D190 F191 L192 Ile Gly Ala Gly Ile Ser Thr Thr Ala Pro Ile Val Leu Leu Arg

Response	Percentage
Doing a good job	70%
Not doing a good job	27%



Response	Percentage
U.S. is a threat to their country's security	51%
U.S. is not a threat to their country's security	46%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	266675	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.796	Depositor
Minimum map value	-0.165	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	485.76, 485.76, 485.76	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.18	0/3190	0.34	0/4446
1	D	0.23	0/3255	0.37	0/4538
1	F	0.24	0/3255	0.36	0/4538
1	H	0.25	0/3251	0.36	0/4533
1	N	0.11	0/3120	0.33	0/4347
1	r	0.08	0/561	0.32	0/782
1	s	0.09	0/571	0.34	0/796
1	t	0.12	0/596	0.42	0/831
1	u	0.13	0/596	0.42	0/831
1	v	0.29	0/640	0.51	0/891
2	O	0.33	0/405	0.39	0/563
2	P	0.30	0/362	0.49	0/504
2	Q	0.12	0/327	0.40	0/455
2	R	0.09	0/327	0.28	0/455
2	S	0.07	0/327	0.20	0/455
2	T	0.15	0/405	0.33	0/563
2	U	0.11	0/405	0.34	0/563
3	V	0.11	0/382	0.28	0/531
3	W	0.11	0/393	0.32	0/548
3	X	0.10	0/388	0.25	0/541
3	Y	0.11	0/387	0.24	0/538
4	Z	0.16	0/1846	0.35	0/2566
5	a	0.12	0/2203	0.40	0/3067
5	b	0.14	0/2232	0.36	0/3107
5	c	0.15	0/2212	0.37	0/3079
5	d	0.15	0/2226	0.37	0/3097
5	e	0.15	0/2212	0.42	0/3079
5	f	0.16	0/2227	0.37	0/3100
5	g	0.15	0/2222	0.37	0/3093
5	h	0.16	0/2227	0.37	0/3100
5	i	0.14	0/2212	0.36	0/3079
5	j	0.13	0/2217	0.34	0/3086
5	k	0.12	0/2212	0.38	0/3079
5	l	0.11	0/2207	0.35	0/3072

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	m	0.10	0/2212	0.37	0/3079
5	n	0.10	0/2257	0.38	0/3142
6	I	0.23	0/3024	0.42	2/4209 (0.0%)
6	K	0.19	0/3034	0.40	1/4223 (0.0%)
7	A	0.17	0/3261	0.39	0/4548
7	C	0.23	0/3241	0.37	0/4520
7	E	0.23	0/3364	0.36	0/4691
7	G	0.23	0/3364	0.36	0/4691
7	M	0.11	0/3300	0.34	0/4602
8	L	0.18	0/4846	0.40	0/6741
9	J	0.21	0/4182	0.42	0/5834
All	All	0.18	0/87683	0.37	3/122133 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	X	0	1
6	I	0	2
6	K	0	3
8	L	0	1
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	79	GLY	N-CA-C	-6.40	98.02	113.18
6	I	80	GLY	N-CA-C	-5.44	101.06	112.04
6	K	79	GLY	N-CA-C	-5.17	100.92	113.18

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	I	442	ARG	Peptide
6	I	665	GLY	Peptide
6	K	249	MET	Peptide
6	K	417	THR	Peptide

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Mol	Chain	Res	Type	Group
6	K	665	GLY	Peptide
8	L	313	THR	Peptide
3	X	637	SER	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	B	3192	0	1417	25	0
1	D	3256	0	1450	19	0
1	F	3256	0	1450	33	0
1	H	3252	0	1447	26	0
1	N	3123	0	1382	19	0
1	r	562	0	254	1	0
1	s	572	0	258	2	0
1	t	597	0	273	2	0
1	u	597	0	273	3	0
1	v	642	0	295	4	0
2	O	406	0	217	3	0
2	P	363	0	185	7	0
2	Q	328	0	153	1	0
2	R	328	0	150	0	0
2	S	328	0	150	1	0
2	T	406	0	217	0	0
2	U	406	0	217	4	0
3	V	384	0	164	1	0
3	W	394	0	169	1	0
3	X	389	0	165	1	0
3	Y	389	0	166	3	0
4	Z	1847	0	848	33	0
5	a	2204	0	971	34	0
5	b	2233	0	984	26	0
5	c	2213	0	976	26	0
5	d	2228	0	981	43	0
5	e	2213	0	976	40	0
5	f	2228	0	982	31	0
5	g	2223	0	980	36	0
5	h	2228	0	982	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	i	2213	0	976	31	0
5	j	2218	0	978	30	0
5	k	2213	0	976	39	0
5	l	2208	0	974	16	0
5	m	2213	0	976	10	0
5	n	2258	0	994	16	0
6	I	3027	0	1327	24	0
6	K	3037	0	1331	22	0
7	A	3264	0	1445	34	0
7	C	3244	0	1438	26	0
7	E	3367	0	1492	15	0
7	G	3367	0	1492	18	0
7	M	3303	0	1464	22	0
8	L	4851	0	2185	35	0
9	J	4186	0	1817	41	0
All	All	87756	0	38997	796	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 6.

