Full wwPDB EM Validation Report

Jan 29, 2022 – 06:16 am GMT

PDB ID	:	7QJB
EMDB ID	:	EMD-14016
Title	:	Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 3-14, homogeneous dataset)
Authors	:	Zupa, E.; Pfeffer, S.
Deposited on	:	2021-12-16
Resolution	:	9.20 Å(reported)
Based on initial models	:	6L81, 6X0U, 7AS4, 6V6S

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

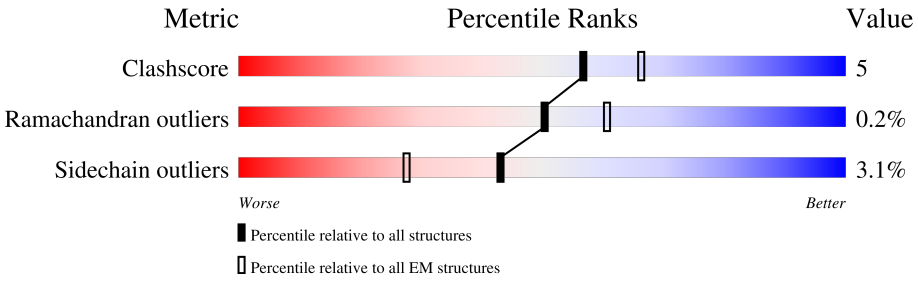
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.20 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	1	451	7% 71% 20% • 7%
1	2	451	10% 71% 19% • 7%
1	Q	451	36% 72% 19% • 7%
1	R	451	25% 73% 18% • 7%
1	S	451	6% 73% 18% • 7%
1	T	451	• 71% 20% • 7%
1	U	451	72% 18% • 7%
1	V	451	72% 19% • 7%

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Mol	Chain	Length	Quality of chain
1	W	451	73% 18% 7%
1	X	451	71% 19% 7%
1	Y	451	72% 19% 7%
1	Z	451	71% 20% 7%
2	e	375	69% 95%
3	D	907	7% 57% 7% 36%
3	F	907	58% 7% 34%
3	H	907	60% 6% 35%
3	N	907	9% 58% 7% 35%
3	a	907	13% 87%
3	h	907	11% 89%
3	j	907	11% 88%
4	C	902	10% 60% 8% 31%
4	E	902	63% 8% 29%
4	G	902	63% 8% 29%
4	M	902	8% 61% 10% 29%
5	I	667	70% 7% 22%
5	K	667	76% 7% 16%
6	J	1024	47% 48%
6	l	1024	10% 89%
7	L	1819	28% 69%
7	c	1819	8% 91%
8	b	82	6% 78% 21%
8	d	82	45% 70% 28%
8	i	82	20% 79% 21%

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Mol	Chain	Length	Quality of chain
8	k	82	79% 21%
8	m	82	78% 21%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 108374 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 Tubulin gamma-1 chain.

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

- Molecule 2 is a protein called actin, cytoplasmic 1.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
4	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		
4	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		
4	M	636	Total	C	N	O	S	0	0
			5186	3342	871	940	33		

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

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

- Molecule 6 is a protein called Gamma-tubulin complex component 5.

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

- Molecule 7 is a protein called Gamma-tubulin complex component 6.

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

- Molecule 8 is a protein called Mitotic-spindle organizing protein 1.

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

- Molecule 9 is water.

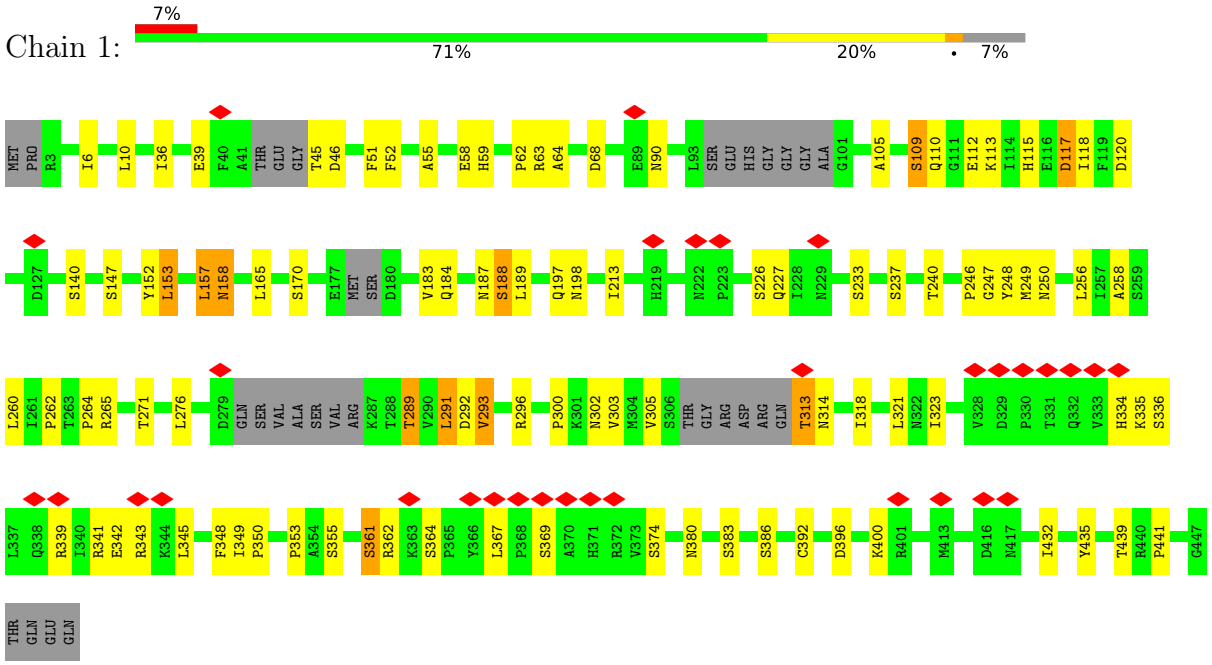
Mol	Chain	Residues	Atoms		AltConf
9	l	6	Total	O	0
			6	6	

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.

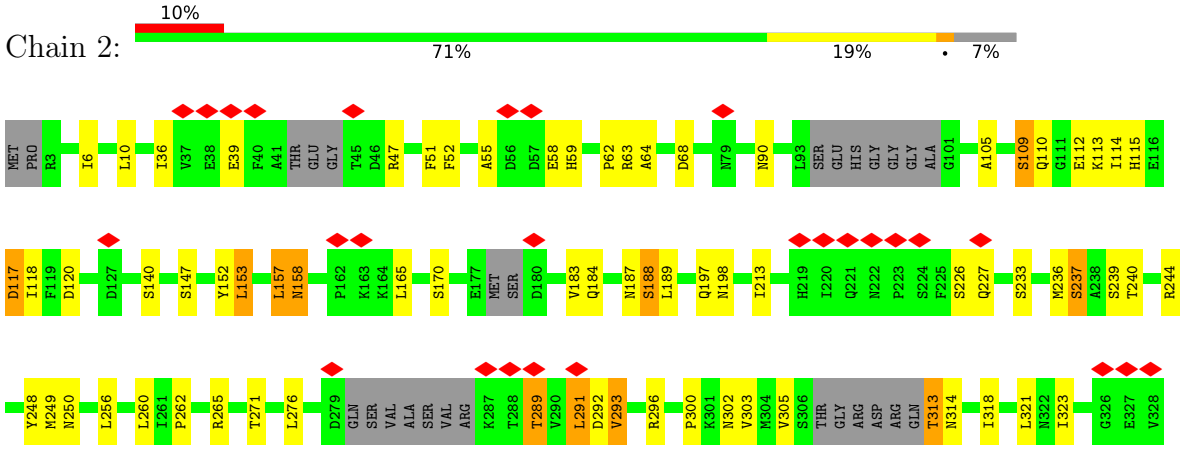
• Molecule 1: Tubulin gamma-1 chain

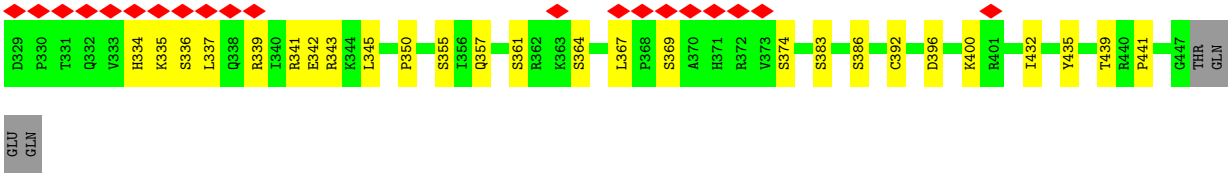
Chain 1:



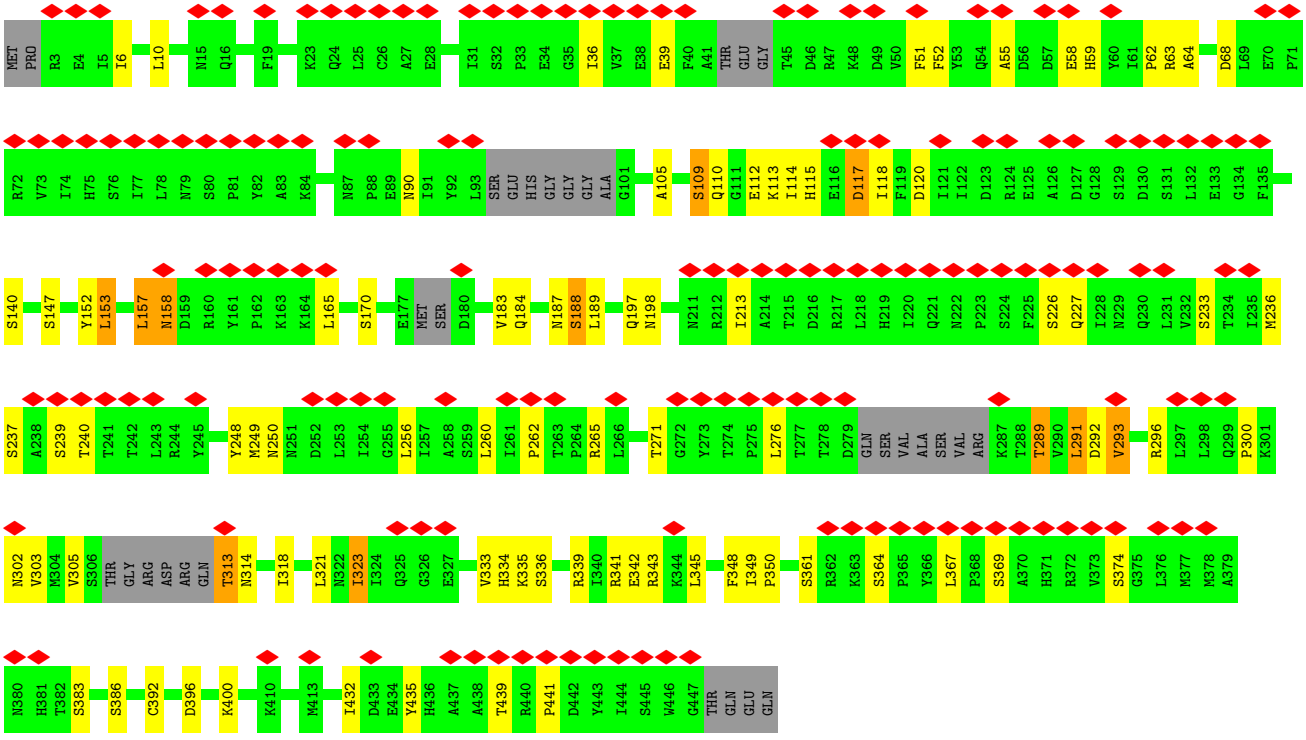
• Molecule 1: Tubulin gamma-1 chain

Chain 2:

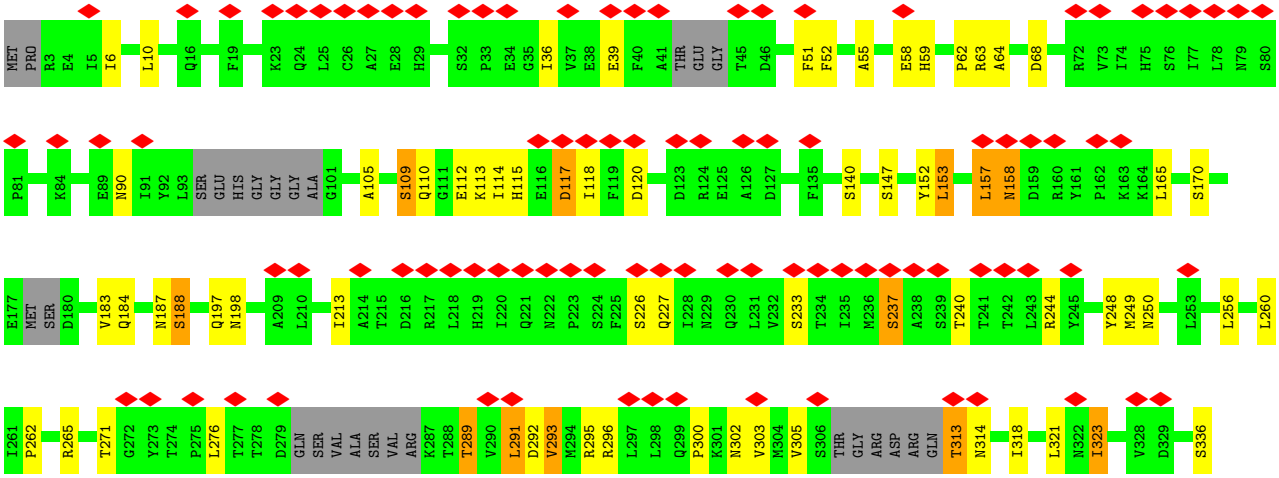


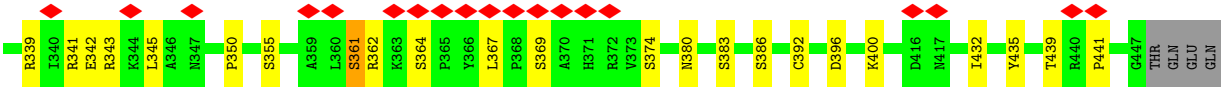


• Molecule 1: Tubulin gamma-1 chain

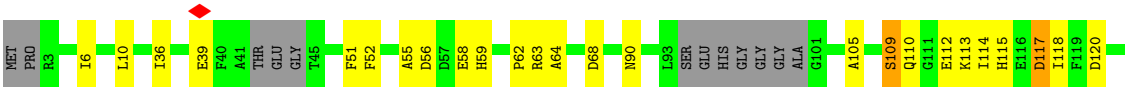


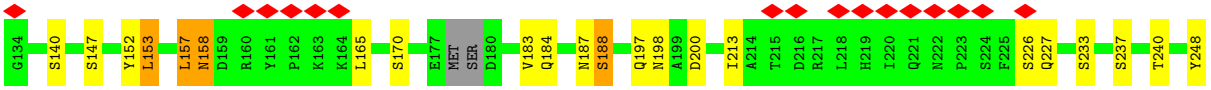
• Molecule 1: Tubulin gamma-1 chain

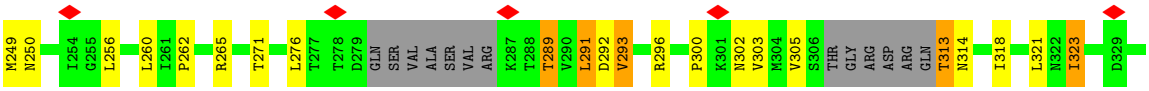


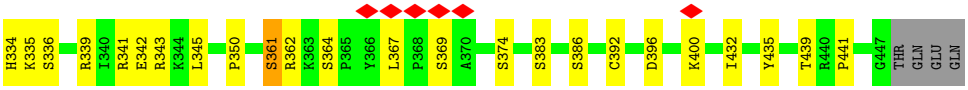


• Molecule 1: Tubulin gamma-1 chain

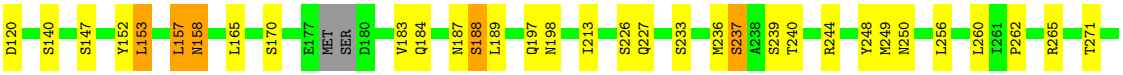


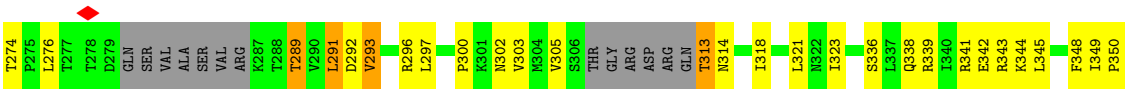


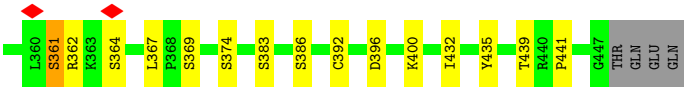




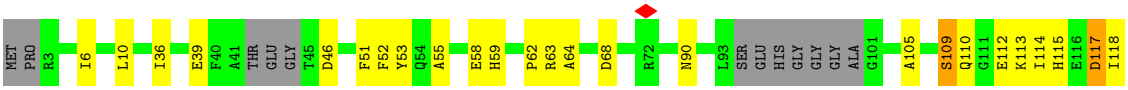
• Molecule 1: Tubulin gamma-1 chain

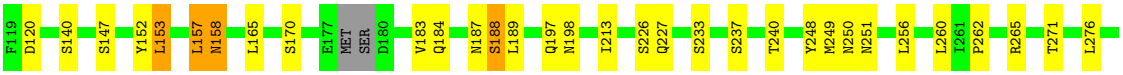


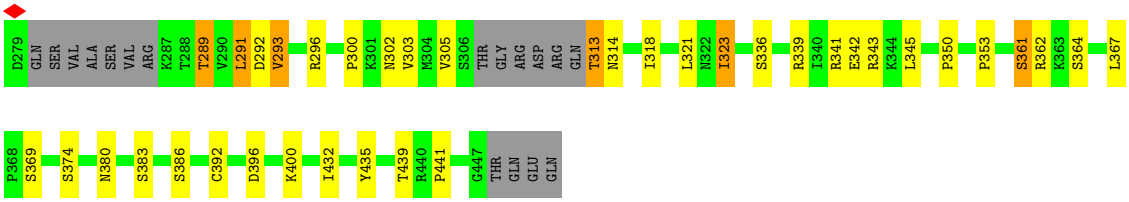




• Molecule 1: Tubulin gamma-1 chain

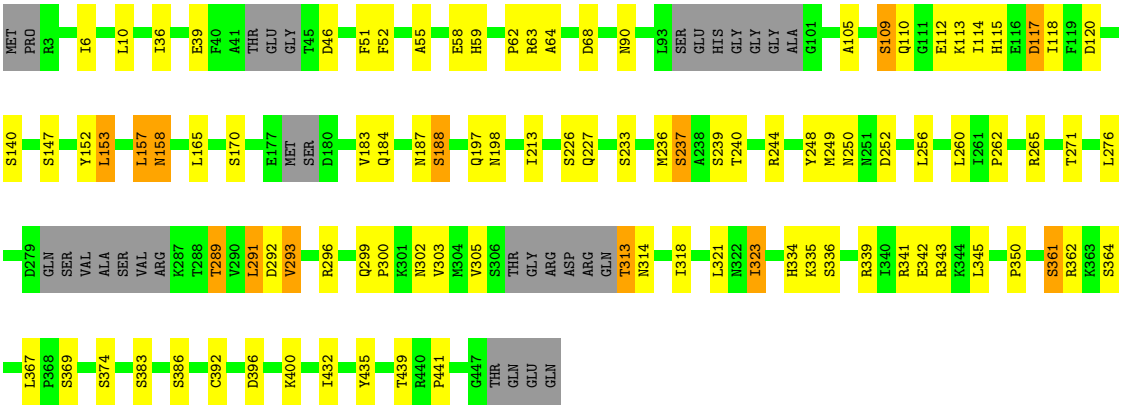






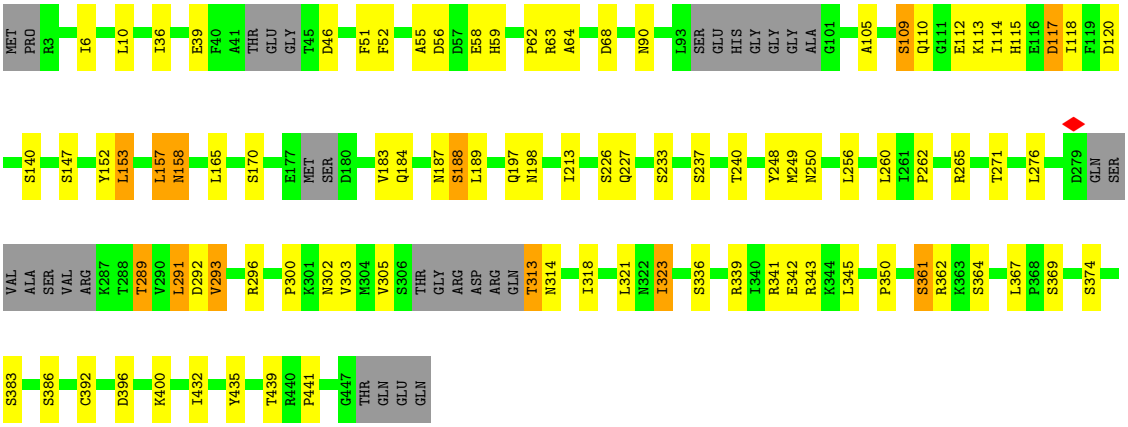
• Molecule 1: Tubulin gamma-1 chain

Chain V:



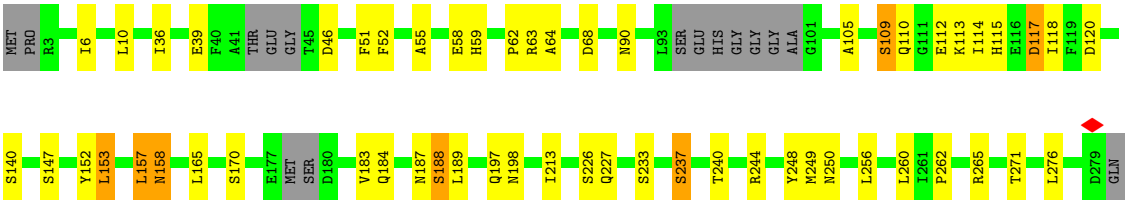
• Molecule 1: Tubulin gamma-1 chain

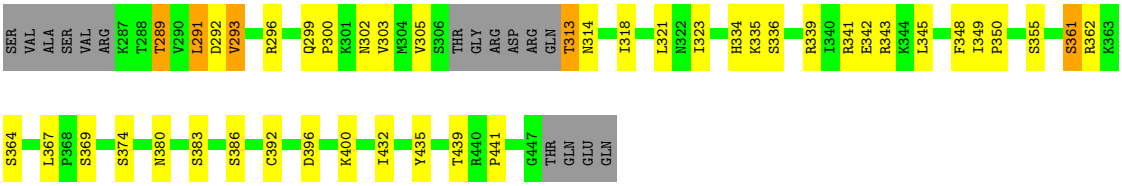
Chain W:



• Molecule 1: Tubulin gamma-1 chain

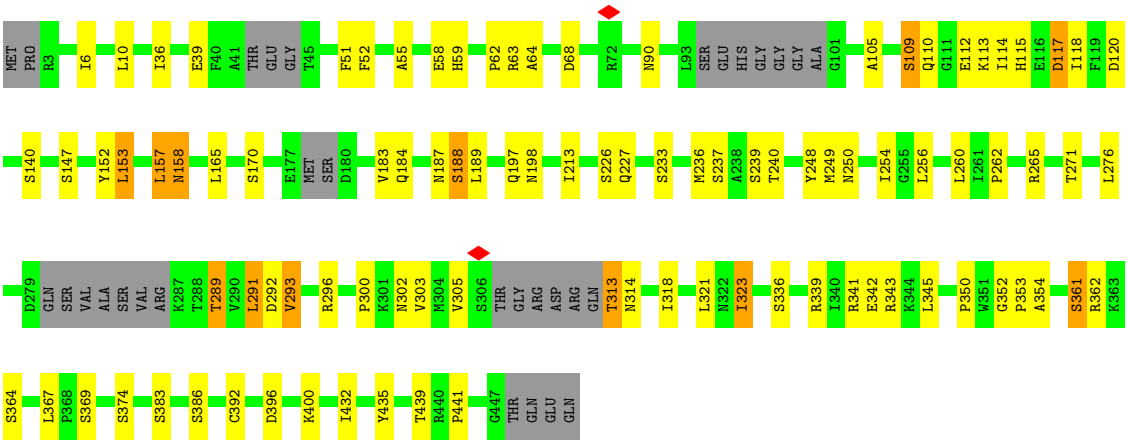
Chain X:





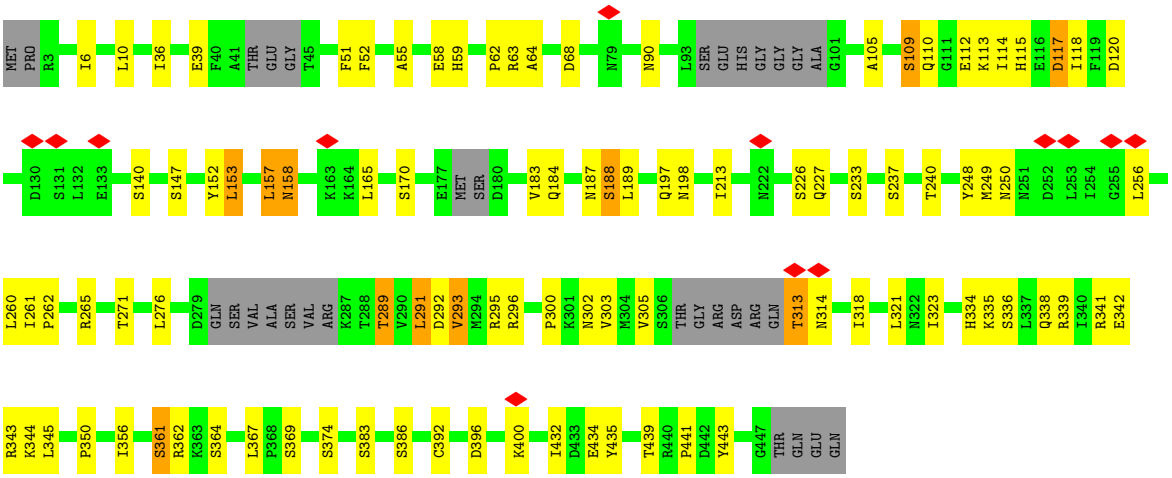
• Molecule 1: Tubulin gamma-1 chain

Chain Y:



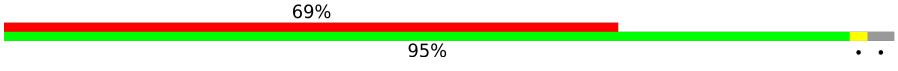
• Molecule 1: Tubulin gamma-1 chain

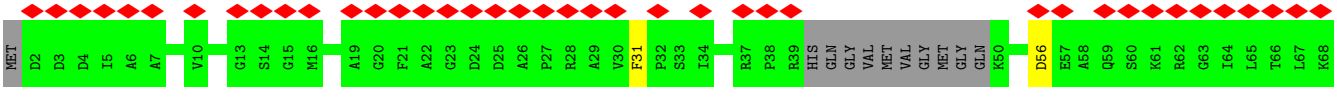
Chain Z:



• Molecule 2: actin, cytoplasmic 1

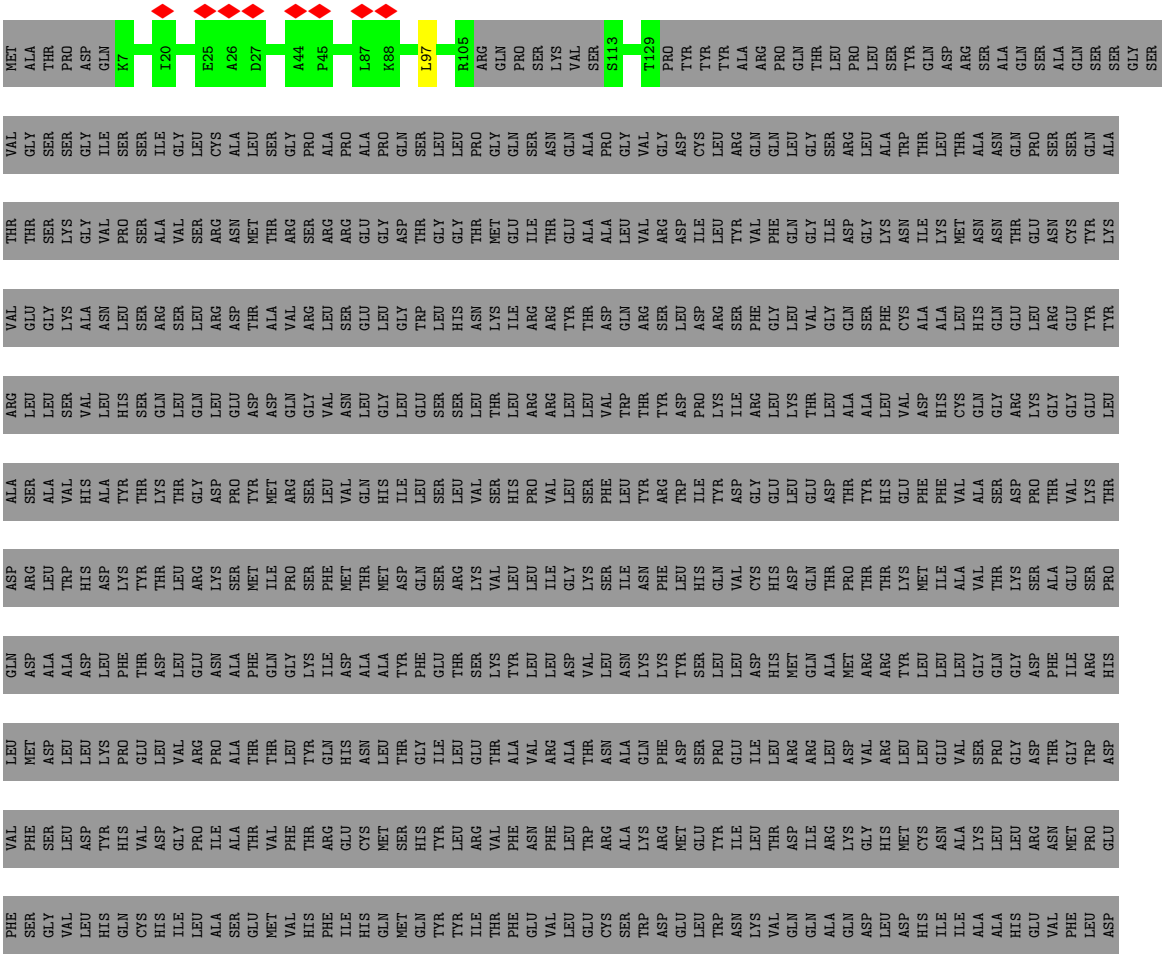
Chain e:

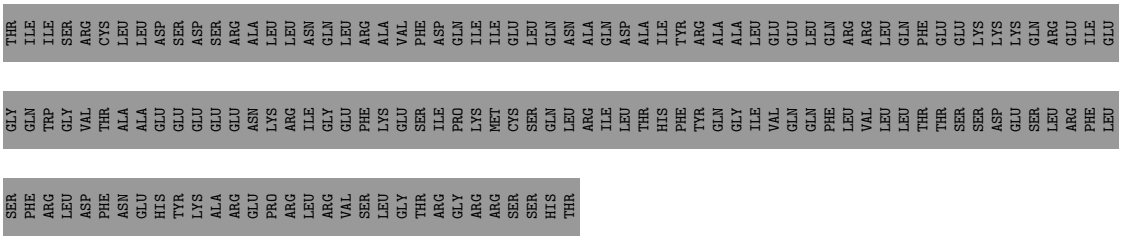




• Molecule 3: Gamma-tubulin complex component 3

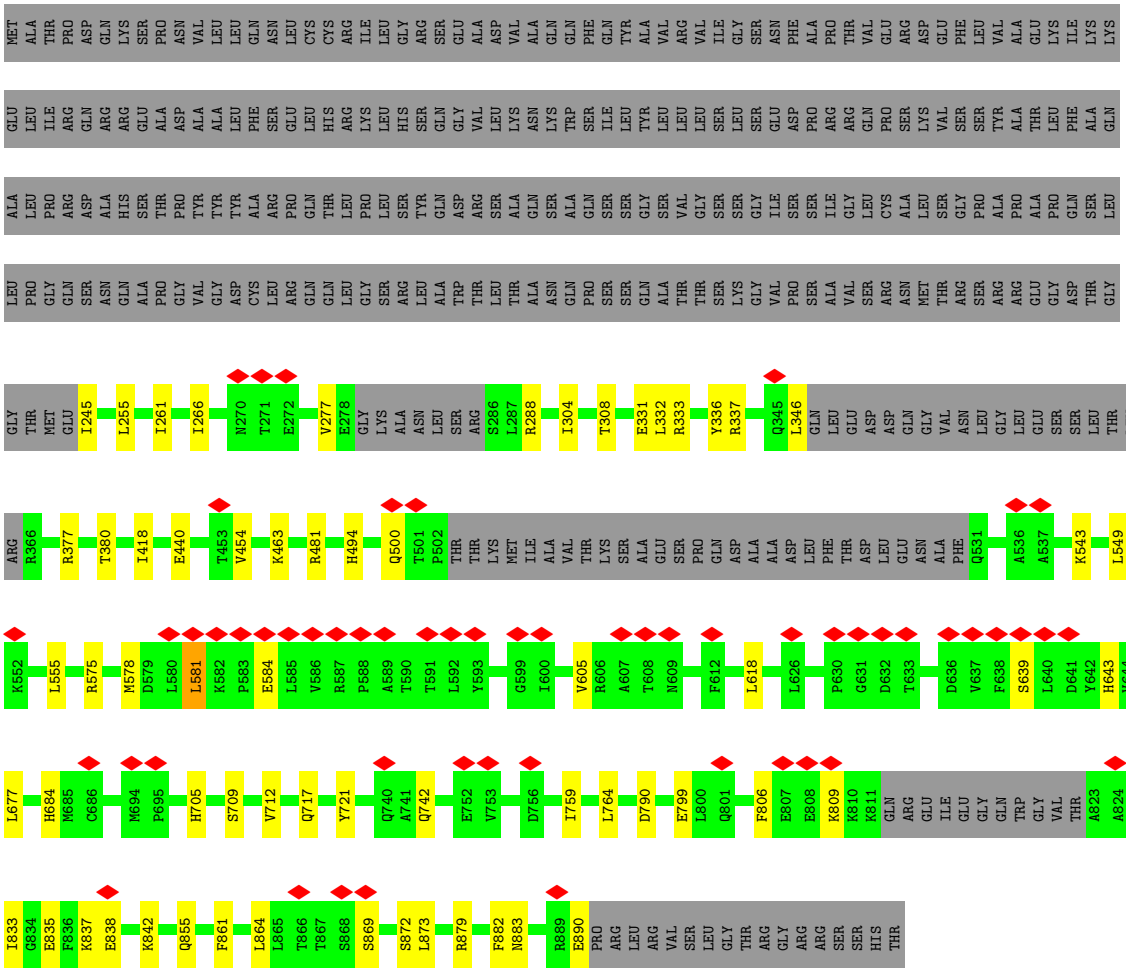
Chain a:





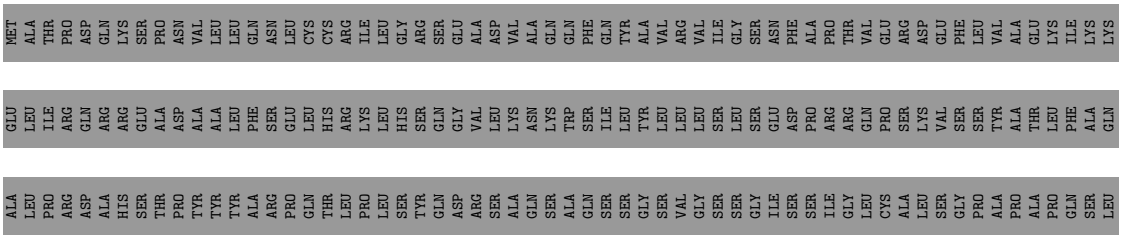
• Molecule 3: Gamma-tubulin complex component 3

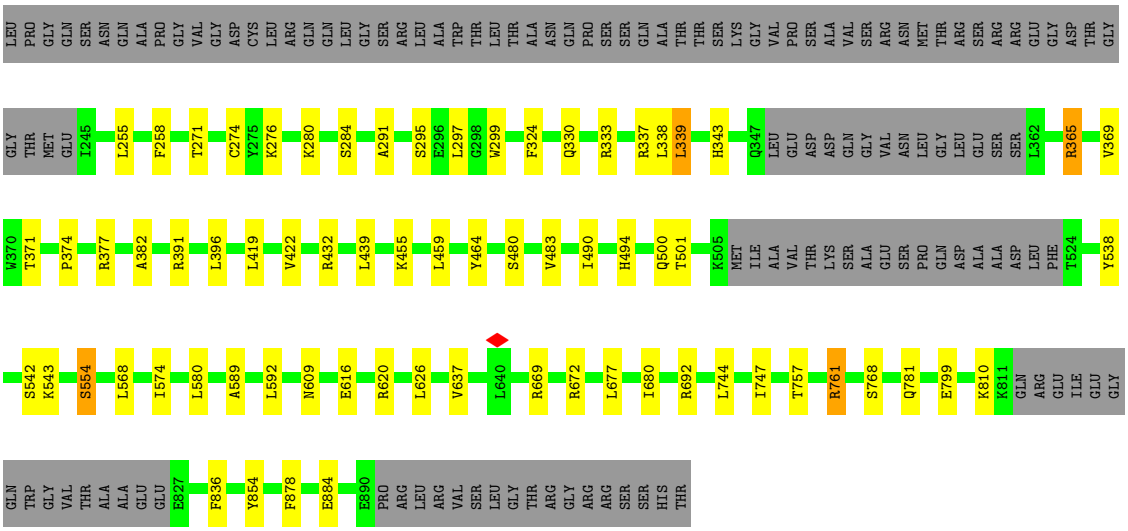
Chain D:



• Molecule 3: Gamma-tubulin complex component 3

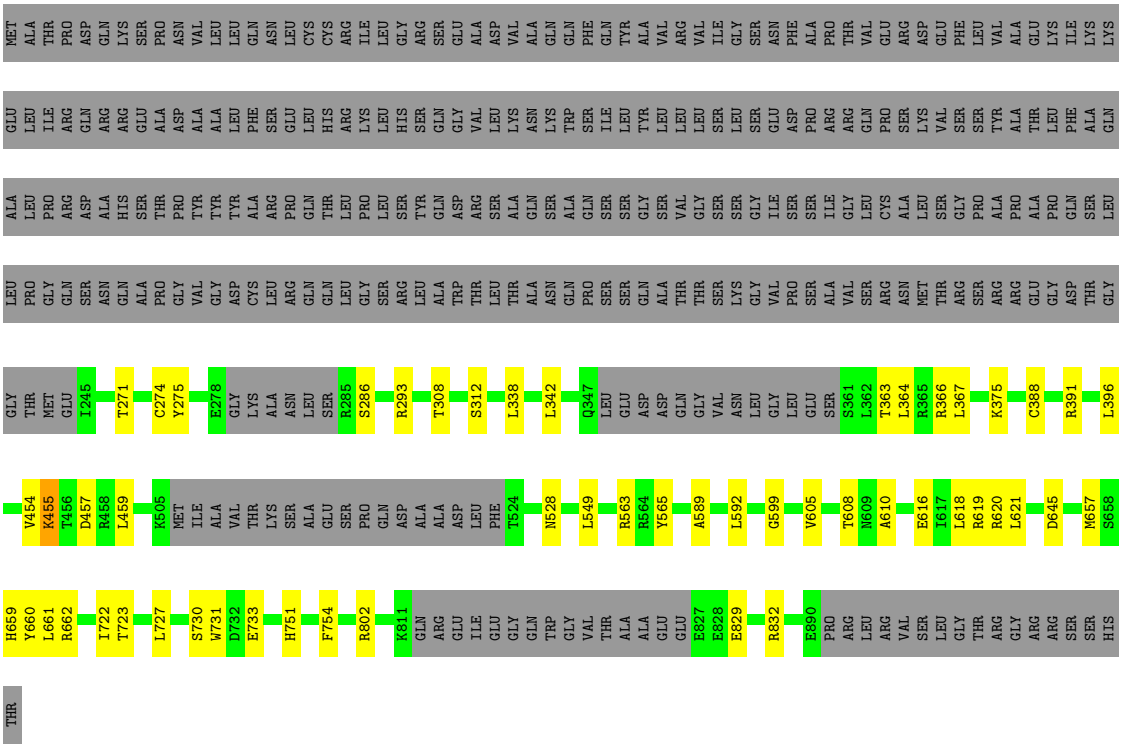
Chain F:





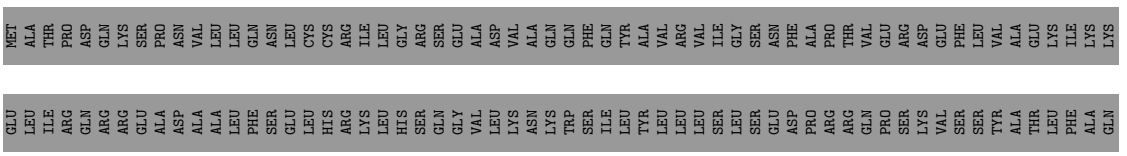
• Molecule 3: Gamma-tubulin complex component 3

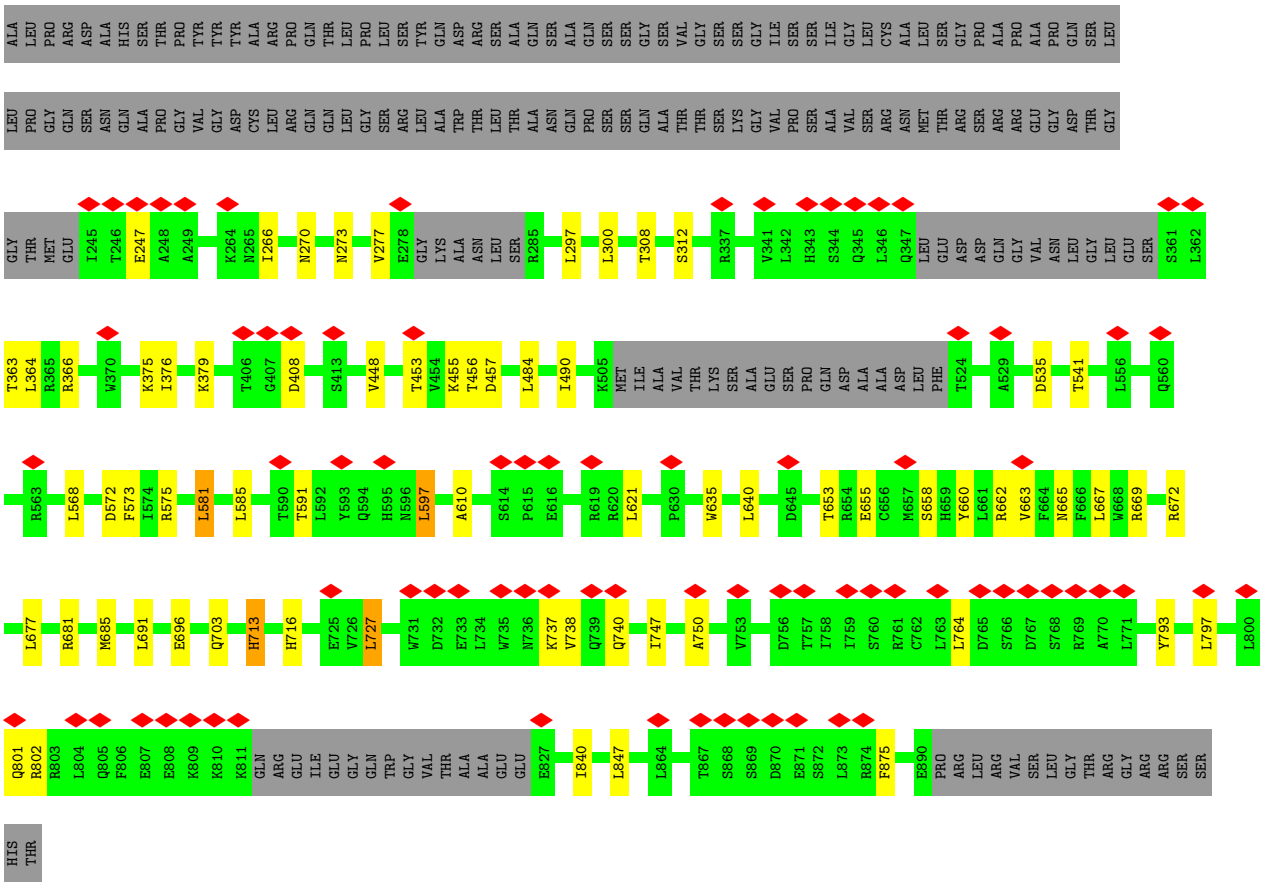
Chain H:



• Molecule 3: Gamma-tubulin complex component 3

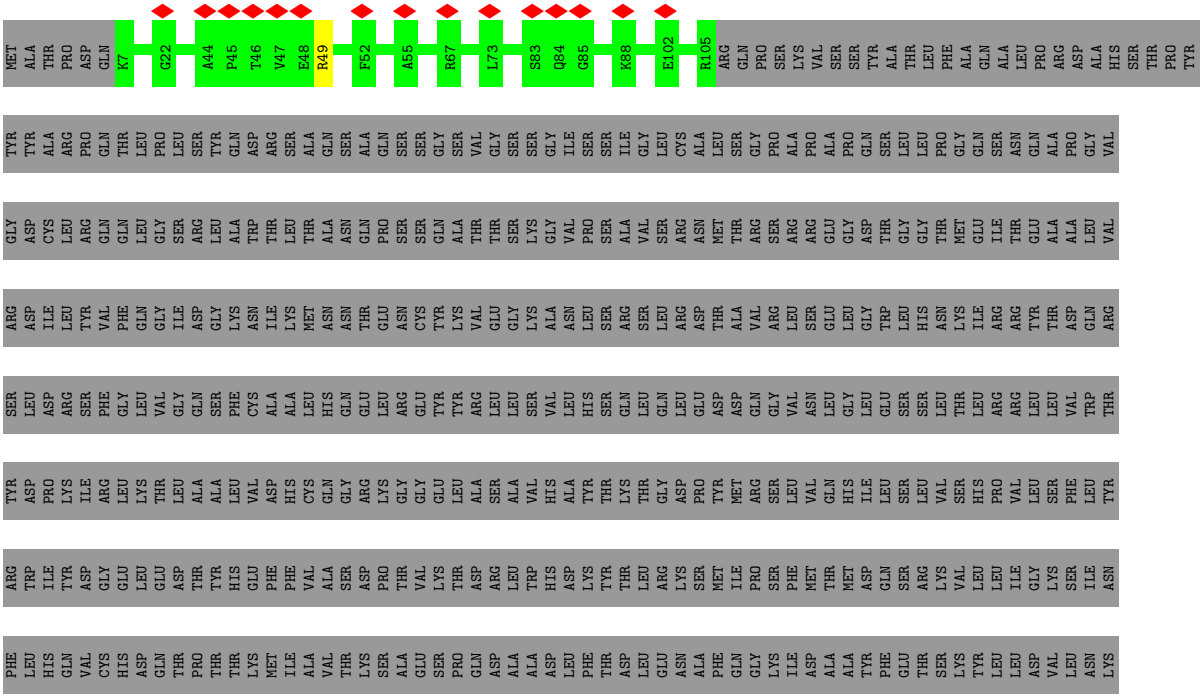
Chain N:

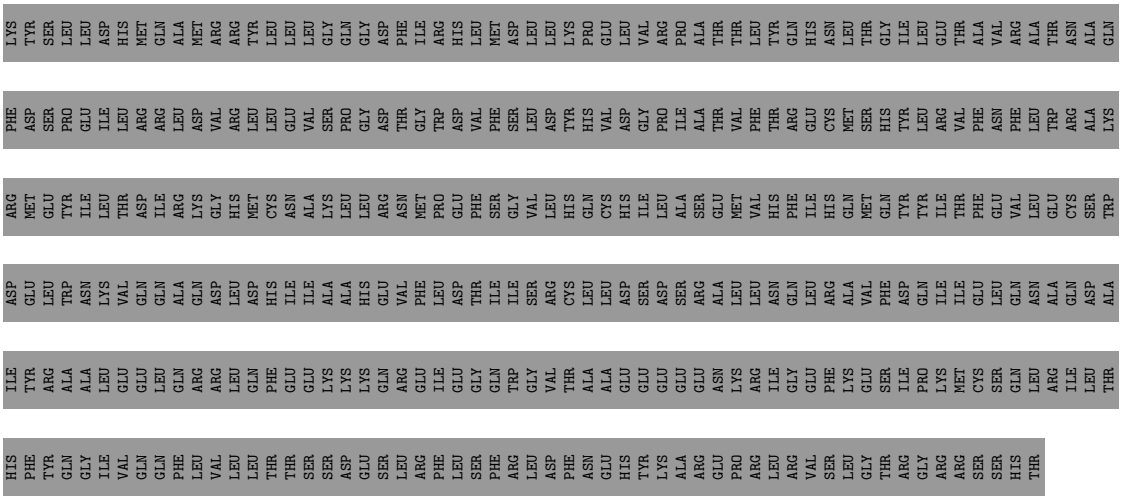




• Molecule 3: Gamma-tubulin complex component 3

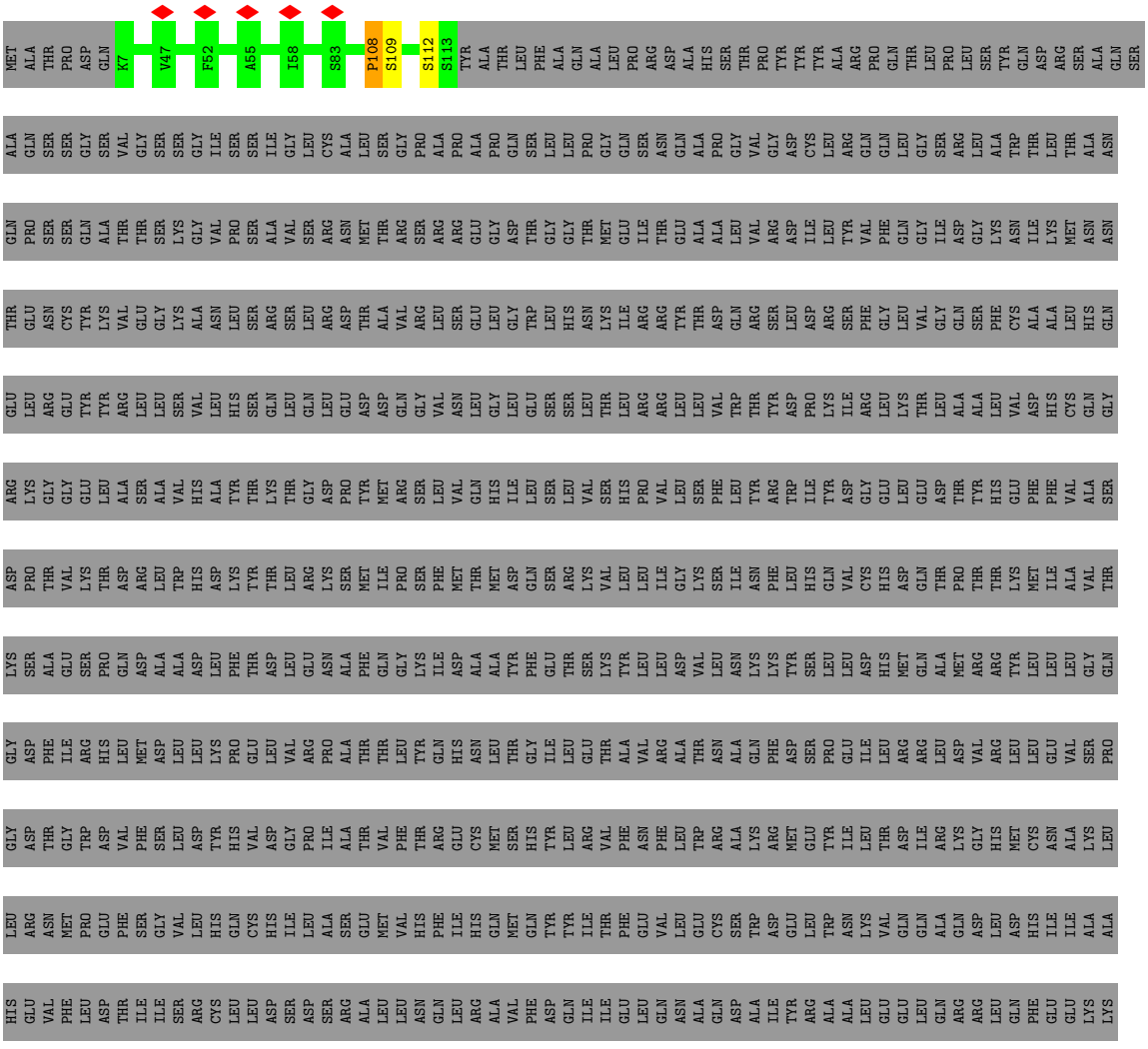
Chain h:

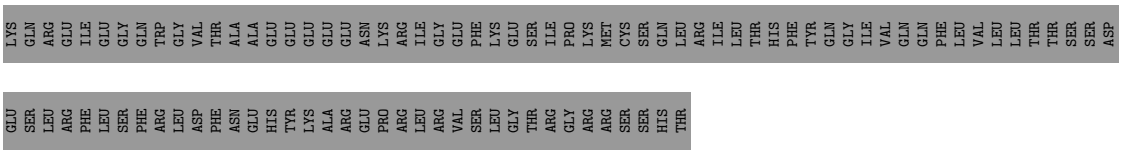




• Molecule 3: Gamma-tubulin complex component 3

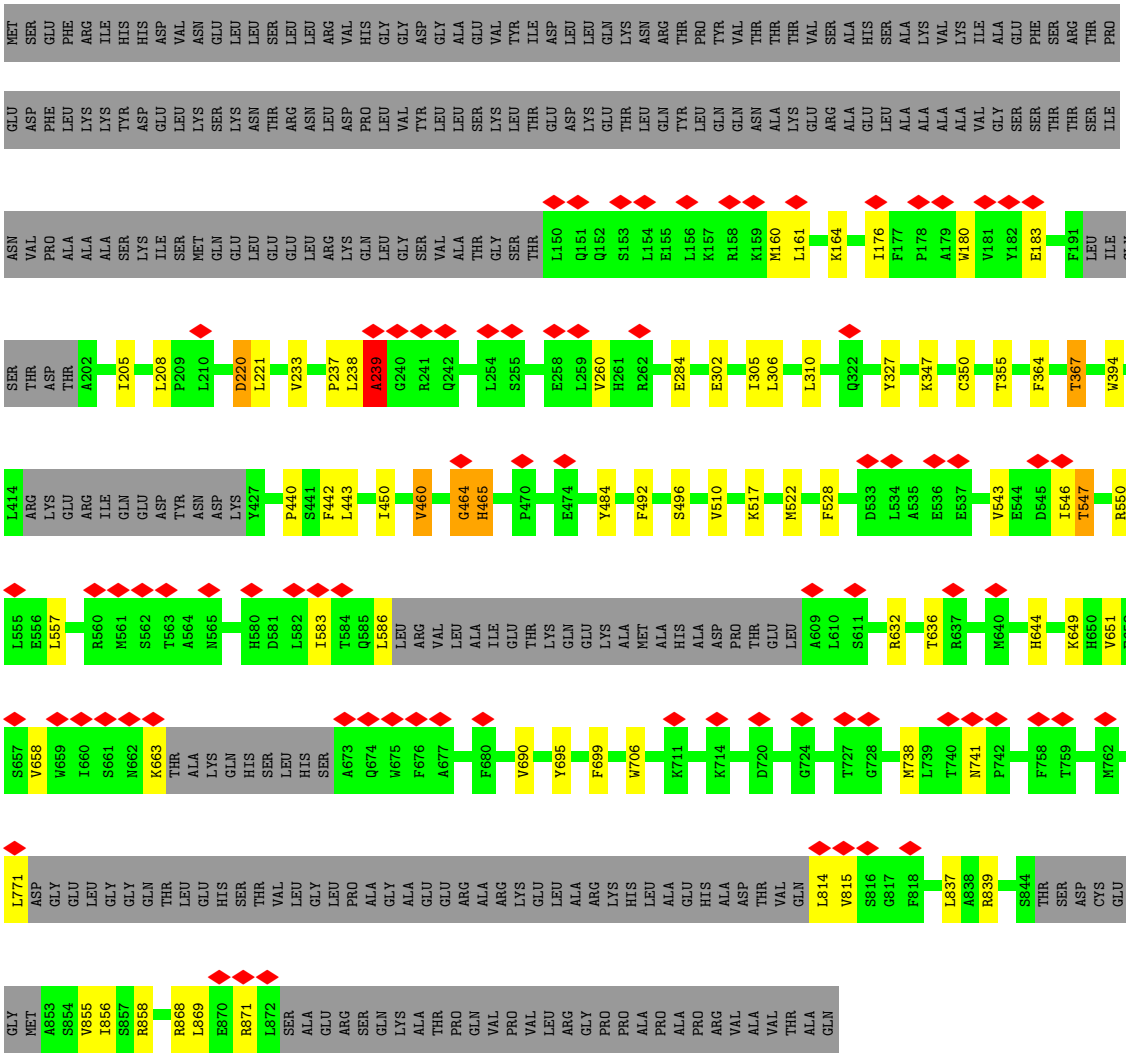
Chain j:





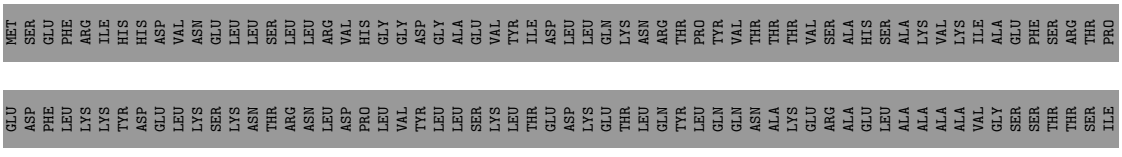
• Molecule 4: Gamma-tubulin complex component 2

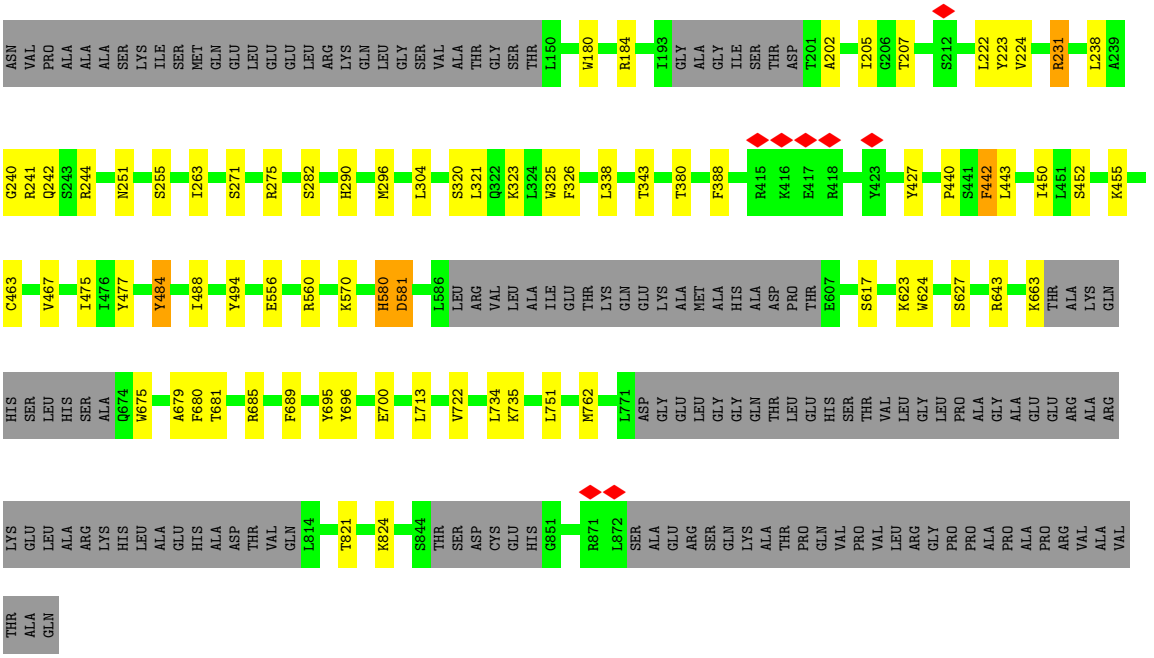
Chain C:



• Molecule 4: Gamma-tubulin complex component 2

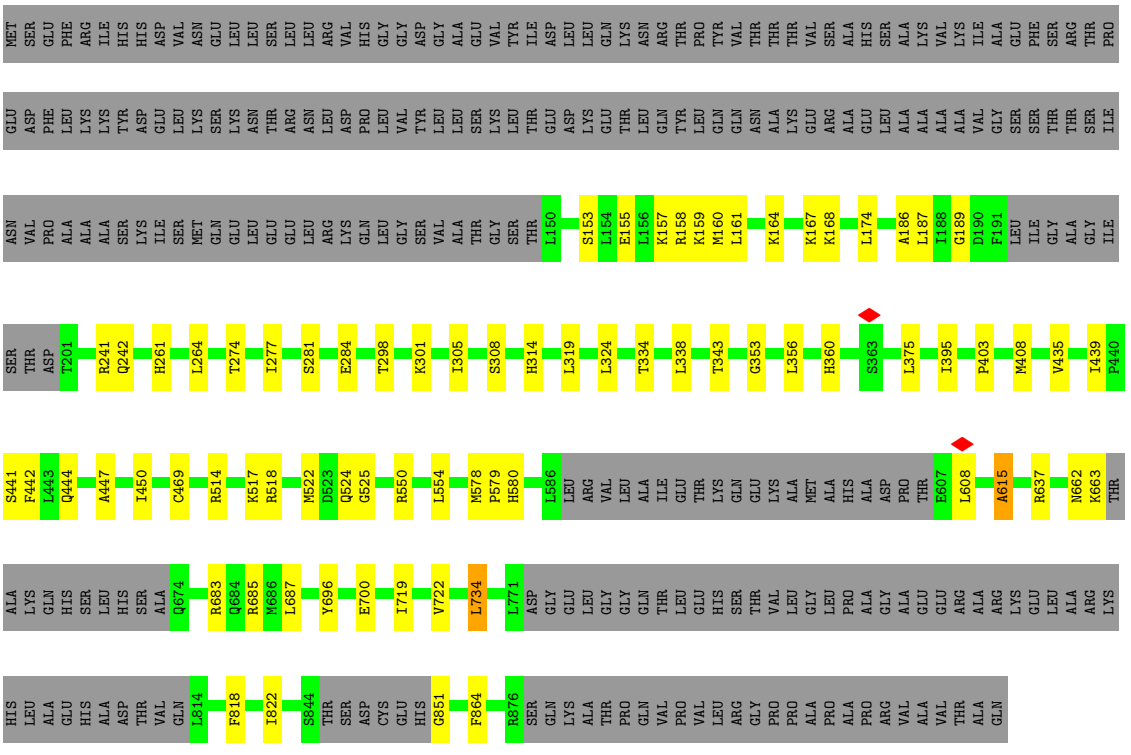
Chain E:





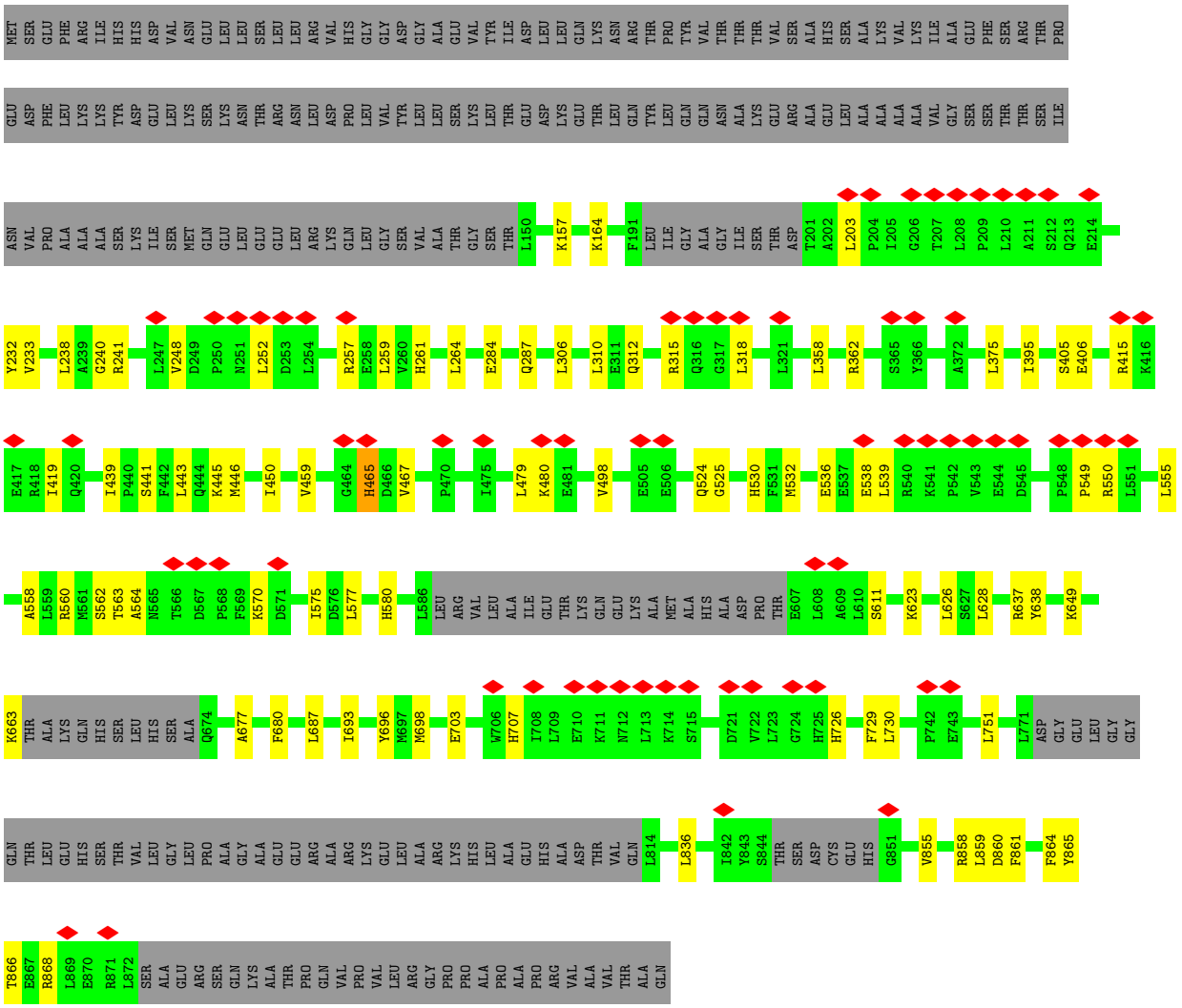
• Molecule 4: Gamma-tubulin complex component 2

Chain G:



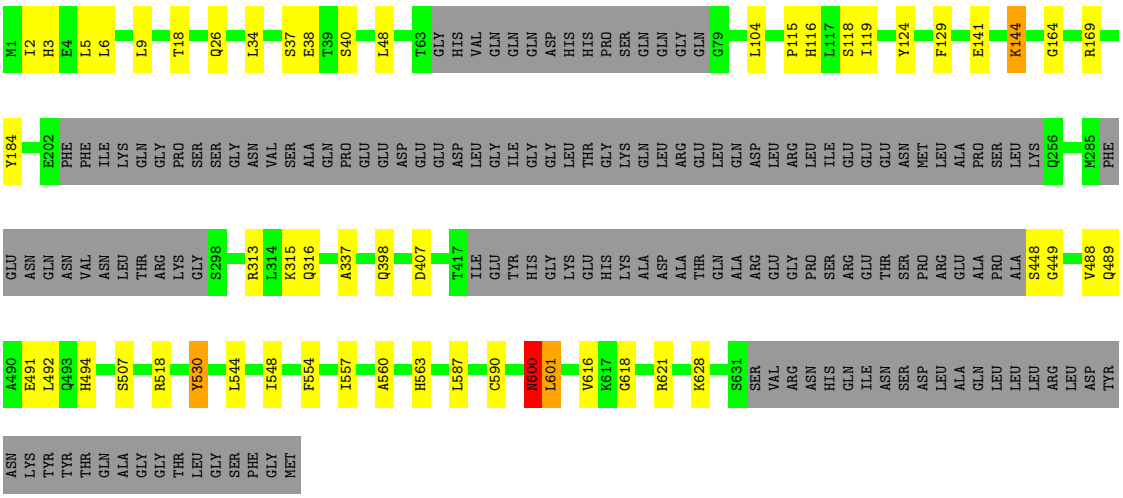
• Molecule 4: Gamma-tubulin complex component 2

Chain M:



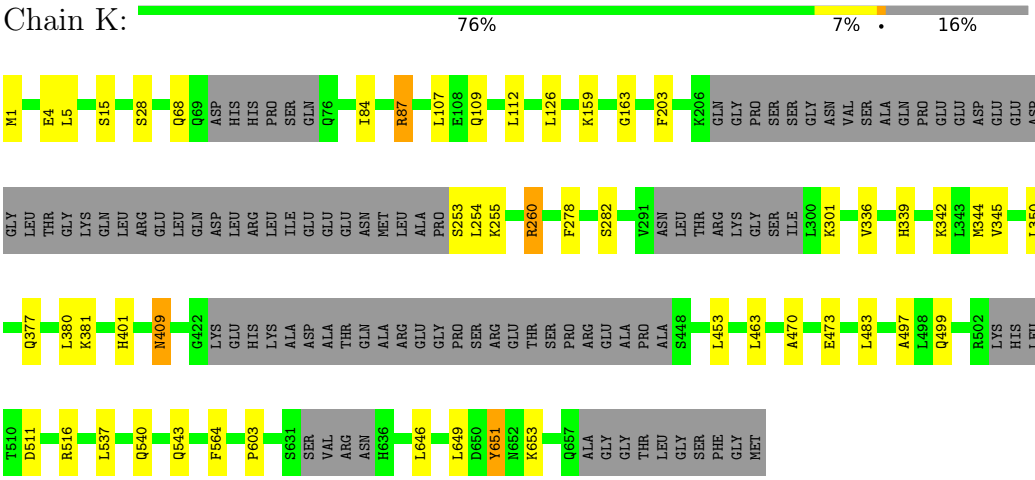
• Molecule 5: Gamma-tubulin complex component 4

Chain I:



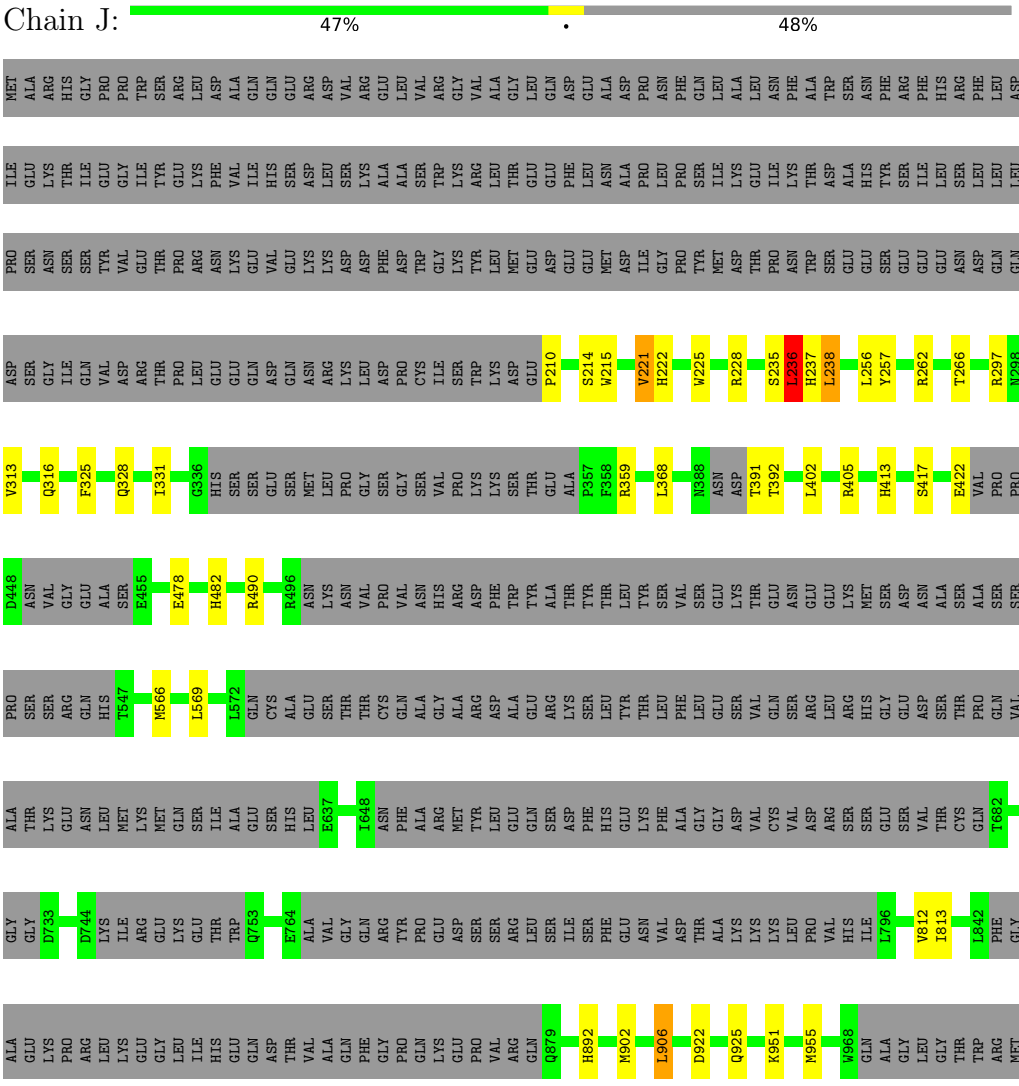
• Molecule 5: Gamma-tubulin complex component 4

Chain K:



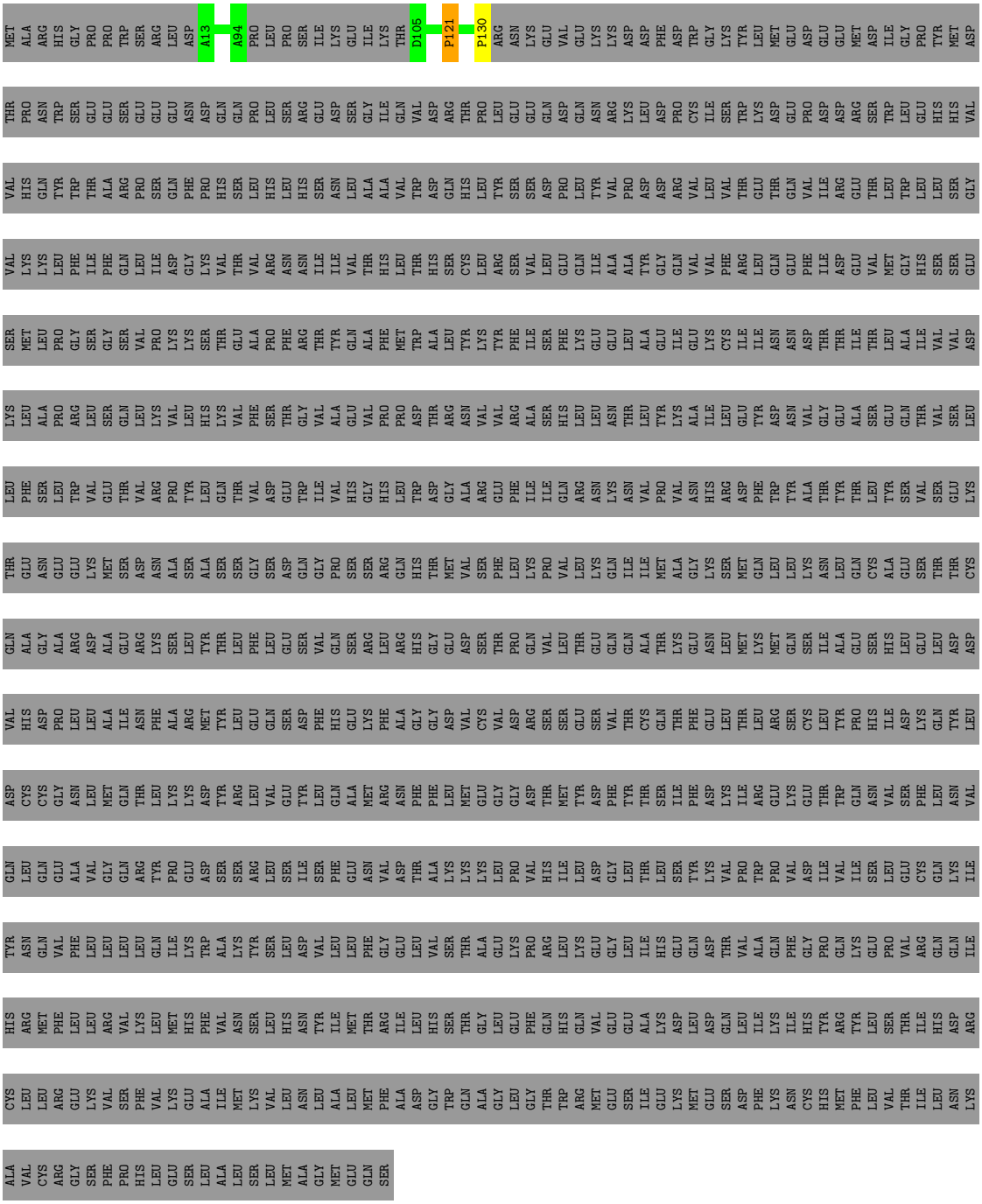
• Molecule 6: Gamma-tubulin complex component 5

Chain J:



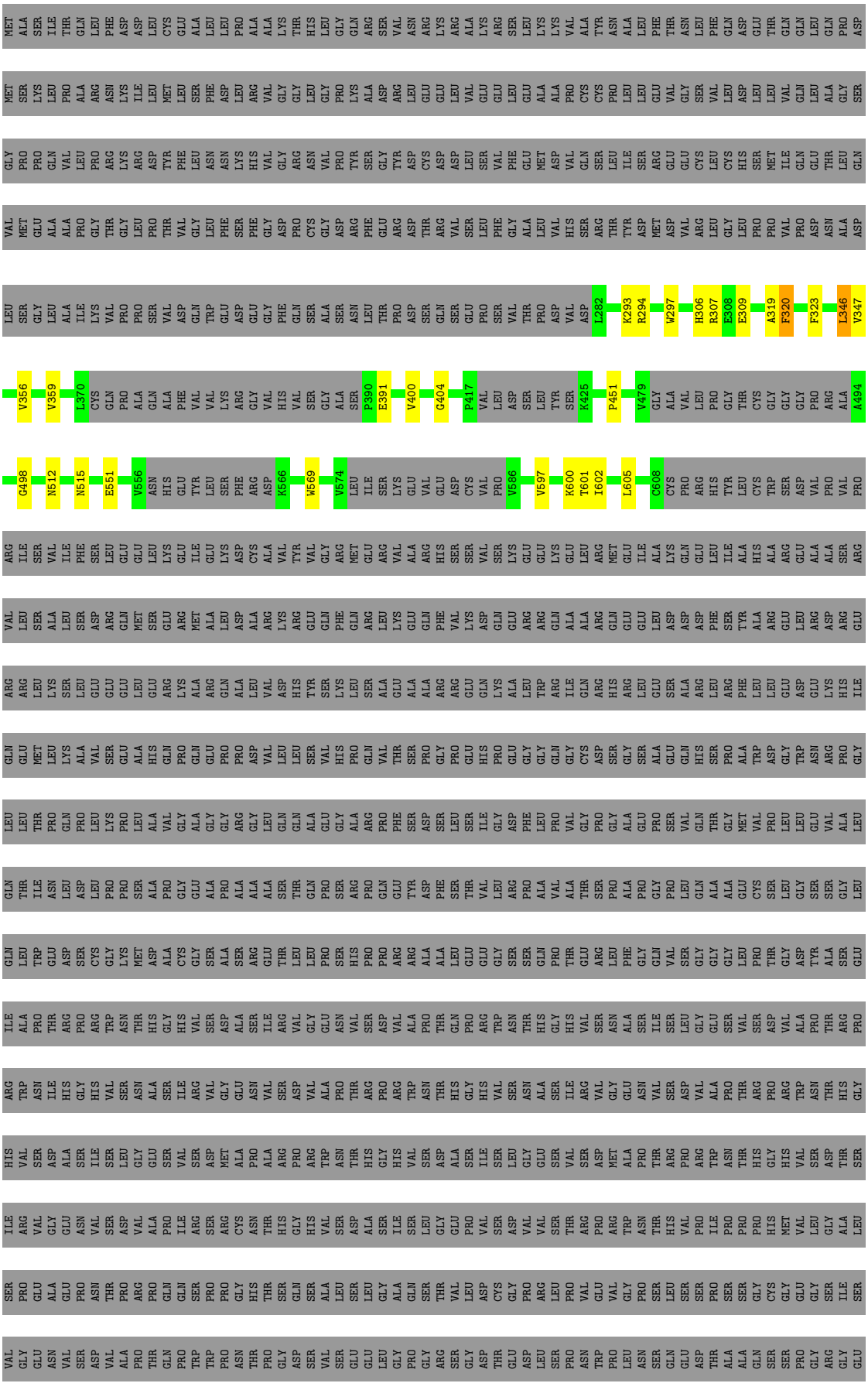
• Molecule 6: Gamma-tubulin complex component 5

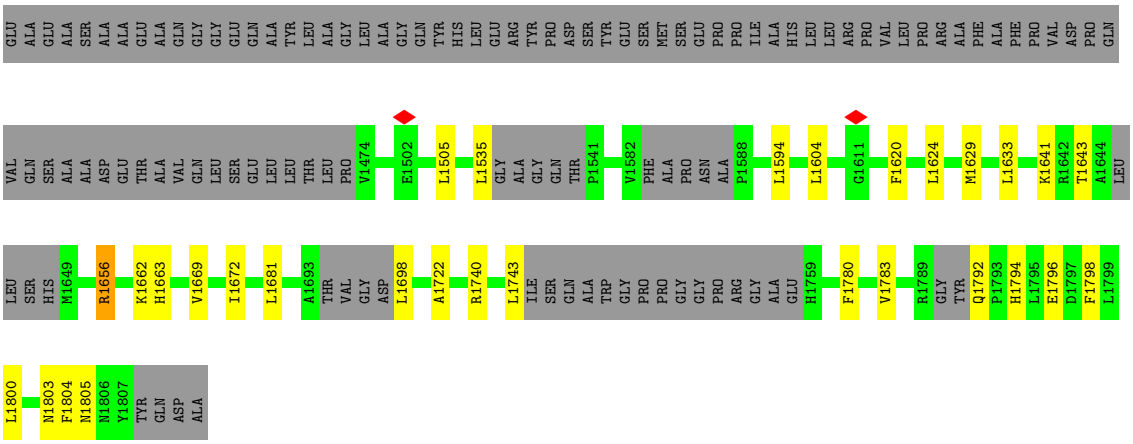
Chain l:



• Molecule 7: Gamma-tubulin complex component 6

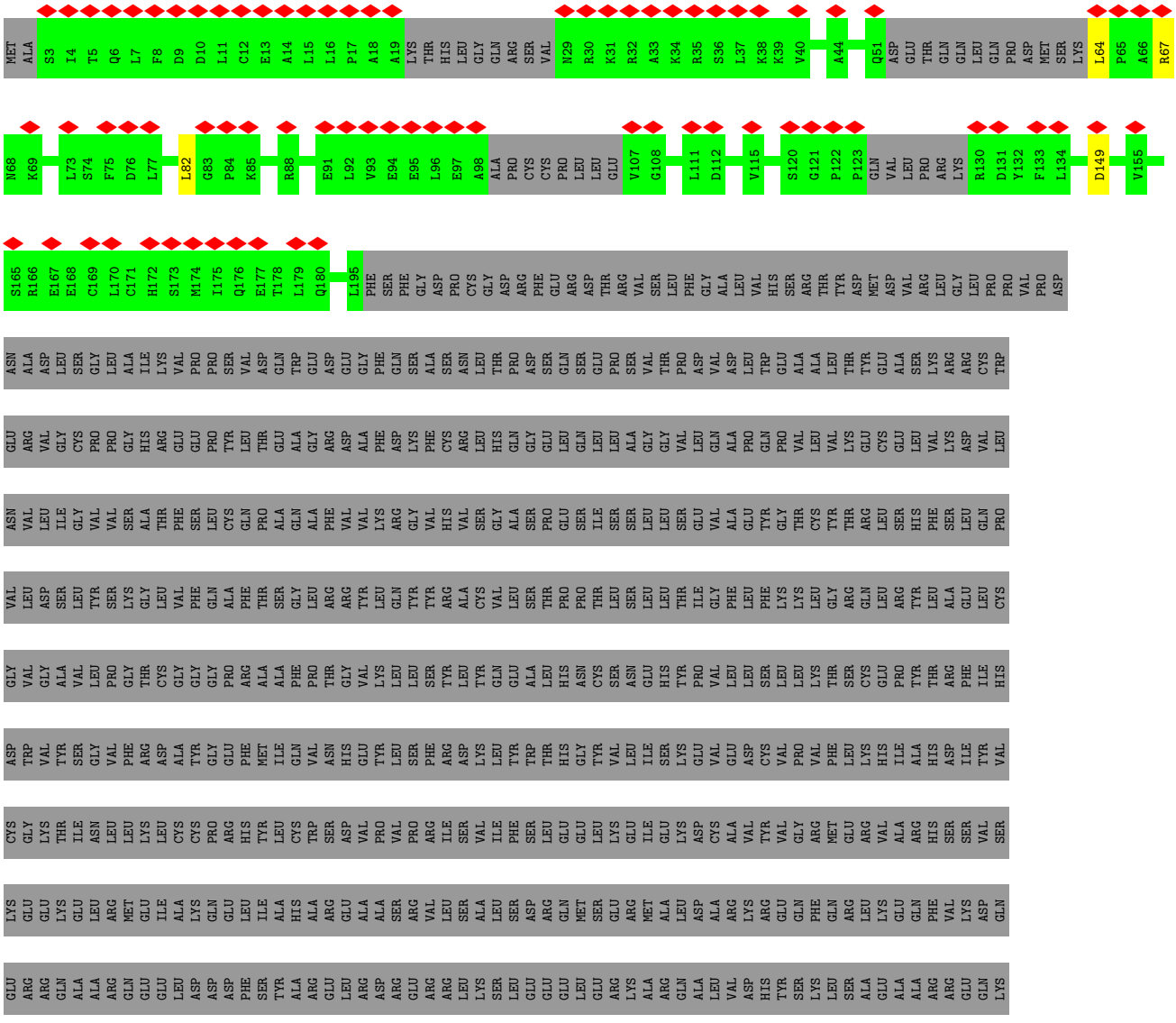
Chain L:

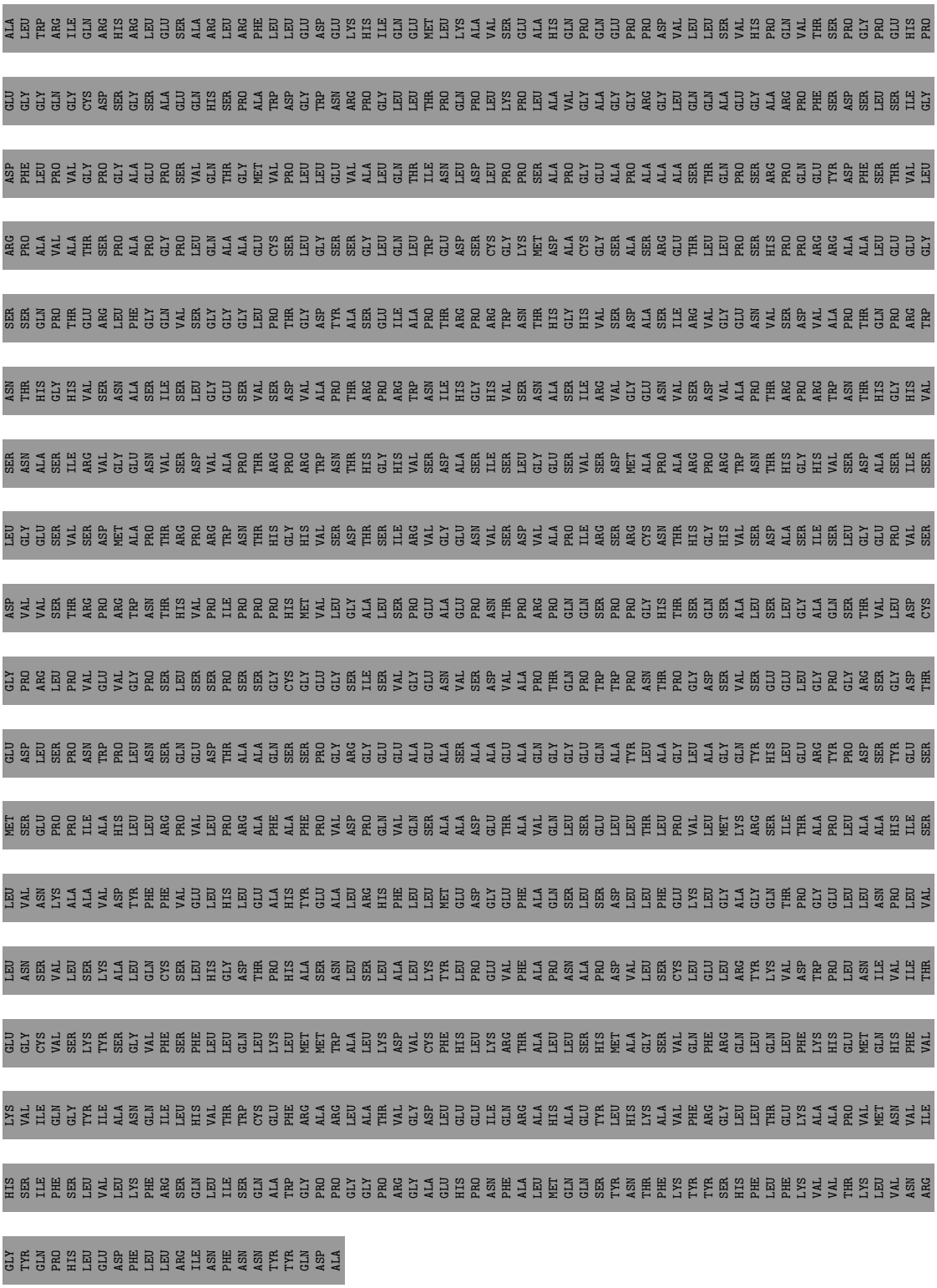

L282
K293
R294
W297
H306
R307
E308
E309
A319
F320
F323
L346
V347
V356
V359
L370
E391
V400
G404
P417
P451
V479
A494
G498
N512
N515
E551
V556
K566
W569
V574
V586
V597
K600
T601
I602
L605
C608
K425
P390



• Molecule 7: Gamma-tubulin complex component 6

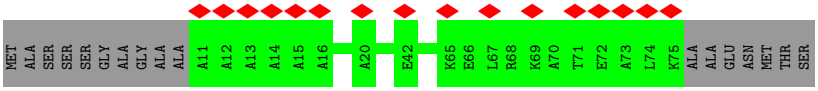
Chain c: 8% 91%





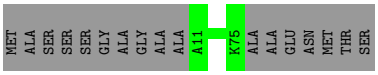
• Molecule 8: Mitotic-spindle organizing protein 1

Chain i:



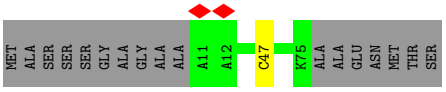
• Molecule 8: Mitotic-spindle organizing protein 1

Chain k:



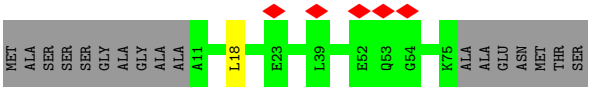
• Molecule 8: Mitotic-spindle organizing protein 1

Chain m:



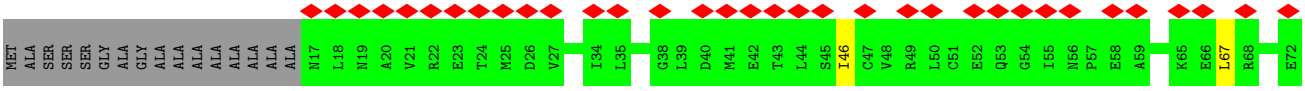
• Molecule 8: Mitotic-spindle organizing protein 1

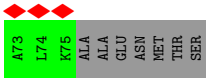
Chain b:



• Molecule 8: Mitotic-spindle organizing protein 1

Chain d:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6456	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	0.170	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0318	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	1	0.30	0/3441	0.53	1/4661 (0.0%)
1	2	0.30	0/3441	0.53	1/4661 (0.0%)
1	Q	0.30	0/3441	0.53	1/4661 (0.0%)
1	R	0.30	0/3441	0.53	1/4661 (0.0%)
1	S	0.30	0/3441	0.53	1/4661 (0.0%)
1	T	0.30	0/3441	0.53	1/4661 (0.0%)
1	U	0.30	0/3441	0.53	1/4661 (0.0%)
1	V	0.30	0/3441	0.53	1/4661 (0.0%)
1	W	0.30	0/3441	0.53	1/4661 (0.0%)
1	X	0.30	0/3441	0.53	1/4661 (0.0%)
1	Y	0.30	0/3441	0.53	1/4661 (0.0%)
1	Z	0.30	0/3441	0.53	1/4661 (0.0%)
2	e	0.56	1/2908 (0.0%)	0.74	3/3938 (0.1%)
3	D	0.39	0/4897	0.67	4/6610 (0.1%)
3	F	0.43	1/5044 (0.0%)	0.67	7/6809 (0.1%)
3	H	0.37	1/5009 (0.0%)	0.61	0/6761
3	N	0.36	0/5009	0.68	6/6761 (0.1%)
3	a	0.36	0/948	0.69	1/1277 (0.1%)
3	h	0.37	0/815	0.63	0/1096
3	j	0.32	0/855	0.62	1/1152 (0.1%)
4	C	0.40	2/5151 (0.0%)	0.67	3/6955 (0.0%)
4	E	0.45	4/5311 (0.1%)	0.68	4/7169 (0.1%)
4	G	0.37	0/5315	0.64	3/7175 (0.0%)
4	M	0.40	0/5295	0.68	3/7147 (0.0%)
5	I	0.41	2/4322 (0.0%)	0.66	3/5853 (0.1%)
5	K	0.46	4/4683 (0.1%)	0.68	6/6338 (0.1%)
6	J	0.40	1/4525 (0.0%)	0.70	4/6119 (0.1%)
6	l	0.35	0/863	0.61	2/1166 (0.2%)
7	L	0.41	1/4697 (0.0%)	0.73	7/6348 (0.1%)
7	c	0.40	0/1235	0.77	2/1664 (0.1%)
8	b	0.44	0/484	0.76	1/653 (0.2%)
8	d	0.34	0/454	0.68	1/611 (0.2%)
8	i	0.36	0/484	0.68	0/653
8	k	0.29	0/484	0.54	0/653

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
8	m	0.35	0/484	0.66	0/653
All	All	0.37	17/110564 (0.0%)	0.63	73/149493 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	2
3	F	0	2
3	H	0	2
3	N	0	1
3	h	0	1
3	j	0	2
4	C	0	3
4	E	0	2
4	G	0	2
4	M	0	1
5	I	0	3
5	K	0	2
6	J	0	4
7	L	0	2
All	All	0	29

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	243	PRO	N-CD	20.70	1.76	1.47
5	K	651	TYR	CD2-CE2	-11.06	1.22	1.39
3	F	299	TRP	CZ3-CH2	9.01	1.54	1.40
4	C	460	VAL	CB-CG2	-7.15	1.37	1.52
4	E	624	TRP	CB-CG	6.75	1.62	1.50
4	C	460	VAL	CB-CG1	-6.70	1.38	1.52
5	I	124	TYR	CD1-CE1	-6.51	1.29	1.39
5	K	651	TYR	CB-CG	-6.38	1.42	1.51
5	K	651	TYR	CD1-CE1	-6.38	1.29	1.39
5	I	530	TYR	CD1-CE1	-6.18	1.30	1.39
6	J	225	TRP	CB-CG	6.01	1.61	1.50
4	E	184	ARG	NE-CZ	6.01	1.40	1.33
4	E	184	ARG	CD-NE	5.94	1.56	1.46
4	E	442	PHE	CD2-CE2	-5.36	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	651	TYR	CG-CD2	-5.18	1.32	1.39
3	H	754	PHE	CD1-CE1	-5.03	1.29	1.39
7	L	320	PHE	CB-CG	-5.03	1.42	1.51

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	727	LEU	CB-CG-CD2	-16.91	82.25	111.00
7	L	1800	LEU	CB-CG-CD1	-13.60	87.87	111.00
4	E	184	ARG	NE-CZ-NH2	-11.72	114.44	120.30
7	L	1800	LEU	CB-CG-CD2	-11.04	92.23	111.00
4	C	460	VAL	CG1-CB-CG2	-10.62	93.91	110.90
4	E	184	ARG	NE-CZ-NH1	10.01	125.30	120.30
7	c	82	LEU	CA-CB-CG	9.28	136.65	115.30
7	L	1681	LEU	CB-CG-CD1	-8.75	96.13	111.00
3	D	581	LEU	CA-CB-CG	8.59	135.06	115.30
6	J	236	LEU	CA-CB-CG	8.25	134.28	115.30
3	N	727	LEU	CA-CB-CG	8.09	133.90	115.30
7	L	1800	LEU	CA-CB-CG	7.95	133.59	115.30
4	M	375	LEU	CB-CG-CD1	-7.54	98.18	111.00
6	J	906	LEU	CA-CB-CG	7.45	132.44	115.30
5	K	651	TYR	CB-CG-CD2	-7.17	116.70	121.00
4	C	220	ASP	CB-CG-OD1	7.13	124.72	118.30
3	F	365	ARG	NE-CZ-NH1	-7.09	116.75	120.30
6	l	121	PRO	N-CA-CB	6.75	111.40	103.30
7	c	64	LEU	CA-CB-CG	6.58	130.43	115.30
3	F	580	LEU	CA-CB-CG	6.57	130.41	115.30
4	M	729	PHE	CB-CG-CD1	-6.55	116.21	120.80
5	K	537	LEU	CA-CB-CG	6.54	130.33	115.30
6	J	238	LEU	CA-CB-CG	6.47	130.19	115.30
4	G	734	LEU	CB-CG-CD1	6.40	121.88	111.00
4	G	554	LEU	CA-CB-CG	6.34	129.88	115.30
2	e	96	VAL	C-N-CA	6.31	137.48	121.70
2	e	185	LEU	CB-CG-CD2	-6.16	100.53	111.00
2	e	56	ASP	CB-CG-OD2	6.13	123.82	118.30
6	l	130	PRO	N-CA-CB	6.06	110.57	103.30
5	K	409	ASN	C-N-CA	5.99	136.68	121.70
3	D	578	MET	CG-SD-CE	5.92	109.68	100.20
7	L	1624	LEU	CB-CG-CD2	-5.89	100.98	111.00
7	L	1656	ARG	NE-CZ-NH1	-5.85	117.38	120.30
5	K	646	LEU	CA-CB-CG	5.82	128.69	115.30
1	X	157	LEU	CA-CB-CG	5.74	128.50	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	b	18	LEU	CA-CB-CG	5.74	128.50	115.30
1	Q	157	LEU	CA-CB-CG	5.74	128.49	115.30
1	U	157	LEU	CA-CB-CG	5.74	128.49	115.30
1	R	157	LEU	CA-CB-CG	5.73	128.49	115.30
1	Z	157	LEU	CA-CB-CG	5.73	128.49	115.30
1	W	157	LEU	CA-CB-CG	5.73	128.48	115.30
1	1	157	LEU	CA-CB-CG	5.73	128.48	115.30
1	2	157	LEU	CA-CB-CG	5.73	128.47	115.30
5	K	463	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	V	157	LEU	CA-CB-CG	5.72	128.46	115.30
1	T	157	LEU	CA-CB-CG	5.72	128.45	115.30
1	Y	157	LEU	CA-CB-CG	5.71	128.44	115.30
1	S	157	LEU	CA-CB-CG	5.71	128.42	115.30
4	E	580	HIS	C-N-CA	5.70	135.95	121.70
3	F	419	LEU	CA-CB-CG	5.63	128.24	115.30
3	D	883	ASN	N-CA-CB	5.61	120.70	110.60
5	I	2	ILE	CG1-CB-CG2	-5.51	99.28	111.40
3	D	790	ASP	CB-CG-OD1	5.48	123.23	118.30
3	N	677	LEU	CB-CG-CD2	-5.47	101.69	111.00
4	G	687	LEU	CA-CB-CG	5.46	127.86	115.30
3	F	377	ARG	NE-CZ-NH1	5.45	123.03	120.30
3	j	108	PRO	N-CA-CB	5.31	109.67	103.30
3	F	299	TRP	CZ3-CH2-CZ2	5.26	127.92	121.60
3	N	597	LEU	CA-CB-CG	5.26	127.41	115.30
5	I	600	ASN	C-N-CA	5.25	134.82	121.70
4	M	259	LEU	CA-CB-CG	5.19	127.25	115.30
4	E	427	TYR	CB-CG-CD1	5.18	124.11	121.00
5	K	68	GLN	CA-CB-CG	5.16	124.74	113.40
3	a	97	LEU	CB-CG-CD2	5.14	119.75	111.00
7	L	1535	LEU	CA-CB-CG	5.14	127.12	115.30
3	N	408	ASP	CB-CG-OD1	5.13	122.92	118.30
4	C	239	ALA	N-CA-CB	5.11	117.25	110.10
8	d	67	LEU	CA-CB-CG	5.11	127.04	115.30
6	J	237	HIS	C-N-CA	5.06	134.34	121.70
3	F	377	ARG	CG-CD-NE	-5.05	101.19	111.80
5	I	104	LEU	CB-CG-CD2	-5.05	102.41	111.00
3	N	581	LEU	CA-CB-CG	5.05	126.91	115.30
3	F	299	TRP	NE1-CE2-CZ2	-5.01	124.89	130.40

