Full wwPDB EM Validation Report ⓘ

Jul 8, 2024 – 02:37 am BST

PDB ID	:	7QJ8
EMDB ID	:	EMD-14013
Title	:	Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 3-14, substoichiometric spokes 1-2)
Authors	:	Zupa, E.; Pfeffer, S.
Deposited on	:	2021-12-16
Resolution	:	8.70 Å(reported)
Based on initial models	:	6L81, 6V6S, 7AS4, 6X0U

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:

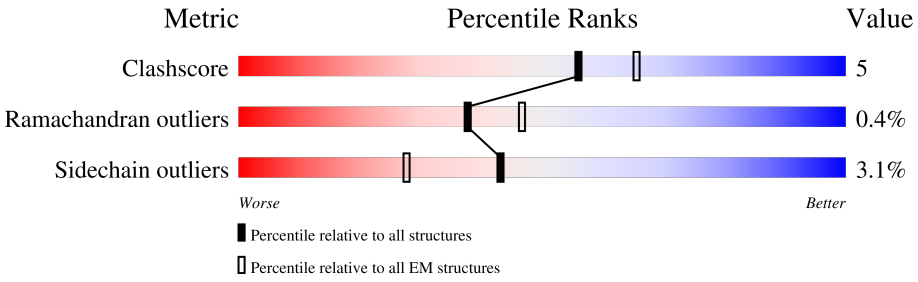
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 8.70 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	J	1024	47% · 48%
1	l	1024	10% 89%
2	1	451	· 69% 22% · 7%
2	2	451	· 70% 21% · 7%
2	Q	451	10% 69% 21% · 7%
2	R	451	6% 70% 21% · 7%
2	S	451	· 70% 21% · 7%
2	T	451	70% 21% · 7%

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Mol	Chain	Length	Quality of chain
2	U	451	70% 21% 7%
2	V	451	71% 21% 7%
2	W	451	71% 20% 7%
2	X	451	71% 21% 7%
2	Y	451	69% 22% 7%
2	Z	451	70% 21% 7%
3	e	375	46% 95%
4	b	82	9% 79% 21%
4	d	82	17% 71% 28%
4	i	82	13% 78% 21%
4	k	82	5% 79% 21%
4	m	82	79% 21%
5	D	907	58% 6% 36%
5	F	907	57% 8% 34%
5	H	907	61% 5% 35%
5	N	907	59% 6% 35%
5	a	907	13% 87%
5	h	907	11% 89%
5	j	907	12% 88%
6	C	902	60% 8% 31%
6	E	902	61% 9% 29%
6	G	902	66% 5% 29%
6	M	902	62% 8% 29%
7	I	667	70% 7% 22%
7	K	667	76% 8% 16%

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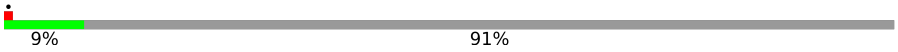
Mol	Chain	Length	Quality of chain
8	L	1819	
8	c	1819	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 108354 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Gamma-tubulin complex component 5.

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

- Molecule 2 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	2	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	Q	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	R	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	S	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	T	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	U	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	V	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	W	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	X	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	Y	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
2	Z	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		

- Molecule 3 is a protein called actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	364	Total	C	N	O	S	0	0
			2847	1803	476	548	20		

- Molecule 4 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
4	i	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
4	k	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
4	m	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
4	d	59	Total	C	N	O	S	0	0
			454	281	79	90	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
5	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		
5	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		
5	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
5	N	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
5	h	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
5	j	107	Total	C	N	O	S	0	0
			843	533	156	152	2		

- Molecule 6 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
6	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		

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

- Molecule 7 is a protein called Gamma-tubulin complex component 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	521	Total 4225	C 2737	N 720	O 750	S 18	0	0
7	K	562	Total 4579	C 2964	N 781	O 816	S 18	0	0

- Molecule 8 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	566	Total 4587	C 3000	N 773	O 789	S 25	0	0
8	c	158	Total 1220	C 771	N 209	O 232	S 8	0	0

- Molecule 9 is water.

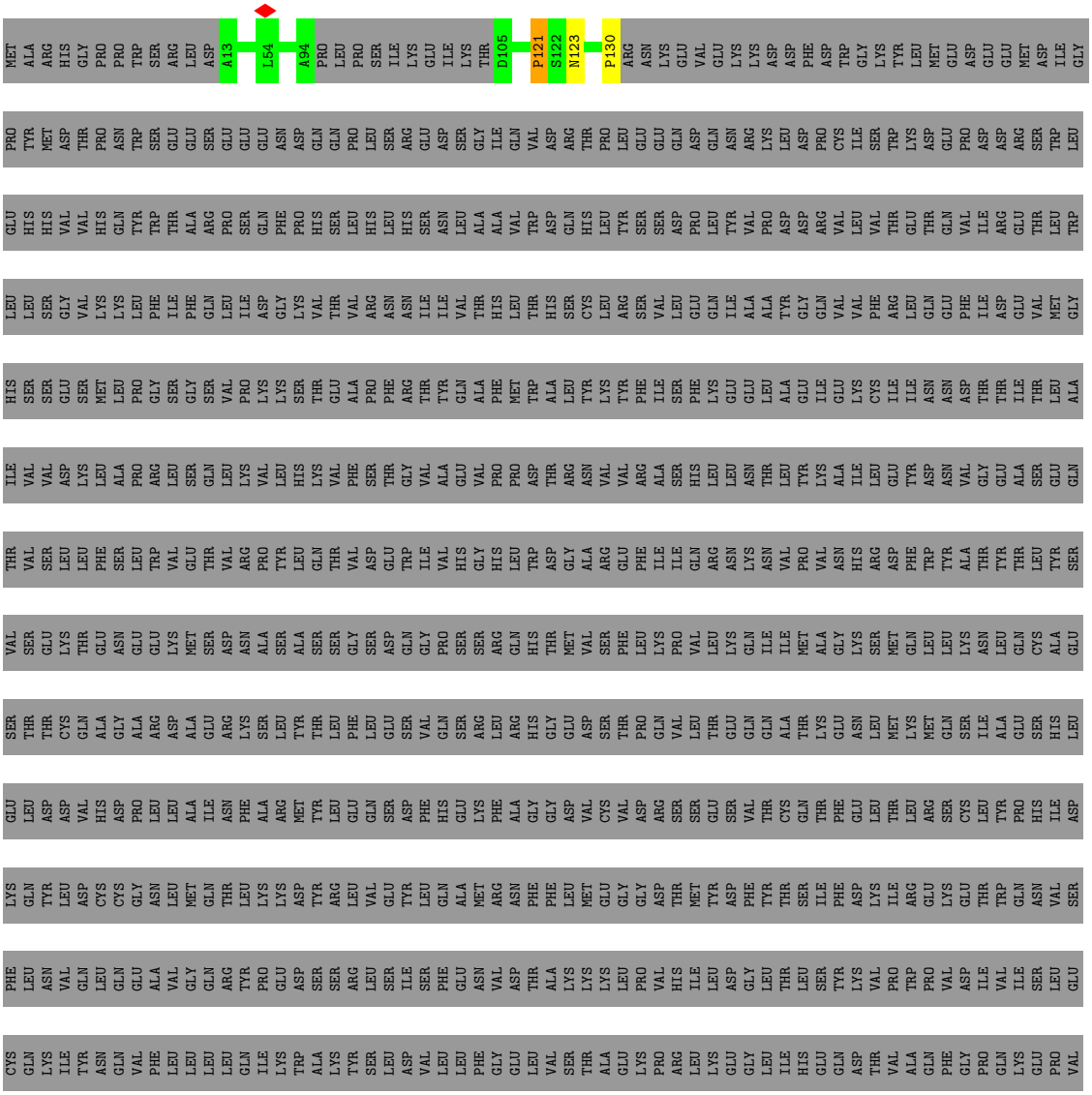
Mol	Chain	Residues	Atoms		AltConf
9	l	5	Total 5	O 5	0
9	m	1	Total 1	O 1	0

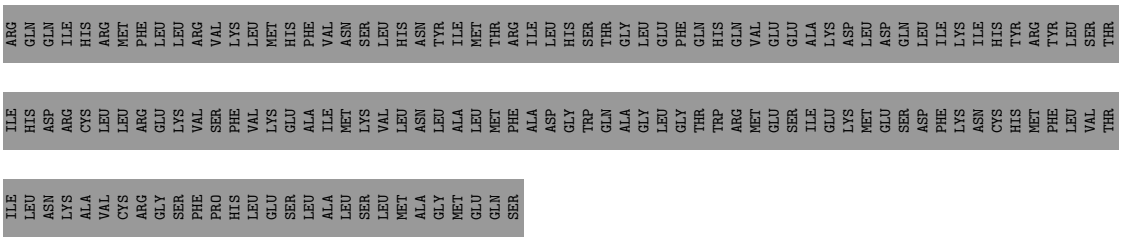
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Gamma-tubulin complex component 5

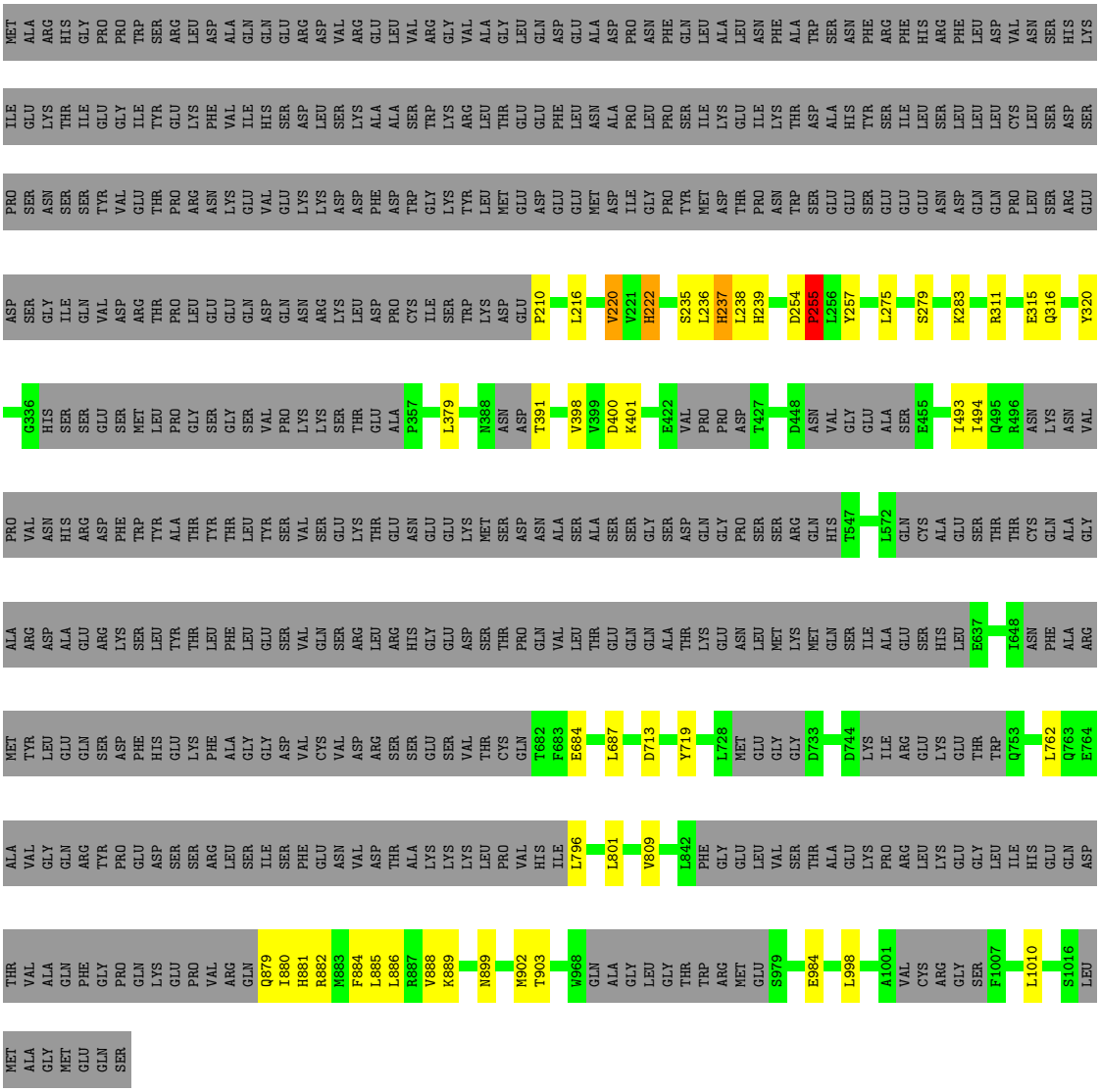
Chain l:





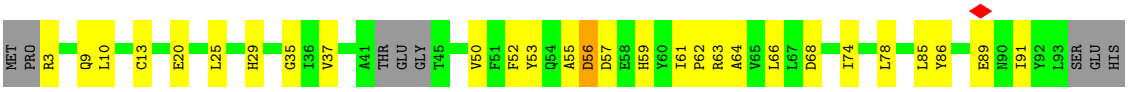
• Molecule 1: Gamma-tubulin complex component 5

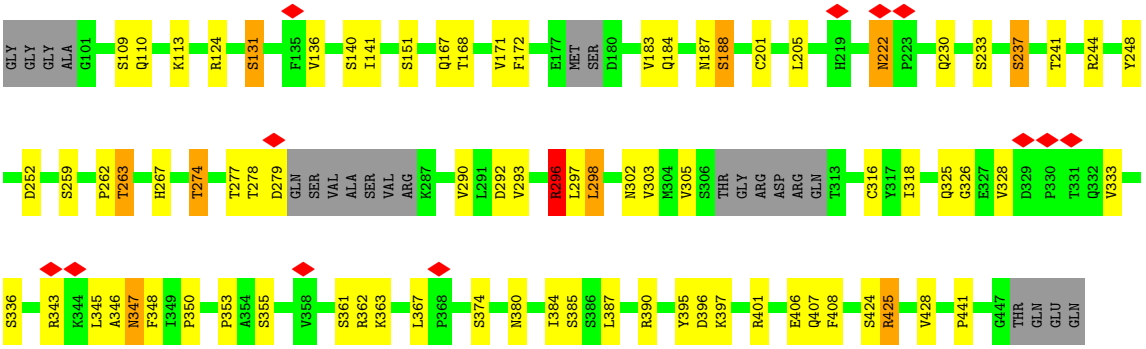
Chain J:



• Molecule 2: Tubulin gamma-1 chain

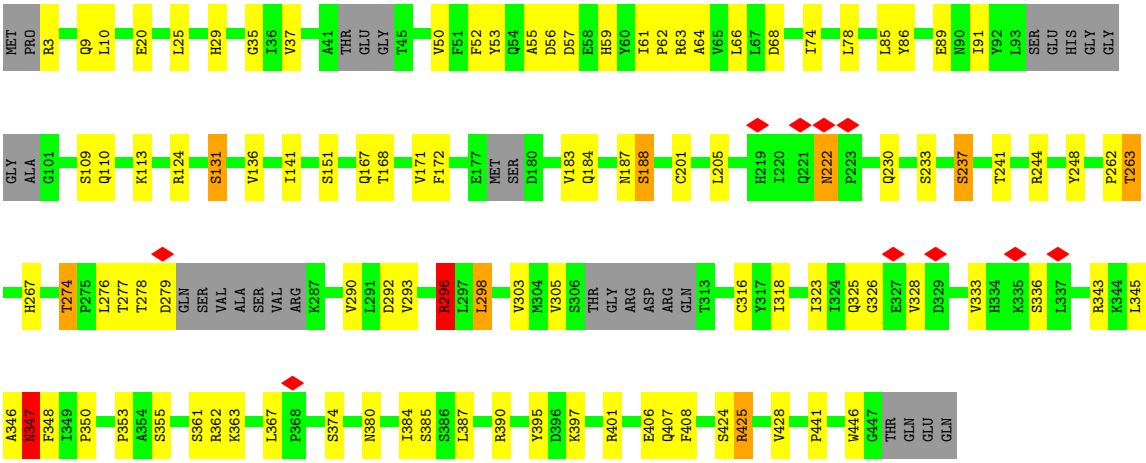
Chain 1:





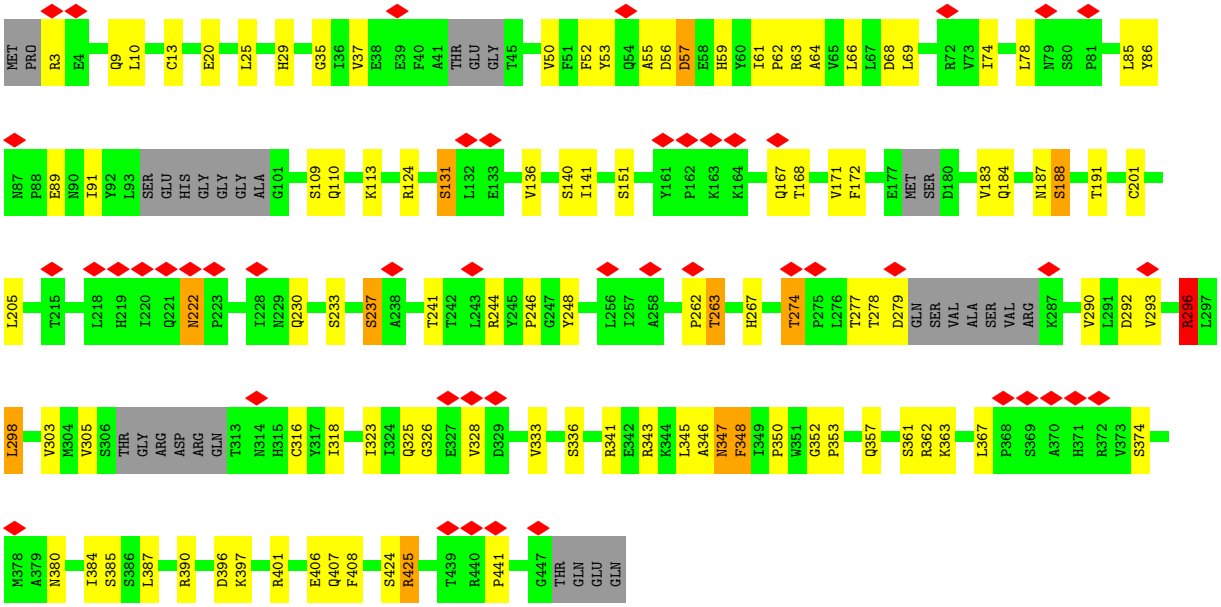
• Molecule 2: Tubulin gamma-1 chain

Chain 2:



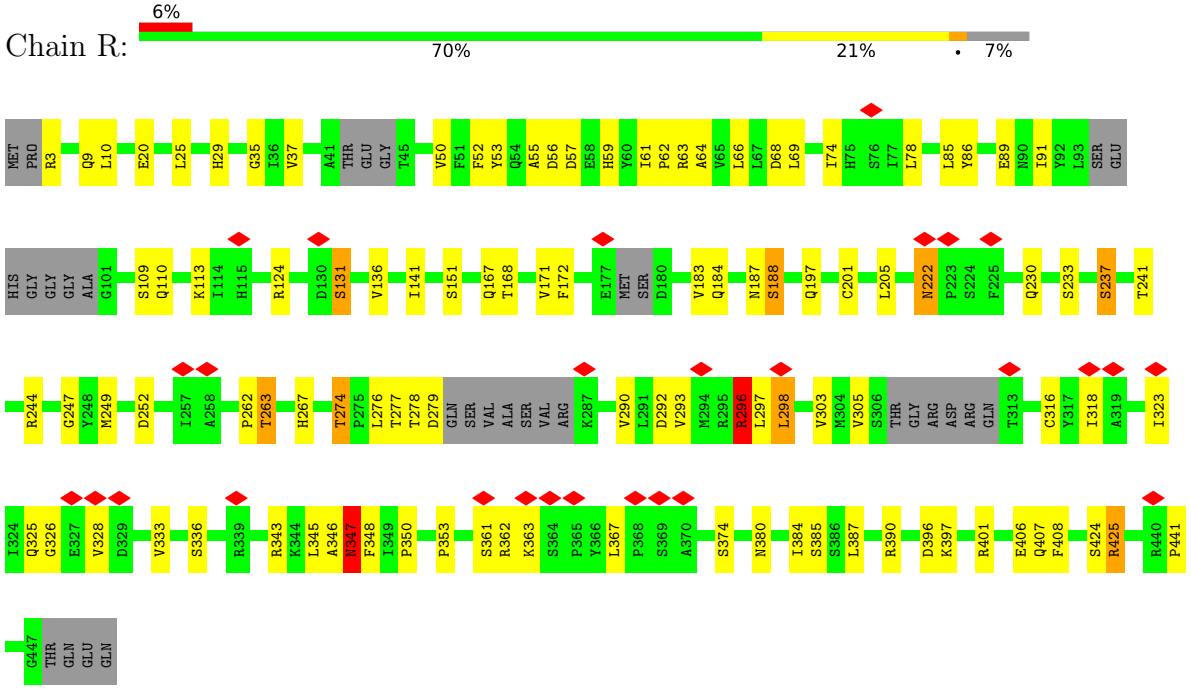
• Molecule 2: Tubulin gamma-1 chain

Chain Q:



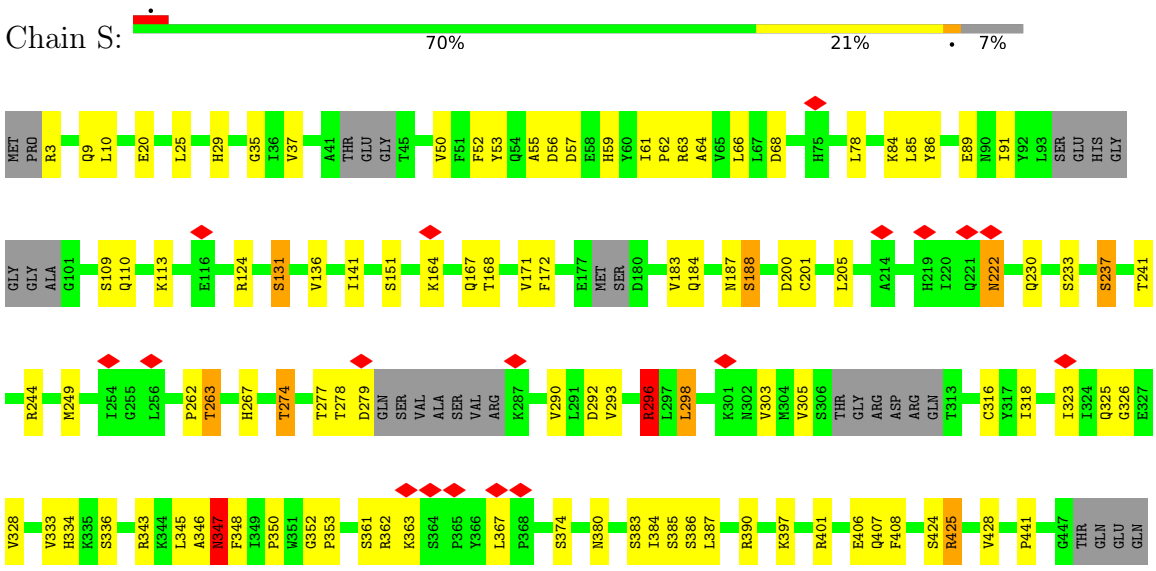
• Molecule 2: Tubulin gamma-1 chain

Chain R:



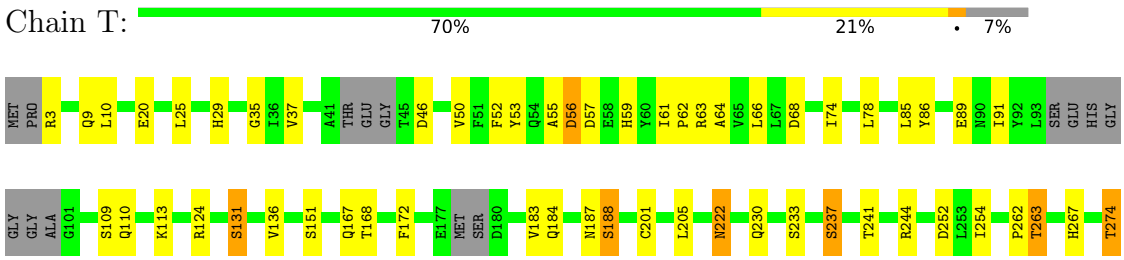
• Molecule 2: Tubulin gamma-1 chain

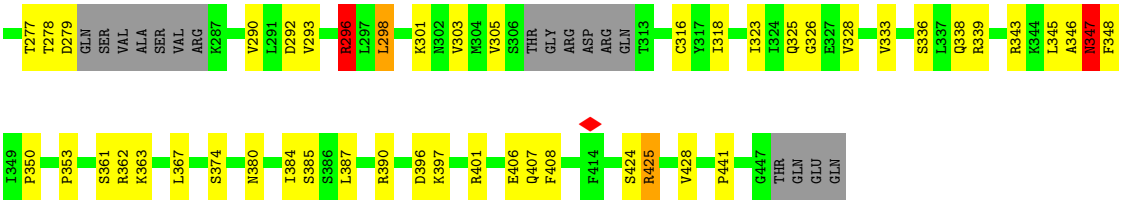
Chain S:



• Molecule 2: Tubulin gamma-1 chain

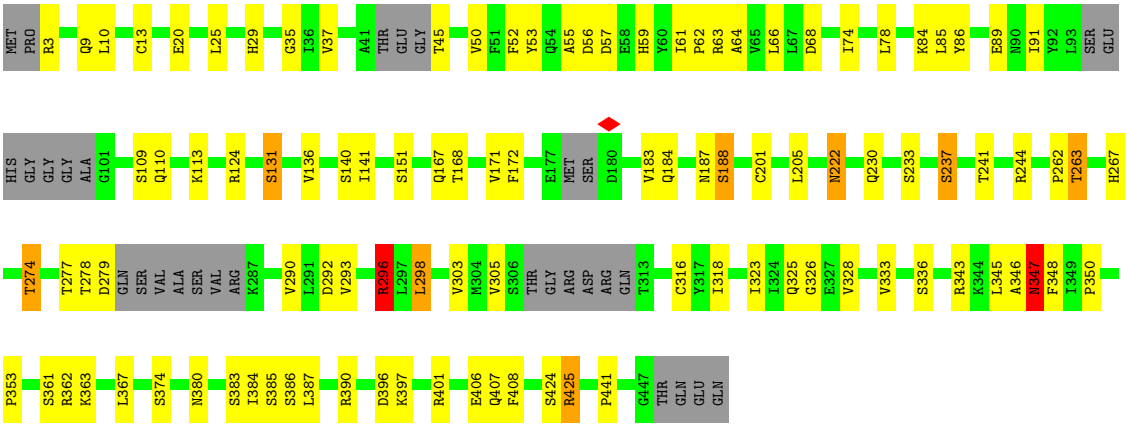
Chain T:





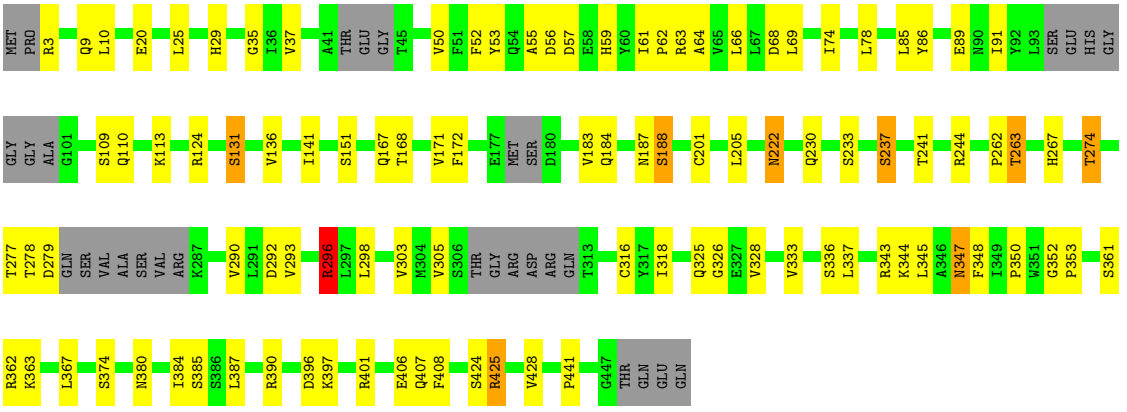
• Molecule 2: Tubulin gamma-1 chain

Chain U:



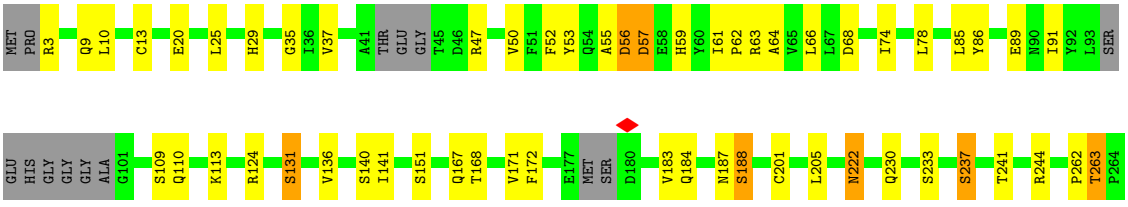
• Molecule 2: Tubulin gamma-1 chain

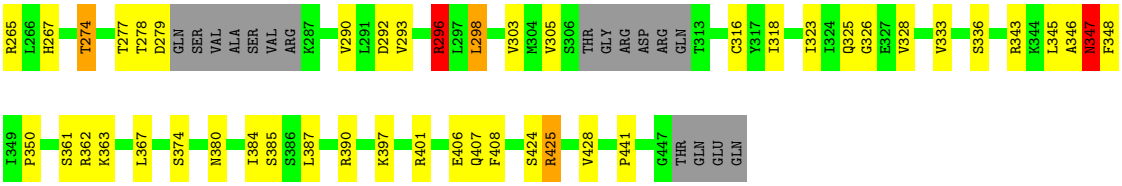
Chain V:



• Molecule 2: Tubulin gamma-1 chain

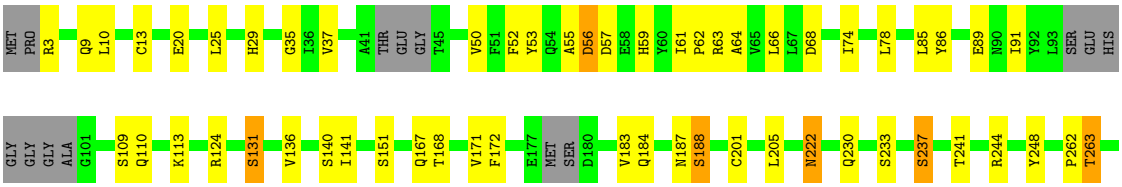
Chain W:

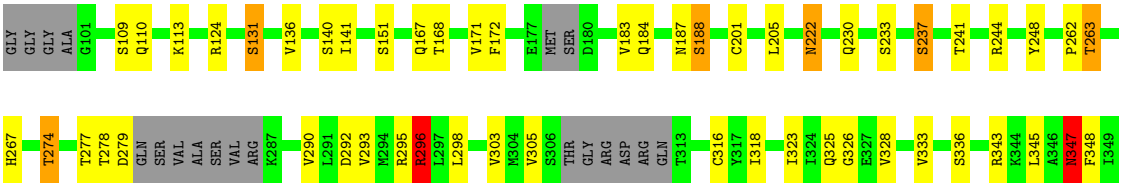


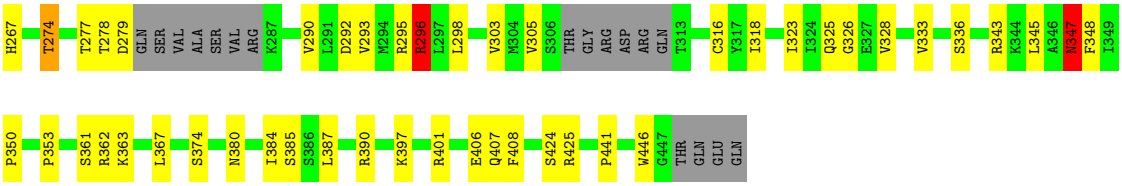


• Molecule 2: Tubulin gamma-1 chain

Chain X:

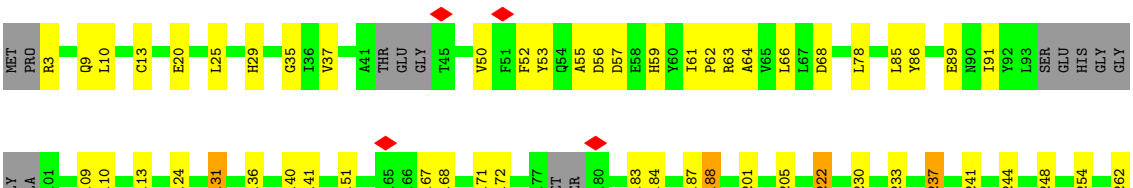


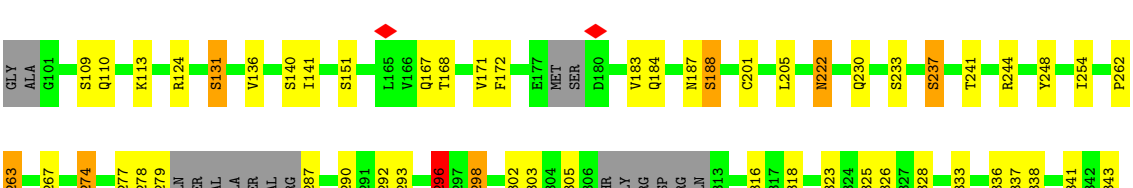


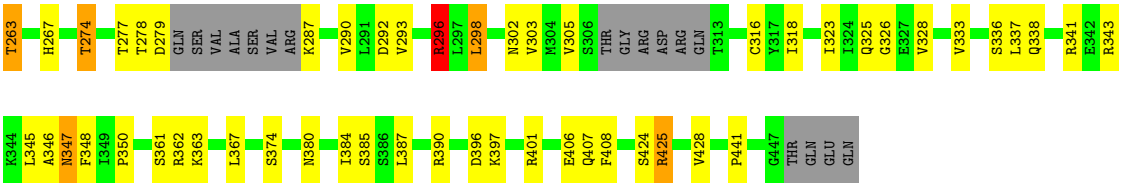


• Molecule 2: Tubulin gamma-1 chain

Chain Y:

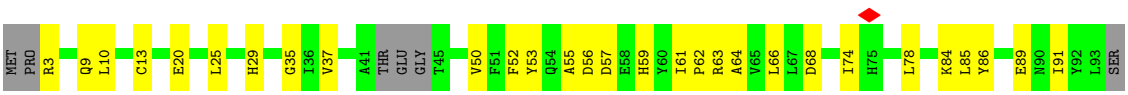


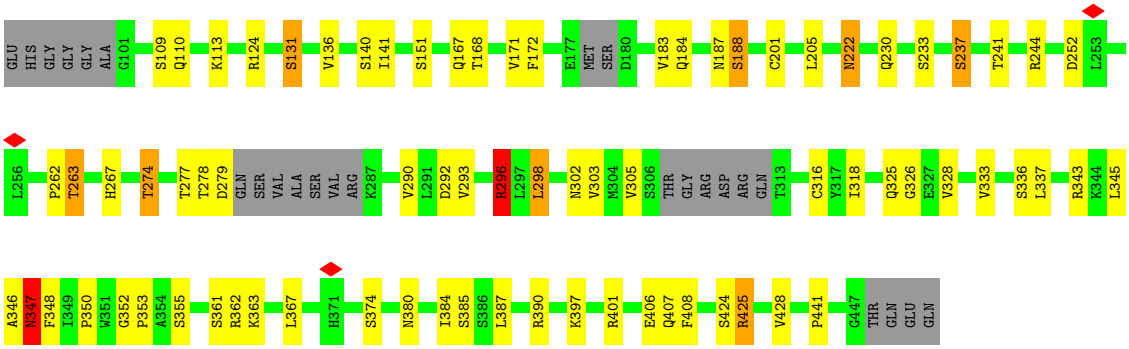




• Molecule 2: Tubulin gamma-1 chain

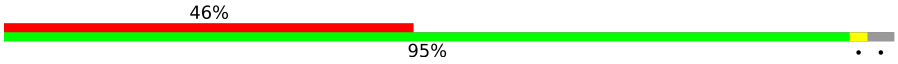
Chain Z:

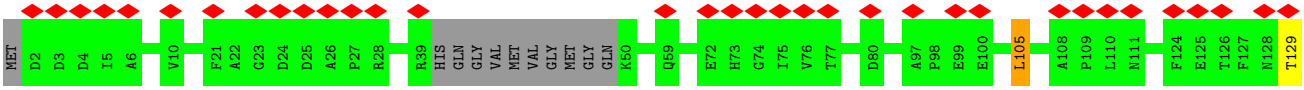


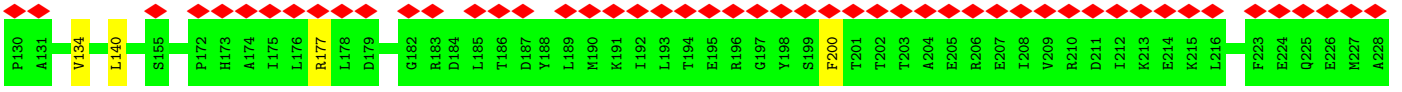


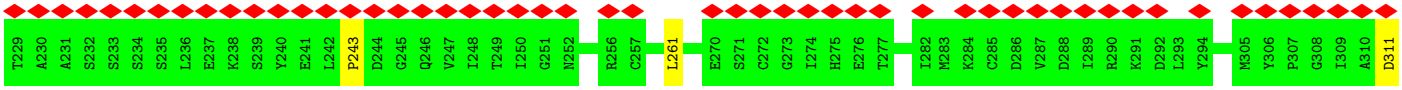
• Molecule 3: actin, cytoplasmic 1

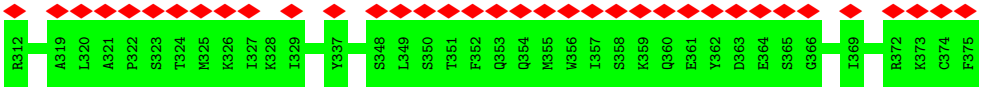
Chain e:





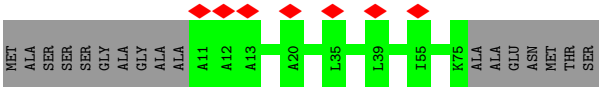






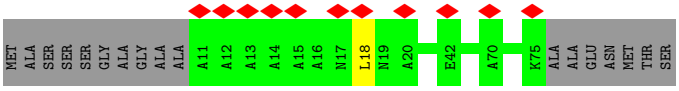
• Molecule 4: Mitotic-spindle organizing protein 1

Chain b:



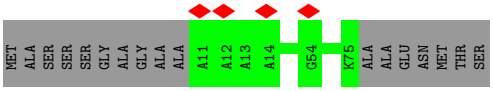
• Molecule 4: Mitotic-spindle organizing protein 1

Chain i:



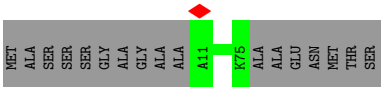
• Molecule 4: Mitotic-spindle organizing protein 1

Chain k:



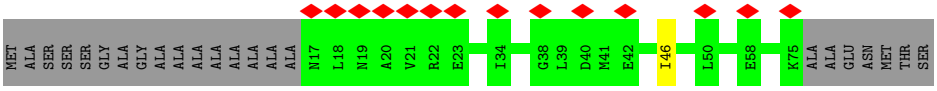
• Molecule 4: Mitotic-spindle organizing protein 1

Chain m:



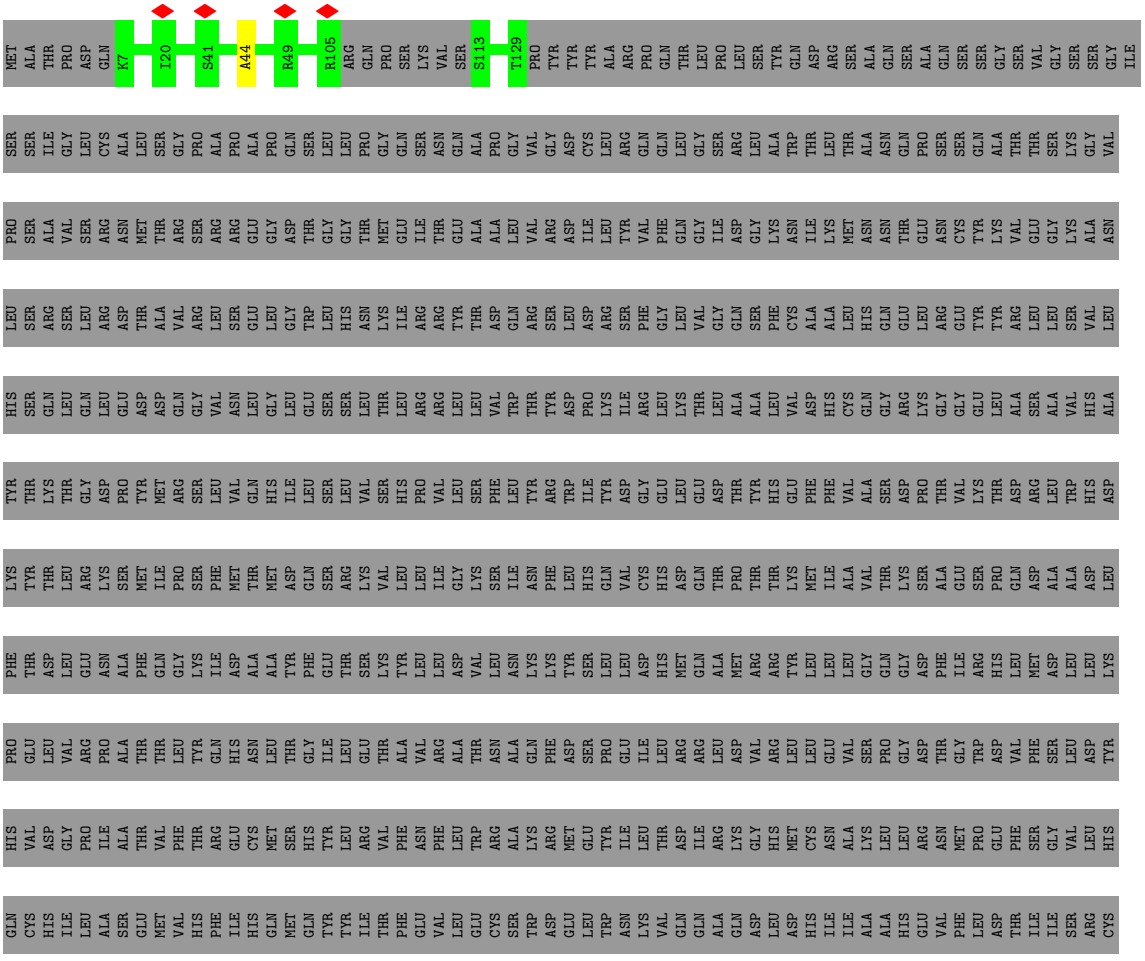
• Molecule 4: Mitotic-spindle organizing protein 1

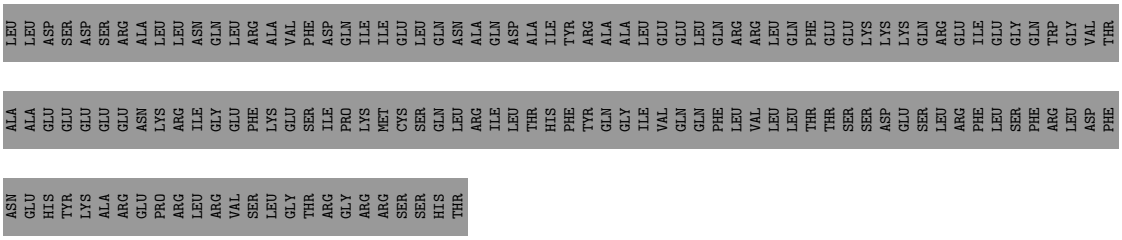
Chain d:



• Molecule 5: Gamma-tubulin complex component 3

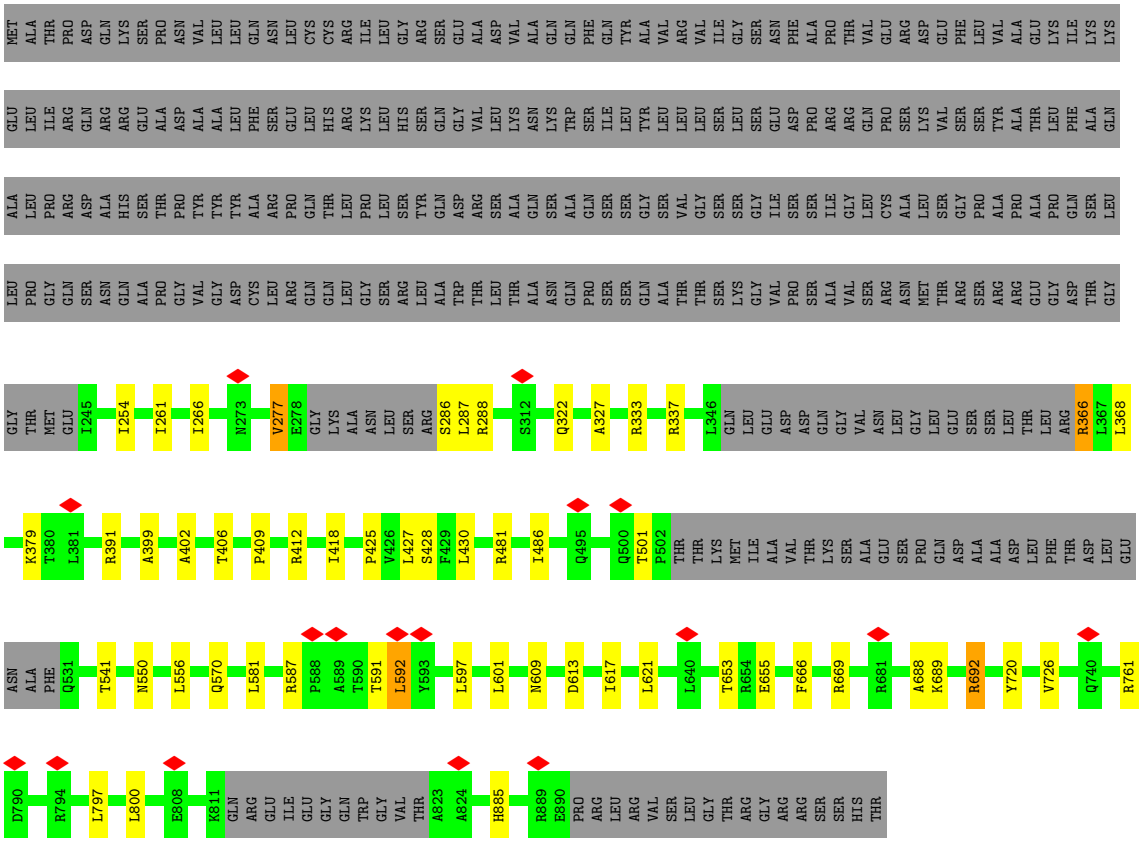
Chain a:





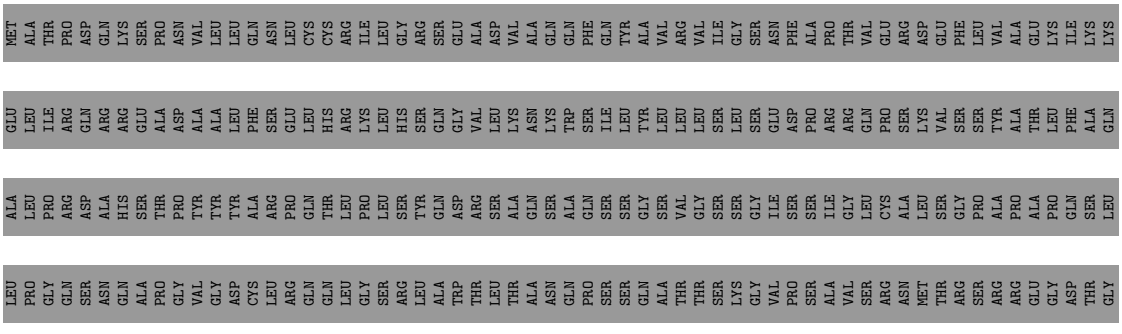
• Molecule 5: Gamma-tubulin complex component 3

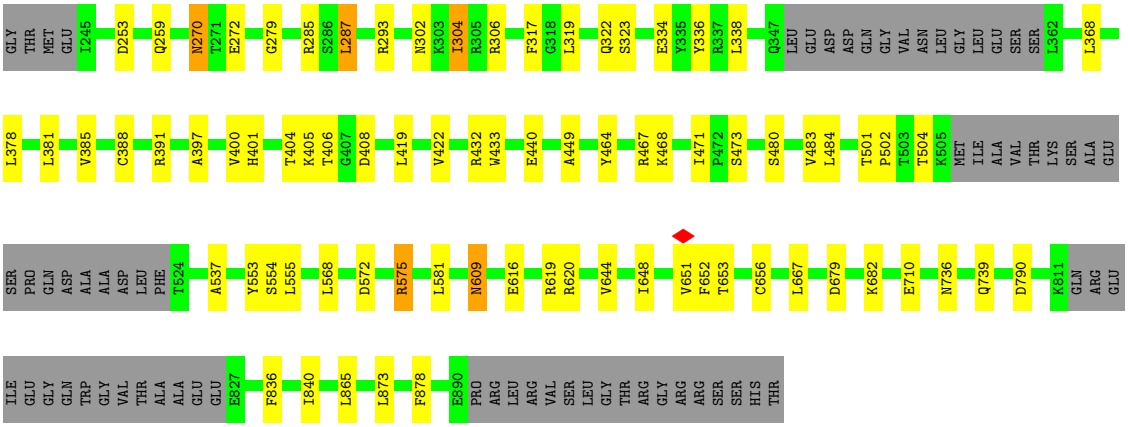
Chain D:



• Molecule 5: Gamma-tubulin complex component 3

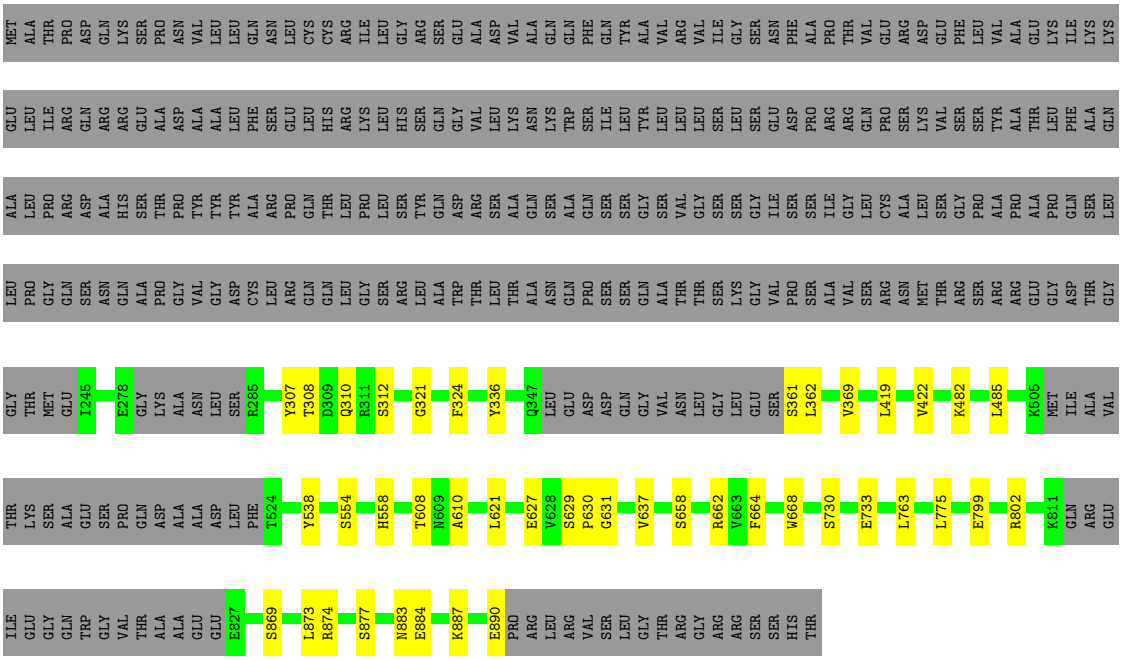
Chain F:





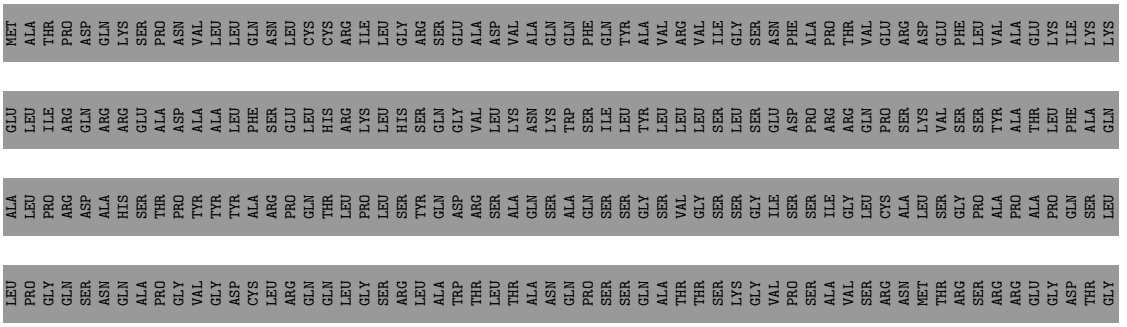
• Molecule 5: Gamma-tubulin complex component 3

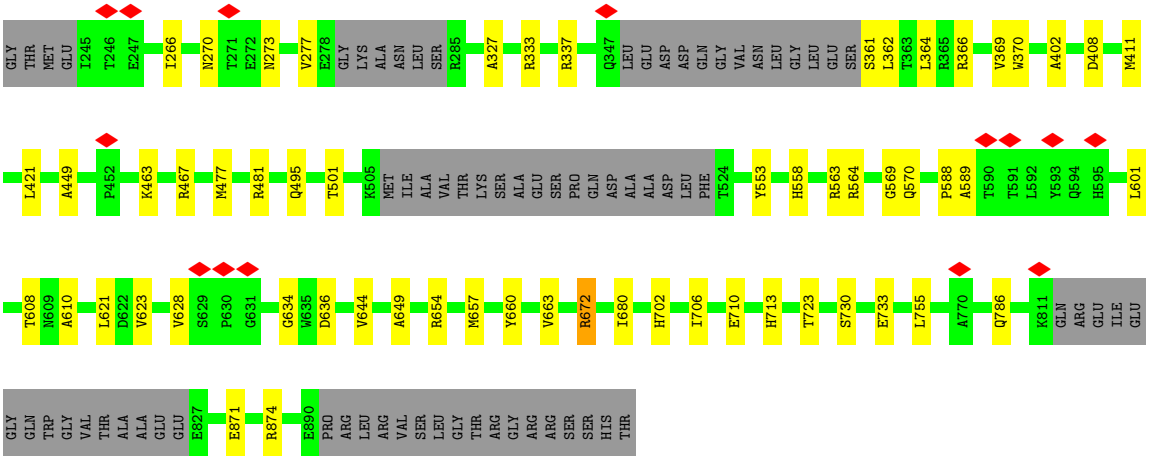
Chain H:



• Molecule 5: Gamma-tubulin complex component 3

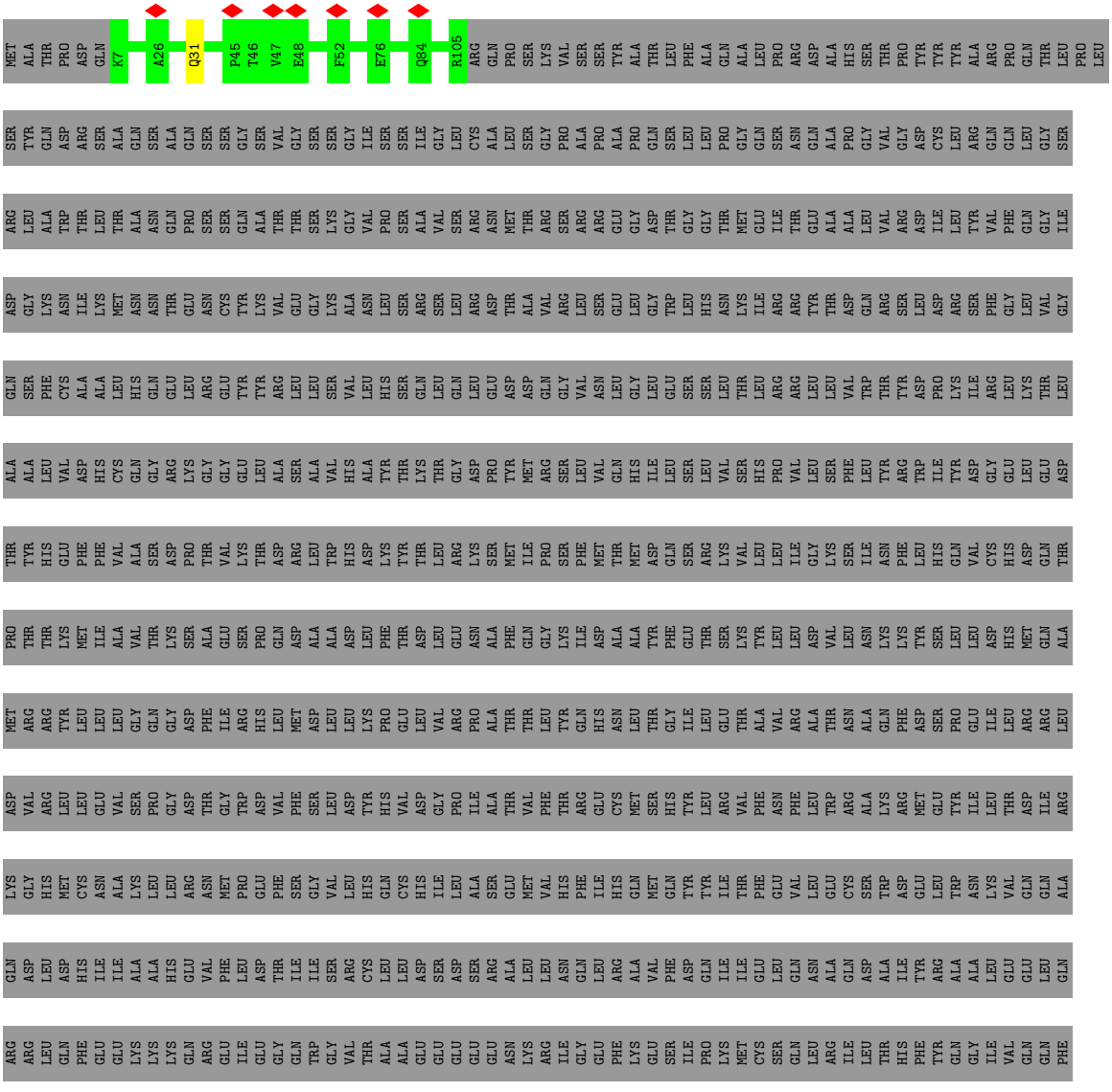
Chain N:





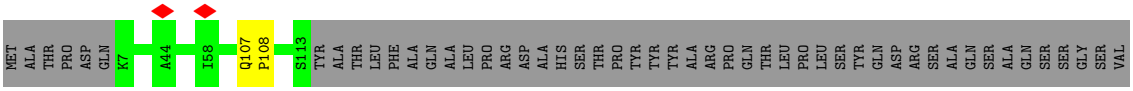
• Molecule 5: Gamma-tubulin complex component 3