All (796) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:MET:HA	1:H:31:TYR:HA	1.56	0.86
4:Z:237:GLU:HA	4:Z:251:GLY:HA2	1.58	0.84
4:Z:36:GLY:HA2	4:Z:67:LEU:HA	1.58	0.83
1:F:24:MET:HA	1:F:31:TYR:HA	1.59	0.83
1:D:24:MET:HA	1:D:31:TYR:HA	1.60	0.83
1:t:4:PRO:O	1:t:6:GLN:N	2.12	0.82
7:M:385:SER:HA	7:M:468:PRO:HA	1.62	0.81
1:B:24:MET:HA	1:B:31:TYR:HA	1.63	0.80
5:a:30:GLY:HA3	5:a:41:ALA:HB2	1.62	0.79
5:e:317:TYR:N	5:e:347:ASN:O	2.16	0.79
5:k:195:LEU:HA	5:k:199:ALA:HB3	1.65	0.78
7:C:262:SER:O	7:C:275:LEU:N	2.18	0.77
5:h:274:THR:O	5:h:375:GLY:N	2.16	0.76
5:i:318:ILE:N	5:i:380:ASN:O	2.18	0.76
7:E:262:SER:O	7:E:275:LEU:N	2.18	0.76
8:L:243:GLY:HA2	7:A:355:TYR:HA	1.68	0.76
5:b:323:ILE:O	5:b:376:LEU:N	2.16	0.75
1:N:642:TYR:O	1:N:646:GLU:N	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:4:GLU:HA	5:k:50:VAL:HA	1.69	0.74
5:g:318:ILE:N	5:g:380:ASN:O	2.21	0.74
5:a:102:ASN:HA	5:a:144:GLY:HA2	1.70	0.73
5:j:318:ILE:N	5:j:380:ASN:O	2.20	0.73
7:A:356:ILE:O	7:A:360:MET:N	2.19	0.73
1:D:277:ASP:O	1:D:281:ASP:N	2.19	0.73
2:P:38:GLY:H	8:L:122:PRO:HA	1.53	0.73
4:Z:36:GLY:N	4:Z:53:TYR:O	2.21	0.73
5:h:53:TYR:O	5:h:61:ILE:N	2.20	0.73
5:g:274:THR:N	5:g:375:GLY:O	2.22	0.72
7:C:264:GLN:N	7:C:273:THR:O	2.23	0.72
8:L:369:SER:O	8:L:378:VAL:N	2.23	0.72
1:H:524:SER:O	1:H:528:LEU:N	2.17	0.72
2:P:32:SER:HA	8:L:121:GLY:HA3	1.71	0.72
5:c:323:ILE:O	5:c:376:LEU:N	2.19	0.72
7:G:262:SER:O	7:G:275:LEU:N	2.20	0.71
9:J:822:MET:O	9:J:827:HIS:N	2.24	0.71
5:c:318:ILE:N	5:c:380:ASN:O	2.24	0.71
5:i:274:THR:N	5:i:375:GLY:O	2.23	0.71
5:f:4:GLU:HA	5:f:50:VAL:HA	1.73	0.71
5:k:318:ILE:N	5:k:380:ASN:O	2.24	0.71
1:N:24:MET:HA	1:N:31:TYR:HA	1.73	0.71
5:f:324:ILE:O	5:f:361:SER:N	2.24	0.70
5:k:272:GLY:O	5:k:377:MET:N	2.22	0.70
7:A:164:LYS:O	7:A:168:LYS:N	2.21	0.70
7:A:262:SER:O	7:A:275:LEU:N	2.22	0.70
5:h:318:ILE:N	5:h:380:ASN:O	2.22	0.70
1:v:123:PRO:O	1:v:125:ASP:N	2.20	0.70
1:N:19:GLY:N	1:N:22:ILE:O	2.25	0.70
5:d:107:GLY:HA3	5:d:148:GLY:HA3	1.73	0.70
5:i:323:ILE:O	5:i:376:LEU:N	2.24	0.70
1:u:4:PRO:O	1:u:6:GLN:N	2.25	0.70
5:g:70:GLU:HA	5:g:97:GLY:HA2	1.74	0.70
9:J:263:VAL:N	9:J:299:ASN:O	2.19	0.70
4:Z:36:GLY:O	4:Z:53:TYR:N	2.19	0.70
5:f:272:GLY:N	5:f:377:MET:O	2.25	0.69
5:l:409:ARG:HA	5:l:415:LYS:HA	1.74	0.69
1:N:515:ILE:O	1:N:520:LEU:N	2.24	0.69
5:l:317:TYR:HA	5:l:381:HIS:HA	1.74	0.69
5:e:141:ILE:N	5:e:171:VAL:O	2.19	0.69
1:F:524:SER:O	1:F:528:LEU:N	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:37:ARG:O	4:Z:66:THR:N	2.24	0.69
7:E:264:GLN:N	7:E:273:THR:O	2.25	0.69
5:f:320:ILE:O	5:f:357:GLN:N	2.26	0.69
5:k:30:GLY:HA3	5:k:41:ALA:HB2	1.73	0.69
5:k:46:ASP:HA	5:k:245:TYR:HA	1.75	0.69
5:d:317:TYR:HA	5:d:381:HIS:HA	1.74	0.69
6:I:294:THR:O	6:I:296:LYS:N	2.25	0.69
9:J:791:LEU:HA	9:J:892:LEU:H	1.57	0.68
2:P:37:THR:N	8:L:121:GLY:O	2.17	0.68
5:d:324:ILE:O	5:d:361:SER:N	2.26	0.68
5:c:5:ILE:N	5:c:50:VAL:O	2.26	0.68
5:i:325:GLN:N	5:i:374:SER:O	2.23	0.68
1:B:203:PHE:O	1:B:223:ARG:N	2.26	0.68
1:B:286:PHE:O	1:B:290:ILE:N	2.22	0.68
5:d:321:LEU:N	5:d:378:MET:O	2.19	0.68
5:h:272:GLY:N	5:h:377:MET:O	2.27	0.68
5:h:324:ILE:O	5:h:361:SER:N	2.26	0.68
5:i:172:PHE:N	5:i:205:LEU:O	2.23	0.68
1:D:23:LYS:O	1:D:32:LYS:N	2.21	0.68
5:b:53:TYR:O	5:b:61:ILE:N	2.23	0.68
7:A:264:GLN:N	7:A:273:THR:O	2.27	0.68
5:d:323:ILE:O	5:d:376:LEU:N	2.24	0.68
5:e:53:TYR:O	5:e:61:ILE:N	2.24	0.67
5:k:317:TYR:HA	5:k:381:HIS:HA	1.76	0.67
5:d:30:GLY:HA3	5:d:41:ALA:HB2	1.76	0.67
7:C:438:GLU:N	7:C:461:THR:O	2.23	0.67
5:e:321:LEU:N	5:e:378:MET:O	2.19	0.67
5:c:274:THR:N	5:c:375:GLY:O	2.27	0.67
5:d:272:GLY:N	5:d:377:MET:O	2.27	0.67
7:M:157:LYS:HA	7:M:313:TYR:HA	1.74	0.67
5:d:318:ILE:N	5:d:380:ASN:O	2.28	0.67
1:H:277:ASP:O	1:H:281:ASP:N	2.23	0.67
1:H:278:LEU:HA	1:H:282:LEU:HA	1.76	0.67
5:e:317:TYR:HA	5:e:381:HIS:HA	1.75	0.67
5:k:324:ILE:HA	5:k:375:GLY:HA2	1.77	0.66
1:H:21:ASN:O	1:H:34:GLU:N	2.23	0.66
9:J:518:LEU:O	9:J:522:LEU:N	2.29	0.66
5:c:325:GLN:N	5:c:374:SER:O	2.24	0.66
5:a:141:ILE:N	5:a:171:VAL:O	2.28	0.66
1:D:203:PHE:O	1:D:223:ARG:N	2.28	0.66
9:J:471:GLN:N	9:J:489:THR:O	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:399:SER:O	6:I:403:VAL:N	2.29	0.66
5:f:53:TYR:O	5:f:61:ILE:N	2.24	0.66
1:B:620:LEU:O	1:B:624:SER:N	2.28	0.66
5:e:195:LEU:HA	5:e:199:ALA:HB3	1.77	0.66
8:L:367:THR:O	8:L:380:LYS:N	2.28	0.66
7:E:438:GLU:N	7:E:461:THR:O	2.26	0.66
5:h:54:GLN:HA	5:h:60:TYR:HA	1.76	0.66
7:E:651:LYS:O	7:E:655:SER:N	2.29	0.66
1:F:277:ASP:O	1:F:281:ASP:N	2.23	0.66
9:J:541:SER:O	9:J:545:LEU:N	2.18	0.65
5:b:274:THR:N	5:b:375:GLY:O	2.29	0.65
5:g:195:LEU:HA	5:g:199:ALA:HB3	1.77	0.65
1:N:23:LYS:O	1:N:32:LYS:N	2.21	0.65
7:C:164:LYS:HA	7:C:432:TYR:HA	1.77	0.65
1:D:620:LEU:O	1:D:624:SER:N	2.29	0.65
1:B:179:SER:O	1:B:183:LEU:N	2.19	0.65
6:K:400:ALA:O	6:K:405:LEU:N	2.28	0.65
5:h:320:ILE:O	5:h:357:GLN:N	2.28	0.65
1:F:205:ALA:N	1:F:221:THR:O	2.27	0.65
4:Z:238:LYS:N	4:Z:250:ILE:O	2.24	0.65
2:O:56:ASN:O	2:O:60:LEU:N	2.22	0.65
1:D:524:SER:O	1:D:528:LEU:N	2.22	0.65
5:g:323:ILE:O	5:g:376:LEU:N	2.29	0.65
9:J:470:ILE:HA	9:J:490:LEU:HA	1.78	0.65
4:Z:37:ARG:HA	4:Z:52:SER:HA	1.79	0.65
7:G:726:MET:O	7:G:731:GLU:N	2.26	0.65
1:F:203:PHE:O	1:F:223:ARG:N	2.29	0.65
1:v:105:ARG:HA	1:v:108:PRO:N	2.12	0.65
1:F:21:ASN:O	1:F:34:GLU:N	2.24	0.65
5:i:317:TYR:HA	5:i:381:HIS:HA	1.79	0.65
9:J:288:GLN:N	9:J:295:THR:O	2.27	0.65
5:b:324:ILE:O	5:b:361:SER:N	2.28	0.64
5:j:272:GLY:N	5:j:377:MET:O	2.29	0.64
6:K:253:SER:O	6:K:256:GLN:N	2.29	0.64
7:G:263:ALA:HA	7:G:274:PHE:HA	1.78	0.64
5:e:318:ILE:N	5:e:380:ASN:O	2.30	0.64
5:f:35:GLY:O	5:f:60:TYR:N	2.29	0.64
5:m:4:GLU:HA	5:m:50:VAL:HA	1.79	0.64
5:e:324:ILE:O	5:e:361:SER:N	2.27	0.64
5:d:53:TYR:O	5:d:61:ILE:N	2.21	0.64
1:B:524:SER:O	1:B:528:LEU:N	2.20	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:5:ILE:N	5:d:50:VAL:O	2.29	0.64
1:H:203:PHE:O	1:H:223:ARG:N	2.30	0.64
5:b:35:GLY:O	5:b:60:TYR:N	2.30	0.64
6:K:294:THR:O	6:K:296:LYS:N	2.27	0.64
7:C:356:ILE:O	7:C:360:MET:N	2.25	0.64
1:H:620:LEU:O	1:H:624:SER:N	2.30	0.64
4:Z:165:ILE:HA	4:Z:170:ALA:HA	1.79	0.64
5:g:53:TYR:O	5:g:61:ILE:N	2.27	0.64
1:H:205:ALA:N	1:H:221:THR:O	2.29	0.64
5:j:317:TYR:HA	5:j:381:HIS:HA	1.79	0.64
7:A:263:ALA:HA	7:A:274:PHE:HA	1.80	0.64
7:E:263:ALA:HA	7:E:274:PHE:HA	1.80	0.64
5:d:323:ILE:N	5:d:376:LEU:O	2.29	0.64
8:L:345:VAL:N	8:L:382:GLY:O	2.20	0.64
1:F:320:ARG:O	1:F:326:GLN:N	2.28	0.63
5:b:325:GLN:N	5:b:374:SER:O	2.22	0.63
5:k:323:ILE:N	5:k:376:LEU:O	2.32	0.63
1:B:23:LYS:O	1:B:32:LYS:N	2.22	0.63
7:C:263:ALA:HA	7:C:274:PHE:HA	1.78	0.63
7:C:651:LYS:O	7:C:655:SER:N	2.32	0.63
1:B:150:GLY:HA3	1:B:226:MET:HA	1.81	0.63
1:D:278:LEU:HA	1:D:282:LEU:HA	1.80	0.63
5:c:195:LEU:HA	5:c:199:ALA:HB3	1.80	0.63
5:e:53:TYR:N	5:e:61:ILE:O	2.25	0.63
5:f:318:ILE:N	5:f:380:ASN:O	2.30	0.62
1:D:21:ASN:O	1:D:34:GLU:N	2.27	0.62
9:J:588:ASP:O	9:J:592:ALA:N	2.24	0.62
7:G:264:GLN:N	7:G:273:THR:O	2.30	0.62
1:F:620:LEU:O	1:F:624:SER:N	2.33	0.62
5:j:323:ILE:O	5:j:376:LEU:N	2.29	0.62
5:j:274:THR:N	5:j:375:GLY:O	2.32	0.62
1:F:382:LEU:N	1:F:393:VAL:O	2.30	0.62
5:m:318:ILE:N	5:m:380:ASN:O	2.29	0.62
5:a:270:MET:N	5:a:379:ALA:O	2.30	0.62
5:a:272:GLY:O	5:a:377:MET:N	2.23	0.62
5:f:323:ILE:N	5:f:376:LEU:O	2.29	0.62
5:l:47:ARG:N	5:l:244:ARG:O	2.27	0.62
7:M:264:GLN:N	7:M:273:THR:O	2.25	0.62
7:C:436:MET:O	7:C:463:VAL:N	2.30	0.62
5:j:325:GLN:N	5:j:374:SER:O	2.25	0.62
7:M:707:ALA:HB1	7:M:790:MET:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:453:ASP:O	7:E:457:ASP:N	2.20	0.62
5:e:35:GLY:O	5:e:60:TYR:N	2.31	0.62
5:d:36:ILE:HA	5:d:59:HIS:HA	1.82	0.62
5:c:317:TYR:HA	5:c:381:HIS:HA	1.81	0.62
6:K:604:ASP:O	6:K:608:ALA:N	2.25	0.61
9:J:621:GLU:O	9:J:625:CYS:N	2.33	0.61
5:e:272:GLY:O	5:e:377:MET:N	2.32	0.61
1:N:418:ARG:HA	9:J:74:ILE:HA	1.82	0.61
5:a:409:ARG:HA	5:a:415:LYS:HA	1.81	0.61
5:d:325:GLN:N	5:d:374:SER:O	2.25	0.61
1:H:184:SER:HA	1:H:270:GLU:CB	2.30	0.61
5:n:269:LEU:HA	5:n:380:ASN:HA	1.83	0.61
7:A:412:SER:O	7:A:416:PHE:N	2.21	0.61
2:O:32:SER:O	2:O:36:ASN:N	2.33	0.61
5:f:323:ILE:O	5:f:376:LEU:N	2.31	0.61
5:f:323:ILE:HA	5:f:359:ALA:HB3	1.82	0.61
5:n:166:VAL:O	5:n:200:ASP:N	2.28	0.61
6:I:269:PRO:O	6:I:273:ALA:N	2.27	0.61
5:g:324:ILE:O	5:g:361:SER:N	2.33	0.61
5:g:141:ILE:N	5:g:171:VAL:O	2.22	0.61
7:C:157:LYS:HA	7:C:313:TYR:HA	1.83	0.61
5:n:134:GLY:HA3	5:n:165:LEU:O	1.99	0.61
1:H:214:ARG:O	1:H:218:ASP:N	2.32	0.61
5:n:270:MET:N	5:n:379:ALA:O	2.34	0.61
5:i:272:GLY:N	5:i:377:MET:O	2.34	0.60
4:Z:132:MET:O	4:Z:357:ILE:N	2.34	0.60
4:Z:150:GLY:O	4:Z:165:ILE:N	2.31	0.60
6:I:400:ALA:O	6:I:405:LEU:N	2.32	0.60
5:f:317:TYR:HA	5:f:381:HIS:HA	1.84	0.60
1:v:123:PRO:C	1:v:125:ASP:H	2.07	0.60
8:L:113:LEU:O	8:L:117:LEU:N	2.35	0.60
5:k:53:TYR:O	5:k:61:ILE:N	2.31	0.60
6:K:654:TYR:O	6:K:659:GLY:N	2.22	0.60
9:J:502:LEU:O	9:J:506:LEU:N	2.35	0.60
5:c:53:TYR:O	5:c:61:ILE:N	2.29	0.60
5:m:317:TYR:HA	5:m:381:HIS:HA	1.83	0.60
5:n:317:TYR:N	5:n:347:ASN:O	2.35	0.60
1:F:23:LYS:O	1:F:32:LYS:N	2.29	0.60
5:h:5:ILE:N	5:h:50:VAL:O	2.33	0.60
1:B:205:ALA:N	1:B:221:THR:O	2.29	0.60
7:M:424:TYR:HA	7:M:496:THR:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:385:SER:O	5:c:389:GLU:N	2.21	0.59
5:e:209:ALA:HB2	5:e:306:SER:H	1.66	0.59
6:K:384:PRO:N	6:K:448:GLY:HA3	2.17	0.59
1:D:205:ALA:N	1:D:221:THR:O	2.27	0.59
6:K:6:LEU:O	6:K:10:SER:N	2.36	0.59
9:J:288:GLN:O	9:J:295:THR:N	2.25	0.59
5:f:172:PHE:N	5:f:205:LEU:O	2.35	0.59
1:B:566:LYS:HA	1:B:576:GLY:O	2.03	0.59
2:U:2:ALA:HB1	6:I:44:ARG:HA	1.84	0.59
5:b:323:ILE:N	5:b:376:LEU:O	2.36	0.59
6:I:343:LEU:O	6:I:348:SER:N	2.36	0.59
5:l:53:TYR:N	5:l:61:ILE:O	2.33	0.58
1:B:382:LEU:N	1:B:393:VAL:O	2.33	0.58
4:Z:38:PRO:HA	4:Z:65:LEU:HA	1.85	0.58
5:a:53:TYR:N	5:a:61:ILE:O	2.27	0.58
7:E:397:ASP:O	7:E:401:GLN:N	2.33	0.58
5:e:320:ILE:O	5:e:357:GLN:N	2.34	0.58
5:b:409:ARG:HA	5:b:415:LYS:HA	1.85	0.58
5:e:323:ILE:N	5:e:376:LEU:O	2.32	0.58
5:h:52:PHE:HA	5:h:62:PRO:HA	1.86	0.58
5:k:434:GLU:O	5:k:438:ALA:N	2.34	0.58
5:d:321:LEU:O	5:d:378:MET:N	2.28	0.58
5:g:272:GLY:N	5:g:377:MET:O	2.36	0.58
6:I:382:THR:O	6:I:448:GLY:N	2.36	0.58
2:P:47:CYS:O	2:P:51:CYS:N	2.30	0.58
5:c:172:PHE:N	5:c:205:LEU:O	2.36	0.58
7:A:651:LYS:O	7:A:655:SER:N	2.37	0.58
1:D:559:ARG:HA	1:D:585:GLU:HA	1.86	0.58
5:c:272:GLY:N	5:c:377:MET:O	2.36	0.57
6:I:20:ASN:O	6:I:24:GLY:N	2.33	0.57
1:H:566:LYS:HA	1:H:576:GLY:O	2.04	0.57
5:e:52:PHE:HA	5:e:62:PRO:HA	1.86	0.57
5:h:323:ILE:HA	5:h:359:ALA:HB3	1.86	0.57
5:n:1:MET:N	1:N:332:HIS:O	2.36	0.57
5:d:10:LEU:HA	5:d:67:LEU:O	2.04	0.57
5:d:323:ILE:HA	5:d:359:ALA:HB3	1.86	0.57
9:J:216:LEU:O	9:J:220:VAL:N	2.33	0.57
5:j:324:ILE:O	5:j:361:SER:N	2.37	0.57
6:I:6:LEU:O	6:I:10:SER:N	2.38	0.57
4:Z:252:ASN:O	4:Z:256:ARG:N	2.21	0.57
4:Z:369:ILE:O	4:Z:373:LYS:N	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:334:PHE:O	9:J:338:GLN:N	2.32	0.57
5:f:321:LEU:O	5:f:378:MET:N	2.30	0.57
5:i:323:ILE:N	5:i:376:LEU:O	2.35	0.57
1:D:163:GLY:HA3	7:C:315:GLN:HA	1.85	0.56
5:g:4:GLU:HA	5:g:50:VAL:HA	1.87	0.56
5:g:5:ILE:N	5:g:50:VAL:O	2.24	0.56
5:b:289:THR:O	5:b:293:VAL:N	2.30	0.56
5:k:1:MET:N	6:K:371:ALA:HB1	2.20	0.56
4:Z:8:LEU:N	4:Z:102:PRO:O	2.30	0.56
5:h:323:ILE:O	5:h:376:LEU:N	2.28	0.56
1:B:116:SER:HA	8:L:232:LEU:H	1.69	0.56
9:J:237:HIS:O	9:J:241:ASN:N	2.34	0.56
4:Z:72:GLU:N	4:Z:75:ILE:O	2.34	0.56
4:Z:202:THR:O	4:Z:206:ARG:N	2.32	0.56
5:m:260:LEU:HA	5:m:319:ALA:HB3	1.86	0.56
6:K:1:MET:O	6:K:5:LEU:N	2.31	0.56
8:L:612:HIS:O	8:L:616:TRP:N	2.39	0.56
1:H:320:ARG:O	1:H:326:GLN:N	2.36	0.56
5:c:324:ILE:O	5:c:361:SER:N	2.38	0.56