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	237	PRO	Peptide
4	C	239	ALA	Peptide
4	C	464	GLY	Peptide
3	D	440	GLU	Peptide
3	D	481	ARG	Peptide
4	E	484	TYR	Peptide
4	E	580	HIS	Peptide
3	F	374	PRO	Peptide
3	F	501	THR	Peptide
4	G	580	HIS	Peptide
4	G	615	ALA	Peptide
3	H	454	VAL	Peptide
3	H	528	ASN	Peptide
5	I	407	ASP	Peptide
5	I	507	SER	Peptide
5	I	600	ASN	Peptide
6	J	235	SER	Peptide
6	J	236	LEU	Mainchain
6	J	256	LEU	Peptide
6	J	726	PHE	Peptide
5	K	253	SER	Peptide,Mainchain
7	L	306	HIS	Peptide
7	L	346	LEU	Peptide
4	M	580	HIS	Peptide
3	N	713	HIS	Sidechain
3	h	49	ARG	Peptide
3	j	108	PRO	Peptide
3	j	112	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3373	0	3325	56	0
1	2	3373	0	3325	56	0
1	Q	3373	0	3325	49	0
1	R	3373	0	3325	48	0
1	S	3373	0	3325	48	0
1	T	3373	0	3325	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	3373	0	3325	53	0
1	V	3373	0	3325	49	0
1	W	3373	0	3325	50	0
1	X	3373	0	3325	53	0
1	Y	3373	0	3325	51	0
1	Z	3373	0	3325	53	0
2	e	2847	0	2810	0	0
3	D	4796	0	4775	37	0
3	F	4941	0	4935	46	0
3	H	4907	0	4896	27	0
3	N	4907	0	4896	44	0
3	a	933	0	953	0	0
3	h	803	0	831	0	0
3	j	843	0	846	0	0
4	C	5044	0	5081	43	0
4	E	5202	0	5241	46	0
4	G	5206	0	5230	44	0
4	M	5186	0	5219	56	0
5	I	4225	0	4259	28	0
5	K	4579	0	4586	31	0
6	J	4429	0	4482	24	0
6	l	847	0	789	0	0
7	L	4587	0	4636	35	0
7	c	1220	0	1231	0	0
8	b	484	0	512	0	0
8	d	454	0	482	0	0
8	i	484	0	512	0	0
8	k	484	0	512	0	0
8	m	484	0	512	0	0
9	l	6	0	0	0	0
All	All	108374	0	108126	995	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 (995) 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)
4:M:638:TYR:HH	4:M:726:HIS:HE2	1.29	0.76
1:T:56:ASP:OD1	1:U:296:ARG:NE	2.19	0.75
4:G:696:TYR:HH	4:G:851:GLY:N	1.84	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:56:ASP:OD2	1:X:299:GLN:NE2	2.22	0.72
5:K:401:HIS:HE1	1:Z:295:ARG:HH12	1.40	0.69
1:1:55:ALA:HB3	1:1:59:HIS:HB2	1.76	0.68
5:K:345:VAL:HA	5:K:350:LEU:HD13	1.75	0.68
1:U:55:ALA:HB3	1:U:59:HIS:HB2	1.76	0.68
1:S:55:ALA:HB3	1:S:59:HIS:HB2	1.76	0.68
1:2:342:GLU:HG3	4:M:549:PRO:HB2	1.73	0.68
1:X:55:ALA:HB3	1:X:59:HIS:HB2	1.76	0.68
1:Z:55:ALA:HB3	1:Z:59:HIS:HB2	1.76	0.68
1:R:55:ALA:HB3	1:R:59:HIS:HB2	1.76	0.68
1:Y:55:ALA:HB3	1:Y:59:HIS:HB2	1.76	0.68
1:2:55:ALA:HB3	1:2:59:HIS:HB2	1.76	0.67
4:E:244:ARG:HE	4:E:275:ARG:HE	1.42	0.67
1:W:55:ALA:HB3	1:W:59:HIS:HB2	1.76	0.67
4:E:696:TYR:O	4:E:700:GLU:HB2	1.95	0.67
1:Q:55:ALA:HB3	1:Q:59:HIS:HB2	1.76	0.67
1:V:55:ALA:HB3	1:V:59:HIS:HB2	1.76	0.67
1:S:56:ASP:OD1	1:T:296:ARG:HD3	1.94	0.67
1:T:55:ALA:HB3	1:T:59:HIS:HB2	1.76	0.66
3:D:806:PHE:HA	3:D:809:LYS:HE3	1.76	0.66
1:1:36:ILE:HD13	1:1:59:HIS:HE1	1.62	0.65
1:V:36:ILE:HD13	1:V:59:HIS:HE1	1.62	0.65
1:S:36:ILE:HD13	1:S:59:HIS:HE1	1.62	0.65
1:2:36:ILE:HD13	1:2:59:HIS:HE1	1.62	0.65
3:N:573:PHE:HB2	3:N:610:ALA:HB2	1.79	0.64
4:G:864:PHE:HB3	1:U:353:PRO:HB3	1.77	0.64
1:Z:36:ILE:HD13	1:Z:59:HIS:HE1	1.62	0.64
4:C:460:VAL:HG23	4:C:465:HIS:CE1	2.33	0.64
1:U:36:ILE:HD13	1:U:59:HIS:HE1	1.62	0.64
1:W:36:ILE:HD13	1:W:59:HIS:HE1	1.62	0.64
1:Y:36:ILE:HD13	1:Y:59:HIS:HE1	1.62	0.64
1:Q:36:ILE:HD13	1:Q:59:HIS:HE1	1.62	0.64
1:T:36:ILE:HD13	1:T:59:HIS:HE1	1.62	0.64
6:J:391:THR:HA	7:L:293:LYS:HG3	1.79	0.63
1:R:36:ILE:HD13	1:R:59:HIS:HE1	1.62	0.63
5:I:398:GLN:NE2	1:X:342:GLU:OE2	2.32	0.63
7:L:1722:ALA:HB2	7:L:1792:GLN:HE22	1.62	0.63
1:X:36:ILE:HD13	1:X:59:HIS:HE1	1.62	0.63
3:F:432:ARG:HH12	3:F:439:LEU:HD12	1.64	0.63
1:U:53:TYR:OH	1:V:299:GLN:NE2	2.24	0.62
4:M:524:GLN:HE21	4:M:564:ALA:HA	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:459:VAL:HG11	4:M:628:LEU:HD11	1.81	0.62
5:K:1:MET:HA	5:K:5:LEU:HD23	1.81	0.62
3:D:245:ILE:HG12	3:D:288:ARG:HH12	1.65	0.62
1:U:300:PRO:HA	1:U:303:VAL:HB	1.82	0.62
1:X:300:PRO:HA	1:X:303:VAL:HB	1.82	0.61
1:Z:300:PRO:HA	1:Z:303:VAL:HB	1.82	0.61
1:T:293:VAL:HA	1:T:296:ARG:HD2	1.83	0.61
1:W:300:PRO:HA	1:W:303:VAL:HB	1.82	0.61
1:1:300:PRO:HA	1:1:303:VAL:HB	1.82	0.61
3:F:391:ARG:HB2	3:F:396:LEU:HD12	1.82	0.61
1:Y:300:PRO:HA	1:Y:303:VAL:HB	1.82	0.61
1:Q:300:PRO:HA	1:Q:303:VAL:HB	1.82	0.61
1:X:293:VAL:HA	1:X:296:ARG:HD2	1.83	0.61
1:2:293:VAL:HA	1:2:296:ARG:HD2	1.83	0.61
4:G:338:LEU:HD21	4:G:375:LEU:HD11	1.82	0.61
1:S:293:VAL:HA	1:S:296:ARG:HD2	1.83	0.61
5:I:618:GLY:HA2	5:I:621:ARG:HE	1.66	0.61
1:R:300:PRO:HA	1:R:303:VAL:HB	1.82	0.60
1:1:264:PRO:HB3	4:M:663:LYS:HG3	1.83	0.60
1:W:158:ASN:ND2	1:W:198:ASN:O	2.35	0.60
1:1:293:VAL:HA	1:1:296:ARG:HD2	1.83	0.60
5:K:339:HIS:HA	5:K:342:LYS:HD2	1.83	0.60
1:S:300:PRO:HA	1:S:303:VAL:HB	1.82	0.60
1:U:158:ASN:ND2	1:U:198:ASN:O	2.35	0.60
1:V:158:ASN:ND2	1:V:198:ASN:O	2.35	0.60
1:Y:293:VAL:HA	1:Y:296:ARG:HD2	1.83	0.60
1:2:300:PRO:HA	1:2:303:VAL:HB	1.82	0.60
5:I:313:ARG:HA	5:I:316:GLN:HE21	1.66	0.60
1:U:293:VAL:HA	1:U:296:ARG:HD2	1.83	0.60
1:X:158:ASN:ND2	1:X:198:ASN:O	2.35	0.60
4:G:167:LYS:HE3	4:G:168:LYS:HG3	1.82	0.60
1:S:158:ASN:ND2	1:S:198:ASN:O	2.35	0.60
1:V:300:PRO:HA	1:V:303:VAL:HB	1.82	0.60
1:W:293:VAL:HA	1:W:296:ARG:HD2	1.83	0.60
1:Z:158:ASN:ND2	1:Z:198:ASN:O	2.35	0.60
3:F:626:LEU:HB2	3:F:637:VAL:HG23	1.84	0.60
3:H:620:ARG:HH12	3:H:645:ASP:H	1.50	0.60
1:T:158:ASN:ND2	1:T:198:ASN:O	2.35	0.60
1:Z:293:VAL:HA	1:Z:296:ARG:HD2	1.83	0.60
1:V:183:VAL:HG13	1:V:187:ASN:HD21	1.67	0.60
1:Y:183:VAL:HG13	1:Y:187:ASN:HD21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:293:VAL:HA	1:V:296:ARG:HD2	1.83	0.60
3:D:266:ILE:HG12	3:D:277:VAL:HG22	1.83	0.59
1:R:183:VAL:HG13	1:R:187:ASN:HD21	1.67	0.59
1:T:300:PRO:HA	1:T:303:VAL:HB	1.82	0.59
1:U:183:VAL:HG13	1:U:187:ASN:HD21	1.67	0.59
1:2:158:ASN:ND2	1:2:198:ASN:O	2.35	0.59
1:2:183:VAL:HG13	1:2:187:ASN:HD21	1.67	0.59
1:S:183:VAL:HG13	1:S:187:ASN:HD21	1.67	0.59
1:1:183:VAL:HG13	1:1:187:ASN:HD21	1.67	0.59
4:E:442:PHE:HE2	4:E:484:TYR:HE2	1.51	0.59
7:L:512:ASN:HD21	7:L:515:ASN:HD22	1.49	0.59
1:Q:293:VAL:HA	1:Q:296:ARG:HD2	1.83	0.59
1:R:293:VAL:HA	1:R:296:ARG:HD2	1.83	0.59
1:Z:183:VAL:HG13	1:Z:187:ASN:HD21	1.67	0.59
1:T:183:VAL:HG13	1:T:187:ASN:HD21	1.67	0.59
1:Y:158:ASN:ND2	1:Y:198:ASN:O	2.35	0.59
1:R:158:ASN:ND2	1:R:198:ASN:O	2.35	0.59
4:C:464:GLY:O	4:C:465:HIS:ND1	2.30	0.59
1:1:247:GLY:O	4:M:525:GLY:N	2.35	0.59
1:U:213:ILE:HG21	1:U:276:LEU:HD22	1.85	0.59
1:W:213:ILE:HG21	1:W:276:LEU:HD22	1.85	0.59
1:X:183:VAL:HG13	1:X:187:ASN:HD21	1.67	0.59
1:X:213:ILE:HG21	1:X:276:LEU:HD22	1.85	0.59
1:2:213:ILE:HG21	1:2:276:LEU:HD22	1.85	0.59
1:2:357:GLN:OE1	3:N:716:HIS:ND1	2.36	0.59
1:S:213:ILE:HG21	1:S:276:LEU:HD22	1.85	0.59
4:C:695:TYR:HB2	4:C:858:ARG:HH22	1.68	0.58
6:J:221:VAL:O	6:J:228:ARG:NH2	2.36	0.58
1:Q:158:ASN:ND2	1:Q:198:ASN:O	2.35	0.58
1:R:213:ILE:HG21	1:R:276:LEU:HD22	1.85	0.58
1:1:158:ASN:ND2	1:1:198:ASN:O	2.35	0.58
1:1:213:ILE:HG21	1:1:276:LEU:HD22	1.85	0.58
1:Q:183:VAL:HG13	1:Q:187:ASN:HD21	1.67	0.58
1:V:350:PRO:HG2	1:V:441:PRO:HG3	1.85	0.58
3:H:363:THR:HB	3:H:366:ARG:H	1.69	0.58
1:S:350:PRO:HG2	1:S:441:PRO:HG3	1.85	0.58
7:L:1663:HIS:ND1	1:Z:261:ILE:O	2.37	0.58
1:2:350:PRO:HG2	1:2:441:PRO:HG3	1.85	0.58
1:Y:350:PRO:HG2	1:Y:441:PRO:HG3	1.85	0.58
4:M:287:GLN:HB2	4:M:406:GLU:HG2	1.86	0.57
1:T:350:PRO:HG2	1:T:441:PRO:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:266:ILE:HG12	3:N:277:VAL:HG12	1.86	0.57
1:W:350:PRO:HG2	1:W:441:PRO:HG3	1.85	0.57
3:H:608:THR:HG23	3:H:610:ALA:H	1.69	0.57
1:T:184:GLN:O	1:T:188:SER:OG	2.23	0.57
1:T:213:ILE:HG21	1:T:276:LEU:HD22	1.85	0.57
1:W:184:GLN:O	1:W:188:SER:OG	2.23	0.57
1:X:184:GLN:O	1:X:188:SER:OG	2.23	0.57
1:X:350:PRO:HG2	1:X:441:PRO:HG3	1.85	0.57
1:Y:213:ILE:HG21	1:Y:276:LEU:HD22	1.85	0.57
1:Q:213:ILE:HG21	1:Q:276:LEU:HD22	1.85	0.57
1:S:260:LEU:HD21	1:S:321:LEU:HB3	1.87	0.57
1:W:183:VAL:HG13	1:W:187:ASN:HD21	1.67	0.57
4:M:560:ARG:HH21	4:M:570:LYS:HD2	1.70	0.57
1:Q:350:PRO:HG2	1:Q:441:PRO:HG3	1.85	0.57
1:Y:184:GLN:O	1:Y:188:SER:OG	2.23	0.57
1:Z:213:ILE:HG21	1:Z:276:LEU:HD22	1.85	0.57
1:2:184:GLN:O	1:2:188:SER:OG	2.23	0.57
5:I:18:THR:OG1	5:I:26:GLN:OE1	2.21	0.57
4:M:536:GLU:HA	4:M:539:LEU:HB2	1.87	0.57
4:E:282:SER:O	4:E:290:HIS:NE2	2.38	0.57
1:T:260:LEU:HD21	1:T:321:LEU:HB3	1.87	0.57
1:U:350:PRO:HG2	1:U:441:PRO:HG3	1.85	0.57
1:V:52:PHE:HA	1:V:62:PRO:HA	1.87	0.57
1:1:350:PRO:HG2	1:1:441:PRO:HG3	1.85	0.57
1:U:260:LEU:HD21	1:U:321:LEU:HB3	1.87	0.57
1:V:213:ILE:HG21	1:V:276:LEU:HD22	1.85	0.57
1:2:355:SER:HB2	3:N:713:HIS:CE1	2.40	0.57
7:L:1656:ARG:NH1	1:Z:434:GLU:OE1	2.38	0.57
1:R:350:PRO:HG2	1:R:441:PRO:HG3	1.85	0.57
1:Z:350:PRO:HG2	1:Z:441:PRO:HG3	1.85	0.57
4:E:231:ARG:NH1	3:F:284:SER:OG	2.38	0.56
1:2:260:LEU:HD21	1:2:321:LEU:HB3	1.87	0.56
1:U:184:GLN:O	1:U:188:SER:OG	2.23	0.56
1:V:184:GLN:O	1:V:188:SER:OG	2.23	0.56
1:Z:184:GLN:O	1:Z:188:SER:OG	2.23	0.56
1:1:45:THR:OG1	4:M:563:THR:OG1	2.23	0.56
4:E:240:GLY:O	4:E:241:ARG:NE	2.37	0.56
4:M:865:TYR:H	4:M:868:ARG:HD2	1.69	0.56
1:Q:64:ALA:O	1:Q:90:ASN:ND2	2.37	0.56
1:T:52:PHE:HA	1:T:62:PRO:HA	1.87	0.56
1:W:64:ALA:O	1:W:90:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:260:LEU:HD21	1:W:321:LEU:HB3	1.87	0.56
1:1:184:GLN:O	1:1:188:SER:OG	2.23	0.56
1:1:260:LEU:HD21	1:1:321:LEU:HB3	1.87	0.56
4:C:440:PRO:HG2	4:C:443:LEU:HB2	1.87	0.56
1:R:260:LEU:HD21	1:R:321:LEU:HB3	1.87	0.56
1:W:341:ARG:NH1	1:W:342:GLU:OE1	2.38	0.56
1:X:226:SER:OG	1:X:227:GLN:NE2	2.39	0.56
1:R:226:SER:OG	1:R:227:GLN:NE2	2.39	0.56
1:T:226:SER:OG	1:T:227:GLN:NE2	2.39	0.56
1:Z:226:SER:OG	1:Z:227:GLN:NE2	2.39	0.56
1:2:52:PHE:HA	1:2:62:PRO:HA	1.87	0.56
1:R:184:GLN:O	1:R:188:SER:OG	2.23	0.56
1:U:226:SER:OG	1:U:227:GLN:NE2	2.39	0.56
1:X:52:PHE:HA	1:X:62:PRO:HA	1.87	0.56
3:H:455:LYS:HE2	3:H:459:LEU:HA	1.88	0.56
4:M:638:TYR:OH	4:M:726:HIS:NE2	2.29	0.56
1:R:341:ARG:NH1	1:R:342:GLU:OE1	2.38	0.56
1:S:184:GLN:O	1:S:188:SER:OG	2.23	0.56
1:S:226:SER:OG	1:S:227:GLN:NE2	2.39	0.56
1:2:226:SER:OG	1:2:227:GLN:NE2	2.39	0.56
7:L:1633:LEU:HD22	7:L:1662:LYS:HZ3	1.69	0.56
1:S:52:PHE:HA	1:S:62:PRO:HA	1.87	0.56
1:Y:226:SER:OG	1:Y:227:GLN:NE2	2.39	0.56
1:2:250:ASN:HB3	1:2:256:LEU:HB2	1.88	0.56
1:U:52:PHE:HA	1:U:62:PRO:HA	1.87	0.56
1:X:260:LEU:HD21	1:X:321:LEU:HB3	1.87	0.56
5:K:653:LYS:HG2	1:Y:350:PRO:HA	1.87	0.56
1:W:56:ASP:HB3	1:X:296:ARG:CG	2.36	0.56
1:Z:52:PHE:HA	1:Z:62:PRO:HA	1.87	0.56
1:2:355:SER:HB2	3:N:713:HIS:NE2	2.20	0.55
1:Q:184:GLN:O	1:Q:188:SER:OG	2.23	0.55
1:W:250:ASN:HB3	1:W:256:LEU:HB2	1.89	0.55
1:Y:250:ASN:HB3	1:Y:256:LEU:HB2	1.88	0.55
1:Y:260:LEU:HD21	1:Y:321:LEU:HB3	1.87	0.55
1:1:64:ALA:O	1:1:90:ASN:ND2	2.37	0.55
1:1:226:SER:OG	1:1:227:GLN:NE2	2.39	0.55
1:Q:52:PHE:HA	1:Q:62:PRO:HA	1.87	0.55
1:Q:250:ASN:HB3	1:Q:256:LEU:HB2	1.88	0.55
1:Y:52:PHE:HA	1:Y:62:PRO:HA	1.87	0.55
4:G:161:LEU:HG	4:G:174:LEU:HD22	1.88	0.55
5:I:448:SER:OG	5:I:449:GLY:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:555:LEU:HD13	4:M:575:ILE:HD11	1.87	0.55
1:T:64:ALA:O	1:T:90:ASN:ND2	2.37	0.55
1:V:260:LEU:HD21	1:V:321:LEU:HB3	1.87	0.55
1:Q:260:LEU:HD21	1:Q:321:LEU:HB3	1.87	0.55
1:S:117:ASP:OD1	1:S:117:ASP:N	2.39	0.55
1:V:117:ASP:OD1	1:V:117:ASP:N	2.39	0.55
1:W:226:SER:OG	1:W:227:GLN:NE2	2.39	0.55
1:Z:117:ASP:OD1	1:Z:117:ASP:N	2.39	0.55
1:V:250:ASN:HB3	1:V:256:LEU:HB2	1.89	0.55
4:M:577:LEU:HD13	4:M:611:SER:HB3	1.88	0.55
1:T:117:ASP:OD1	1:T:117:ASP:N	2.39	0.55
1:V:64:ALA:O	1:V:90:ASN:ND2	2.37	0.55
1:V:226:SER:OG	1:V:227:GLN:NE2	2.39	0.55
1:W:52:PHE:HA	1:W:62:PRO:HA	1.87	0.55
1:X:250:ASN:HB3	1:X:256:LEU:HB2	1.89	0.55
1:1:250:ASN:HB3	1:1:256:LEU:HB2	1.88	0.55
6:J:566:MET:HA	6:J:569:LEU:HD12	1.87	0.55
1:T:250:ASN:HB3	1:T:256:LEU:HB2	1.89	0.55
1:U:117:ASP:N	1:U:117:ASP:OD1	2.39	0.55
1:X:117:ASP:OD1	1:X:117:ASP:N	2.39	0.55
1:Z:260:LEU:HD21	1:Z:321:LEU:HB3	1.87	0.55
1:1:52:PHE:HA	1:1:62:PRO:HA	1.87	0.55
4:M:445:LYS:HB3	4:M:446:MET:HE1	1.88	0.55
3:N:453:THR:OG1	3:N:455:LYS:NZ	2.40	0.55
1:X:341:ARG:NH1	1:X:342:GLU:OE1	2.38	0.55
1:Z:341:ARG:NH1	1:Z:342:GLU:OE1	2.38	0.55
1:Q:226:SER:OG	1:Q:227:GLN:NE2	2.39	0.55
3:F:554:SER:O	3:F:554:SER:OG	2.24	0.54
3:F:799:GLU:HG2	3:F:836:PHE:CZ	2.43	0.54
3:H:589:ALA:HA	3:H:592:LEU:HG	1.90	0.54
1:Q:117:ASP:OD1	1:Q:117:ASP:N	2.39	0.54
1:R:117:ASP:N	1:R:117:ASP:OD1	2.39	0.54
1:Y:341:ARG:NH1	1:Y:342:GLU:OE1	2.38	0.54
4:M:855:VAL:HA	4:M:858:ARG:HG2	1.88	0.54
1:R:52:PHE:HA	1:R:62:PRO:HA	1.87	0.54
1:S:250:ASN:HB3	1:S:256:LEU:HB2	1.88	0.54
1:Y:117:ASP:OD1	1:Y:117:ASP:N	2.40	0.54
3:N:662:ARG:HB3	3:N:764:LEU:HD21	1.89	0.54
3:N:801:GLN:OE1	3:N:802:ARG:NH2	2.40	0.54
3:F:799:GLU:HG2	3:F:836:PHE:HZ	1.72	0.54
1:Z:250:ASN:HB3	1:Z:256:LEU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:839:ARG:HG3	4:C:871:ARG:HH22	1.73	0.54
4:M:703:GLU:HG3	4:M:707:HIS:CE1	2.43	0.54
1:2:341:ARG:NH1	1:2:342:GLU:OE1	2.38	0.54
3:H:723:THR:HA	3:H:727:LEU:HG	1.89	0.54
1:U:250:ASN:HB3	1:U:256:LEU:HB2	1.88	0.54
5:K:107:LEU:HD11	5:K:126:LEU:HD21	1.90	0.54
3:N:581:LEU:HD11	3:N:597:LEU:HD12	1.90	0.53
4:C:658:VAL:HG23	4:C:765:PHE:HD1	1.73	0.53
1:S:64:ALA:O	1:S:90:ASN:ND2	2.37	0.53
4:C:350:CYS:HG	4:C:355:THR:HG1	1.55	0.53
4:G:353:GLY:HA2	4:G:356:LEU:HD12	1.91	0.53
4:G:578:MET:H	4:G:615:ALA:HB1	1.72	0.53
1:2:248:TYR:CE1	3:N:727:LEU:HD21	2.43	0.53
1:Q:110:GLN:HA	1:Q:113:LYS:HE3	1.91	0.53
1:S:341:ARG:NH1	1:S:342:GLU:OE1	2.38	0.53
1:2:64:ALA:O	1:2:90:ASN:ND2	2.37	0.53
4:E:663:LYS:NZ	1:S:200:ASP:OD1	2.39	0.53
4:G:160:MET:HG3	4:G:284:GLU:HB2	1.89	0.53
5:I:492:LEU:HD11	5:I:590:CYS:HB3	1.89	0.53
1:R:250:ASN:HB3	1:R:256:LEU:HB2	1.88	0.53
1:1:110:GLN:HA	1:1:113:LYS:HE3	1.91	0.53
4:G:153:SER:OG	4:G:157:LYS:NZ	2.40	0.53
4:M:233:VAL:HG12	4:M:248:VAL:HA	1.91	0.53
1:Y:105:ALA:O	1:Y:109:SER:OG	2.27	0.53
7:L:1656:ARG:NH2	1:Z:443:TYR:OH	2.42	0.53
7:L:1663:HIS:CG	1:Z:262:PRO:HA	2.43	0.53
1:U:105:ALA:O	1:U:109:SER:OG	2.27	0.53
1:Z:110:GLN:HA	1:Z:113:LYS:HE3	1.91	0.53
1:1:117:ASP:OD1	1:1:117:ASP:N	2.40	0.53
1:2:110:GLN:HA	1:2:113:LYS:HE3	1.91	0.53
1:S:110:GLN:HA	1:S:113:LYS:HE3	1.91	0.53
1:X:64:ALA:O	1:X:90:ASN:ND2	2.37	0.53
1:R:110:GLN:HA	1:R:113:LYS:HE3	1.91	0.52
1:U:341:ARG:NH1	1:U:342:GLU:OE1	2.38	0.52
1:W:105:ALA:O	1:W:109:SER:OG	2.27	0.52
1:1:341:ARG:NH1	1:1:342:GLU:OE1	2.38	0.52
1:2:105:ALA:O	1:2:109:SER:OG	2.27	0.52
4:C:442:PHE:HB2	4:C:484:TYR:OH	2.09	0.52
1:T:105:ALA:O	1:T:109:SER:OG	2.27	0.52
1:W:117:ASP:N	1:W:117:ASP:OD1	2.40	0.52
3:D:304:ILE:HG12	3:D:332:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:110:GLN:HA	1:V:113:LYS:HE3	1.91	0.52
1:1:105:ALA:O	1:1:109:SER:OG	2.27	0.52
5:I:548:ILE:HD12	5:I:557:ILE:HG23	1.92	0.52
1:Q:341:ARG:NH1	1:Q:342:GLU:OE1	2.38	0.52
1:Z:64:ALA:O	1:Z:90:ASN:ND2	2.37	0.52
1:1:45:THR:HG1	4:M:563:THR:HG1	1.58	0.52
3:D:643:HIS:NE2	3:D:645:ASP:OD1	2.41	0.52
1:S:313:THR:OG1	1:S:314:ASN:N	2.43	0.52
1:T:313:THR:OG1	1:T:314:ASN:N	2.43	0.52
1:V:105:ALA:O	1:V:109:SER:OG	2.27	0.52
1:X:110:GLN:HA	1:X:113:LYS:HE3	1.91	0.52
1:Y:313:THR:OG1	1:Y:314:ASN:N	2.43	0.52
1:2:117:ASP:N	1:2:117:ASP:OD1	2.39	0.52
1:2:337:LEU:HD23	3:N:875:PHE:CZ	2.45	0.52
1:T:341:ARG:NH1	1:T:342:GLU:OE1	2.38	0.52
1:Y:64:ALA:O	1:Y:90:ASN:ND2	2.37	0.52
1:Q:313:THR:OG1	1:Q:314:ASN:N	2.43	0.52
1:Z:105:ALA:O	1:Z:109:SER:OG	2.27	0.52
7:L:597:VAL:HA	7:L:600:LYS:HE2	1.92	0.52
7:L:1643:THR:HG21	7:L:1743:LEU:HD21	1.91	0.52
1:S:105:ALA:O	1:S:109:SER:OG	2.27	0.52
1:U:313:THR:OG1	1:U:314:ASN:N	2.43	0.52
3:H:829:GLU:HA	3:H:832:ARG:HB2	1.92	0.52
7:L:498:GLY:HA3	7:L:551:GLU:HB2	1.91	0.52
1:Q:105:ALA:O	1:Q:109:SER:OG	2.27	0.52
1:R:105:ALA:O	1:R:109:SER:OG	2.27	0.52
7:L:356:VAL:HG13	7:L:400:VAL:HG11	1.91	0.52
1:V:341:ARG:NH1	1:V:342:GLU:OE1	2.38	0.52
1:Y:110:GLN:HA	1:Y:113:LYS:HE3	1.91	0.52
4:C:161:LEU:HG	4:C:284:GLU:HG3	1.91	0.51
4:M:164:LYS:HD2	4:M:405:SER:H	1.75	0.51
1:V:383:SER:O	1:V:386:SER:OG	2.28	0.51
1:Q:383:SER:O	1:Q:386:SER:OG	2.28	0.51
1:Z:313:THR:OG1	1:Z:314:ASN:N	2.43	0.51
1:2:313:THR:OG1	1:2:314:ASN:N	2.43	0.51
3:F:455:LYS:HA	3:F:459:LEU:HB2	1.92	0.51
1:Q:336:SER:OG	1:Q:339:ARG:NH1	2.44	0.51
1:W:336:SER:OG	1:W:339:ARG:NH1	2.44	0.51
1:X:105:ALA:O	1:X:109:SER:OG	2.27	0.51
1:1:313:THR:OG1	1:1:314:ASN:N	2.43	0.51
7:L:602:ILE:HD13	7:L:605:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:110:GLN:HA	1:T:113:LYS:HE3	1.91	0.51
1:U:110:GLN:HA	1:U:113:LYS:HE3	1.91	0.51
1:V:313:THR:OG1	1:V:314:ASN:N	2.43	0.51
1:X:313:THR:OG1	1:X:314:ASN:N	2.43	0.51
3:D:869:SER:HB3	3:D:873:LEU:HD23	1.93	0.51
4:C:522:MET:HB3	1:Q:248:TYR:CE1	2.46	0.51
6:J:210:PRO:N	6:J:214:SER:HG	2.09	0.51
1:S:383:SER:O	1:S:386:SER:OG	2.28	0.51
1:X:336:SER:OG	1:X:339:ARG:NH1	2.44	0.51
3:D:549:LEU:HB3	3:D:555:LEU:HG	1.93	0.51
5:I:184:TYR:HD2	5:I:315:LYS:HB3	1.76	0.51
1:R:313:THR:OG1	1:R:314:ASN:N	2.43	0.51
1:V:197:GLN:HA	1:V:265:ARG:HH22	1.76	0.51
1:V:336:SER:OG	1:V:339:ARG:NH1	2.44	0.51
1:W:197:GLN:HA	1:W:265:ARG:HH22	1.76	0.51
1:Z:336:SER:OG	1:Z:339:ARG:NH1	2.44	0.51
1:Z:383:SER:O	1:Z:386:SER:OG	2.28	0.51
4:E:380:THR:HB	4:E:477:TYR:HE2	1.76	0.51
4:G:685:ARG:HG2	1:U:353:PRO:HG2	1.93	0.51
1:S:197:GLN:HA	1:S:265:ARG:HH22	1.76	0.51
1:W:110:GLN:HA	1:W:113:LYS:HE3	1.91	0.51
1:W:383:SER:O	1:W:386:SER:OG	2.28	0.51
1:X:197:GLN:HA	1:X:265:ARG:HH22	1.76	0.51
1:Y:197:GLN:HA	1:Y:265:ARG:HH22	1.76	0.51
1:2:47:ARG:HH11	3:N:575:ARG:HH21	1.59	0.51
6:J:478:GLU:O	6:J:482:HIS:HB2	2.10	0.51
1:2:336:SER:OG	1:2:339:ARG:NH1	2.44	0.51
4:E:581:ASP:HA	4:E:643:ARG:HH12	1.77	0.51
4:M:530:HIS:CD2	4:M:562:SER:HB3	2.45	0.51
3:N:621:LEU:HD11	3:N:640:LEU:HD13	1.92	0.51
1:S:336:SER:OG	1:S:339:ARG:NH1	2.44	0.50
1:T:336:SER:OG	1:T:339:ARG:NH1	2.44	0.50
1:Z:197:GLN:HA	1:Z:265:ARG:HH22	1.76	0.50
3:D:838:GLU:OE1	3:D:842:LYS:NZ	2.40	0.50
3:F:757:THR:O	3:F:761:ARG:NE	2.40	0.50
1:1:336:SER:OG	1:1:339:ARG:NH1	2.44	0.50
3:D:331:GLU:HG3	3:D:418:ILE:HD11	1.93	0.50
3:D:759:ILE:HG23	3:D:764:LEU:HD23	1.94	0.50
4:G:662:ASN:HD21	4:G:683:ARG:HH12	1.57	0.50
6:J:392:THR:H	7:L:293:LYS:HZ3	1.60	0.50
3:N:655:GLU:O	3:N:658:SER:OG	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:660:TYR:HA	3:N:663:VAL:HG12	1.93	0.50
1:R:336:SER:OG	1:R:339:ARG:NH1	2.44	0.50
1:2:197:GLN:HA	1:2:265:ARG:HH22	1.76	0.50
5:K:4:GLU:HG2	7:L:320:PHE:CE1	2.47	0.50
5:K:499:GLN:O	5:K:516:ARG:NH1	2.44	0.50
1:R:383:SER:O	1:R:386:SER:OG	2.28	0.50
1:U:336:SER:OG	1:U:339:ARG:NH1	2.44	0.50
1:Y:383:SER:O	1:Y:386:SER:OG	2.28	0.50
4:E:623:LYS:O	4:E:627:SER:N	2.45	0.50
4:G:522:MET:HB2	1:U:248:TYR:CE1	2.46	0.50
1:T:383:SER:O	1:T:386:SER:OG	2.28	0.50
1:1:197:GLN:HA	1:1:265:ARG:HH22	1.76	0.50
1:2:383:SER:O	1:2:386:SER:OG	2.28	0.50
3:F:878:PHE:HD2	1:T:338:GLN:HE22	1.59	0.50
4:M:157:LYS:HA	4:M:284:GLU:HG3	1.94	0.50
1:S:6:ILE:HG12	1:S:63:ARG:HB3	1.94	0.50
1:T:197:GLN:HA	1:T:265:ARG:HH22	1.76	0.50
4:C:644:HIS:CE1	4:C:738:MET:HB2	2.47	0.50
1:W:313:THR:OG1	1:W:314:ASN:N	2.43	0.50
1:X:383:SER:O	1:X:386:SER:OG	2.28	0.50
1:Y:336:SER:OG	1:Y:339:ARG:NH1	2.44	0.50
3:N:737:LYS:HA	3:N:740:GLN:HE21	1.77	0.50
1:R:6:ILE:HG12	1:R:63:ARG:HB3	1.94	0.50
1:U:64:ALA:O	1:U:90:ASN:ND2	2.37	0.50
1:W:6:ILE:HG12	1:W:63:ARG:HB3	1.94	0.50
1:X:6:ILE:HG12	1:X:63:ARG:HB3	1.94	0.50
1:Q:6:ILE:HG12	1:Q:63:ARG:HB3	1.94	0.50
1:R:64:ALA:O	1:R:90:ASN:ND2	2.37	0.50
1:U:197:GLN:HA	1:U:265:ARG:HH22	1.76	0.50
1:Q:197:GLN:HA	1:Q:265:ARG:HH22	1.76	0.49
1:V:6:ILE:HG12	1:V:63:ARG:HB3	1.94	0.49
4:M:538:GLU:HG2	4:M:550:ARG:CZ	2.42	0.49
1:X:112:GLU:O	1:X:115:HIS:ND1	2.45	0.49
4:G:514:ARG:HA	4:G:517:LYS:HG2	1.92	0.49
7:L:601:THR:HG23	7:L:1698:LEU:HD13	1.94	0.49
1:R:112:GLU:O	1:R:115:HIS:ND1	2.45	0.49
1:T:6:ILE:HG12	1:T:63:ARG:HB3	1.94	0.49
1:1:383:SER:O	1:1:386:SER:OG	2.28	0.49
1:2:6:ILE:HG12	1:2:63:ARG:HB3	1.94	0.49
1:R:197:GLN:HA	1:R:265:ARG:HH22	1.76	0.49
3:F:274:CYS:SG	3:F:276:LYS:NZ	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:855:GLN:HB3	3:D:890:GLU:HG3	1.95	0.49
4:E:388:PHE:HD2	4:E:475:ILE:HD12	1.77	0.49
5:I:118:SER:OG	5:I:119:ILE:N	2.45	0.49
3:N:572:ASP:HA	3:N:575:ARG:NH1	2.28	0.49
1:W:56:ASP:HB3	1:X:296:ARG:HG3	1.93	0.49
4:E:320:SER:OG	4:E:321:LEU:N	2.46	0.49
7:L:1669:VAL:HA	7:L:1672:ILE:HG22	1.95	0.49
1:Y:112:GLU:O	1:Y:115:HIS:ND1	2.45	0.49
1:U:383:SER:O	1:U:386:SER:OG	2.28	0.49
6:J:313:VAL:O	6:J:316:GLN:HG2	2.13	0.49
5:K:470:ALA:O	5:K:473:GLU:HG2	2.12	0.49
1:V:112:GLU:O	1:V:115:HIS:ND1	2.45	0.49
1:1:6:ILE:HG12	1:1:63:ARG:HB3	1.94	0.48
1:1:112:GLU:O	1:1:115:HIS:ND1	2.46	0.48
4:C:221:LEU:HD11	4:C:260:VAL:HG22	1.95	0.48
3:D:581:LEU:HD12	3:D:584:GLU:HB3	1.93	0.48
4:M:860:ASP:HB3	4:M:866:THR:HB	1.95	0.48
3:N:270:ASN:HD21	3:N:273:ASN:HB2	1.78	0.48
1:U:6:ILE:HG12	1:U:63:ARG:HB3	1.94	0.48
1:Y:158:ASN:OD1	1:Y:158:ASN:N	2.46	0.48
4:E:222:LEU:HB3	3:F:365:ARG:HH22	1.78	0.48
4:E:475:ILE:HD13	4:E:484:TYR:HB3	1.94	0.48
4:E:734:LEU:HB3	4:E:735:LYS:HZ2	1.78	0.48
3:F:589:ALA:HA	3:F:592:LEU:HD13	1.93	0.48
4:G:155:GLU:HG3	4:G:158:ARG:HH21	1.78	0.48
4:G:525:GLY:HA3	1:U:251:ASN:HD22	1.77	0.48
3:H:388:CYS:HB3	3:H:396:LEU:HD11	1.95	0.48
6:J:902:MET:HA	6:J:906:LEU:HD23	1.94	0.48
1:W:112:GLU:O	1:W:115:HIS:ND1	2.45	0.48
3:N:456:THR:OG1	3:N:457:ASP:N	2.45	0.48
1:Q:158:ASN:N	1:Q:158:ASN:OD1	2.46	0.48
1:U:112:GLU:O	1:U:115:HIS:ND1	2.46	0.48
4:C:394:TRP:HB2	4:C:400:ILE:HD12	1.95	0.48
4:C:543:VAL:HA	4:C:546:ILE:HD12	1.93	0.48
4:E:467:VAL:O	4:E:494:TYR:OH	2.25	0.48
3:F:669:ARG:HG2	3:F:672:ARG:HH22	1.78	0.48
4:G:298:THR:HA	4:G:301:LYS:HD3	1.94	0.48
1:W:158:ASN:OD1	1:W:158:ASN:N	2.46	0.48
1:Z:112:GLU:O	1:Z:115:HIS:ND1	2.46	0.48
4:E:205:ILE:HG23	4:E:207:THR:H	1.78	0.48
4:C:738:MET:HA	4:C:741:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:6:ILE:HG12	1:Z:63:ARG:HB3	1.94	0.48
3:D:721:TYR:OH	3:D:872:SER:OG	2.26	0.48
3:N:448:VAL:HG22	3:N:484:LEU:HD12	1.96	0.48
1:U:158:ASN:OD1	1:U:158:ASN:N	2.46	0.48
1:Y:6:ILE:HG12	1:Y:63:ARG:HB3	1.94	0.48
1:Z:158:ASN:OD1	1:Z:158:ASN:N	2.46	0.48
4:C:528:PHE:HB3	4:C:649:LYS:HE2	1.95	0.48
3:N:308:THR:O	3:N:312:SER:OG	2.27	0.48
1:V:158:ASN:N	1:V:158:ASN:OD1	2.46	0.48
1:1:158:ASN:N	1:1:158:ASN:OD1	2.46	0.47
4:E:304:LEU:HG	3:F:369:VAL:HG22	1.96	0.47
4:M:677:ALA:HA	4:M:680:PHE:CD2	2.50	0.47
1:S:158:ASN:N	1:S:158:ASN:OD1	2.46	0.47
3:D:308:THR:HG21	3:D:332:LEU:HD22	1.97	0.47
4:E:242:GLN:HB2	4:E:343:THR:HB	1.96	0.47
3:H:605:VAL:HG11	3:H:618:LEU:HD11	1.96	0.47
1:X:158:ASN:N	1:X:158:ASN:OD1	2.46	0.47
1:2:158:ASN:OD1	1:2:158:ASN:N	2.46	0.47
1:T:112:GLU:O	1:T:115:HIS:ND1	2.45	0.47
1:2:291:LEU:HD21	4:M:560:ARG:HH12	1.79	0.47
4:C:868:ARG:HG3	4:C:869:LEU:HD23	1.96	0.47
4:G:395:ILE:HD11	4:G:450:ILE:HG23	1.96	0.47
3:H:391:ARG:HB2	3:H:396:LEU:HD13	1.96	0.47
5:K:497:ALA:HB2	1:Y:254:ILE:HD11	1.97	0.47
7:L:569:TRP:NE1	7:L:600:LYS:HD2	2.30	0.47
3:N:376:ILE:HA	3:N:379:LYS:HG2	1.97	0.47
3:N:691:LEU:HD11	3:N:797:LEU:HG	1.96	0.47
1:R:158:ASN:OD1	1:R:158:ASN:N	2.46	0.47
4:E:238:LEU:HD21	4:E:241:ARG:HB2	1.97	0.47
4:E:440:PRO:HD2	4:E:443:LEU:HD12	1.96	0.47
3:F:494:HIS:CD2	3:F:500:GLN:HA	2.49	0.47
3:N:535:ASP:N	3:N:535:ASP:OD1	2.45	0.47
1:Q:112:GLU:O	1:Q:115:HIS:ND1	2.45	0.47
1:Z:189:LEU:HD12	1:Z:189:LEU:HA	1.78	0.47
3:F:297:LEU:HD22	3:F:371:THR:HG22	1.96	0.47
7:L:1629:MET:HB2	7:L:1669:VAL:HG11	1.96	0.47
3:N:738:VAL:HG12	3:N:747:ILE:HG23	1.97	0.47
3:F:255:LEU:HD11	3:F:343:HIS:HB2	1.97	0.47
3:F:609:ASN:ND2	1:T:49:ASP:OD2	2.38	0.47
4:G:242:GLN:HG3	4:G:343:THR:HA	1.97	0.47
5:I:337:ALA:HB1	5:I:554:PHE:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:158:ASN:OD1	1:T:158:ASN:N	2.46	0.47
5:K:511:ASP:HB3	5:K:603:PRO:HB3	1.97	0.46
3:D:333:ARG:HG2	4:E:326:PHE:HB2	1.97	0.46
4:G:314:HIS:HB2	4:G:319:LEU:HD23	1.97	0.46
3:H:616:GLU:OE1	3:H:619:ARG:NH1	2.44	0.46
5:K:380:LEU:HD22	5:K:453:LEU:HD11	1.97	0.46
7:L:1505:LEU:HD22	7:L:1604:LEU:HD22	1.96	0.46
4:M:312:GLN:HG3	3:N:364:LEU:HD12	1.97	0.46
