Full wwPDB EM Validation Report

Jan 29, 2022 – 06:22 am GMT

PDB ID	:	7QJ9
EMDB ID	:	EMD-14014
Title	:	Structure of recombinant human gamma-Tubulin Ring Complex 10-spoked assembly intermediate (spokes 3-12, homogeneous dataset)
Authors	:	Zupa, E.; Pfeffer, S.
Deposited on	:	2021-12-16
Resolution	:	8.10 Å(reported)
Based on initial models	:	6L81, 6V6S, 7AS4, 6X0U

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

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

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

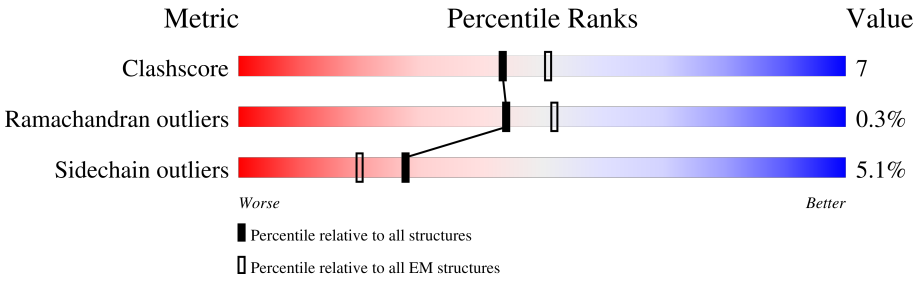
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 8.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	J	1024	45% 7% 48%
1	l	1024	10% 89%
2	e	375	68% 95%
3	b	82	78% 21%
3	d	82	23% 71% 28%
3	i	82	27% 78% 21%
3	k	82	77% 21%
3	m	82	78% 21%

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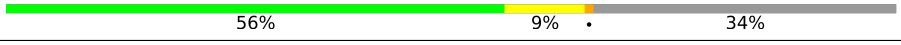
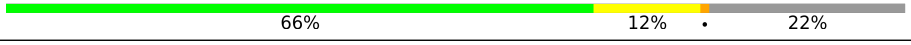
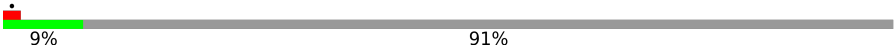
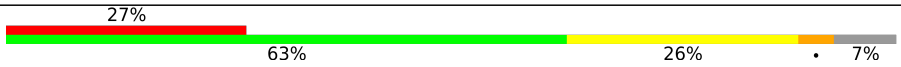
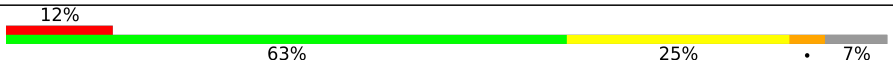
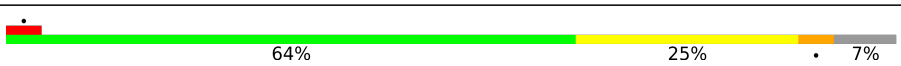
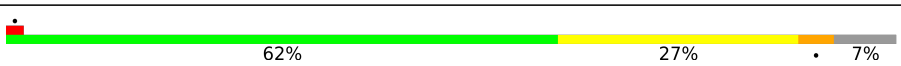
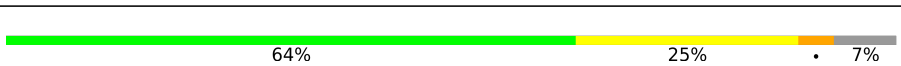
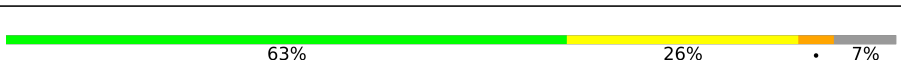
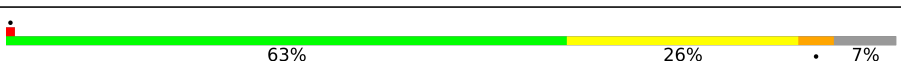
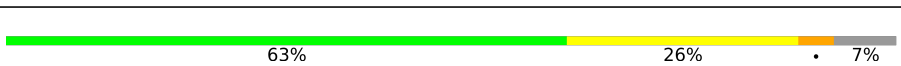
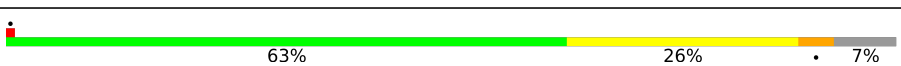
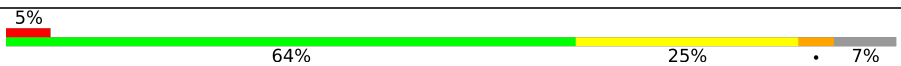
Mol	Chain	Length	Quality of chain
4	D	907	
4	F	907	
4	H	907	
4	a	907	
4	h	907	
4	j	907	
5	C	902	
5	E	902	
5	G	902	
6	I	667	
6	K	667	
7	L	1819	
7	c	1819	
8	Q	451	
8	R	451	
8	S	451	
8	T	451	
8	U	451	
8	V	451	
8	W	451	
8	X	451	
8	Y	451	
8	Z	451	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 91535 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 4 is a protein called Gamma-tubulin complex component 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
4	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		
4	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
4	h	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
4	j	107	Total	C	N	O	S	0	0
			843	533	156	152	2		

- Molecule 5 is a protein called Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
5	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		
5	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		

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

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

- 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 Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		
8	R	420	Total	C	N	O	S	0	0
			3373	2134	586	638	15		

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

- Molecule 9 is water.

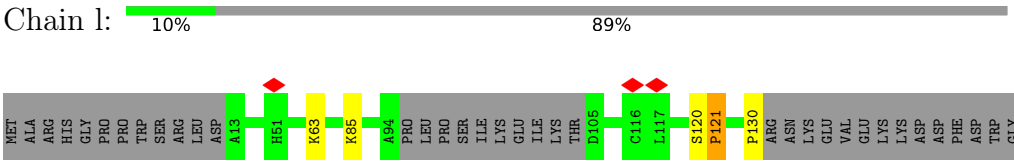
Mol	Chain	Residues	Atoms		AltConf
9	l	6	Total	O	0
			6	6	

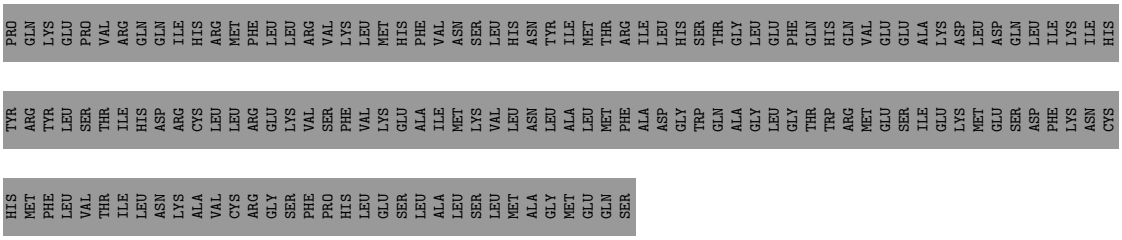
3 Residue-property plots (i)

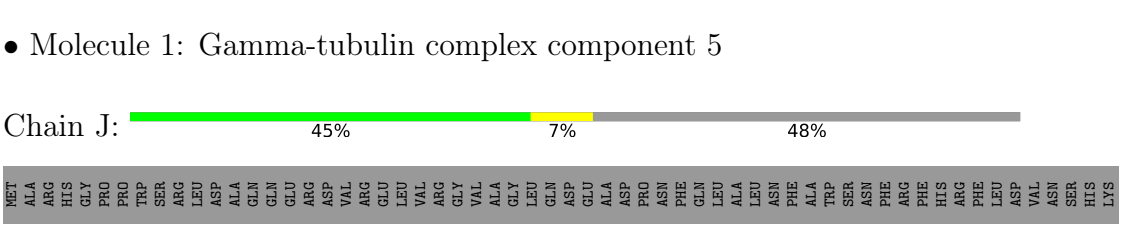
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

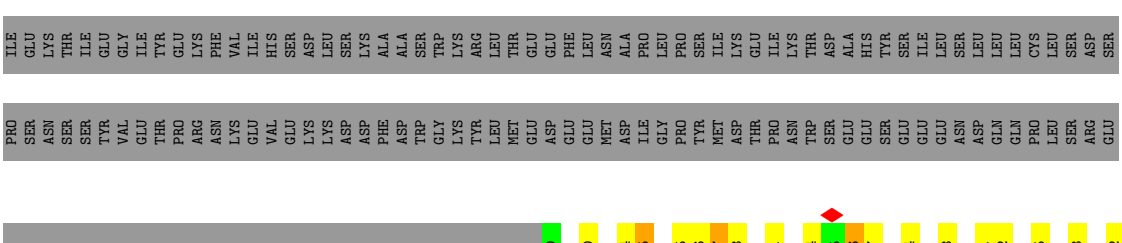
- Molecule 1: Gamma-tubulin complex component 5

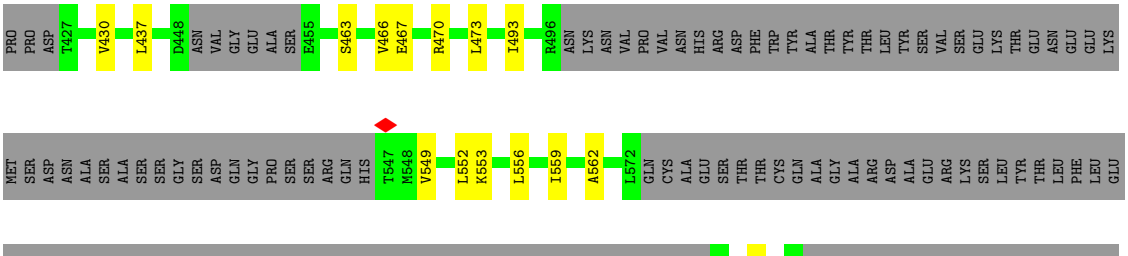
Chain l:

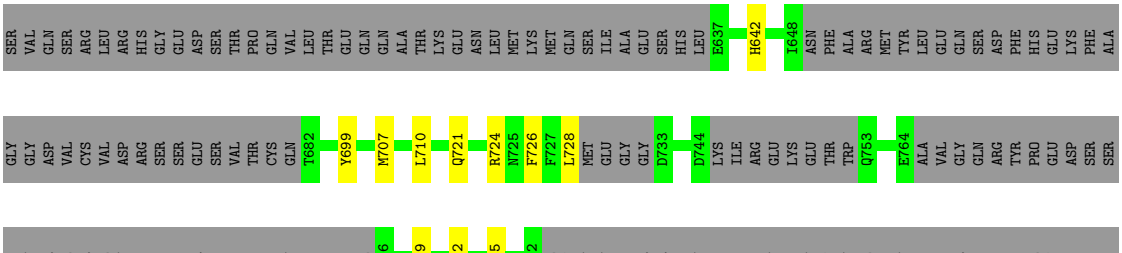


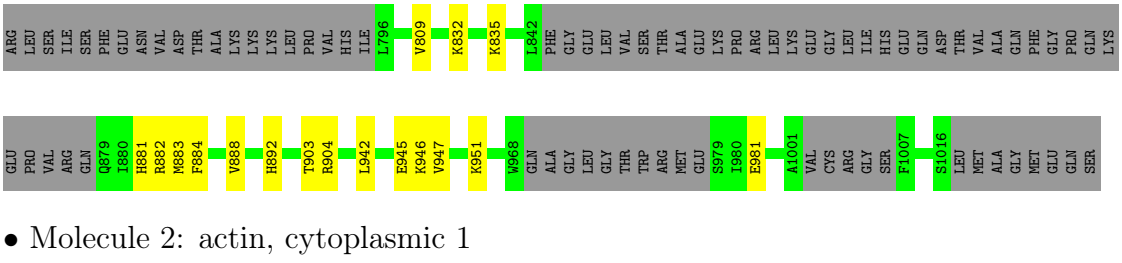


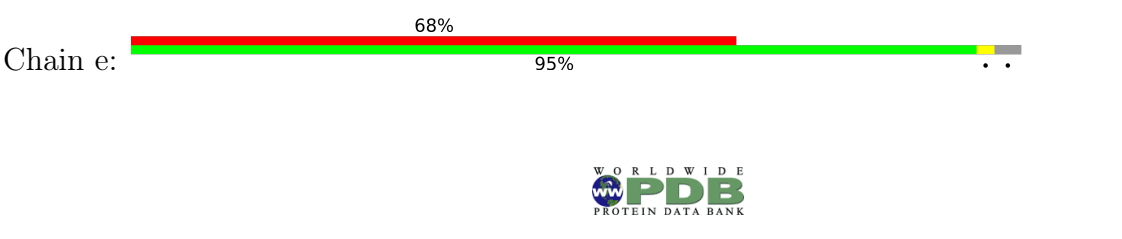












• Molecule 1: Gamma-tubulin complex component 5

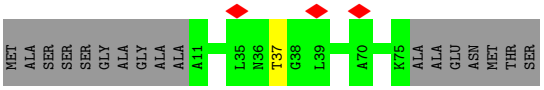
Chain J:

• Molecule 2: actin, cytoplasmic 1

Chain e:

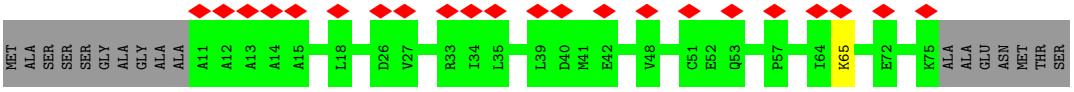
• Molecule 3: Mitotic-spindle organizing protein 1

Chain b:



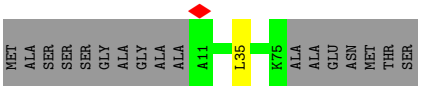
• Molecule 3: Mitotic-spindle organizing protein 1

Chain i:



• Molecule 3: Mitotic-spindle organizing protein 1

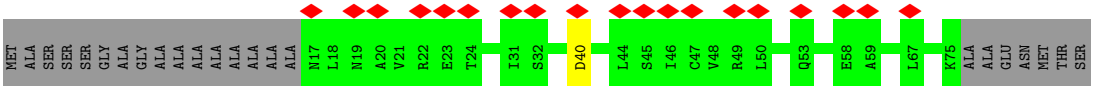
Chain m:



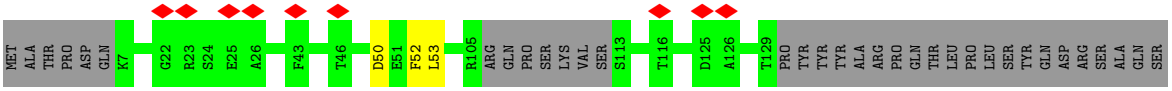
• Molecule 3: Mitotic-spindle organizing protein 1

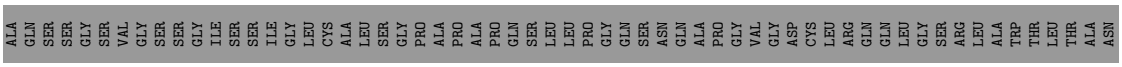
Chain k:

• Molecule 3: Mitotic-spindle organizing protein 1



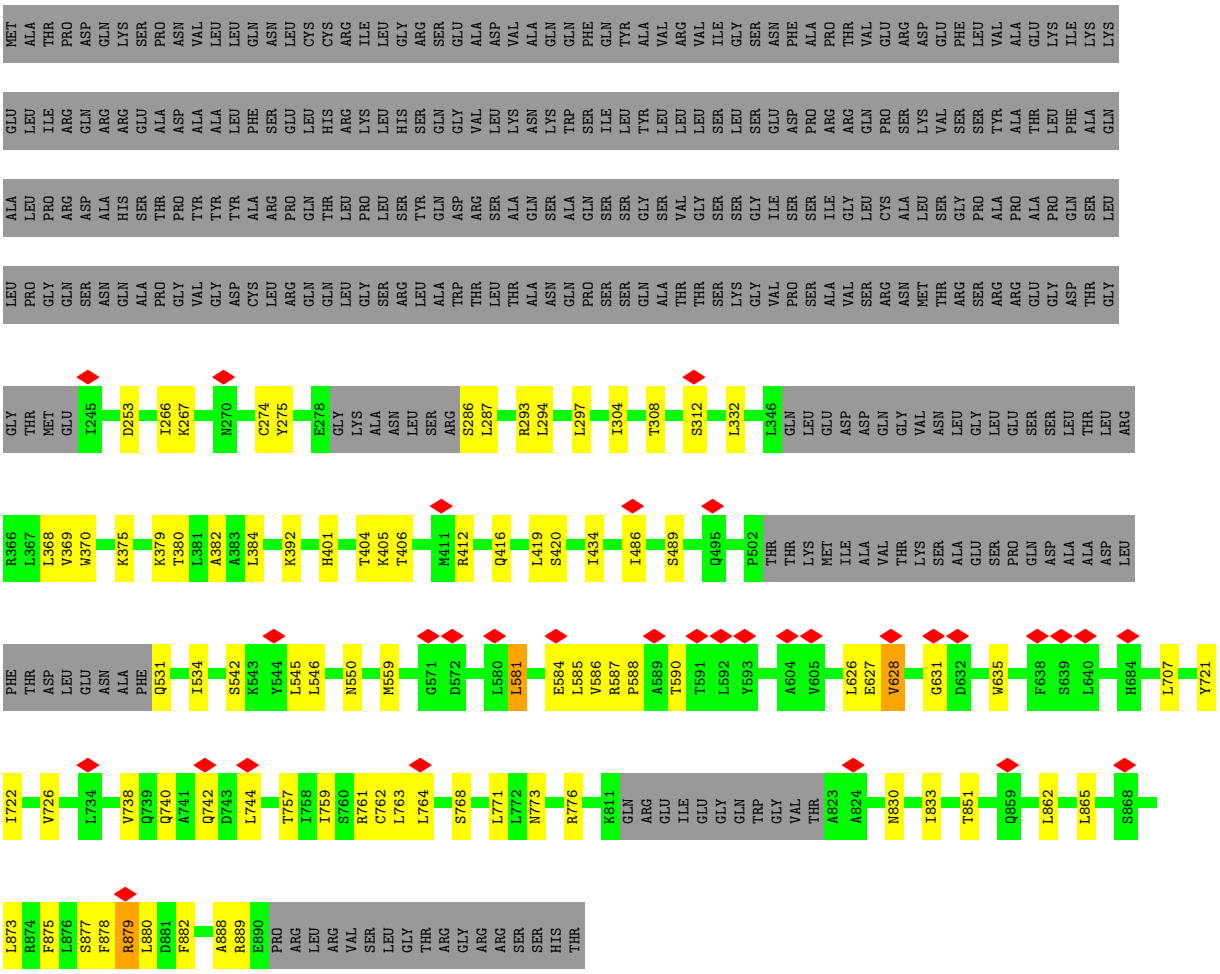
• Molecule 4: Gamma-tubulin complex component 3





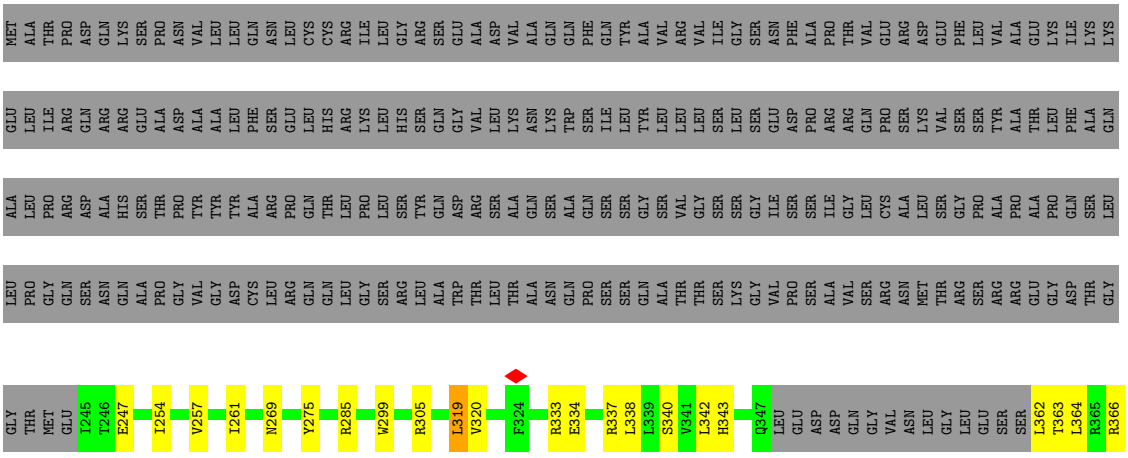
• Molecule 4: Gamma-tubulin complex component 3

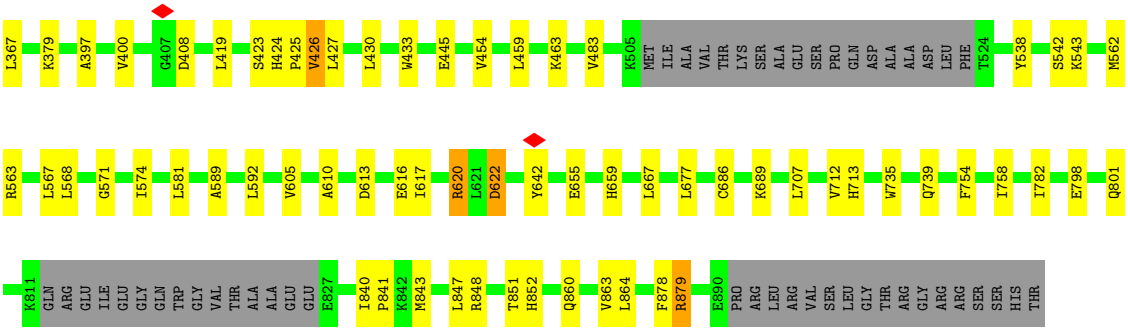
Chain D:



• Molecule 4: Gamma-tubulin complex component 3

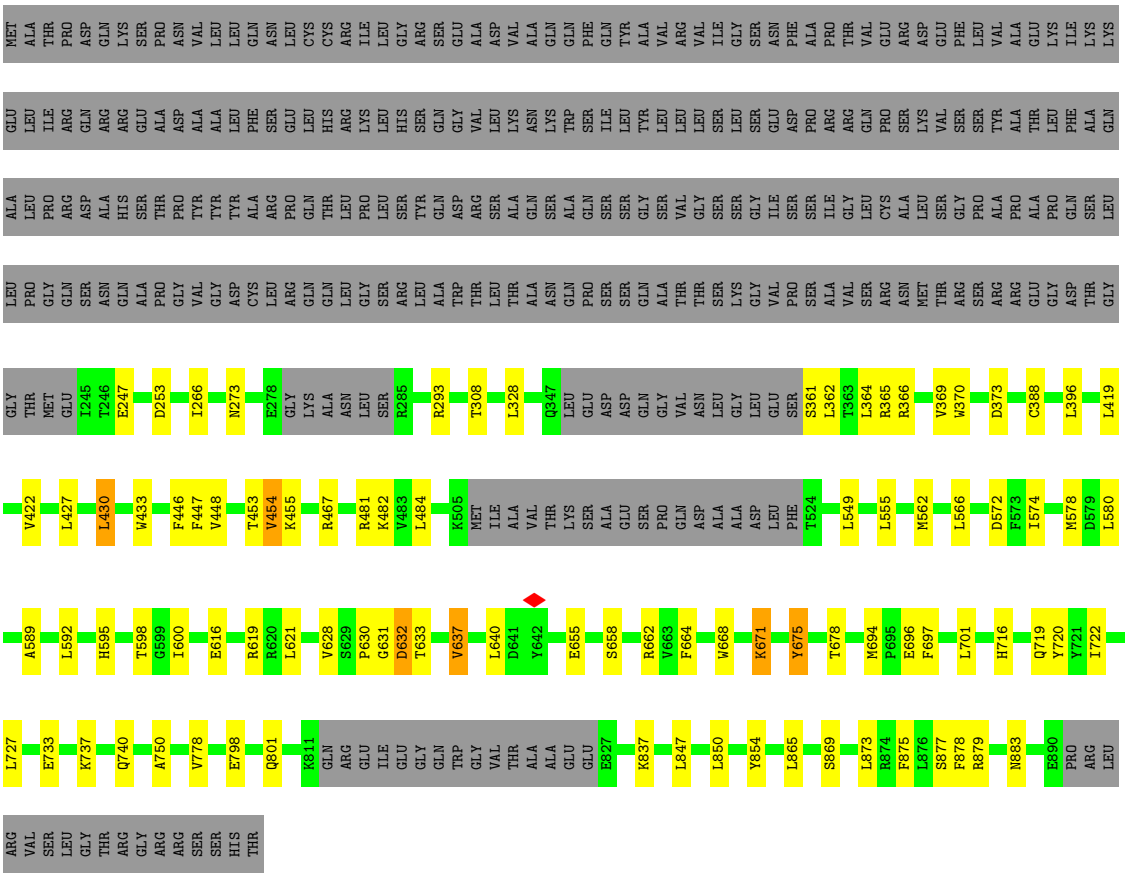
Chain F:





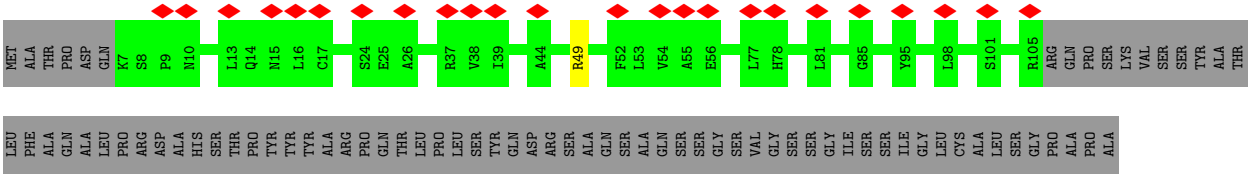
• Molecule 4: Gamma-tubulin complex component 3

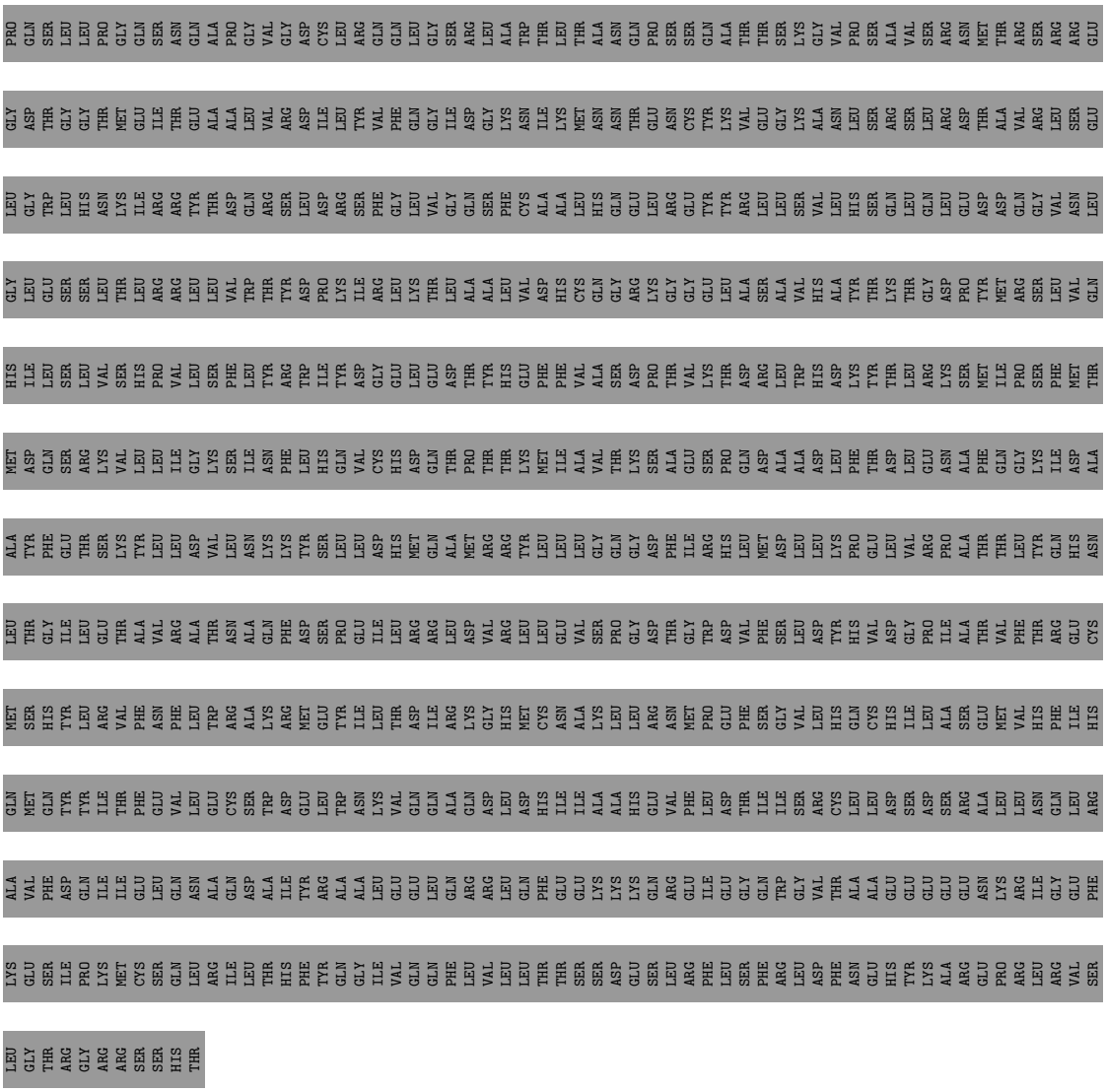
Chain H:



• Molecule 4: Gamma-tubulin complex component 3

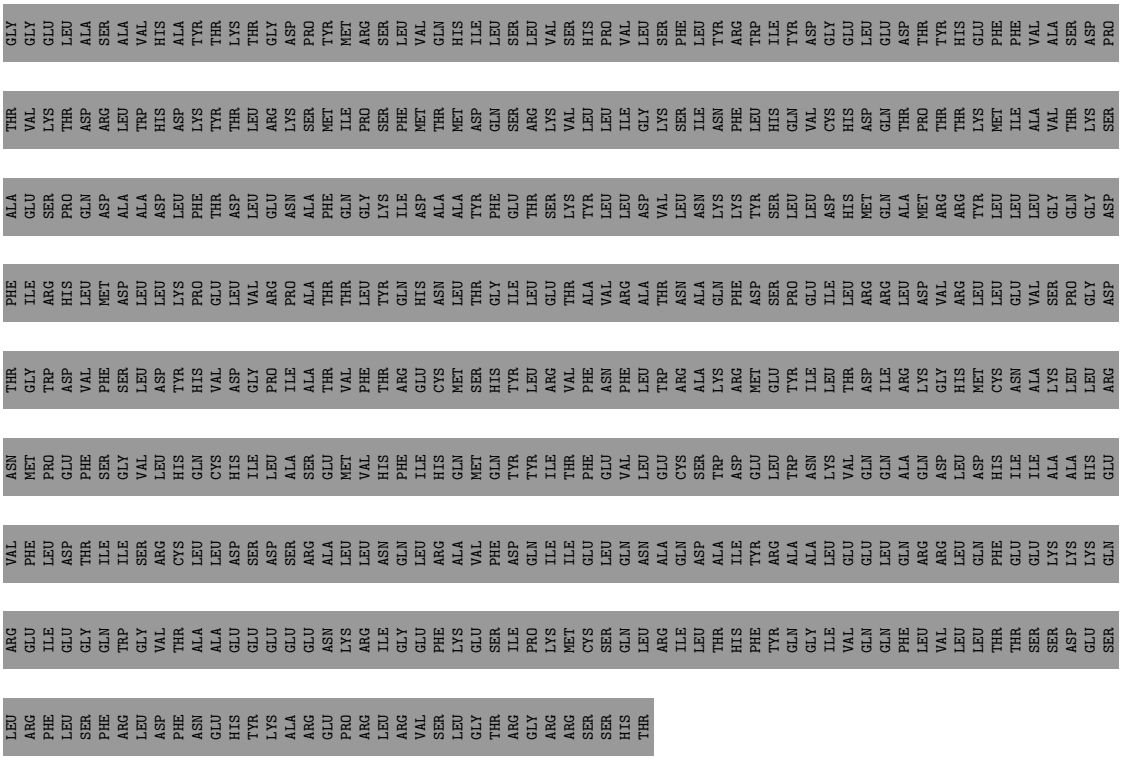
Chain h:





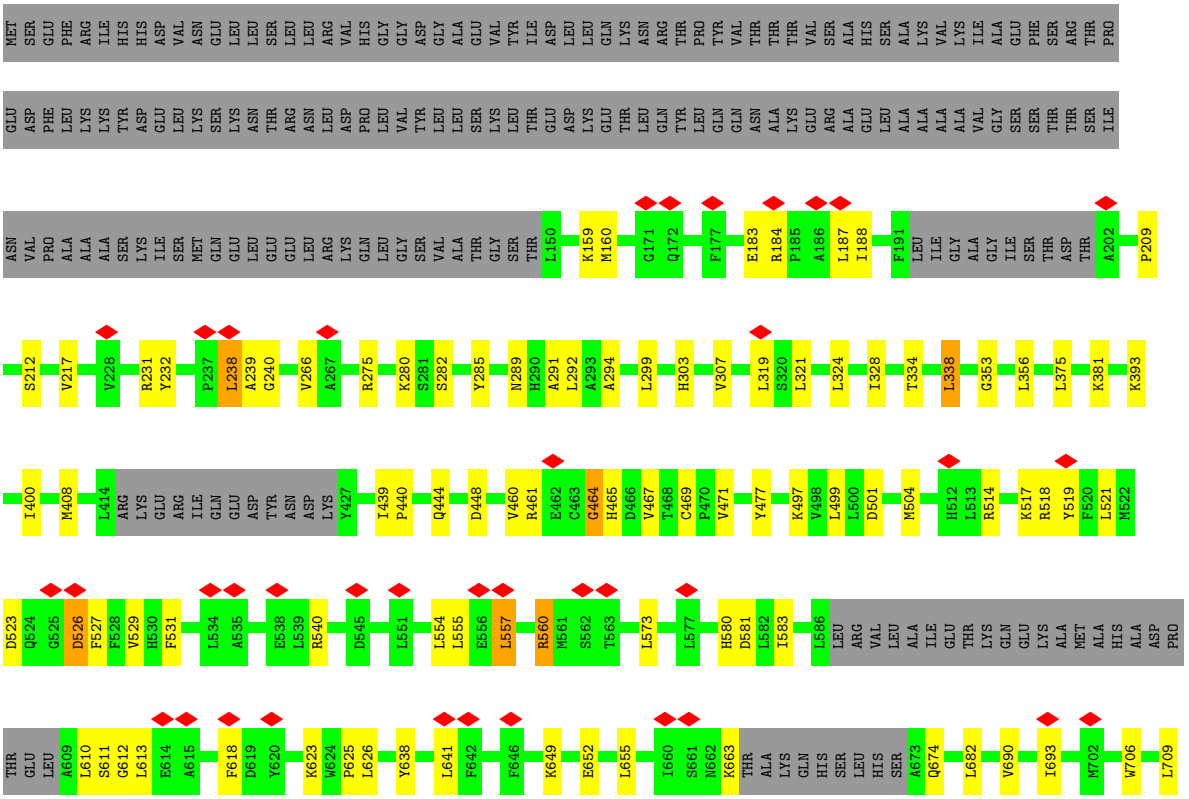
• Molecule 4: Gamma-tubulin complex component 3

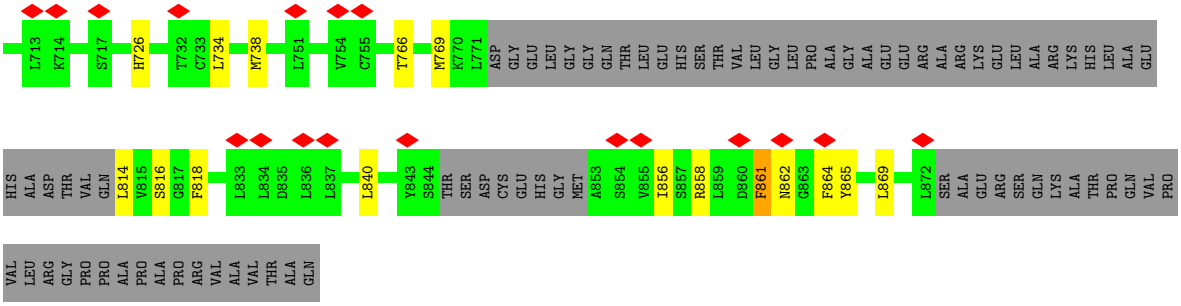
Chain j:



• Molecule 5: Gamma-tubulin complex component 2

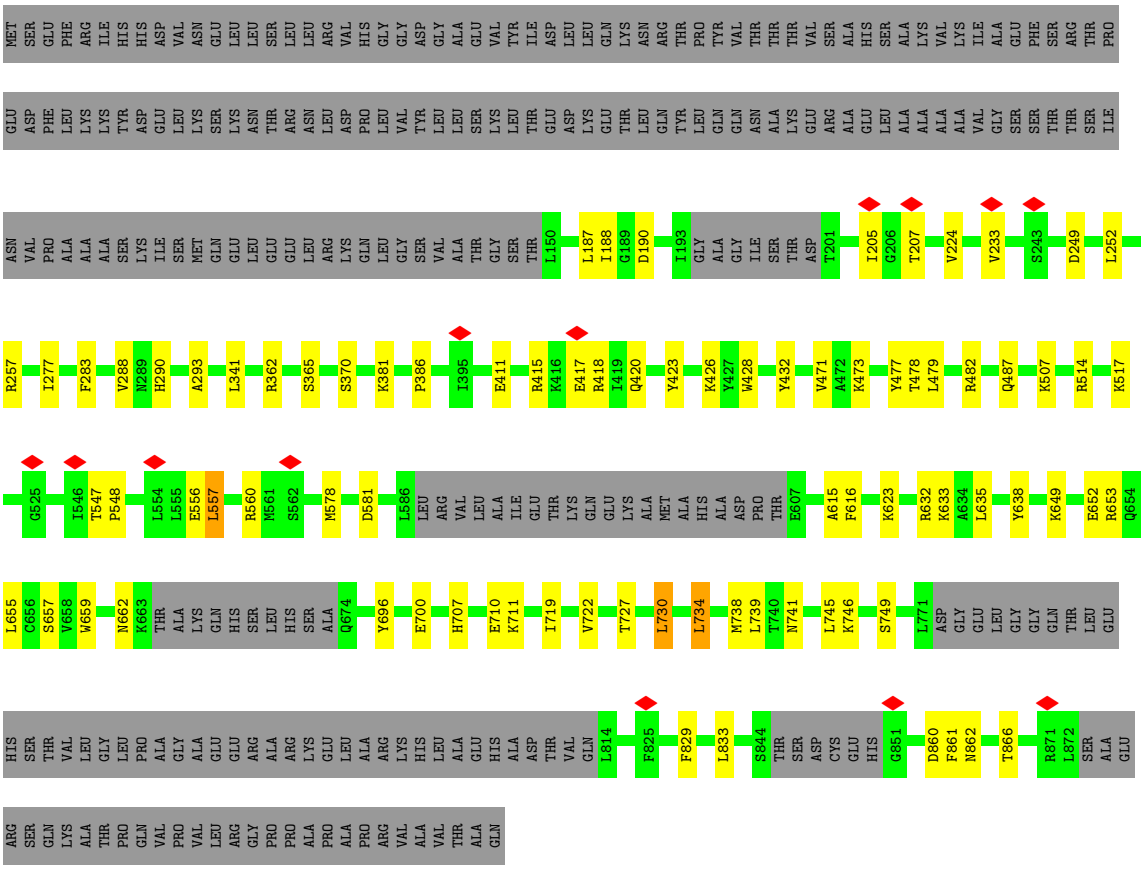
Chain C:





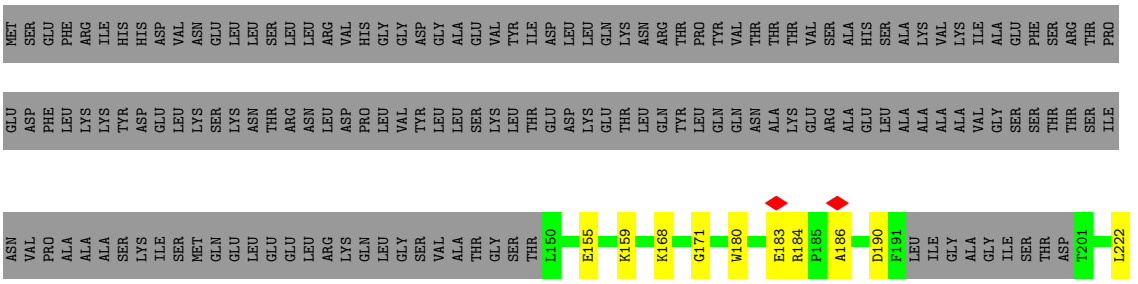
• Molecule 5: Gamma-tubulin complex component 2

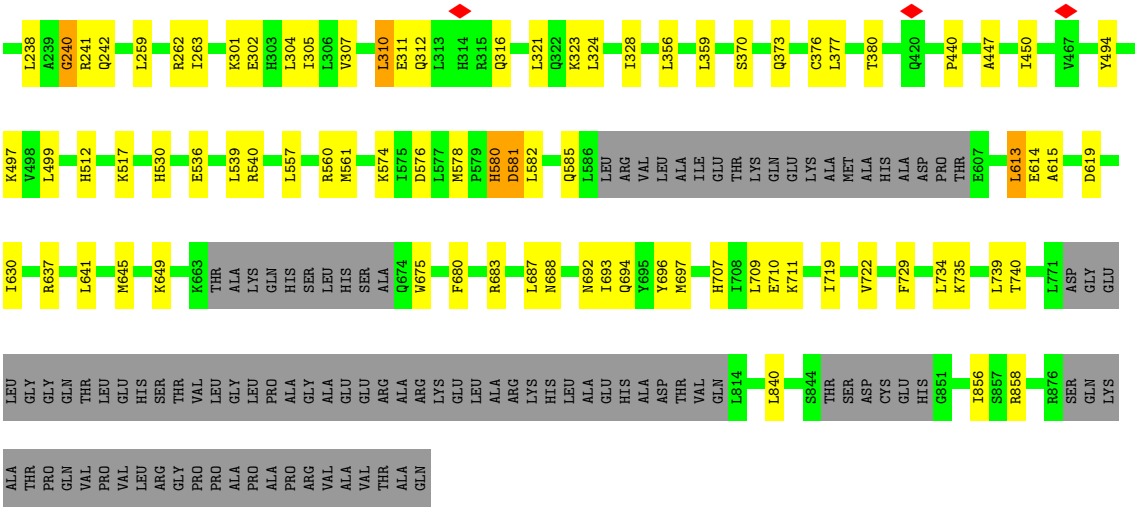
Chain E:



• Molecule 5: Gamma-tubulin complex component 2

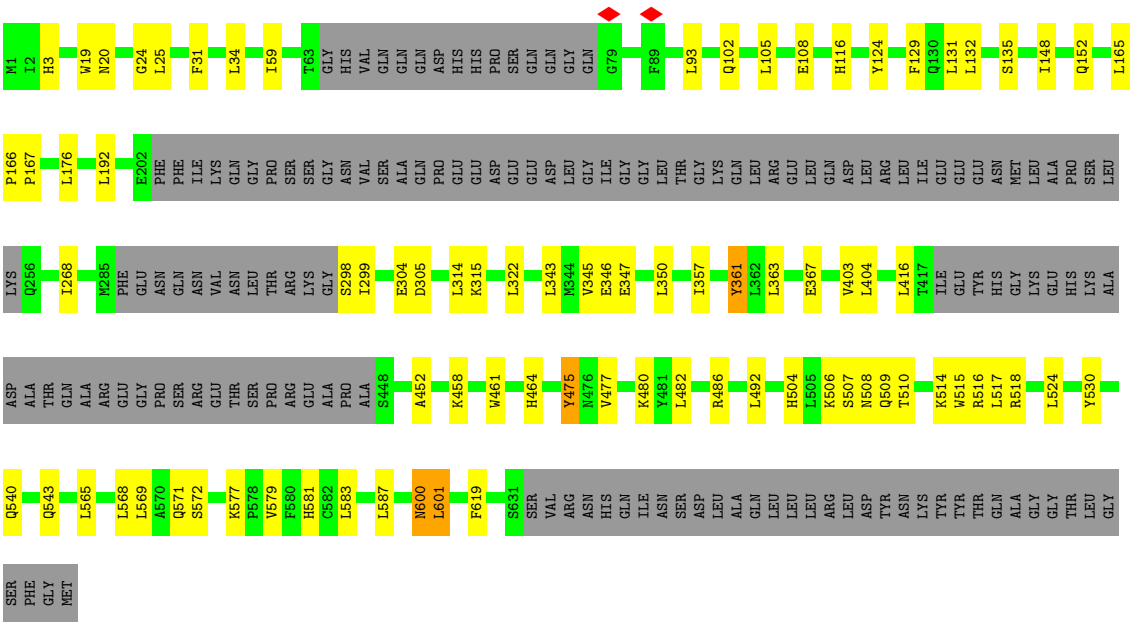
Chain G:





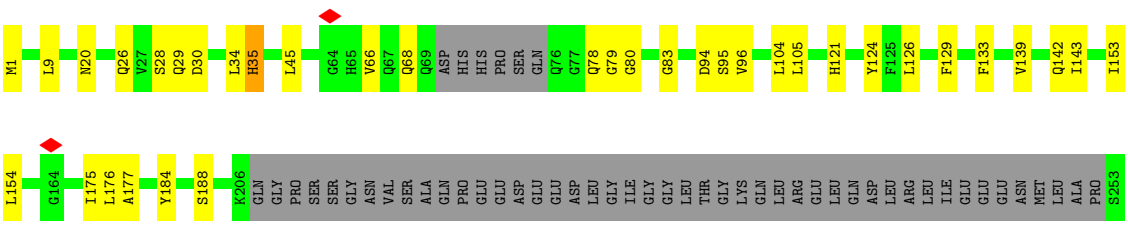
• Molecule 6: Gamma-tubulin complex component 4

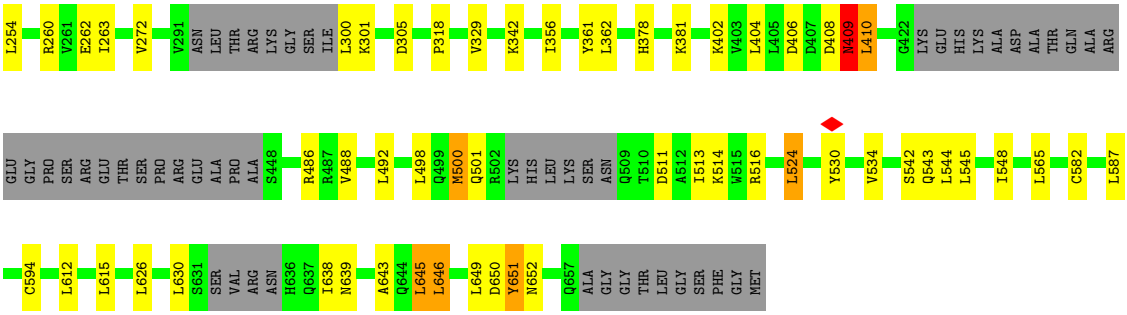
Chain I:



• Molecule 6: Gamma-tubulin complex component 4

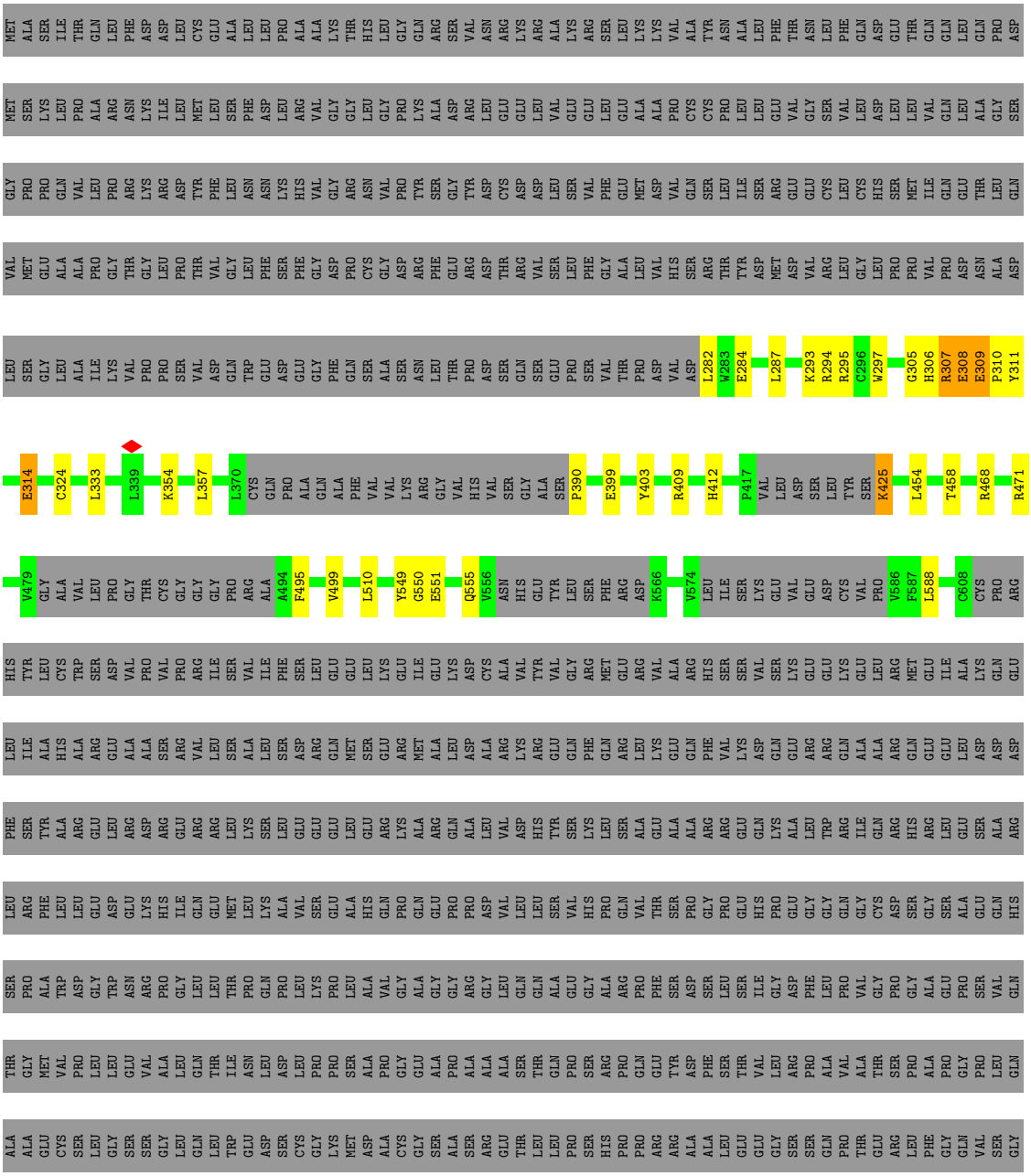
Chain K:

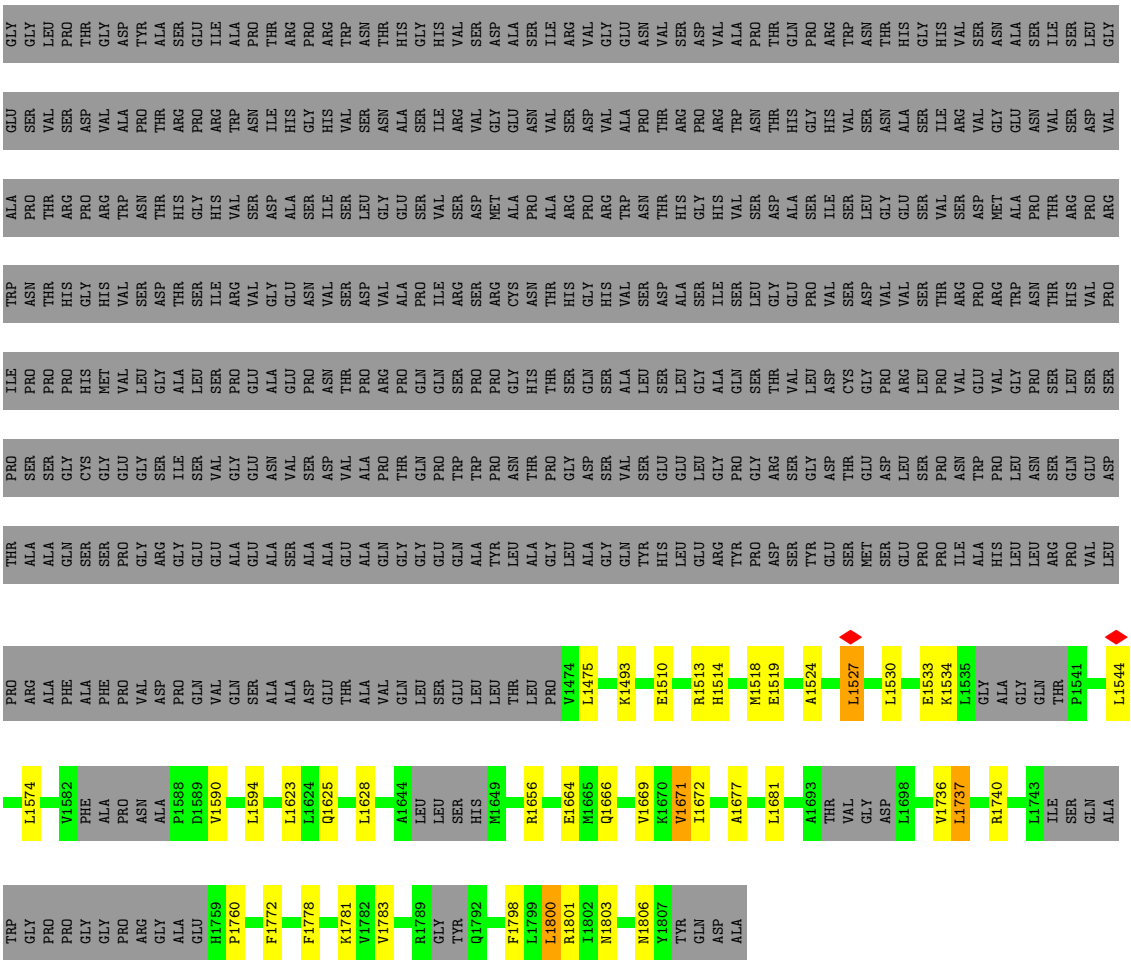




• Molecule 7: Gamma-tubulin complex component 6

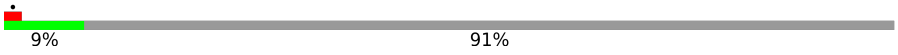
Chain L: 27% 69%

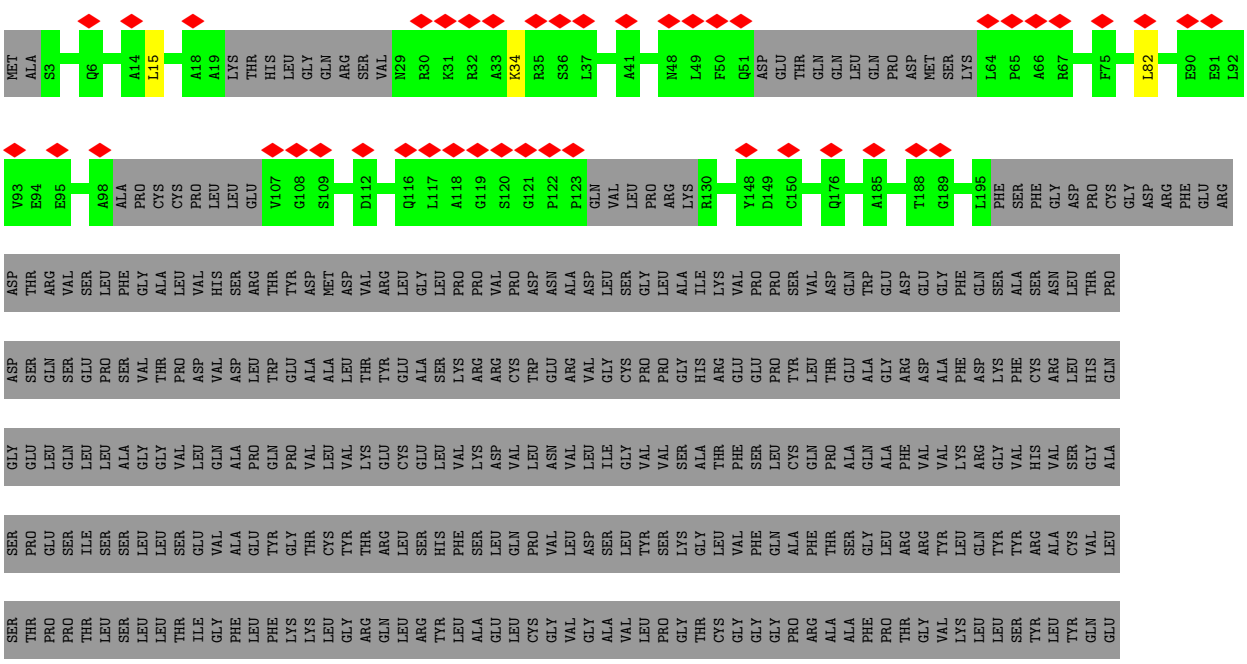


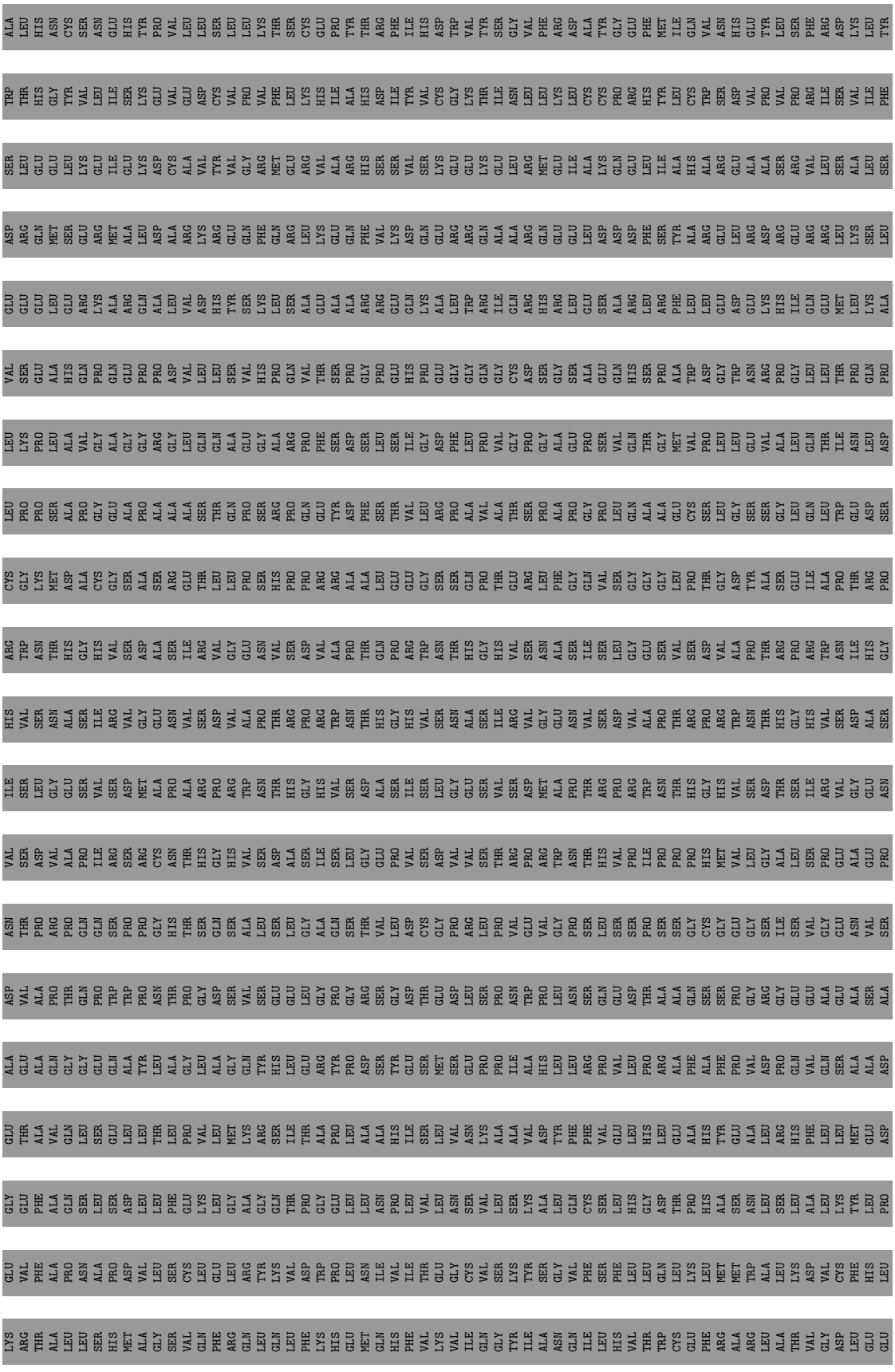


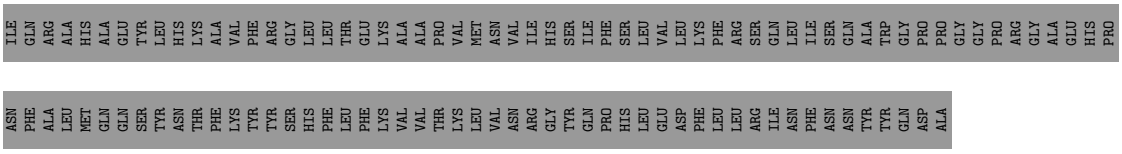
• Molecule 7: Gamma-tubulin complex component 6

Chain c:



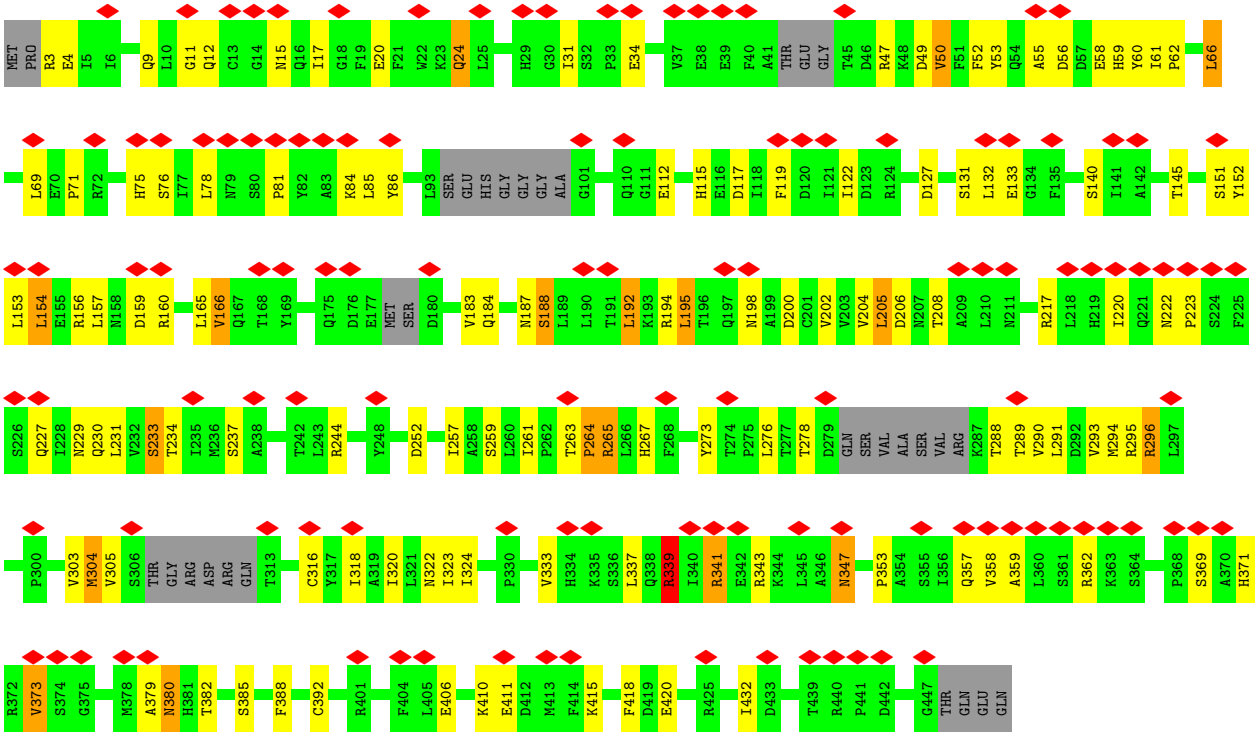



ALA LEU HIS ASN CYS SER ASN GLU HIS TYR PRO VAL LEU LEU SER LEU LEU LYS THR SER CYS GLU PRO TYR THR ARG PHE ILE HIS ASP TRP VAL TYR SER GLY VAL PHE ARG ASP ALA TYR GLY GLU PHE MET ILE GLN VAL ASN HIS GLU TYR LEU SER PHE ARG ASP LYS LEU TYR
TRP THR HIS GLY TYR VAL LEU ILE SER LYS GLU VAL GLU ASP CYS VAL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



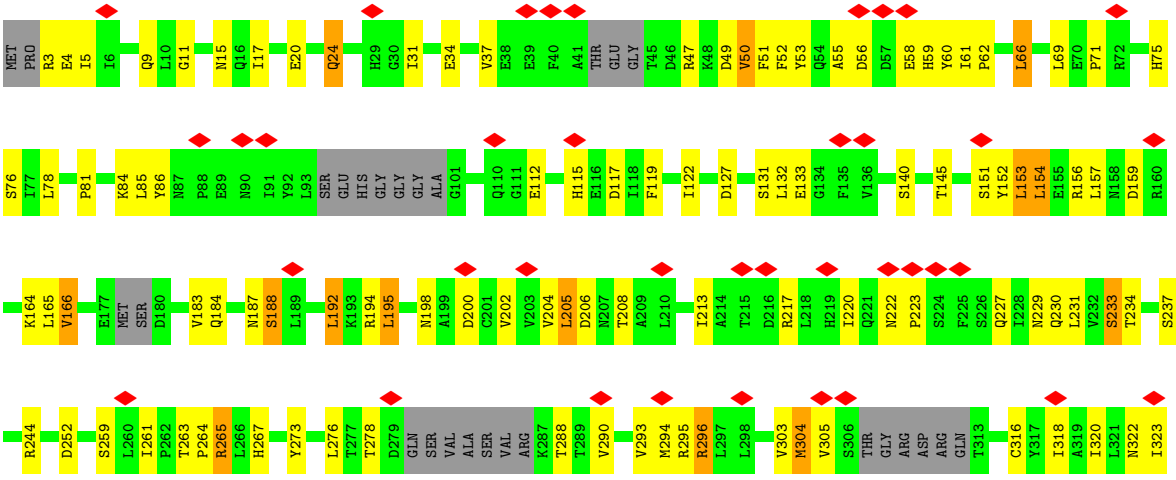
• Molecule 8: Tubulin gamma-1 chain

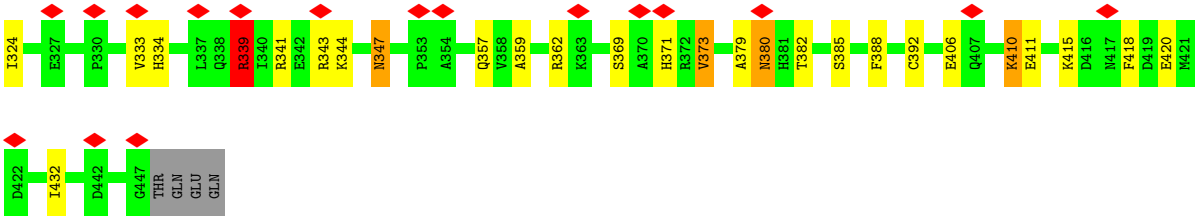
Chain Q:



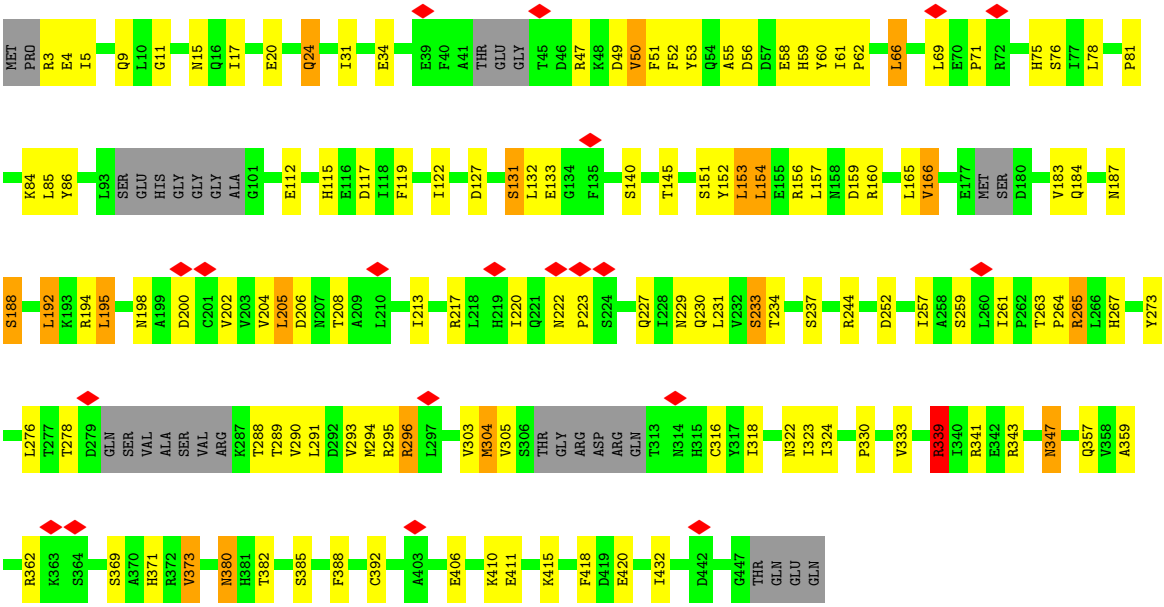
• Molecule 8: Tubulin gamma-1 chain

Chain R:

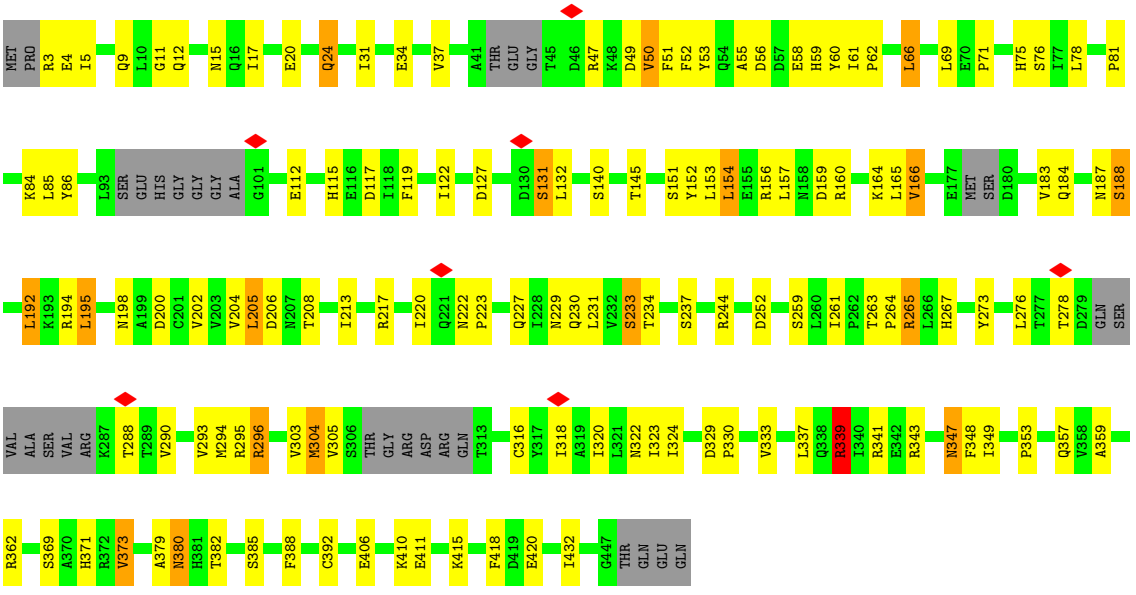




• Molecule 8: Tubulin gamma-1 chain

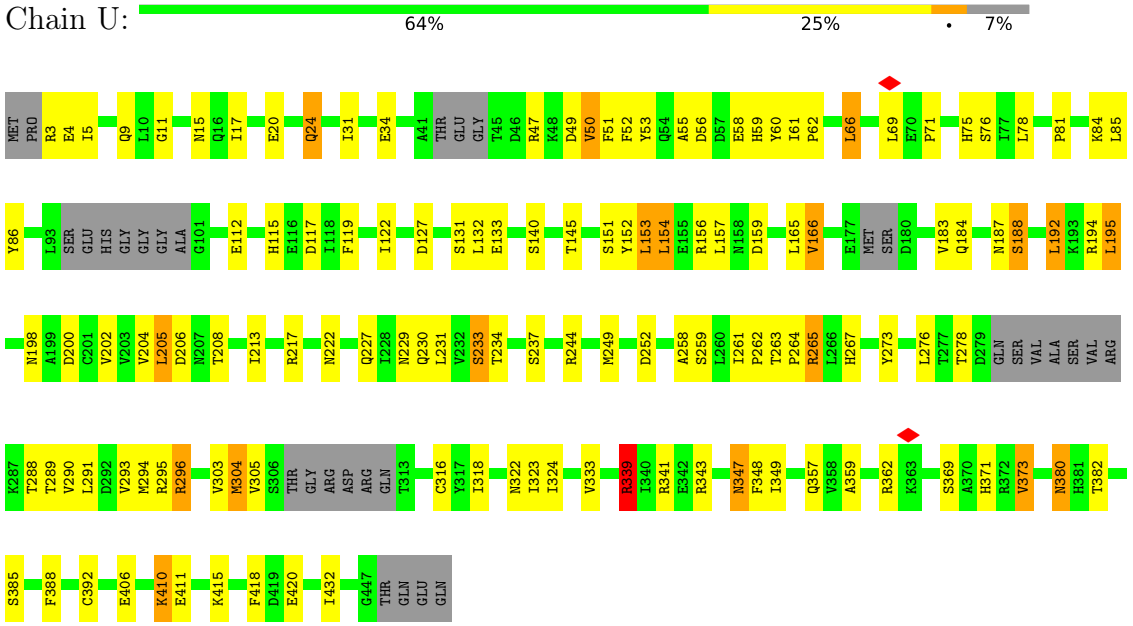


• Molecule 8: Tubulin gamma-1 chain



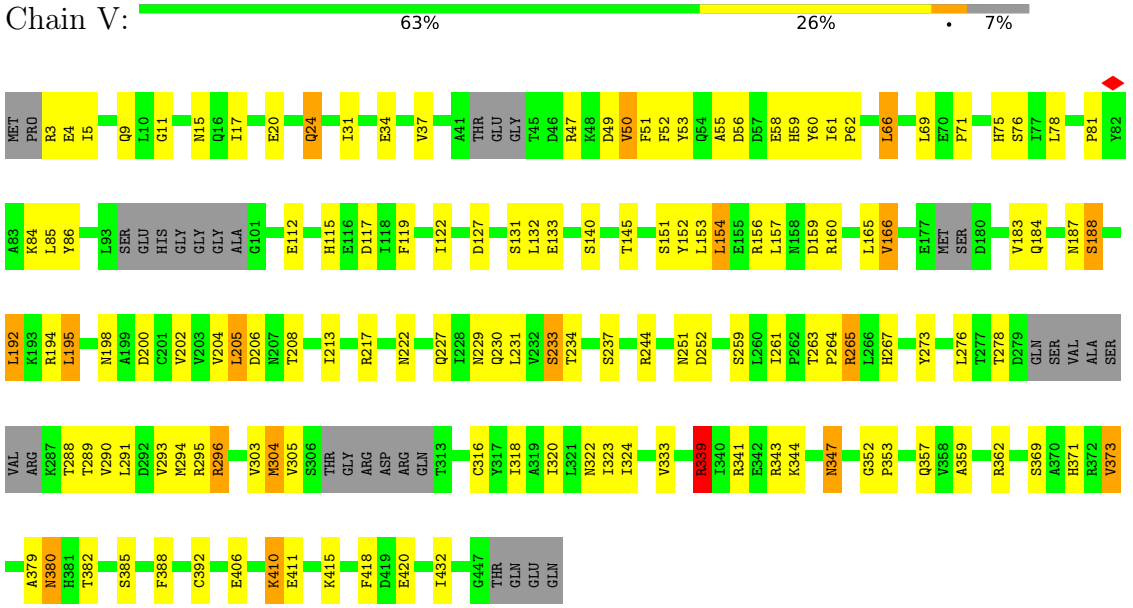
• Molecule 8: Tubulin gamma-1 chain

Chain U:



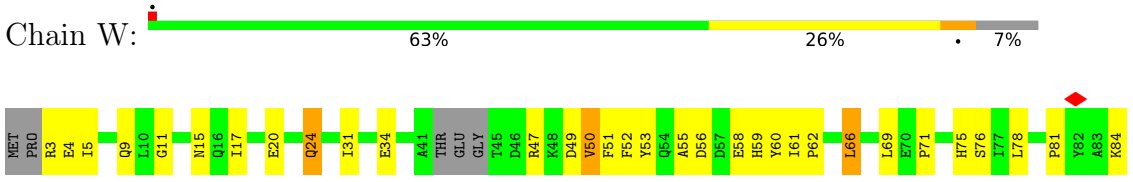
• Molecule 8: Tubulin gamma-1 chain

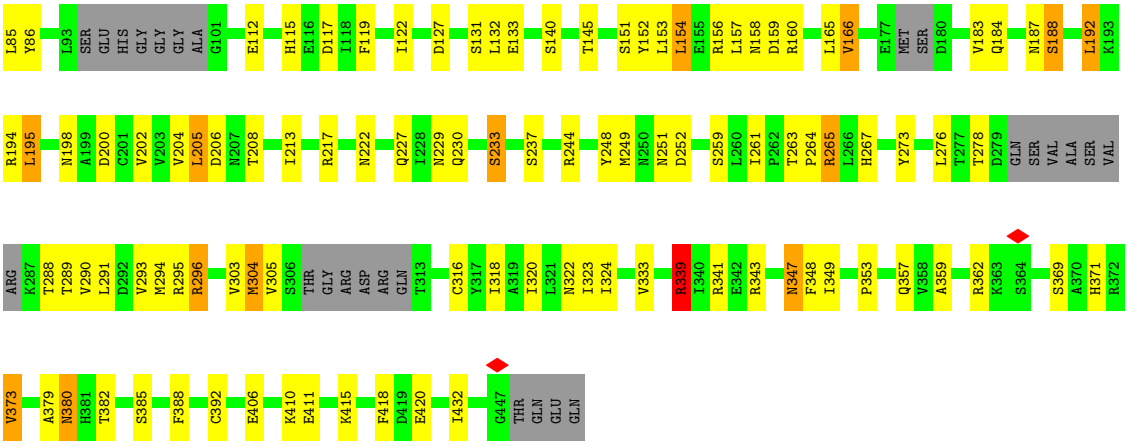
Chain V:



• Molecule 8: Tubulin gamma-1 chain

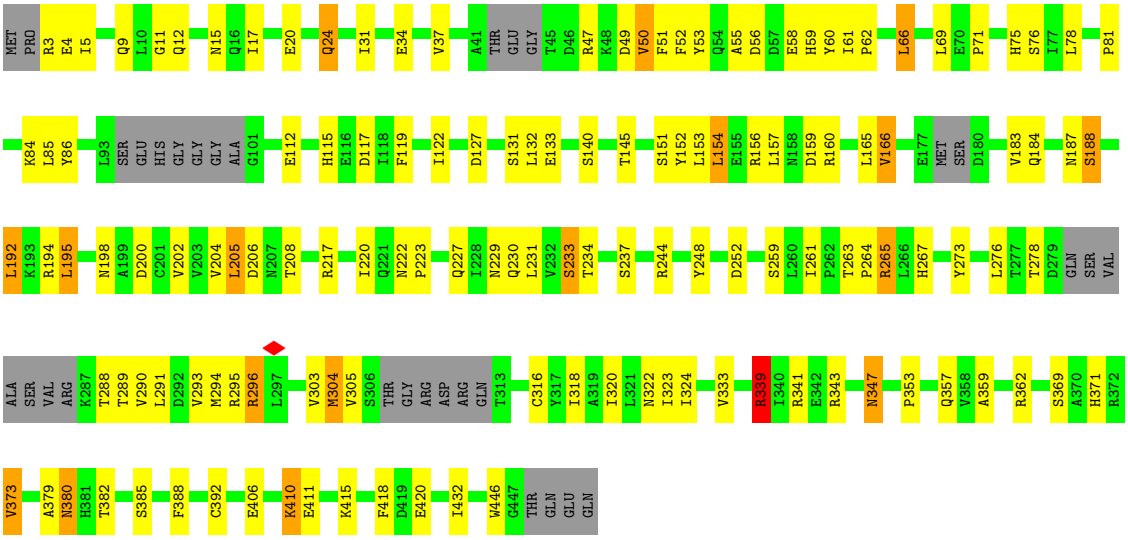
Chain W:





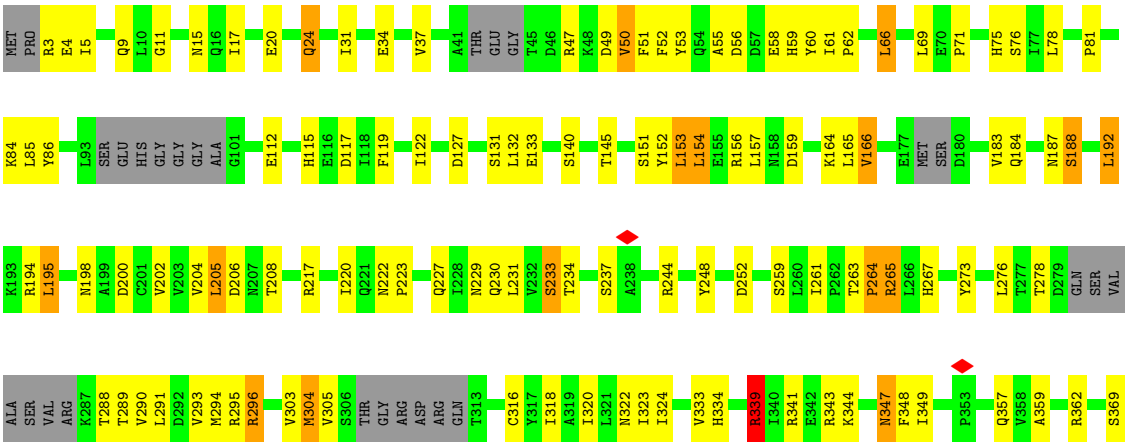
• Molecule 8: Tubulin gamma-1 chain

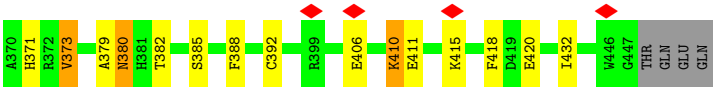
Chain X:



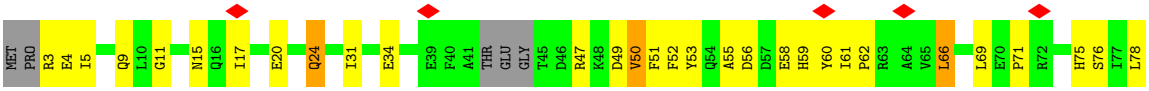
• Molecule 8: Tubulin gamma-1 chain

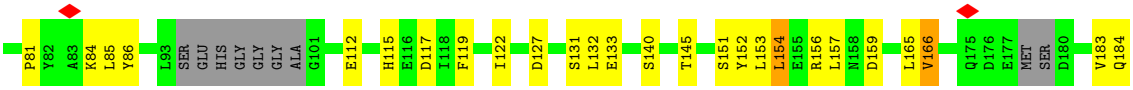
Chain Y:

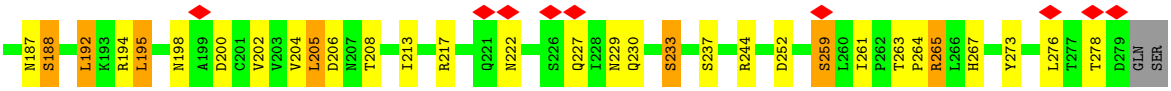


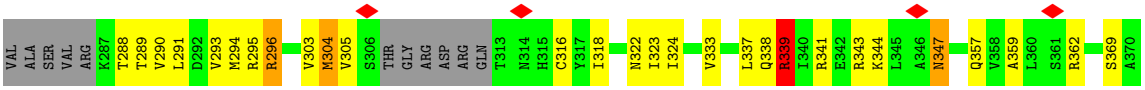


• Molecule 8: Tubulin gamma-1 chain









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21860	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	0.329	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0299	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	J	0.47	3/4525 (0.1%)	0.73	2/6119 (0.0%)
1	l	0.39	0/863	0.71	2/1166 (0.2%)
2	e	0.54	1/2908 (0.0%)	0.74	3/3938 (0.1%)
3	b	0.40	0/484	0.69	0/653
3	d	0.43	0/454	0.80	1/611 (0.2%)
3	i	0.41	0/484	0.70	0/653
3	k	0.41	0/484	0.63	1/653 (0.2%)
3	m	0.34	0/484	0.67	1/653 (0.2%)
4	D	0.39	0/4897	0.71	3/6610 (0.0%)
4	F	0.38	0/5044	0.66	4/6809 (0.1%)
4	H	0.45	1/5009 (0.0%)	0.70	2/6761 (0.0%)
4	a	0.45	0/948	0.75	1/1277 (0.1%)
4	h	0.37	0/815	0.65	1/1096 (0.1%)
4	j	0.36	0/855	0.70	2/1152 (0.2%)
5	C	0.42	0/5151	0.73	8/6955 (0.1%)
5	E	0.41	1/5311 (0.0%)	0.68	3/7169 (0.0%)
5	G	0.41	0/5315	0.69	3/7175 (0.0%)
6	I	0.49	1/4322 (0.0%)	0.71	4/5853 (0.1%)
6	K	0.49	3/4683 (0.1%)	0.78	15/6338 (0.2%)
7	L	0.41	1/4697 (0.0%)	0.69	7/6348 (0.1%)
7	c	0.40	0/1235	0.77	2/1664 (0.1%)
8	Q	0.35	0/3441	0.66	3/4661 (0.1%)
8	R	0.35	0/3441	0.66	3/4661 (0.1%)
8	S	0.35	0/3441	0.66	3/4661 (0.1%)
8	T	0.35	0/3441	0.66	3/4661 (0.1%)
8	U	0.35	0/3441	0.66	3/4661 (0.1%)
8	V	0.35	0/3441	0.66	3/4661 (0.1%)
8	W	0.35	0/3441	0.66	3/4661 (0.1%)
8	X	0.35	0/3441	0.66	3/4661 (0.1%)
8	Y	0.35	0/3441	0.66	3/4661 (0.1%)
8	Z	0.35	0/3441	0.66	3/4661 (0.1%)
All	All	0.40	11/93378 (0.0%)	0.69	95/126263 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	4
2	e	0	1
4	D	0	1
4	F	0	1
4	H	0	5
5	C	0	1
5	E	0	1
5	G	0	3
6	I	0	2
6	K	0	4
8	Q	0	2
8	R	0	2
8	S	0	2
8	T	0	2
8	U	0	2
8	V	0	2
8	W	0	2
8	X	0	2
8	Y	0	2
8	Z	0	2
All	All	0	43

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	243	PRO	N-CD	18.00	1.73	1.47
6	I	361	TYR	CD2-CE2	-9.36	1.25	1.39
6	K	651	TYR	CB-CG	-7.87	1.39	1.51
6	K	651	TYR	CD1-CE1	-7.14	1.28	1.39
6	K	651	TYR	CD2-CE2	-6.94	1.28	1.39
4	H	675	TYR	CD1-CE1	-6.54	1.29	1.39
1	J	224	TYR	CD2-CE2	-5.67	1.30	1.39
7	L	1671	VAL	CB-CG2	-5.43	1.41	1.52
1	J	224	TYR	CE2-CZ	-5.35	1.31	1.38
1	J	225	TRP	CG-CD1	-5.22	1.29	1.36
5	E	471	VAL	CB-CG1	-5.19	1.42	1.52

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	S	339	ARG	NE-CZ-NH2	11.98	126.29	120.30
8	V	339	ARG	NE-CZ-NH2	11.97	126.28	120.30
8	T	339	ARG	NE-CZ-NH2	11.96	126.28	120.30
8	W	339	ARG	NE-CZ-NH2	11.92	126.26	120.30
8	Z	339	ARG	NE-CZ-NH2	11.91	126.26	120.30
8	X	339	ARG	NE-CZ-NH2	11.91	126.25	120.30
8	U	339	ARG	NE-CZ-NH2	11.87	126.23	120.30
8	Y	339	ARG	NE-CZ-NH2	11.86	126.23	120.30
8	Q	339	ARG	NE-CZ-NH2	11.86	126.23	120.30
8	R	339	ARG	NE-CZ-NH2	11.85	126.23	120.30
6	K	524	LEU	CB-CG-CD1	-10.12	93.79	111.00
4	D	581	LEU	CA-CB-CG	9.20	136.46	115.30
6	K	646	LEU	CB-CG-CD2	8.22	124.97	111.00
7	c	82	LEU	CA-CB-CG	7.87	133.40	115.30
7	L	1544	LEU	CA-CB-CG	7.14	131.72	115.30
5	E	557	LEU	CA-CB-CG	7.11	131.65	115.30
7	L	1800	LEU	CB-CG-CD2	-7.09	98.95	111.00
5	C	557	LEU	CB-CG-CD2	-7.07	98.97	111.00
6	K	154	LEU	CA-CB-CG	7.00	131.39	115.30
6	I	475	TYR	CA-CB-CG	6.73	126.18	113.40
7	L	1527	LEU	CA-CB-CG	6.69	130.68	115.30
6	K	254	LEU	CA-CB-CG	6.52	130.30	115.30
8	U	117	ASP	CB-CG-OD1	6.45	124.10	118.30
8	T	117	ASP	CB-CG-OD1	6.43	124.08	118.30
8	Q	117	ASP	CB-CG-OD1	6.41	124.07	118.30
5	C	557	LEU	CA-CB-CG	6.40	130.03	115.30
6	K	176	LEU	CA-CB-CG	6.40	130.02	115.30
7	L	1737	LEU	CA-CB-CG	6.40	130.01	115.30
8	Y	117	ASP	CB-CG-OD1	6.39	124.05	118.30
8	Z	117	ASP	CB-CG-OD1	6.38	124.04	118.30
8	V	117	ASP	CB-CG-OD1	6.38	124.04	118.30
8	W	117	ASP	CB-CG-OD1	6.37	124.03	118.30
8	S	117	ASP	CB-CG-OD1	6.34	124.01	118.30
8	X	117	ASP	CB-CG-OD1	6.34	124.01	118.30
7	L	1800	LEU	CA-CB-CG	6.33	129.86	115.30
8	R	117	ASP	CB-CG-OD1	6.33	124.00	118.30
2	e	11	ASP	CB-CG-OD1	6.29	123.96	118.30
6	I	124	TYR	CB-CG-CD1	-6.26	117.25	121.00
4	D	293	ARG	NE-CZ-NH1	6.24	123.42	120.30
6	K	651	TYR	CA-CB-CG	-6.21	101.59	113.40
4	F	879	ARG	CG-CD-NE	6.12	124.66	111.80
5	C	560	ARG	NE-CZ-NH1	-6.10	117.25	120.30
4	D	879	ARG	NE-CZ-NH1	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	l	130	PRO	N-CA-CB	6.06	110.58	103.30
5	C	682	LEU	CB-CG-CD1	-6.01	100.79	111.00
1	l	121	PRO	N-CA-CB	6.00	110.50	103.30
6	K	615	LEU	CA-CB-CG	5.93	128.95	115.30
8	T	339	ARG	NE-CZ-NH1	-5.83	117.39	120.30
6	K	651	TYR	CB-CG-CD1	-5.82	117.51	121.00
8	S	339	ARG	NE-CZ-NH1	-5.76	117.42	120.30
5	C	464	GLY	C-N-CA	5.74	136.04	121.70
2	e	171	LEU	CA-CB-CG	5.73	128.48	115.30
8	R	339	ARG	NE-CZ-NH1	-5.73	117.43	120.30
8	Q	339	ARG	NE-CZ-NH1	-5.73	117.44	120.30
8	X	339	ARG	NE-CZ-NH1	-5.72	117.44	120.30
8	W	339	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	J	224	TYR	OH-CZ-CE2	-5.70	104.71	120.10
8	Y	339	ARG	NE-CZ-NH1	-5.69	117.45	120.30
8	Z	339	ARG	NE-CZ-NH1	-5.69	117.46	120.30
8	V	339	ARG	NE-CZ-NH1	-5.68	117.46	120.30
5	E	734	LEU	CA-CB-CG	5.66	128.31	115.30
8	U	339	ARG	NE-CZ-NH1	-5.62	117.49	120.30
7	c	15	LEU	CA-CB-CG	5.60	128.19	115.30
4	a	53	LEU	CA-CB-CG	5.59	128.16	115.30
2	e	65	LEU	CA-CB-CG	5.57	128.11	115.30
4	h	49	ARG	NE-CZ-NH1	-5.55	117.53	120.30
6	I	124	TYR	CB-CG-CD2	5.53	124.32	121.00
5	G	310	LEU	CA-CB-CG	5.53	128.01	115.30
6	K	524	LEU	CB-CG-CD2	5.49	120.33	111.00
4	j	104	PRO	C-N-CA	5.45	135.32	121.70
4	H	430	LEU	CA-CB-CG	5.44	127.81	115.30
6	I	176	LEU	CA-CB-CG	5.43	127.80	115.30
3	d	40	ASP	CB-CG-OD1	5.43	123.19	118.30
5	C	869	LEU	CA-CB-CG	5.42	127.78	115.30
4	j	108	PRO	N-CA-CB	5.40	109.78	103.30
4	H	455	LYS	CA-CB-CG	5.39	125.26	113.40
3	m	35	LEU	CA-CB-CG	5.39	127.69	115.30
7	L	282	LEU	CA-CB-CG	5.34	127.57	115.30
5	E	730	LEU	CA-CB-CG	5.33	127.56	115.30
6	K	410	LEU	CA-CB-CG	5.33	127.55	115.30
4	F	319	LEU	CA-CB-CG	5.30	127.49	115.30
6	K	645	LEU	CB-CG-CD2	-5.29	102.01	111.00
6	K	545	LEU	CA-CB-CG	5.28	127.44	115.30
6	K	565	LEU	CB-CG-CD1	-5.26	102.05	111.00
7	L	333	LEU	CA-CB-CG	5.26	127.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	k	63	VAL	CA-CB-CG2	5.22	118.73	110.90
6	K	645	LEU	CA-CB-CG	5.18	127.21	115.30
4	F	408	ASP	CB-CG-OD1	5.17	122.96	118.30
4	F	581	LEU	CA-CB-CG	5.15	127.14	115.30
5	C	338	LEU	CB-CG-CD1	-5.13	102.28	111.00
5	C	238	LEU	CA-CB-CG	5.08	126.98	115.30
5	G	580	HIS	C-N-CA	5.02	134.26	121.70
6	K	646	LEU	CB-CA-C	5.01	119.72	110.20
1	J	305	LEU	CA-CB-CG	5.01	126.82	115.30
5	G	613	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	464	GLY	Peptide
4	D	888	ALA	Peptide
5	E	370	SER	Peptide
4	F	269	ASN	Peptide
5	G	240	GLY	Peptide
5	G	580	HIS	Peptide
5	G	581	ASP	Mainchain
4	H	453	THR	Peptide
4	H	454	VAL	Peptide,Mainchain
4	H	637	VAL	Peptide
4	H	740	GLN	Peptide
6	I	600	ASN	Peptide
6	I	601	LEU	Peptide
1	J	235	SER	Peptide
1	J	237	HIS	Peptide
1	J	256	LEU	Peptide
1	J	726	PHE	Peptide
6	K	28	SER	Peptide
6	K	408	ASP	Peptide
6	K	409	ASN	Mainchain
6	K	638	ILE	Peptide
8	Q	264	PRO	Peptide
8	Q	406	GLU	Peptide
8	R	264	PRO	Peptide
8	R	406	GLU	Peptide
8	S	264	PRO	Peptide
8	S	406	GLU	Peptide