5:f:272:GLY:O	5:f:377:MET:N	2.33	0.56
9:J:525:ALA:O	9:J:527:SER:N	2.39	0.56
5:c:326:GLY:N	5:c:361:SER:O	2.33	0.56
5:j:107:GLY:HA3	5:j:148:GLY:HA3	1.87	0.56
5:k:47:ARG:N	5:k:244:ARG:O	2.35	0.56
5:d:274:THR:O	5:d:375:GLY:N	2.26	0.56
3:X:584:LEU:HA	3:Y:584:LEU:H	1.70	0.56
4:Z:35:VAL:HA	4:Z:54:VAL:HA	1.87	0.56
1:N:337:LEU:O	1:N:341:LEU:N	2.21	0.56
5:d:274:THR:N	5:d:375:GLY:O	2.35	0.56
7:G:248:ASP:O	7:G:252:VAL:N	2.33	0.56
7:A:567:LEU:O	7:A:640:GLY:N	2.39	0.56
5:e:321:LEU:O	5:e:378:MET:N	2.30	0.56
5:d:241:THR:O	5:d:245:TYR:N	2.31	0.56
7:M:356:ILE:O	7:M:360:MET:N	2.30	0.56
1:F:278:LEU:HA	1:F:282:LEU:HA	1.88	0.55
1:H:23:LYS:O	1:H:32:LYS:N	2.25	0.55
5:g:8:LEU:O	5:g:138:CYS:N	2.24	0.55
7:A:385:SER:HA	7:A:469:SER:H	1.71	0.55
5:b:36:ILE:HA	5:b:59:HIS:HA	1.88	0.55
5:j:53:TYR:O	5:j:61:ILE:N	2.25	0.55
1:N:407:VAL:HA	1:N:504:ILE:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:332:ALA:HB1	9:J:338:GLN:HA	1.87	0.55
5:k:11:GLY:N	5:k:67:LEU:O	2.40	0.55
5:k:166:VAL:O	5:k:200:ASP:N	2.32	0.55
4:Z:301:GLY:N	4:Z:335:ARG:O	2.39	0.55
5:e:137:LEU:O	5:e:169:TYR:N	2.31	0.55
6:I:18:THR:N	6:I:26:GLN:O	2.40	0.55
1:D:214:ARG:O	1:D:218:ASP:N	2.35	0.55
1:F:305:LEU:O	1:F:310:SER:N	2.40	0.55
1:F:566:LYS:HA	1:F:576:GLY:O	2.06	0.55
5:c:323:ILE:N	5:c:376:LEU:O	2.36	0.55
7:M:252:VAL:C	7:M:295:ALA:HB1	2.32	0.55
5:h:172:PHE:N	5:h:205:LEU:O	2.40	0.55
5:k:405:LEU:O	5:k:409:ARG:N	2.36	0.55
5:d:10:LEU:N	5:d:138:CYS:O	2.36	0.55
9:J:499:VAL:O	9:J:503:LYS:N	2.41	0.54
9:J:727:GLU:O	9:J:743:GLY:HA3	2.08	0.54
7:A:249:LEU:O	7:A:253:LEU:N	2.31	0.54
4:Z:70:PRO:O	4:Z:77:THR:N	2.32	0.54
1:B:159:TYR:HA	7:A:175:PRO:HA	1.88	0.54
1:D:409:THR:O	1:D:413:MET:N	2.25	0.54
5:h:3:ARG:HA	5:h:131:SER:O	2.07	0.54
5:i:325:GLN:O	5:i:374:SER:N	2.29	0.54
6:K:74:SER:HA	6:K:200:HIS:HA	1.89	0.54
5:b:274:THR:O	5:b:375:GLY:N	2.19	0.54
5:k:241:THR:O	5:k:245:TYR:N	2.35	0.54
7:C:740:ASN:O	7:C:744:ALA:N	2.41	0.54
1:H:318:MET:O	1:H:323:LEU:N	2.40	0.54
5:k:316:CYS:O	5:k:382:THR:N	2.25	0.54
5:l:30:GLY:HA3	5:l:41:ALA:HB2	1.89	0.54
1:F:409:THR:O	1:F:413:MET:N	2.25	0.54
5:a:100:ALA:CB	5:a:148:GLY:HA3	2.38	0.54
2:P:38:GLY:H	8:L:122:PRO:CA	2.20	0.54
6:K:358:LYS:O	6:K:364:GLY:N	2.38	0.54
7:A:319:ALA:HB1	7:A:410:ALA:HB1	1.90	0.53
4:Z:131:ALA:HA	4:Z:358:SER:HA	1.91	0.53
5:n:11:GLY:N	5:n:67:LEU:O	2.41	0.53
1:N:127:THR:O	1:N:131:LYS:N	2.39	0.53
5:c:241:THR:O	5:c:245:TYR:N	2.33	0.53
9:J:471:GLN:O	9:J:489:THR:N	2.37	0.53
5:b:241:THR:O	5:b:245:TYR:N	2.31	0.53
9:J:473:ASN:N	9:J:487:THR:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:55:ALA:N	5:b:59:HIS:O	2.40	0.53
7:E:726:MET:O	7:E:731:GLU:N	2.36	0.53
2:S:76:ALA:HB1	1:s:113:SER:HA	1.90	0.53
5:d:30:GLY:O	5:d:38:GLU:N	2.31	0.53
2:U:10:ALA:HB2	6:I:29:GLN:HA	1.91	0.53
5:b:172:PHE:N	5:b:205:LEU:O	2.40	0.53
5:f:138:CYS:HA	5:f:169:TYR:O	2.08	0.53
5:j:7:THR:O	5:j:65:VAL:N	2.26	0.53
5:d:320:ILE:O	5:d:357:GLN:N	2.35	0.53
7:G:438:GLU:O	7:G:461:THR:N	2.38	0.53
8:L:1577:LYS:N	8:L:1593:CYS:O	2.29	0.53
5:h:274:THR:N	5:h:375:GLY:O	2.38	0.52
1:N:13:VAL:O	1:N:54:GLY:HA3	2.08	0.52
7:G:438:GLU:N	7:G:461:THR:O	2.30	0.52
8:L:588:LEU:O	8:L:592:ALA:N	2.43	0.52
7:M:657:ILE:HA	7:M:751:LEU:HA	1.90	0.52
5:g:274:THR:O	5:g:375:GLY:N	2.27	0.52
5:i:317:TYR:O	5:i:348:PHE:HA	2.09	0.52
5:d:8:LEU:O	5:d:138:CYS:N	2.28	0.52
8:L:311:TYR:O	8:L:314:GLU:N	2.40	0.52
5:a:141:ILE:H	5:a:171:VAL:C	2.16	0.52
5:g:55:ALA:N	5:g:59:HIS:O	2.42	0.52
5:j:241:THR:O	5:j:245:TYR:N	2.34	0.52
2:P:32:SER:CA	8:L:121:GLY:HA3	2.39	0.52
5:i:289:THR:O	5:i:293:VAL:N	2.30	0.52
5:k:291:LEU:HA	5:k:336:SER:HA	1.92	0.52
5:k:324:ILE:O	5:k:361:SER:N	2.42	0.52
7:M:314:GLY:HA2	7:M:432:TYR:CB	2.39	0.52
9:J:535:ARG:O	9:J:539:ARG:N	2.41	0.52
4:Z:11:ASP:N	4:Z:18:LYS:O	2.33	0.52
5:f:321:LEU:N	5:f:378:MET:O	2.24	0.52
5:k:323:ILE:O	5:k:376:LEU:N	2.40	0.52
1:B:162:THR:HA	7:A:311:PHE:CB	2.40	0.52
5:d:141:ILE:N	5:d:171:VAL:O	2.30	0.52
6:I:532:GLN:O	6:I:537:GLU:N	2.34	0.52
1:D:479:THR:O	1:D:484:GLU:N	2.43	0.52
5:a:1:MET:N	7:A:558:HIS:O	2.40	0.52
1:r:108:PRO:O	1:r:110:LYS:N	2.43	0.52
9:J:721:ARG:O	9:J:749:LYS:N	2.41	0.52
6:K:20:ASN:O	6:K:24:GLY:N	2.33	0.51
5:j:172:PHE:N	5:j:205:LEU:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:g:168:THR:N	5:g:201:CYS:O	2.40	0.51
5:j:57:ASP:N	5:k:285:VAL:O	2.43	0.51
7:M:468:PRO:O	7:M:472:GLN:N	2.43	0.51
5:b:102:ASN:HA	5:b:144:GLY:N	2.25	0.51
5:i:324:ILE:O	5:i:361:SER:N	2.41	0.51
5:j:434:GLU:O	5:j:438:ALA:N	2.39	0.51
5:m:166:VAL:O	5:m:200:ASP:N	2.38	0.51
4:Z:144:ALA:HB2	4:Z:342:GLY:HA2	1.91	0.51
5:j:323:ILE:N	5:j:376:LEU:O	2.42	0.51
5:d:53:TYR:N	5:d:61:ILE:O	2.32	0.51
1:D:22:ILE:HA	1:D:33:VAL:HA	1.92	0.51
7:E:740:ASN:O	7:E:744:ALA:N	2.44	0.51
5:e:10:LEU:N	5:e:138:CYS:O	2.32	0.51
5:i:323:ILE:HA	5:i:359:ALA:HB3	1.93	0.51
8:L:106:GLU:O	8:L:110:VAL:N	2.40	0.51
2:U:2:ALA:CB	6:I:44:ARG:HA	2.40	0.51
5:g:385:SER:O	5:g:389:GLU:N	2.28	0.51
5:k:326:GLY:N	5:k:361:SER:O	2.44	0.51
7:A:586:ALA:O	7:A:590:SER:N	2.43	0.51
5:a:100:ALA:HB2	5:a:148:GLY:HA3	1.93	0.51
5:g:172:PHE:N	5:g:205:LEU:O	2.44	0.51
5:h:70:GLU:HA	5:h:97:GLY:HA2	1.93	0.51
6:K:343:LEU:O	6:K:348:SER:N	2.43	0.51
5:d:209:ALA:HB2	5:d:306:SER:H	1.75	0.51
5:e:8:LEU:O	5:e:138:CYS:N	2.32	0.50
7:G:571:VAL:H	7:G:637:ALA:HB1	1.76	0.50
9:J:430:SER:O	9:J:434:VAL:N	2.34	0.50
9:J:517:GLN:O	9:J:521:ASN:CB	2.58	0.50
5:a:10:LEU:HA	5:a:67:LEU:O	2.11	0.50
5:a:214:ALA:O	5:a:220:ILE:N	2.33	0.50
6:I:253:SER:O	6:I:256:GLN:N	2.44	0.50
1:H:112:LEU:C	1:H:114:LEU:H	2.19	0.50
5:a:317:TYR:N	5:a:347:ASN:O	2.30	0.50
1:H:205:ALA:O	1:H:221:THR:N	2.29	0.50
5:a:52:PHE:HA	5:a:62:PRO:HA	1.92	0.50
4:Z:20:GLY:HA3	4:Z:28:ARG:H	1.76	0.50
5:h:323:ILE:N	5:h:376:LEU:O	2.39	0.50
1:B:19:GLY:N	1:B:22:ILE:O	2.45	0.50
9:J:723:SER:N	9:J:747:SER:O	2.33	0.50
7:A:341:LEU:O	7:A:346:LEU:N	2.38	0.50
5:c:3:ARG:HA	5:c:131:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:c:141:ILE:N	5:c:171:VAL:O	2.35	0.50
5:i:46:ASP:HA	5:i:244:ARG:O	2.12	0.50
1:F:310:SER:O	1:F:314:HIS:N	2.34	0.49
5:j:320:ILE:O	5:j:357:GLN:N	2.41	0.49
5:k:10:LEU:O	5:k:146:GLY:HA2	2.12	0.49
5:l:209:ALA:HB2	5:l:306:SER:N	2.27	0.49
5:n:6:ILE:O	5:n:136:VAL:N	2.30	0.49
5:n:163:LYS:HA	1:N:439:GLY:HA2	1.94	0.49
7:A:762:LEU:O	7:A:767:LEU:N	2.45	0.49
9:J:522:LEU:O	9:J:524:CYS:N	2.42	0.49
1:F:191:TYR:CB	1:F:266:THR:HA	2.43	0.49
5:k:35:GLY:O	5:k:60:TYR:N	2.45	0.49
7:C:619:ALA:HB1	7:C:624:GLN:C	2.38	0.49
2:U:10:ALA:HB2	6:I:30:ASP:H	1.77	0.49
5:a:48:LYS:O	5:a:52:PHE:N	2.24	0.49
5:f:325:GLN:HA	5:f:361:SER:O	2.13	0.49
5:h:55:ALA:N	5:h:59:HIS:O	2.44	0.49
5:k:14:GLY:CA	5:k:139:HIS:HA	2.42	0.49
1:N:578:THR:O	1:N:582:GLU:N	2.33	0.49
7:A:381:GLY:N	7:A:434:GLU:HA	2.28	0.49
5:h:53:TYR:N	5:h:61:ILE:O	2.40	0.49
8:L:295:ARG:H	9:J:368:THR:CB	2.26	0.49
1:F:341:LEU:HA	1:F:390:GLY:HA3	1.93	0.49
5:a:71:PRO:N	5:a:97:GLY:HA2	2.27	0.49
1:B:214:ARG:O	1:B:218:ASP:N	2.35	0.49
3:W:637:SER:O	3:W:639:ASN:N	2.46	0.49
5:f:322:ASN:O	5:f:359:ALA:N	2.24	0.49
5:n:14:GLY:HA3	5:n:139:HIS:HA	1.95	0.49
7:C:567:LEU:O	7:C:640:GLY:N	2.45	0.49
5:g:53:TYR:N	5:g:61:ILE:O	2.34	0.48
8:L:179:LEU:O	8:L:183:GLU:N	2.46	0.48
8:L:349:GLU:O	8:L:351:GLU:N	2.45	0.48
7:C:567:LEU:HA	7:C:640:GLY:HA3	1.95	0.48
1:D:595:SER:O	1:D:599:MET:N	2.30	0.48
5:a:269:LEU:HA	5:a:380:ASN:HA	1.95	0.48
5:e:4:GLU:HA	5:e:50:VAL:HA	1.94	0.48
1:B:341:LEU:HA	1:B:390:GLY:HA3	1.95	0.48
7:E:381:GLY:HA3	7:E:466:GLN:O	2.13	0.48
5:a:214:ALA:O	5:a:219:HIS:N	2.47	0.48
5:b:282:VAL:O	5:b:370:ALA:HB1	2.14	0.48
5:a:46:ASP:HA	5:a:244:ARG:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:320:ILE:HA	5:e:379:ALA:HA	1.96	0.48
1:B:310:SER:O	1:B:314:HIS:N	2.33	0.48
1:F:22:ILE:HA	1:F:33:VAL:HA	1.94	0.48
1:F:205:ALA:O	1:F:221:THR:N	2.28	0.48
1:F:214:ARG:O	1:F:218:ASP:N	2.35	0.48
1:H:22:ILE:HA	1:H:33:VAL:HA	1.95	0.48
5:a:385:SER:O	5:a:389:GLU:N	2.27	0.48
5:h:272:GLY:O	5:h:377:MET:N	2.36	0.48
1:H:455:GLY:HA2	5:h:448:THR:HA	1.95	0.48
5:e:434:GLU:O	5:e:438:ALA:N	2.36	0.48
6:K:157:VAL:O	6:K:161:SER:N	2.47	0.48
1:F:112:LEU:C	1:F:114:LEU:H	2.22	0.48
1:H:595:SER:O	1:H:599:MET:N	2.35	0.48
4:Z:19:ALA:O	4:Z:28:ARG:N	2.47	0.48
5:e:438:ALA:HA	5:e:443:TYR:CB	2.44	0.48
5:g:241:THR:O	5:g:245:TYR:N	2.41	0.48
5:h:137:LEU:O	5:h:169:TYR:N	2.35	0.48
7:C:161:LEU:N	7:C:312:GLU:O	2.46	0.48
9:J:627:THR:O	9:J:631:THR:N	2.25	0.48
6:I:16:ILE:O	6:I:28:SER:N	2.26	0.48
1:H:25:ASN:N	1:H:30:CYS:O	2.39	0.48
5:c:53:TYR:N	5:c:61:ILE:O	2.41	0.48
5:g:274:THR:C	5:g:375:GLY:H	2.20	0.48
5:f:107:GLY:HA3	5:f:148:GLY:HA3	1.95	0.48
7:A:272:ARG:N	7:A:296:ALA:HB1	2.29	0.48
6:I:632:VAL:O	6:I:636:GLN:N	2.47	0.48
5:e:272:GLY:N	5:e:377:MET:O	2.43	0.47
5:d:35:GLY:O	5:d:60:TYR:N	2.47	0.47
7:E:619:ALA:HB1	7:E:624:GLN:C	2.39	0.47
7:M:157:LYS:HA	7:M:313:TYR:CA	2.44	0.47
5:a:289:THR:O	5:a:293:VAL:N	2.34	0.47
5:b:53:TYR:N	5:b:61:ILE:O	2.38	0.47
5:f:52:PHE:HA	5:f:62:PRO:HA	1.95	0.47
5:i:274:THR:O	5:i:375:GLY:N	2.33	0.47
5:n:259:SER:O	5:n:319:ALA:HB1	2.14	0.47
5:d:195:LEU:HA	5:d:199:ALA:HB3	1.96	0.47
7:A:618:LEU:HA	7:A:767:LEU:O	2.13	0.47
5:f:241:THR:O	5:f:245:TYR:N	2.36	0.47
5:k:8:LEU:O	5:k:138:CYS:N	2.35	0.47
7:G:740:ASN:O	7:G:744:ALA:N	2.48	0.47
8:L:244:LEU:N	7:A:355:TYR:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:k:317:TYR:O	5:k:348:PHE:HA	2.14	0.47
1:B:25:ASN:N	1:B:30:CYS:O	2.38	0.47
1:N:207:ASP:N	1:N:219:LYS:O	2.34	0.47
8:L:349:GLU:O	8:L:352:LEU:N	2.47	0.47
5:g:10:LEU:N	5:g:138:CYS:O	2.41	0.47
5:i:274:THR:C	5:i:375:GLY:H	2.20	0.47
5:j:4:GLU:HA	5:j:50:VAL:HA	1.97	0.47
5:m:55:ALA:HB1	5:n:217:ARG:HA	1.95	0.47
8:L:210:THR:O	8:L:215:PHE:N	2.36	0.47
7:E:436:MET:O	7:E:463:VAL:N	2.41	0.47
1:F:478:ILE:O	1:F:483:LEU:N	2.31	0.47
5:e:325:GLN:HA	5:e:361:SER:O	2.14	0.47
5:j:136:VAL:HA	5:j:167:GLN:O	2.14	0.47
9:J:469:ILE:O	9:J:491:TYR:N	2.30	0.47
7:A:309:SER:HA	7:A:318:HIS:HA	1.96	0.47
5:f:324:ILE:N	5:f:359:ALA:O	2.29	0.47
5:g:321:LEU:N	5:g:378:MET:O	2.24	0.47
5:g:434:GLU:O	5:g:438:ALA:N	2.44	0.47
5:i:324:ILE:HA	5:i:375:GLY:HA2	1.95	0.47
7:G:179:ALA:O	7:G:183:GLU:N	2.43	0.47
1:F:25:ASN:N	1:F:30:CYS:O	2.41	0.47
5:e:5:ILE:N	5:e:50:VAL:O	2.26	0.47
7:A:619:ALA:HB1	7:A:624:GLN:C	2.40	0.47
5:j:195:LEU:HA	5:j:199:ALA:HB3	1.97	0.47
5:k:322:ASN:HA	5:k:377:MET:HA	1.97	0.46
5:i:53:TYR:O	5:i:61:ILE:N	2.36	0.46
5:i:320:ILE:O	5:i:357:GLN:N	2.33	0.46
5:l:52:PHE:HA	5:l:63:ARG:H	1.81	0.46
1:B:493:LYS:O	1:B:497:ALA:N	2.49	0.46
5:d:320:ILE:HA	5:d:379:ALA:HA	1.98	0.46
7:A:610:LEU:H	7:A:642:GLU:CB	2.28	0.46
1:H:337:LEU:O	1:H:341:LEU:N	2.33	0.46
5:b:324:ILE:HA	5:b:375:GLY:HA2	1.97	0.46
5:c:321:LEU:O	5:c:378:MET:N	2.37	0.46
9:J:324:VAL:O	9:J:328:GLN:N	2.48	0.46
1:F:341:LEU:O	1:F:390:GLY:N	2.48	0.46
5:g:325:GLN:HA	5:g:361:SER:O	2.15	0.46
5:i:7:THR:O	5:i:65:VAL:N	2.29	0.46
5:k:11:GLY:HA2	5:k:68:ASP:HA	1.98	0.46
8:L:20:LYS:O	8:L:22:HIS:N	2.49	0.46
5:g:102:ASN:HA	5:g:144:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:i:409:ARG:HA	5:i:415:LYS:HA	1.97	0.46
5:j:317:TYR:N	5:j:347:ASN:O	2.47	0.46
5:l:52:PHE:HA	5:l:62:PRO:HA	1.98	0.46
6:K:269:PRO:O	6:K:273:ALA:N	2.39	0.46
7:G:397:ASP:O	7:G:401:GLN:N	2.39	0.46
5:g:325:GLN:N	5:g:374:SER:O	2.34	0.46
5:i:321:LEU:O	5:i:378:MET:N	2.33	0.46
5:j:4:GLU:O	5:j:132:LEU:HA	2.15	0.46
1:u:1:MET:O	1:u:3:THR:N	2.48	0.46
4:Z:144:ALA:HB2	4:Z:342:GLY:CA	2.46	0.46
5:c:102:ASN:HA	5:c:144:GLY:N	2.31	0.46
5:l:4:GLU:HA	5:l:50:VAL:HA	1.98	0.46
5:d:272:GLY:O	5:d:377:MET:N	2.44	0.46
4:Z:166:TYR:N	4:Z:169:TYR:O	2.31	0.46
5:f:51:PHE:O	5:f:63:ARG:N	2.43	0.46
5:k:14:GLY:HA3	5:k:139:HIS:HA	1.97	0.46
1:t:112:SER:C	1:t:114:TYR:H	2.24	0.46