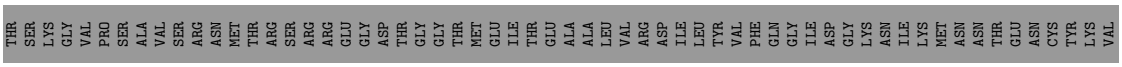
Chain h:



• Molecule 5: Gamma-tubulin complex component 3

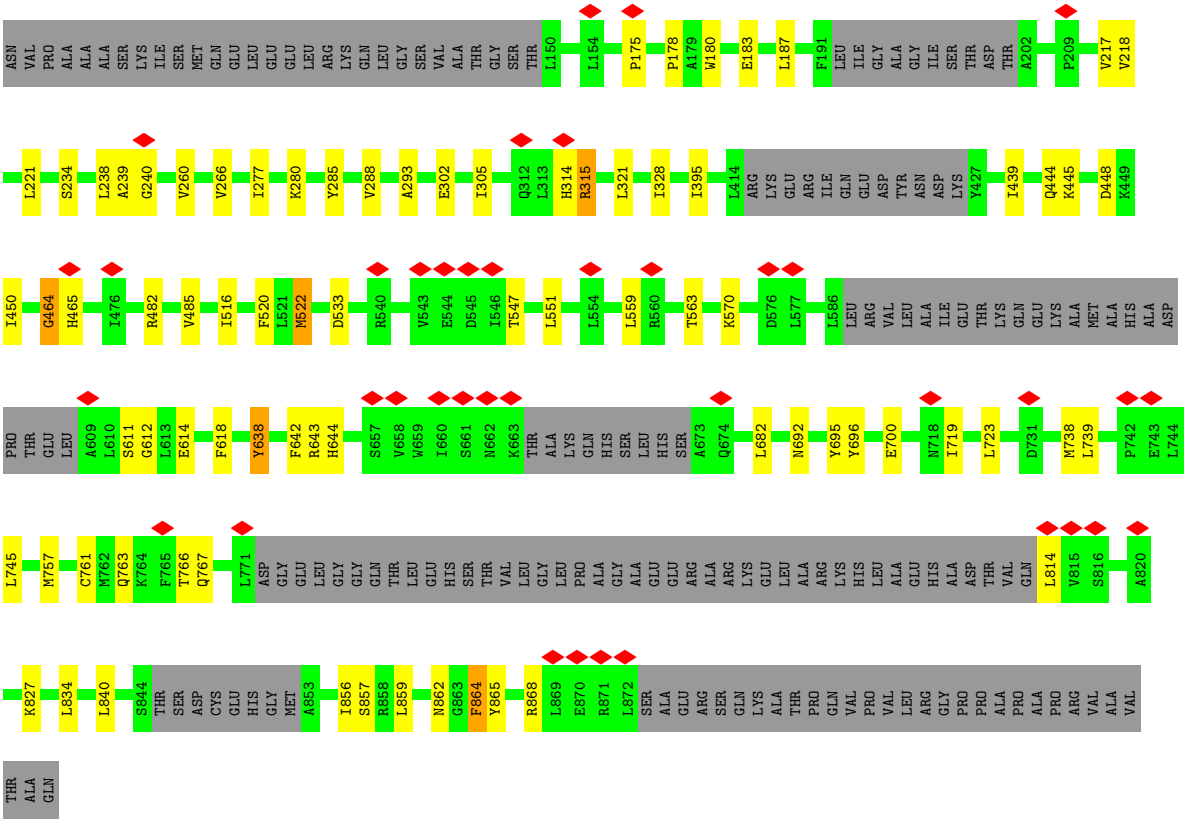
Chain j:





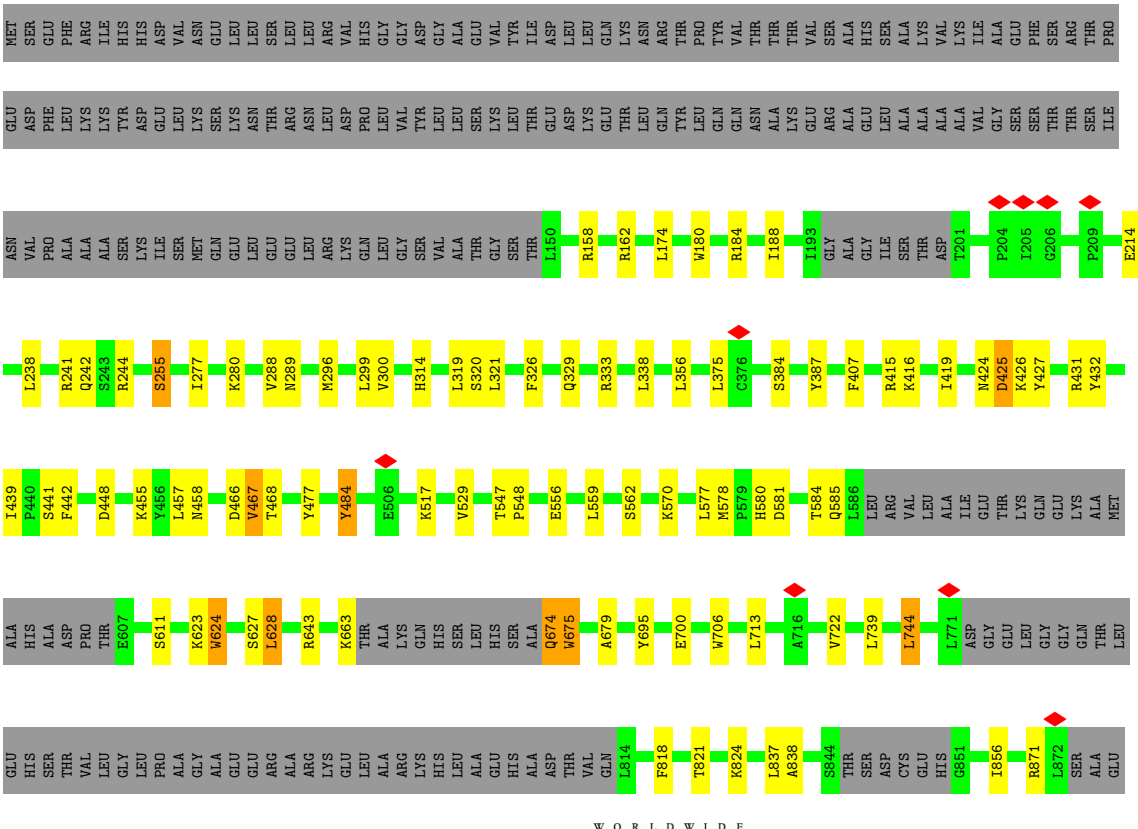
• Molecule 6: Gamma-tubulin complex component 2

Chain C:



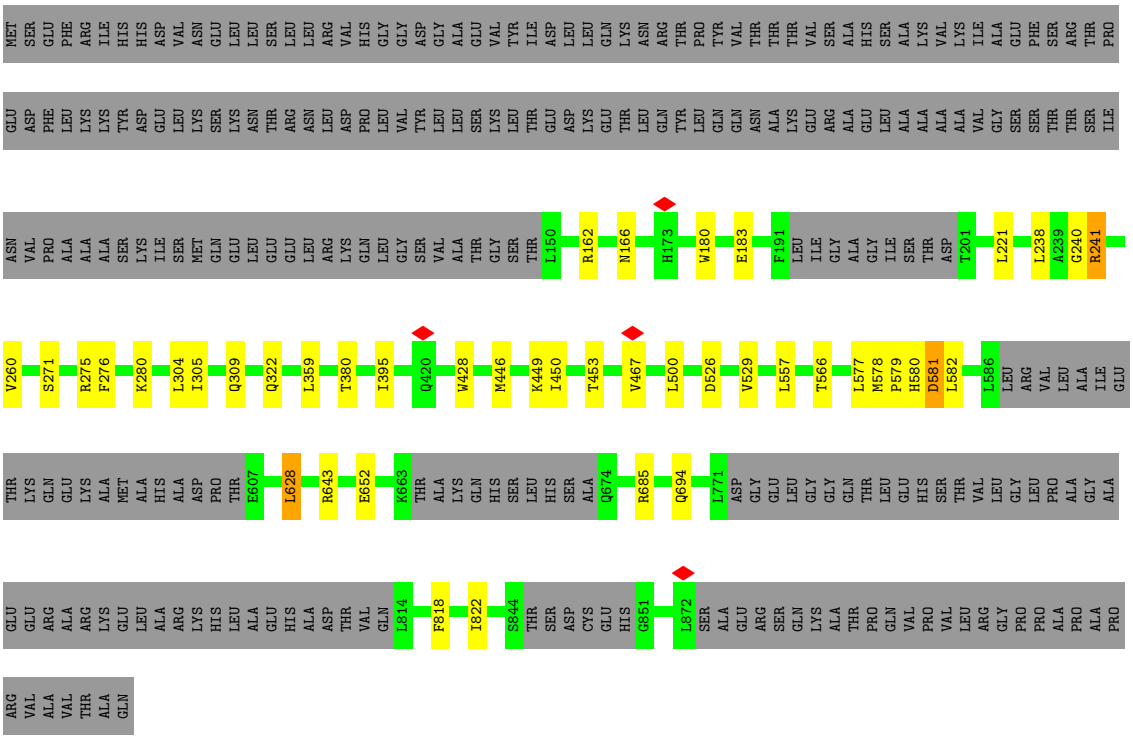
• Molecule 6: Gamma-tubulin complex component 2

Chain E:



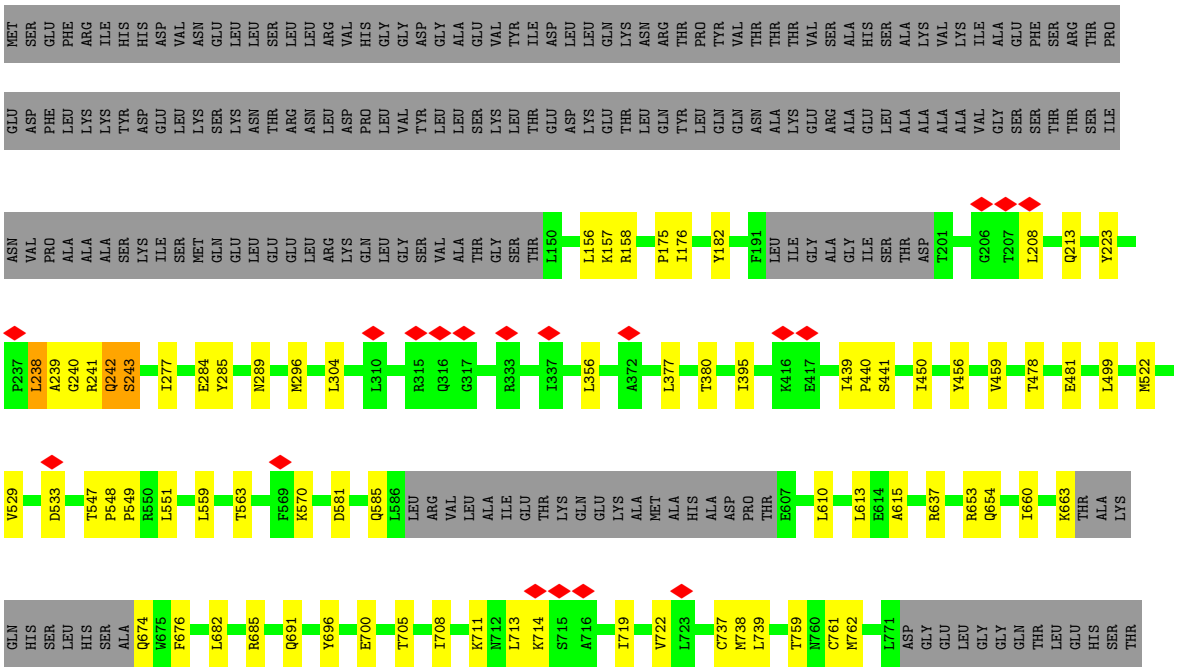
• Molecule 6: Gamma-tubulin complex component 2

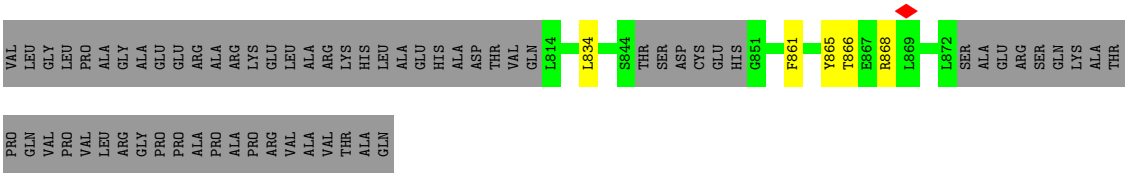
Chain G:



• Molecule 6: Gamma-tubulin complex component 2

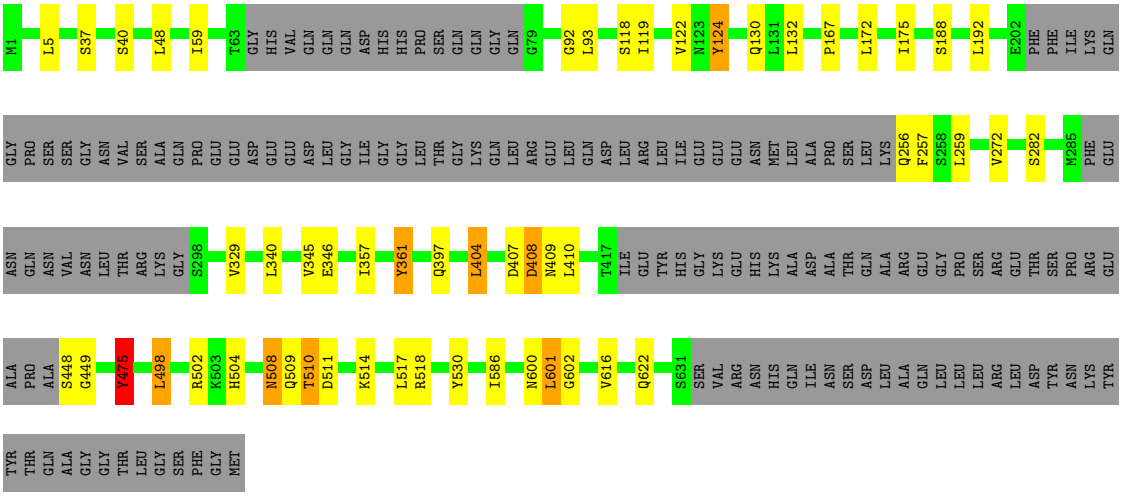
Chain M:





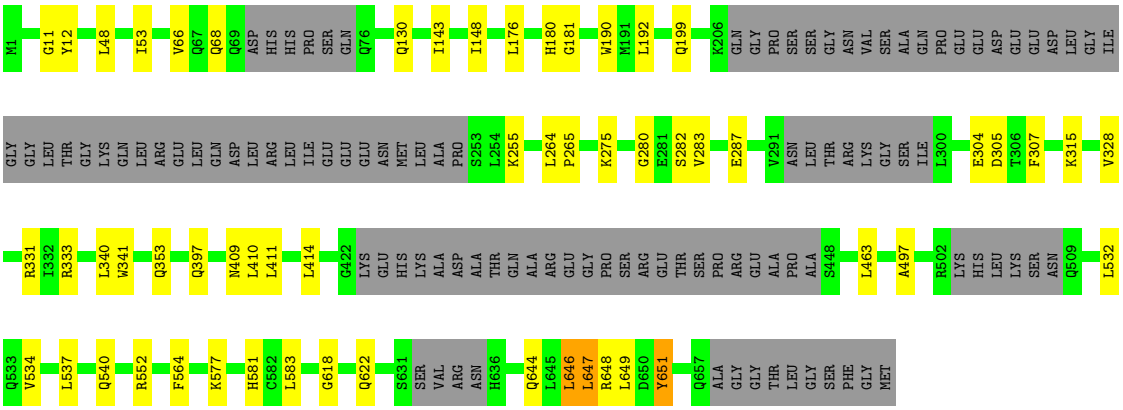
• Molecule 7: Gamma-tubulin complex component 4

Chain I:



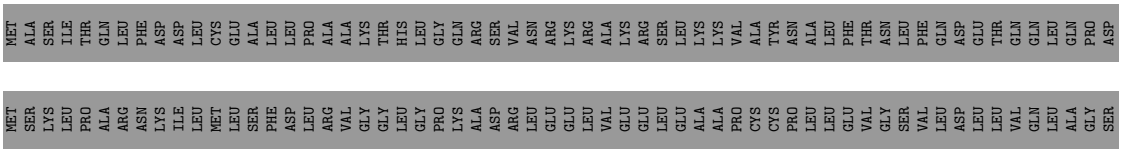
• Molecule 7: Gamma-tubulin complex component 4

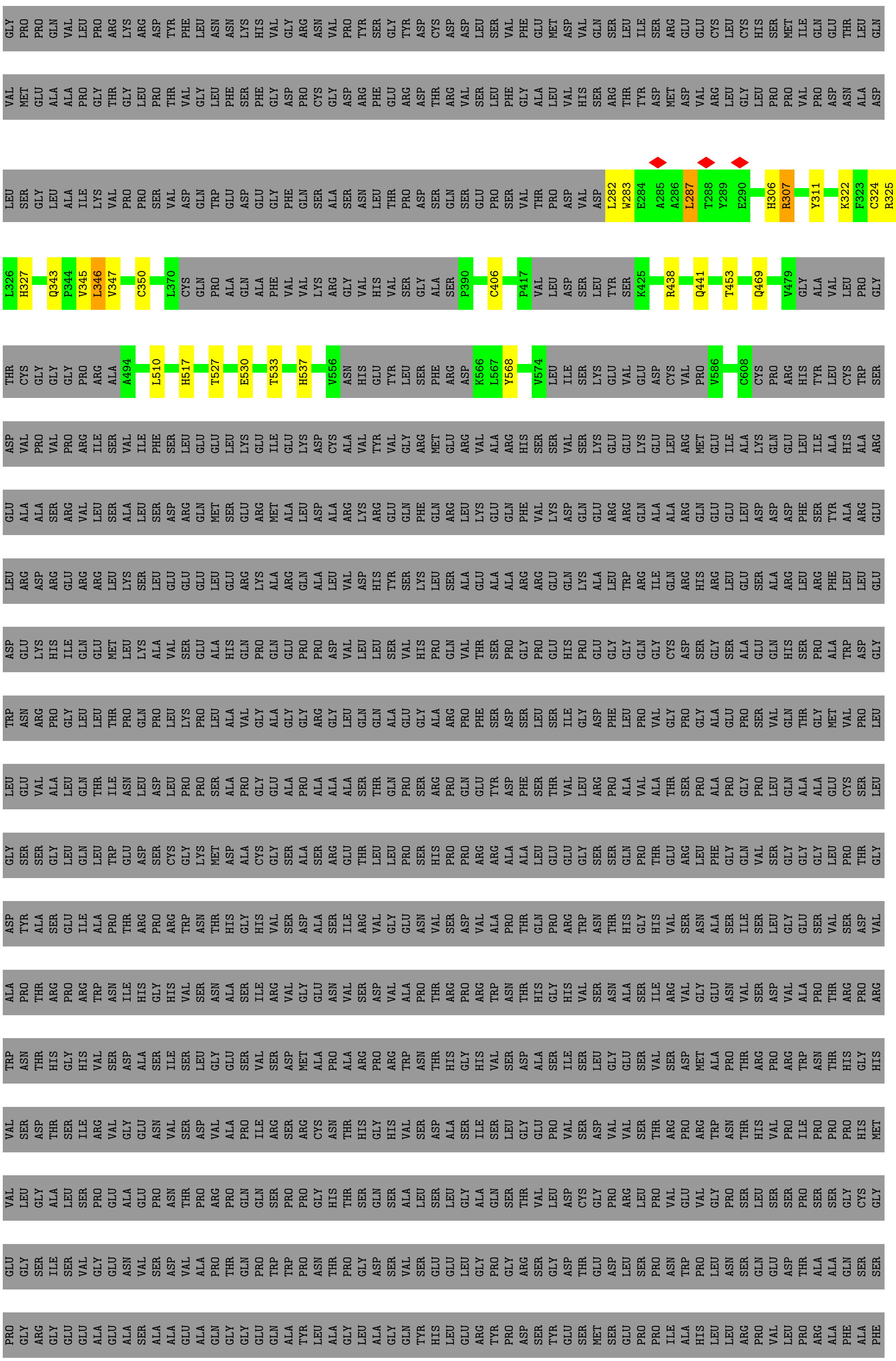
Chain K:

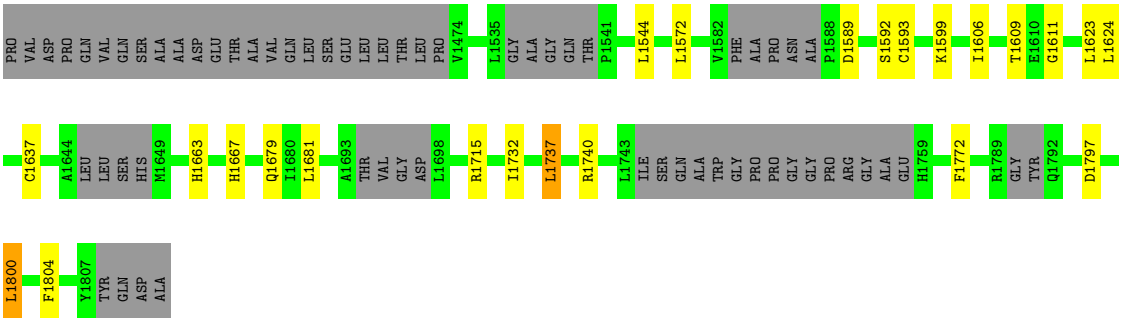


• Molecule 8: Gamma-tubulin complex component 6

Chain L:

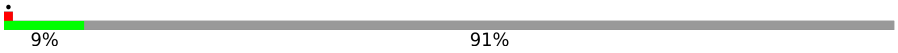


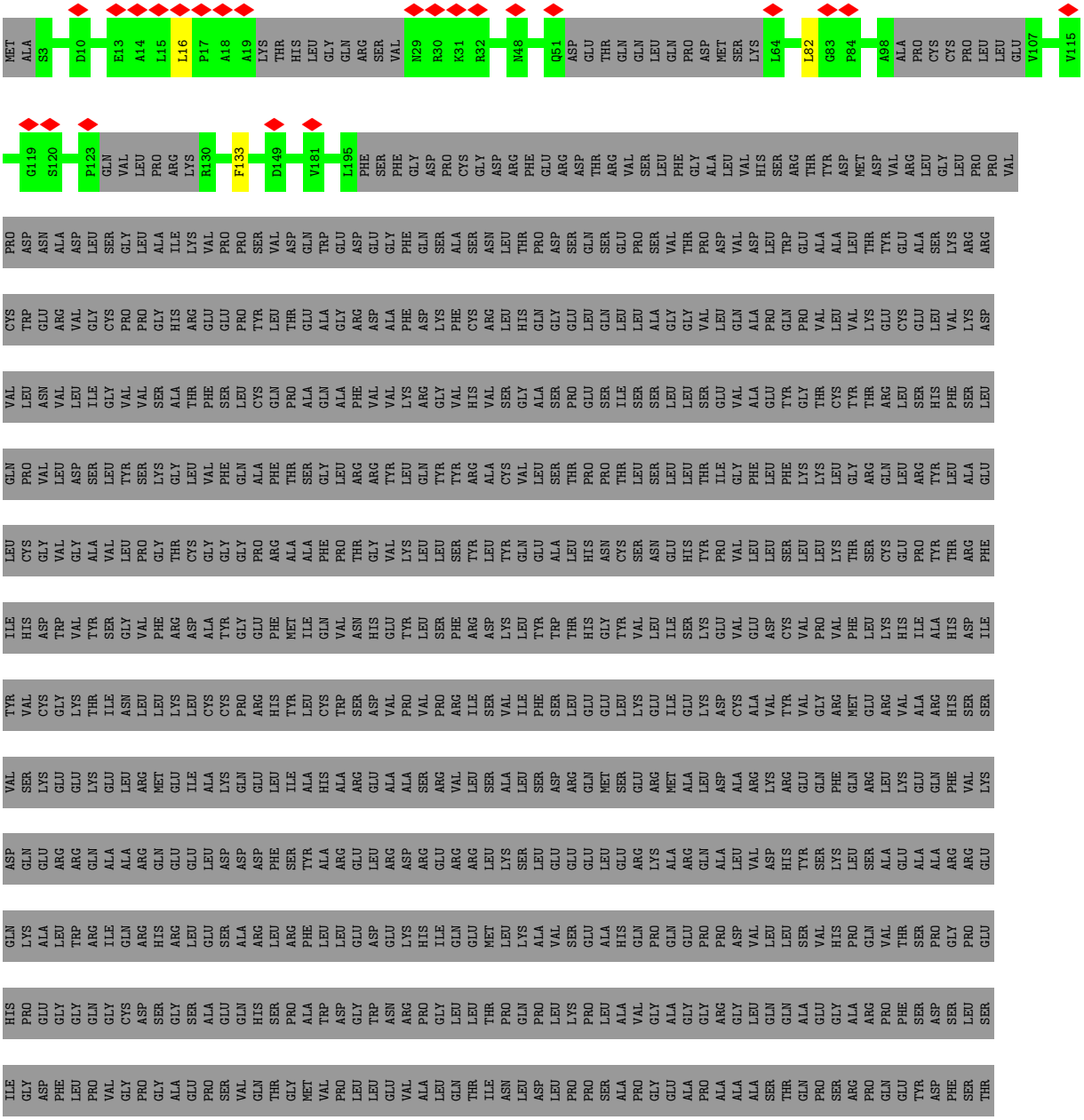

L282
W283
E284
A285
A286
L287
T288
Y289
E290
H306
R307
Y311
K322
F323
C324
R325
L326
H327
Q343
P344
V345
L346
V347
C350
L370
P390
C406
P417
K425
R438
Q441
T453
Q469
V479
A494
L510
H517
T527
E530
T533
H537
V556
K566
L567
Y568
V574
V586
C608



• Molecule 8: Gamma-tubulin complex component 6

Chain c:





VAL LEU ARG PRO ALA VAL ALA THR SER PRO ALA PRO GLY PRO LEU GLN ALA ALA GLU CYS SER LEU GLY SER SER GLY LEU GLN LEU TRP GLU ASP SER CYS GLY LYS MET ASP ALA CYS GLY SER ALA SER ARG GLU THR LEU LEU PRO SER HIS PRO PRO ARG ARG ALA ALA LEU GLU

GLU GLY SER SER GLN PRO THR GLU ARG LEU PHE GLY GLN VAL SER GLY GLY GLY LEU PRO THR GLY ASP TYR ALA SER GLU ILE ALA PRO THR ARG PRO ARG TRP ASN THR HIS GLY HIS VAL SER ASP ALA SER ILE ARG VAL GLY GLU ASN VAL SER ASP VAL ALA PRO THR GLN PRO

ARG TRP ASN THR HIS GLY HIS VAL SER ASN ALA SER ILE SER LEU GLY GLU SER VAL SER ASP VAL ALA PRO THR ARG PRO ARG TRP ASN ILE HIS GLY HIS VAL SER ASN ALA SER ILE ARG VAL GLY GLU ASN VAL SER ASP VAL ALA PRO THR ARG PRO ARG TRP ASN THR HIS GLY

HIS VAL SER ASN ALA SER ILE ARG VAL GLY GLU ASN VAL SER ASP VAL ALA PRO THR ARG PRO ARG TRP ASN THR HIS GLY HIS VAL SER ASP ALA SER ILE SER LEU GLY GLU SER VAL SER ASP MET ALA PRO ALA ARG PRO ARG TRP ASN THR HIS GLY HIS VAL SER ASP ALA SER

ILE SER LEU GLY GLU SER VAL SER ASP MET ALA PRO THR ARG PRO ARG TRP ASN THR HIS GLY HIS VAL SER ASP THR SER ILE ARG VAL GLY GLU ASN VAL SER ASP VAL ALA PRO ILE ARG SER ARG CYS ASN THR HIS GLY HIS VAL SER ASP ALA SER ILE SER LEU GLY GLU PRO

VAL SER ASP VAL VAL SER THR ARG PRO ARG TRP ASN THR HIS VAL PRO ILE PRO PRO PRO HIS MET VAL LEU GLY ALA LEU SER PRO GLU ALA GLU PRO ASN THR PRO ARG PRO GLN GLN SER PRO PRO GLY HIS THR SER GLN SER ALA LEU SER LEU GLY ALA GLN SER THR VAL LEU

ASP CYS GLY PRO ARG LEU PRO VAL GLU VAL GLY PRO SER LEU SER SER PRO SER SER GLY CYS GLY GLU GLY SER ILE SER VAL GLY GLU ASN VAL SER ASP VAL ALA PRO THR GLN PRO TRP TRP PRO ASN THR PRO GLY ASP SER VAL SER GLU GLU LEU GLY PRO GLY ARG SER GLY

ASP THR GLU ASP LEU SER PRO ASN TRP PRO LEU ASN SER GLN GLU ASP THR ALA ALA GLN SER SER PRO GLY ARG GLY GLU GLU ALA GLU ALA SER ALA ALA GLU ALA GLN GLY GLY GLU GLN ALA TYR LEU ALA GLY LEU ALA GLY GLN TYR HIS LEU GLU ARG TYR PRO ASP SER TYR

GLU SER MET SER GLU PRO PRO ILE ALA HIS LEU LEU ARG PRO VAL LEU PRO ARG ALA PHE ALA PHE PRO VAL ASP PRO GLN VAL GLN SER ALA ALA ASP GLU THR ALA VAL GLN LEU SER GLU LEU THR LEU PRO VAL LEU MET LYS ARG SER ILE THR ALA PRO LEU ALA ALA HIS