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Mol	Chain	Res	Type	Group
8	T	264	PRO	Peptide
8	T	406	GLU	Peptide
8	U	264	PRO	Peptide
8	U	406	GLU	Peptide
8	V	264	PRO	Peptide
8	V	406	GLU	Peptide
8	W	264	PRO	Peptide
8	W	406	GLU	Peptide
8	X	264	PRO	Peptide
8	X	406	GLU	Peptide
8	Y	264	PRO	Peptide
8	Y	406	GLU	Peptide
8	Z	264	PRO	Peptide
8	Z	406	GLU	Peptide
2	e	200	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4429	0	4482	43	0
1	l	847	0	789	0	0
2	e	2847	0	2810	0	0
3	b	484	0	512	0	0
3	d	454	0	482	0	0
3	i	484	0	512	0	0
3	k	484	0	512	0	0
3	m	484	0	512	0	0
4	D	4796	0	4775	50	0
4	F	4941	0	4935	48	0
4	H	4907	0	4896	59	0
4	a	933	0	953	0	0
4	h	803	0	831	0	0
4	j	843	0	846	0	0
5	C	5044	0	5081	67	0
5	E	5202	0	5241	51	0
5	G	5206	0	5230	61	0
6	I	4225	0	4259	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	4579	0	4586	53	0
7	L	4587	0	4636	48	0
7	c	1220	0	1231	0	0
8	Q	3373	0	3325	67	0
8	R	3373	0	3325	70	0
8	S	3373	0	3325	64	0
8	T	3373	0	3325	71	0
8	U	3373	0	3325	68	0
8	V	3373	0	3325	73	0
8	W	3373	0	3325	70	0
8	X	3373	0	3325	70	0
8	Y	3373	0	3325	73	0
8	Z	3373	0	3325	66	0
9	l	6	0	0	0	0
All	All	91535	0	91361	1146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1146) 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:F:879:ARG:HD2	8:T:337:LEU:HD23	1.58	0.83
8:W:56:ASP:HB2	8:X:296:ARG:HD2	1.62	0.81
5:E:734:LEU:HB2	5:E:739:LEU:HD11	1.69	0.75
5:G:560:ARG:HB2	8:V:339:ARG:HE	1.52	0.74
5:E:696:TYR:O	5:E:700:GLU:HB2	1.89	0.71
5:C:159:LYS:NZ	5:C:160:MET:SD	2.64	0.70
4:H:865:LEU:HD22	4:H:877:SER:HB3	1.72	0.70
5:E:381:LYS:HG2	5:E:477:TYR:HB3	1.73	0.69
1:J:238:LEU:H	1:J:241:ASN:HB3	1.56	0.69
4:H:253:ASP:HB3	4:H:266:ILE:HG22	1.76	0.68
6:K:78:GLN:HE21	6:K:80:GLY:H	1.42	0.67
6:I:540:GLN:HG3	6:I:571:GLN:HE22	1.59	0.67
4:H:572:ASP:OD1	8:V:251:ASN:ND2	2.28	0.67
1:J:272:ARG:HH12	1:J:387:ILE:HG13	1.60	0.67
5:G:238:LEU:HG	5:G:240:GLY:H	1.60	0.67
4:D:862:LEU:HD21	4:D:880:LEU:HB3	1.77	0.67
8:S:347:ASN:N	8:S:347:ASN:OD1	2.29	0.66
8:T:347:ASN:OD1	8:T:347:ASN:N	2.29	0.66
8:W:347:ASN:OD1	8:W:347:ASN:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:347:ASN:OD1	8:V:347:ASN:N	2.29	0.66
4:H:364:LEU:HD22	4:H:370:TRP:HE1	1.60	0.66
5:C:706:TRP:HA	5:C:709:LEU:HD12	1.77	0.66
5:G:370:SER:HA	5:G:373:GLN:HG2	1.78	0.66
8:X:47:ARG:HD3	8:X:50:VAL:HG13	1.79	0.65
8:Y:347:ASN:OD1	8:Y:347:ASN:N	2.29	0.65
8:Z:347:ASN:OD1	8:Z:347:ASN:N	2.29	0.65
8:R:347:ASN:OD1	8:R:347:ASN:N	2.29	0.65
8:U:47:ARG:HD3	8:U:50:VAL:HG13	1.79	0.65
8:W:47:ARG:HD3	8:W:50:VAL:HG13	1.79	0.65
4:F:840:ILE:HG13	4:F:841:PRO:HD3	1.79	0.65
5:G:222:LEU:HD11	4:H:365:ARG:HH12	1.60	0.65
8:U:347:ASN:N	8:U:347:ASN:OD1	2.29	0.65
8:Q:347:ASN:OD1	8:Q:347:ASN:N	2.29	0.65
8:Y:47:ARG:HD3	8:Y:50:VAL:HG13	1.79	0.65
6:I:361:TYR:CE2	6:I:475:TYR:HB3	2.31	0.64
8:S:47:ARG:HD3	8:S:50:VAL:HG13	1.79	0.64
8:V:295:ARG:HB3	8:V:296:ARG:HH21	1.63	0.64
8:X:295:ARG:HB3	8:X:296:ARG:HH21	1.63	0.64
8:T:47:ARG:HD3	8:T:50:VAL:HG13	1.79	0.64
8:U:295:ARG:HB3	8:U:296:ARG:HH21	1.63	0.64
8:V:47:ARG:HD3	8:V:50:VAL:HG13	1.79	0.64
8:R:47:ARG:HD3	8:R:50:VAL:HG13	1.79	0.64
8:Q:47:ARG:HD3	8:Q:50:VAL:HG13	1.79	0.64
8:Z:47:ARG:HD3	8:Z:50:VAL:HG13	1.79	0.64
8:W:263:THR:HG1	8:W:265:ARG:HH11	1.45	0.63
8:T:295:ARG:HB3	8:T:296:ARG:HH21	1.63	0.63
4:F:343:HIS:HB3	5:G:323:LYS:HZ1	1.63	0.63
6:K:406:ASP:OD2	8:Z:339:ARG:NH1	2.30	0.63
8:Z:295:ARG:HB3	8:Z:296:ARG:HH21	1.63	0.63
4:D:763:LEU:HD21	4:D:873:LEU:HD11	1.81	0.63
8:R:295:ARG:HB3	8:R:296:ARG:HH21	1.63	0.63
8:S:295:ARG:HB3	8:S:296:ARG:HH21	1.63	0.63
5:C:527:PHE:O	5:C:531:PHE:HB2	1.98	0.63
5:C:862:ASN:HB2	5:C:864:PHE:HE2	1.64	0.63
1:J:467:GLU:HG3	1:J:470:ARG:HH22	1.63	0.63
8:W:295:ARG:HB3	8:W:296:ARG:HH21	1.63	0.63
8:X:347:ASN:N	8:X:347:ASN:OD1	2.29	0.63
6:I:367:GLU:OE1	8:W:251:ASN:ND2	2.28	0.62
5:G:359:LEU:HB3	5:G:380:THR:HG22	1.80	0.62
8:Q:295:ARG:HB3	8:Q:296:ARG:HH21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:773:ASN:HA	4:D:776:ARG:HE	1.63	0.62
8:Y:343:ARG:O	8:Y:343:ARG:NH2	2.33	0.62
8:Y:295:ARG:HB3	8:Y:296:ARG:HH21	1.63	0.62
5:E:860:ASP:HB3	5:E:866:THR:HG22	1.82	0.62
8:R:343:ARG:NH2	8:R:343:ARG:O	2.33	0.62
4:D:759:ILE:HA	4:D:764:LEU:HD21	1.82	0.61
4:D:830:ASN:HA	4:D:833:ILE:HD12	1.81	0.61
6:I:540:GLN:OE1	6:I:543:GLN:NE2	2.33	0.61
8:V:343:ARG:O	8:V:343:ARG:NH2	2.33	0.61
8:X:343:ARG:O	8:X:343:ARG:NH2	2.33	0.61
6:I:504:HIS:CE1	8:W:158:ASN:HD21	2.18	0.61
8:W:343:ARG:NH2	8:W:343:ARG:O	2.33	0.61
8:Z:183:VAL:HG13	8:Z:187:ASN:HD21	1.66	0.61
8:U:343:ARG:NH2	8:U:343:ARG:O	2.33	0.60
7:L:1800:LEU:HD21	8:Z:337:LEU:HB3	1.83	0.60
8:U:183:VAL:HG13	8:U:187:ASN:HD21	1.66	0.60
7:L:1736:VAL:HG12	7:L:1740:ARG:HH11	1.67	0.60
7:L:1803:ASN:ND2	7:L:1806:ASN:O	2.34	0.60
8:V:183:VAL:HG13	8:V:187:ASN:HD21	1.66	0.60
5:C:862:ASN:HA	8:Q:341:ARG:HG2	1.83	0.60
8:R:183:VAL:HG13	8:R:187:ASN:HD21	1.66	0.60
8:Y:183:VAL:HG13	8:Y:187:ASN:HD21	1.66	0.60
8:Q:411:GLU:HB3	8:Q:418:PHE:HE2	1.67	0.60
8:T:183:VAL:HG13	8:T:187:ASN:HD21	1.66	0.60
8:X:411:GLU:HB3	8:X:418:PHE:HE2	1.67	0.60
8:T:411:GLU:HB3	8:T:418:PHE:HE2	1.67	0.60
8:Y:411:GLU:HB3	8:Y:418:PHE:HE2	1.67	0.60
5:G:447:ALA:HA	5:G:450:ILE:HD12	1.82	0.60
8:Q:183:VAL:HG13	8:Q:187:ASN:HD21	1.67	0.60
8:Q:343:ARG:O	8:Q:343:ARG:NH2	2.33	0.60
5:G:574:LYS:HG2	5:G:619:ASP:HB3	1.82	0.60
8:T:343:ARG:O	8:T:343:ARG:NH2	2.33	0.60
8:Z:343:ARG:NH2	8:Z:343:ARG:O	2.33	0.60
5:G:613:LEU:HD12	5:G:614:GLU:HG3	1.84	0.59
5:G:710:GLU:HB2	5:G:711:LYS:HZ2	1.67	0.59
8:S:343:ARG:O	8:S:343:ARG:NH2	2.33	0.59
5:C:291:ALA:HA	5:C:294:ALA:HB3	1.84	0.59
5:C:560:ARG:HB2	8:R:339:ARG:HE	1.67	0.59
8:R:411:GLU:HB3	8:R:418:PHE:HE2	1.67	0.59
6:I:458:LYS:HE3	6:I:461:TRP:HZ2	1.68	0.59
6:I:486:ARG:NH1	8:W:248:TYR:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:183:VAL:HG13	8:W:187:ASN:HD21	1.67	0.59
8:X:183:VAL:HG13	8:X:187:ASN:HD21	1.67	0.59
8:Z:263:THR:OG1	8:Z:265:ARG:NH1	2.36	0.59
8:Z:411:GLU:HB3	8:Z:418:PHE:HE2	1.67	0.59
1:J:404:PRO:HB2	1:J:405:ARG:HH11	1.67	0.59
7:L:324:CYS:HG	7:L:390:PRO:N	2.01	0.59
8:W:263:THR:OG1	8:W:265:ARG:NH1	2.36	0.59
8:Q:263:THR:OG1	8:Q:265:ARG:NH1	2.36	0.59
8:R:263:THR:OG1	8:R:265:ARG:NH1	2.36	0.59
8:S:263:THR:OG1	8:S:265:ARG:NH1	2.36	0.59
5:C:738:MET:SD	5:C:738:MET:N	2.75	0.59
5:E:205:ILE:HG23	5:E:207:THR:H	1.66	0.59
8:S:183:VAL:HG13	8:S:187:ASN:HD21	1.66	0.59
4:D:401:HIS:O	4:D:405:LYS:NZ	2.36	0.58
5:G:494:TYR:HA	5:G:497:LYS:HE2	1.85	0.58
8:W:411:GLU:HB3	8:W:418:PHE:HE2	1.67	0.58
5:G:557:LEU:O	8:V:339:ARG:NH1	2.36	0.58
4:H:433:TRP:HE1	4:H:484:LEU:HA	1.69	0.58
1:J:225:TRP:HE1	6:K:35:HIS:CG	2.20	0.58
8:S:411:GLU:HB3	8:S:418:PHE:HE2	1.67	0.58
8:T:263:THR:OG1	8:T:265:ARG:NH1	2.36	0.58
8:U:411:GLU:HB3	8:U:418:PHE:HE2	1.67	0.58
4:F:454:VAL:HG12	4:F:459:LEU:HD22	1.86	0.58
5:G:688:ASN:HD21	8:U:357:GLN:HE22	1.51	0.58
8:Z:166:VAL:HG13	8:Z:200:ASP:H	1.69	0.58
6:I:357:ILE:O	6:I:361:TYR:HB3	2.03	0.58
8:R:166:VAL:HG13	8:R:200:ASP:H	1.69	0.57
8:V:411:GLU:HB3	8:V:418:PHE:HE2	1.67	0.57
8:Y:166:VAL:HG13	8:Y:200:ASP:H	1.69	0.57
8:V:166:VAL:HG13	8:V:200:ASP:H	1.69	0.57
5:E:652:GLU:HA	5:E:655:LEU:HD12	1.84	0.57
8:U:166:VAL:HG13	8:U:200:ASP:H	1.69	0.57
8:S:166:VAL:HG13	8:S:200:ASP:H	1.69	0.57
5:C:448:ASP:N	5:C:448:ASP:OD1	2.37	0.57
8:T:227:GLN:HA	8:T:230:GLN:HG2	1.86	0.57
8:U:263:THR:OG1	8:U:265:ARG:NH1	2.36	0.57
8:U:323:ILE:HG13	8:U:359:ALA:HB3	1.87	0.57
8:V:227:GLN:HA	8:V:230:GLN:HG2	1.86	0.57
8:V:323:ILE:HG13	8:V:359:ALA:HB3	1.87	0.57
5:E:738:MET:SD	5:E:738:MET:N	2.78	0.57
4:F:677:LEU:HB2	4:F:782:ILE:HD11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:737:LYS:NZ	4:H:750:ALA:O	2.36	0.57
8:U:227:GLN:HA	8:U:230:GLN:HG2	1.86	0.57
5:C:840:LEU:HB3	5:C:856:ILE:HD11	1.87	0.57
5:E:224:VAL:HG21	5:E:233:VAL:HG13	1.85	0.57
4:D:542:SER:HA	4:D:545:LEU:HD12	1.86	0.57
6:K:650:ASP:HB3	6:K:651:TYR:CZ	2.40	0.57
8:X:166:VAL:HG13	8:X:200:ASP:H	1.69	0.57
8:X:263:THR:OG1	8:X:265:ARG:NH1	2.36	0.57
5:G:307:VAL:O	4:H:365:ARG:NH1	2.37	0.57
6:K:513:ILE:HA	6:K:516:ARG:HD2	1.86	0.57
8:Q:323:ILE:HG13	8:Q:359:ALA:HB3	1.87	0.57
8:S:227:GLN:HA	8:S:230:GLN:HG2	1.86	0.57
6:I:129:PHE:HA	6:I:132:LEU:HB2	1.86	0.57
8:V:263:THR:OG1	8:V:265:ARG:NH1	2.36	0.57
8:W:166:VAL:HG13	8:W:200:ASP:H	1.69	0.57
4:D:865:LEU:HD11	4:D:873:LEU:HB3	1.86	0.56
8:Y:263:THR:OG1	8:Y:265:ARG:NH1	2.36	0.56
8:Z:323:ILE:HG13	8:Z:359:ALA:HB3	1.87	0.56
8:Q:227:GLN:HA	8:Q:230:GLN:HG2	1.86	0.56
8:W:56:ASP:HB2	8:X:296:ARG:CD	2.33	0.56
5:C:580:HIS:HB3	5:C:583:ILE:HG22	1.87	0.56
5:C:862:ASN:HB2	5:C:864:PHE:CE2	2.41	0.56
5:E:741:ASN:HD22	5:E:745:LEU:H	1.51	0.56
4:F:454:VAL:HB	4:F:463:LYS:HD2	1.87	0.56
8:Q:166:VAL:HG13	8:Q:200:ASP:H	1.69	0.56
8:R:227:GLN:HA	8:R:230:GLN:HG2	1.86	0.56
8:W:323:ILE:HG13	8:W:359:ALA:HB3	1.87	0.56
8:X:323:ILE:HG13	8:X:359:ALA:HB3	1.87	0.56
8:Y:323:ILE:HG13	8:Y:359:ALA:HB3	1.87	0.56
1:J:942:LEU:HB3	1:J:951:LYS:HD3	1.88	0.56
5:E:653:ARG:HH12	5:E:657:SER:HB3	1.69	0.56
5:G:687:LEU:HD11	8:U:258:ALA:HB1	1.88	0.56
8:S:323:ILE:HG13	8:S:359:ALA:HB3	1.87	0.56
4:F:860:GLN:HE21	4:F:864:LEU:HG	1.70	0.56
6:I:514:LYS:HG2	6:I:516:ARG:H	1.70	0.56
8:V:318:ILE:HD11	8:V:382:THR:HG23	1.88	0.56
8:W:227:GLN:HA	8:W:230:GLN:HG2	1.86	0.56
8:Y:53:TYR:O	8:Y:61:ILE:N	2.38	0.56
8:Y:227:GLN:HA	8:Y:230:GLN:HG2	1.86	0.56
8:U:229:ASN:O	8:U:233:SER:OG	2.23	0.56
4:F:333:ARG:HH21	4:F:334:GLU:HG3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:227:GLN:HA	8:Z:230:GLN:HG2	1.86	0.56
8:Z:229:ASN:O	8:Z:233:SER:OG	2.23	0.56
8:U:318:ILE:HD11	8:U:382:THR:HG23	1.88	0.56
8:Y:318:ILE:HD11	8:Y:382:THR:HG23	1.88	0.56
5:C:393:LYS:HD2	5:C:400:ILE:HD12	1.86	0.56
8:R:323:ILE:HG13	8:R:359:ALA:HB3	1.87	0.55
8:T:323:ILE:HG13	8:T:359:ALA:HB3	1.87	0.55
8:W:4:GLU:OE2	8:W:47:ARG:NH2	2.40	0.55
8:T:166:VAL:HG13	8:T:200:ASP:H	1.69	0.55
8:U:4:GLU:OE2	8:U:47:ARG:NH2	2.40	0.55
8:X:227:GLN:HA	8:X:230:GLN:HG2	1.86	0.55
4:H:720:TYR:HE2	8:V:357:GLN:HB3	1.71	0.55
8:X:4:GLU:OE2	8:X:47:ARG:NH2	2.40	0.55
8:Y:4:GLU:OE2	8:Y:47:ARG:NH2	2.40	0.55
8:Z:318:ILE:HB	8:Z:380:ASN:HB3	1.89	0.55
5:G:321:LEU:HA	5:G:324:LEU:HD12	1.88	0.55
4:H:589:ALA:HA	4:H:592:LEU:HG	1.88	0.55
8:R:318:ILE:HD11	8:R:382:THR:HG23	1.88	0.55
8:T:4:GLU:OE2	8:T:47:ARG:NH2	2.40	0.55
6:K:45:LEU:HD22	6:K:126:LEU:HD23	1.89	0.55
8:V:4:GLU:OE2	8:V:47:ARG:NH2	2.40	0.55
8:X:318:ILE:HD11	8:X:382:THR:HG23	1.88	0.55
8:Z:4:GLU:OE2	8:Z:47:ARG:NH2	2.40	0.55
4:D:489:SER:HB2	4:D:545:LEU:HD21	1.88	0.55
8:R:4:GLU:OE2	8:R:47:ARG:NH2	2.40	0.55
8:S:4:GLU:OE2	8:S:47:ARG:NH2	2.40	0.55
8:T:318:ILE:HB	8:T:380:ASN:HB3	1.89	0.55
8:Z:318:ILE:HD11	8:Z:382:THR:HG23	1.88	0.55
6:K:105:LEU:HD11	7:L:458:THR:HG22	1.87	0.55
8:X:318:ILE:HB	8:X:380:ASN:HB3	1.89	0.55
6:K:514:LYS:HE3	6:K:612:LEU:HD21	1.88	0.55
8:S:318:ILE:HB	8:S:380:ASN:HB3	1.89	0.55
8:Y:318:ILE:HB	8:Y:380:ASN:HB3	1.89	0.55
1:J:272:ARG:HE	7:L:308:GLU:HG3	1.72	0.55
1:J:881:HIS:CE1	8:X:446:TRP:HB3	2.42	0.55
7:L:1514:HIS:HA	7:L:1519:GLU:H	1.72	0.55
8:W:318:ILE:HD11	8:W:382:THR:HG23	1.88	0.55
8:X:53:TYR:O	8:X:61:ILE:N	2.37	0.55
8:Y:229:ASN:O	8:Y:233:SER:OG	2.23	0.55
8:Z:47:ARG:HG2	8:Z:49:ASP:H	1.72	0.55
4:H:427:LEU:HA	4:H:430:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:4:GLU:OE2	8:Q:47:ARG:NH2	2.40	0.54
8:T:318:ILE:HD11	8:T:382:THR:HG23	1.88	0.54
8:V:47:ARG:HG2	8:V:49:ASP:H	1.73	0.54
8:W:47:ARG:HG2	8:W:49:ASP:H	1.72	0.54
6:K:356:ILE:HD11	6:K:410:LEU:HD13	1.88	0.54
8:R:53:TYR:O	8:R:61:ILE:N	2.37	0.54
8:Y:47:ARG:HG2	8:Y:49:ASP:H	1.73	0.54
6:I:404:LEU:HD21	8:W:47:ARG:HG3	1.89	0.54
4:F:622:ASP:OD2	4:F:622:ASP:N	2.40	0.54
8:Q:47:ARG:HG2	8:Q:49:ASP:H	1.73	0.54
8:S:47:ARG:HG2	8:S:49:ASP:H	1.73	0.54
8:X:229:ASN:O	8:X:233:SER:OG	2.23	0.54
5:E:187:LEU:HD22	4:F:379:LYS:HD3	1.90	0.54
5:E:417:GLU:HG2	5:E:418:ARG:HG3	1.90	0.54
8:Q:318:ILE:HB	8:Q:380:ASN:HB3	1.89	0.54
8:R:318:ILE:HB	8:R:380:ASN:HB3	1.89	0.54
8:R:47:ARG:HG2	8:R:49:ASP:H	1.73	0.54
8:S:318:ILE:HD11	8:S:382:THR:HG23	1.88	0.54
8:W:318:ILE:HB	8:W:380:ASN:HB3	1.89	0.54
5:C:334:THR:HG23	5:C:375:LEU:HD22	1.89	0.54
4:D:762:CYS:SG	4:D:763:LEU:N	2.81	0.54
5:G:301:LYS:NZ	4:H:373:ASP:OD1	2.40	0.54
4:D:253:ASP:HB3	4:D:266:ILE:HG22	1.90	0.54
8:U:318:ILE:HB	8:U:380:ASN:HB3	1.89	0.54
8:T:47:ARG:HG2	8:T:49:ASP:H	1.72	0.54
5:E:249:ASP:HB2	5:E:252:LEU:HD23	1.89	0.54
5:E:557:LEU:HA	8:T:339:ARG:NH1	2.23	0.54
8:V:318:ILE:HB	8:V:380:ASN:HB3	1.89	0.54
4:H:869:SER:HB3	4:H:873:LEU:HG	1.90	0.53
5:G:180:TRP:HA	5:G:183:GLU:HG2	1.89	0.53
8:Q:252:ASP:OD1	8:Q:252:ASP:N	2.42	0.53
8:Q:318:ILE:HD11	8:Q:382:THR:HG23	1.88	0.53
7:L:510:LEU:HG	7:L:1475:LEU:H	1.74	0.53
6:K:260:ARG:HB3	6:K:262:GLU:HG2	1.90	0.53
5:C:581:ASP:HB2	5:C:610:LEU:HD11	1.90	0.53
4:F:677:LEU:HD21	4:F:712:VAL:HG22	1.90	0.53
6:I:192:LEU:HD12	6:I:304:GLU:HG2	1.90	0.53
1:J:287:PHE:HB3	1:J:294:VAL:HG23	1.91	0.53
8:X:53:TYR:N	8:X:61:ILE:O	2.42	0.53
5:C:231:ARG:NH2	5:C:232:TYR:OH	2.38	0.53
1:J:832:LYS:HD2	1:J:835:LYS:HZ1	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:847:LEU:HA	4:H:850:LEU:HD12	1.91	0.53
6:K:582:CYS:HB3	6:K:626:LEU:HD12	1.90	0.53
7:L:293:LYS:HZ3	7:L:295:ARG:HD3	1.74	0.53
8:Q:53:TYR:N	8:Q:61:ILE:O	2.42	0.53
8:S:184:GLN:O	8:S:188:SER:OG	2.27	0.53
8:W:184:GLN:O	8:W:188:SER:OG	2.27	0.53
7:L:311:TYR:H	7:L:314:GLU:HB2	1.74	0.53
8:U:53:TYR:O	8:U:61:ILE:N	2.37	0.53
8:X:47:ARG:HG2	8:X:49:ASP:H	1.73	0.53
5:C:641:LEU:HG	5:C:734:LEU:HD13	1.90	0.53
4:F:424:HIS:HA	4:F:427:LEU:HG	1.90	0.53
4:F:613:ASP:HB3	4:F:617:ILE:HD11	1.90	0.53
6:I:577:LYS:O	6:I:581:HIS:ND1	2.41	0.53
8:Q:184:GLN:O	8:Q:188:SER:OG	2.27	0.53
8:W:53:TYR:N	8:W:61:ILE:O	2.42	0.53
8:R:184:GLN:O	8:R:188:SER:OG	2.27	0.52
8:Z:184:GLN:O	8:Z:188:SER:OG	2.27	0.52
1:J:391:THR:HA	7:L:293:LYS:HZ1	1.73	0.52
8:X:184:GLN:O	8:X:188:SER:OG	2.27	0.52
6:I:102:GLN:HE22	6:I:105:LEU:HD23	1.74	0.52
6:I:416:LEU:HG	6:I:452:ALA:HB1	1.91	0.52
8:Z:53:TYR:O	8:Z:61:ILE:N	2.38	0.52
8:S:229:ASN:O	8:S:233:SER:OG	2.23	0.52
8:U:47:ARG:HG2	8:U:49:ASP:H	1.72	0.52
8:U:184:GLN:O	8:U:188:SER:OG	2.27	0.52
8:W:81:PRO:HA	8:W:84:LYS:HE2	1.92	0.52
8:W:229:ASN:O	8:W:233:SER:OG	2.23	0.52
7:L:294:ARG:HG2	7:L:305:GLY:HA3	1.92	0.52
7:L:1510:GLU:HA	7:L:1513:ARG:HD3	1.92	0.52
8:Q:278:THR:HA	8:Q:371:HIS:HE1	1.75	0.52
8:U:56:ASP:O	8:U:58:GLU:N	2.43	0.52
8:U:278:THR:HA	8:U:371:HIS:HE1	1.75	0.52
5:E:277:ILE:HA	5:E:293:ALA:HB1	1.92	0.52
4:H:448:VAL:HG22	4:H:484:LEU:HD12	1.91	0.52
4:H:878:PHE:HB2	4:H:879:ARG:HH22	1.75	0.52
7:L:1677:ALA:HA	7:L:1681:LEU:HD12	1.92	0.52
8:Q:62:PRO:HD2	8:Q:86:TYR:HB3	1.92	0.52
8:S:278:THR:HA	8:S:371:HIS:HE1	1.75	0.52
8:X:50:VAL:HG21	8:X:244:ARG:HG2	1.92	0.52
5:C:319:LEU:HD21	5:C:324:LEU:HD13	1.91	0.52
5:C:526:ASP:N	5:C:526:ASP:OD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:268:ILE:HG12	6:I:322:LEU:HD11	1.91	0.52
6:I:403:VAL:HG22	6:I:404:LEU:HG	1.91	0.52
8:R:53:TYR:N	8:R:61:ILE:O	2.42	0.52
8:T:62:PRO:HD2	8:T:86:TYR:HB3	1.92	0.52
8:T:184:GLN:O	8:T:188:SER:OG	2.27	0.52
8:U:50:VAL:HG21	8:U:244:ARG:HG2	1.92	0.52
8:V:184:GLN:O	8:V:188:SER:OG	2.27	0.52
8:Z:62:PRO:HD2	8:Z:86:TYR:HB3	1.92	0.52
5:C:623:LYS:HG3	5:C:625:PRO:HG2	1.92	0.52
8:S:53:TYR:O	8:S:61:ILE:N	2.38	0.52
8:V:62:PRO:HD2	8:V:86:TYR:HB3	1.92	0.52
8:W:62:PRO:HD2	8:W:86:TYR:HB3	1.92	0.52
8:Y:278:THR:HA	8:Y:371:HIS:HE1	1.75	0.52
5:G:585:GLN:HE22	5:G:739:LEU:HD12	1.75	0.52
4:H:798:GLU:HA	4:H:801:GLN:HE21	1.75	0.52
8:R:278:THR:HA	8:R:371:HIS:HE1	1.75	0.52
8:T:229:ASN:O	8:T:233:SER:OG	2.23	0.52
8:V:81:PRO:HA	8:V:84:LYS:HE2	1.92	0.52
8:W:50:VAL:HG21	8:W:244:ARG:HG2	1.92	0.52
8:Y:53:TYR:N	8:Y:61:ILE:O	2.42	0.52
4:H:419:LEU:HA	4:H:422:VAL:HG22	1.92	0.51
8:R:81:PRO:HA	8:R:84:LYS:HE2	1.92	0.51
8:S:50:VAL:HG21	8:S:244:ARG:HG2	1.92	0.51
8:S:81:PRO:HA	8:S:84:LYS:HE2	1.92	0.51
8:T:81:PRO:HA	8:T:84:LYS:HE2	1.92	0.51
8:Z:53:TYR:N	8:Z:61:ILE:O	2.42	0.51
4:H:247:GLU:HG3	4:H:366:ARG:HH12	1.75	0.51
4:H:664:PHE:O	4:H:668:TRP:HB2	2.10	0.51
8:Q:81:PRO:HA	8:Q:84:LYS:HE2	1.92	0.51
5:C:674:GLN:O	8:Q:265:ARG:NH2	2.43	0.51
4:F:562:MET:HA	4:F:642:TYR:HE1	1.75	0.51
8:R:62:PRO:HD2	8:R:86:TYR:HB3	1.92	0.51
8:Z:81:PRO:HA	8:Z:84:LYS:HE2	1.92	0.51
4:D:581:LEU:HG	4:D:585:LEU:HG	1.91	0.51
8:Q:53:TYR:O	8:Q:61:ILE:N	2.38	0.51
8:R:20:GLU:OE2	8:R:24:GLN:NE2	2.44	0.51
8:S:53:TYR:N	8:S:61:ILE:O	2.42	0.51
4:H:694:MET:HG3	4:H:696:GLU:HG2	1.91	0.51
8:T:20:GLU:OE2	8:T:24:GLN:NE2	2.44	0.51
8:U:71:PRO:O	8:U:75:HIS:NE2	2.44	0.51
8:V:53:TYR:O	8:V:61:ILE:N	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:71:PRO:O	8:V:75:HIS:NE2	2.44	0.51
8:X:20:GLU:OE2	8:X:24:GLN:NE2	2.44	0.51
8:Y:81:PRO:HA	8:Y:84:LYS:HE2	1.92	0.51
8:Z:388:PHE:HB2	8:Z:432:ILE:HD11	1.93	0.51
5:E:710:GLU:HB2	5:E:711:LYS:HZ2	1.75	0.51
1:J:430:VAL:HG23	1:J:493:ILE:HA	1.93	0.51
8:R:50:VAL:HG21	8:R:244:ARG:HG2	1.92	0.51
8:S:388:PHE:HB2	8:S:432:ILE:HD11	1.93	0.51
8:U:81:PRO:HA	8:U:84:LYS:HE2	1.92	0.51
8:V:388:PHE:HB2	8:V:432:ILE:HD11	1.92	0.51
8:X:62:PRO:HD2	8:X:86:TYR:HB3	1.92	0.51
8:X:278:THR:HA	8:X:371:HIS:HE1	1.75	0.51
8:Y:20:GLU:OE2	8:Y:24:GLN:NE2	2.44	0.51
4:H:778:VAL:HG23	4:H:854:TYR:HE1	1.75	0.51
6:K:404:LEU:HD22	8:Z:339:ARG:HH12	1.76	0.51
8:W:278:THR:HA	8:W:371:HIS:HE1	1.75	0.51
8:Q:388:PHE:HB2	8:Q:432:ILE:HD11	1.93	0.51
8:U:388:PHE:HB2	8:U:432:ILE:HD11	1.93	0.51
8:Y:71:PRO:O	8:Y:75:HIS:NE2	2.44	0.51
8:T:278:THR:HA	8:T:371:HIS:HE1	1.75	0.51
8:U:62:PRO:HD2	8:U:86:TYR:HB3	1.92	0.51
8:V:50:VAL:HG21	8:V:244:ARG:HG2	1.92	0.51
8:V:53:TYR:N	8:V:61:ILE:O	2.42	0.51
8:V:252:ASP:OD1	8:V:252:ASP:N	2.41	0.51
8:V:278:THR:HA	8:V:371:HIS:HE1	1.75	0.51
8:Z:213:ILE:HD13	8:Z:304:MET:HE3	1.93	0.51
8:Z:278:THR:HA	8:Z:371:HIS:HE1	1.75	0.51
5:G:719:ILE:HA	5:G:722:VAL:HG22	1.93	0.51