1:N:179:SER:O	1:N:183:LEU:N	2.35	0.46
7:G:249:LEU:O	7:G:253:LEU:N	2.35	0.46
7:G:701:ALA:O	7:G:705:ALA:N	2.48	0.46
4:Z:240:TYR:N	4:Z:248:ILE:O	2.31	0.46
5:k:104:TRP:CB	5:k:187:ASN:HA	2.46	0.46
5:m:52:PHE:HA	5:m:62:PRO:HA	1.97	0.46
1:B:337:LEU:O	1:B:341:LEU:N	2.30	0.46
7:M:248:ASP:CB	7:M:258:GLY:HA3	2.46	0.46
7:A:248:ASP:O	7:A:252:VAL:N	2.34	0.45
5:a:52:PHE:HA	5:a:63:ARG:H	1.81	0.45
5:c:49:ASP:HA	5:c:52:PHE:O	2.16	0.45
1:B:566:LYS:HA	1:B:576:GLY:C	2.41	0.45
7:E:356:ILE:O	7:E:360:MET:N	2.35	0.45
5:h:317:TYR:O	5:h:348:PHE:HA	2.16	0.45
5:k:351:TRP:O	6:K:662:GLY:HA3	2.17	0.45
5:l:57:ASP:N	5:m:287:LYS:O	2.47	0.45
5:l:320:ILE:O	5:l:356:ILE:HA	2.16	0.45
1:B:249:LEU:O	1:B:255:ASP:N	2.30	0.45
7:G:619:ALA:HB1	7:G:624:GLN:C	2.41	0.45
7:M:262:SER:O	7:M:275:LEU:N	2.31	0.45
5:l:318:ILE:N	5:l:380:ASN:O	2.45	0.45
1:H:19:GLY:N	1:H:22:ILE:O	2.50	0.45
2:P:32:SER:CB	8:L:121:GLY:HA3	2.46	0.45
1:F:493:LYS:O	1:F:497:ALA:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:h:325:GLN:HA	5:h:361:SER:O	2.16	0.45
7:M:316:VAL:H	7:M:434:GLU:CB	2.30	0.45
7:C:164:LYS:HA	7:C:431:PRO:O	2.16	0.45
5:c:70:GLU:HA	5:c:97:GLY:O	2.16	0.45
5:j:317:TYR:O	5:j:348:PHE:HA	2.17	0.45
8:L:553:MET:O	8:L:576:ILE:N	2.26	0.45
5:m:5:ILE:N	5:m:50:VAL:O	2.42	0.45
6:I:359:ASP:HA	6:I:364:GLY:HA3	1.99	0.45
5:j:325:GLN:HA	5:j:361:SER:O	2.16	0.45
5:k:202:VAL:O	5:k:268:PHE:HA	2.17	0.45
5:b:61:ILE:HA	5:b:85:LEU:O	2.18	0.45
5:i:438:ALA:HA	5:i:443:TYR:CB	2.47	0.45
8:L:20:LYS:C	8:L:22:HIS:H	2.26	0.45
7:M:567:LEU:CB	7:M:641:LEU:H	2.30	0.45
5:b:100:ALA:HB3	5:b:144:GLY:HA3	1.99	0.44
5:l:274:THR:O	5:l:375:GLY:N	2.50	0.44
7:G:453:ASP:O	7:G:457:ASP:N	2.31	0.44
7:C:610:LEU:H	7:C:642:GLU:CB	2.30	0.44
5:a:49:ASP:HA	5:a:52:PHE:O	2.17	0.44
5:g:137:LEU:O	5:g:169:TYR:N	2.26	0.44
5:k:10:LEU:O	5:k:14:GLY:HA3	2.17	0.44
4:Z:148:THR:O	4:Z:168:GLY:N	2.29	0.44
5:f:55:ALA:N	5:f:59:HIS:O	2.47	0.44
5:n:53:TYR:O	5:n:61:ILE:N	2.39	0.44
6:K:383:PRO:HA	6:K:448:GLY:HA3	1.98	0.44
7:C:381:GLY:HA3	7:C:466:GLN:O	2.17	0.44
7:A:740:ASN:O	7:A:744:ALA:N	2.50	0.44
7:C:157:LYS:HA	7:C:313:TYR:CA	2.46	0.44
5:f:30:GLY:HA3	5:f:41:ALA:HB2	2.00	0.44
5:f:274:THR:O	5:f:375:GLY:N	2.42	0.44
3:V:584:LEU:H	3:Y:588:GLN:CB	2.30	0.44
7:M:604:ASP:N	7:M:645:SER:O	2.35	0.44
7:C:249:LEU:O	7:C:253:LEU:N	2.35	0.44
9:J:72:PHE:O	9:J:77:ASP:N	2.50	0.44
1:F:12:TYR:O	1:F:17:ILE:N	2.34	0.44
5:e:214:ALA:O	5:e:219:HIS:N	2.50	0.44
5:h:102:ASN:HA	5:h:144:GLY:N	2.32	0.44
5:h:434:GLU:O	5:h:438:ALA:N	2.39	0.44
5:d:172:PHE:N	5:d:205:LEU:O	2.50	0.44
5:d:325:GLN:O	5:d:374:SER:N	2.42	0.44
7:G:604:ASP:O	7:G:645:SER:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:438:GLU:N	7:A:461:THR:O	2.33	0.44
7:E:544:ILE:O	7:E:548:PHE:N	2.50	0.44
7:E:604:ASP:O	7:E:645:SER:N	2.47	0.44
1:D:25:ASN:N	1:D:30:CYS:O	2.41	0.44
5:b:320:ILE:O	5:b:357:GLN:N	2.51	0.44
5:c:319:ALA:O	5:c:380:ASN:N	2.39	0.44
5:g:52:PHE:HA	5:g:63:ARG:H	1.83	0.44
1:N:361:VAL:HA	1:N:366:ALA:HB3	1.99	0.44
1:F:108:GLN:C	1:F:110:VAL:H	2.25	0.44
5:e:49:ASP:HA	5:e:52:PHE:O	2.18	0.44
5:i:138:CYS:HA	5:i:169:TYR:O	2.18	0.44
5:n:7:THR:O	5:n:64:ALA:HA	2.17	0.44
7:C:262:SER:N	7:C:275:LEU:O	2.41	0.44
7:C:341:LEU:O	7:C:346:LEU:N	2.45	0.44
9:J:119:ASP:N	2:Q:19:LEU:O	2.31	0.44
5:g:320:ILE:O	5:g:356:ILE:HA	2.17	0.44
5:i:174:ASN:HA	5:i:208:THR:N	2.33	0.44
1:v:44:ALA:H	2:O:56:ASN:CB	2.31	0.44
6:K:532:GLN:O	6:K:537:GLU:N	2.40	0.44
8:L:346:LEU:HA	8:L:384:HIS:O	2.17	0.44
4:Z:71:ILE:HA	4:Z:76:VAL:HA	1.99	0.43
5:i:325:GLN:HA	5:i:361:SER:O	2.18	0.43
5:l:340:ILE:O	5:l:344:LYS:N	2.51	0.43
5:m:205:LEU:HA	5:m:304:MET:O	2.17	0.43
5:n:252:ASP:O	5:n:256:LEU:N	2.48	0.43
1:D:493:LYS:O	1:D:497:ALA:N	2.51	0.43
4:Z:150:GLY:N	4:Z:165:ILE:O	2.37	0.43
5:a:171:VAL:HA	5:a:205:LEU:O	2.18	0.43
6:K:338:GLU:HA	6:K:551:ARG:O	2.18	0.43
5:d:8:LEU:HA	5:d:65:VAL:O	2.19	0.43
7:C:452:ASN:O	7:C:454:LYS:N	2.50	0.43
4:Z:229:THR:O	4:Z:233:SER:N	2.49	0.43
5:e:209:ALA:HB2	5:e:306:SER:N	2.32	0.43
5:i:53:TYR:N	5:i:61:ILE:O	2.45	0.43
5:i:321:LEU:N	5:i:378:MET:O	2.28	0.43
6:K:421:HIS:N	6:K:441:PRO:O	2.47	0.43
7:M:416:PHE:CB	7:M:503:ILE:H	2.32	0.43
1:D:337:LEU:O	1:D:341:LEU:N	2.30	0.43
5:g:52:PHE:HA	5:g:62:PRO:HA	1.99	0.43
5:j:325:GLN:O	5:j:374:SER:N	2.23	0.43
8:L:371:CYS:N	8:L:376:ALA:O	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:GLN:C	1:H:110:VAL:H	2.27	0.43
5:a:108:PHE:HA	5:a:152:TYR:HA	2.01	0.43
5:e:52:PHE:HA	5:e:63:ARG:H	1.83	0.43
5:d:52:PHE:HA	5:d:62:PRO:HA	2.00	0.43
6:I:380:LEU:HA	6:I:448:GLY:HA3	2.00	0.43
8:L:406:CYS:HA	8:L:481:ALA:HB2	2.00	0.43
7:C:616:ARG:HA	7:C:628:MET:CB	2.48	0.43
4:Z:260:ALA:HA	4:Z:263:GLN:O	2.18	0.43
8:L:365:SER:N	8:L:368:PHE:O	2.51	0.43
7:M:272:ARG:N	7:M:296:ALA:HB1	2.34	0.43
5:e:241:THR:O	5:e:245:TYR:N	2.33	0.43
5:l:325:GLN:N	5:l:374:SER:O	2.42	0.43
5:a:260:LEU:HA	5:a:319:ALA:HB3	2.00	0.43
5:i:385:SER:O	5:i:389:GLU:N	2.27	0.43
5:k:409:ARG:HA	5:k:415:LYS:HA	2.01	0.43
5:d:319:ALA:O	5:d:380:ASN:N	2.38	0.43
7:A:438:GLU:O	7:A:461:THR:N	2.43	0.43
5:a:11:GLY:HA3	5:a:146:GLY:N	2.34	0.43
5:b:10:LEU:HA	5:b:67:LEU:O	2.19	0.43
5:b:272:GLY:N	5:b:377:MET:O	2.52	0.43
1:H:187:TYR:CB	1:H:269:ALA:HB3	2.49	0.42
1:F:337:LEU:O	1:F:341:LEU:N	2.25	0.42
5:a:140:SER:HA	5:a:171:VAL:H	1.85	0.42
5:f:49:ASP:HA	5:f:52:PHE:O	2.18	0.42
7:M:544:ILE:O	7:M:548:PHE:N	2.51	0.42
7:M:602:LYS:O	7:M:647:ASP:N	2.36	0.42
7:A:157:LYS:HA	7:A:313:TYR:CA	2.49	0.42
7:A:437:VAL:HA	7:A:461:THR:O	2.19	0.42
5:b:5:ILE:N	5:b:50:VAL:O	2.53	0.42
5:c:209:ALA:HB2	5:c:306:SER:H	1.84	0.42
5:g:289:THR:O	5:g:293:VAL:N	2.32	0.42
1:N:150:GLY:HA2	1:N:228:PRO:HA	2.01	0.42
7:G:659:ASN:O	7:G:663:LEU:N	2.30	0.42
8:L:1558:LEU:HA	8:L:1564:GLY:HA3	2.02	0.42
7:C:453:ASP:O	7:C:457:ASP:N	2.26	0.42
6:K:399:SER:O	6:K:403:VAL:N	2.45	0.42
5:d:9:GLN:CB	5:d:15:ASN:HA	2.48	0.42
9:J:223:GLN:O	9:J:226:THR:N	2.48	0.42
9:J:531:GLN:C	9:J:533:GLY:H	2.26	0.42
7:G:571:VAL:N	7:G:637:ALA:HB1	2.35	0.42
1:s:112:SER:C	1:s:114:TYR:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:325:GLN:HA	5:d:361:SER:O	2.20	0.42
6:I:358:LYS:O	6:I:364:GLY:N	2.51	0.42
1:F:40:SER:O	1:F:44:ARG:N	2.44	0.42
1:H:341:LEU:HA	1:H:390:GLY:HA3	2.00	0.42
5:a:26:CYS:O	5:a:30:GLY:N	2.53	0.42
5:f:61:ILE:HA	5:f:85:LEU:O	2.20	0.42
5:f:409:ARG:O	5:f:415:LYS:HA	2.20	0.42
5:g:174:ASN:HA	5:g:208:THR:H	1.84	0.42
5:d:322:ASN:O	5:d:359:ALA:N	2.29	0.42
5:c:320:ILE:O	5:c:356:ILE:HA	2.20	0.42
5:e:215:THR:O	5:e:219:HIS:HA	2.19	0.42
1:u:3:THR:O	1:u:4:PRO:C	2.63	0.42
6:I:206:LYS:O	6:I:258:SER:N	2.40	0.42
5:g:323:ILE:N	5:g:376:LEU:O	2.44	0.42
5:k:274:THR:O	5:k:375:GLY:N	2.53	0.42
5:e:51:PHE:O	5:e:63:ARG:N	2.50	0.42
5:l:405:LEU:O	5:l:409:ARG:N	2.44	0.42
9:J:577:ALA:O	9:J:581:LEU:N	2.31	0.42
7:A:157:LYS:HA	7:A:313:TYR:HA	2.02	0.42
5:e:102:ASN:C	5:e:144:GLY:HA3	2.45	0.41
5:e:214:ALA:O	5:e:220:ILE:N	2.37	0.41
5:j:142:ALA:HB2	5:j:173:PRO:CB	2.50	0.41
9:J:472:ARG:HA	9:J:488:TYR:HA	2.01	0.41
5:j:100:ALA:HB3	5:j:144:GLY:C	2.45	0.41
5:j:104:TRP:CB	5:j:187:ASN:HA	2.50	0.41
5:n:438:ALA:HA	5:n:443:TYR:CB	2.50	0.41
4:Z:219:VAL:O	4:Z:308:GLY:HA3	2.19	0.41
5:e:30:GLY:HA3	5:e:41:ALA:HB2	2.02	0.41
5:j:61:ILE:HA	5:j:85:LEU:O	2.20	0.41
1:F:455:GLY:HA2	5:f:448:THR:HA	2.02	0.41
5:g:30:GLY:HA3	5:g:41:ALA:HB2	2.02	0.41
5:e:322:ASN:O	5:e:359:ALA:N	2.33	0.41
1:N:14:PHE:HA	1:N:54:GLY:HA3	2.02	0.41
5:d:3:ARG:HA	5:d:131:SER:O	2.21	0.41
5:d:43:GLU:C	5:d:45:THR:H	2.29	0.41
1:H:493:LYS:O	1:H:497:ALA:N	2.53	0.41
5:e:317:TYR:O	5:e:348:PHE:HA	2.21	0.41
5:j:321:LEU:N	5:j:378:MET:O	2.34	0.41
8:L:311:TYR:HA	9:J:220:VAL:O	2.21	0.41
5:g:209:ALA:HB1	5:g:306:SER:H	1.86	0.41
8:L:1652:SER:HA	8:L:1756:GLY:HA3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:TRP:HA	1:F:194:GLU:O	2.20	0.41
5:a:51:PHE:O	5:a:63:ARG:N	2.50	0.41
5:c:35:GLY:O	5:c:60:TYR:N	2.54	0.41
5:g:8:LEU:N	5:g:136:VAL:O	2.28	0.41
5:i:70:GLU:HA	5:i:97:GLY:HA2	2.03	0.41
5:k:438:ALA:HA	5:k:443:TYR:CB	2.51	0.41
5:d:322:ASN:N	5:d:357:GLN:O	2.36	0.41
7:M:412:SER:O	7:M:416:PHE:N	2.34	0.41
7:M:779:LEU:HA	7:M:857:PHE:HA	2.03	0.41
7:C:544:ILE:O	7:C:548:PHE:N	2.54	0.41
7:A:161:LEU:N	7:A:312:GLU:O	2.53	0.41
6:I:508:GLN:O	6:I:666:MET:HA	2.21	0.41
6:I:652:LYS:O	6:I:656:GLN:N	2.39	0.41
1:F:105:GLU:CB	1:F:117:SER:HA	2.51	0.41
5:e:273:TYR:HA	5:e:376:LEU:HA	2.02	0.41
5:f:4:GLU:O	5:f:133:GLU:N	2.34	0.41
5:a:325:GLN:HA	5:a:361:SER:O	2.20	0.40
5:i:136:VAL:HA	5:i:167:GLN:O	2.21	0.40
1:B:112:LEU:C	1:B:114:LEU:H	2.28	0.40
6:K:385:THR:H	6:K:388:THR:CB	2.34	0.40
8:L:368:PHE:HA	8:L:378:VAL:O	2.21	0.40
9:J:723:SER:O	9:J:747:SER:N	2.26	0.40
5:e:324:ILE:N	5:e:359:ALA:O	2.33	0.40
5:j:35:GLY:O	5:j:60:TYR:N	2.31	0.40
5:k:206:ASP:CB	5:k:306:SER:H	2.34	0.40
5:a:11:GLY:HA3	5:a:146:GLY:HA2	2.04	0.40
5:b:325:GLN:HA	5:b:361:SER:O	2.22	0.40
5:h:138:CYS:HA	5:h:169:TYR:O	2.21	0.40
5:h:317:TYR:HA	5:h:381:HIS:HA	2.03	0.40
1:B:205:ALA:O	1:B:221:THR:N	2.30	0.40
1:N:345:ALA:N	1:N:388:ASP:O	2.48	0.40
5:b:272:GLY:HA2	5:b:304:MET:H	1.86	0.40
5:d:102:ASN:HA	5:d:144:GLY:N	2.37	0.40
7:A:636:LEU:O	7:A:638:LEU:N	2.55	0.40
1:F:19:GLY:N	1:F:22:ILE:O	2.54	0.40
5:a:100:ALA:HB1	5:a:103:ASN:O	2.22	0.40
5:d:100:ALA:HB3	5:d:144:GLY:C	2.46	0.40
3:Y:660:PHE:C	8:L:230:LEU:HA	2.47	0.40
9:J:935:LEU:O	9:J:939:ALA:N	2.55	0.40
6:I:622:SER:CB	6:I:661:LEU:H	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	640/907 (71%)	628 (98%)	12 (2%)	0	100	100
1	D	655/907 (72%)	644 (98%)	11 (2%)	0	100	100
1	F	655/907 (72%)	644 (98%)	11 (2%)	0	100	100
1	H	654/907 (72%)	642 (98%)	12 (2%)	0	100	100
1	N	624/907 (69%)	617 (99%)	7 (1%)	0	100	100
1	r	111/907 (12%)	102 (92%)	5 (4%)	4 (4%)	2	20
1	s	113/907 (12%)	104 (92%)	5 (4%)	4 (4%)	3	20
1	t	118/907 (13%)	103 (87%)	9 (8%)	6 (5%)	1	15
1	u	118/907 (13%)	103 (87%)	8 (7%)	7 (6%)	1	14
1	v	125/907 (14%)	111 (89%)	9 (7%)	5 (4%)	2	18
2	O	80/82 (98%)	80 (100%)	0	0	100	100
2	P	71/82 (87%)	71 (100%)	0	0	100	100
2	Q	64/82 (78%)	64 (100%)	0	0	100	100
2	R	64/82 (78%)	64 (100%)	0	0	100	100
2	S	64/82 (78%)	64 (100%)	0	0	100	100
2	T	80/82 (98%)	80 (100%)	0	0	100	100
2	U	80/82 (98%)	80 (100%)	0	0	100	100
3	V	73/660 (11%)	73 (100%)	0	0	100	100
3	W	77/660 (12%)	76 (99%)	0	1 (1%)	9	41
3	X	76/660 (12%)	75 (99%)	1 (1%)	0	100	100
3	Y	74/660 (11%)	73 (99%)	1 (1%)	0	100	100
4	Z	373/375 (100%)	365 (98%)	8 (2%)	0	100	100
5	a	444/457 (97%)	437 (98%)	7 (2%)	0	100	100
5	b	450/457 (98%)	442 (98%)	8 (2%)	0	100	100
5	c	446/457 (98%)	439 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	448/457 (98%)	440 (98%)	8 (2%)	0	100	100
5	e	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	f	449/457 (98%)	441 (98%)	8 (2%)	0	100	100
5	g	448/457 (98%)	440 (98%)	8 (2%)	0	100	100
5	h	449/457 (98%)	441 (98%)	8 (2%)	0	100	100
5	i	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	j	447/457 (98%)	439 (98%)	8 (2%)	0	100	100
5	k	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	l	445/457 (97%)	438 (98%)	7 (2%)	0	100	100
5	m	446/457 (98%)	438 (98%)	8 (2%)	0	100	100
5	n	455/457 (100%)	448 (98%)	7 (2%)	0	100	100
6	I	606/667 (91%)	586 (97%)	19 (3%)	1 (0%)	43	78
6	K	608/667 (91%)	589 (97%)	15 (2%)	4 (1%)	18	55
7	A	651/930 (70%)	640 (98%)	11 (2%)	0	100	100
7	C	647/930 (70%)	637 (98%)	10 (2%)	0	100	100
7	E	672/930 (72%)	661 (98%)	11 (2%)	0	100	100
7	G	672/930 (72%)	661 (98%)	11 (2%)	0	100	100
7	M	659/930 (71%)	650 (99%)	9 (1%)	0	100	100
8	L	972/1811 (54%)	923 (95%)	45 (5%)	4 (0%)	30	67
9	J	834/1024 (81%)	807 (97%)	23 (3%)	4 (0%)	24	63
All	All	17575/27876 (63%)	17174 (98%)	361 (2%)	40 (0%)	44	78