ILE SER LEU VAL ASN LYS ALA ALA VAL ASP TYR PHE PHE VAL GLU LEU HIS LEU GLU ALA HIS TYR GLU ALA LEU ARG HIS PHE LEU LEU MET GLU ASP GLY GLU PHE ALA GLN SER LEU SER ASP LEU LEU PHE GLU LYS LEU GLY ALA GLY GLN THR PRO GLY GLU LEU LEU ASN PRO

LEU VAL LEU ASN SER VAL LEU SER LYS ALA LEU GLN CYS SER LEU HIS GLY ASP THR PRO HIS ALA SER ASN LEU SER LEU ALA LEU LYS TYR LEU PRO GLU VAL PHE ALA PRO ASN ALA PRO ASP VAL LEU SER CYS LEU GLU LEU ARG TYR LYS VAL ASP TRP PRO LEU ASN ILE VAL

ILE THR GLU GLY CYS VAL SER LYS TYR SER GLY VAL PHE SER PHE LEU LEU GLN LEU LYS LEU MET MET TRP ALA LEU LYS ASP VAL CYS PHE HIS LEU LYS ARG THR ALA LEU LEU SER HIS MET ALA GLY SER VAL GLN PHE ARG GLN LEU GLN LEU PHE LYS HIS GLU MET GLN HIS

PHE VAL LYS VAL ILE GLN GLY TYR ILE ALA ASN GLN ILE LEU HIS VAL THR TRP CYS GLU PHE ARG ALA ARG LEU ALA THR VAL GLY ASP LEU GLU GLU ILE GLN ARG ALA HIS ALA GLU TYR LEU HIS LYS ALA VAL PHE ARG GLY LEU LEU THR GLU LYS ALA ALA PRO VAL MET ASN

VAL ILE HIS SER ILE PHE SER LEU VAL LEU LYS PHE ARG SER GLN LEU ILE SER GLN ALA TRP GLY PRO PRO GLY GLY PRO ARG GLY ALA GLU HIS PRO ASN PHE ALA LEU MET GLN GLN SER TYR ASN THR PHE LYS TYR TYR SER HIS PHE LEU PHE LYS VAL VAL THR LYS LEU VAL

ASN ARG GLY TYR GLN PRO HIS LEU GLU ASP PHE LEU LEU ARG ILE ASN PHE ASN ASN TYR TYR GLN ASP ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.160	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0357	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	J	0.39	0/4525	0.68	5/6119 (0.1%)
1	l	0.33	0/863	0.63	2/1166 (0.2%)
2	1	0.30	0/3441	0.54	1/4661 (0.0%)
2	2	0.30	0/3441	0.54	1/4661 (0.0%)
2	Q	0.30	0/3441	0.54	1/4661 (0.0%)
2	R	0.30	0/3441	0.54	1/4661 (0.0%)
2	S	0.30	0/3441	0.54	1/4661 (0.0%)
2	T	0.30	0/3441	0.54	1/4661 (0.0%)
2	U	0.30	0/3441	0.54	1/4661 (0.0%)
2	V	0.30	0/3441	0.54	1/4661 (0.0%)
2	W	0.30	0/3441	0.54	1/4661 (0.0%)
2	X	0.30	0/3441	0.54	1/4661 (0.0%)
2	Y	0.30	0/3441	0.54	1/4661 (0.0%)
2	Z	0.30	0/3441	0.54	1/4661 (0.0%)
3	e	0.53	1/2908 (0.0%)	0.76	5/3938 (0.1%)
4	b	0.35	0/484	0.69	0/653
4	d	0.37	0/454	0.68	0/611
4	i	0.30	0/484	0.58	1/653 (0.2%)
4	k	0.31	0/484	0.59	0/653
4	m	0.32	0/484	0.61	0/653
5	D	0.38	0/4897	0.66	4/6610 (0.1%)
5	F	0.37	1/5044 (0.0%)	0.65	4/6809 (0.1%)
5	H	0.35	0/5009	0.59	1/6761 (0.0%)
5	N	0.35	0/5009	0.63	3/6761 (0.0%)
5	a	0.32	0/948	0.60	0/1277
5	h	0.33	0/815	0.57	0/1096
5	j	0.32	0/855	0.60	0/1152
6	C	0.42	3/5151 (0.1%)	0.68	4/6955 (0.1%)
6	E	0.50	8/5311 (0.2%)	0.71	6/7169 (0.1%)
6	G	0.37	0/5295	0.62	1/7147 (0.0%)
6	M	0.41	1/5295 (0.0%)	0.69	3/7147 (0.0%)
7	I	0.44	3/4322 (0.1%)	0.67	7/5853 (0.1%)
7	K	0.39	1/4683 (0.0%)	0.67	5/6338 (0.1%)
8	L	0.38	1/4697 (0.0%)	0.68	7/6348 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
8	c	0.36	0/1235	0.72	2/1664 (0.1%)
All	All	0.36	19/110544 (0.0%)	0.62	72/149465 (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
1	J	0	2
1	l	0	1
2	1	0	4
2	2	0	4
2	Q	0	4
2	R	0	4
2	S	0	4
2	T	0	4
2	U	0	4
2	V	0	4
2	W	0	4
2	X	0	4
2	Y	0	4
2	Z	0	4
5	D	0	2
5	F	0	2
5	N	0	1
5	j	0	1
6	C	0	2
6	E	0	4
6	G	0	3
6	M	0	4
7	I	0	4
7	K	0	1
8	L	0	1
8	c	0	1
All	All	0	77

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	243	PRO	N-CD	17.57	1.72	1.47
6	E	624	TRP	CB-CG	8.40	1.65	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	624	TRP	CE3-CZ3	-8.22	1.24	1.38
6	E	624	TRP	CD1-NE1	-8.03	1.24	1.38
6	E	624	TRP	CG-CD1	7.80	1.47	1.36
7	I	361	TYR	CD2-CE2	-7.53	1.28	1.39
7	I	124	TYR	CD1-CE1	-7.48	1.28	1.39
7	I	530	TYR	CD2-CE2	-7.12	1.28	1.39
6	M	182	TYR	CD1-CE1	-6.92	1.28	1.39
6	E	624	TRP	CZ2-CH2	-6.65	1.24	1.37
8	L	406	CYS	CB-SG	-5.62	1.72	1.81
5	F	575	ARG	CG-CD	5.61	1.66	1.51
6	C	638	TYR	CB-CG	-5.61	1.43	1.51
6	E	624	TRP	CZ3-CH2	-5.44	1.31	1.40
6	E	624	TRP	CE2-CZ2	5.38	1.48	1.39
6	E	415	ARG	CG-CD	5.36	1.65	1.51
7	K	651	TYR	CD1-CE1	5.33	1.47	1.39
6	C	864	PHE	CB-CG	-5.02	1.42	1.51
6	C	638	TYR	CD2-CE2	-5.01	1.31	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	624	TRP	CE3-CZ3-CH2	9.79	131.97	121.20
5	D	692	ARG	NE-CZ-NH2	-9.52	115.54	120.30
8	c	82	LEU	CA-CB-CG	9.46	137.05	115.30
7	I	361	TYR	CB-CG-CD2	-9.07	115.56	121.00
1	J	236	LEU	CA-CB-CG	8.80	135.53	115.30
5	D	368	LEU	CA-CB-CG	8.09	133.92	115.30
5	N	621	LEU	CB-CG-CD1	-7.67	97.96	111.00
8	L	1681	LEU	CB-CG-CD1	-7.66	97.97	111.00
3	e	105	LEU	CB-CG-CD2	-7.37	98.47	111.00
5	F	581	LEU	CA-CB-CG	7.35	132.21	115.30
6	E	624	TRP	CG-CD2-CE3	7.23	140.40	133.90
1	l	121	PRO	N-CA-CB	6.93	111.62	103.30
7	K	651	TYR	CB-CG-CD2	-6.91	116.85	121.00
3	e	105	LEU	CB-CG-CD1	6.88	122.69	111.00
5	F	790	ASP	CB-CG-OD2	6.84	124.45	118.30
8	L	1544	LEU	CA-CB-CG	6.82	130.98	115.30
6	E	624	TRP	CB-CG-CD2	6.81	135.45	126.60
6	E	415	ARG	NE-CZ-NH2	6.75	123.68	120.30
7	I	361	TYR	CB-CG-CD1	6.75	125.05	121.00
8	L	1624	LEU	CA-CB-CG	6.75	130.82	115.30
7	I	361	TYR	CZ-CE2-CD2	6.31	125.48	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	296	ARG	NE-CZ-NH1	-6.29	117.15	120.30
2	1	296	ARG	NE-CZ-NH1	-6.23	117.18	120.30
2	R	296	ARG	NE-CZ-NH1	-6.22	117.19	120.30
2	Z	296	ARG	NE-CZ-NH1	-6.22	117.19	120.30
2	U	296	ARG	NE-CZ-NH1	-6.20	117.20	120.30
2	W	296	ARG	NE-CZ-NH1	-6.20	117.20	120.30
2	2	296	ARG	NE-CZ-NH1	-6.19	117.20	120.30
8	c	16	LEU	CB-CG-CD1	-6.18	100.49	111.00
2	S	296	ARG	NE-CZ-NH1	-6.17	117.22	120.30
2	Q	296	ARG	NE-CZ-NH1	-6.16	117.22	120.30
2	T	296	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	l	130	PRO	N-CA-CB	6.13	110.66	103.30
2	V	296	ARG	NE-CZ-NH1	-6.11	117.25	120.30
2	Y	296	ARG	NE-CZ-NH1	-6.06	117.27	120.30
5	H	621	LEU	CA-CB-CG	6.04	129.19	115.30
5	N	672	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	J	235	SER	C-N-CA	6.04	136.79	121.70
1	J	400	ASP	CB-CG-OD2	6.02	123.72	118.30
7	I	475	TYR	CA-CB-CG	5.95	124.70	113.40
5	F	287	LEU	CA-CB-CG	5.92	128.91	115.30
7	K	651	TYR	CA-CB-CG	5.91	124.63	113.40
8	L	287	LEU	CB-CG-CD1	-5.87	101.01	111.00
6	M	182	TYR	CB-CG-CD1	-5.79	117.52	121.00
7	I	498	LEU	CA-CB-CG	5.69	128.38	115.30
6	C	464	GLY	C-N-CA	5.68	135.90	121.70
7	K	12	TYR	CB-CG-CD2	-5.63	117.62	121.00
6	C	522	MET	CG-SD-CE	5.56	109.09	100.20
3	e	134	VAL	CG1-CB-CG2	-5.54	102.04	110.90
8	L	282	LEU	CA-CB-CG	5.50	127.95	115.30
8	L	1800	LEU	CB-CG-CD1	-5.50	101.66	111.00
8	L	1737	LEU	CB-CG-CD1	-5.40	101.81	111.00
7	K	646	LEU	CB-CG-CD2	5.34	120.08	111.00
6	E	299	LEU	CB-CG-CD2	-5.34	101.92	111.00
6	C	315	ARG	NE-CZ-NH1	-5.31	117.64	120.30
6	M	674	GLN	C-N-CA	5.25	134.83	121.70
6	M	156	LEU	CA-CB-CG	5.24	127.35	115.30
6	E	744	LEU	CA-CB-CG	5.19	127.23	115.30
5	N	621	LEU	CB-CG-CD2	5.13	119.72	111.00
5	F	253	ASP	CB-CG-OD2	5.12	122.91	118.30
4	i	18	LEU	CA-CB-CG	5.12	127.08	115.30
5	D	592	LEU	CA-CB-CG	5.12	127.07	115.30
6	C	682	LEU	CB-CG-CD2	-5.10	102.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	361	TYR	CD1-CE1-CZ	-5.06	115.25	119.80
1	J	885	LEU	CA-CB-CG	-5.05	103.67	115.30
5	D	366	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	J	796	LEU	CA-CB-CG	5.05	126.91	115.30
3	e	140	LEU	CA-CB-CG	5.04	126.90	115.30
7	I	404	LEU	CB-CG-CD2	-5.03	102.44	111.00
3	e	311	ASP	CB-CG-OD2	5.02	122.82	118.30
6	G	500	LEU	CA-CB-CG	5.01	126.81	115.30
7	K	583	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (77) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	347	ASN	Peptide
2	1	406	GLU	Peptide
2	1	55	ALA	Peptide
2	1	86	TYR	Peptide
2	2	347	ASN	Peptide
2	2	406	GLU	Peptide
2	2	55	ALA	Peptide
2	2	86	TYR	Peptide
6	C	238	LEU	Peptide
6	C	464	GLY	Peptide
5	D	481	ARG	Peptide
5	D	501	THR	Peptide
6	E	424	ASN	Peptide
6	E	425	ASP	Peptide
6	E	484	TYR	Peptide
6	E	580	HIS	Peptide
5	F	272	GLU	Peptide
5	F	609	ASN	Peptide
6	G	240	GLY	Peptide
6	G	580	HIS	Peptide
6	G	581	ASP	Mainchain
7	I	407	ASP	Peptide
7	I	600	ASN	Peptide
7	I	601	LEU	Mainchain
7	I	602	GLY	Peptide
1	J	210	PRO	Peptide
1	J	255	PRO	Peptide
7	K	410	LEU	Peptide