1:U:289:THR:HG23	1:U:292:ASP:HB2	1.97	0.46
5:I:3:HIS:HB3	7:L:297:TRP:CH2	2.50	0.46
5:K:1:MET:H1	7:L:323:PHE:HZ	1.64	0.46
5:K:540:GLN:HE21	5:K:564:PHE:HA	1.80	0.46
3:N:737:LYS:HG3	3:N:750:ALA:HB1	1.98	0.46
1:T:289:THR:HG23	1:T:292:ASP:HB2	1.98	0.46
1:T:396:ASP:HB3	1:T:400:LYS:HE2	1.98	0.46
1:Z:289:THR:HG23	1:Z:292:ASP:HB2	1.98	0.46
6:J:262:ARG:HH11	6:J:301:ILE:HD12	1.79	0.46
1:S:112:GLU:O	1:S:115:HIS:ND1	2.46	0.46
1:2:47:ARG:NH1	3:N:575:ARG:HH21	2.12	0.46
1:2:112:GLU:O	1:2:115:HIS:ND1	2.45	0.46
4:G:164:LYS:HB2	4:G:174:LEU:HD21	1.97	0.46
6:J:892:HIS:HE1	1:X:355:SER:HB2	1.81	0.46
1:Q:289:THR:HG23	1:Q:292:ASP:HB2	1.97	0.46
1:Q:396:ASP:HB3	1:Q:400:LYS:HE2	1.98	0.46
1:S:289:THR:HG23	1:S:292:ASP:HB2	1.98	0.46
1:V:289:THR:HG23	1:V:292:ASP:HB2	1.98	0.46
1:W:289:THR:HG23	1:W:292:ASP:HB2	1.98	0.46
1:2:337:LEU:HD23	3:N:875:PHE:HZ	1.79	0.46
4:C:180:TRP:HA	4:C:183:GLU:HG3	1.98	0.46
4:C:492:PHE:O	4:C:496:SER:OG	2.27	0.46
4:E:680:PHE:HB3	1:S:262:PRO:O	2.15	0.46
3:F:768:SER:O	3:F:768:SER:OG	2.31	0.46
5:I:164:GLY:H	5:I:169:ARG:HD2	1.79	0.46
1:R:248:TYR:HD2	1:R:249:MET:HG2	1.81	0.46
1:S:396:ASP:HB3	1:S:400:LYS:HE2	1.98	0.46
4:C:160:MET:O	4:C:164:LYS:HG2	2.15	0.46
3:D:832:ARG:HA	3:D:835:GLU:HG3	1.98	0.46
5:K:483:LEU:HD12	5:K:483:LEU:HA	1.81	0.46
4:M:558:ALA:O	4:M:562:SER:OG	2.26	0.46
1:2:248:TYR:HD2	1:2:249:MET:HG2	1.81	0.46
1:2:396:ASP:HB3	1:2:400:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:684:HIS:CE1	3:D:705:HIS:HA	2.51	0.46
4:E:244:ARG:HD2	4:E:271:SER:HB3	1.97	0.46
4:E:713:LEU:HD22	4:E:722:VAL:HG13	1.97	0.46
7:L:1780:PHE:HB2	7:L:1803:ASN:HD22	1.81	0.46
5:I:488:VAL:HG21	5:I:587:LEU:HD22	1.97	0.46
4:M:467:VAL:HG21	4:M:498:VAL:HG11	1.98	0.46
1:Q:248:TYR:HD2	1:Q:249:MET:HG2	1.81	0.46
1:T:248:TYR:HD2	1:T:249:MET:HG2	1.81	0.46
3:F:439:LEU:HD22	3:F:464:TYR:HE1	1.82	0.45
4:G:168:LYS:HE3	4:G:403:PRO:HA	1.97	0.45
5:I:37:SER:O	5:I:40:SER:OG	2.33	0.45
5:K:15:SER:OG	7:L:391:GLU:OE2	2.32	0.45
5:K:301:LYS:NZ	5:K:336:VAL:HA	2.32	0.45
3:N:490:ILE:HD13	3:N:541:THR:HG22	1.97	0.45
4:E:442:PHE:CE2	4:E:484:TYR:HE2	2.33	0.45
3:H:659:HIS:HA	3:H:662:ARG:HD3	1.97	0.45
3:H:802:ARG:HE	3:H:832:ARG:HE	1.64	0.45
4:G:719:ILE:HA	4:G:722:VAL:HG22	1.99	0.45
6:J:812:VAL:HG23	6:J:813:ILE:HG12	1.98	0.45
5:K:649:LEU:CB	1:Y:341:ARG:HH21	2.29	0.45
1:X:396:ASP:HB3	1:X:400:LYS:HE2	1.98	0.45
1:Y:289:THR:HG23	1:Y:292:ASP:HB2	1.98	0.45
1:1:248:TYR:HD2	1:1:249:MET:HG2	1.81	0.45
1:R:396:ASP:HB3	1:R:400:LYS:HE2	1.98	0.45
1:Z:248:TYR:HD2	1:Z:249:MET:HG2	1.81	0.45
1:Z:303:VAL:HG12	1:Z:305:VAL:H	1.81	0.45
4:C:770:LYS:HG3	4:C:771:LEU:HG	1.99	0.45
3:D:454:VAL:HG13	3:D:463:LYS:HG3	1.99	0.45
1:S:248:TYR:HD2	1:S:249:MET:HG2	1.81	0.45
1:V:303:VAL:HG12	1:V:305:VAL:H	1.81	0.45
1:X:248:TYR:HD2	1:X:249:MET:HG2	1.81	0.45
1:X:303:VAL:HG12	1:X:305:VAL:H	1.81	0.45
1:1:396:ASP:HB3	1:1:400:LYS:HE2	1.98	0.45
4:E:263:ILE:HD11	4:E:325:TRP:HB2	1.98	0.45
3:F:339:LEU:H	3:F:339:LEU:HG	1.48	0.45
7:L:1641:LYS:HA	7:L:1641:LYS:HD3	1.76	0.45
1:U:248:TYR:HD2	1:U:249:MET:HG2	1.81	0.45
1:Y:303:VAL:HG12	1:Y:305:VAL:H	1.82	0.45
1:Z:396:ASP:HB3	1:Z:400:LYS:HE2	1.98	0.45
1:1:262:PRO:HG3	1:1:318:ILE:HG21	1.99	0.45
3:D:261:ILE:HD13	4:E:255:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:444:GLN:HA	4:G:447:ALA:HB2	1.99	0.45
6:J:266:THR:HA	6:J:302:VAL:HG13	1.97	0.45
1:R:289:THR:HG23	1:R:292:ASP:HB2	1.98	0.45
1:W:56:ASP:HB3	1:X:296:ARG:HG2	1.99	0.45
1:Y:396:ASP:HB3	1:Y:400:LYS:HE2	1.98	0.45
4:C:557:LEU:HD13	1:R:295:ARG:HH12	1.82	0.45
4:C:632:ARG:HE	4:C:636:THR:HG23	1.82	0.45
1:Q:262:PRO:HG3	1:Q:318:ILE:HG21	1.99	0.45
1:W:262:PRO:HG3	1:W:318:ILE:HG21	1.99	0.45
1:1:276:LEU:HD23	1:1:276:LEU:HA	1.83	0.45
1:1:289:THR:HG23	1:1:292:ASP:HB2	1.98	0.45
1:2:291:LEU:HD13	1:2:339:ARG:HB3	1.99	0.45
3:D:377:ARG:O	3:D:380:THR:OG1	2.32	0.45
4:G:277:ILE:O	4:G:281:SER:OG	2.29	0.45
4:G:663:LYS:NZ	1:U:265:ARG:HH12	2.14	0.45
5:K:84:ILE:HA	5:K:87:ARG:HE	1.81	0.45
7:L:1792:GLN:HE21	7:L:1794:HIS:CE1	2.34	0.45
3:N:653:THR:HG23	3:N:655:GLU:H	1.82	0.45
3:N:703:GLN:HE21	3:N:847:LEU:HD23	1.81	0.45
1:R:276:LEU:HD23	1:R:276:LEU:HA	1.83	0.45
1:T:262:PRO:HG3	1:T:318:ILE:HG21	1.99	0.45
1:U:396:ASP:HB3	1:U:400:LYS:HE2	1.98	0.45
1:W:396:ASP:HB3	1:W:400:LYS:HE2	1.98	0.45
4:E:323:LYS:HA	4:E:326:PHE:CE1	2.51	0.45
3:H:274:CYS:SG	3:H:275:TYR:N	2.89	0.45
5:I:548:ILE:HD12	5:I:557:ILE:HD12	1.98	0.45
3:N:375:LYS:HG3	3:N:379:LYS:HE3	1.99	0.45
1:U:189:LEU:HD12	1:U:189:LEU:HA	1.78	0.45
1:U:262:PRO:HG3	1:U:318:ILE:HG21	1.99	0.45
1:V:396:ASP:HB3	1:V:400:LYS:HE2	1.98	0.45
1:W:248:TYR:HD2	1:W:249:MET:HG2	1.81	0.45
1:Y:276:LEU:HD23	1:Y:276:LEU:HA	1.83	0.45
3:D:639:SER:HA	3:D:664:PHE:CE1	2.52	0.44
3:F:692:ARG:NH1	1:T:197:GLN:HB3	2.32	0.44
7:L:1783:VAL:HG21	7:L:1798:PHE:HD2	1.82	0.44
1:T:303:VAL:HG12	1:T:305:VAL:H	1.81	0.44
1:U:291:LEU:HD13	1:U:339:ARG:HB3	1.99	0.44
1:V:291:LEU:HD13	1:V:339:ARG:HB3	1.99	0.44
1:2:289:THR:HG23	1:2:292:ASP:HB2	1.97	0.44
1:2:303:VAL:HG12	1:2:305:VAL:H	1.81	0.44
1:2:342:GLU:HB3	4:M:550:ARG:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:522:MET:HB3	1:Q:248:TYR:HE1	1.81	0.44
5:I:5:LEU:HD11	5:I:119:ILE:HD12	1.97	0.44
1:Q:291:LEU:HD13	1:Q:339:ARG:HB3	1.99	0.44
1:R:303:VAL:HG12	1:R:305:VAL:H	1.81	0.44
1:X:189:LEU:HD12	1:X:189:LEU:HA	1.78	0.44
1:X:289:THR:HG23	1:X:292:ASP:HB2	1.98	0.44
1:1:343:ARG:HG3	1:1:345:LEU:HB2	2.00	0.44
4:E:556:GLU:O	4:E:560:ARG:HG2	2.18	0.44
4:E:679:ALA:HB1	4:E:762:MET:HG3	1.99	0.44
6:J:922:ASP:HB3	6:J:925:GLN:HG2	1.98	0.44
1:X:262:PRO:HG3	1:X:318:ILE:HG21	1.99	0.44
1:Y:291:LEU:HD13	1:Y:339:ARG:HB3	1.99	0.44
4:E:296:MET:HG2	4:E:338:LEU:HD22	1.98	0.44
4:E:452:SER:HA	4:E:455:LYS:HB3	1.99	0.44
3:F:884:GLU:OE1	1:T:344:LYS:NZ	2.49	0.44
1:1:303:VAL:HG12	1:1:305:VAL:H	1.81	0.44
1:2:39:GLU:N	1:2:39:GLU:OE1	2.51	0.44
3:H:308:THR:O	3:H:312:SER:OG	2.32	0.44
1:U:39:GLU:OE1	1:U:39:GLU:N	2.51	0.44
1:V:39:GLU:N	1:V:39:GLU:OE1	2.51	0.44
1:V:262:PRO:HG3	1:V:318:ILE:HG21	1.99	0.44
1:Y:189:LEU:HA	1:Y:189:LEU:HD12	1.78	0.44
1:Y:248:TYR:HD2	1:Y:249:MET:HG2	1.81	0.44
1:Z:291:LEU:HD13	1:Z:339:ARG:HB3	1.99	0.44
1:1:109:SER:H	1:1:109:SER:HG	1.52	0.44
1:1:291:LEU:HD13	1:1:339:ARG:HB3	1.99	0.44
1:2:262:PRO:HG3	1:2:318:ILE:HG21	1.99	0.44
4:G:439:ILE:HG22	4:G:441:SER:H	1.83	0.44
3:H:730:SER:O	3:H:733:GLU:HG2	2.18	0.44
1:Q:39:GLU:N	1:Q:39:GLU:OE1	2.51	0.44
1:U:276:LEU:HD23	1:U:276:LEU:HA	1.83	0.44
1:W:291:LEU:HD13	1:W:339:ARG:HB3	1.99	0.44
1:W:303:VAL:HG12	1:W:305:VAL:H	1.82	0.44
1:X:291:LEU:HD13	1:X:339:ARG:HB3	1.99	0.44
1:Z:262:PRO:HG3	1:Z:318:ILE:HG21	1.99	0.44
1:Z:343:ARG:HG3	1:Z:345:LEU:HB2	2.00	0.44
1:1:353:PRO:HB3	4:M:864:PHE:O	2.18	0.44
4:E:380:THR:HB	4:E:477:TYR:CE2	2.53	0.44
3:F:258:PHE:HB3	3:F:339:LEU:HD22	2.00	0.44
6:J:215:TRP:HE1	7:L:319:ALA:HB2	1.81	0.44
5:K:278:PHE:O	5:K:282:SER:OG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:359:VAL:HG12	7:L:404:GLY:HA3	2.00	0.44
4:M:439:ILE:HG22	4:M:441:SER:H	1.82	0.44
1:S:39:GLU:OE1	1:S:39:GLU:N	2.51	0.44
1:S:323:ILE:HD13	1:S:323:ILE:HA	1.91	0.44
1:V:248:TYR:HD2	1:V:249:MET:HG2	1.81	0.44
3:D:677:LEU:HD21	3:D:712:VAL:HA	1.99	0.44
4:E:821:THR:HA	4:E:824:LYS:HG2	1.99	0.44
4:G:186:ALA:HB1	3:H:293:ARG:HG2	1.99	0.44
5:K:358:LYS:HA	5:K:362:LEU:HD12	1.99	0.44
4:M:358:LEU:HG	4:M:362:ARG:HE	1.82	0.44
1:Q:303:VAL:HG12	1:Q:305:VAL:H	1.81	0.44
1:U:51:PHE:HZ	1:U:240:THR:HG21	1.83	0.44
1:W:68:ASP:OD1	1:W:68:ASP:N	2.51	0.44
1:X:39:GLU:N	1:X:39:GLU:OE1	2.51	0.44
3:D:255:LEU:HD13	3:D:346:LEU:HD22	2.00	0.44
3:F:494:HIS:HD2	3:F:500:GLN:HA	1.82	0.44
3:F:543:LYS:HD2	3:F:543:LYS:HA	1.78	0.44
1:Q:51:PHE:HZ	1:Q:240:THR:HG21	1.83	0.44
1:Q:323:ILE:HD13	1:Q:323:ILE:HA	1.91	0.44
1:Y:39:GLU:N	1:Y:39:GLU:OE1	2.51	0.44
1:Y:343:ARG:HG3	1:Y:345:LEU:HB2	2.00	0.44
1:2:68:ASP:OD1	1:2:68:ASP:N	2.51	0.43
4:C:443:LEU:HD22	4:C:450:ILE:HD11	2.00	0.43
3:F:330:GLN:HA	3:F:333:ARG:HE	1.82	0.43
5:I:48:LEU:HD11	5:I:129:PHE:HB2	2.00	0.43
5:K:344:MET:HG2	5:K:350:LEU:HD11	2.00	0.43
3:N:247:GLU:OE2	3:N:366:ARG:NH1	2.51	0.43
1:T:39:GLU:N	1:T:39:GLU:OE1	2.51	0.43
1:T:68:ASP:OD1	1:T:68:ASP:N	2.51	0.43
1:T:291:LEU:HD13	1:T:339:ARG:HB3	1.99	0.43
3:D:717:GLN:HB3	3:D:879:ARG:HB3	2.00	0.43
5:K:540:GLN:OE1	5:K:543:GLN:NE2	2.50	0.43
4:M:395:ILE:HD11	4:M:450:ILE:HG23	2.00	0.43
1:S:51:PHE:HZ	1:S:240:THR:HG21	1.83	0.43
1:S:262:PRO:HG3	1:S:318:ILE:HG21	1.99	0.43
1:S:291:LEU:HD13	1:S:339:ARG:HB3	1.99	0.43
1:U:303:VAL:HG12	1:U:305:VAL:H	1.81	0.43
1:W:51:PHE:HZ	1:W:240:THR:HG21	1.83	0.43
1:X:343:ARG:HG3	1:X:345:LEU:HB2	2.00	0.43
1:Y:262:PRO:HG3	1:Y:318:ILE:HG21	1.99	0.43
1:Z:39:GLU:OE1	1:Z:39:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:68:ASP:OD1	1:Z:68:ASP:N	2.51	0.43
1:1:246:PRO:HB2	4:M:524:GLN:HG3	2.01	0.43
1:2:51:PHE:HZ	1:2:240:THR:HG21	1.83	0.43
3:F:490:ILE:HG12	3:F:494:HIS:CE1	2.54	0.43
3:F:677:LEU:HA	3:F:680:ILE:HD12	2.00	0.43
1:R:262:PRO:HG3	1:R:318:ILE:HG21	1.99	0.43
1:S:303:VAL:HG12	1:S:305:VAL:H	1.82	0.43
1:X:51:PHE:HZ	1:X:240:THR:HG21	1.83	0.43
4:C:699:PHE:HB3	1:Q:333:VAL:HG21	1.99	0.43
3:D:861:PHE:HA	3:D:864:LEU:HD12	1.99	0.43
4:G:189:GLY:H	4:G:274:THR:HG21	1.82	0.43
3:N:581:LEU:HG	3:N:585:LEU:HG	1.99	0.43
1:X:118:ILE:HD12	1:X:153:LEU:HD11	2.01	0.43
3:D:709:SER:HA	3:D:712:VAL:HG12	2.00	0.43
3:H:563:ARG:HD3	3:H:731:TRP:CD2	2.54	0.43
5:I:6:LEU:HD23	5:I:9:LEU:HD21	2.00	0.43
4:M:415:ARG:HD2	4:M:419:ILE:HD13	2.01	0.43
1:R:291:LEU:HD13	1:R:339:ARG:HB3	1.99	0.43
1:R:343:ARG:HG3	1:R:345:LEU:HB2	2.00	0.43
1:V:68:ASP:N	1:V:68:ASP:OD1	2.51	0.43
1:1:39:GLU:N	1:1:39:GLU:OE1	2.51	0.43
5:K:203:PHE:H	5:K:260:ARG:HH12	1.66	0.43
5:K:651:TYR:CE2	1:Y:354:ALA:HB3	2.54	0.43
7:L:1594:LEU:HG	7:L:1620:PHE:HE2	1.83	0.43
1:S:118:ILE:HD12	1:S:153:LEU:HD11	2.01	0.43
1:T:118:ILE:HD12	1:T:153:LEU:HD11	2.01	0.43
1:U:118:ILE:HD12	1:U:153:LEU:HD11	2.01	0.43
1:U:343:ARG:HG3	1:U:345:LEU:HB2	2.00	0.43
1:V:118:ILE:HD12	1:V:153:LEU:HD11	2.01	0.43
3:D:333:ARG:HB3	3:D:337:ARG:HH22	1.84	0.43
3:D:543:LYS:NZ	3:D:742:GLN:OE1	2.48	0.43
4:M:637:ARG:HB2	4:M:730:LEU:HD21	2.01	0.43
1:Q:68:ASP:N	1:Q:68:ASP:OD1	2.51	0.43
1:S:343:ARG:HG3	1:S:345:LEU:HB2	2.00	0.43
1:W:39:GLU:N	1:W:39:GLU:OE1	2.51	0.43
1:W:118:ILE:HD12	1:W:153:LEU:HD11	2.01	0.43
1:1:189:LEU:HD12	1:1:189:LEU:HA	1.78	0.43
4:C:460:VAL:H	4:C:460:VAL:HG12	1.55	0.43
5:I:518:ARG:HE	5:I:616:VAL:HG12	1.83	0.43
6:J:222:HIS:O	6:J:228:ARG:NE	2.52	0.43
1:R:68:ASP:OD1	1:R:68:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:112:GLU:HA	1:S:152:TYR:CZ	2.54	0.43
1:V:51:PHE:HZ	1:V:240:THR:HG21	1.83	0.43
1:V:323:ILE:HD13	1:V:323:ILE:HA	1.91	0.43
1:2:112:GLU:HA	1:2:152:TYR:CZ	2.54	0.43
4:C:306:LEU:O	4:C:310:LEU:HG	2.18	0.43
3:H:722:ILE:HG22	3:H:727:LEU:HD23	2.00	0.43
7:L:1796:GLU:OE2	1:Z:338:GLN:NE2	2.52	0.43
4:M:698:MET:HE2	4:M:698:MET:HB2	1.85	0.43
1:Q:118:ILE:HD12	1:Q:153:LEU:HD11	2.01	0.43
1:T:51:PHE:HZ	1:T:240:THR:HG21	1.83	0.43
1:T:343:ARG:HG3	1:T:345:LEU:HB2	2.00	0.43
1:V:343:ARG:HG3	1:V:345:LEU:HB2	2.00	0.43
1:2:343:ARG:HG3	1:2:345:LEU:HB2	2.00	0.43
1:R:39:GLU:N	1:R:39:GLU:OE1	2.51	0.43
1:S:68:ASP:N	1:S:68:ASP:OD1	2.51	0.43
1:W:343:ARG:HG3	1:W:345:LEU:HB2	2.00	0.43
1:Y:323:ILE:HD13	1:Y:323:ILE:HA	1.91	0.43
1:Z:118:ILE:HD12	1:Z:153:LEU:HD11	2.01	0.43
4:C:663:LYS:HB3	4:C:663:LYS:HE3	1.80	0.42
4:C:837:LEU:HB3	4:C:856:ILE:HG12	2.01	0.42
3:D:721:TYR:OH	3:D:872:SER:O	2.36	0.42
3:F:490:ILE:HG12	3:F:494:HIS:HE1	1.84	0.42
6:J:402:LEU:HD13	6:J:405:ARG:HG3	2.01	0.42
5:K:159:LYS:HA	5:K:159:LYS:HD3	1.80	0.42
1:T:348:PHE:HB3	1:T:349:ILE:H	1.71	0.42
1:U:68:ASP:OD1	1:U:68:ASP:N	2.51	0.42
1:U:323:ILE:HD13	1:U:323:ILE:HA	1.91	0.42
1:X:68:ASP:N	1:X:68:ASP:OD1	2.51	0.42
1:Z:51:PHE:HZ	1:Z:240:THR:HG21	1.83	0.42
1:1:68:ASP:N	1:1:68:ASP:OD1	2.51	0.42
4:G:319:LEU:HD11	4:G:324:LEU:HB2	1.99	0.42
5:I:491:GLU:HA	5:I:494:HIS:CE1	2.54	0.42
4:M:443:LEU:HD22	4:M:450:ILE:HD11	2.00	0.42
3:N:635:TRP:CG	3:N:672:ARG:HG3	2.54	0.42
1:1:432:ILE:HD13	1:1:435:TYR:HD2	1.84	0.42
5:I:489:GLN:HB3	5:I:530:TYR:OH	2.19	0.42
4:M:261:HIS:HA	4:M:264:LEU:HD12	2.02	0.42
4:M:693:ILE:HD13	4:M:859:LEU:HD11	2.00	0.42
1:R:112:GLU:HA	1:R:152:TYR:CZ	2.54	0.42
1:R:118:ILE:HD12	1:R:153:LEU:HD11	2.01	0.42
1:W:112:GLU:HA	1:W:152:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:276:LEU:HD11	1:2:302:ASN:HA	2.02	0.42
4:C:302:GLU:HA	4:C:305:ILE:HD12	2.02	0.42
3:D:494:HIS:CD2	3:D:500:GLN:HA	2.54	0.42
5:I:601:LEU:HD23	5:I:601:LEU:HA	1.77	0.42
5:I:628:LYS:HD2	5:I:628:LYS:HA	1.87	0.42
5:K:651:TYR:HE2	1:Y:354:ALA:HB3	1.83	0.42
4:M:479:LEU:HG	4:M:480:LYS:HG2	2.00	0.42
4:M:623:LYS:H	4:M:626:LEU:HB2	1.85	0.42
1:Q:112:GLU:HA	1:Q:152:TYR:CZ	2.54	0.42
1:T:189:LEU:HD12	1:T:189:LEU:HA	1.78	0.42
1:1:51:PHE:HZ	1:1:240:THR:HG21	1.83	0.42
4:C:205:ILE:HD12	4:C:208:LEU:HD12	2.01	0.42
4:C:651:VAL:HG23	4:C:690:VAL:HG11	2.01	0.42
3:D:833:ILE:O	3:D:837:LYS:HG2	2.20	0.42
4:E:681:THR:O	4:E:685:ARG:HG3	2.20	0.42
4:G:579:PRO:HA	4:G:608:LEU:HG	2.01	0.42
1:T:112:GLU:HA	1:T:152:TYR:CZ	2.54	0.42
1:V:432:ILE:HD13	1:V:435:TYR:HD2	1.85	0.42
1:W:432:ILE:HD13	1:W:435:TYR:HD2	1.85	0.42
1:Y:68:ASP:OD1	1:Y:68:ASP:N	2.51	0.42
3:F:568:LEU:HD23	3:F:574:ILE:HG21	2.02	0.42
4:G:637:ARG:HD3	4:G:734:LEU:HD22	2.02	0.42
5:I:141:GLU:HA	5:I:144:LYS:HG3	2.02	0.42
1:R:51:PHE:HZ	1:R:240:THR:HG21	1.83	0.42
1:T:432:ILE:HD13	1:T:435:TYR:HD2	1.85	0.42
1:W:276:LEU:HD11	1:W:302:ASN:HA	2.02	0.42
4:C:220:ASP:HB2	4:C:233:VAL:HG12	2.02	0.42
4:G:408:MET:O	4:G:435:VAL:N	2.51	0.42
6:J:331:ILE:HD11	6:J:368:LEU:HD12	2.02	0.42
1:R:113:LYS:HG3	1:R:114:ILE:HG23	2.02	0.42
1:V:112:GLU:HA	1:V:152:TYR:CZ	2.54	0.42
1:X:112:GLU:HA	1:X:152:TYR:CZ	2.54	0.42
1:Y:51:PHE:HZ	1:Y:240:THR:HG21	1.83	0.42
1:Z:112:GLU:HA	1:Z:152:TYR:CZ	2.54	0.42
1:2:432:ILE:HD13	1:2:435:TYR:HD2	1.85	0.42
4:G:167:LYS:HE2	4:G:167:LYS:HB3	1.90	0.42
6:J:325:PHE:O	6:J:328:GLN:HG3	2.19	0.42
5:K:649:LEU:C	5:K:651:TYR:H	2.23	0.42
1:Q:343:ARG:HG3	1:Q:345:LEU:HB2	2.00	0.42
1:Q:348:PHE:HB3	1:Q:349:ILE:H	1.70	0.42
1:Q:432:ILE:HD13	1:Q:435:TYR:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:113:LYS:HG3	1:T:114:ILE:HG23	2.02	0.42
1:U:113:LYS:HG3	1:U:114:ILE:HG23	2.02	0.42
1:U:276:LEU:HD11	1:U:302:ASN:HA	2.02	0.42
1:U:432:ILE:HD13	1:U:435:TYR:HD2	1.85	0.42
1:2:189:LEU:HD12	1:2:189:LEU:HA	1.78	0.42
4:C:547:THR:HG21	4:C:550:ARG:CZ	2.49	0.42
3:F:480:SER:HA	3:F:483:VAL:HG22	2.02	0.42
4:G:305:ILE:O	4:G:308:SER:OG	2.38	0.42
3:N:568:LEU:HD13	3:N:667:LEU:HB3	2.01	0.42
1:Q:113:LYS:HG3	1:Q:114:ILE:HG23	2.02	0.42
1:R:276:LEU:HD11	1:R:302:ASN:HA	2.02	0.42
1:R:432:ILE:HD13	1:R:435:TYR:HD2	1.85	0.42
1:U:112:GLU:HA	1:U:152:TYR:CZ	2.54	0.42
1:1:46:ASP:OD1	1:1:46:ASP:N	2.53	0.42
1:1:118:ILE:HD12	1:1:153:LEU:HD11	2.01	0.42
3:F:744:LEU:HA	3:F:747:ILE:HD12	2.01	0.42
3:H:657:MET:O	3:H:661:LEU:HG	2.19	0.42
1:Q:276:LEU:HD23	1:Q:276:LEU:HA	1.83	0.42
1:Q:276:LEU:HD11	1:Q:302:ASN:HA	2.02	0.42
1:X:276:LEU:HD11	1:X:302:ASN:HA	2.02	0.42
4:G:550:ARG:CZ	1:V:342:GLU:HB3	2.50	0.41
4:G:696:TYR:O	4:G:700:GLU:HB2	2.20	0.41
3:H:549:LEU:HD23	3:H:549:LEU:HA	1.92	0.41
3:H:565:TYR:HB3	3:H:621:LEU:HD12	2.02	0.41
4:M:315:ARG:NH2	3:N:363:THR:OG1	2.52	0.41
1:Q:189:LEU:HD12	1:Q:189:LEU:HA	1.78	0.41
1:S:432:ILE:HD13	1:S:435:TYR:HD2	1.85	0.41
1:X:46:ASP:OD1	1:X:46:ASP:N	2.53	0.41
4:C:364:PHE:HA	4:C:367:THR:HG23	2.02	0.41
3:D:332:LEU:HG	3:D:336:TYR:HE2	1.84	0.41
4:E:689:PHE:HE2	4:E:751:LEU:HD13	1.85	0.41
3:F:781:GLN:HE22	3:F:854:TYR:HA	1.85	0.41
6:J:297:ARG:HG2	6:J:299:ASN:H	1.85	0.41
4:M:696:TYR:HB2	4:M:858:ARG:HD3	2.02	0.41
3:N:665:ASN:HD21	3:N:669:ARG:HE	1.68	0.41
1:X:113:LYS:HG3	1:X:114:ILE:HG23	2.02	0.41
1:Z:432:ILE:HD13	1:Z:435:TYR:HD2	1.85	0.41
1:1:265:ARG:NH1	4:M:663:LYS:HZ1	2.18	0.41
1:1:355:SER:HA	4:M:861:PHE:HB3	2.03	0.41
4:C:583:ILE:HA	4:C:586:LEU:HD22	2.03	0.41
4:G:663:LYS:HE3	4:G:663:LYS:HB2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:338:LEU:O	3:H:342:LEU:HG	2.20	0.41
5:I:34:LEU:HD13	5:I:38:GLU:HG2	2.02	0.41
6:J:413:HIS:O	6:J:417:SER:OG	2.34	0.41
1:S:113:LYS:HG3	1:S:114:ILE:HG23	2.02	0.41
1:S:276:LEU:HD11	1:S:302:ASN:HA	2.02	0.41
1:T:361:SER:OG	1:T:362:ARG:N	2.54	0.41
1:X:361:SER:OG	1:X:362:ARG:N	2.54	0.41
1:Y:118:ILE:HD12	1:Y:153:LEU:HD11	2.01	0.41
1:Z:113:LYS:HG3	1:Z:114:ILE:HG23	2.02	0.41
4:C:176:ILE:HA	4:C:284:GLU:OE2	2.20	0.41
3:F:324:PHE:CD2	3:F:422:VAL:HG21	2.55	0.41
4:M:751:LEU:HD13	4:M:836:LEU:HD13	2.02	0.41
4:M:865:TYR:H	4:M:868:ARG:HH11	1.67	0.41
1:X:432:ILE:HD13	1:X:435:TYR:HD2	1.84	0.41
1:Y:112:GLU:HA	1:Y:152:TYR:CZ	2.54	0.41
1:Y:276:LEU:HD11	1:Y:302:ASN:HA	2.02	0.41
1:1:112:GLU:HA	1:1:152:TYR:CZ	2.54	0.41
3:D:671:LYS:HE2	1:R:248:TYR:OH	2.21	0.41
3:D:799:GLU:HG2	3:D:832:ARG:HE	1.86	0.41
4:G:360:HIS:CE1	4:G:442:PHE:HB3	2.55	0.41
6:J:359:ARG:HD2	5:K:163:GLY:HA2	2.02	0.41
6:J:951:LYS:HE2	6:J:955:MET:HG2	2.01	0.41
7:L:346:LEU:HA	7:L:347:VAL:HA	1.68	0.41
4:C:310:LEU:HD22	4:C:327:TYR:CD2	2.56	0.41
4:E:205:ILE:HA	4:E:251:ASN:HD21	1.85	0.41
3:F:291:ALA:O	3:F:295:SER:OG	2.32	0.41
1:U:361:SER:OG	1:U:362:ARG:N	2.54	0.41
1:V:252:ASP:OD1	1:V:252:ASP:N	2.54	0.41
1:W:113:LYS:HG3	1:W:114:ILE:HG23	2.02	0.41
1:W:189:LEU:HD12	1:W:189:LEU:HA	1.78	0.41
1:W:361:SER:OG	1:W:362:ARG:N	2.54	0.41
1:1:348:PHE:HB3	1:1:349:ILE:H	1.71	0.41
1:2:118:ILE:HD12	1:2:153:LEU:HD11	2.01	0.41
1:Y:113:LYS:HG3	1:Y:114:ILE:HG23	2.02	0.41
1:Y:432:ILE:HD13	1:Y:435:TYR:HD2	1.85	0.41
4:E:700:GLU:OE2	1:S:334:HIS:HB3	2.21	0.41
3:H:364:LEU:HB2	3:H:367:LEU:HD23	2.02	0.41
1:V:276:LEU:HD11	1:V:302:ASN:HA	2.02	0.41
1:W:46:ASP:OD1	1:W:46:ASP:N	2.53	0.41
1:Y:361:SER:OG	1:Y:362:ARG:N	2.54	0.41
3:D:605:VAL:HG11	3:D:618:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:882:PHE:HB3	1:R:355:SER:OG	2.20	0.41
4:E:180:TRP:CH2	3:F:382:ALA:HB1	2.55	0.41
4:E:180:TRP:HH2	3:F:382:ALA:HB1	1.85	0.41
4:E:223:TYR:HA	3:F:365:ARG:NH1	2.35	0.41
4:E:450:ILE:HG12	4:E:488:ILE:HD13	2.02	0.41
3:F:538:TYR:O	3:F:542:SER:OG	2.32	0.41
4:G:155:GLU:O	4:G:159:LYS:HG2	2.20	0.41
4:G:187:LEU:HD12	3:H:375:LYS:HE3	2.03	0.41
4:G:261:HIS:HA	4:G:264:LEU:HD12	2.03	0.41
4:G:334:THR:O	4:G:338:LEU:HG	2.21	0.41
5:I:544:LEU:O	5:I:548:ILE:HG12	2.21	0.41
7:L:1804:PHE:CE2	1:Z:341:ARG:HB2	2.56	0.41
4:M:306:LEU:O	4:M:310:LEU:HG	2.20	0.41
4:M:532:MET:SD	4:M:649:LYS:HG3	2.61	0.41
4:M:539:LEU:HD23	4:M:539:LEU:HA	1.85	0.41
1:S:361:SER:OG	1:S:362:ARG:N	2.54	0.41
1:V:113:LYS:HG3	1:V:114:ILE:HG23	2.02	0.41
1:V:334:HIS:HE1	1:V:335:LYS:HE2	1.86	0.41
1:Y:352:GLY:HA2	1:Y:353:PRO:HD3	1.90	0.41
1:Z:276:LEU:HD11	1:Z:302:ASN:HA	2.02	0.41
1:1:258:ALA:HB1	4:M:687:LEU:HD13	2.02	0.41
1:1:318:ILE:HB	1:1:380:ASN:HB3	2.03	0.41
3:H:599:GLY:HA3	1:W:342:GLU:HG3	2.03	0.41
6:J:490:ARG:HA	6:J:490:ARG:HD2	1.88	0.41
7:L:1805:ASN:HD22	1:Z:344:LYS:HD3	1.85	0.41
3:N:247:GLU:HB3	3:N:366:ARG:HH11	1.86	0.41
1:Q:236:MET:O	1:Q:239:SER:OG	2.39	0.41
1:T:236:MET:O	1:T:239:SER:OG	2.39	0.41
1:T:237:SER:O	1:T:244:ARG:NH2	2.54	0.41
1:Y:236:MET:O	1:Y:239:SER:OG	2.39	0.41
1:Z:276:LEU:HD23	1:Z:276:LEU:HA	1.83	0.41
1:1:334:HIS:HE1	1:1:335:LYS:HE2	1.86	0.40
1:1:361:SER:OG	1:1:362:ARG:N	2.54	0.40
1:2:113:LYS:HG3	1:2:114:ILE:HG23	2.02	0.40
1:2:237:SER:O	1:2:244:ARG:NH2	2.55	0.40
1:2:276:LEU:HA	1:2:276:LEU:HD23	1.83	0.40
4:C:517:LYS:HE3	4:C:706:TRP:CD1	2.56	0.40
4:C:814:LEU:HB3	4:C:815:VAL:H	1.63	0.40
4:C:855:VAL:HA	4:C:858:ARG:HG2	2.03	0.40
4:E:560:ARG:HH22	4:E:570:LYS:HD2	1.85	0.40
3:N:696:GLU:HG3	3:N:840:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:276:LEU:HD11	1:T:302:ASN:HA	2.02	0.40
1:V:361:SER:OG	1:V:362:ARG:N	2.54	0.40
1:W:276:LEU:HD23	1:W:276:LEU:HA	1.83	0.40
1:Z:361:SER:OG	1:Z:362:ARG:N	2.54	0.40
1:1:276:LEU:HD11	1:1:302:ASN:HA	2.02	0.40
1:2:334:HIS:HE1	1:2:335:LYS:HE2	1.86	0.40
3:D:333:ARG:HB3	3:D:337:ARG:NH2	2.37	0.40
3:F:324:PHE:HD2	3:F:422:VAL:HG21	1.86	0.40
4:G:518:ARG:NH1	4:G:524:GLN:OE1	2.53	0.40
3:H:660:TYR:OH	3:H:751:HIS:NE2	2.28	0.40
5:I:115:PRO:HG2	5:I:116:HIS:ND1	2.36	0.40
5:I:560:ALA:HA	5:I:563:HIS:CD2	2.56	0.40
6:J:422:GLU:HG3	6:J:432:ARG:HH21	1.85	0.40
5:K:109:GLN:HA	5:K:112:LEU:HD12	2.02	0.40
4:M:203:LEU:H	4:M:232:TYR:HE1	1.70	0.40
1:R:318:ILE:HB	1:R:380:ASN:HB3	2.03	0.40
1:V:236:MET:O	1:V:239:SER:OG	2.39	0.40
1:W:323:ILE:HD13	1:W:323:ILE:HA	1.91	0.40
1:X:237:SER:O	1:X:244:ARG:NH2	2.55	0.40
4:E:695:TYR:HE1	1:S:249:MET:HG3	1.86	0.40
3:F:280:LYS:HD2	3:F:280:LYS:HA	1.94	0.40
3:F:836:PHE:HD1	3:F:836:PHE:HA	1.70	0.40
3:N:297:LEU:HA	3:N:300:LEU:HD12	2.04	0.40
3:N:793:TYR:HB3	3:N:797:LEU:HD12	2.03	0.40
1:V:46:ASP:OD1	1:V:46:ASP:N	2.53	0.40
1:V:237:SER:O	1:V:244:ARG:NH2	2.55	0.40
1:X:318:ILE:HB	1:X:380:ASN:HB3	2.03	0.40
1:X:334:HIS:HE1	1:X:335:LYS:HE2	1.86	0.40
1:X:348:PHE:HB3	1:X:349:ILE:H	1.71	0.40
4:C:350:CYS:SG	4:C:355:THR:OG1	2.69	0.40
4:E:202:ALA:HB2	4:E:231:ARG:HH21	1.86	0.40
3:F:616:GLU:O	3:F:620:ARG:HG2	2.21	0.40
4:G:818:PHE:O	4:G:822:ILE:HG12	2.22	0.40
7:L:1804:PHE:HB3	1:Z:356:ILE:H	1.86	0.40
4:M:252:LEU:HB3	4:M:257:ARG:HD2	2.02	0.40
1:Q:334:HIS:HE1	1:Q:335:LYS:HE2	1.86	0.40
1:R:323:ILE:HD13	1:R:323:ILE:HA	1.91	0.40
1:R:361:SER:OG	1:R:362:ARG:N	2.54	0.40
1:T:274:THR:HB	1:T:297:LEU:HD13	2.04	0.40
1:U:46:ASP:OD1	1:U:46:ASP:N	2.53	0.40
1:U:318:ILE:HB	1:U:380:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:334:HIS:HE1	1:Z:335:LYS:HE2	1.86	0.40
1:2:236:MET:O	1:2:239:SER:OG	2.40	0.40
3:F:810:LYS:HA	3:F:810:LYS:HD2	1.89	0.40
5:K:377:GLN:O	5:K:381:LYS:HB2	2.22	0.40
4:M:238:LEU:HG	4:M:240:GLY:H	1.86	0.40
3:N:681:ARG:O	3:N:685:MET:HG2	2.21	0.40
1:R:237:SER:O	1:R:244:ARG:NH2	2.55	0.40
1:S:334:HIS:HE1	1:S:335:LYS:HE2	1.86	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	1	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	2	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	Q	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	R	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	S	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	T	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	U	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	V	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	W	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	X	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	Y	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	Z	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
2	e	360/375 (96%)	345 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	571/907 (63%)	546 (96%)	25 (4%)	0	100	100
3	F	591/907 (65%)	556 (94%)	35 (6%)	0	100	100
3	H	584/907 (64%)	557 (95%)	25 (4%)	2 (0%)	41	77
3	N	584/907 (64%)	568 (97%)	16 (3%)	0	100	100
3	a	112/907 (12%)	108 (96%)	4 (4%)	0	100	100
3	h	97/907 (11%)	93 (96%)	4 (4%)	0	100	100
3	j	105/907 (12%)	94 (90%)	10 (10%)	1 (1%)	15	55
4	C	606/902 (67%)	571 (94%)	32 (5%)	3 (0%)	29	69
4	E	626/902 (69%)	577 (92%)	48 (8%)	1 (0%)	47	81
4	G	628/902 (70%)	585 (93%)	43 (7%)	0	100	100
4	M	624/902 (69%)	591 (95%)	31 (5%)	2 (0%)	41	77
5	I	511/667 (77%)	482 (94%)	27 (5%)	2 (0%)	34	72
5	K	548/667 (82%)	525 (96%)	20 (4%)	3 (0%)	29	69
6	J	506/1024 (49%)	472 (93%)	31 (6%)	3 (1%)	25	66
6	l	104/1024 (10%)	96 (92%)	7 (7%)	1 (1%)	15	55
7	L	540/1819 (30%)	501 (93%)	36 (7%)	3 (1%)	25	66
7	c	148/1819 (8%)	139 (94%)	9 (6%)	0	100	100
8	b	63/82 (77%)	63 (100%)	0	0	100	100
8	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
8	i	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
8	k	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
8	m	63/82 (77%)	63 (100%)	0	0	100	100
All	All	13050/23174 (56%)	12341 (95%)	688 (5%)	21 (0%)	50	81