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	638	VAL
1	r	109	SER
1	s	109	SER
1	s	111	VAL
1	t	5	ASP
1	t	109	SER
1	t	111	VAL
1	u	5	ASP
1	u	111	VAL
1	v	108	PRO

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Mol	Chain	Res	Type
6	K	295	ARG
6	K	447	SER
8	L	351	GLU
6	I	295	ARG
1	r	111	VAL
1	r	113	SER
1	s	113	SER
1	t	6	GLN
1	t	113	SER
1	u	6	GLN
1	u	109	SER
1	u	113	SER
1	v	124	ARG
1	v	125	ASP
6	K	250	LEU
8	L	417	PRO
9	J	221	VAL
1	r	110	LYS
1	t	110	LYS
1	u	110	LYS
8	L	1454	GLN
9	J	223	GLN
9	J	526	GLU
1	s	110	LYS
6	K	445	PRO
1	u	4	PRO
1	v	119	ALA
1	v	123	PRO
8	L	309	GLU
9	J	616	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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	L	2
1	v	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	v	106:ARG	C	107:GLN	N	8.98
1	L	123:PRO	C	124:GLN	N	5.52
1	L	311:TYR	C	312:LEU	N	3.84

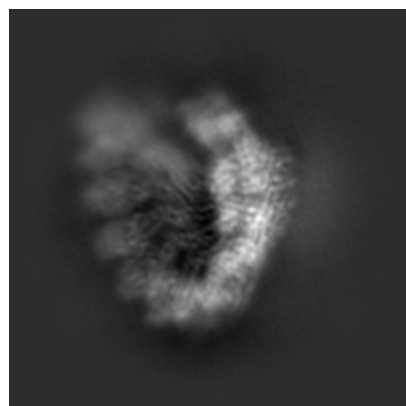
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53400. These allow visual inspection of the internal detail of the map and identification of artifacts.