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Mol	Chain	Res	Type	Group
8	L	306	HIS	Peptide
6	M	239	ALA	Peptide
6	M	240	GLY	Peptide
6	M	242	GLN	Peptide
6	M	866	THR	Peptide
5	N	501	THR	Peptide
2	Q	347	ASN	Peptide
2	Q	406	GLU	Peptide
2	Q	55	ALA	Peptide
2	Q	86	TYR	Peptide
2	R	347	ASN	Peptide
2	R	406	GLU	Peptide
2	R	55	ALA	Peptide
2	R	86	TYR	Peptide
2	S	347	ASN	Peptide
2	S	406	GLU	Peptide
2	S	55	ALA	Peptide
2	S	86	TYR	Peptide
2	T	347	ASN	Peptide
2	T	406	GLU	Peptide
2	T	55	ALA	Peptide
2	T	86	TYR	Peptide
2	U	347	ASN	Peptide
2	U	406	GLU	Peptide
2	U	55	ALA	Peptide
2	U	86	TYR	Peptide
2	V	347	ASN	Peptide
2	V	406	GLU	Peptide
2	V	55	ALA	Peptide
2	V	86	TYR	Peptide
2	W	347	ASN	Peptide
2	W	406	GLU	Peptide
2	W	55	ALA	Peptide
2	W	86	TYR	Peptide
2	X	347	ASN	Peptide
2	X	406	GLU	Peptide
2	X	55	ALA	Peptide
2	X	86	TYR	Peptide
2	Y	347	ASN	Peptide
2	Y	406	GLU	Peptide
2	Y	55	ALA	Peptide
2	Y	86	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	Z	347	ASN	Peptide
2	Z	406	GLU	Peptide
2	Z	55	ALA	Peptide
2	Z	86	TYR	Peptide
8	c	133	PHE	Peptide
5	j	107	GLN	Peptide
1	l	123	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4429	0	4482	25	0
1	l	847	0	789	0	0
2	1	3373	0	3325	60	0
2	2	3373	0	3325	54	0
2	Q	3373	0	3325	59	0
2	R	3373	0	3325	56	0
2	S	3373	0	3325	56	0
2	T	3373	0	3325	57	0
2	U	3373	0	3325	56	0
2	V	3373	0	3325	53	0
2	W	3373	0	3325	56	0
2	X	3373	0	3325	55	0
2	Y	3373	0	3325	55	0
2	Z	3373	0	3325	57	0
3	e	2847	0	2810	0	0
4	b	484	0	512	0	0
4	d	454	0	482	0	0
4	i	484	0	512	0	0
4	k	484	0	512	0	0
4	m	484	0	512	0	0
5	D	4796	0	4775	39	0
5	F	4941	0	4935	46	0
5	H	4907	0	4896	24	0
5	N	4907	0	4896	33	0
5	a	933	0	953	0	0
5	h	803	0	831	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	j	843	0	846	0	0
6	C	5044	0	5081	46	0
6	E	5202	0	5241	57	0
6	G	5186	0	5219	24	0
6	M	5186	0	5219	41	0
7	I	4225	0	4259	32	0
7	K	4579	0	4586	34	0
8	L	4587	0	4636	26	0
8	c	1220	0	1231	0	0
9	l	5	0	0	0	0
9	m	1	0	0	0	0
All	All	108354	0	108115	1019	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1019) 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:T:56:ASP:OD1	2:U:296:ARG:NH1	1.96	0.98
7:I:48:LEU:HD21	7:I:130:GLN:HG2	1.64	0.79
7:K:646:LEU:HG	2:Y:338:GLN:HE22	1.44	0.79
7:I:361:TYR:HE2	7:I:475:TYR:HB3	1.48	0.79
7:I:357:ILE:O	7:I:361:TYR:HB3	1.84	0.77
5:D:692:ARG:HH22	2:R:197:GLN:HA	1.51	0.76
6:M:304:LEU:HB3	5:N:369:VAL:HG12	1.67	0.75
6:C:522:MET:SD	2:Q:248:TYR:OH	2.45	0.73
5:F:616:GLU:HG3	5:F:619:ARG:HH11	1.54	0.73
1:J:684:GLU:H	1:J:687:LEU:HB3	1.56	0.71
2:W:56:ASP:O	2:X:295:ARG:NH1	2.24	0.71
7:K:649:LEU:HB3	2:Y:341:ARG:HH21	1.56	0.70
7:I:361:TYR:CE2	7:I:475:TYR:HB3	2.26	0.70
5:F:553:TYR:HB3	5:F:648:ILE:HD11	1.74	0.69
2:2:136:VAL:HG23	2:2:167:GLN:HB3	1.75	0.69
2:Q:136:VAL:HG23	2:Q:167:GLN:HB3	1.75	0.69
2:W:136:VAL:HG23	2:W:167:GLN:HB3	1.75	0.69
6:C:696:TYR:O	6:C:700:GLU:HB2	1.93	0.69
2:T:136:VAL:HG23	2:T:167:GLN:HB3	1.75	0.69
2:V:136:VAL:HG23	2:V:167:GLN:HB3	1.75	0.69
5:N:563:ARG:HH22	5:N:569:GLY:HA3	1.58	0.69
8:L:527:THR:HA	8:L:530:GLU:HG2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:136:VAL:HG23	2:R:167:GLN:HB3	1.75	0.68
2:W:56:ASP:C	2:X:296:ARG:HH12	1.95	0.68
2:U:136:VAL:HG23	2:U:167:GLN:HB3	1.75	0.68
2:X:136:VAL:HG23	2:X:167:GLN:HB3	1.75	0.68
2:S:136:VAL:HG23	2:S:167:GLN:HB3	1.75	0.68
2:Z:136:VAL:HG23	2:Z:167:GLN:HB3	1.75	0.68
2:1:136:VAL:HG23	2:1:167:GLN:HB3	1.75	0.67
2:Y:136:VAL:HG23	2:Y:167:GLN:HB3	1.75	0.67
5:F:259:GLN:NE2	6:G:322:GLN:OE1	2.28	0.67
2:1:248:TYR:OH	6:M:522:MET:SD	2.51	0.67
5:D:322:GLN:HG2	6:E:333:ARG:HH22	1.61	0.66
2:W:56:ASP:O	2:X:296:ARG:NH1	2.20	0.66
6:E:581:ASP:O	6:E:643:ARG:NH1	2.29	0.65
5:N:601:LEU:HD22	5:N:623:VAL:HG13	1.78	0.65
5:H:307:TYR:HA	5:H:310:GLN:HE21	1.62	0.65
6:M:158:ARG:HH12	6:M:176:ILE:HG21	1.61	0.65
6:C:315:ARG:HH12	5:D:366:ARG:HB3	1.61	0.64
7:K:532:LEU:HD22	7:K:644:GLN:HG2	1.80	0.64
5:D:266:ILE:HG12	5:D:277:VAL:HB	1.79	0.64
6:C:395:ILE:HD11	6:C:450:ILE:HG23	1.81	0.63
7:I:132:LEU:HG	7:I:167:PRO:HB3	1.81	0.63
5:F:878:PHE:HD2	2:T:338:GLN:HE22	1.47	0.63
5:F:620:ARG:HH21	5:F:644:VAL:HA	1.63	0.63
8:L:1663:HIS:CG	2:Z:262:PRO:HA	2.34	0.62
6:C:533:ASP:OD2	2:Q:3:ARG:NH2	2.32	0.62
2:W:3:ARG:N	2:W:131:SER:HG	1.98	0.62
5:F:304:ILE:HD12	5:F:381:LEU:HD13	1.79	0.62
5:F:865:LEU:HD11	5:F:873:LEU:HD22	1.81	0.62
8:L:1797:ASP:HA	8:L:1800:LEU:HD23	1.81	0.62
6:C:644:HIS:HB2	6:C:739:LEU:HD21	1.82	0.62
5:F:736:ASN:HA	5:F:739:GLN:HE21	1.64	0.62
2:X:3:ARG:N	2:X:131:SER:HG	1.98	0.62
2:1:3:ARG:NH1	6:M:529:VAL:O	2.33	0.62
5:F:401:HIS:HD2	5:F:419:LEU:HD21	1.65	0.62
6:G:221:LEU:HD11	6:G:260:VAL:HG22	1.82	0.62
6:C:187:LEU:HD22	5:D:379:LYS:HE3	1.82	0.61
2:S:3:ARG:N	2:S:131:SER:HG	1.98	0.61
7:K:192:LEU:HD11	7:K:307:PHE:HB2	1.81	0.61
2:Y:3:ARG:N	2:Y:131:SER:HG	1.98	0.61
5:D:570:GLN:NE2	2:R:247:GLY:O	2.33	0.61
2:T:3:ARG:N	2:T:131:SER:HG	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:292:ASP:O	2:W:296:ARG:HB2	2.01	0.61
5:D:486:ILE:HG23	5:D:541:THR:HG21	1.82	0.61
2:Q:292:ASP:O	2:Q:296:ARG:HB2	2.01	0.61
2:1:292:ASP:O	2:1:296:ARG:HB2	2.01	0.61
8:L:283:TRP:O	8:L:287:LEU:HB2	1.99	0.61
2:2:3:ARG:N	2:2:131:SER:HG	1.98	0.61
2:Y:318:ILE:HB	2:Y:380:ASN:HB3	1.83	0.61
6:M:585:GLN:OE1	6:M:637:ARG:NH2	2.34	0.61
2:Z:318:ILE:HB	2:Z:380:ASN:HB3	1.83	0.61
2:R:3:ARG:N	2:R:131:SER:HG	1.98	0.60
2:R:292:ASP:O	2:R:296:ARG:HB2	2.01	0.60
2:S:292:ASP:O	2:S:296:ARG:HB2	2.01	0.60
2:1:3:ARG:N	2:1:131:SER:HG	1.98	0.60
2:2:292:ASP:O	2:2:296:ARG:HB2	2.01	0.60
8:L:1732:ILE:HG23	8:L:1772:PHE:HE1	1.64	0.60
2:Q:3:ARG:N	2:Q:131:SER:HG	1.98	0.60
2:U:3:ARG:N	2:U:131:SER:HG	1.98	0.60
2:X:292:ASP:O	2:X:296:ARG:HB2	2.01	0.60
2:T:292:ASP:O	2:T:296:ARG:HB2	2.01	0.60
2:V:292:ASP:O	2:V:296:ARG:HB2	2.01	0.60
2:Z:292:ASP:O	2:Z:296:ARG:HB2	2.01	0.60
2:V:3:ARG:N	2:V:131:SER:HG	1.99	0.60
2:W:318:ILE:HB	2:W:380:ASN:HB3	1.83	0.60
2:Y:292:ASP:O	2:Y:296:ARG:HB2	2.01	0.60
2:T:318:ILE:HB	2:T:380:ASN:HB3	1.83	0.60
5:N:477:MET:HG3	5:N:481:ARG:HE	1.65	0.60
2:Z:3:ARG:N	2:Z:131:SER:HG	1.99	0.60
7:K:397:GLN:HE22	7:K:411:LEU:HB3	1.66	0.60
2:U:318:ILE:HB	2:U:380:ASN:HB3	1.83	0.60
2:2:318:ILE:HB	2:2:380:ASN:HB3	1.83	0.60
5:F:304:ILE:HA	5:F:385:VAL:HG11	1.84	0.60
7:I:272:VAL:HG13	7:I:329:VAL:HG11	1.83	0.60
6:M:696:TYR:O	6:M:700:GLU:HB3	2.01	0.60
2:R:318:ILE:HB	2:R:380:ASN:HB3	1.83	0.59
2:U:292:ASP:O	2:U:296:ARG:HB2	2.01	0.59
2:Q:318:ILE:HB	2:Q:380:ASN:HB3	1.83	0.59
2:1:3:ARG:N	2:1:131:SER:OG	2.36	0.59
2:1:318:ILE:HB	2:1:380:ASN:HB3	1.83	0.59
7:I:404:LEU:HD11	2:W:47:ARG:HG3	1.85	0.59
2:S:3:ARG:N	2:S:131:SER:OG	2.36	0.59
2:2:3:ARG:N	2:2:131:SER:OG	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:318:ILE:HB	2:S:380:ASN:HB3	1.83	0.59
6:G:577:LEU:HG	6:G:579:PRO:HD3	1.84	0.59
2:T:3:ARG:N	2:T:131:SER:OG	2.36	0.59
2:V:318:ILE:HB	2:V:380:ASN:HB3	1.83	0.59
7:I:404:LEU:HD21	2:W:47:ARG:HA	1.85	0.59
6:M:547:THR:HG22	6:M:549:PRO:HD2	1.84	0.59
2:Y:3:ARG:N	2:Y:131:SER:OG	2.36	0.59
2:V:3:ARG:N	2:V:131:SER:OG	2.36	0.58
2:X:318:ILE:HB	2:X:380:ASN:HB3	1.83	0.58
6:E:556:GLU:HG2	2:T:339:ARG:HE	1.68	0.58
5:F:504:THR:HG21	5:F:537:ALA:HA	1.85	0.58
2:Q:3:ARG:N	2:Q:131:SER:OG	2.36	0.58
2:V:326:GLY:HA2	2:V:363:LYS:HD3	1.85	0.58
2:W:3:ARG:N	2:W:131:SER:OG	2.36	0.58
2:Z:66:LEU:HB3	2:Z:91:ILE:HA	1.85	0.58
6:E:188:ILE:HG22	6:E:244:ARG:HH22	1.67	0.58
6:M:285:TYR:O	6:M:289:ASN:ND2	2.36	0.58
2:R:3:ARG:N	2:R:131:SER:OG	2.36	0.58
2:X:3:ARG:N	2:X:131:SER:OG	2.36	0.58
2:Z:3:ARG:N	2:Z:131:SER:OG	2.36	0.58
2:S:66:LEU:HB3	2:S:91:ILE:HA	1.85	0.58
1:J:255:PRO:HD2	1:J:257:TYR:H	1.68	0.58
2:T:66:LEU:HB3	2:T:91:ILE:HA	1.85	0.58
6:E:174:LEU:HD11	5:F:405:LYS:HD2	1.85	0.58
5:F:270:ASN:HD21	5:F:302:ASN:HD22	1.52	0.58
2:U:3:ARG:N	2:U:131:SER:OG	2.36	0.58
5:F:609:ASN:ND2	2:T:46:ASP:O	2.36	0.58
2:U:66:LEU:HB3	2:U:91:ILE:HA	1.85	0.58
6:E:314:HIS:HB2	6:E:319:LEU:HD23	1.85	0.58
5:F:682:LYS:HB2	2:T:254:ILE:HD11	1.85	0.58
8:L:438:ARG:NH1	8:L:441:GLN:OE1	2.37	0.58
2:R:326:GLY:HA2	2:R:363:LYS:HD3	1.85	0.58
2:W:66:LEU:HB3	2:W:91:ILE:HA	1.85	0.58
2:1:353:PRO:HG2	6:M:685:ARG:HG2	1.85	0.57
2:U:326:GLY:HA2	2:U:363:LYS:HD3	1.85	0.57
2:X:326:GLY:HA2	2:X:363:LYS:HD3	1.85	0.57
2:2:66:LEU:HB3	2:2:91:ILE:HA	1.85	0.57
6:C:614:GLU:HA	6:C:643:ARG:HH12	1.69	0.57
6:M:478:THR:OG1	6:M:481:GLU:O	2.22	0.57
2:Q:66:LEU:HB3	2:Q:91:ILE:HA	1.85	0.57
2:V:66:LEU:HB3	2:V:91:ILE:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:66:LEU:HB3	2:Y:91:ILE:HA	1.85	0.57
2:S:326:GLY:HA2	2:S:363:LYS:HD3	1.85	0.57
2:Y:326:GLY:HA2	2:Y:363:LYS:HD3	1.85	0.57
5:H:308:THR:O	5:H:312:SER:OG	2.21	0.57
2:T:326:GLY:HA2	2:T:363:LYS:HD3	1.85	0.57
2:X:66:LEU:HB3	2:X:91:ILE:HA	1.85	0.57
2:2:326:GLY:HA2	2:2:363:LYS:HD3	1.85	0.57
2:Q:326:GLY:HA2	2:Q:363:LYS:HD3	1.85	0.57
7:I:92:GLY:HA3	7:I:175:ILE:HG12	1.86	0.57
7:K:48:LEU:HD21	7:K:130:GLN:HA	1.87	0.57
5:F:555:LEU:HD13	5:F:651:VAL:HG21	1.87	0.57
5:H:883:ASN:HD21	2:V:350:PRO:HA	1.68	0.57
8:L:324:CYS:HA	8:L:327:HIS:CE1	2.40	0.57
2:W:326:GLY:HA2	2:W:363:LYS:HD3	1.85	0.57
2:Z:326:GLY:HA2	2:Z:363:LYS:HD3	1.85	0.56
2:1:66:LEU:HB3	2:1:91:ILE:HA	1.85	0.56
2:R:66:LEU:HB3	2:R:91:ILE:HA	1.85	0.56
2:1:233:SER:O	2:1:237:SER:OG	2.24	0.56
2:1:326:GLY:HA2	2:1:363:LYS:HD3	1.85	0.56
6:G:395:ILE:HD11	6:G:450:ILE:HG23	1.88	0.56
2:V:303:VAL:HG12	2:V:305:VAL:H	1.71	0.56
2:2:303:VAL:HG12	2:2:305:VAL:H	1.71	0.56
8:L:1589:ASP:H	8:L:1737:LEU:HD13	1.69	0.56
5:F:432:ARG:HH12	5:F:440:GLU:H	1.52	0.56
2:R:233:SER:O	2:R:237:SER:OG	2.24	0.56
2:S:233:SER:O	2:S:237:SER:OG	2.24	0.56
2:Y:233:SER:O	2:Y:237:SER:OG	2.24	0.56
2:2:233:SER:O	2:2:237:SER:OG	2.24	0.56
2:U:303:VAL:HG12	2:U:305:VAL:H	1.71	0.56
2:1:303:VAL:HG12	2:1:305:VAL:H	1.71	0.56
6:C:738:MET:HG3	6:C:745:LEU:HD13	1.88	0.56
5:F:464:TYR:HB3	5:F:484:LEU:HD11	1.88	0.56
6:E:439:ILE:HG22	6:E:441:SER:H	1.71	0.56
2:S:303:VAL:HG12	2:S:305:VAL:H	1.71	0.56
6:E:277:ILE:HD11	6:E:296:MET:HG3	1.87	0.55
2:R:303:VAL:HG12	2:R:305:VAL:H	1.71	0.55
2:X:303:VAL:HG12	2:X:305:VAL:H	1.71	0.55
2:Z:52:PHE:HA	2:Z:62:PRO:HA	1.88	0.55
6:M:696:TYR:O	6:M:700:GLU:CB	2.55	0.55
2:S:52:PHE:HA	2:S:62:PRO:HA	1.89	0.55
2:U:233:SER:O	2:U:237:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:52:PHE:HA	2:X:62:PRO:HA	1.89	0.55
2:Z:233:SER:O	2:Z:237:SER:OG	2.24	0.55
8:L:1592:SER:OG	8:L:1593:CYS:N	2.38	0.55
2:T:303:VAL:HG12	2:T:305:VAL:H	1.71	0.55
2:U:52:PHE:HA	2:U:62:PRO:HA	1.89	0.55
2:Z:303:VAL:HG12	2:Z:305:VAL:H	1.71	0.55
5:D:550:ASN:HD21	5:D:556:LEU:HD22	1.72	0.55
2:R:52:PHE:HA	2:R:62:PRO:HA	1.88	0.55
2:T:52:PHE:HA	2:T:62:PRO:HA	1.89	0.55
2:V:52:PHE:HA	2:V:62:PRO:HA	1.88	0.55
2:2:446:TRP:HB3	5:N:702:HIS:CG	2.42	0.55
5:D:254:ILE:HG13	5:D:366:ARG:HH22	1.72	0.55
5:D:666:PHE:HA	5:D:669:ARG:HE	1.72	0.55
2:W:52:PHE:HA	2:W:62:PRO:HA	1.88	0.55
5:F:378:LEU:HD13	5:F:381:LEU:HD11	1.88	0.55
1:J:881:HIS:CE1	2:X:446:TRP:HD1	2.25	0.55
2:Q:233:SER:O	2:Q:237:SER:OG	2.24	0.55
2:V:233:SER:O	2:V:237:SER:OG	2.24	0.55
8:L:1800:LEU:HD11	2:Z:337:LEU:HG	1.90	0.54
2:W:233:SER:O	2:W:237:SER:OG	2.24	0.54
2:X:233:SER:O	2:X:237:SER:OG	2.24	0.54
6:C:520:PHE:HB3	6:C:642:PHE:HB2	1.89	0.54
6:M:682:LEU:HD13	6:M:685:ARG:HH11	1.72	0.54
2:Q:52:PHE:HA	2:Q:62:PRO:HA	1.88	0.54
2:Q:303:VAL:HG12	2:Q:305:VAL:H	1.71	0.54
2:T:233:SER:O	2:T:237:SER:OG	2.24	0.54
2:1:259:SER:HB3	6:M:691:GLN:HE22	1.72	0.54
5:D:427:LEU:HA	5:D:430:LEU:HD12	1.89	0.54
5:D:601:LEU:HD21	5:D:621:LEU:HD21	1.90	0.54
6:G:271:SER:OG	6:G:275:ARG:NH2	2.41	0.54
2:1:52:PHE:HA	2:1:62:PRO:HA	1.89	0.54
2:2:355:SER:HB2	5:N:713:HIS:NE2	2.23	0.54
5:N:266:ILE:HG12	5:N:277:VAL:HG22	1.89	0.54
2:Q:57:ASP:OD2	2:R:276:LEU:HB3	2.08	0.54
2:Y:303:VAL:HG12	2:Y:305:VAL:H	1.71	0.54
2:2:52:PHE:HA	2:2:62:PRO:HA	1.89	0.54
7:K:534:VAL:HG21	2:Y:248:TYR:HE2	1.71	0.54
2:Y:52:PHE:HA	2:Y:62:PRO:HA	1.88	0.54
6:C:445:LYS:HD3	6:C:482:ARG:HH12	1.73	0.54
7:I:188:SER:O	7:I:192:LEU:HB2	2.08	0.54
5:F:419:LEU:HA	5:F:422:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:222:ASN:OD1	2:1:222:ASN:N	2.41	0.54
6:C:834:LEU:HD13	6:C:868:ARG:HH11	1.73	0.54
5:H:608:THR:HG23	5:H:610:ALA:H	1.72	0.54
2:W:303:VAL:HG12	2:W:305:VAL:H	1.71	0.54
2:Y:222:ASN:N	2:Y:222:ASN:OD1	2.41	0.54
7:K:618:GLY:O	7:K:622:GLN:NE2	2.41	0.54
2:U:222:ASN:OD1	2:U:222:ASN:N	2.41	0.53
2:W:241:THR:HB	2:W:325:GLN:HE22	1.74	0.53
2:Z:222:ASN:OD1	2:Z:222:ASN:N	2.41	0.53
5:N:636:ASP:OD1	5:N:672:ARG:NH1	2.42	0.53
2:U:241:THR:HB	2:U:325:GLN:HE22	1.74	0.53
2:W:66:LEU:HD22	2:W:91:ILE:HG23	1.91	0.53
2:X:237:SER:O	2:X:241:THR:OG1	2.25	0.53
2:1:241:THR:HB	2:1:325:GLN:HE22	1.73	0.53
5:D:885:HIS:CG	2:R:353:PRO:HA	2.43	0.53
6:E:214:GLU:OE2	6:E:320:SER:OG	2.26	0.53
5:H:664:PHE:O	5:H:668:TRP:HB2	2.09	0.53
2:Q:241:THR:HB	2:Q:325:GLN:HE22	1.73	0.53
2:T:241:THR:HB	2:T:325:GLN:HE22	1.73	0.53
2:X:66:LEU:HD22	2:X:91:ILE:HG23	1.91	0.53
2:1:66:LEU:HD22	2:1:91:ILE:HG23	1.91	0.53
2:2:241:THR:HB	2:2:325:GLN:HE22	1.73	0.53
2:S:66:LEU:HD22	2:S:91:ILE:HG23	1.91	0.53
2:S:241:THR:HB	2:S:325:GLN:HE22	1.73	0.53
2:X:222:ASN:OD1	2:X:222:ASN:N	2.41	0.53
2:Z:241:THR:HB	2:Z:325:GLN:HE22	1.73	0.53
2:2:66:LEU:HD22	2:2:91:ILE:HG23	1.91	0.53
5:F:653:THR:HG1	5:F:656:CYS:HG	1.56	0.53
2:V:222:ASN:OD1	2:V:222:ASN:N	2.41	0.53
7:I:5:LEU:HD11	7:I:122:VAL:HG21	1.90	0.53
2:Q:222:ASN:OD1	2:Q:222:ASN:N	2.41	0.53
2:T:66:LEU:HD22	2:T:91:ILE:HG23	1.91	0.53
2:Y:241:THR:HB	2:Y:325:GLN:HE22	1.73	0.53
2:Z:184:GLN:O	2:Z:188:SER:OG	2.27	0.53
2:2:222:ASN:N	2:2:222:ASN:OD1	2.41	0.53
2:R:66:LEU:HD22	2:R:91:ILE:HG23	1.91	0.53
2:U:66:LEU:HD22	2:U:91:ILE:HG23	1.91	0.53
2:W:222:ASN:N	2:W:222:ASN:OD1	2.41	0.53
6:C:757:MET:HA	6:C:761:CYS:HB3	1.91	0.53
2:Q:184:GLN:O	2:Q:188:SER:OG	2.27	0.53
2:X:241:THR:HB	2:X:325:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:554:SER:O	5:H:558:HIS:ND1	2.33	0.53
2:R:222:ASN:N	2:R:222:ASN:OD1	2.41	0.53
2:U:184:GLN:O	2:U:188:SER:OG	2.27	0.53
2:Y:37:VAL:HG12	2:Y:59:HIS:HD2	1.74	0.53
2:Y:66:LEU:HD22	2:Y:91:ILE:HG23	1.91	0.53
2:2:184:GLN:O	2:2:188:SER:OG	2.27	0.52
6:E:559:LEU:HD21	6:E:570:LYS:HD2	1.91	0.52
1:J:889:LYS:HA	2:X:353:PRO:HG2	1.91	0.52
8:L:568:TYR:HB3	8:L:1606:ILE:HD13	1.91	0.52
2:S:37:VAL:HG12	2:S:59:HIS:HD2	1.74	0.52
7:K:143:ILE:HA	7:K:148:ILE:HD12	1.91	0.52
6:M:737:CYS:SG	6:M:738:MET:N	2.81	0.52
2:V:184:GLN:O	2:V:188:SER:OG	2.27	0.52
2:Y:361:SER:OG	2:Y:362:ARG:N	2.43	0.52
2:2:37:VAL:HG12	2:2:59:HIS:HD2	1.74	0.52
5:D:261:ILE:HG21	6:E:255:SER:HB3	1.92	0.52
6:E:387:TYR:HE2	6:E:407:PHE:HD1	1.56	0.52
7:K:66:VAL:HG13	7:K:68:GLN:H	1.74	0.52
5:D:286:SER:OG	5:D:287:LEU:N	2.39	0.52
2:S:361:SER:OG	2:S:362:ARG:N	2.43	0.52
2:T:361:SER:OG	2:T:362:ARG:N	2.43	0.52
6:E:585:GLN:HE21	6:E:744:LEU:HD21	1.74	0.52
2:Q:37:VAL:HG12	2:Q:59:HIS:HD2	1.74	0.52
2:V:37:VAL:HG12	2:V:59:HIS:HD2	1.74	0.52
2:1:184:GLN:O	2:1:188:SER:OG	2.27	0.52
5:H:419:LEU:HA	5:H:422:VAL:HG22	1.92	0.52
7:I:408:ASP:HB2	7:I:410:LEU:H	1.74	0.52
2:1:37:VAL:HG12	2:1:59:HIS:HD2	1.74	0.52
6:E:448:ASP:N	6:E:448:ASP:OD2	2.43	0.52
5:F:619:ARG:HH12	5:F:620:ARG:HH11	1.57	0.52
2:T:222:ASN:N	2:T:222:ASN:OD1	2.41	0.52
2:X:37:VAL:HG12	2:X:59:HIS:HD2	1.74	0.52
2:1:353:PRO:HG3	6:M:865:TYR:CD2	2.45	0.52
6:C:180:TRP:HA	6:C:183:GLU:HB2	1.92	0.52
2:R:184:GLN:O	2:R:188:SER:OG	2.27	0.52
2:R:241:THR:HB	2:R:325:GLN:HE22	1.74	0.52
2:W:361:SER:OG	2:W:362:ARG:N	2.43	0.52
2:2:361:SER:OG	2:2:362:ARG:N	2.43	0.52
7:K:199:GLN:NE2	8:L:510:LEU:O	2.43	0.52
2:S:222:ASN:OD1	2:S:222:ASN:N	2.41	0.52
2:U:37:VAL:HG12	2:U:59:HIS:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:361:SER:OG	2:X:362:ARG:N	2.43	0.52
2:Y:184:GLN:O	2:Y:188:SER:OG	2.27	0.52
2:2:290:VAL:HG23	2:2:336:SER:HB2	1.92	0.52
2:R:37:VAL:HG12	2:R:59:HIS:HD2	1.74	0.52
2:V:66:LEU:HD22	2:V:91:ILE:HG23	1.91	0.52
2:Y:290:VAL:HG23	2:Y:336:SER:HB2	1.92	0.52
2:Z:66:LEU:HD22	2:Z:91:ILE:HG23	1.91	0.52
2:Q:66:LEU:HD22	2:Q:91:ILE:HG23	1.91	0.51
2:S:290:VAL:HG23	2:S:336:SER:HB2	1.92	0.51
2:U:361:SER:OG	2:U:362:ARG:N	2.43	0.51
7:K:192:LEU:HD22	7:K:304:GLU:HG2	1.92	0.51
2:R:290:VAL:HG23	2:R:336:SER:HB2	1.92	0.51
2:V:241:THR:HB	2:V:325:GLN:HE22	1.74	0.51
2:W:184:GLN:O	2:W:188:SER:OG	2.27	0.51
6:G:428:TRP:CD1	6:G:628:LEU:HB3	2.46	0.51
2:U:290:VAL:HG23	2:U:336:SER:HB2	1.92	0.51
2:X:184:GLN:O	2:X:188:SER:OG	2.27	0.51
5:F:433:TRP:HZ2	5:F:484:LEU:HD12	1.75	0.51
7:I:37:SER:O	7:I:40:SER:OG	2.29	0.51
7:K:353:GLN:HG3	7:K:463:LEU:HD13	1.93	0.51
2:T:37:VAL:HG12	2:T:59:HIS:HD2	1.74	0.51
2:W:53:TYR:HB2	2:W:63:ARG:HG2	1.93	0.51
6:C:763:GLN:HG3	6:C:766:THR:H	1.75	0.51
2:T:53:TYR:HB2	2:T:63:ARG:HG2	1.93	0.51
2:V:361:SER:OG	2:V:362:ARG:N	2.43	0.51
2:X:290:VAL:HG23	2:X:336:SER:HB2	1.92	0.51
2:Z:290:VAL:HG23	2:Z:336:SER:HB2	1.92	0.51
8:L:1609:THR:HG22	8:L:1611:GLY:H	1.76	0.51
2:Y:53:TYR:HB2	2:Y:63:ARG:HG2	1.93	0.51
2:Z:361:SER:OG	2:Z:362:ARG:N	2.43	0.51
2:1:361:SER:OG	2:1:362:ARG:N	2.43	0.51
2:2:53:TYR:HB2	2:2:63:ARG:HG2	1.93	0.51
5:D:726:VAL:HG13	5:D:761:ARG:HB2	1.93	0.51
2:Q:361:SER:OG	2:Q:362:ARG:N	2.43	0.51
2:R:53:TYR:HB2	2:R:63:ARG:HG2	1.93	0.51
2:W:37:VAL:HG12	2:W:59:HIS:HD2	1.74	0.51
2:Z:37:VAL:HG12	2:Z:59:HIS:HD2	1.74	0.51
2:T:184:GLN:O	2:T:188:SER:OG	2.27	0.51
2:Z:53:TYR:HB2	2:Z:63:ARG:HG2	1.93	0.51
2:1:53:TYR:HB2	2:1:63:ARG:HG2	1.93	0.51
2:1:290:VAL:HG23	2:1:336:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:439:ILE:HD12	6:C:444:GLN:HE22	1.76	0.51
5:F:449:ALA:HB2	5:F:467:ARG:HB2	1.92	0.51
2:T:237:SER:O	2:T:241:THR:OG1	2.25	0.51
2:U:53:TYR:HB2	2:U:63:ARG:HG2	1.93	0.51
5:H:631:GLY:HA3	5:H:637:VAL:HG23	1.93	0.50
1:J:316:GLN:NE2	1:J:320:TYR:OH	2.31	0.50
1:J:899:ASN:O	1:J:903:THR:OG1	2.28	0.50
7:K:176:LEU:HG	7:K:180:HIS:CE1	2.46	0.50
2:S:184:GLN:O	2:S:188:SER:OG	2.27	0.50
2:X:35:GLY:HA2	2:X:85:LEU:HD12	1.94	0.50
7:I:345:VAL:HG23	7:I:346:GLU:HG3	1.92	0.50
2:Q:290:VAL:HG23	2:Q:336:SER:HB2	1.92	0.50
2:Y:35:GLY:HA2	2:Y:85:LEU:HD12	1.94	0.50
6:C:266:VAL:HG21	6:C:328:ILE:HD12	1.93	0.50
2:V:290:VAL:HG23	2:V:336:SER:HB2	1.92	0.50
2:Q:53:TYR:HB2	2:Q:63:ARG:HG2	1.93	0.50
2:V:53:TYR:HB2	2:V:63:ARG:HG2	1.93	0.50
2:R:361:SER:OG	2:R:362:ARG:N	2.43	0.50
2:W:35:GLY:HA2	2:W:85:LEU:HD12	1.93	0.50
2:T:35:GLY:HA2	2:T:85:LEU:HD12	1.94	0.50
2:T:290:VAL:HG23	2:T:336:SER:HB2	1.92	0.50
2:V:35:GLY:HA2	2:V:85:LEU:HD12	1.93	0.50
6:E:695:TYR:HE1	2:S:249:MET:HG3	1.76	0.49
7:I:397:GLN:HB3	7:I:409:ASN:HD22	1.75	0.49
6:M:377:LEU:O	6:M:380:THR:OG1	2.31	0.49
5:N:608:THR:HG23	5:N:610:ALA:H	1.77	0.49
2:S:53:TYR:HB2	2:S:63:ARG:HG2	1.93	0.49
2:U:35:GLY:HA2	2:U:85:LEU:HD12	1.94	0.49
2:W:290:VAL:HG23	2:W:336:SER:HB2	1.92	0.49
5:D:613:ASP:HB2	5:D:617:ILE:HD11	1.93	0.49
1:J:220:VAL:HG13	8:L:311:TYR:HA	1.94	0.49
2:Z:35:GLY:HA2	2:Z:85:LEU:HD12	1.94	0.49
2:2:35:GLY:HA2	2:2:85:LEU:HD12	1.94	0.49
2:S:124:ARG:HG3	2:T:301:LYS:NZ	2.27	0.49
2:X:53:TYR:HB2	2:X:63:ARG:HG2	1.93	0.49
6:C:563:THR:HG21	2:Q:246:PRO:HG3	1.94	0.49
6:E:280:LYS:HD2	6:E:289:ASN:HD21	1.76	0.49
2:1:35:GLY:HA2	2:1:85:LEU:HD12	1.94	0.49
5:F:259:GLN:HG2	5:F:336:TYR:HE1	1.76	0.49
5:F:279:GLY:HA3	5:F:287:LEU:HD11	1.94	0.49
5:N:564:ARG:HB3	5:N:570:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:35:GLY:HA2	2:Q:85:LEU:HD12	1.94	0.49
2:1:237:SER:O	2:1:241:THR:OG1	2.25	0.49
5:D:333:ARG:HG3	6:E:329:GLN:HG3	1.95	0.49
6:E:432:TYR:OH	6:E:458:ASN:ND2	2.36	0.49
5:H:884:GLU:OE2	2:V:344:LYS:NZ	2.45	0.49
5:N:270:ASN:HD22	5:N:273:ASN:HB2	1.78	0.49
5:F:710:GLU:HG2	2:T:353:PRO:HG2	1.94	0.49
7:K:192:LEU:HD21	7:K:307:PHE:HD2	1.77	0.49
7:K:540:GLN:HE21	7:K:564:PHE:HA	1.78	0.49
2:R:35:GLY:HA2	2:R:85:LEU:HD12	1.94	0.49
2:2:248:TYR:HD2	5:N:723:THR:HG23	1.78	0.49
5:D:720:TYR:HE1	2:R:249:MET:HG3	1.78	0.49
7:K:176:LEU:O	7:K:180:HIS:ND1	2.45	0.49
6:M:277:ILE:HD11	6:M:296:MET:HB3	1.95	0.49
2:T:262:PRO:HG3	2:T:318:ILE:HG21	1.95	0.49
6:E:837:LEU:HD22	6:E:856:ILE:HG12	1.94	0.49
5:F:432:ARG:NH1	5:F:440:GLU:OE1	2.45	0.49
7:I:282:SER:HB3	7:I:340:LEU:HD11	1.95	0.49
6:M:834:LEU:HD11	6:M:868:ARG:HB2	1.94	0.49
2:X:262:PRO:HG3	2:X:318:ILE:HG21	1.95	0.49
2:Z:262:PRO:HG3	2:Z:318:ILE:HG21	1.95	0.49
2:Q:387:LEU:HA	2:Q:390:ARG:HD3	1.95	0.49
2:W:387:LEU:HA	2:W:390:ARG:HD3	1.95	0.49
7:I:508:ASN:C	7:I:510:THR:H	2.17	0.48
6:C:221:LEU:HD11	6:C:260:VAL:HG22	1.95	0.48
6:G:526:ASP:HA	6:G:529:VAL:HG12	1.95	0.48
2:U:262:PRO:HG3	2:U:318:ILE:HG21	1.95	0.48
2:W:262:PRO:HG3	2:W:318:ILE:HG21	1.95	0.48
5:F:554:SER:O	5:F:554:SER:OG	2.31	0.48
6:G:578:MET:HG3	6:G:643:ARG:HD3	1.94	0.48
5:H:627:GLU:HB2	5:H:630:PRO:HG2	1.94	0.48
2:S:35:GLY:HA2	2:S:85:LEU:HD12	1.94	0.48
2:Y:387:LEU:HA	2:Y:390:ARG:HD3	1.95	0.48
2:1:56:ASP:HB3	2:2:276:LEU:HD22	1.94	0.48
5:F:317:PHE:HB3	5:F:322:GLN:HE21	1.77	0.48
1:J:398:VAL:HA	1:J:401:LYS:HE2	1.94	0.48
2:Q:262:PRO:HG3	2:Q:318:ILE:HG21	1.95	0.48
2:V:262:PRO:HG3	2:V:318:ILE:HG21	1.95	0.48
2:Z:387:LEU:HA	2:Z:390:ARG:HD3	1.95	0.48
2:2:237:SER:O	2:2:241:THR:OG1	2.25	0.48
6:G:566:THR:HG22	2:U:45:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:554:SER:O	5:H:554:SER:OG	2.30	0.48
6:M:175:PRO:HG3	5:N:402:ALA:HB1	1.94	0.48
2:X:387:LEU:HA	2:X:390:ARG:HD3	1.95	0.48
2:Y:262:PRO:HG3	2:Y:318:ILE:HG21	1.95	0.48
6:G:305:ILE:HG22	6:G:309:GLN:HE21	1.78	0.48
8:L:1572:LEU:HD22	8:L:1599:LYS:H	1.79	0.48
2:S:347:ASN:OD1	2:S:347:ASN:N	2.47	0.48
2:T:347:ASN:OD1	2:T:347:ASN:N	2.47	0.48
2:U:387:LEU:HA	2:U:390:ARG:HD3	1.95	0.48
5:H:887:LYS:HA	5:H:890:GLU:HB2	1.96	0.48
2:V:407:GLN:NE2	2:V:408:PHE:O	2.47	0.48
6:C:175:PRO:HB3	5:D:402:ALA:HB1	1.95	0.48
6:C:187:LEU:HA	5:D:379:LYS:HE2	1.96	0.48
5:D:406:THR:HG23	5:D:412:ARG:HG2	1.96	0.48
2:R:237:SER:O	2:R:241:THR:OG1	2.25	0.48
2:1:387:LEU:HA	2:1:390:ARG:HD3	1.95	0.48
2:Z:237:SER:O	2:Z:241:THR:OG1	2.25	0.48
6:C:302:GLU:HA	6:C:305:ILE:HD12	1.96	0.47
5:F:568:LEU:HD22	5:F:667:LEU:HG	1.95	0.47
8:L:1667:HIS:CE1	2:Z:355:SER:H	2.32	0.47
2:U:347:ASN:OD1	2:U:347:ASN:N	2.47	0.47
2:1:262:PRO:HG3	2:1:318:ILE:HG21	1.95	0.47
2:2:407:GLN:NE2	2:2:408:PHE:O	2.47	0.47
7:K:283:VAL:O	7:K:287:GLU:HB2	2.14	0.47
2:1:237:SER:O	2:1:244:ARG:NH2	2.48	0.47
6:C:862:ASN:HB2	6:C:864:PHE:CZ	2.49	0.47
2:Z:237:SER:O	2:Z:244:ARG:NH2	2.48	0.47
2:1:407:GLN:NE2	2:1:408:PHE:O	2.47	0.47
2:2:387:LEU:HA	2:2:390:ARG:HD3	1.95	0.47
6:G:446:MET:SD	6:G:446:MET:N	2.87	0.47
2:V:237:SER:O	2:V:244:ARG:NH2	2.48	0.47
2:W:407:GLN:NE2	2:W:408:PHE:O	2.47	0.47
2:2:262:PRO:HG3	2:2:318:ILE:HG21	1.95	0.47
5:D:587:ARG:HH12	5:D:592:LEU:HB2	1.79	0.47
6:M:533:ASP:OD2	6:M:653:ARG:NH2	2.48	0.47
5:N:333:ARG:HE	5:N:337:ARG:HH11	1.62	0.47
2:Q:237:SER:O	2:Q:244:ARG:NH2	2.48	0.47
2:V:387:LEU:HA	2:V:390:ARG:HD3	1.95	0.47
2:Y:407:GLN:NE2	2:Y:408:PHE:O	2.47	0.47
2:Z:347:ASN:OD1	2:Z:347:ASN:N	2.47	0.47
6:C:559:LEU:HD21	6:C:570:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:644:HIS:HE1	6:C:738:MET:HB2	1.79	0.47
6:E:416:LYS:H	6:E:419:ILE:HB	1.80	0.47
2:T:387:LEU:HA	2:T:390:ARG:HD3	1.95	0.47
2:T:407:GLN:NE2	2:T:408:PHE:O	2.47	0.47
2:2:68:ASP:OD2	2:2:68:ASP:N	2.48	0.47
6:C:482:ARG:HD2	6:C:485:VAL:HG21	1.97	0.47
6:E:517:LYS:HZ2	6:E:706:TRP:HE1	1.62	0.47
5:F:302:ASN:O	5:F:306:ARG:HB2	2.15	0.47
6:G:238:LEU:HD11	6:G:241:ARG:HH21	1.79	0.47
6:M:223:TYR:OH	5:N:366:ARG:NH2	2.47	0.47
6:M:713:LEU:HD22	6:M:722:VAL:HG13	1.96	0.47
2:R:68:ASP:OD2	2:R:68:ASP:N	2.48	0.47
2:S:262:PRO:HG3	2:S:318:ILE:HG21	1.95	0.47
2:S:387:LEU:HA	2:S:390:ARG:HD3	1.95	0.47
2:U:237:SER:O	2:U:241:THR:OG1	2.25	0.47
2:U:407:GLN:NE2	2:U:408:PHE:O	2.47	0.47
2:2:347:ASN:OD1	2:2:347:ASN:N	2.47	0.47
2:R:387:LEU:HA	2:R:390:ARG:HD3	1.95	0.47
6:E:442:PHE:CE1	6:E:484:TYR:HE1	2.33	0.47
2:Y:384:ILE:HD12	2:Y:387:LEU:HD12	1.97	0.47
6:C:857:SER:O	2:Q:341:ARG:NE	2.48	0.47
2:R:237:SER:O	2:R:244:ARG:NH2	2.48	0.47
2:W:68:ASP:OD2	2:W:68:ASP:N	2.48	0.47
2:Z:407:GLN:NE2	2:Z:408:PHE:O	2.47	0.47
2:1:384:ILE:HD12	2:1:387:LEU:HD12	1.97	0.46
2:2:89:GLU:O	2:2:124:ARG:NH2	2.48	0.46
6:C:234:SER:HG	5:D:286:SER:N	2.13	0.46
5:N:361:SER:OG	5:N:362:LEU:N	2.48	0.46
2:R:407:GLN:NE2	2:R:408:PHE:O	2.47	0.46
2:S:89:GLU:O	2:S:124:ARG:NH2	2.48	0.46
2:X:68:ASP:OD2	2:X:68:ASP:N	2.48	0.46
2:Y:89:GLU:O	2:Y:124:ARG:NH2	2.49	0.46
2:2:274:THR:HG21	2:2:293:VAL:HG12	1.97	0.46
6:M:559:LEU:HD11	6:M:570:LYS:HB2	1.97	0.46
2:Q:68:ASP:OD2	2:Q:68:ASP:N	2.48	0.46
2:R:262:PRO:HG3	2:R:318:ILE:HG21	1.95	0.46
2:W:237:SER:O	2:W:244:ARG:NH2	2.48	0.46
2:1:68:ASP:OD2	2:1:68:ASP:N	2.48	0.46