1:J:728:LEU:HA	8:X:248:TYR:CE1	2.45	0.51
8:Q:20:GLU:OE2	8:Q:24:GLN:NE2	2.44	0.51
8:S:20:GLU:OE2	8:S:24:GLN:NE2	2.44	0.51
8:U:20:GLU:OE2	8:U:24:GLN:NE2	2.44	0.51
8:X:388:PHE:HB2	8:X:432:ILE:HD11	1.93	0.51
8:Y:388:PHE:HB2	8:Y:432:ILE:HD11	1.93	0.51
4:D:304:ILE:HD11	4:D:382:ALA:HA	1.91	0.50
5:G:840:LEU:HG	5:G:856:ILE:HD11	1.92	0.50
8:Y:62:PRO:HD2	8:Y:86:TYR:HB3	1.92	0.50
7:L:1514:HIS:CD2	7:L:1519:GLU:HB3	2.46	0.50
8:T:50:VAL:HG21	8:T:244:ARG:HG2	1.92	0.50
8:W:20:GLU:OE2	8:W:24:GLN:NE2	2.44	0.50
8:Z:20:GLU:OE2	8:Z:24:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:305:ASP:N	6:K:305:ASP:OD1	2.44	0.50
6:K:639:ASN:HB2	8:Y:334:HIS:NE2	2.26	0.50
8:Q:50:VAL:HG21	8:Q:244:ARG:HG2	1.92	0.50
8:S:213:ILE:HD13	8:S:304:MET:HE3	1.92	0.50
8:T:53:TYR:O	8:T:61:ILE:N	2.38	0.50
8:V:20:GLU:OE2	8:V:24:GLN:NE2	2.44	0.50
8:X:81:PRO:HA	8:X:84:LYS:HE2	1.92	0.50
8:Y:50:VAL:HG21	8:Y:244:ARG:HG2	1.92	0.50
4:F:320:VAL:HG12	4:F:425:PRO:HB2	1.92	0.50
1:J:225:TRP:HE1	6:K:35:HIS:CD2	2.28	0.50
6:K:260:ARG:HB2	6:K:263:ILE:HG22	1.93	0.50
6:K:645:LEU:HB2	6:K:646:LEU:HD22	1.94	0.50
8:X:71:PRO:O	8:X:75:HIS:NE2	2.44	0.50
8:Y:184:GLN:O	8:Y:188:SER:OG	2.27	0.50
8:Z:156:ARG:NH2	8:Z:159:ASP:OD2	2.45	0.50
5:E:420:GLN:H	5:E:423:TYR:HB3	1.75	0.50
5:G:560:ARG:HB2	8:V:339:ARG:NE	2.23	0.50
8:Q:71:PRO:O	8:Q:75:HIS:NE2	2.44	0.50
8:Q:156:ARG:NH2	8:Q:159:ASP:OD2	2.45	0.50
8:R:229:ASN:O	8:R:233:SER:OG	2.23	0.50
8:S:62:PRO:HD2	8:S:86:TYR:HB3	1.92	0.50
8:S:156:ARG:NH2	8:S:159:ASP:OD2	2.45	0.50
8:U:156:ARG:NH2	8:U:159:ASP:OD2	2.45	0.50
8:X:322:ASN:ND2	8:X:357:GLN:O	2.45	0.50
8:Z:322:ASN:ND2	8:Z:357:GLN:O	2.45	0.50
8:T:322:ASN:ND2	8:T:357:GLN:O	2.45	0.50
8:V:156:ARG:NH2	8:V:159:ASP:OD2	2.45	0.50
8:W:322:ASN:ND2	8:W:357:GLN:O	2.45	0.50
5:E:514:ARG:HG2	5:E:517:LYS:HE3	1.94	0.50
6:I:504:HIS:HE1	8:W:158:ASN:HD21	1.60	0.50
1:J:882:ARG:HH21	1:J:981:GLU:HA	1.77	0.50
8:U:322:ASN:ND2	8:U:357:GLN:O	2.45	0.50
8:V:322:ASN:ND2	8:V:357:GLN:O	2.45	0.50
8:W:53:TYR:O	8:W:61:ILE:N	2.37	0.50
8:X:415:LYS:HG3	8:X:418:PHE:H	1.77	0.50
8:Y:322:ASN:ND2	8:Y:357:GLN:O	2.45	0.50
8:Z:71:PRO:O	8:Z:75:HIS:NE2	2.44	0.50
5:C:861:PHE:CE1	8:Q:337:LEU:HG	2.47	0.50
5:E:578:MET:HE2	5:E:616:PHE:H	1.77	0.50
8:Q:339:ARG:HG2	8:Q:339:ARG:HH21	1.77	0.50
8:W:252:ASP:OD1	8:W:252:ASP:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:388:PHE:HB2	8:W:432:ILE:HD11	1.93	0.50
8:Z:50:VAL:HG21	8:Z:244:ARG:HG2	1.92	0.50
5:E:288:VAL:HG22	5:E:386:PRO:HG2	1.94	0.50
4:H:446:PHE:O	4:H:467:ARG:NH1	2.44	0.50
8:R:156:ARG:NH2	8:R:159:ASP:OD2	2.45	0.50
8:R:322:ASN:ND2	8:R:357:GLN:O	2.45	0.50
8:S:322:ASN:ND2	8:S:357:GLN:O	2.45	0.50
1:J:305:LEU:HD22	1:J:310:LEU:HD13	1.94	0.49
8:S:71:PRO:O	8:S:75:HIS:NE2	2.44	0.49
8:S:339:ARG:HH21	8:S:339:ARG:HG2	1.77	0.49
8:S:415:LYS:HG3	8:S:418:PHE:H	1.77	0.49
8:T:71:PRO:O	8:T:75:HIS:NE2	2.44	0.49
8:Y:415:LYS:HE3	8:Y:420:GLU:HG3	1.95	0.49
8:U:415:LYS:HG3	8:U:418:PHE:H	1.77	0.49
8:V:415:LYS:HG3	8:V:418:PHE:H	1.77	0.49
8:W:71:PRO:O	8:W:75:HIS:NE2	2.44	0.49
8:Z:415:LYS:HE3	8:Z:420:GLU:HG3	1.95	0.49
8:R:56:ASP:O	8:R:58:GLU:N	2.43	0.49
8:R:71:PRO:O	8:R:75:HIS:NE2	2.44	0.49
8:T:156:ARG:NH2	8:T:159:ASP:OD2	2.45	0.49
8:T:388:PHE:HB2	8:T:432:ILE:HD11	1.92	0.49
8:V:339:ARG:HG2	8:V:339:ARG:HH21	1.77	0.49
8:W:156:ARG:NH2	8:W:159:ASP:OD2	2.45	0.49
8:Y:156:ARG:NH2	8:Y:159:ASP:OD2	2.45	0.49
4:D:297:LEU:HG	4:D:375:LYS:HE3	1.93	0.49
1:J:947:VAL:HA	1:J:951:LYS:HG2	1.93	0.49
8:V:47:ARG:HE	8:V:49:ASP:HB3	1.78	0.49
8:Y:415:LYS:HG3	8:Y:418:PHE:H	1.77	0.49
4:D:721:TYR:HD1	4:D:875:PHE:HD2	1.59	0.49
4:F:655:GLU:O	4:F:659:HIS:ND1	2.46	0.49
8:Q:56:ASP:O	8:Q:58:GLU:N	2.43	0.49
8:Q:322:ASN:ND2	8:Q:357:GLN:O	2.45	0.49
8:Q:415:LYS:HG3	8:Q:418:PHE:H	1.77	0.49
8:R:388:PHE:HB2	8:R:432:ILE:HD11	1.93	0.49
8:U:339:ARG:HH21	8:U:339:ARG:HG2	1.77	0.49
8:X:415:LYS:HE3	8:X:420:GLU:HG3	1.94	0.49
4:D:587:ARG:NH1	4:D:588:PRO:O	2.46	0.49
1:J:272:ARG:NH1	1:J:387:ILE:HG13	2.27	0.49
8:R:339:ARG:HH21	8:R:339:ARG:HG2	1.77	0.49
8:V:229:ASN:O	8:V:233:SER:OG	2.23	0.49
5:G:263:ILE:HD12	5:G:328:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:561:MET:N	8:V:339:ARG:HH11	2.10	0.49
7:L:409:ARG:HA	7:L:412:HIS:CE1	2.48	0.49
8:R:47:ARG:HE	8:R:49:ASP:HB3	1.78	0.49
8:R:415:LYS:HE3	8:R:420:GLU:HG3	1.95	0.49
8:W:339:ARG:HG2	8:W:339:ARG:HH21	1.77	0.49
8:X:156:ARG:NH2	8:X:159:ASP:OD2	2.45	0.49
8:Y:56:ASP:O	8:Y:58:GLU:N	2.43	0.49
8:Y:252:ASP:OD1	8:Y:252:ASP:N	2.41	0.49
4:D:559:MET:HE1	4:D:738:VAL:HG21	1.95	0.49
4:F:397:ALA:HA	4:F:400:VAL:HG22	1.95	0.49
4:H:878:PHE:HB2	4:H:879:ARG:NH2	2.28	0.49
8:U:415:LYS:HE3	8:U:420:GLU:HG3	1.95	0.49
8:Z:56:ASP:O	8:Z:58:GLU:N	2.43	0.49
4:F:319:LEU:N	4:F:445:GLU:OE2	2.28	0.49
7:L:294:ARG:HE	7:L:306:HIS:N	2.11	0.49
8:T:339:ARG:HG2	8:T:339:ARG:HH21	1.77	0.49
8:T:415:LYS:HG3	8:T:418:PHE:H	1.77	0.49
8:W:415:LYS:HE3	8:W:420:GLU:HG3	1.95	0.49
8:X:339:ARG:HG2	8:X:339:ARG:HH21	1.77	0.49
5:C:282:SER:HB2	5:C:285:TYR:HD1	1.76	0.49
5:C:638:TYR:OH	5:C:726:HIS:NE2	2.46	0.49
8:R:415:LYS:HG3	8:R:418:PHE:H	1.77	0.49
8:V:213:ILE:HD13	8:V:304:MET:HE3	1.95	0.49
8:W:47:ARG:HE	8:W:49:ASP:HB3	1.78	0.49
5:C:231:ARG:HH11	4:D:287:LEU:HB3	1.78	0.48
4:D:740:GLN:O	4:D:742:GLN:NE2	2.45	0.48
4:H:630:PRO:O	4:H:632:ASP:N	2.45	0.48
8:Q:47:ARG:HE	8:Q:49:ASP:HB3	1.78	0.48
8:V:56:ASP:O	8:V:58:GLU:N	2.43	0.48
8:V:415:LYS:HE3	8:V:420:GLU:HG3	1.95	0.48
8:Y:237:SER:O	8:Y:244:ARG:NH2	2.43	0.48
4:D:404:THR:HG21	4:D:419:LEU:HD13	1.95	0.48
4:D:531:GLN:HA	4:D:534:ILE:HG22	1.94	0.48
5:G:735:LYS:HA	5:G:740:THR:HB	1.94	0.48
8:S:56:ASP:O	8:S:58:GLU:N	2.43	0.48
8:S:415:LYS:HE3	8:S:420:GLU:HG3	1.94	0.48
8:T:47:ARG:HE	8:T:49:ASP:HB3	1.78	0.48
8:T:237:SER:O	8:T:244:ARG:NH2	2.43	0.48
8:Z:237:SER:O	8:Z:244:ARG:NH2	2.43	0.48
8:Z:324:ILE:HD11	8:Z:373:VAL:HG12	1.96	0.48
4:F:247:GLU:OE1	4:F:366:ARG:NH2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:562:ALA:HB2	1:J:699:TYR:HD1	1.78	0.48
8:T:53:TYR:N	8:T:61:ILE:O	2.42	0.48
8:W:415:LYS:HG3	8:W:418:PHE:H	1.77	0.48
8:Z:415:LYS:HG3	8:Z:418:PHE:H	1.77	0.48
5:E:719:ILE:HA	5:E:722:VAL:HG22	1.95	0.48
7:L:1533:GLU:HB2	7:L:1534:LYS:HZ2	1.79	0.48
8:Q:415:LYS:HE3	8:Q:420:GLU:HG3	1.95	0.48
8:T:213:ILE:HD13	8:T:304:MET:HE3	1.95	0.48
8:U:324:ILE:HD11	8:U:373:VAL:HG12	1.96	0.48
8:V:237:SER:O	8:V:244:ARG:NH2	2.43	0.48
8:X:56:ASP:O	8:X:58:GLU:N	2.43	0.48
8:Y:324:ILE:HD11	8:Y:373:VAL:HG12	1.96	0.48
5:C:517:LYS:HA	5:C:521:LEU:HD13	1.96	0.48
5:G:688:ASN:ND2	8:U:357:GLN:HE22	2.11	0.48
7:L:354:LYS:HA	7:L:357:LEU:HD12	1.95	0.48
8:W:237:SER:O	8:W:244:ARG:NH2	2.43	0.48
8:Z:339:ARG:HH21	8:Z:339:ARG:HG2	1.77	0.48
4:D:721:TYR:CE1	4:D:875:PHE:HB3	2.49	0.48
4:D:721:TYR:HE1	4:D:875:PHE:HB3	1.78	0.48
4:H:733:GLU:O	4:H:737:LYS:HG2	2.13	0.48
8:U:47:ARG:HE	8:U:49:ASP:HB3	1.78	0.48
8:Z:47:ARG:HE	8:Z:49:ASP:HB3	1.78	0.48
4:D:586:VAL:HG12	4:D:635:TRP:HE1	1.77	0.48
7:L:1656:ARG:NH2	8:Z:443:TYR:OH	2.46	0.48
7:L:1800:LEU:HD22	8:Z:338:GLN:HG3	1.94	0.48
8:Q:324:ILE:HD11	8:Q:373:VAL:HG12	1.96	0.48
8:T:56:ASP:O	8:T:58:GLU:N	2.43	0.48
8:U:237:SER:O	8:U:244:ARG:NH2	2.42	0.48
6:K:139:VAL:HA	6:K:142:GLN:HE21	1.79	0.48
7:L:1590:VAL:HG13	7:L:1737:LEU:HD23	1.96	0.48
8:W:324:ILE:HD11	8:W:373:VAL:HG12	1.96	0.48
8:S:47:ARG:HE	8:S:49:ASP:HB3	1.78	0.48
8:T:415:LYS:HE3	8:T:420:GLU:HG3	1.95	0.48
8:U:53:TYR:N	8:U:61:ILE:O	2.42	0.48
8:X:47:ARG:HE	8:X:49:ASP:HB3	1.78	0.48
4:D:768:SER:HA	4:D:771:LEU:HD13	1.96	0.47
4:F:798:GLU:HA	4:F:801:GLN:HE21	1.79	0.47
1:J:553:LYS:HA	1:J:556:LEU:HD12	1.96	0.47
6:K:272:VAL:HG23	6:K:329:VAL:HG11	1.95	0.47
4:D:773:ASN:HD22	4:D:776:ARG:HE	1.61	0.47
6:K:488:VAL:HG21	6:K:587:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:499:VAL:HB	7:L:551:GLU:HG2	1.97	0.47
8:Y:47:ARG:HE	8:Y:49:ASP:HB3	1.78	0.47
6:I:518:ARG:HD2	6:I:619:PHE:HD1	1.79	0.47
8:Q:229:ASN:O	8:Q:233:SER:OG	2.23	0.47
5:G:540:ARG:HA	5:G:613:LEU:HD23	1.97	0.47
8:S:252:ASP:OD1	8:S:252:ASP:N	2.41	0.47
8:X:237:SER:O	8:X:244:ARG:NH2	2.43	0.47
4:D:406:THR:HG23	4:D:412:ARG:HG2	1.97	0.47
4:D:707:LEU:HD13	4:D:851:THR:HG22	1.95	0.47
5:E:341:LEU:HD21	5:E:362:ARG:HG3	1.97	0.47
4:F:426:VAL:HG22	4:F:430:LEU:HD13	1.96	0.47
8:Y:9:GLN:HG3	8:Y:66:LEU:HA	1.97	0.47
5:C:611:SER:OG	5:C:612:GLY:N	2.47	0.47
4:H:361:SER:OG	4:H:362:LEU:N	2.46	0.47
1:J:268:THR:HA	1:J:271:ILE:HD12	1.96	0.47
8:R:4:GLU:O	8:R:133:GLU:N	2.47	0.47
8:T:9:GLN:HG3	8:T:66:LEU:HA	1.97	0.47
8:T:324:ILE:HD11	8:T:373:VAL:HG12	1.96	0.47
8:V:324:ILE:HD11	8:V:373:VAL:HG12	1.96	0.47
5:G:311:GLU:HB2	4:H:365:ARG:HH11	1.80	0.47
5:G:512:HIS:HE1	5:G:630:ILE:HD12	1.79	0.47
5:G:693:ILE:HA	5:G:696:TYR:CE1	2.50	0.47
7:L:550:GLY:HA2	7:L:555:GLN:HE21	1.79	0.47
7:L:1664:GLU:HG3	7:L:1772:PHE:HE2	1.80	0.47
8:T:231:LEU:O	8:T:234:THR:OG1	2.30	0.47
8:U:119:PHE:HA	8:U:122:ILE:HD12	1.97	0.47
5:C:187:LEU:HD21	4:D:379:LYS:HD3	1.96	0.47
5:C:814:LEU:HD22	5:C:818:PHE:HD1	1.80	0.47
5:G:241:ARG:HG3	5:G:242:GLN:H	1.79	0.47
8:Q:9:GLN:HG3	8:Q:66:LEU:HA	1.97	0.47
8:R:324:ILE:HD11	8:R:373:VAL:HG12	1.96	0.47
5:C:649:LYS:HE2	5:C:649:LYS:HB3	1.63	0.47
4:D:369:VAL:HG23	4:D:370:TRP:HD1	1.80	0.47
4:H:447:PHE:O	4:H:467:ARG:N	2.44	0.47
6:I:59:ILE:HD11	6:I:93:LEU:HG	1.97	0.47
6:K:20:ASN:HD22	6:K:26:GLN:HE22	1.62	0.47
8:W:9:GLN:HG3	8:W:66:LEU:HA	1.97	0.47
8:W:119:PHE:HA	8:W:122:ILE:HD12	1.97	0.47
8:Y:339:ARG:HG2	8:Y:339:ARG:HH21	1.77	0.47
4:H:481:ARG:HB3	4:H:482:LYS:HZ2	1.80	0.46
6:K:498:LEU:HD12	6:K:501:GLN:HE21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:GLN:HG3	8:U:66:LEU:HA	1.97	0.46
8:V:410:LYS:H	8:V:410:LYS:HG2	1.51	0.46
8:X:119:PHE:HA	8:X:122:ILE:HD12	1.97	0.46
8:X:324:ILE:HD11	8:X:373:VAL:HG12	1.96	0.46
8:Q:119:PHE:HA	8:Q:122:ILE:HD12	1.97	0.46
8:S:324:ILE:HD11	8:S:373:VAL:HG12	1.96	0.46
4:D:590:THR:HG21	4:D:631:GLY:HA2	1.96	0.46
4:D:757:THR:O	4:D:761:ARG:HG2	2.16	0.46
1:J:883:MET:SD	1:J:883:MET:N	2.88	0.46
8:Q:237:SER:O	8:Q:244:ARG:NH2	2.43	0.46
8:U:231:LEU:O	8:U:234:THR:OG1	2.30	0.46
5:G:561:MET:HB2	8:V:339:ARG:HH12	1.81	0.46
6:I:19:TRP:HA	6:I:25:LEU:H	1.81	0.46
5:G:637:ARG:HB3	5:G:734:LEU:HD11	1.97	0.46
5:G:707:HIS:O	5:G:711:LYS:NZ	2.39	0.46
6:I:357:ILE:O	6:I:361:TYR:CB	2.64	0.46
1:J:556:LEU:HA	1:J:559:ILE:HD12	1.96	0.46
6:K:630:LEU:HG	6:K:645:LEU:HD21	1.96	0.46
7:L:1513:ARG:HG3	7:L:1514:HIS:CD2	2.51	0.46
8:R:119:PHE:HA	8:R:122:ILE:HD12	1.97	0.46
8:U:410:LYS:H	8:U:410:LYS:HG2	1.51	0.46
8:V:119:PHE:HA	8:V:122:ILE:HD12	1.97	0.46
8:Z:52:PHE:HB3	8:Z:60:TYR:HB3	1.98	0.46
6:K:643:ALA:HB2	8:Y:334:HIS:HD1	1.81	0.46
8:R:9:GLN:HG3	8:R:66:LEU:HA	1.97	0.46
8:S:119:PHE:HA	8:S:122:ILE:HD12	1.97	0.46
8:Y:52:PHE:HB3	8:Y:60:TYR:HB3	1.98	0.46
4:F:433:TRP:CD1	4:F:483:VAL:HG22	2.51	0.46
5:G:693:ILE:HD12	5:G:696:TYR:HE1	1.81	0.46
6:K:121:HIS:HA	6:K:124:TYR:CE1	2.51	0.46
7:L:1669:VAL:HA	7:L:1672:ILE:HG22	1.96	0.46
8:Q:205:LEU:HA	8:Q:305:VAL:HG22	1.98	0.46
8:U:252:ASP:OD1	8:U:252:ASP:N	2.42	0.46
8:W:213:ILE:HD13	8:W:304:MET:HE3	1.97	0.46
5:C:231:ARG:HG2	4:D:286:SER:HB3	1.98	0.46
1:J:552:LEU:HG	1:J:556:LEU:HG	1.98	0.46
6:K:378:HIS:HA	6:K:381:LYS:HG2	1.97	0.46
6:K:542:SER:OG	6:K:543:GLN:NE2	2.48	0.46
8:Q:3:ARG:HH11	8:Q:132:LEU:H	1.64	0.46
8:X:9:GLN:HG3	8:X:66:LEU:HA	1.97	0.46
8:Z:119:PHE:HA	8:Z:122:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:434:ILE:HG22	4:D:486:ILE:HD11	1.98	0.46
5:E:746:LYS:O	5:E:749:SER:OG	2.29	0.46
4:H:578:MET:SD	4:H:671:LYS:HD3	2.56	0.46
4:H:580:LEU:HB3	4:H:600:ILE:HD11	1.97	0.46
1:J:282:LYS:HG3	1:J:283:LYS:HG2	1.98	0.46
1:J:884:PHE:O	1:J:888:VAL:HG23	2.16	0.46
8:T:52:PHE:HB3	8:T:60:TYR:HB3	1.98	0.46
8:U:192:LEU:HA	8:U:195:LEU:HB2	1.98	0.46
8:U:202:VAL:HG12	8:U:204:VAL:HG12	1.98	0.46
8:V:205:LEU:HA	8:V:305:VAL:HG22	1.98	0.46
8:Z:55:ALA:N	8:Z:59:HIS:O	2.49	0.46
8:Z:202:VAL:HG12	8:Z:204:VAL:HG12	1.98	0.46
5:C:183:GLU:HB3	5:C:184:ARG:HH11	1.81	0.46
5:E:478:THR:OG1	5:E:482:ARG:HA	2.16	0.46
5:E:727:THR:HA	5:E:730:LEU:HG	1.98	0.46
4:F:571:GLY:H	4:F:574:ILE:HD12	1.80	0.46
4:H:430:LEU:HD23	4:H:446:PHE:HE1	1.81	0.46
1:J:707:MET:HA	1:J:710:LEU:HG	1.98	0.46
8:R:252:ASP:OD1	8:R:252:ASP:N	2.41	0.46
8:S:3:ARG:HH11	8:S:132:LEU:H	1.64	0.46
8:W:52:PHE:HB3	8:W:60:TYR:HB3	1.98	0.46
8:W:192:LEU:HA	8:W:195:LEU:HB2	1.98	0.46
8:X:3:ARG:HH11	8:X:132:LEU:H	1.64	0.46
8:X:4:GLU:O	8:X:133:GLU:N	2.47	0.46
8:Z:4:GLU:O	8:Z:133:GLU:N	2.47	0.46
4:F:538:TYR:O	4:F:542:SER:OG	2.27	0.45
4:F:848:ARG:HH21	4:F:852:HIS:CE1	2.34	0.45
5:G:694:GLN:HE22	8:U:249:MET:HG2	1.81	0.45
4:H:655:GLU:O	4:H:658:SER:OG	2.33	0.45
4:H:697:PHE:HB3	4:H:701:LEU:HD23	1.97	0.45
6:I:345:VAL:HG23	6:I:346:GLU:HG3	1.98	0.45
1:J:892:HIS:CD2	8:X:353:PRO:HB2	2.51	0.45
1:J:903:THR:OG1	1:J:904:ARG:N	2.49	0.45
7:L:1666:GLN:HE22	8:Z:259:SER:HA	1.81	0.45
8:S:9:GLN:HG3	8:S:66:LEU:HA	1.97	0.45
8:S:52:PHE:HB3	8:S:60:TYR:HB3	1.98	0.45
8:W:3:ARG:HH11	8:W:132:LEU:H	1.64	0.45
8:Z:3:ARG:HH11	8:Z:132:LEU:H	1.64	0.45
6:K:511:ASP:HA	6:K:514:LYS:HE2	1.98	0.45
8:S:205:LEU:HA	8:S:305:VAL:HG22	1.98	0.45
8:U:153:LEU:HD13	8:U:153:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:9:GLN:HG3	8:V:66:LEU:HA	1.97	0.45
8:V:202:VAL:HG12	8:V:204:VAL:HG12	1.98	0.45
8:V:231:LEU:O	8:V:234:THR:OG1	2.30	0.45
8:W:56:ASP:O	8:W:58:GLU:N	2.43	0.45
8:X:52:PHE:HB3	8:X:60:TYR:HB3	1.98	0.45
8:Y:202:VAL:HG12	8:Y:204:VAL:HG12	1.98	0.45
5:E:632:ARG:CZ	5:E:633:LYS:HG2	2.46	0.45
6:K:409:ASN:O	6:K:410:LEU:HG	2.16	0.45
6:K:649:LEU:HD13	6:K:652:ASN:HA	1.98	0.45
8:R:303:VAL:HG12	8:R:305:VAL:H	1.82	0.45
8:S:4:GLU:O	8:S:133:GLU:N	2.47	0.45
8:S:69:LEU:HD23	8:S:145:THR:HB	1.98	0.45
8:S:303:VAL:HG12	8:S:305:VAL:H	1.82	0.45
8:T:252:ASP:OD1	8:T:252:ASP:N	2.41	0.45
8:U:205:LEU:HA	8:U:305:VAL:HG22	1.98	0.45
8:Y:55:ALA:N	8:Y:59:HIS:O	2.49	0.45
8:Z:9:GLN:HG3	8:Z:66:LEU:HA	1.97	0.45
4:F:568:LEU:HD13	4:F:667:LEU:HB3	1.98	0.45
6:I:31:PHE:HB2	6:I:34:LEU:HG	1.98	0.45
1:J:466:VAL:HG13	1:J:642:HIS:HE1	1.81	0.45
7:L:293:LYS:HA	7:L:293:LYS:HD2	1.74	0.45
8:Q:55:ALA:N	8:Q:59:HIS:O	2.49	0.45
8:Q:303:VAL:HG12	8:Q:305:VAL:H	1.82	0.45
8:Y:192:LEU:HA	8:Y:195:LEU:HB2	1.98	0.45
4:D:581:LEU:HD12	4:D:584:GLU:HB2	1.99	0.45
5:E:507:LYS:HZ2	5:E:623:LYS:HE3	1.81	0.45
5:G:576:ASP:OD1	5:G:576:ASP:N	2.49	0.45
6:I:350:LEU:HD13	6:I:464:HIS:CE1	2.52	0.45
1:J:721:GLN:HA	1:J:724:ARG:HE	1.81	0.45
1:J:832:LYS:HD2	1:J:835:LYS:NZ	2.31	0.45
1:J:835:LYS:HE2	1:J:835:LYS:HB2	1.67	0.45
8:Q:202:VAL:HG12	8:Q:204:VAL:HG12	1.98	0.45
8:R:3:ARG:HH11	8:R:132:LEU:H	1.64	0.45
8:R:69:LEU:HD23	8:R:145:THR:HB	1.98	0.45
8:T:119:PHE:HA	8:T:122:ILE:HD12	1.97	0.45
8:Y:119:PHE:HA	8:Y:122:ILE:HD12	1.97	0.45
5:C:299:LEU:HD22	5:C:338:LEU:HD11	1.98	0.45
8:U:303:VAL:HG12	8:U:305:VAL:H	1.82	0.45
6:K:544:LEU:O	6:K:548:ILE:HG12	2.17	0.45
8:R:205:LEU:HA	8:R:305:VAL:HG22	1.98	0.45
8:W:69:LEU:HD23	8:W:145:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:4:GLU:O	8:Y:133:GLU:N	2.47	0.45
8:Z:3:ARG:HB3	8:Z:4:GLU:H	1.51	0.45
5:C:519:TYR:HB3	5:C:618:PHE:HE1	1.82	0.45
4:H:621:LEU:HD11	4:H:640:LEU:HD21	1.98	0.45
6:I:477:VAL:HA	6:I:480:LYS:HD2	1.98	0.45
8:S:273:TYR:N	8:S:304:MET:SD	2.90	0.45
8:T:202:VAL:HG12	8:T:204:VAL:HG12	1.98	0.45
8:T:303:VAL:HG12	8:T:305:VAL:H	1.82	0.45
8:W:303:VAL:HG12	8:W:305:VAL:H	1.82	0.45
5:C:501:ASP:HA	5:C:504:MET:HG2	1.98	0.45
6:I:298:SER:OG	6:I:299:ILE:N	2.50	0.45
6:K:143:ILE:HD12	6:K:153:ILE:HG12	1.98	0.45
7:L:425:LYS:HZ2	7:L:549:TYR:HE2	1.64	0.45
8:R:231:LEU:O	8:R:234:THR:OG1	2.30	0.45
8:U:3:ARG:HH11	8:U:132:LEU:H	1.64	0.45
8:U:213:ILE:HD13	8:U:304:MET:HE3	1.98	0.45
8:Y:273:TYR:N	8:Y:304:MET:SD	2.90	0.45
8:Z:303:VAL:HG12	8:Z:305:VAL:H	1.82	0.45
5:E:556:GLU:O	5:E:560:ARG:NH1	2.50	0.45
6:K:500:MET:HA	8:Y:264:PRO:HG3	1.97	0.45
8:Q:192:LEU:HA	8:Q:195:LEU:HB2	1.98	0.45
8:V:4:GLU:O	8:V:133:GLU:N	2.47	0.45
8:Y:69:LEU:HD23	8:Y:145:THR:HB	1.98	0.45
8:Y:303:VAL:HG12	8:Y:305:VAL:H	1.82	0.45
8:Z:69:LEU:HD23	8:Z:145:THR:HB	1.98	0.45
5:E:707:HIS:O	5:E:711:LYS:NZ	2.45	0.44
8:Q:34:GLU:HG3	8:Q:84:LYS:HE3	1.99	0.44
8:Q:52:PHE:HB3	8:Q:60:TYR:HB3	1.98	0.44
8:T:3:ARG:HH11	8:T:132:LEU:H	1.64	0.44
8:V:3:ARG:HH11	8:V:132:LEU:H	1.64	0.44
8:V:34:GLU:HG3	8:V:84:LYS:HE3	1.99	0.44
8:V:52:PHE:HB3	8:V:60:TYR:HB3	1.98	0.44
8:W:34:GLU:HG3	8:W:84:LYS:HE3	1.99	0.44
8:W:202:VAL:HG12	8:W:204:VAL:HG12	1.98	0.44
8:X:192:LEU:HA	8:X:195:LEU:HB2	1.98	0.44
8:X:202:VAL:HG12	8:X:204:VAL:HG12	1.98	0.44
8:X:273:TYR:N	8:X:304:MET:SD	2.90	0.44
5:C:663:LYS:NZ	8:Q:264:PRO:HB3	2.33	0.44
4:F:860:GLN:HA	4:F:863:VAL:HG12	1.99	0.44
5:G:356:LEU:HG	5:G:440:PRO:HB3	1.99	0.44
5:G:376:CYS:SG	5:G:377:LEU:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:875:PHE:O	4:H:879:ARG:NH2	2.50	0.44
6:I:20:ASN:H	6:I:24:GLY:HA2	1.82	0.44
8:R:192:LEU:HA	8:R:195:LEU:HB2	1.98	0.44
8:S:192:LEU:HA	8:S:195:LEU:HB2	1.98	0.44
8:W:205:LEU:HA	8:W:305:VAL:HG22	1.98	0.44
8:Z:34:GLU:HG3	8:Z:84:LYS:HE3	1.99	0.44
5:E:188:ILE:HG22	5:E:190:ASP:H	1.82	0.44
5:E:659:TRP:HA	5:E:662:ASN:HD21	1.82	0.44
4:F:563:ARG:HA	4:F:567:LEU:HD13	1.99	0.44
4:H:308:THR:HG21	4:H:328:LEU:HD22	1.99	0.44
8:Q:69:LEU:HD23	8:Q:145:THR:HB	1.98	0.44
8:V:303:VAL:HG12	8:V:305:VAL:H	1.82	0.44
8:Y:3:ARG:HH11	8:Y:132:LEU:H	1.64	0.44
8:Y:34:GLU:HG3	8:Y:84:LYS:HE3	1.99	0.44
8:Y:205:LEU:HA	8:Y:305:VAL:HG22	1.98	0.44
4:F:605:VAL:HG13	4:F:610:ALA:HB3	2.00	0.44
8:R:52:PHE:HB3	8:R:60:TYR:HB3	1.98	0.44
8:S:202:VAL:HG12	8:S:204:VAL:HG12	1.98	0.44
8:U:273:TYR:N	8:U:304:MET:SD	2.90	0.44
8:W:4:GLU:O	8:W:133:GLU:N	2.47	0.44
8:X:69:LEU:HD23	8:X:145:THR:HB	1.98	0.44
8:Z:273:TYR:N	8:Z:304:MET:SD	2.90	0.44
5:C:469:CYS:HB3	5:C:471:VAL:HG12	2.00	0.44
5:C:690:VAL:HA	5:C:693:ILE:HG22	1.98	0.44