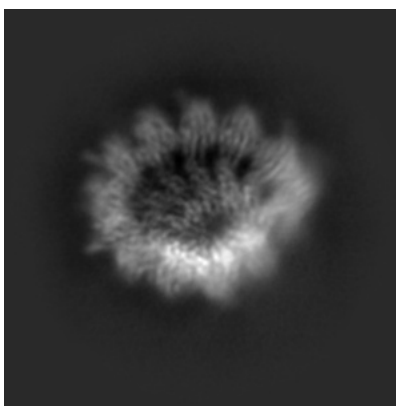
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

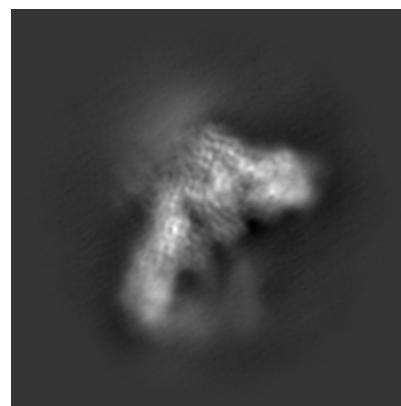
6.1.1 Primary map



X

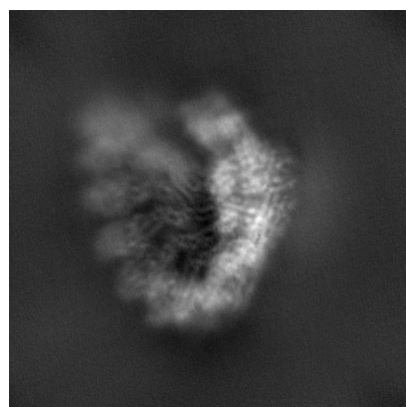


Y

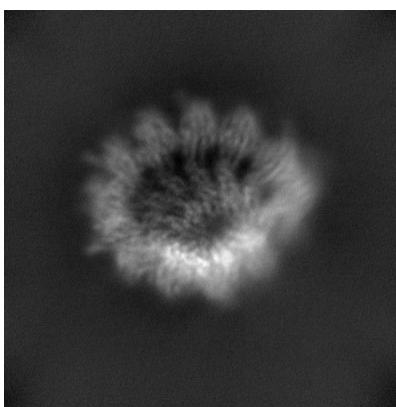


Z

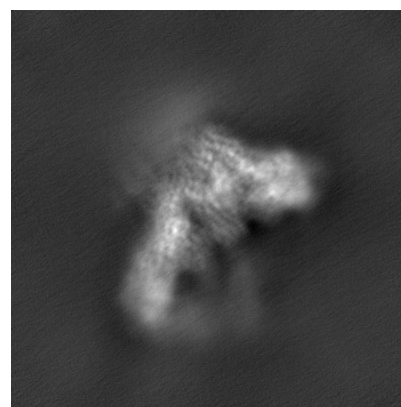
6.1.2 Raw map



X



Y

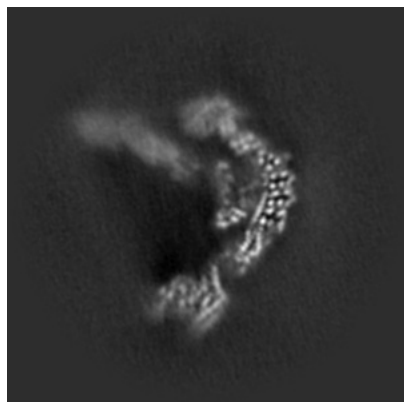


Z

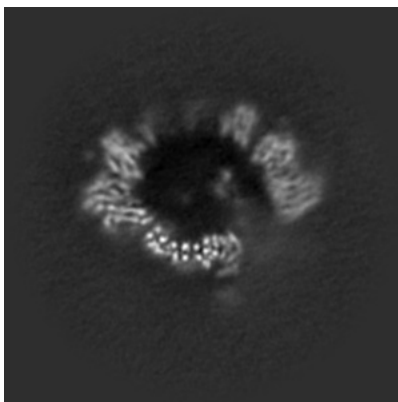
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

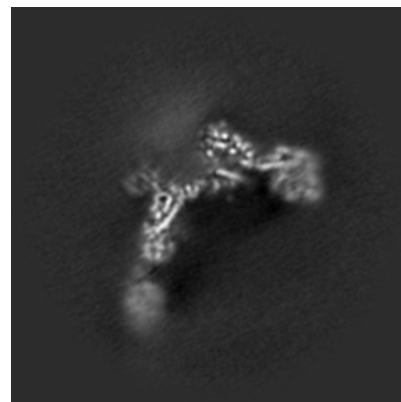
6.2.1 Primary map



X Index: 184

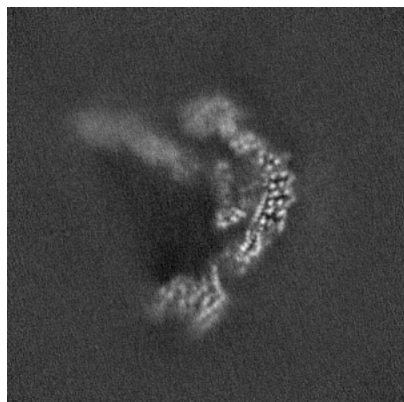


Y Index: 184

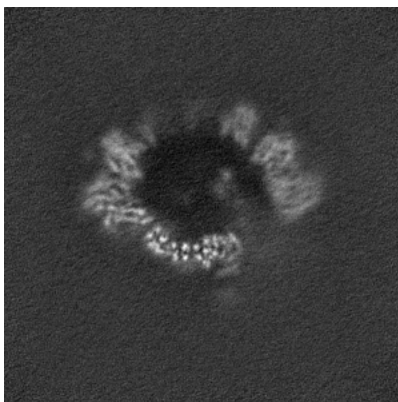


Z Index: 184

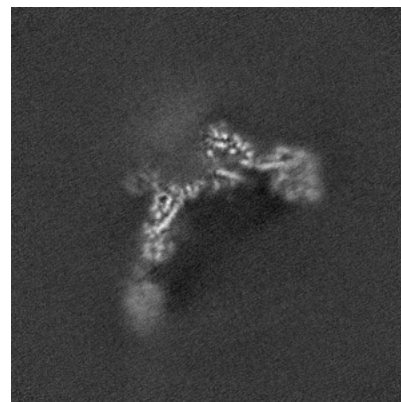
6.2.2 Raw map



X Index: 184



Y Index: 184

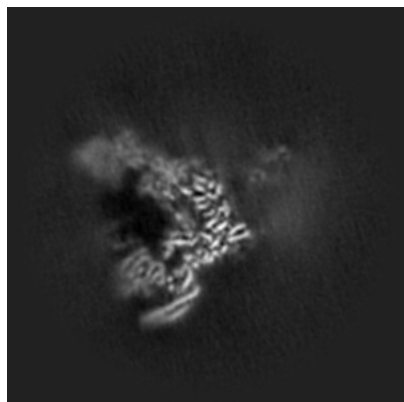


Z Index: 184

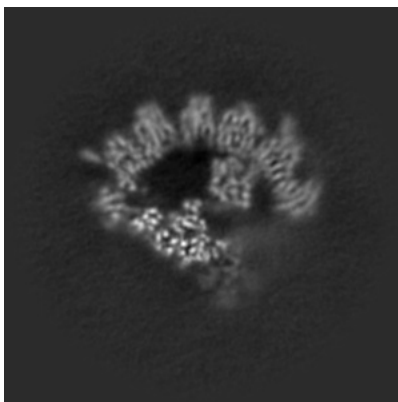
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

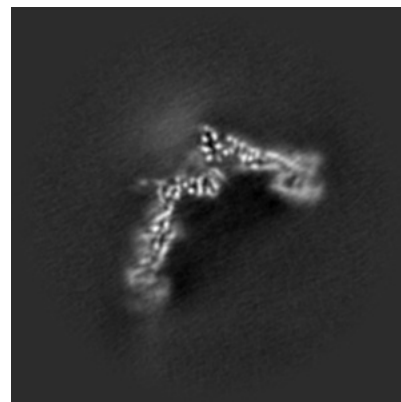
6.3.1 Primary map



X Index: 149

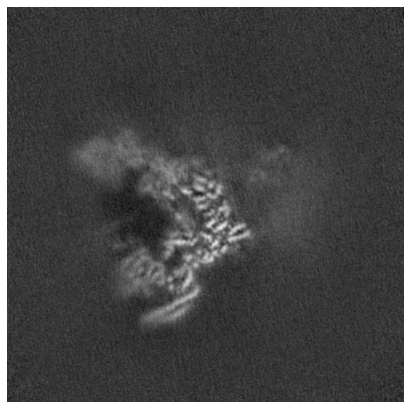


Y Index: 196

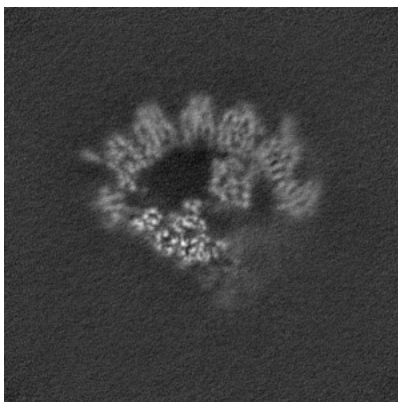


Z Index: 175

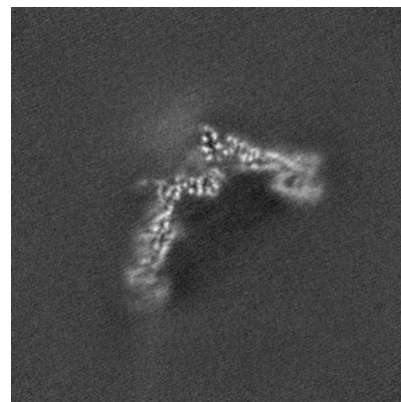
6.3.2 Raw map



X Index: 149



Y Index: 196

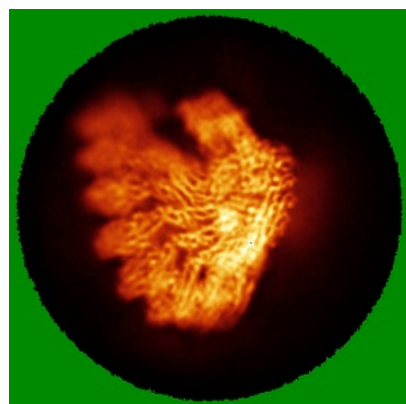


Z Index: 175

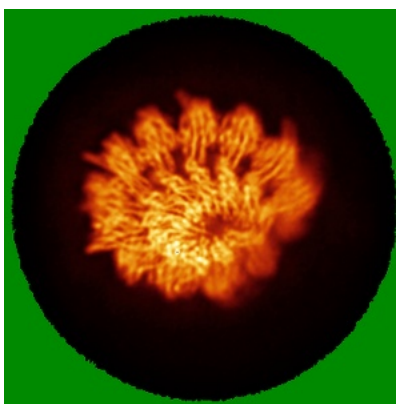
The images above show the largest variance slices of the map in three orthogonal directions.

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

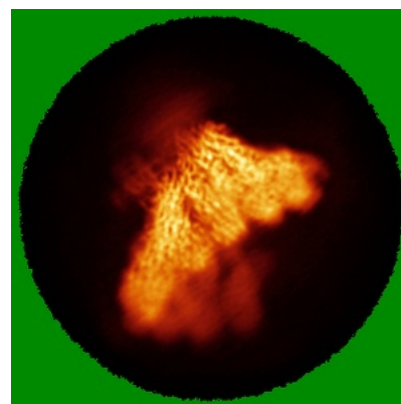
6.4.1 Primary map



X

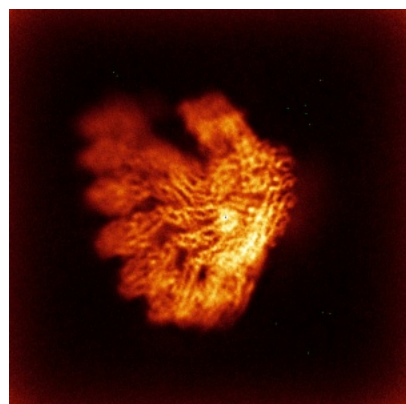


Y

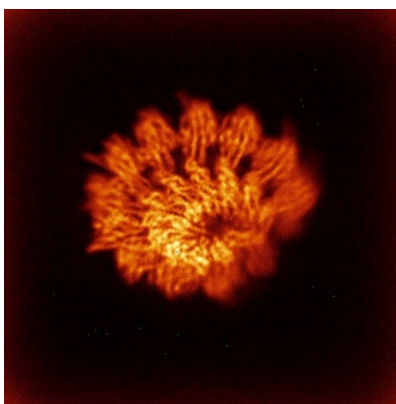


Z

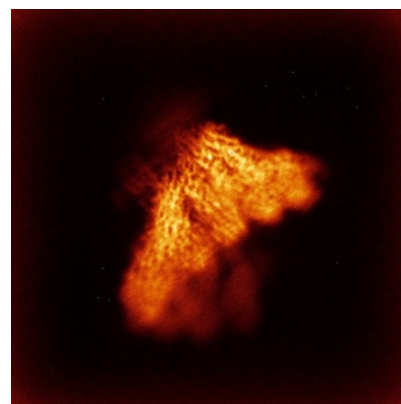
6.4.2 Raw map



X



Y

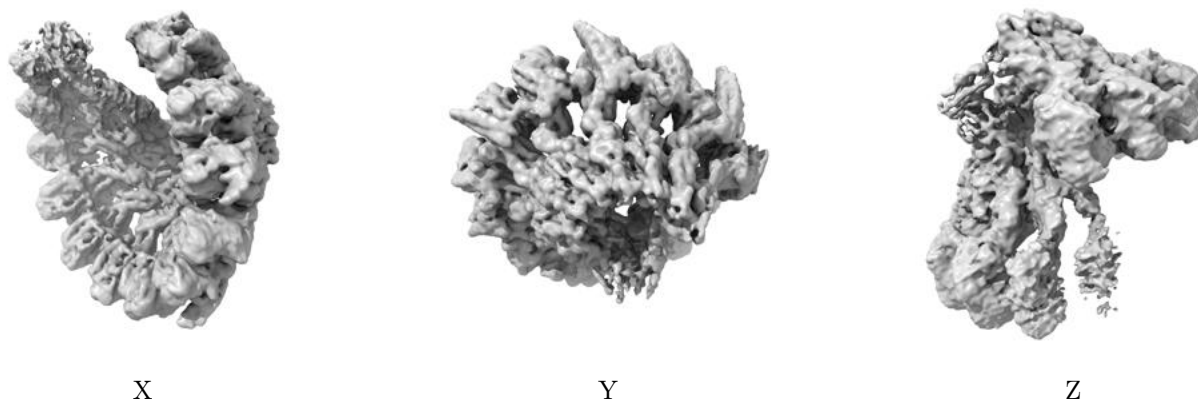


Z

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.