2:2:384:ILE:HD12	2:2:387:LEU:HD12	1.97	0.46
7:I:511:ASP:H	7:I:514:LYS:HG2	1.80	0.46
6:M:581:ASP:HB2	6:M:615:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:384:ILE:HD12	2:S:387:LEU:HD12	1.97	0.46
2:U:274:THR:HG21	2:U:293:VAL:HG12	1.97	0.46
2:W:292:ASP:HA	2:W:296:ARG:HH21	1.81	0.46
2:X:89:GLU:O	2:X:124:ARG:NH2	2.48	0.46
2:Y:68:ASP:OD2	2:Y:68:ASP:N	2.48	0.46
2:1:274:THR:HG21	2:1:293:VAL:HG12	1.97	0.46
7:K:647:LEU:HD22	2:Y:337:LEU:HD23	1.97	0.46
2:Q:89:GLU:O	2:Q:124:ARG:NH2	2.49	0.46
2:T:68:ASP:OD2	2:T:68:ASP:N	2.48	0.46
2:U:237:SER:O	2:U:244:ARG:NH2	2.48	0.46
2:W:274:THR:HG21	2:W:293:VAL:HG12	1.97	0.46
2:X:407:GLN:NE2	2:X:408:PHE:O	2.47	0.46
2:1:172:PHE:N	2:1:205:LEU:O	2.49	0.46
5:D:689:LYS:HA	5:D:692:ARG:NE	2.31	0.46
6:E:427:TYR:OH	6:E:455:LYS:O	2.31	0.46
2:U:292:ASP:HA	2:U:296:ARG:HH21	1.81	0.46
2:V:89:GLU:O	2:V:124:ARG:NH2	2.49	0.46
2:W:89:GLU:O	2:W:124:ARG:NH2	2.49	0.46
2:X:384:ILE:HD12	2:X:387:LEU:HD12	1.97	0.46
2:Z:89:GLU:O	2:Z:124:ARG:NH2	2.48	0.46
2:1:89:GLU:O	2:1:124:ARG:NH2	2.49	0.46
6:G:162:ARG:O	6:G:166:ASN:ND2	2.48	0.46
1:J:902:MET:HG3	2:X:248:TYR:CE2	2.51	0.46
7:K:341:TRP:CE2	7:K:552:ARG:HA	2.51	0.46
8:L:533:THR:O	8:L:537:HIS:HB2	2.15	0.46
6:M:761:CYS:SG	6:M:762:MET:N	2.89	0.46
2:R:89:GLU:O	2:R:124:ARG:NH2	2.48	0.46
2:R:292:ASP:HA	2:R:296:ARG:HH21	1.81	0.46
2:T:323:ILE:HD12	2:T:323:ILE:HA	1.81	0.46
6:E:628:LEU:H	6:E:628:LEU:HG	1.56	0.46
2:T:172:PHE:N	2:T:205:LEU:O	2.49	0.46
2:X:56:ASP:OD1	2:Y:287:LYS:HD2	2.16	0.46
2:Y:292:ASP:HA	2:Y:296:ARG:HH21	1.81	0.46
2:2:172:PHE:N	2:2:205:LEU:O	2.49	0.46
2:2:353:PRO:HD2	5:N:710:GLU:HG2	1.97	0.46
6:E:529:VAL:O	2:S:3:ARG:NH1	2.49	0.46
7:I:357:ILE:O	7:I:361:TYR:CB	2.62	0.46
7:I:498:LEU:HA	7:I:502:ARG:HB2	1.97	0.46
2:Q:292:ASP:HA	2:Q:296:ARG:HH21	1.81	0.46
2:R:384:ILE:HD12	2:R:387:LEU:HD12	1.97	0.46
2:S:237:SER:O	2:S:241:THR:OG1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:292:ASP:HA	2:S:296:ARG:HH21	1.81	0.46
2:T:237:SER:O	2:T:244:ARG:NH2	2.48	0.46
2:U:68:ASP:N	2:U:68:ASP:OD2	2.48	0.46
2:V:274:THR:HG21	2:V:293:VAL:HG12	1.97	0.46
2:X:292:ASP:HA	2:X:296:ARG:HH21	1.81	0.46
6:E:457:LEU:HD22	6:E:467:VAL:HG12	1.97	0.46
5:H:730:SER:HA	5:H:733:GLU:HG3	1.98	0.46
2:Q:384:ILE:HD12	2:Q:387:LEU:HD12	1.97	0.46
2:S:274:THR:HG21	2:S:293:VAL:HG12	1.97	0.46
2:T:274:THR:HG21	2:T:293:VAL:HG12	1.97	0.46
2:U:89:GLU:O	2:U:124:ARG:NH2	2.48	0.46
2:V:68:ASP:OD2	2:V:68:ASP:N	2.48	0.46
2:Y:172:PHE:N	2:Y:205:LEU:O	2.49	0.46
2:Z:384:ILE:HD12	2:Z:387:LEU:HD12	1.97	0.46
6:E:238:LEU:HD23	6:E:244:ARG:H	1.80	0.46
2:U:172:PHE:N	2:U:205:LEU:O	2.49	0.46
2:U:323:ILE:HD12	2:U:323:ILE:HA	1.81	0.46
5:D:425:PRO:O	5:D:428:SER:OG	2.33	0.45
5:F:397:ALA:O	5:F:473:SER:OG	2.33	0.45
5:H:482:LYS:HD2	5:H:538:TYR:CZ	2.51	0.45
1:J:275:LEU:HA	1:J:379:LEU:HD12	1.97	0.45
1:J:879:GLN:HB3	1:J:880:ILE:HD12	1.98	0.45
2:T:89:GLU:O	2:T:124:ARG:NH2	2.48	0.45
2:X:237:SER:O	2:X:244:ARG:NH2	2.48	0.45
2:2:237:SER:O	2:2:244:ARG:NH2	2.48	0.45
6:E:338:LEU:HD11	6:E:375:LEU:HD21	1.97	0.45
7:K:176:LEU:HG	7:K:180:HIS:HE1	1.81	0.45
6:M:705:THR:HA	6:M:708:ILE:HG22	1.98	0.45
2:W:347:ASN:OD1	2:W:347:ASN:N	2.47	0.45
2:Y:237:SER:O	2:Y:244:ARG:NH2	2.48	0.45
2:Z:274:THR:HG21	2:Z:293:VAL:HG12	1.97	0.45
2:2:292:ASP:HA	2:2:296:ARG:HH21	1.81	0.45
5:D:254:ILE:HB	5:D:366:ARG:HH12	1.81	0.45
6:E:427:TYR:CD2	6:E:431:ARG:HD3	2.51	0.45
5:N:364:LEU:HD13	5:N:370:TRP:HE1	1.81	0.45
2:T:292:ASP:HA	2:T:296:ARG:HH21	1.81	0.45
2:T:384:ILE:HD12	2:T:387:LEU:HD12	1.97	0.45
2:V:384:ILE:HD12	2:V:387:LEU:HD12	1.97	0.45
2:Y:274:THR:HG21	2:Y:293:VAL:HG12	1.97	0.45
6:E:241:ARG:HH21	6:E:242:GLN:NE2	2.15	0.45
1:J:879:GLN:N	1:J:879:GLN:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:882:ARG:NH2	1:J:984:GLU:OE2	2.50	0.45
7:K:577:LYS:O	7:K:581:HIS:HB2	2.15	0.45
2:Q:407:GLN:NE2	2:Q:408:PHE:O	2.47	0.45
2:S:323:ILE:HD12	2:S:323:ILE:HA	1.81	0.45
2:W:384:ILE:HD12	2:W:387:LEU:HD12	1.97	0.45
2:X:274:THR:HG21	2:X:293:VAL:HG12	1.97	0.45
2:Z:68:ASP:N	2:Z:68:ASP:OD2	2.48	0.45
6:E:427:TYR:HB3	6:E:624:TRP:HZ2	1.80	0.45
5:F:480:SER:HA	5:F:483:VAL:HG22	1.98	0.45
8:L:322:LYS:HG3	8:L:325:ARG:NH2	2.31	0.45
2:S:68:ASP:OD2	2:S:68:ASP:N	2.48	0.45
6:M:654:GLN:HB3	6:M:759:THR:HG21	1.98	0.45
2:Q:274:THR:HG21	2:Q:293:VAL:HG12	1.97	0.45
2:R:274:THR:HG21	2:R:293:VAL:HG12	1.97	0.45
2:U:384:ILE:HD12	2:U:387:LEU:HD12	1.97	0.45
6:C:865:TYR:CD1	2:Q:353:PRO:HG3	2.52	0.45
5:H:321:GLY:HA2	5:H:324:PHE:HB3	1.99	0.45
8:L:1679:GLN:HB3	8:L:1715:ARG:HB3	1.99	0.45
6:M:499:LEU:HD23	6:M:719:ILE:HG13	1.98	0.45
2:S:237:SER:O	2:S:244:ARG:NH2	2.48	0.45
5:F:406:THR:HG22	5:F:408:ASP:H	1.81	0.45
7:I:256:GLN:HB3	7:I:257:PHE:H	1.67	0.45
7:I:397:GLN:HB3	7:I:409:ASN:ND2	2.32	0.45
2:U:343:ARG:HG3	2:U:345:LEU:HB2	1.99	0.45
2:V:172:PHE:N	2:V:205:LEU:O	2.49	0.45
2:W:29:HIS:HE1	2:W:244:ARG:HD2	1.82	0.45
2:1:296:ARG:HH11	2:1:296:ARG:HD3	1.59	0.45
2:1:343:ARG:HG3	2:1:345:LEU:HB2	1.99	0.45
7:I:504:HIS:HD2	2:W:265:ARG:HH12	1.65	0.45
6:M:157:LYS:HG2	6:M:284:GLU:HG3	1.99	0.45
5:N:680:ILE:HD11	5:N:786:GLN:HA	1.98	0.45
2:Z:292:ASP:HA	2:Z:296:ARG:HH21	1.81	0.45
2:1:292:ASP:HA	2:1:296:ARG:HH21	1.81	0.45
6:C:551:LEU:HA	6:C:551:LEU:HD12	1.80	0.45
6:E:241:ARG:HH21	6:E:242:GLN:HE22	1.63	0.45
2:R:343:ARG:HG3	2:R:345:LEU:HB2	1.99	0.45
2:W:343:ARG:HG3	2:W:345:LEU:HB2	1.99	0.45
6:C:218:VAL:HG13	6:C:314:HIS:NE2	2.31	0.44
6:G:276:PHE:CE1	6:G:280:LYS:HG3	2.51	0.44
6:M:456:TYR:HA	6:M:459:VAL:HG22	1.98	0.44
2:S:262:PRO:HG2	2:S:263:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:29:HIS:HE1	2:V:244:ARG:HD2	1.82	0.44
2:V:296:ARG:HH11	2:V:296:ARG:HD3	1.59	0.44
2:Y:343:ARG:HG3	2:Y:345:LEU:HB2	1.99	0.44
2:2:29:HIS:HE1	2:2:244:ARG:HD2	1.82	0.44
2:2:343:ARG:HG3	2:2:345:LEU:HB2	1.99	0.44
5:F:388:CYS:HA	5:F:391:ARG:HE	1.82	0.44
6:G:529:VAL:HG22	2:U:3:ARG:HH12	1.82	0.44
6:M:208:LEU:O	6:M:213:GLN:NE2	2.50	0.44
2:R:347:ASN:OD1	2:R:347:ASN:N	2.47	0.44
2:W:57:ASP:HA	2:X:296:ARG:NH1	2.32	0.44
2:X:183:VAL:HG13	2:X:187:ASN:HD21	1.83	0.44
2:X:343:ARG:HG3	2:X:345:LEU:HB2	1.99	0.44
2:Z:172:PHE:N	2:Z:205:LEU:O	2.49	0.44
1:J:391:THR:N	8:L:307:ARG:HH12	2.16	0.44
2:Q:29:HIS:HE1	2:Q:244:ARG:HD2	1.82	0.44
2:R:172:PHE:N	2:R:205:LEU:O	2.49	0.44
2:S:183:VAL:HG13	2:S:187:ASN:HD21	1.83	0.44
2:V:277:THR:HG22	2:V:279:ASP:H	1.83	0.44
2:W:277:THR:HG22	2:W:279:ASP:H	1.83	0.44
6:C:719:ILE:HG22	6:C:723:LEU:HD23	1.99	0.44
5:D:277:VAL:HG13	5:D:288:ARG:HD2	2.00	0.44
6:E:296:MET:HE2	6:E:300:VAL:HG23	2.00	0.44
7:K:328:VAL:HG23	7:K:331:ARG:HH21	1.81	0.44
2:Q:277:THR:HG22	2:Q:279:ASP:H	1.83	0.44
2:S:407:GLN:NE2	2:S:408:PHE:O	2.47	0.44
2:T:277:THR:HG22	2:T:279:ASP:H	1.83	0.44
2:V:292:ASP:HA	2:V:296:ARG:HH21	1.81	0.44
2:W:183:VAL:HG13	2:W:187:ASN:HD21	1.83	0.44
6:C:611:SER:OG	6:C:612:GLY:N	2.50	0.44
2:Q:262:PRO:HG2	2:Q:263:THR:HG22	2.00	0.44
2:R:262:PRO:HG2	2:R:263:THR:HG22	2.00	0.44
2:1:277:THR:HG22	2:1:279:ASP:H	1.83	0.44
6:C:516:ILE:HG23	6:C:638:TYR:CE2	2.53	0.44
6:C:520:PHE:CZ	6:C:618:PHE:HB2	2.52	0.44
6:E:288:VAL:HG11	6:E:356:LEU:HD12	2.00	0.44
6:M:548:PRO:HA	6:M:551:LEU:HD12	1.99	0.44
2:R:277:THR:HG22	2:R:279:ASP:H	1.83	0.44
2:U:396:ASP:OD2	2:U:425:ARG:NH2	2.47	0.44
2:Y:350:PRO:HG2	2:Y:441:PRO:HG3	2.00	0.44
6:E:158:ARG:HB3	6:E:162:ARG:HH21	1.82	0.44
5:N:327:ALA:HB2	5:N:421:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:183:VAL:HG13	2:Q:187:ASN:HD21	1.83	0.44
2:T:262:PRO:HG2	2:T:263:THR:HG22	2.00	0.44
2:U:29:HIS:HE1	2:U:244:ARG:HD2	1.82	0.44
2:W:350:PRO:HG2	2:W:441:PRO:HG3	2.00	0.44
2:X:172:PHE:N	2:X:205:LEU:O	2.49	0.44
2:X:262:PRO:HG2	2:X:263:THR:HG22	2.00	0.44
8:L:1804:PHE:CD1	2:Z:355:SER:HB3	2.52	0.44
2:R:323:ILE:HD12	2:R:323:ILE:HA	1.81	0.44
2:T:343:ARG:HG3	2:T:345:LEU:HB2	1.99	0.44
2:U:262:PRO:HG2	2:U:263:THR:HG22	2.00	0.44
2:Z:29:HIS:HE1	2:Z:244:ARG:HD2	1.82	0.44
2:1:183:VAL:HG13	2:1:187:ASN:HD21	1.83	0.44
2:1:355:SER:OG	6:M:861:PHE:HB3	2.18	0.44
2:2:262:PRO:HG2	2:2:263:THR:HG22	1.99	0.44
6:E:663:LYS:NZ	2:S:164:LYS:O	2.40	0.44
6:E:663:LYS:NZ	2:S:200:ASP:OD1	2.51	0.44
5:H:361:SER:OG	5:H:362:LEU:N	2.50	0.44
2:T:396:ASP:OD2	2:T:425:ARG:NH2	2.47	0.44
2:V:183:VAL:HG13	2:V:187:ASN:HD21	1.83	0.44
2:Z:262:PRO:HG2	2:Z:263:THR:HG22	2.00	0.44
2:1:29:HIS:HE1	2:1:244:ARG:HD2	1.82	0.43
2:1:350:PRO:HG2	2:1:441:PRO:HG3	2.00	0.43
2:2:323:ILE:HD12	2:2:323:ILE:HA	1.81	0.43
6:G:359:LEU:HB3	6:G:380:THR:HG22	2.00	0.43
2:R:183:VAL:HG13	2:R:187:ASN:HD21	1.83	0.43
2:S:29:HIS:HE1	2:S:244:ARG:HD2	1.82	0.43
2:T:29:HIS:HE1	2:T:244:ARG:HD2	1.82	0.43
5:D:337:ARG:HB2	6:E:326:PHE:CE1	2.53	0.43
5:D:581:LEU:HD21	5:D:597:LEU:HD23	2.00	0.43
6:G:529:VAL:O	2:U:3:ARG:NH1	2.51	0.43
7:K:275:LYS:HB3	7:K:333:ARG:HG3	2.00	0.43
7:K:497:ALA:HB2	2:Y:254:ILE:HD11	1.99	0.43
2:W:172:PHE:N	2:W:205:LEU:O	2.49	0.43
2:W:262:PRO:HG2	2:W:263:THR:HG22	2.00	0.43
2:X:347:ASN:OD1	2:X:347:ASN:N	2.47	0.43
2:2:183:VAL:HG13	2:2:187:ASN:HD21	1.83	0.43
7:I:448:SER:OG	7:I:449:GLY:N	2.50	0.43
1:J:283:LYS:HD2	1:J:283:LYS:HA	1.78	0.43
7:K:11:GLY:HA2	7:K:53:ILE:HG12	2.00	0.43
6:M:610:LEU:HB3	6:M:613:LEU:HD13	2.00	0.43
2:Q:343:ARG:HG3	2:Q:345:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:29:HIS:HE1	2:R:244:ARG:HD2	1.82	0.43
2:T:296:ARG:HH11	2:T:296:ARG:HD3	1.59	0.43
2:Y:277:THR:HG22	2:Y:279:ASP:H	1.83	0.43
2:Z:183:VAL:HG13	2:Z:187:ASN:HD21	1.83	0.43
2:Z:277:THR:HG22	2:Z:279:ASP:H	1.83	0.43
5:D:688:ALA:O	5:D:692:ARG:HG3	2.17	0.43
5:N:654:ARG:HA	5:N:657:MET:HG2	2.00	0.43
2:R:20:GLU:OE1	2:R:230:GLN:NE2	2.52	0.43
2:R:69:LEU:HD12	2:R:69:LEU:HA	1.88	0.43
2:S:20:GLU:OE1	2:S:230:GLN:NE2	2.52	0.43
2:S:277:THR:HG22	2:S:279:ASP:H	1.83	0.43
2:T:183:VAL:HG13	2:T:187:ASN:HD21	1.83	0.43
2:V:396:ASP:OD2	2:V:425:ARG:NH2	2.47	0.43
2:W:20:GLU:OE1	2:W:230:GLN:NE2	2.52	0.43
2:Y:237:SER:O	2:Y:241:THR:OG1	2.25	0.43
2:1:297:LEU:HD12	2:1:297:LEU:HA	1.91	0.43
6:E:821:THR:HA	6:E:824:LYS:HG2	2.00	0.43
7:I:498:LEU:HD11	7:I:517:LEU:HD22	2.00	0.43
8:L:350:CYS:HB2	8:L:453:THR:HG21	1.99	0.43
2:U:183:VAL:HG13	2:U:187:ASN:HD21	1.83	0.43
2:V:343:ARG:HG3	2:V:345:LEU:HB2	1.99	0.43
2:1:262:PRO:HG2	2:1:263:THR:HG22	2.00	0.43
6:E:180:TRP:O	6:E:184:ARG:HG2	2.18	0.43
6:E:713:LEU:HD22	6:E:722:VAL:HG13	2.00	0.43
6:G:449:LYS:O	6:G:453:THR:OG1	2.30	0.43
2:Z:343:ARG:HG3	2:Z:345:LEU:HB2	1.99	0.43
2:1:110:GLN:HA	2:1:113:LYS:HE3	2.01	0.43
2:2:277:THR:HG22	2:2:279:ASP:H	1.83	0.43
6:C:692:ASN:HD22	6:C:859:LEU:HD23	1.82	0.43
5:D:409:PRO:HA	5:D:412:ARG:HB2	2.01	0.43
6:E:320:SER:OG	6:E:321:LEU:N	2.51	0.43
6:E:674:GLN:HB2	6:E:675:TRP:H	1.62	0.43
5:F:400:VAL:HG11	5:F:422:VAL:HG21	1.99	0.43
8:L:469:GLN:HA	8:L:517:HIS:CE1	2.53	0.43
2:Q:110:GLN:HA	2:Q:113:LYS:HE3	2.01	0.43
2:S:172:PHE:N	2:S:205:LEU:O	2.49	0.43
2:T:110:GLN:HA	2:T:113:LYS:HE3	2.01	0.43
2:U:110:GLN:HA	2:U:113:LYS:HE3	2.01	0.43
2:U:277:THR:HG22	2:U:279:ASP:H	1.83	0.43
2:X:29:HIS:HE1	2:X:244:ARG:HD2	1.82	0.43
2:Z:110:GLN:HA	2:Z:113:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:350:PRO:HG2	2:T:441:PRO:HG3	2.00	0.43
2:Y:29:HIS:HE1	2:Y:244:ARG:HD2	1.82	0.43
2:Y:262:PRO:HG2	2:Y:263:THR:HG22	1.99	0.43
2:Z:350:PRO:HG2	2:Z:441:PRO:HG3	2.00	0.43
2:2:350:PRO:HG2	2:2:441:PRO:HG3	2.00	0.43
6:C:695:TYR:HE2	2:Q:357:GLN:HB3	1.84	0.43
6:E:578:MET:HG2	6:E:584:THR:HG21	2.00	0.43
5:N:408:ASP:HB3	5:N:411:MET:HB2	2.01	0.43
2:Q:350:PRO:HG2	2:Q:441:PRO:HG3	2.00	0.43
2:X:277:THR:HG22	2:X:279:ASP:H	1.83	0.43
6:E:585:GLN:HB2	6:E:739:LEU:HD12	2.01	0.43
6:E:623:LYS:O	6:E:627:SER:N	2.52	0.43
5:H:658:SER:O	5:H:662:ARG:HG3	2.19	0.43
5:N:660:TYR:HA	5:N:663:VAL:HG22	2.01	0.43
2:Q:69:LEU:HD12	2:Q:69:LEU:HA	1.88	0.43
2:U:20:GLU:OE1	2:U:230:GLN:NE2	2.52	0.43
2:V:262:PRO:HG2	2:V:263:THR:HG22	2.00	0.43
2:W:237:SER:O	2:W:241:THR:OG1	2.25	0.43
6:C:280:LYS:HD2	6:C:285:TYR:CE2	2.54	0.42
6:C:448:ASP:OD1	6:C:448:ASP:N	2.52	0.42
6:E:427:TYR:HD1	6:E:628:LEU:HD22	1.84	0.42
6:E:679:ALA:HB2	6:E:818:PHE:CE2	2.53	0.42
1:J:311:ARG:O	1:J:315:GLU:HB2	2.19	0.42
7:K:282:SER:HB2	7:K:340:LEU:HD21	2.01	0.42
5:N:589:ALA:HB1	5:N:628:VAL:HG12	2.00	0.42
5:N:755:LEU:HA	5:N:755:LEU:HD13	1.86	0.42
2:Q:172:PHE:N	2:Q:205:LEU:O	2.49	0.42
2:R:110:GLN:HA	2:R:113:LYS:HE3	2.01	0.42
2:V:69:LEU:HD12	2:V:69:LEU:HA	1.88	0.42
2:X:350:PRO:HG2	2:X:441:PRO:HG3	2.00	0.42
6:C:178:PRO:HB3	6:C:180:TRP:CE2	2.54	0.42
6:G:180:TRP:HA	6:G:183:GLU:HB2	2.01	0.42
8:L:1804:PHE:HD1	2:Z:355:SER:HB3	1.82	0.42
6:M:660:ILE:HA	6:M:663:LYS:HA	2.01	0.42
6:M:711:LYS:HA	6:M:714:LYS:HG2	2.01	0.42
5:N:449:ALA:HB2	5:N:467:ARG:HD2	2.00	0.42
5:N:730:SER:HA	5:N:733:GLU:HG3	2.01	0.42
2:S:350:PRO:HG2	2:S:441:PRO:HG3	2.00	0.42
5:D:587:ARG:HH22	5:D:591:THR:HB	1.84	0.42
2:S:110:GLN:HA	2:S:113:LYS:HE3	2.01	0.42
2:S:343:ARG:HG3	2:S:345:LEU:HB2	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:352:GLY:HA2	2:S:353:PRO:HD3	1.88	0.42
2:V:237:SER:O	2:V:241:THR:OG1	2.25	0.42
2:V:350:PRO:HG2	2:V:441:PRO:HG3	2.00	0.42
2:W:110:GLN:HA	2:W:113:LYS:HE3	2.01	0.42
6:E:442:PHE:HE1	6:E:484:TYR:HE1	1.66	0.42
5:F:468:LYS:HA	5:F:471:ILE:HG13	2.01	0.42
6:G:818:PHE:O	6:G:822:ILE:HG12	2.20	0.42
7:I:118:SER:OG	7:I:119:ILE:N	2.53	0.42
5:N:463:LYS:HE2	5:N:495:GLN:HE22	1.83	0.42
2:R:350:PRO:HG2	2:R:441:PRO:HG3	2.00	0.42
2:X:141:ILE:H	2:X:171:VAL:HG22	1.85	0.42
2:Z:20:GLU:OE1	2:Z:230:GLN:NE2	2.52	0.42
2:1:141:ILE:H	2:1:171:VAL:HG22	1.84	0.42
2:2:9:GLN:HE21	2:2:64:ALA:HB1	1.85	0.42
2:2:110:GLN:HA	2:2:113:LYS:HE3	2.01	0.42
5:D:797:LEU:HA	5:D:800:LEU:HG	2.01	0.42
6:M:395:ILE:HD11	6:M:450:ILE:HG23	2.02	0.42
2:U:350:PRO:HG2	2:U:441:PRO:HG3	2.00	0.42
5:F:319:LEU:O	5:F:323:SER:OG	2.37	0.42
1:J:237:HIS:O	1:J:239:HIS:N	2.53	0.42
2:Q:20:GLU:OE1	2:Q:230:GLN:NE2	2.52	0.42
2:U:141:ILE:H	2:U:171:VAL:HG22	1.85	0.42
2:Y:9:GLN:HE21	2:Y:64:ALA:HB1	1.85	0.42
2:Y:323:ILE:HD12	2:Y:323:ILE:HA	1.81	0.42
5:F:334:GLU:O	5:F:338:LEU:HD13	2.19	0.42
5:H:763:LEU:HD12	5:H:775:LEU:HD22	2.02	0.42
5:H:869:SER:HB3	5:H:873:LEU:HD13	2.01	0.42
7:I:172:LEU:HD23	7:I:175:ILE:HD12	2.01	0.42
6:M:739:LEU:HD13	6:M:739:LEU:HA	1.83	0.42
2:Q:237:SER:O	2:Q:241:THR:OG1	2.25	0.42
2:V:141:ILE:H	2:V:171:VAL:HG22	1.85	0.42
2:W:141:ILE:H	2:W:171:VAL:HG22	1.85	0.42
2:Y:141:ILE:H	2:Y:171:VAL:HG22	1.85	0.42
2:Y:183:VAL:HG13	2:Y:187:ASN:HD21	1.83	0.42
2:Z:9:GLN:HE21	2:Z:64:ALA:HB1	1.85	0.42
2:Z:37:VAL:HG12	2:Z:59:HIS:CD2	2.54	0.42
7:I:59:ILE:HD11	7:I:93:LEU:HG	2.00	0.42
2:R:9:GLN:HE21	2:R:64:ALA:HB1	1.85	0.42
2:S:383:SER:O	2:S:386:SER:OG	2.29	0.42
2:T:20:GLU:OE1	2:T:230:GLN:NE2	2.52	0.42
2:T:37:VAL:HG12	2:T:59:HIS:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:397:LYS:HE2	2:U:401:ARG:HH11	1.85	0.42
2:Y:110:GLN:HA	2:Y:113:LYS:HE3	2.01	0.42
2:Y:397:LYS:HE2	2:Y:401:ARG:HH11	1.85	0.42
5:D:653:THR:HG22	5:D:655:GLU:H	1.85	0.42
6:E:577:LEU:HD13	6:E:611:SER:HB2	2.01	0.42
5:H:485:LEU:HD12	5:H:485:LEU:HA	1.93	0.42
7:K:305:ASP:N	7:K:305:ASP:OD2	2.53	0.42
5:N:871:GLU:HG2	5:N:874:ARG:NH2	2.34	0.42
2:Q:396:ASP:OD2	2:Q:425:ARG:NH2	2.47	0.42
2:Z:141:ILE:H	2:Z:171:VAL:HG22	1.85	0.42
2:S:37:VAL:HG12	2:S:59:HIS:CD2	2.54	0.42
2:W:397:LYS:HE2	2:W:401:ARG:HH11	1.85	0.42
2:Z:397:LYS:HE2	2:Z:401:ARG:HH11	1.85	0.42
2:1:298:LEU:HD21	2:1:346:ALA:HB2	2.02	0.41
5:F:644:VAL:HG11	5:F:652:PHE:HB2	2.02	0.41
6:G:304:LEU:HB3	5:H:369:VAL:HG22	2.01	0.41
7:K:264:LEU:HD12	7:K:265:PRO:HD2	2.01	0.41
2:R:141:ILE:H	2:R:171:VAL:HG22	1.84	0.41
2:W:9:GLN:HE21	2:W:64:ALA:HB1	1.85	0.41
2:X:20:GLU:OE1	2:X:230:GLN:NE2	2.52	0.41
2:X:323:ILE:HD12	2:X:323:ILE:HA	1.81	0.41
2:2:141:ILE:H	2:2:171:VAL:HG22	1.85	0.41
6:C:520:PHE:HB2	6:C:638:TYR:CZ	2.55	0.41
6:E:427:TYR:HE1	6:E:628:LEU:HD13	1.85	0.41
7:I:586:ILE:HD13	7:I:622:GLN:HE21	1.85	0.41
1:J:886:LEU:HA	1:J:886:LEU:HD13	1.68	0.41
2:Q:66:LEU:HD21	2:Q:74:ILE:HG12	2.03	0.41
2:R:298:LEU:HD21	2:R:346:ALA:HB2	2.03	0.41
2:S:141:ILE:H	2:S:171:VAL:HG22	1.85	0.41
2:T:66:LEU:HD21	2:T:74:ILE:HG12	2.03	0.41
2:W:66:LEU:HD21	2:W:74:ILE:HG12	2.03	0.41
2:X:110:GLN:HA	2:X:113:LYS:HE3	2.01	0.41
2:Y:20:GLU:OE1	2:Y:230:GLN:NE2	2.52	0.41
2:Z:66:LEU:HD21	2:Z:74:ILE:HG12	2.03	0.41
2:1:66:LEU:HD21	2:1:74:ILE:HG12	2.02	0.41
2:Q:37:VAL:HG12	2:Q:59:HIS:CD2	2.54	0.41
2:Q:352:GLY:HA2	2:Q:353:PRO:HD3	1.88	0.41
2:R:37:VAL:HG12	2:R:59:HIS:CD2	2.54	0.41
2:U:298:LEU:HD21	2:U:346:ALA:HB2	2.02	0.41
2:V:20:GLU:OE1	2:V:230:GLN:NE2	2.52	0.41
2:V:110:GLN:HA	2:V:113:LYS:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:298:LEU:HD21	2:W:346:ALA:HB2	2.03	0.41
2:2:66:LEU:HD21	2:2:74:ILE:HG12	2.03	0.41
6:E:466:ASP:OD1	6:E:466:ASP:N	2.49	0.41
6:G:685:ARG:HD3	2:U:353:PRO:HG2	2.02	0.41
7:I:404:LEU:HD23	7:I:404:LEU:HA	1.76	0.41
6:M:439:ILE:HG22	6:M:441:SER:H	1.84	0.41
2:R:396:ASP:OD2	2:R:425:ARG:NH2	2.47	0.41
2:R:397:LYS:HE2	2:R:401:ARG:HH11	1.85	0.41
2:S:9:GLN:HE21	2:S:64:ALA:HB1	1.85	0.41
2:U:13:CYS:HB2	2:U:140:SER:HB3	2.03	0.41
2:X:66:LEU:HD21	2:X:74:ILE:HG12	2.03	0.41
6:C:277:ILE:HG12	6:C:293:ALA:HB1	2.01	0.41
5:H:336:TYR:HB2	7:I:124:TYR:CD1	2.55	0.41
1:J:275:LEU:O	1:J:279:SER:OG	2.35	0.41
2:Q:397:LYS:HE2	2:Q:401:ARG:HH11	1.85	0.41
2:R:66:LEU:HD21	2:R:74:ILE:HG12	2.02	0.41
2:W:53:TYR:N	2:W:61:ILE:O	2.54	0.41
2:X:13:CYS:HB2	2:X:140:SER:HB3	2.03	0.41
2:Y:296:ARG:HB2	2:Y:296:ARG:HE	1.72	0.41
5:D:609:ASN:HD22	5:D:609:ASN:HA	1.63	0.41
1:J:762:LEU:HD22	1:J:801:LEU:HD11	2.03	0.41
2:Q:53:TYR:N	2:Q:61:ILE:O	2.54	0.41
2:Q:298:LEU:HD21	2:Q:346:ALA:HB2	2.02	0.41
2:R:53:TYR:N	2:R:61:ILE:O	2.54	0.41
2:R:297:LEU:HD12	2:R:297:LEU:HA	1.91	0.41
2:U:383:SER:O	2:U:386:SER:OG	2.29	0.41
2:V:397:LYS:HE2	2:V:401:ARG:HH11	1.85	0.41
2:W:425:ARG:HA	2:W:428:VAL:HG12	2.03	0.41
2:Y:298:LEU:HD21	2:Y:346:ALA:HB2	2.02	0.41
2:1:20:GLU:OE1	2:1:230:GLN:NE2	2.52	0.41
2:2:296:ARG:HB2	2:2:296:ARG:HE	1.72	0.41
6:E:700:GLU:OE1	2:S:334:HIS:HB3	2.20	0.41
1:J:493:ILE:HG13	1:J:494:ILE:HG12	2.03	0.41
7:K:648:ARG:HG3	7:K:649:LEU:HD23	2.02	0.41
2:S:53:TYR:N	2:S:61:ILE:O	2.54	0.41
2:S:425:ARG:HA	2:S:428:VAL:HG12	2.03	0.41
2:U:84:LYS:HB2	2:U:84:LYS:HE3	1.90	0.41
2:X:53:TYR:N	2:X:61:ILE:O	2.54	0.41
2:1:425:ARG:HA	2:1:428:VAL:HG12	2.03	0.41
6:C:840:LEU:HB2	6:C:856:ILE:HD11	2.02	0.41
6:E:547:THR:HA	6:E:548:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:679:ASP:HA	5:F:682:LYS:HB3	2.03	0.41
5:F:836:PHE:O	5:F:840:ILE:HG12	2.20	0.41
6:M:238:LEU:HA	6:M:238:LEU:HD12	1.68	0.41
2:Q:141:ILE:H	2:Q:171:VAL:HG22	1.85	0.41
2:1:53:TYR:N	2:1:61:ILE:O	2.54	0.41
2:1:396:ASP:OD2	2:1:425:ARG:NH2	2.47	0.41
2:2:397:LYS:HE2	2:2:401:ARG:HH11	1.85	0.41
2:2:425:ARG:HA	2:2:428:VAL:HG12	2.03	0.41
6:C:864:PHE:CZ	2:Q:348:PHE:HD1	2.39	0.41
5:D:327:ALA:HB1	5:D:418:ILE:HA	2.03	0.41
5:F:619:ARG:HH12	5:F:620:ARG:NH1	2.18	0.41
1:J:884:PHE:O	1:J:888:VAL:HG23	2.21	0.41
7:K:190:TRP:CH2	7:K:280:GLY:HA3	2.56	0.41
6:M:356:LEU:HG	6:M:440:PRO:HB3	2.03	0.41
5:N:644:VAL:HG11	5:N:649:ALA:HB2	2.02	0.41
2:Q:187:ASN:O	2:Q:191:THR:OG1	2.33	0.41
2:T:53:TYR:N	2:T:61:ILE:O	2.54	0.41
2:V:425:ARG:HA	2:V:428:VAL:HG12	2.03	0.41
2:W:37:VAL:HG12	2:W:59:HIS:CD2	2.54	0.41
2:X:9:GLN:HE21	2:X:64:ALA:HB1	1.85	0.41
2:X:37:VAL:HG12	2:X:59:HIS:CD2	2.54	0.41
2:X:397:LYS:HE2	2:X:401:ARG:HH11	1.85	0.41
2:Y:396:ASP:OD2	2:Y:425:ARG:NH2	2.47	0.41
2:Y:425:ARG:HA	2:Y:428:VAL:HG12	2.03	0.41
2:Z:53:TYR:N	2:Z:61:ILE:O	2.54	0.41
2:Z:298:LEU:HD21	2:Z:346:ALA:HB2	2.02	0.41
2:1:9:GLN:HE21	2:1:64:ALA:HB1	1.85	0.41
2:1:37:VAL:HG12	2:1:59:HIS:CD2	2.54	0.41
2:2:298:LEU:HD21	2:2:346:ALA:HB2	2.03	0.41
6:E:384:SER:OG	6:E:477:TYR:HB3	2.21	0.41
6:G:652:GLU:HG2	6:G:694:GLN:HE22	1.86	0.41
1:J:719:TYR:HD1	1:J:809:VAL:HG21	1.85	0.41
7:K:181:GLY:HA2	7:K:315:LYS:HG3	2.02	0.41
2:T:425:ARG:HA	2:T:428:VAL:HG12	2.03	0.41
2:U:9:GLN:HE21	2:U:64:ALA:HB1	1.85	0.41
2:U:53:TYR:N	2:U:61:ILE:O	2.54	0.41
2:V:352:GLY:HA2	2:V:353:PRO:HD3	1.88	0.41
2:Y:13:CYS:HB2	2:Y:140:SER:HB3	2.03	0.41
6:C:767:GLN:HE21	6:C:814:LEU:HG	1.85	0.40
6:E:180:TRP:O	6:E:184:ARG:NH1	2.54	0.40
5:H:874:ARG:O	5:H:877:SER:OG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:518:ARG:HD3	7:I:616:VAL:HG12	2.01	0.40
2:S:397:LYS:HE2	2:S:401:ARG:HH11	1.85	0.40
2:U:37:VAL:HG12	2:U:59:HIS:CD2	2.54	0.40
2:V:37:VAL:HG12	2:V:59:HIS:CD2	2.54	0.40
2:Z:84:LYS:HB2	2:Z:84:LYS:HE3	1.90	0.40
2:1:395:TYR:HE2	2:1:425:ARG:HG3	1.87	0.40
2:2:20:GLU:OE1	2:2:230:GLN:NE2	2.52	0.40
6:E:838:ALA:HB3	6:E:871:ARG:HH21	1.86	0.40
6:G:557:LEU:HD21	2:V:343:ARG:HD3	2.03	0.40
5:N:706:ILE:O	5:N:710:GLU:HG3	2.21	0.40
2:T:298:LEU:HD21	2:T:346:ALA:HB2	2.03	0.40
2:W:13:CYS:HB2	2:W:140:SER:HB3	2.03	0.40
2:1:397:LYS:HE2	2:1:401:ARG:HH11	1.85	0.40
2:2:53:TYR:N	2:2:61:ILE:O	2.54	0.40
1:J:216:LEU:HD22	1:J:222:HIS:NE2	2.36	0.40
8:L:1623:LEU:HD12	8:L:1623:LEU:HA	1.94	0.40
5:N:588:PRO:HA	5:N:634:GLY:H	1.86	0.40
2:Q:9:GLN:HE21	2:Q:64:ALA:HB1	1.85	0.40
2:S:298:LEU:HD21	2:S:346:ALA:HB2	2.03	0.40
2:T:9:GLN:HE21	2:T:64:ALA:HB1	1.85	0.40
2:T:252:ASP:OD1	2:T:252:ASP:N	2.55	0.40
2:U:66:LEU:HD21	2:U:74:ILE:HG12	2.02	0.40
2:V:9:GLN:HE21	2:V:64:ALA:HB1	1.85	0.40
2:V:337:LEU:HD12	2:V:337:LEU:HA	1.94	0.40
2:Y:53:TYR:N	2:Y:61:ILE:O	2.54	0.40
2:Z:252:ASP:OD1	2:Z:252:ASP:N	2.55	0.40
2:1:296:ARG:HG3	2:1:302:ASN:ND2	2.37	0.40
5:D:689:LYS:HA	5:D:692:ARG:HE	1.86	0.40
5:F:293:ARG:HD3	5:F:368:LEU:HD22	2.03	0.40
7:K:411:LEU:HD13	7:K:414:LEU:HD12	2.03	0.40
8:L:346:LEU:HD13	8:L:347:VAL:HA	2.02	0.40
5:N:553:TYR:O	5:N:558:HIS:HE1	2.04	0.40
2:Q:13:CYS:HB2	2:Q:140:SER:HB3	2.03	0.40
2:Q:323:ILE:HD12	2:Q:323:ILE:HA	1.81	0.40
2:R:252:ASP:OD1	2:R:252:ASP:N	2.55	0.40
2:V:53:TYR:N	2:V:61:ILE:O	2.54	0.40
2:V:66:LEU:HD21	2:V:74:ILE:HG12	2.03	0.40
2:Y:296:ARG:HG3	2:Y:302:ASN:ND2	2.37	0.40
2:Z:296:ARG:HG3	2:Z:302:ASN:ND2	2.37	0.40
2:Z:425:ARG:HA	2:Z:428:VAL:HG12	2.03	0.40
2:1:13:CYS:HB2	2:1:140:SER:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:252:ASP:OD1	2:1:252:ASP:N	2.55	0.40
2:2:395:TYR:HE2	2:2:425:ARG:HG3	1.87	0.40
6:C:217:VAL:HG12	6:C:321:LEU:HD21	2.03	0.40
5:D:391:ARG:HH21	5:D:399:ALA:HB2	1.85	0.40
5:F:572:ASP:O	5:F:575:ARG:HG3	2.22	0.40
5:H:799:GLU:HG2	5:H:802:ARG:HH11	1.85	0.40
1:J:998:LEU:HD11	1:J:1010:LEU:HB3	2.03	0.40
7:K:255:LYS:HD2	7:K:255:LYS:HA	1.87	0.40
2:S:84:LYS:HE3	2:S:84:LYS:HB2	1.90	0.40
2:T:397:LYS:HE2	2:T:401:ARG:HH11	1.85	0.40
2:W:323:ILE:HD12	2:W:323:ILE:HA	1.81	0.40
2:Z:13:CYS:HB2	2:Z:140:SER:HB3	2.03	0.40
2:Z:352:GLY:HA2	2:Z:353:PRO:HD3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	506/1024 (49%)	467 (92%)	35 (7%)	4 (1%)	19	60
1	l	104/1024 (10%)	94 (90%)	9 (9%)	1 (1%)	15	55
2	1	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	2	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	Q	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	R	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	S	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	T	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	U	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	V	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	W	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	X	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	Y	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
2	Z	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	29	69
3	e	360/375 (96%)	339 (94%)	21 (6%)	0	100	100
4	b	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	d	57/82 (70%)	57 (100%)	0	0	100	100
4	i	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	k	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
4	m	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	D	571/907 (63%)	547 (96%)	24 (4%)	0	100	100
5	F	591/907 (65%)	556 (94%)	32 (5%)	3 (0%)	29	69
5	H	584/907 (64%)	565 (97%)	19 (3%)	0	100	100
5	N	584/907 (64%)	565 (97%)	19 (3%)	0	100	100
5	a	112/907 (12%)	108 (96%)	3 (3%)	1 (1%)	17	57
5	h	97/907 (11%)	95 (98%)	2 (2%)	0	100	100
5	j	105/907 (12%)	97 (92%)	7 (7%)	1 (1%)	15	55
6	C	606/902 (67%)	577 (95%)	26 (4%)	3 (0%)	29	69
6	E	626/902 (69%)	577 (92%)	47 (8%)	2 (0%)	41	77
6	G	624/902 (69%)	589 (94%)	32 (5%)	3 (0%)	29	69
6	M	624/902 (69%)	591 (95%)	28 (4%)	5 (1%)	19	60
7	I	511/667 (77%)	473 (93%)	32 (6%)	6 (1%)	13	50
7	K	548/667 (82%)	526 (96%)	21 (4%)	1 (0%)	47	81
8	L	540/1819 (30%)	493 (91%)	44 (8%)	3 (1%)	25	66
8	c	148/1819 (8%)	139 (94%)	9 (6%)	0	100	100
All	All	13046/23174 (56%)	12322 (94%)	667 (5%)	57 (0%)	38	72