4:D:332:LEU:HD23	4:D:332:LEU:HA	1.68	0.44
8:R:273:TYR:N	8:R:304:MET:SD	2.90	0.44
8:T:205:LEU:HA	8:T:305:VAL:HG22	1.98	0.44
8:V:69:LEU:HD23	8:V:145:THR:HB	1.98	0.44
8:V:192:LEU:HA	8:V:195:LEU:HB2	1.98	0.44
8:V:273:TYR:N	8:V:304:MET:SD	2.90	0.44
8:X:34:GLU:HG3	8:X:84:LYS:HE3	1.99	0.44
8:X:205:LEU:HA	8:X:305:VAL:HG22	1.98	0.44
8:X:252:ASP:OD1	8:X:252:ASP:N	2.41	0.44
5:C:461:ARG:HD3	5:C:467:VAL:HG21	2.00	0.44
5:C:766:THR:HG23	5:C:769:MET:H	1.82	0.44
4:F:419:LEU:O	4:F:423:SER:OG	2.23	0.44
8:T:192:LEU:HA	8:T:195:LEU:HB2	1.98	0.44
8:T:273:TYR:N	8:T:304:MET:SD	2.90	0.44
8:V:160:ARG:HD2	8:V:160:ARG:HA	1.82	0.44
8:W:273:TYR:N	8:W:304:MET:SD	2.90	0.44
8:X:303:VAL:HG12	8:X:305:VAL:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:192:LEU:HA	8:Z:195:LEU:HB2	1.98	0.44
5:C:217:VAL:HG23	5:C:321:LEU:HD21	2.00	0.44
4:D:726:VAL:HA	4:D:761:ARG:HD3	1.98	0.44
8:Q:273:TYR:N	8:Q:304:MET:SD	2.90	0.44
8:R:202:VAL:HG12	8:R:204:VAL:HG12	1.98	0.44
8:U:52:PHE:HB3	8:U:60:TYR:HB3	1.98	0.44
5:C:280:LYS:HE3	5:C:289:ASN:HB3	2.00	0.44
6:K:129:PHE:HB3	6:K:133:PHE:CE2	2.53	0.44
8:U:34:GLU:HG3	8:U:84:LYS:HE3	1.99	0.44
8:X:55:ALA:N	8:X:59:HIS:O	2.49	0.44
4:D:546:LEU:HD23	4:D:744:LEU:HD23	1.98	0.44
4:F:589:ALA:HA	4:F:592:LEU:HG	2.00	0.44
4:H:589:ALA:HB2	4:H:637:VAL:HG21	1.99	0.44
6:K:486:ARG:HB2	6:K:530:TYR:HE2	1.83	0.44
8:S:154:LEU:HD23	8:S:198:ASN:HB2	2.00	0.44
8:T:34:GLU:HG3	8:T:84:LYS:HE3	1.99	0.44
8:U:69:LEU:HD23	8:U:145:THR:HB	1.98	0.44
8:X:160:ARG:HD2	8:X:160:ARG:HA	1.83	0.44
8:Z:205:LEU:HA	8:Z:305:VAL:HG22	1.98	0.44
5:C:555:LEU:HD21	5:C:573:LEU:HG	1.99	0.43
5:C:865:TYR:HE1	8:Q:353:PRO:HG3	1.83	0.43
4:H:595:HIS:HA	4:H:598:THR:HG22	1.99	0.43
6:K:534:VAL:HG21	8:Y:248:TYR:HE2	1.83	0.43
8:Q:4:GLU:O	8:Q:133:GLU:N	2.47	0.43
8:R:261:ILE:HG12	8:R:267:HIS:HA	2.00	0.43
8:X:410:LYS:H	8:X:410:LYS:HG2	1.51	0.43
5:C:527:PHE:O	5:C:531:PHE:CB	2.66	0.43
4:D:546:LEU:O	4:D:550:ASN:ND2	2.51	0.43
4:F:364:LEU:HB2	4:F:367:LEU:HD12	1.98	0.43
5:G:709:LEU:HD13	5:G:729:PHE:HB2	1.99	0.43
7:L:468:ARG:HA	7:L:471:ARG:HD3	2.00	0.43
8:T:69:LEU:HD23	8:T:145:THR:HB	1.98	0.43
8:X:154:LEU:HD23	8:X:198:ASN:HB2	2.00	0.43
8:X:261:ILE:HG12	8:X:267:HIS:HA	2.00	0.43
8:Y:261:ILE:HG12	8:Y:267:HIS:HA	2.00	0.43
8:Z:252:ASP:OD1	8:Z:252:ASP:N	2.41	0.43
5:C:209:PRO:O	5:C:212:SER:OG	2.26	0.43
6:I:116:HIS:HE1	1:J:237:HIS:CD2	2.36	0.43
8:R:55:ALA:N	8:R:59:HIS:O	2.49	0.43
8:U:4:GLU:O	8:U:133:GLU:N	2.47	0.43
8:V:344:LYS:HD3	8:V:344:LYS:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:261:ILE:HG12	8:W:267:HIS:HA	2.01	0.43
5:C:560:ARG:HB2	8:R:339:ARG:HH11	1.82	0.43
5:E:507:LYS:NZ	5:E:623:LYS:HE3	2.32	0.43
7:L:1625:GLN:HA	7:L:1628:LEU:HD12	2.00	0.43
8:S:34:GLU:HG3	8:S:84:LYS:HE3	1.99	0.43
5:C:518:ARG:HA	5:C:523:ASP:HB3	2.01	0.43
5:C:554:LEU:HA	5:C:557:LEU:HG	2.00	0.43
8:S:151:SER:HB2	8:S:194:ARG:HG2	2.01	0.43
8:T:261:ILE:HG12	8:T:267:HIS:HA	2.00	0.43
4:H:574:ILE:O	4:H:578:MET:HG2	2.17	0.43
6:I:165:LEU:HA	6:I:166:PRO:HD3	1.80	0.43
8:T:154:LEU:HD23	8:T:198:ASN:HB2	2.00	0.43
8:T:348:PHE:HB3	8:T:349:ILE:H	1.69	0.43
8:U:3:ARG:HB3	8:U:4:GLU:H	1.51	0.43
8:W:151:SER:HB2	8:W:194:ARG:HG2	2.01	0.43
5:C:460:VAL:HG12	5:C:499:LEU:HD13	1.99	0.43
5:C:623:LYS:HE2	5:C:626:LEU:HG	2.01	0.43
4:D:875:PHE:HA	4:D:878:PHE:HB3	1.99	0.43
8:R:34:GLU:HG3	8:R:84:LYS:HE3	1.99	0.43
8:R:37:VAL:N	8:R:58:GLU:O	2.49	0.43
8:R:154:LEU:HD23	8:R:198:ASN:HB2	2.00	0.43
8:R:344:LYS:HD3	8:R:344:LYS:HA	1.82	0.43
8:W:160:ARG:HA	8:W:160:ARG:HD2	1.83	0.43
8:X:12:GLN:H	8:X:12:GLN:HG2	1.68	0.43
4:D:308:THR:O	4:D:312:SER:OG	2.37	0.43
4:D:380:THR:O	4:D:384:LEU:HG	2.19	0.43
4:F:616:GLU:O	4:F:620:ARG:HG2	2.18	0.43
4:F:843:MET:O	4:F:847:LEU:HG	2.19	0.43
4:H:883:ASN:ND2	8:V:352:GLY:O	2.52	0.43
6:K:96:VAL:HG21	6:K:175:ILE:HG13	2.01	0.43
7:L:1594:LEU:HD23	7:L:1594:LEU:HA	1.89	0.43
8:Q:154:LEU:HD23	8:Q:198:ASN:HB2	2.00	0.43
8:U:348:PHE:HB3	8:U:349:ILE:H	1.70	0.43
8:X:151:SER:HB2	8:X:194:ARG:HG2	2.01	0.43
5:E:741:ASN:HD22	5:E:745:LEU:N	2.16	0.43
4:F:362:LEU:HB3	4:F:363:THR:H	1.61	0.43
4:H:447:PHE:HA	4:H:467:ARG:HB3	2.01	0.43
7:L:284:GLU:HA	7:L:287:LEU:HD12	2.01	0.43
8:X:37:VAL:N	8:X:58:GLU:O	2.49	0.43
5:G:155:GLU:O	5:G:159:LYS:HG2	2.18	0.43
6:I:509:GLN:HB3	6:I:510:THR:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:364:PHE:O	1:J:368:LEU:HG	2.19	0.43
8:R:237:SER:O	8:R:244:ARG:NH2	2.43	0.43
8:Y:154:LEU:HD23	8:Y:198:ASN:HB2	2.00	0.43
5:C:266:VAL:HG21	5:C:328:ILE:HD13	2.00	0.42
4:D:722:ILE:HD13	4:D:726:VAL:HG21	2.00	0.42
5:E:557:LEU:HD13	8:T:339:ARG:CZ	2.49	0.42
5:E:560:ARG:HB2	8:T:339:ARG:HH11	1.83	0.42
5:E:578:MET:HE2	5:E:615:ALA:HA	2.01	0.42
5:G:696:TYR:CE2	5:G:697:MET:HG3	2.54	0.42
7:L:399:GLU:OE2	7:L:403:TYR:OH	2.34	0.42
7:L:1518:MET:HB2	7:L:1623:LEU:HD21	2.00	0.42
8:R:278:THR:HG23	8:R:371:HIS:ND1	2.34	0.42
8:S:231:LEU:O	8:S:234:THR:OG1	2.30	0.42
8:T:12:GLN:H	8:T:12:GLN:HG2	1.68	0.42
8:V:151:SER:HB2	8:V:194:ARG:HG2	2.01	0.42
8:V:154:LEU:HD23	8:V:198:ASN:HB2	2.00	0.42
8:W:154:LEU:HD23	8:W:198:ASN:HB2	2.00	0.42
8:Z:151:SER:HB2	8:Z:194:ARG:HG2	2.01	0.42
5:C:816:SER:O	5:C:816:SER:OG	2.32	0.42
5:E:547:THR:HA	5:E:548:PRO:HD3	1.93	0.42
5:G:692:ASN:HA	5:G:858:ARG:HH22	1.85	0.42
4:H:388:CYS:HB3	4:H:396:LEU:HG	2.01	0.42
6:I:3:HIS:CG	7:L:297:TRP:HE1	2.37	0.42
8:Q:278:THR:HG23	8:Q:371:HIS:ND1	2.34	0.42
8:S:115:HIS:HB3	8:S:152:TYR:HE2	1.85	0.42
8:U:278:THR:HG23	8:U:371:HIS:ND1	2.34	0.42
8:V:3:ARG:HB3	8:V:4:GLU:H	1.51	0.42
8:V:261:ILE:HG12	8:V:267:HIS:HA	2.00	0.42
8:Y:348:PHE:HB3	8:Y:349:ILE:H	1.70	0.42
8:Z:261:ILE:HG12	8:Z:267:HIS:HA	2.00	0.42
4:H:549:LEU:HD12	4:H:555:LEU:HD21	2.02	0.42
4:H:722:ILE:O	4:H:727:LEU:HG	2.19	0.42
8:X:278:THR:HG23	8:X:371:HIS:ND1	2.34	0.42
8:Y:37:VAL:N	8:Y:58:GLU:O	2.49	0.42
4:F:686:CYS:HA	4:F:689:LYS:HD3	2.01	0.42
5:G:536:GLU:HA	5:G:539:LEU:HB2	2.01	0.42
4:H:716:HIS:HA	4:H:719:GLN:HE21	1.83	0.42
6:I:524:LEU:HD22	8:W:353:PRO:HB2	2.01	0.42
7:L:284:GLU:HA	7:L:287:LEU:HB2	2.02	0.42
8:Q:231:LEU:O	8:Q:234:THR:OG1	2.30	0.42
8:T:278:THR:HG23	8:T:371:HIS:ND1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:278:THR:HG23	8:W:371:HIS:ND1	2.34	0.42
4:H:616:GLU:HG2	4:H:619:ARG:HH11	1.83	0.42
6:K:184:TYR:O	6:K:188:SER:OG	2.26	0.42
6:K:651:TYR:CE1	8:Y:348:PHE:HB2	2.54	0.42
8:Q:11:GLY:O	8:Q:15:ASN:ND2	2.52	0.42
8:R:151:SER:HB2	8:R:194:ARG:HG2	2.01	0.42
8:U:154:LEU:HD23	8:U:198:ASN:HB2	2.00	0.42
8:U:261:ILE:HG12	8:U:267:HIS:HA	2.00	0.42
8:V:11:GLY:O	8:V:15:ASN:ND2	2.52	0.42
8:V:278:THR:HG23	8:V:371:HIS:ND1	2.34	0.42
8:W:115:HIS:HB3	8:W:152:TYR:HE2	1.85	0.42
8:Z:154:LEU:HD23	8:Z:198:ASN:HB2	2.00	0.42
5:G:312:GLN:NE2	5:G:316:GLN:HE21	2.17	0.42
8:Q:151:SER:HB2	8:Q:194:ARG:HG2	2.01	0.42
8:Q:261:ILE:HG12	8:Q:267:HIS:HA	2.00	0.42
8:R:11:GLY:O	8:R:15:ASN:ND2	2.52	0.42
8:T:151:SER:HB2	8:T:194:ARG:HG2	2.01	0.42
8:W:11:GLY:O	8:W:15:ASN:ND2	2.52	0.42
5:C:540:ARG:HA	5:C:613:LEU:HD11	2.02	0.42
5:G:302:GLU:HA	5:G:305:ILE:HD12	2.01	0.42
5:G:311:GLU:HB2	4:H:365:ARG:NH1	2.34	0.42
7:L:1783:VAL:HG21	7:L:1798:PHE:CD1	2.54	0.42
8:S:11:GLY:O	8:S:15:ASN:ND2	2.52	0.42
8:T:115:HIS:HB3	8:T:152:TYR:HE2	1.85	0.42
8:Z:11:GLY:O	8:Z:15:ASN:ND2	2.52	0.42
1:J:275:LEU:HA	1:J:278:LEU:HD12	2.01	0.42
6:K:524:LEU:HA	6:K:524:LEU:HD12	1.83	0.42
8:R:115:HIS:HB3	8:R:152:TYR:HE2	1.85	0.42
8:R:164:LYS:HD3	8:R:164:LYS:HA	1.84	0.42
8:S:55:ALA:N	8:S:59:HIS:O	2.49	0.42
8:S:237:SER:O	8:S:244:ARG:NH2	2.43	0.42
8:S:261:ILE:HG12	8:S:267:HIS:HA	2.00	0.42
8:T:3:ARG:HB3	8:T:4:GLU:H	1.51	0.42
8:V:55:ALA:N	8:V:59:HIS:O	2.49	0.42
8:X:11:GLY:O	8:X:15:ASN:ND2	2.52	0.42
5:E:365:SER:O	5:E:365:SER:OG	3.63	0.42
5:E:411:GLU:HG2	5:E:432:TYR:HE1	1.85	0.42
5:G:186:ALA:HB1	4:H:293:ARG:HA	2.01	0.42
6:K:639:ASN:HB2	8:Y:334:HIS:CE1	2.54	0.42
8:Q:12:GLN:H	8:Q:12:GLN:HG2	1.68	0.42
8:Q:115:HIS:HB3	8:Q:152:TYR:HE2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:5:ILE:HB	8:T:51:PHE:HE1	1.85	0.42
8:T:329:ASP:HA	8:T:330:PRO:HD3	1.91	0.42
8:U:55:ALA:N	8:U:59:HIS:O	2.49	0.42
8:Y:11:GLY:O	8:Y:15:ASN:ND2	2.52	0.42
8:Y:278:THR:HG23	8:Y:371:HIS:ND1	2.34	0.42
8:Z:344:LYS:HA	8:Z:344:LYS:HD3	1.82	0.42
5:C:526:ASP:HA	5:C:529:VAL:HG22	2.02	0.42
4:D:294:LEU:HD23	4:D:294:LEU:HA	1.83	0.42
4:F:305:ARG:HH22	5:G:262:ARG:HD3	1.85	0.42
5:G:578:MET:H	5:G:615:ALA:HB1	1.85	0.42
1:J:291:ASP:N	1:J:291:ASP:OD1	2.51	0.42
6:K:66:VAL:HG13	6:K:68:GLN:H	1.84	0.42
7:L:1530:LEU:HD23	7:L:1530:LEU:HA	1.94	0.42
8:R:213:ILE:HD13	8:R:304:MET:HE3	2.02	0.42
8:S:5:ILE:HB	8:S:51:PHE:HE1	1.85	0.42
8:U:5:ILE:HB	8:U:51:PHE:HE1	1.85	0.42
8:Y:151:SER:HB2	8:Y:194:ARG:HG2	2.01	0.42
5:C:188:ILE:HG21	5:C:275:ARG:HG2	2.03	0.41
5:C:353:GLY:HA3	5:C:440:PRO:HD3	2.02	0.41
5:E:861:PHE:CD2	5:E:862:ASN:HB2	2.55	0.41
4:F:707:LEU:HD22	4:F:851:THR:HG22	2.02	0.41
6:I:565:LEU:O	6:I:569:LEU:HG	2.20	0.41
6:I:568:LEU:O	6:I:572:SER:OG	2.21	0.41
6:K:9:LEU:HD23	6:K:104:LEU:HD22	2.01	0.41
6:K:177:ALA:HB2	6:K:318:PRO:HA	2.02	0.41
8:Q:160:ARG:HD2	8:Q:160:ARG:HA	1.82	0.41
8:R:5:ILE:HB	8:R:51:PHE:HE1	1.85	0.41
8:S:278:THR:HG23	8:S:371:HIS:ND1	2.34	0.41
8:U:151:SER:HB2	8:U:194:ARG:HG2	2.01	0.41
8:Z:115:HIS:HB3	8:Z:152:TYR:HE2	1.85	0.41
8:Z:278:THR:HG23	8:Z:371:HIS:ND1	2.34	0.41
4:F:275:TYR:HE1	4:F:299:TRP:HB2	1.84	0.41
6:K:94:ASP:OD1	6:K:95:SER:N	2.53	0.41
8:S:289:THR:HG23	8:S:291:LEU:HB3	2.03	0.41
8:T:11:GLY:O	8:T:15:ASN:ND2	2.52	0.41
8:T:55:ALA:N	8:T:59:HIS:O	2.49	0.41
8:V:115:HIS:HB3	8:V:152:TYR:HE2	1.85	0.41
8:V:289:THR:HG23	8:V:291:LEU:HB3	2.02	0.41
5:C:557:LEU:HA	8:R:339:ARG:NE	2.35	0.41
4:D:416:GLN:HE22	4:D:420:SER:HB3	1.85	0.41
5:G:499:LEU:HD23	5:G:719:ILE:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:645:MET:HB3	5:G:649:LYS:HZ3	1.85	0.41
5:G:709:LEU:HD22	5:G:729:PHE:CG	2.55	0.41
6:I:132:LEU:HA	6:I:132:LEU:HD23	1.83	0.41
1:J:254:ASP:HA	1:J:256:LEU:HD13	2.01	0.41
1:J:264:LEU:HD13	1:J:301:ILE:HG23	2.02	0.41
8:T:164:LYS:HD3	8:T:164:LYS:HA	1.84	0.41
8:U:289:THR:HG23	8:U:291:LEU:HB3	2.03	0.41
8:W:348:PHE:HB3	8:W:349:ILE:H	1.70	0.41
5:C:858:ARG:HH11	8:Q:358:VAL:HG11	1.85	0.41
6:I:131:LEU:HD22	6:I:167:PRO:HB2	2.02	0.41
6:I:515:TRP:CE2	6:I:517:LEU:HA	2.55	0.41
8:Y:5:ILE:HB	8:Y:51:PHE:HE1	1.85	0.41
5:C:356:LEU:HB2	5:C:440:PRO:HB3	2.02	0.41
5:G:259:LEU:O	5:G:263:ILE:HG12	2.21	0.41
5:G:304:LEU:HA	5:G:307:VAL:HG22	2.03	0.41
4:H:578:MET:HG2	4:H:578:MET:H	1.62	0.41
4:H:675:TYR:HA	4:H:678:THR:HG22	2.03	0.41
8:R:410:LYS:H	8:R:410:LYS:HG2	1.51	0.41
8:S:153:LEU:HD13	8:S:153:LEU:HA	1.82	0.41
8:U:11:GLY:O	8:U:15:ASN:ND2	2.52	0.41
8:X:3:ARG:HB3	8:X:4:GLU:H	1.51	0.41
8:X:115:HIS:HB3	8:X:152:TYR:HE2	1.85	0.41
8:Z:5:ILE:HB	8:Z:51:PHE:HE1	1.85	0.41
5:E:473:LYS:HE3	5:E:487:GLN:HB3	2.03	0.41
4:F:261:ILE:HG13	5:G:262:ARG:HH22	1.85	0.41
4:F:735:TRP:O	4:F:739:GLN:HG2	2.21	0.41
1:J:437:LEU:HD22	1:J:549:VAL:HG11	2.03	0.41
6:K:300:LEU:HB3	6:K:301:LYS:H	1.61	0.41
7:L:1524:ALA:HA	7:L:1527:LEU:HG	2.03	0.41
8:S:160:ARG:HD2	8:S:160:ARG:HA	1.83	0.41
8:W:55:ALA:N	8:W:59:HIS:O	2.49	0.41
8:X:5:ILE:HB	8:X:51:PHE:HE1	1.85	0.41
8:Y:344:LYS:HA	8:Y:344:LYS:HD3	1.82	0.41
4:D:865:LEU:HG	4:D:877:SER:HB2	2.02	0.41
5:E:653:ARG:NH1	5:E:657:SER:HB3	2.36	0.41
7:L:307:ARG:O	7:L:309:GLU:HG3	2.20	0.41
8:R:320:ILE:HG23	8:R:379:ALA:HB2	2.03	0.41
8:W:5:ILE:HB	8:W:51:PHE:HE1	1.85	0.41
8:Y:231:LEU:O	8:Y:234:THR:OG1	2.30	0.41
8:Y:320:ILE:HG23	8:Y:379:ALA:HB2	2.03	0.41
8:Y:410:LYS:H	8:Y:410:LYS:HG2	1.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:337:ARG:O	4:F:340:SER:OG	2.29	0.41
5:G:683:ARG:NH2	8:U:262:PRO:O	2.53	0.41
6:I:131:LEU:O	6:I:135:SER:OG	2.28	0.41
7:L:454:LEU:HD22	7:L:458:THR:HG21	2.02	0.41
7:L:1574:LEU:HD12	7:L:1574:LEU:HA	1.95	0.41
8:R:3:ARG:HB3	8:R:4:GLU:H	1.51	0.41
8:T:320:ILE:HG23	8:T:379:ALA:HB2	2.03	0.41
8:V:5:ILE:HB	8:V:51:PHE:HE1	1.85	0.41
5:C:439:ILE:HD11	5:C:444:GLN:HA	2.03	0.41
5:C:652:GLU:O	5:C:655:LEU:HG	2.21	0.41
4:D:274:CYS:SG	4:D:275:TYR:N	2.92	0.41
4:F:543:LYS:HD2	4:F:543:LYS:HA	1.91	0.41
4:F:754:PHE:O	4:F:758:ILE:HG12	2.21	0.41
5:G:184:ARG:NH1	4:H:273:ASN:OD1	2.53	0.41
4:H:369:VAL:HG13	4:H:370:TRP:CD1	2.56	0.41
4:H:562:MET:HG3	4:H:566:LEU:HD12	2.02	0.41
6:I:148:ILE:HG23	6:I:152:GLN:HB2	2.03	0.41
6:I:568:LEU:HA	6:I:571:GLN:NE2	2.36	0.41
6:I:583:LEU:O	6:I:587:LEU:HG	2.21	0.41
6:K:361:TYR:HB2	6:K:362:LEU:HD12	2.01	0.41
7:L:588:LEU:HA	7:L:588:LEU:HD12	1.85	0.41
7:L:1736:VAL:O	7:L:1740:ARG:HD3	2.21	0.41
8:Q:257:ILE:HD13	8:Q:257:ILE:HA	1.93	0.41
8:Q:320:ILE:HG23	8:Q:379:ALA:HB2	2.03	0.41
8:S:257:ILE:HD13	8:S:257:ILE:HA	1.93	0.41
8:T:3:ARG:HH11	8:T:131:SER:HA	1.86	0.41
8:T:37:VAL:N	8:T:58:GLU:O	2.49	0.41
8:V:320:ILE:HG23	8:V:379:ALA:HB2	2.03	0.41
8:Y:3:ARG:HB3	8:Y:4:GLU:H	1.51	0.41
8:Y:115:HIS:HB3	8:Y:152:TYR:HE2	1.85	0.41
5:C:303:HIS:O	5:C:307:VAL:HG23	2.20	0.41
5:C:381:LYS:HG3	5:C:477:TYR:HB3	2.03	0.41
4:D:368:LEU:HA	4:D:368:LEU:HD13	1.74	0.41
5:E:252:LEU:HD11	5:E:257:ARG:HB3	2.03	0.41
5:E:415:ARG:HD2	5:E:415:ARG:HA	1.92	0.41
5:E:426:LYS:HE2	5:E:428:TRP:CZ3	2.56	0.41
5:E:745:LEU:HD12	5:E:745:LEU:HA	1.96	0.41
5:E:829:PHE:O	5:E:833:LEU:HG	2.21	0.41
6:I:579:VAL:O	6:I:583:LEU:HG	2.21	0.41
6:K:650:ASP:HB3	6:K:651:TYR:CE2	2.55	0.41
7:L:1671:VAL:HG23	7:L:1801:ARG:HH21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:153:LEU:HD13	8:R:153:LEU:HA	1.82	0.41
8:S:220:ILE:HB	8:S:223:PRO:HD2	2.03	0.41
8:T:160:ARG:HD2	8:T:160:ARG:HA	1.82	0.41
8:Y:164:LYS:HA	8:Y:164:LYS:HD3	1.84	0.41
8:Y:192:LEU:HA	8:Y:192:LEU:HD13	1.96	0.41
8:Y:220:ILE:HB	8:Y:223:PRO:HD2	2.03	0.41
8:Z:410:LYS:H	8:Z:410:LYS:HG2	1.51	0.41
4:F:254:ILE:HD12	4:F:257:VAL:HB	2.03	0.40
5:G:168:LYS:HG2	5:G:171:GLY:H	1.85	0.40
4:H:865:LEU:HD21	4:H:873:LEU:O	2.21	0.40
6:I:363:LEU:HD12	6:I:482:LEU:HG	2.03	0.40
1:J:283:LYS:HA	1:J:283:LYS:HD2	1.96	0.40
8:Q:220:ILE:HB	8:Q:223:PRO:HD2	2.03	0.40
8:V:352:GLY:HA2	8:V:353:PRO:HD3	1.94	0.40
5:E:479:LEU:HD12	5:E:479:LEU:HA	1.94	0.40
4:F:338:LEU:O	4:F:342:LEU:HG	2.22	0.40
4:F:878:PHE:HB3	4:F:879:ARG:HE	1.86	0.40
4:H:481:ARG:HD2	4:H:482:LYS:HZ1	1.87	0.40
6:I:305:ASP:OD1	6:I:305:ASP:N	2.55	0.40
1:J:378:GLU:O	1:J:382:ILE:HG12	2.21	0.40
6:K:30:ASP:HA	6:K:34:LEU:HD11	2.03	0.40
6:K:79:GLY:HA2	6:K:83:GLY:HA3	2.04	0.40
8:V:37:VAL:N	8:V:58:GLU:O	2.49	0.40
8:X:220:ILE:HB	8:X:223:PRO:HD2	2.03	0.40
8:X:320:ILE:HG23	8:X:379:ALA:HB2	2.03	0.40
5:C:238:LEU:HD23	5:C:239:ALA:H	1.85	0.40
5:C:408:MET:HG2	5:C:439:ILE:HA	2.03	0.40
4:D:875:PHE:CE1	8:R:334:HIS:HB2	2.56	0.40
5:E:283:PHE:HA	5:E:290:HIS:NE2	2.36	0.40
5:E:635:LEU:HA	5:E:638:TYR:HB2	2.04	0.40
5:E:707:HIS:CG	8:S:330:PRO:HG2	2.56	0.40
4:H:837:LYS:HD2	4:H:837:LYS:HA	1.81	0.40
8:R:220:ILE:HB	8:R:223:PRO:HD2	2.03	0.40
4:D:879:ARG:HH12	4:D:882:PHE:HD2	1.68	0.40
4:F:713:HIS:CG	8:T:353:PRO:HB2	2.57	0.40
5:G:530:HIS:HE1	8:U:3:ARG:HG2	1.87	0.40
4:H:658:SER:O	4:H:662:ARG:HG3	2.21	0.40
6:I:343:LEU:O	6:I:347:GLU:HG3	2.22	0.40
6:I:530:TYR:HE2	8:W:249:MET:HB2	1.87	0.40
1:J:721:GLN:HA	1:J:724:ARG:NE	2.36	0.40
6:K:492:LEU:HD22	6:K:594:CYS:SG	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1778:PHE:HA	7:L:1781:LYS:HE2	2.03	0.40
8:R:295:ARG:HB3	8:R:296:ARG:NH2	2.35	0.40
8:U:115:HIS:HB3	8:U:152:TYR:HE2	1.85	0.40
8:W:289:THR:HG23	8:W:291:LEU:HB3	2.03	0.40
8:X:231:LEU:O	8:X:234:THR:OG1	2.30	0.40
8:X:289:THR:HG23	8:X:291:LEU:HB3	2.03	0.40
8:Y:153:LEU:HD13	8:Y:153:LEU:HA	1.82	0.40
8:Z:289:THR:HG23	8:Z:291:LEU:HB3	2.03	0.40
5:C:289:ASN:HA	5:C:292:LEU:HB2	2.04	0.40
5:G:680:PHE:HA	5:G:683:ARG:HE	1.87	0.40
6:I:108:GLU:H	6:I:108:GLU:HG3	1.69	0.40
6:I:314:LEU:HD13	6:I:314:LEU:HA	1.88	0.40
6:K:342:LYS:HE2	6:K:342:LYS:HB2	1.90	0.40
6:K:500:MET:H	6:K:500:MET:HG3	1.73	0.40
8:Q:289:THR:HG23	8:Q:291:LEU:HB3	2.03	0.40
8:S:3:ARG:HH11	8:S:131:SER:HA	1.87	0.40
8:T:220:ILE:HB	8:T:223:PRO:HD2	2.03	0.40
8:W:320:ILE:HG23	8:W:379:ALA:HB2	2.03	0.40
8:X:160:ARG:HD2	8:X:160:ARG:HH11	1.77	0.40
8:Y:289:THR:HG23	8:Y:291:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	506/1024 (49%)	464 (92%)	38 (8%)	4 (1%)	19 60
1	l	104/1024 (10%)	97 (93%)	5 (5%)	2 (2%)	8 38
2	e	360/375 (96%)	345 (96%)	15 (4%)	0	100 100
3	b	63/82 (77%)	61 (97%)	2 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	d	57/82 (70%)	56 (98%)	1 (2%)	0	100	100
3	i	63/82 (77%)	63 (100%)	0	0	100	100
3	k	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
3	m	63/82 (77%)	63 (100%)	0	0	100	100
4	D	571/907 (63%)	552 (97%)	17 (3%)	2 (0%)	34	72
4	F	591/907 (65%)	561 (95%)	30 (5%)	0	100	100
4	H	584/907 (64%)	557 (95%)	23 (4%)	4 (1%)	22	63
4	a	112/907 (12%)	109 (97%)	3 (3%)	0	100	100
4	h	97/907 (11%)	94 (97%)	3 (3%)	0	100	100
4	j	105/907 (12%)	99 (94%)	6 (6%)	0	100	100
5	C	606/902 (67%)	575 (95%)	28 (5%)	3 (0%)	29	69
5	E	626/902 (69%)	587 (94%)	38 (6%)	1 (0%)	47	81
5	G	628/902 (70%)	596 (95%)	29 (5%)	3 (0%)	29	69
6	I	511/667 (77%)	484 (95%)	25 (5%)	2 (0%)	34	72
6	K	548/667 (82%)	530 (97%)	16 (3%)	2 (0%)	34	72
7	L	540/1819 (30%)	495 (92%)	38 (7%)	7 (1%)	12	48
7	c	148/1819 (8%)	142 (96%)	6 (4%)	0	100	100
8	Q	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	R	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	S	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	T	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	U	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	V	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	W	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	X	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	Y	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
8	Z	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
All	All	11026/20463 (54%)	10451 (95%)	545 (5%)	30 (0%)	44	77