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	239	ALA
4	C	465	HIS
4	E	581	ASP
3	H	455	LYS
5	I	601	LEU
6	J	236	LEU
6	J	238	LEU

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Mol	Chain	Res	Type
5	K	254	LEU
7	L	307	ARG
4	M	241	ARG
6	l	121	PRO
5	K	255	LYS
7	L	451	PRO
4	C	238	LEU
3	H	457	ASP
6	J	257	TYR
5	K	409	ASN
7	L	309	GLU
5	I	600	ASN
4	M	465	HIS
3	j	109	SER

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	1	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	2	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	Q	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	R	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	S	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	T	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	U	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	V	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	W	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	X	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	Y	376/400 (94%)	348 (93%)	28 (7%)	13	38
1	Z	376/400 (94%)	348 (93%)	28 (7%)	13	38
2	e	310/318 (98%)	307 (99%)	3 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	525/798 (66%)	524 (100%)	1 (0%)	93 96
3	F	542/798 (68%)	536 (99%)	6 (1%)	73 84
3	H	539/798 (68%)	537 (100%)	2 (0%)	91 94
3	N	539/798 (68%)	538 (100%)	1 (0%)	93 96
3	a	101/798 (13%)	101 (100%)	0	100 100
3	h	88/798 (11%)	88 (100%)	0	100 100
3	j	88/798 (11%)	88 (100%)	0	100 100
4	C	556/791 (70%)	552 (99%)	4 (1%)	84 90
4	E	574/791 (73%)	569 (99%)	5 (1%)	78 87
4	G	572/791 (72%)	570 (100%)	2 (0%)	92 95
4	M	572/791 (72%)	570 (100%)	2 (0%)	92 95
5	I	472/594 (80%)	471 (100%)	1 (0%)	93 96
5	K	509/594 (86%)	506 (99%)	3 (1%)	86 92
6	J	498/933 (53%)	497 (100%)	1 (0%)	93 96
6	l	84/933 (9%)	84 (100%)	0	100 100
7	L	501/1546 (32%)	499 (100%)	2 (0%)	91 94
7	c	135/1546 (9%)	133 (98%)	2 (2%)	65 80
8	b	53/62 (86%)	53 (100%)	0	100 100
8	d	53/62 (86%)	52 (98%)	1 (2%)	57 75
8	i	53/62 (86%)	53 (100%)	0	100 100
8	k	53/62 (86%)	53 (100%)	0	100 100
8	m	53/62 (86%)	52 (98%)	1 (2%)	57 75
All	All	11982/20324 (59%)	11609 (97%)	373 (3%)	43 62

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	LEU
1	1	58	GLU
1	1	109	SER
1	1	117	ASP
1	1	120	ASP
1	1	140	SER
1	1	147	SER

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Mol	Chain	Res	Type
1	1	153	LEU
1	1	157	LEU
1	1	158	ASN
1	1	165	LEU
1	1	170	SER
1	1	188	SER
1	1	233	SER
1	1	237	SER
1	1	271	THR
1	1	289	THR
1	1	291	LEU
1	1	293	VAL
1	1	313	THR
1	1	323	ILE
1	1	361	SER
1	1	364	SER
1	1	367	LEU
1	1	369	SER
1	1	374	SER
1	1	392	CYS
1	1	439	THR
1	2	10	LEU
1	2	58	GLU
1	2	109	SER
1	2	117	ASP
1	2	120	ASP
1	2	140	SER
1	2	147	SER
1	2	153	LEU
1	2	157	LEU
1	2	158	ASN
1	2	165	LEU
1	2	170	SER
1	2	188	SER
1	2	233	SER
1	2	237	SER
1	2	271	THR
1	2	289	THR
1	2	291	LEU
1	2	293	VAL
1	2	313	THR
1	2	323	ILE

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Mol	Chain	Res	Type
1	2	361	SER
1	2	364	SER
1	2	367	LEU
1	2	369	SER
1	2	374	SER
1	2	392	CYS
1	2	439	THR
2	e	31	PHE
2	e	196	ARG
2	e	289	ILE
4	C	347	LYS
4	C	367	THR
4	C	510	VAL
4	C	547	THR
3	D	575	ARG
4	E	224	VAL
4	E	231	ARG
4	E	463	CYS
4	E	617	SER
4	E	675	TRP
3	F	271	THR
3	F	337	ARG
3	F	338	LEU
3	F	339	LEU
3	F	554	SER
3	F	761	ARG
4	G	241	ARG
4	G	469	CYS
3	H	271	THR
3	H	286	SER
5	I	144	LYS
6	J	221	VAL
5	K	28	SER
5	K	87	ARG
5	K	260	ARG
7	L	294	ARG
7	L	1740	ARG
4	M	318	LEU
4	M	465	HIS
3	N	591	THR
1	Q	10	LEU
1	Q	58	GLU

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Mol	Chain	Res	Type
1	Q	109	SER
1	Q	117	ASP
1	Q	120	ASP
1	Q	140	SER
1	Q	147	SER
1	Q	153	LEU
1	Q	157	LEU
1	Q	158	ASN
1	Q	165	LEU
1	Q	170	SER
1	Q	188	SER
1	Q	233	SER
1	Q	237	SER
1	Q	271	THR
1	Q	289	THR
1	Q	291	LEU
1	Q	293	VAL
1	Q	313	THR
1	Q	323	ILE
1	Q	361	SER
1	Q	364	SER
1	Q	367	LEU
1	Q	369	SER
1	Q	374	SER
1	Q	392	CYS
1	Q	439	THR
1	R	10	LEU
1	R	58	GLU
1	R	109	SER
1	R	117	ASP
1	R	120	ASP
1	R	140	SER
1	R	147	SER
1	R	153	LEU
1	R	157	LEU
1	R	158	ASN
1	R	165	LEU
1	R	170	SER
1	R	188	SER
1	R	233	SER
1	R	237	SER
1	R	271	THR

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Mol	Chain	Res	Type
1	R	289	THR
1	R	291	LEU
1	R	293	VAL
1	R	313	THR
1	R	323	ILE
1	R	361	SER
1	R	364	SER
1	R	367	LEU
1	R	369	SER
1	R	374	SER
1	R	392	CYS
1	R	439	THR
1	S	10	LEU
1	S	58	GLU
1	S	109	SER
1	S	117	ASP
1	S	120	ASP
1	S	140	SER
1	S	147	SER
1	S	153	LEU
1	S	157	LEU
1	S	158	ASN
1	S	165	LEU
1	S	170	SER
1	S	188	SER
1	S	233	SER
1	S	237	SER
1	S	271	THR
1	S	289	THR
1	S	291	LEU
1	S	293	VAL
1	S	313	THR
1	S	323	ILE
1	S	361	SER
1	S	364	SER
1	S	367	LEU
1	S	369	SER
1	S	374	SER
1	S	392	CYS
1	S	439	THR
1	T	10	LEU
1	T	58	GLU

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Mol	Chain	Res	Type
1	T	109	SER
1	T	117	ASP
1	T	120	ASP
1	T	140	SER
1	T	147	SER
1	T	153	LEU
1	T	157	LEU
1	T	158	ASN
1	T	165	LEU
1	T	170	SER
1	T	188	SER
1	T	233	SER
1	T	237	SER
1	T	271	THR
1	T	289	THR
1	T	291	LEU
1	T	293	VAL
1	T	313	THR
1	T	323	ILE
1	T	361	SER
1	T	364	SER
1	T	367	LEU
1	T	369	SER
1	T	374	SER
1	T	392	CYS
1	T	439	THR
1	U	10	LEU
1	U	58	GLU
1	U	109	SER
1	U	117	ASP
1	U	120	ASP
1	U	140	SER
1	U	147	SER
1	U	153	LEU
1	U	157	LEU
1	U	158	ASN
1	U	165	LEU
1	U	170	SER
1	U	188	SER
1	U	233	SER
1	U	237	SER
1	U	271	THR

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Mol	Chain	Res	Type
1	U	289	THR
1	U	291	LEU
1	U	293	VAL
1	U	313	THR
1	U	323	ILE
1	U	361	SER
1	U	364	SER
1	U	367	LEU
1	U	369	SER
1	U	374	SER
1	U	392	CYS
1	U	439	THR
1	V	10	LEU
1	V	58	GLU
1	V	109	SER
1	V	117	ASP
1	V	120	ASP
1	V	140	SER
1	V	147	SER
1	V	153	LEU
1	V	157	LEU
1	V	158	ASN
1	V	165	LEU
1	V	170	SER
1	V	188	SER
1	V	233	SER
1	V	237	SER
1	V	271	THR
1	V	289	THR
1	V	291	LEU
1	V	293	VAL
1	V	313	THR
1	V	323	ILE
1	V	361	SER
1	V	364	SER
1	V	367	LEU
1	V	369	SER
1	V	374	SER
1	V	392	CYS
1	V	439	THR
1	W	10	LEU
1	W	58	GLU