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	121	PRO
6	C	239	ALA
6	C	465	HIS

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Mol	Chain	Res	Type
6	E	425	ASP
6	G	241	ARG
6	G	581	ASP
7	I	408	ASP
7	I	509	GLN
7	I	601	LEU
1	J	237	HIS
1	J	238	LEU
6	M	241	ARG
6	M	243	SER
5	j	108	PRO
2	1	347	ASN
2	1	348	PHE
2	2	347	ASN
2	2	348	PHE
6	E	426	LYS
5	F	270	ASN
7	I	510	THR
8	L	307	ARG
6	M	676	PHE
2	Q	347	ASN
2	Q	348	PHE
2	R	347	ASN
2	R	348	PHE
2	S	347	ASN
2	S	348	PHE
2	T	347	ASN
2	T	348	PHE
2	U	347	ASN
2	U	348	PHE
2	V	347	ASN
2	V	348	PHE
2	W	347	ASN
2	W	348	PHE
2	X	347	ASN
2	X	348	PHE
2	Y	347	ASN
2	Y	348	PHE
2	Z	347	ASN
2	Z	348	PHE
6	G	582	LEU
7	I	259	LEU

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Mol	Chain	Res	Type
1	J	255	PRO
8	L	345	VAL
5	a	44	ALA
6	M	238	LEU
6	M	242	GLN
6	C	240	GLY
7	I	508	ASN
7	K	409	ASN
8	L	343	GLN
5	F	501	THR
1	J	713	ASP
5	F	502	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	498/933 (53%)	495 (99%)	3 (1%)	86 92
1	l	84/933 (9%)	84 (100%)	0	100 100
2	1	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	2	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	Q	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	R	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	S	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	T	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	U	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	V	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	W	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	X	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	Y	376/400 (94%)	348 (93%)	28 (7%)	13 38
2	Z	376/400 (94%)	348 (93%)	28 (7%)	13 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	e	310/318 (98%)	305 (98%)	5 (2%)	62 79
4	b	53/62 (86%)	53 (100%)	0	100 100
4	d	53/62 (86%)	52 (98%)	1 (2%)	57 75
4	i	53/62 (86%)	53 (100%)	0	100 100
4	k	53/62 (86%)	53 (100%)	0	100 100
4	m	53/62 (86%)	53 (100%)	0	100 100
5	D	525/798 (66%)	524 (100%)	1 (0%)	93 96
5	F	542/798 (68%)	539 (99%)	3 (1%)	86 92
5	H	539/798 (68%)	538 (100%)	1 (0%)	93 96
5	N	539/798 (68%)	539 (100%)	0	100 100
5	a	101/798 (13%)	101 (100%)	0	100 100
5	h	88/798 (11%)	87 (99%)	1 (1%)	73 84
5	j	88/798 (11%)	88 (100%)	0	100 100
6	C	556/791 (70%)	553 (100%)	3 (0%)	88 93
6	E	574/791 (73%)	567 (99%)	7 (1%)	71 83
6	G	572/791 (72%)	570 (100%)	2 (0%)	92 95
6	M	572/791 (72%)	570 (100%)	2 (0%)	92 95
7	I	472/594 (80%)	471 (100%)	1 (0%)	93 96
7	K	509/594 (86%)	506 (99%)	3 (1%)	86 92
8	L	501/1546 (32%)	498 (99%)	3 (1%)	86 92
8	c	135/1546 (9%)	135 (100%)	0	100 100
All	All	11982/20324 (59%)	11610 (97%)	372 (3%)	43 62

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	10	LEU
2	1	25	LEU
2	1	50	VAL
2	1	56	ASP
2	1	57	ASP
2	1	78	LEU
2	1	109	SER
2	1	131	SER
2	1	151	SER

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Mol	Chain	Res	Type
2	1	168	THR
2	1	188	SER
2	1	201	CYS
2	1	222	ASN
2	1	237	SER
2	1	263	THR
2	1	267	HIS
2	1	274	THR
2	1	278	THR
2	1	296	ARG
2	1	298	LEU
2	1	316	CYS
2	1	328	VAL
2	1	333	VAL
2	1	367	LEU
2	1	374	SER
2	1	385	SER
2	1	424	SER
2	1	425	ARG
2	2	10	LEU
2	2	25	LEU
2	2	50	VAL
2	2	56	ASP
2	2	57	ASP
2	2	78	LEU
2	2	109	SER
2	2	131	SER
2	2	151	SER
2	2	168	THR
2	2	188	SER
2	2	201	CYS
2	2	222	ASN
2	2	237	SER
2	2	263	THR
2	2	267	HIS
2	2	274	THR
2	2	278	THR
2	2	296	ARG
2	2	298	LEU
2	2	316	CYS
2	2	328	VAL
2	2	333	VAL

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Mol	Chain	Res	Type
2	2	367	LEU
2	2	374	SER
2	2	385	SER
2	2	424	SER
2	2	425	ARG
3	e	105	LEU
3	e	129	THR
3	e	177	ARG
3	e	200	PHE
3	e	261	LEU
6	C	288	VAL
6	C	547	THR
6	C	827	LYS
5	D	277	VAL
6	E	255	SER
6	E	467	VAL
6	E	468	THR
6	E	562	SER
6	E	628	LEU
6	E	674	GLN
6	E	675	TRP
5	F	285	ARG
5	F	304	ILE
5	F	404	THR
6	G	467	VAL
6	G	628	LEU
5	H	629	SER
7	I	475	TYR
1	J	220	VAL
1	J	222	HIS
1	J	254	ASP
7	K	537	LEU
7	K	647	LEU
7	K	651	TYR
8	L	346	LEU
8	L	1637	CYS
8	L	1740	ARG
6	M	243	SER
6	M	563	THR
2	Q	10	LEU
2	Q	25	LEU
2	Q	50	VAL

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Mol	Chain	Res	Type
2	Q	56	ASP
2	Q	57	ASP
2	Q	78	LEU
2	Q	109	SER
2	Q	131	SER
2	Q	151	SER
2	Q	168	THR
2	Q	188	SER
2	Q	201	CYS
2	Q	222	ASN
2	Q	237	SER
2	Q	263	THR
2	Q	267	HIS
2	Q	274	THR
2	Q	278	THR
2	Q	296	ARG
2	Q	298	LEU
2	Q	316	CYS
2	Q	328	VAL
2	Q	333	VAL
2	Q	367	LEU
2	Q	374	SER
2	Q	385	SER
2	Q	424	SER
2	Q	425	ARG
2	R	10	LEU
2	R	25	LEU
2	R	50	VAL
2	R	56	ASP
2	R	57	ASP
2	R	78	LEU
2	R	109	SER
2	R	131	SER
2	R	151	SER
2	R	168	THR
2	R	188	SER
2	R	201	CYS
2	R	222	ASN
2	R	237	SER
2	R	263	THR
2	R	267	HIS
2	R	274	THR

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Mol	Chain	Res	Type
2	R	278	THR
2	R	296	ARG
2	R	298	LEU
2	R	316	CYS
2	R	328	VAL
2	R	333	VAL
2	R	367	LEU
2	R	374	SER
2	R	385	SER
2	R	424	SER
2	R	425	ARG
2	S	10	LEU
2	S	25	LEU
2	S	50	VAL
2	S	56	ASP
2	S	57	ASP
2	S	78	LEU
2	S	109	SER
2	S	131	SER
2	S	151	SER
2	S	168	THR
2	S	188	SER
2	S	201	CYS
2	S	222	ASN
2	S	237	SER
2	S	263	THR
2	S	267	HIS
2	S	274	THR
2	S	278	THR
2	S	296	ARG
2	S	298	LEU
2	S	316	CYS
2	S	328	VAL
2	S	333	VAL
2	S	367	LEU
2	S	374	SER
2	S	385	SER
2	S	424	SER
2	S	425	ARG
2	T	10	LEU
2	T	25	LEU
2	T	50	VAL

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Mol	Chain	Res	Type
2	T	56	ASP
2	T	57	ASP
2	T	78	LEU
2	T	109	SER
2	T	131	SER
2	T	151	SER
2	T	168	THR
2	T	188	SER
2	T	201	CYS
2	T	222	ASN
2	T	237	SER
2	T	263	THR
2	T	267	HIS
2	T	274	THR
2	T	278	THR
2	T	296	ARG
2	T	298	LEU
2	T	316	CYS
2	T	328	VAL
2	T	333	VAL
2	T	367	LEU
2	T	374	SER
2	T	385	SER
2	T	424	SER
2	T	425	ARG
2	U	10	LEU
2	U	25	LEU
2	U	50	VAL
2	U	56	ASP
2	U	57	ASP
2	U	78	LEU
2	U	109	SER
2	U	131	SER
2	U	151	SER
2	U	168	THR
2	U	188	SER
2	U	201	CYS
2	U	222	ASN
2	U	237	SER
2	U	263	THR
2	U	267	HIS
2	U	274	THR

Continued on next page...

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Mol	Chain	Res	Type
2	U	278	THR
2	U	296	ARG
2	U	298	LEU
2	U	316	CYS
2	U	328	VAL
2	U	333	VAL
2	U	367	LEU
2	U	374	SER
2	U	385	SER
2	U	424	SER
2	U	425	ARG
2	V	10	LEU
2	V	25	LEU
2	V	50	VAL
2	V	56	ASP
2	V	57	ASP
2	V	78	LEU
2	V	109	SER
2	V	131	SER
2	V	151	SER
2	V	168	THR
2	V	188	SER
2	V	201	CYS
2	V	222	ASN
2	V	237	SER
2	V	263	THR
2	V	267	HIS
2	V	274	THR
2	V	278	THR
2	V	296	ARG
2	V	298	LEU
2	V	316	CYS
2	V	328	VAL
2	V	333	VAL
2	V	367	LEU
2	V	374	SER
2	V	385	SER
2	V	424	SER
2	V	425	ARG
2	W	10	LEU
2	W	25	LEU
2	W	50	VAL

Continued on next page...

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Mol	Chain	Res	Type
2	W	56	ASP
2	W	57	ASP
2	W	78	LEU
2	W	109	SER
2	W	131	SER
2	W	151	SER
2	W	168	THR
2	W	188	SER
2	W	201	CYS
2	W	222	ASN
2	W	237	SER
2	W	263	THR
2	W	267	HIS
2	W	274	THR
2	W	278	THR
2	W	296	ARG
2	W	298	LEU
2	W	316	CYS
2	W	328	VAL
2	W	333	VAL
2	W	367	LEU
2	W	374	SER
2	W	385	SER
2	W	424	SER
2	W	425	ARG
2	X	10	LEU
2	X	25	LEU
2	X	50	VAL
2	X	56	ASP
2	X	57	ASP
2	X	78	LEU
2	X	109	SER
2	X	131	SER
2	X	151	SER
2	X	168	THR
2	X	188	SER
2	X	201	CYS
2	X	222	ASN
2	X	237	SER
2	X	263	THR
2	X	267	HIS
2	X	274	THR

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Mol	Chain	Res	Type
2	X	278	THR
2	X	296	ARG
2	X	298	LEU
2	X	316	CYS
2	X	328	VAL
2	X	333	VAL
2	X	367	LEU
2	X	374	SER
2	X	385	SER
2	X	424	SER
2	X	425	ARG
2	Y	10	LEU
2	Y	25	LEU
2	Y	50	VAL
2	Y	56	ASP
2	Y	57	ASP
2	Y	78	LEU
2	Y	109	SER
2	Y	131	SER
2	Y	151	SER
2	Y	168	THR
2	Y	188	SER
2	Y	201	CYS
2	Y	222	ASN
2	Y	237	SER
2	Y	263	THR
2	Y	267	HIS
2	Y	274	THR
2	Y	278	THR
2	Y	296	ARG
2	Y	298	LEU
2	Y	316	CYS
2	Y	328	VAL
2	Y	333	VAL
2	Y	367	LEU
2	Y	374	SER
2	Y	385	SER
2	Y	424	SER
2	Y	425	ARG
2	Z	10	LEU
2	Z	25	LEU
2	Z	50	VAL

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Mol	Chain	Res	Type
2	Z	56	ASP
2	Z	57	ASP
2	Z	78	LEU
2	Z	109	SER
2	Z	131	SER
2	Z	151	SER
2	Z	168	THR
2	Z	188	SER
2	Z	201	CYS
2	Z	222	ASN
2	Z	237	SER
2	Z	263	THR
2	Z	267	HIS
2	Z	274	THR
2	Z	278	THR
2	Z	296	ARG
2	Z	298	LEU
2	Z	316	CYS
2	Z	328	VAL
2	Z	333	VAL
2	Z	367	LEU
2	Z	374	SER
2	Z	385	SER
2	Z	424	SER
2	Z	425	ARG
5	h	31	GLN
4	d	46	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (179) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	29	HIS
2	1	59	HIS
2	1	167	GLN
2	1	229	ASN
2	1	325	GLN
2	1	338	GLN
2	2	29	HIS
2	2	59	HIS
2	2	167	GLN
2	2	229	ASN
2	2	251	ASN

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Mol	Chain	Res	Type
2	2	325	GLN
2	2	334	HIS
2	2	338	GLN
3	e	12	ASN
3	e	88	HIS
3	e	111	ASN
3	e	115	ASN
3	e	296	ASN
5	a	120	GLN
6	C	151	GLN
6	C	444	GLN
6	C	524	GLN
6	C	585	GLN
6	C	644	HIS
6	C	694	GLN
6	C	823	ASN
5	D	259	GLN
5	D	343	HIS
5	D	401	HIS
5	D	444	HIS
5	D	494	HIS
5	D	576	HIS
5	D	609	ASN
5	D	684	HIS
5	D	687	ASN
5	D	883	ASN
6	E	236	GLN
6	E	242	GLN
6	E	289	ASN
6	E	309	GLN
6	E	412	HIS
6	E	438	GLN
6	E	565	ASN
6	E	585	GLN
6	E	631	ASN
6	E	741	ASN
5	F	269	ASN
5	F	302	ASN
5	F	322	GLN
5	F	330	GLN
5	F	609	ASN
5	F	713	HIS

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Mol	Chain	Res	Type
5	F	739	GLN
5	F	781	GLN
5	F	855	GLN
6	G	166	ASN
6	G	309	GLN
6	G	329	GLN
6	G	438	GLN
6	G	694	GLN
6	G	741	ASN
6	G	862	ASN
5	H	310	GLN
5	H	774	GLN
5	H	805	GLN
5	H	859	GLN
5	H	883	ASN
7	I	123	ASN
7	I	186	GLN
7	I	316	GLN
7	I	327	GLN
7	I	370	GLN
7	I	398	GLN
7	I	476	ASN
7	I	504	HIS
7	I	571	GLN
7	I	622	GLN
1	J	269	GLN
1	J	328	GLN
1	J	362	GLN
1	J	456	GLN
1	J	567	GLN
1	J	879	GLN
1	J	881	HIS
1	J	892	HIS
1	J	895	ASN
7	K	65	HIS
7	K	68	GLN
7	K	121	HIS
7	K	378	HIS
7	K	397	GLN
7	K	409	ASN
7	K	476	ASN
7	K	540	GLN

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Mol	Chain	Res	Type
8	L	327	HIS
8	L	340	GLN
8	L	507	GLN
8	L	512	ASN
8	L	517	HIS
8	L	603	ASN
8	L	1568	HIS
8	L	1657	GLN
8	L	1659	GLN
8	L	1679	GLN
8	L	1742	GLN
8	L	1770	ASN
6	M	465	HIS
6	M	493	ASN
6	M	688	ASN
6	M	691	GLN
6	M	760	ASN
5	N	479	GLN
5	N	531	GLN
5	N	687	ASN
5	N	702	HIS
2	Q	29	HIS
2	Q	59	HIS
2	Q	167	GLN
2	Q	229	ASN
2	Q	251	ASN
2	Q	325	GLN
2	Q	334	HIS
2	R	29	HIS
2	R	59	HIS
2	R	167	GLN
2	R	229	ASN
2	R	325	GLN
2	S	29	HIS
2	S	59	HIS
2	S	167	GLN
2	S	229	ASN
2	S	325	GLN
2	S	338	GLN
2	T	29	HIS
2	T	59	HIS
2	T	167	GLN

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Mol	Chain	Res	Type
2	T	219	HIS
2	T	229	ASN
2	T	325	GLN
2	T	338	GLN
2	U	29	HIS
2	U	59	HIS
2	U	167	GLN
2	U	229	ASN
2	U	325	GLN
2	V	29	HIS
2	V	59	HIS
2	V	167	GLN
2	V	229	ASN
2	V	325	GLN
2	W	29	HIS
2	W	59	HIS
2	W	167	GLN
2	W	197	GLN
2	W	229	ASN
2	W	325	GLN
2	X	29	HIS
2	X	59	HIS
2	X	167	GLN
2	X	229	ASN
2	X	251	ASN
2	X	325	GLN
2	Y	29	HIS
2	Y	59	HIS
2	Y	167	GLN
2	Y	229	ASN
2	Y	325	GLN
2	Y	338	GLN
2	Z	29	HIS
2	Z	59	HIS
2	Z	167	GLN
2	Z	229	ASN
2	Z	325	GLN
2	Z	338	GLN
4	d	53	GLN
8	c	29	ASN
8	c	161	GLN
5	j	84	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

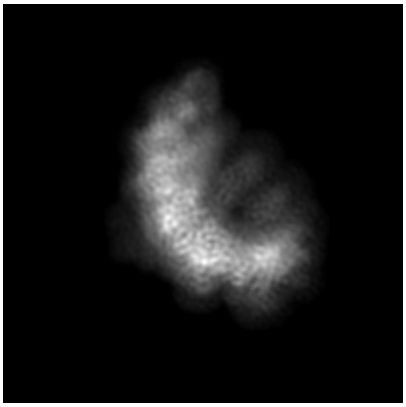
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14013. These allow visual inspection of the internal detail of the map and identification of artifacts.