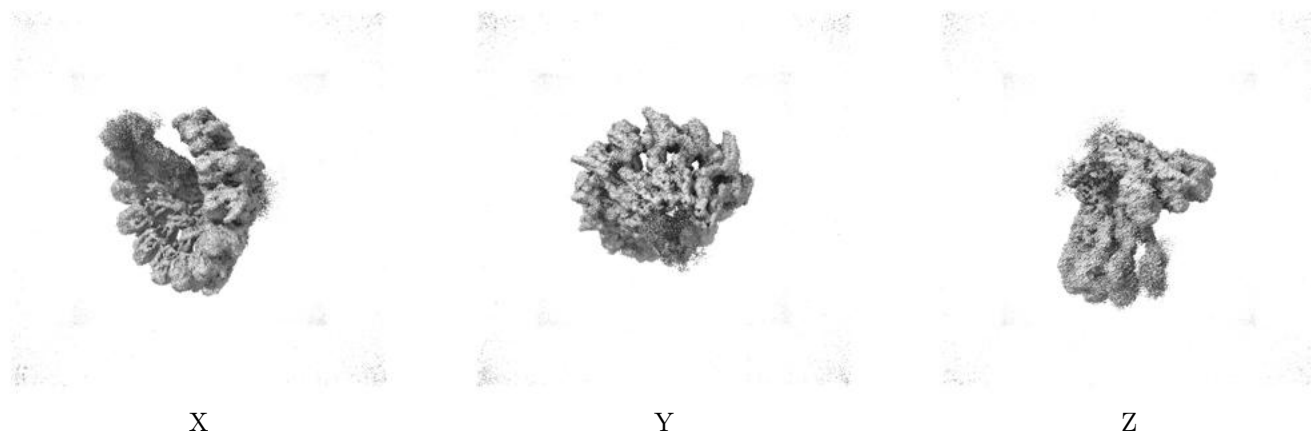
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

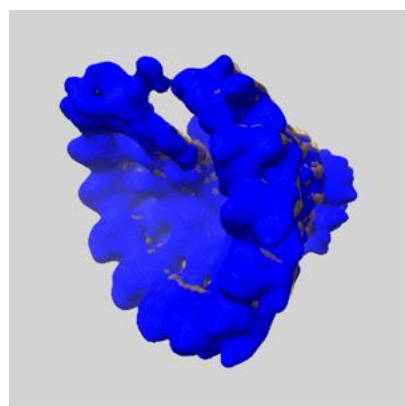
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

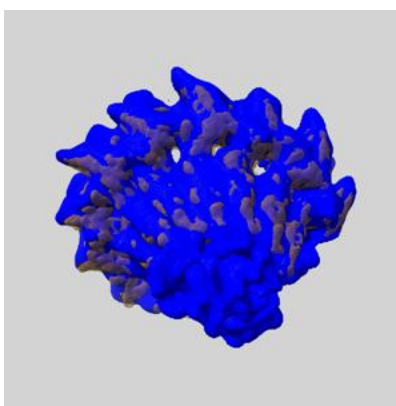
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

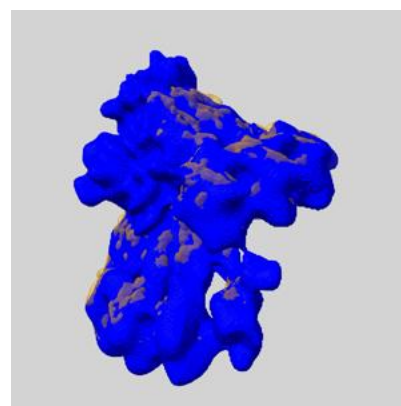
6.6.1 emd_53400_msk_1.map [i](#)



X



Y

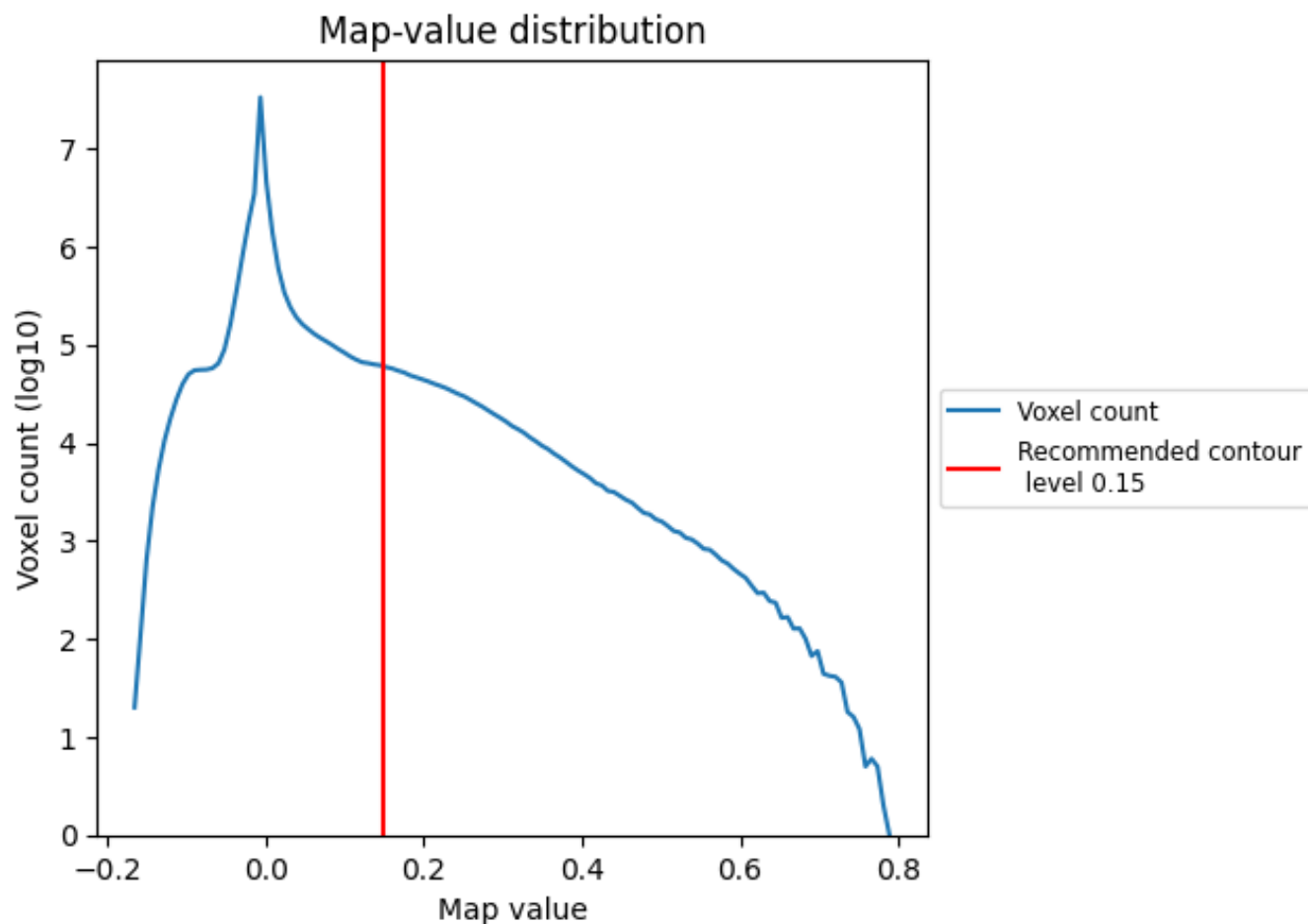


Z

7 Map analysis [i](#)

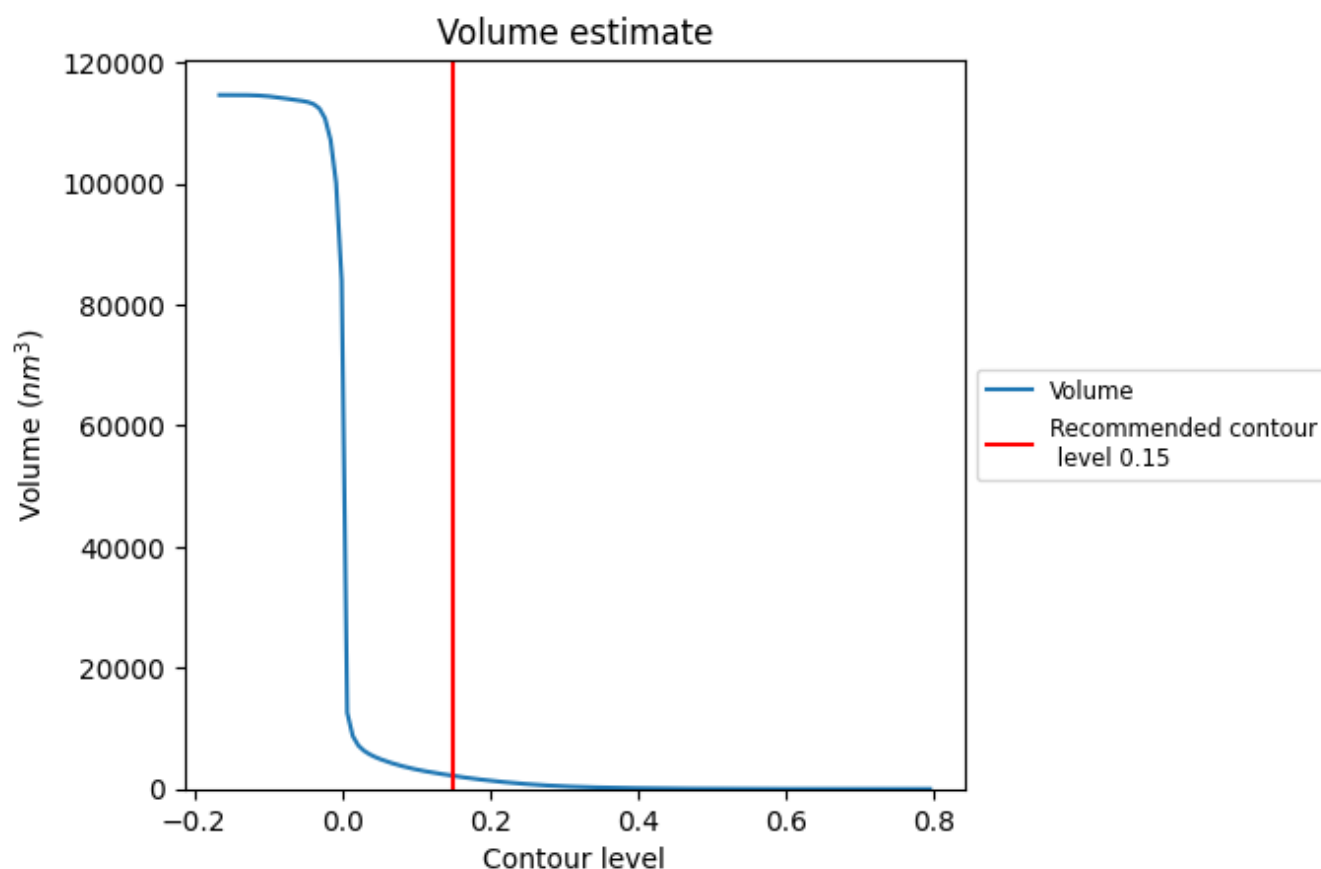
This section contains the results of statistical analysis of the map.

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.

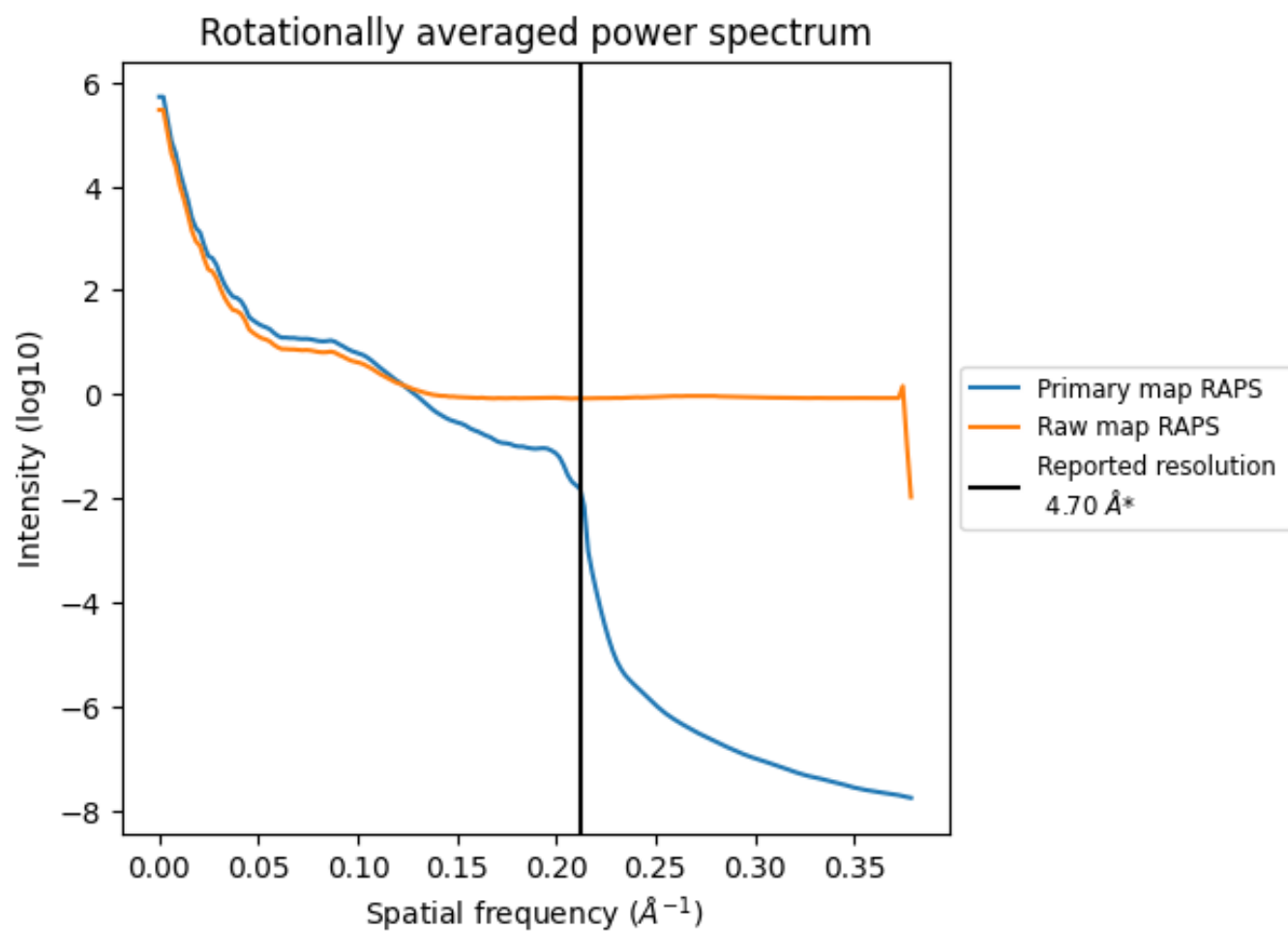
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2190 nm³; this corresponds to an approximate mass of 1978 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](#)