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Mol	Chain	Res	Type
1	W	109	SER
1	W	117	ASP
1	W	120	ASP
1	W	140	SER
1	W	147	SER
1	W	153	LEU
1	W	157	LEU
1	W	158	ASN
1	W	165	LEU
1	W	170	SER
1	W	188	SER
1	W	233	SER
1	W	237	SER
1	W	271	THR
1	W	289	THR
1	W	291	LEU
1	W	293	VAL
1	W	313	THR
1	W	323	ILE
1	W	361	SER
1	W	364	SER
1	W	367	LEU
1	W	369	SER
1	W	374	SER
1	W	392	CYS
1	W	439	THR
1	X	10	LEU
1	X	58	GLU
1	X	109	SER
1	X	117	ASP
1	X	120	ASP
1	X	140	SER
1	X	147	SER
1	X	153	LEU
1	X	157	LEU
1	X	158	ASN
1	X	165	LEU
1	X	170	SER
1	X	188	SER
1	X	233	SER
1	X	237	SER
1	X	271	THR

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Mol	Chain	Res	Type
1	X	289	THR
1	X	291	LEU
1	X	293	VAL
1	X	313	THR
1	X	323	ILE
1	X	361	SER
1	X	364	SER
1	X	367	LEU
1	X	369	SER
1	X	374	SER
1	X	392	CYS
1	X	439	THR
1	Y	10	LEU
1	Y	58	GLU
1	Y	109	SER
1	Y	117	ASP
1	Y	120	ASP
1	Y	140	SER
1	Y	147	SER
1	Y	153	LEU
1	Y	157	LEU
1	Y	158	ASN
1	Y	165	LEU
1	Y	170	SER
1	Y	188	SER
1	Y	233	SER
1	Y	237	SER
1	Y	271	THR
1	Y	289	THR
1	Y	291	LEU
1	Y	293	VAL
1	Y	313	THR
1	Y	323	ILE
1	Y	361	SER
1	Y	364	SER
1	Y	367	LEU
1	Y	369	SER
1	Y	374	SER
1	Y	392	CYS
1	Y	439	THR
1	Z	10	LEU
1	Z	58	GLU

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Mol	Chain	Res	Type
1	Z	109	SER
1	Z	117	ASP
1	Z	120	ASP
1	Z	140	SER
1	Z	147	SER
1	Z	153	LEU
1	Z	157	LEU
1	Z	158	ASN
1	Z	165	LEU
1	Z	170	SER
1	Z	188	SER
1	Z	233	SER
1	Z	237	SER
1	Z	271	THR
1	Z	289	THR
1	Z	291	LEU
1	Z	293	VAL
1	Z	313	THR
1	Z	323	ILE
1	Z	361	SER
1	Z	364	SER
1	Z	367	LEU
1	Z	369	SER
1	Z	374	SER
1	Z	392	CYS
1	Z	439	THR
8	m	47	CYS
8	d	46	ILE
7	c	67	ARG
7	c	149	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	187	ASN
1	1	227	GLN
1	1	229	ASN
1	1	267	HIS
1	2	187	ASN
1	2	227	GLN
1	2	229	ASN
1	2	267	HIS

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Mol	Chain	Res	Type
2	e	78	ASN
2	e	88	HIS
2	e	263	GLN
2	e	296	ASN
3	a	84	GLN
4	C	329	GLN
4	C	360	HIS
4	C	639	GLN
4	C	644	HIS
4	C	650	HIS
4	C	718	ASN
4	C	741	ASN
4	C	763	GLN
3	D	500	GLN
3	D	594	GLN
3	D	684	HIS
3	D	705	HIS
3	D	773	ASN
3	D	789	GLN
3	D	852	HIS
4	E	691	GLN
3	F	302	ASN
3	F	322	GLN
3	F	329	HIS
3	F	345	GLN
3	F	491	ASN
3	F	528	ASN
3	F	705	HIS
3	F	713	HIS
3	F	773	ASN
4	G	165	GLN
4	G	314	HIS
4	G	430	GLN
4	G	530	HIS
4	G	639	GLN
4	G	691	GLN
4	G	741	ASN
3	H	401	HIS
3	H	479	GLN
3	H	665	ASN
3	H	684	HIS
5	I	142	GLN

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Mol	Chain	Res	Type
5	I	316	GLN
5	I	533	GLN
6	J	708	GLN
6	J	879	GLN
6	J	881	HIS
6	J	892	HIS
6	J	925	GLN
5	K	82	HIS
5	K	393	ASN
5	K	401	HIS
5	K	460	GLN
5	K	540	GLN
5	K	543	GLN
5	K	561	HIS
5	K	567	ASN
7	L	343	GLN
7	L	512	ASN
7	L	1492	ASN
7	L	1605	ASN
7	L	1792	GLN
7	L	1803	ASN
7	L	1805	ASN
7	L	1806	ASN
4	M	530	HIS
4	M	565	ASN
4	M	654	GLN
4	M	741	ASN
3	N	322	GLN
3	N	343	HIS
3	N	345	GLN
3	N	500	GLN
3	N	560	GLN
3	N	665	ASN
3	N	684	HIS
3	N	687	ASN
3	N	693	ASN
3	N	703	GLN
3	N	740	GLN
3	N	805	GLN
3	N	830	ASN
3	N	855	GLN
3	N	859	GLN

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Mol	Chain	Res	Type
1	Q	187	ASN
1	Q	227	GLN
1	Q	229	ASN
1	Q	267	HIS
1	R	187	ASN
1	R	227	GLN
1	R	229	ASN
1	R	267	HIS
1	S	187	ASN
1	S	227	GLN
1	S	229	ASN
1	S	267	HIS
1	T	187	ASN
1	T	227	GLN
1	T	229	ASN
1	T	267	HIS
1	T	338	GLN
1	U	187	ASN
1	U	227	GLN
1	U	229	ASN
1	U	251	ASN
1	U	267	HIS
1	V	187	ASN
1	V	227	GLN
1	V	229	ASN
1	V	267	HIS
1	W	187	ASN
1	W	227	GLN
1	W	229	ASN
1	W	267	HIS
1	X	187	ASN
1	X	227	GLN
1	X	229	ASN
1	X	267	HIS
1	X	299	GLN
1	Y	187	ASN
1	Y	227	GLN
1	Y	229	ASN
1	Y	267	HIS
1	Z	187	ASN
1	Z	227	GLN
1	Z	229	ASN

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Mol	Chain	Res	Type
1	Z	267	HIS
1	Z	315	HIS
1	Z	338	GLN
3	h	84	GLN
8	d	17	ASN
7	c	43	ASN
7	c	51	GLN
3	j	42	ASN
6	l	15	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.

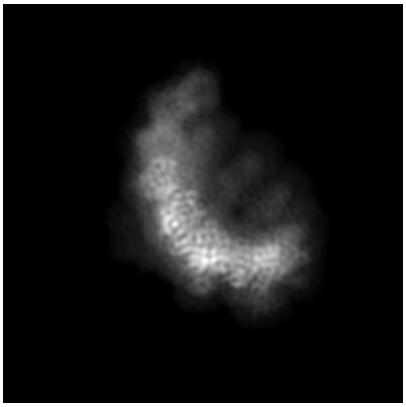
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14016. These allow visual inspection of the internal detail of the map and identification of artifacts.

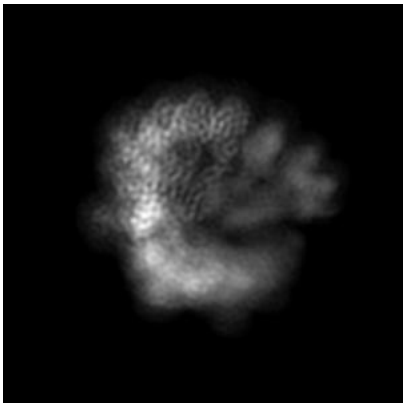
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

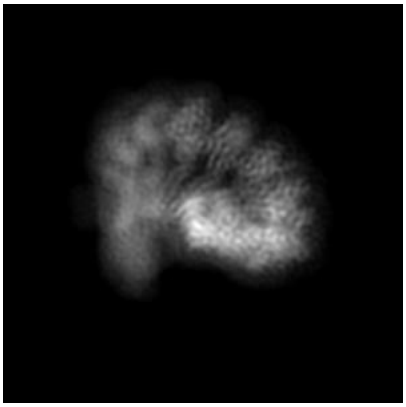
6.1.1 Primary map



X



Y

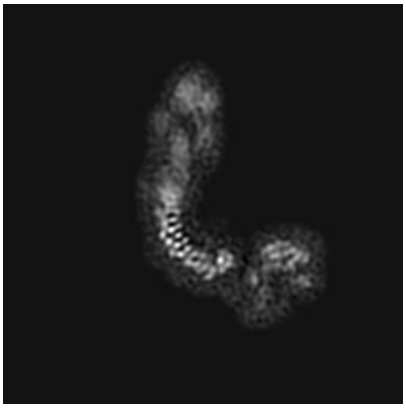


Z

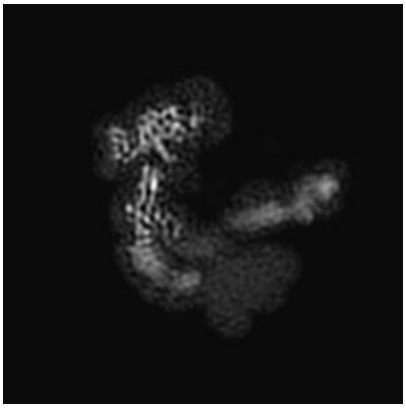
The images above show the map projected in three orthogonal directions.

6.2 Central slices

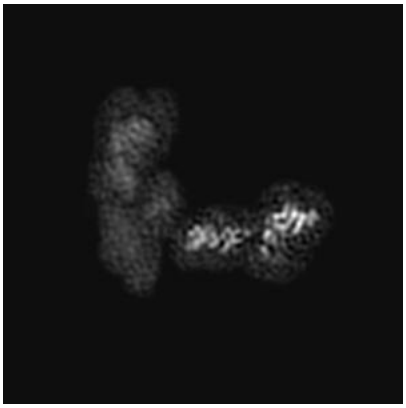
6.2.1 Primary map



X Index: 100



Y Index: 100



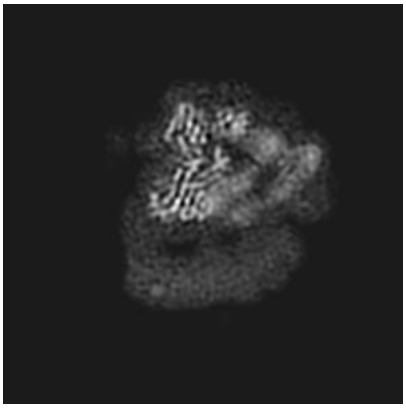
Z Index: 100

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

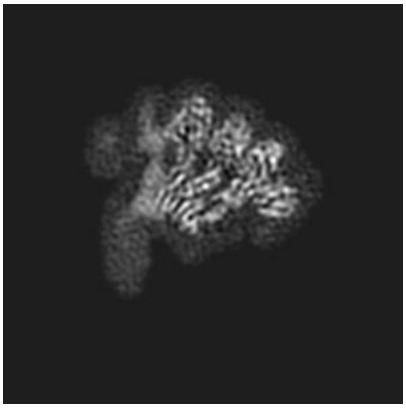
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 134



Y Index: 84

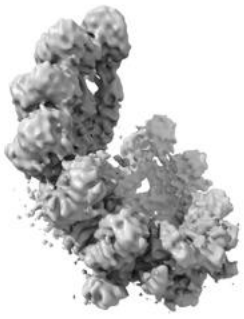


Z Index: 72

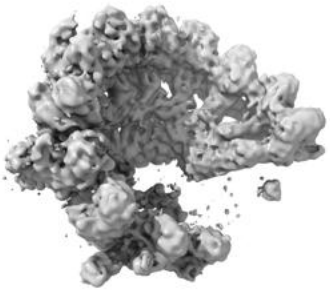
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

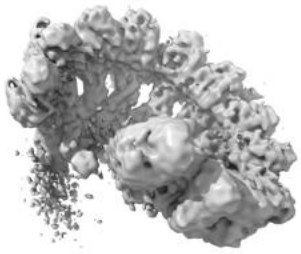
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0318. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

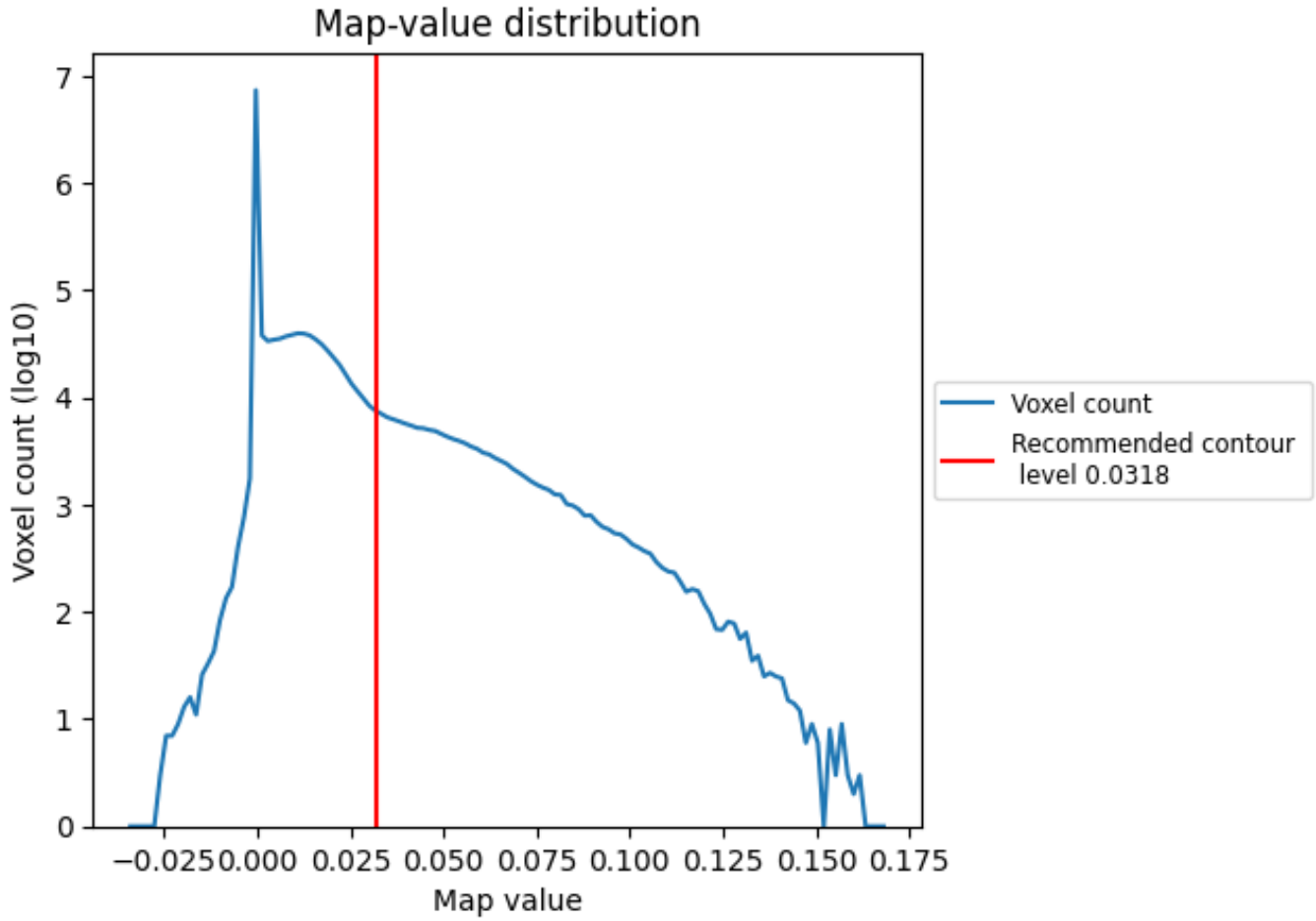
6.5 Mask visualisation (i)

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

7 Map analysis

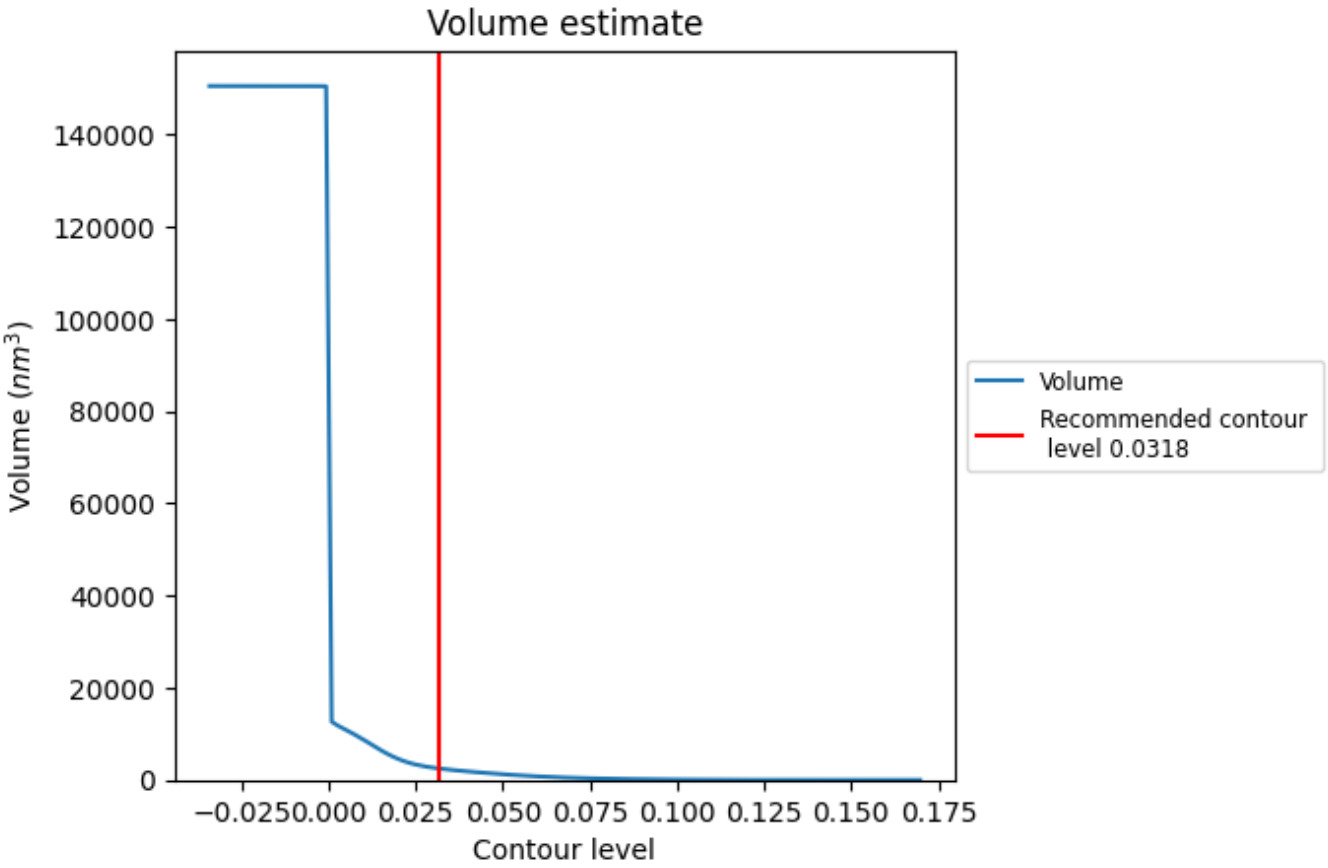
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

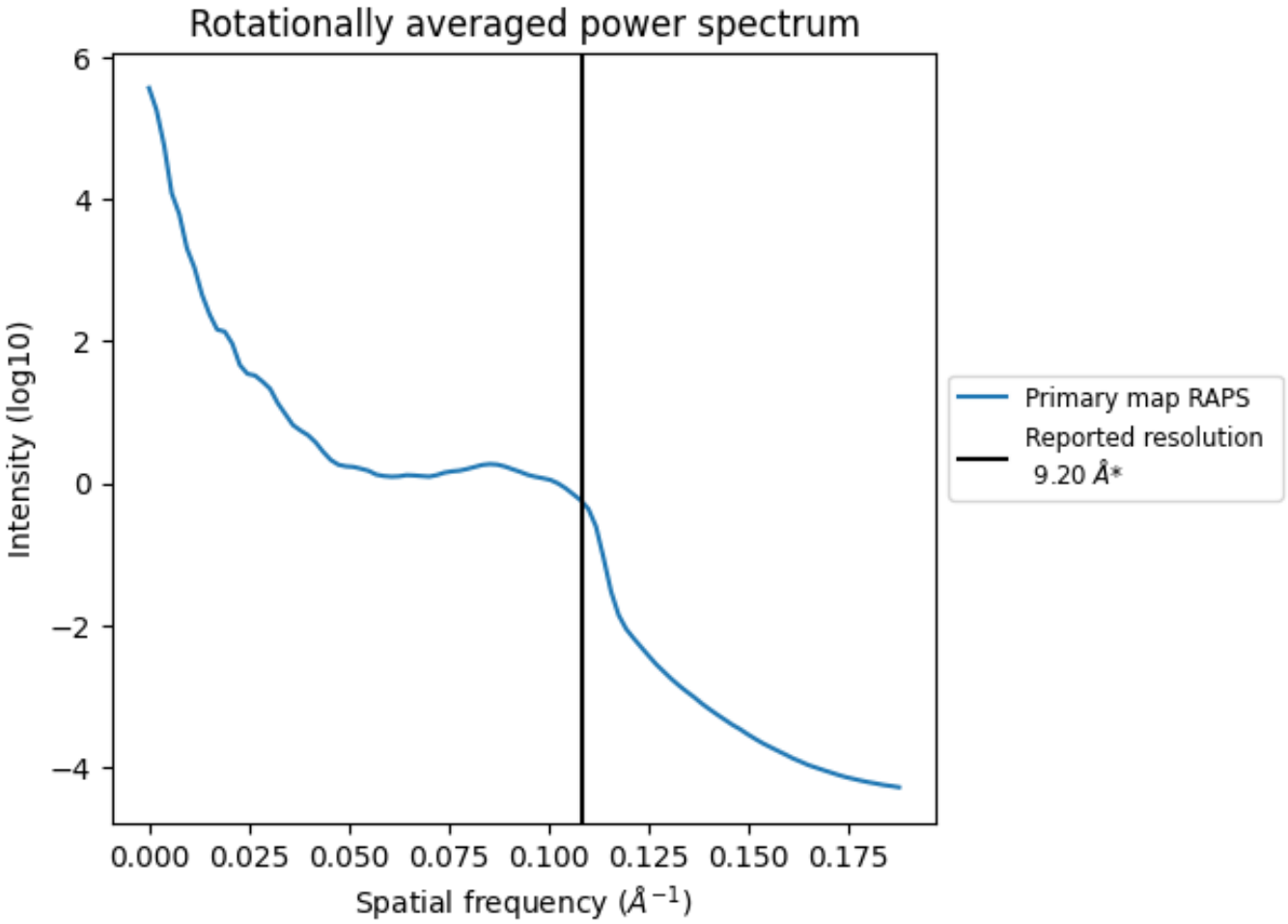
7.2 Volume estimate



The volume at the recommended contour level is 2484 nm^3; this corresponds to an approximate mass of 2244 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 0.109 Å^{-1}

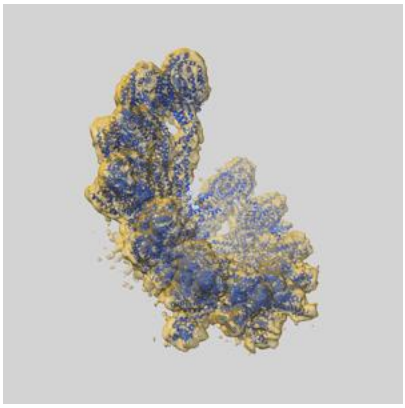
8 Fourier-Shell correlation

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

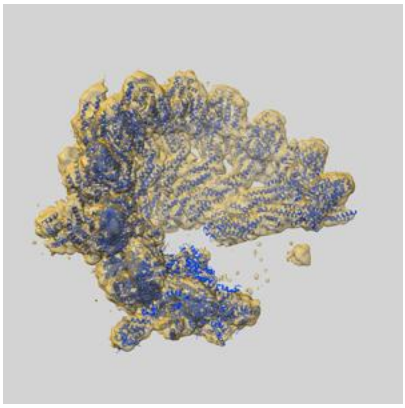
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14016 and PDB model 7QJB. Per-residue inclusion information can be found in section 3 on page 8.

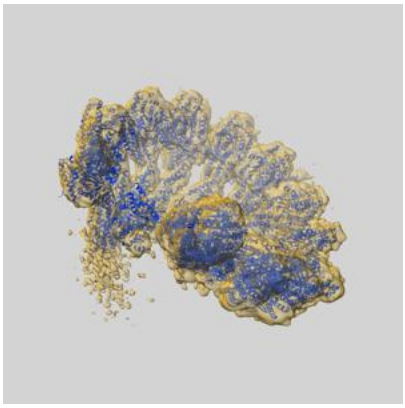
9.1 Map-model overlay



X



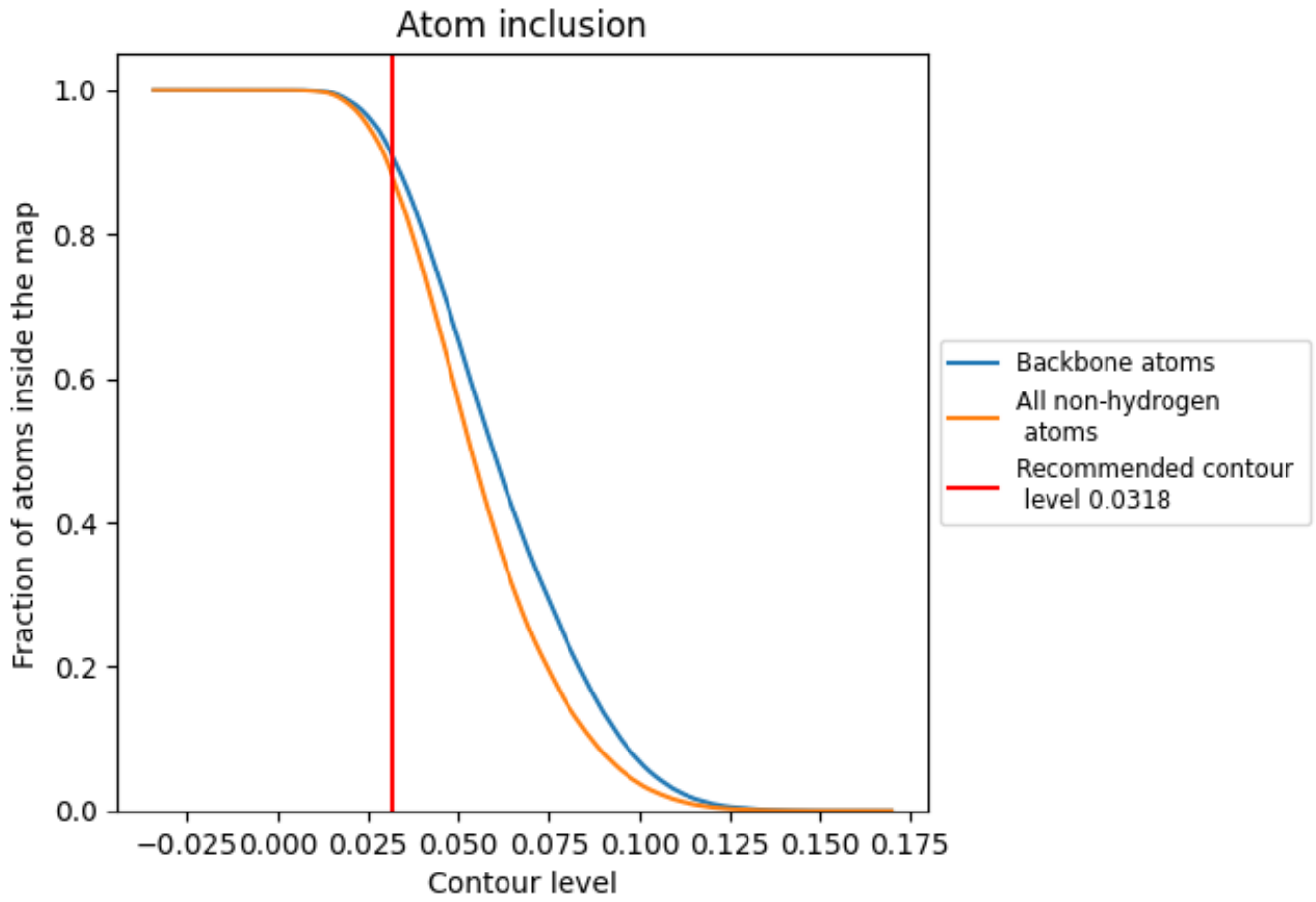
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0318 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.