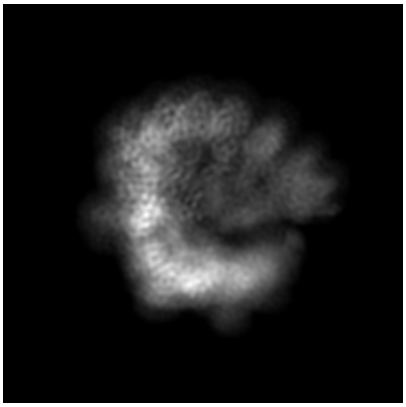
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

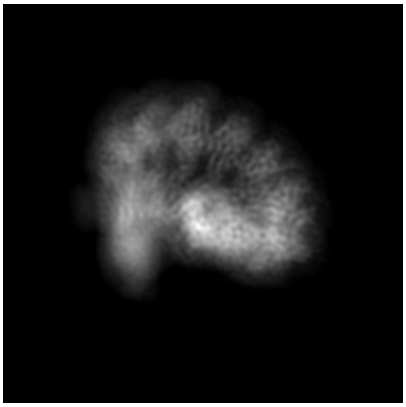
6.1.1 Primary map



X



Y

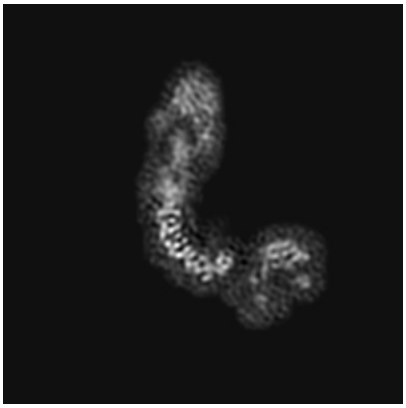


Z

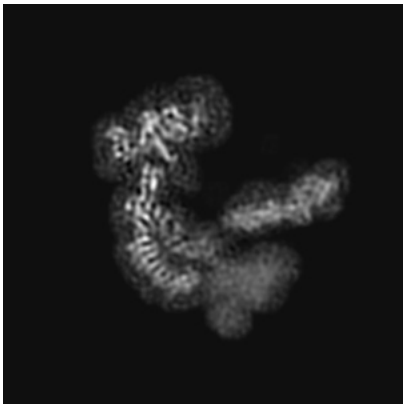
The images above show the map projected in three orthogonal directions.

6.2 Central slices

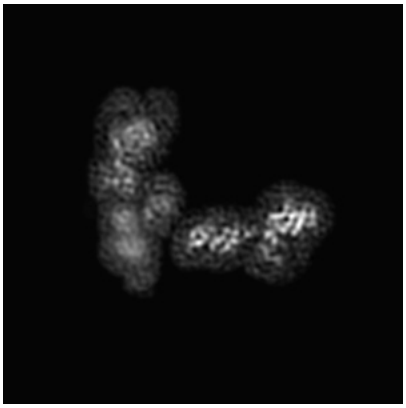
6.2.1 Primary map



X Index: 100



Y Index: 100

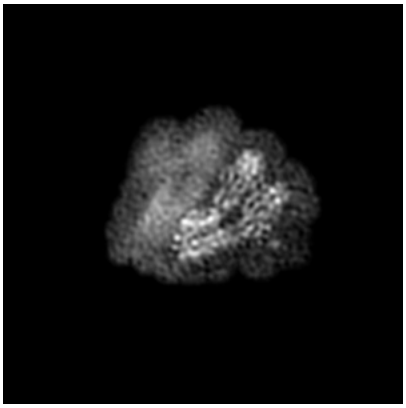


Z Index: 100

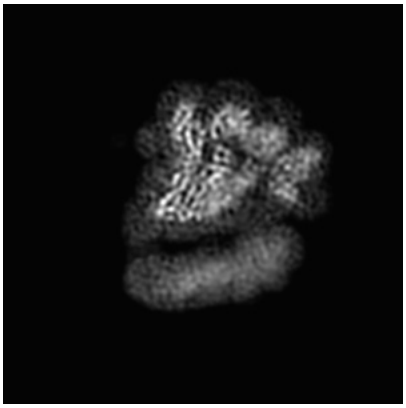
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

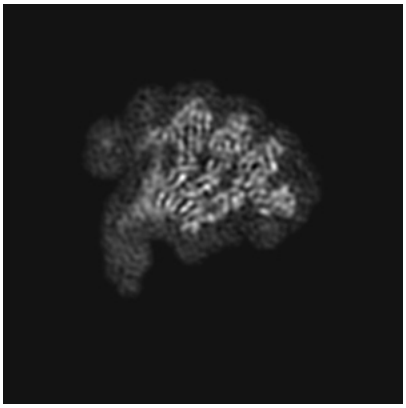
6.3.1 Primary map



X Index: 63



Y Index: 82

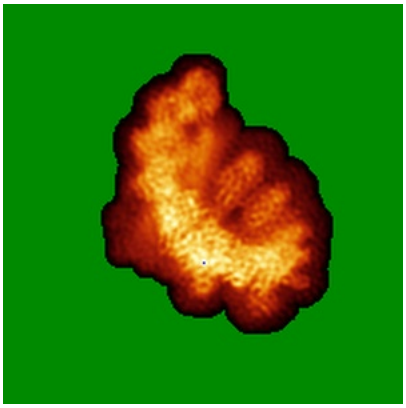


Z Index: 71

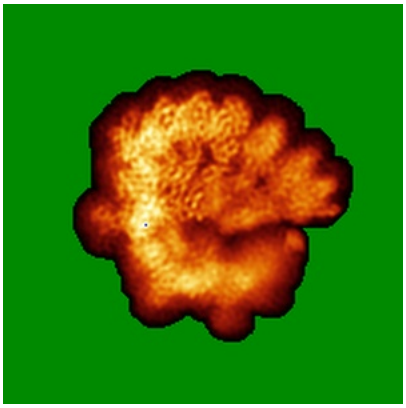
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

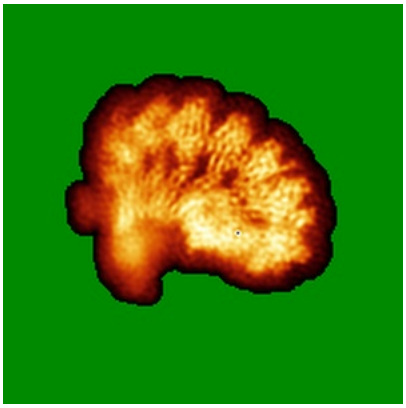
6.4.1 Primary map



X



Y



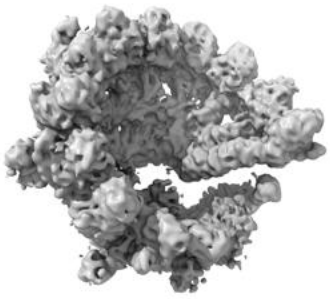
Z

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

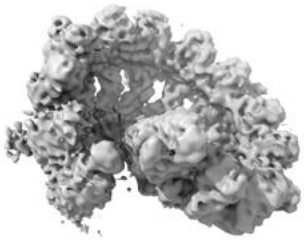
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0357. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

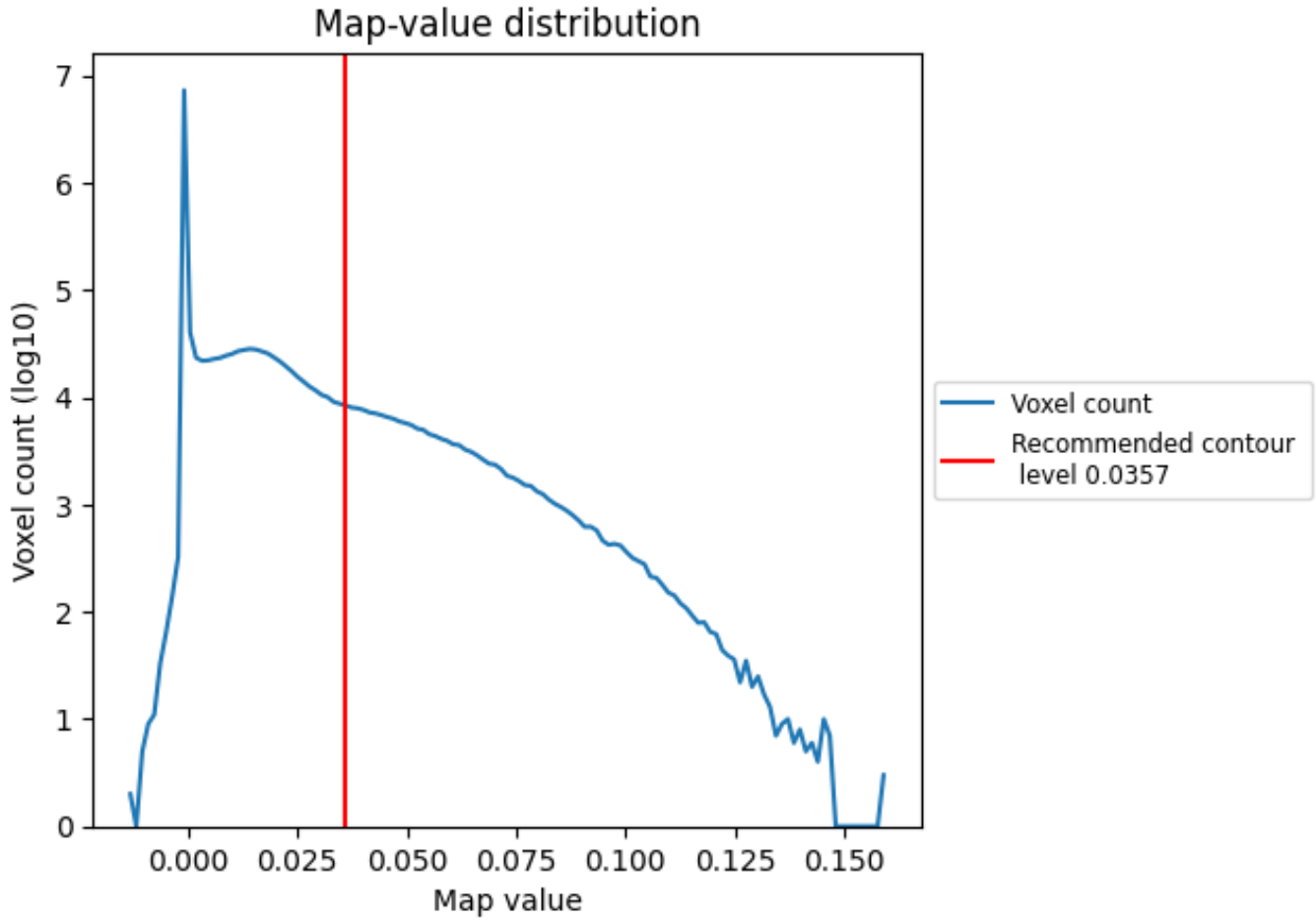
6.6 Mask visualisation (i)

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

7 Map analysis

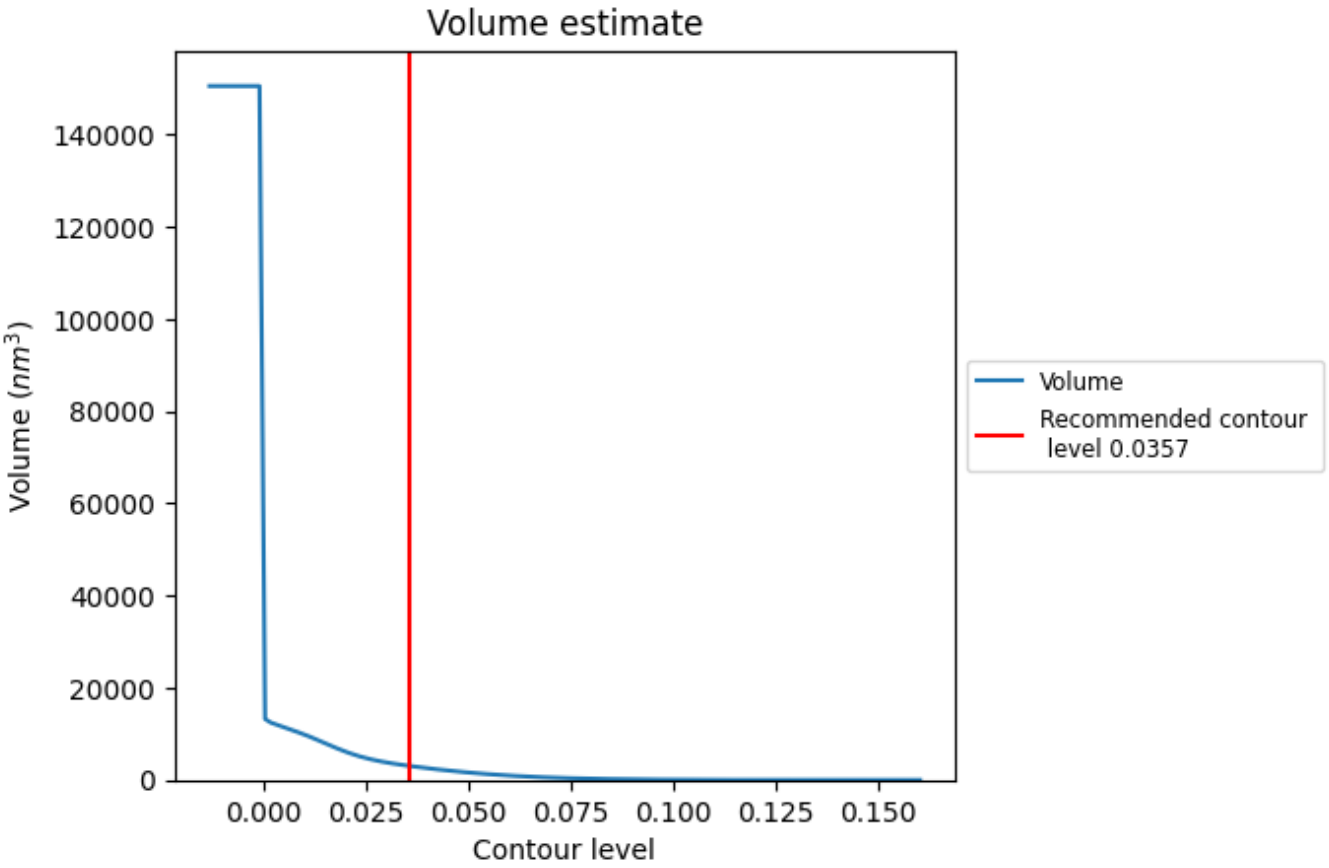
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

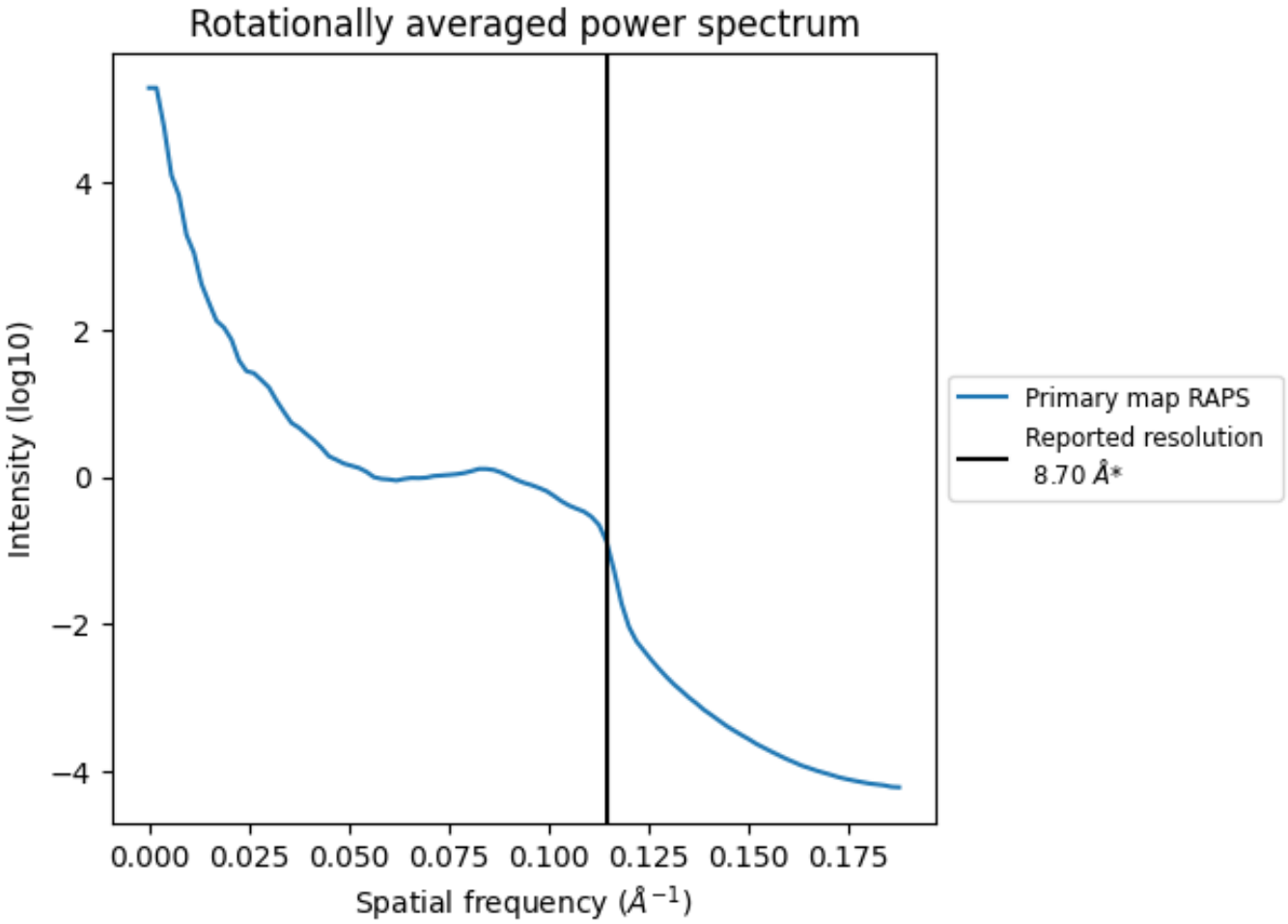
7.2 Volume estimate



The volume at the recommended contour level is 3032 nm^3; this corresponds to an approximate mass of 2739 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 0.115 Å^{-1}

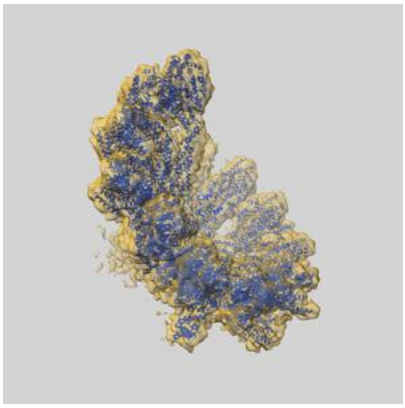
8 Fourier-Shell correlation (i)

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

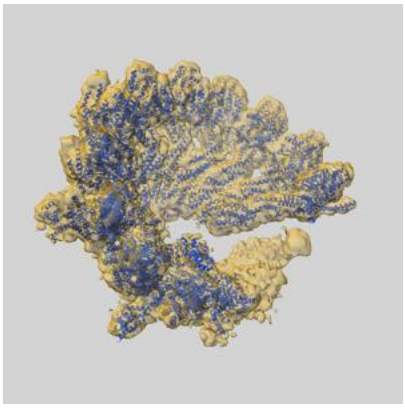
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14013 and PDB model 7QJ8. Per-residue inclusion information can be found in section 3 on page 8.

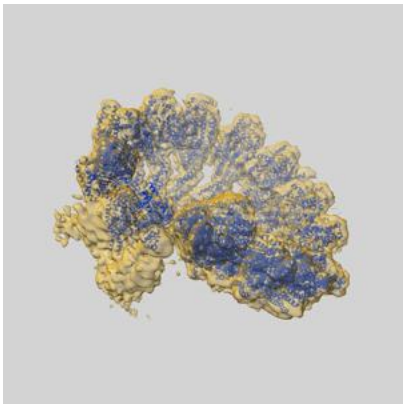
9.1 Map-model overlay



X



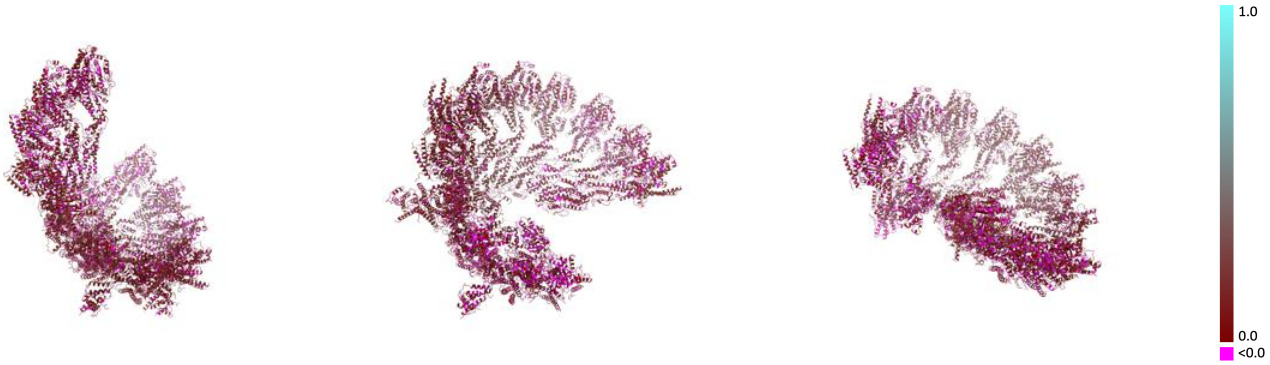
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0357 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.

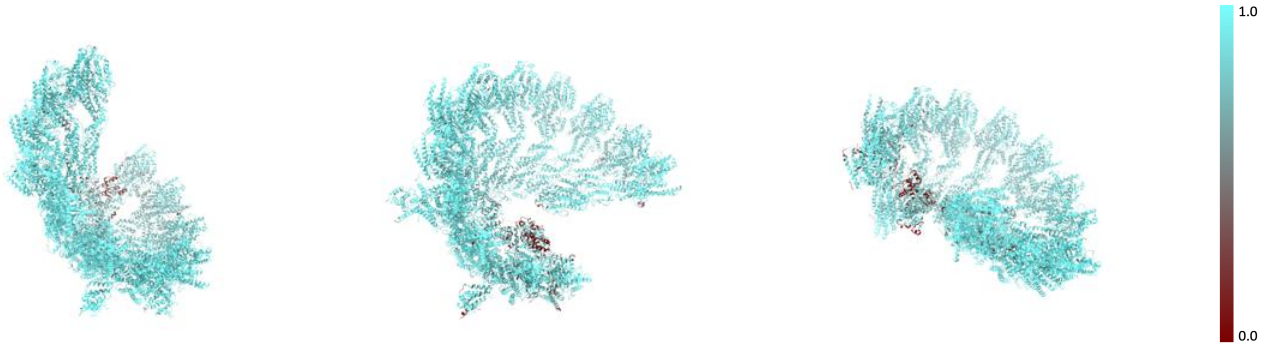
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

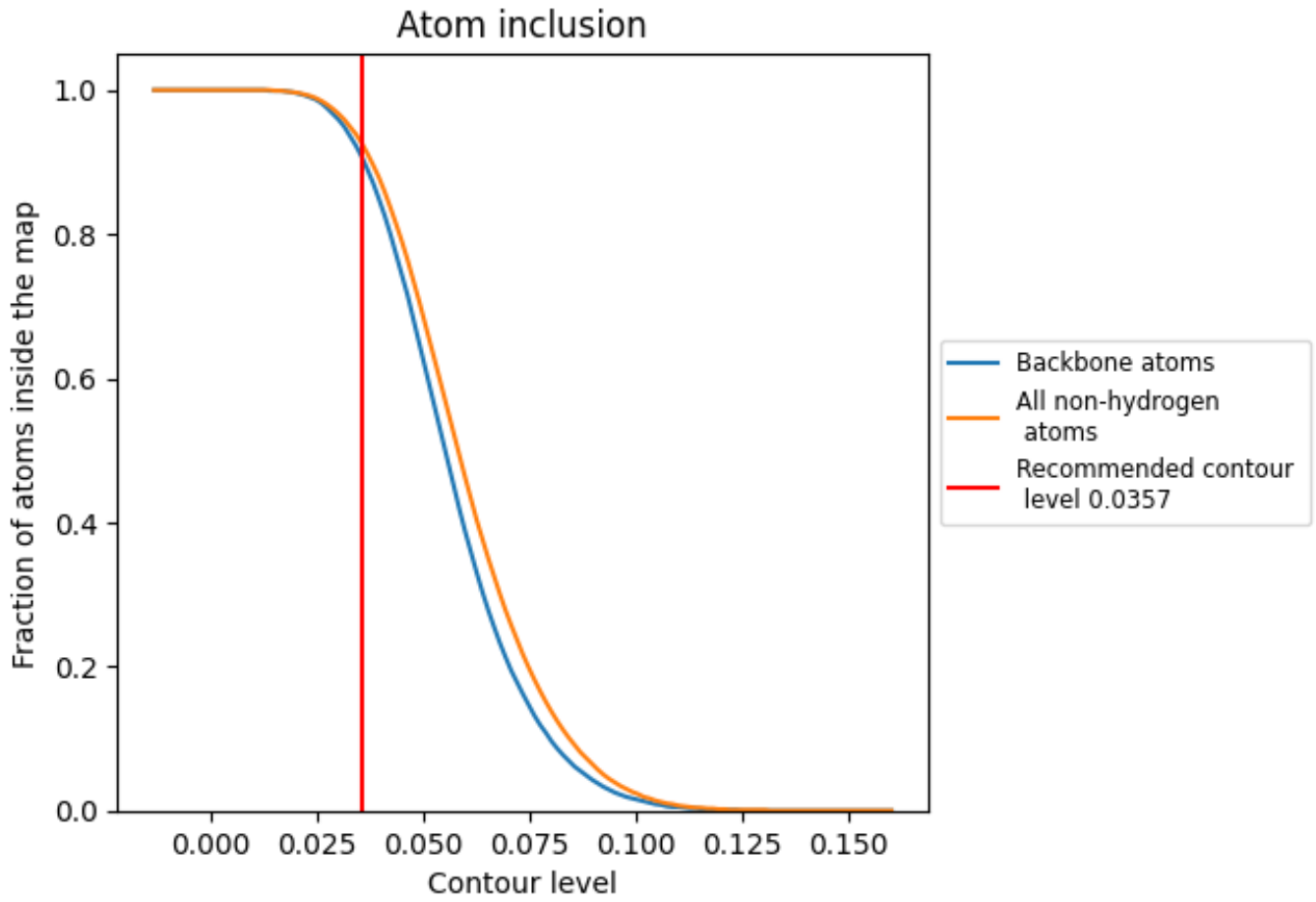
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.0357).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 93% 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 (0.0357) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9260	0.1050
1	0.9240	0.0670
2	0.9390	0.0750
C	0.9030	0.0870
D	0.9190	0.1100
E	0.9520	0.1010
F	0.9600	0.1250
G	0.9560	0.1330
H	0.9680	0.1350
I	0.9680	0.1400
J	0.9730	0.1460
K	0.9710	0.1320
L	0.9830	0.0990
M	0.9260	0.0900
N	0.9460	0.1030
Q	0.8470	0.0540
R	0.8860	0.0770
S	0.9280	0.0590
T	0.9660	0.1110
U	0.9640	0.1100
V	0.9820	0.1320
W	0.9700	0.1220
X	0.9710	0.1210
Y	0.9580	0.0940
Z	0.9700	0.0730
a	0.8440	0.1280
b	0.7960	0.1200
c	0.7270	0.0940
d	0.6860	0.1270
e	0.4850	0.0500
h	0.8470	0.0900
i	0.8070	0.0920
j	0.9220	0.1250
k	0.9220	0.1360
l	0.9560	0.1250
m	0.9580	0.1540