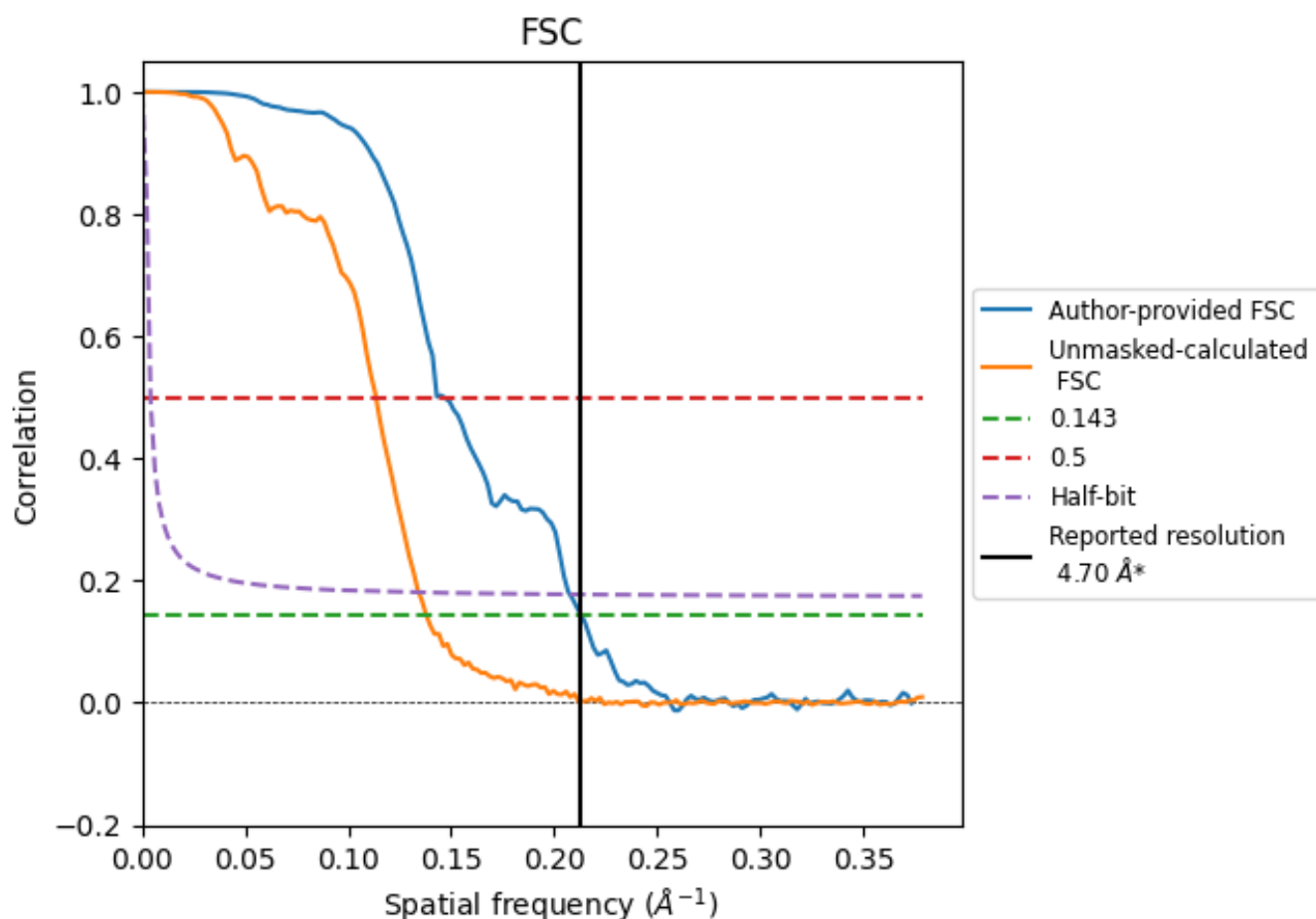


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

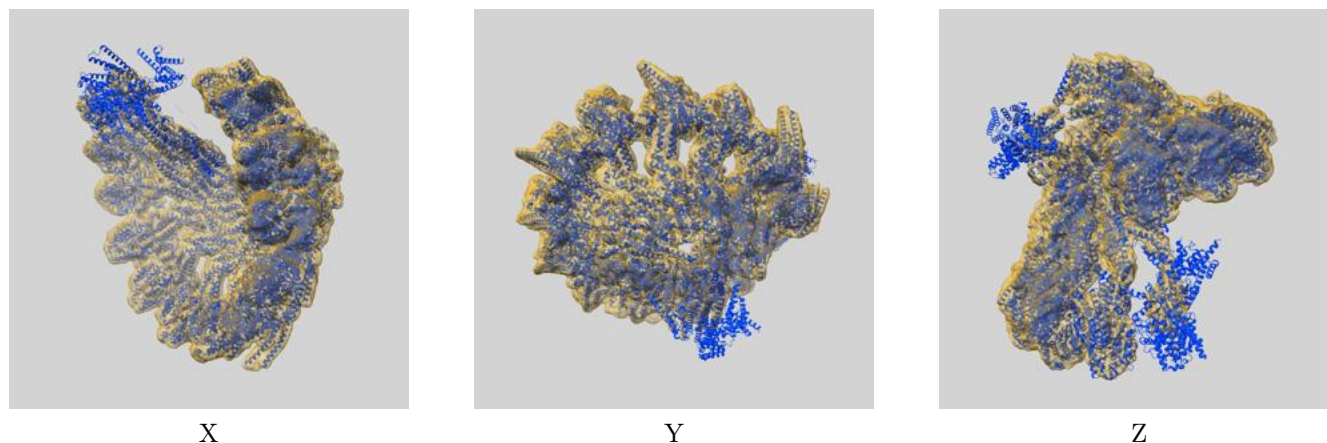
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.69	6.82	4.81
Unmasked-calculated*	7.25	8.80	7.45

*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 7.25 differs from the reported value 4.7 by more than 10 %

9 Map-model fit [i](#)

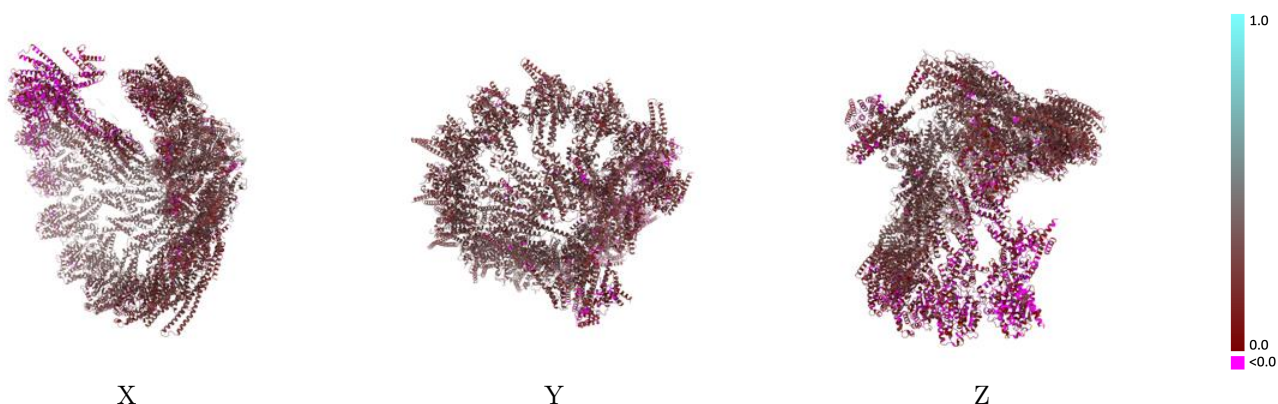
This section contains information regarding the fit between EMDB map EMD-53400 and PDB model 9QVN. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



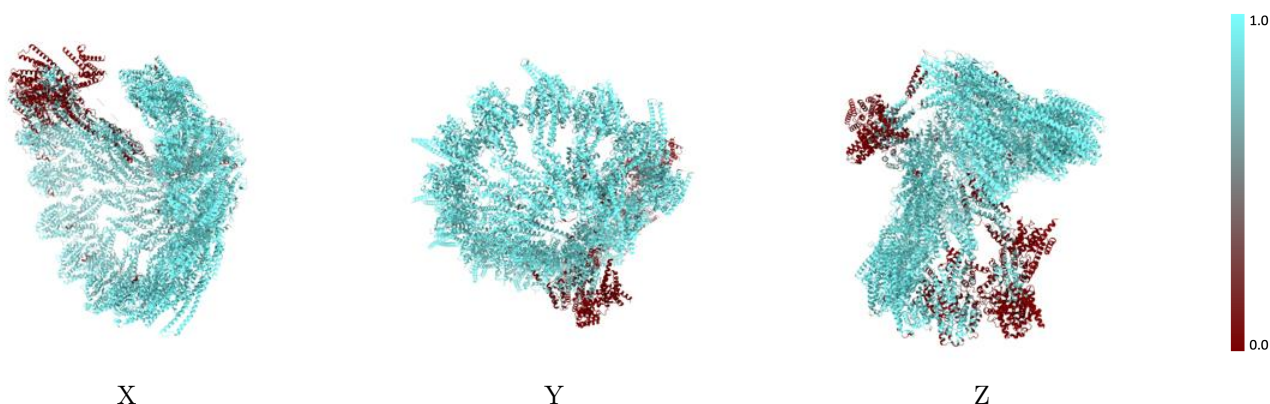
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



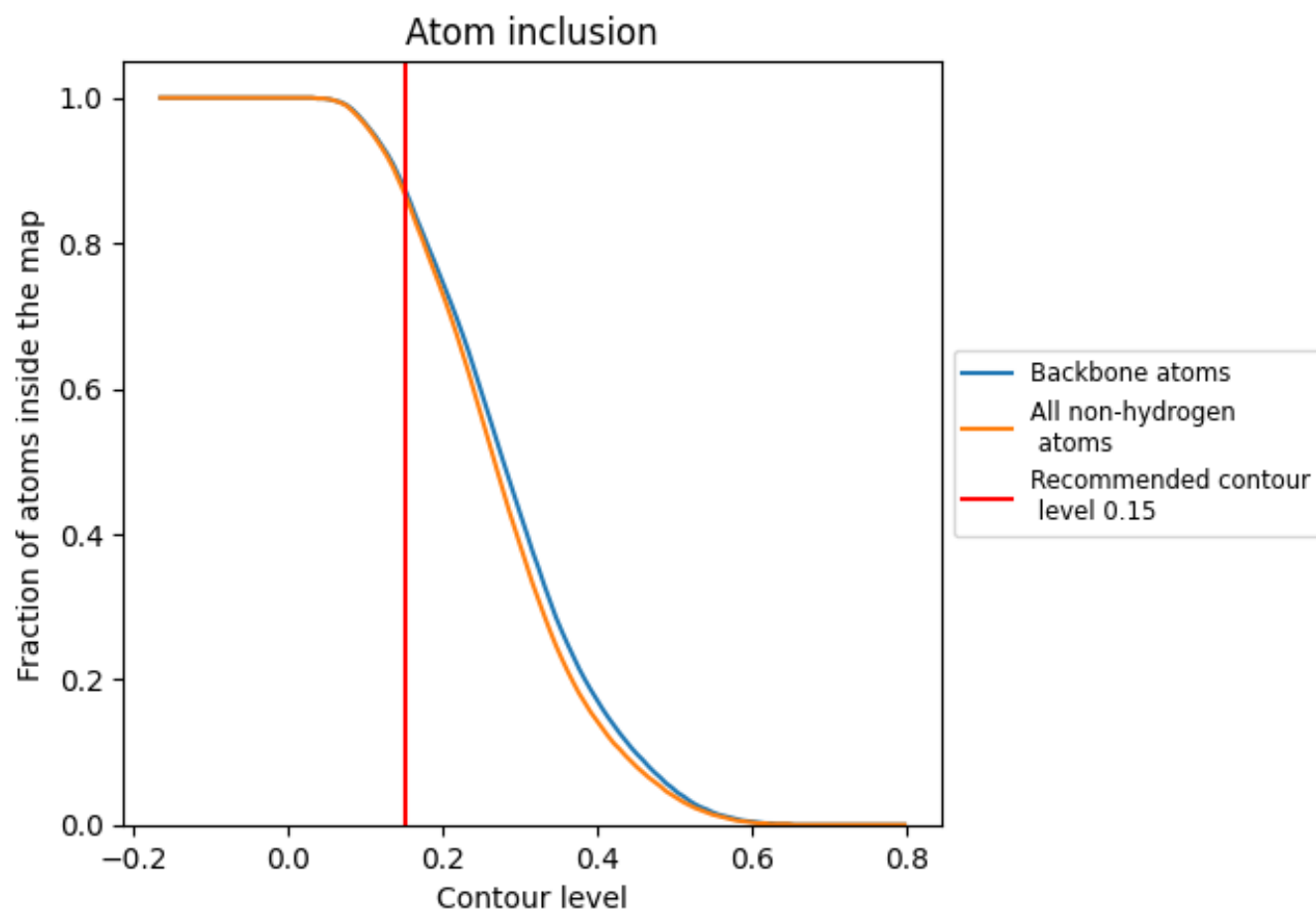
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.2270
A	 0.9740	 0.2350
B	 0.9840	 0.2660
C	 0.9860	 0.2760
D	 0.9860	 0.2780
E	 0.9780	 0.2830
F	 0.9920	 0.2860
G	 0.9860	 0.2790
H	 0.9970	 0.2950
I	 0.9990	 0.2850
J	 0.8500	 0.2510
K	 0.9940	 0.2540
L	 0.9690	 0.2470
M	 0.7240	 0.1350
N	 0.4040	 0.0870
O	 0.8990	 0.2870
P	 0.9810	 0.2800
Q	 0.0000	 0.0710
R	 0.0000	 0.1830
S	 0.0000	 0.1520
T	 0.7780	 0.2340
U	 0.4700	 0.2380
V	 0.5650	 0.2420
W	 0.4310	 0.2260
X	 0.3910	 0.2160
Y	 0.5730	 0.2340
Z	 0.9720	 0.2750
a	 0.9740	 0.1620
b	 0.9840	 0.2180
c	 0.9820	 0.2450
d	 0.9860	 0.2350
e	 0.9890	 0.2280
f	 0.9970	 0.2640
g	 0.9730	 0.2480
h	 0.9920	 0.2820



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Chain	Atom inclusion	Q-score
i	 0.9830	 0.2480
j	 0.9770	 0.2270
k	 0.9720	 0.1480
l	 0.8940	 0.1090
m	 0.5730	 0.0610
n	 0.0860	 0.0490
r	 0.0000	 0.1660
s	 0.0090	 0.1350
t	 0.4120	 0.2310
u	 0.5490	 0.2660
v	 0.9910	 0.3160