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	121	PRO

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Mol	Chain	Res	Type
5	C	465	HIS
5	G	581	ASP
4	H	454	VAL
4	H	632	ASP
6	I	601	LEU
1	J	236	LEU
6	K	29	GLN
6	K	409	ASN
7	L	308	GLU
5	G	582	LEU
5	G	675	TRP
4	H	631	GLY
4	H	633	THR
6	I	600	ASN
4	D	628	VAL
4	D	889	ARG
5	E	581	ASP
1	l	120	SER
1	J	257	TYR
1	J	946	LYS
7	L	307	ARG
7	L	309	GLU
5	C	861	PHE
1	J	945	GLU
7	L	314	GLU
7	L	495	PHE
7	L	1760	PRO
7	L	310	PRO
5	C	240	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	J	498/933 (53%)	493 (99%)	5 (1%)	76 86
1	l	84/933 (9%)	82 (98%)	2 (2%)	49 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	e	310/318 (98%)	306 (99%)	4 (1%)	69 81
3	b	53/62 (86%)	52 (98%)	1 (2%)	57 75
3	d	53/62 (86%)	53 (100%)	0	100 100
3	i	53/62 (86%)	52 (98%)	1 (2%)	57 75
3	k	53/62 (86%)	51 (96%)	2 (4%)	33 57
3	m	53/62 (86%)	53 (100%)	0	100 100
4	D	525/798 (66%)	520 (99%)	5 (1%)	76 86
4	F	542/798 (68%)	538 (99%)	4 (1%)	84 90
4	H	539/798 (68%)	537 (100%)	2 (0%)	91 94
4	a	101/798 (13%)	99 (98%)	2 (2%)	55 74
4	h	88/798 (11%)	88 (100%)	0	100 100
4	j	88/798 (11%)	88 (100%)	0	100 100
5	C	556/791 (70%)	553 (100%)	3 (0%)	88 93
5	E	574/791 (73%)	573 (100%)	1 (0%)	93 96
5	G	572/791 (72%)	568 (99%)	4 (1%)	84 90
6	I	472/594 (80%)	467 (99%)	5 (1%)	73 84
6	K	509/594 (86%)	505 (99%)	4 (1%)	81 89
7	L	501/1546 (32%)	499 (100%)	2 (0%)	91 94
7	c	135/1546 (9%)	134 (99%)	1 (1%)	84 90
8	Q	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	R	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	S	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	T	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	U	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	V	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	W	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	X	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	Y	376/400 (94%)	329 (88%)	47 (12%)	4 19
8	Z	376/400 (94%)	329 (88%)	47 (12%)	4 19
All	All	10119/17935 (56%)	9601 (95%)	518 (5%)	27 48

All (518) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	l	63	LYS
1	l	85	LYS
2	e	152	VAL
2	e	162	THR
2	e	165	ILE
2	e	291	LYS
3	b	37	THR
4	a	50	ASP
4	a	52	PHE
5	C	497	LYS
5	C	514	ARG
5	C	526	ASP
4	D	267	LYS
4	D	392	LYS
4	D	626	LEU
4	D	627	GLU
4	D	628	VAL
5	E	649	LYS
4	F	285	ARG
4	F	426	VAL
4	F	620	ARG
4	F	622	ASP
5	G	190	ASP
5	G	310	LEU
5	G	517	LYS
5	G	641	LEU
4	H	628	VAL
4	H	671	LYS
6	I	315	LYS
6	I	492	LEU
6	I	506	LYS
6	I	507	SER
6	I	508	ASN
1	J	220	VAL
1	J	369	TYR
1	J	463	SER
1	J	473	LEU
1	J	809	VAL
6	K	1	MET
6	K	35	HIS
6	K	402	LYS
6	K	500	MET
7	L	425	LYS

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Mol	Chain	Res	Type
7	L	1493	LYS
3	i	65	LYS
8	Q	17	ILE
8	Q	24	GLN
8	Q	31	ILE
8	Q	50	VAL
8	Q	66	LEU
8	Q	76	SER
8	Q	78	LEU
8	Q	85	LEU
8	Q	112	GLU
8	Q	127	ASP
8	Q	131	SER
8	Q	140	SER
8	Q	153	LEU
8	Q	154	LEU
8	Q	157	LEU
8	Q	165	LEU
8	Q	166	VAL
8	Q	188	SER
8	Q	192	LEU
8	Q	195	LEU
8	Q	205	LEU
8	Q	206	ASP
8	Q	208	THR
8	Q	217	ARG
8	Q	222	ASN
8	Q	233	SER
8	Q	259	SER
8	Q	265	ARG
8	Q	276	LEU
8	Q	288	THR
8	Q	290	VAL
8	Q	293	VAL
8	Q	294	MET
8	Q	296	ARG
8	Q	304	MET
8	Q	316	CYS
8	Q	333	VAL
8	Q	339	ARG
8	Q	341	ARG
8	Q	347	ASN

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Mol	Chain	Res	Type
8	Q	362	ARG
8	Q	369	SER
8	Q	373	VAL
8	Q	380	ASN
8	Q	385	SER
8	Q	392	CYS
8	Q	410	LYS
8	R	17	ILE
8	R	24	GLN
8	R	31	ILE
8	R	50	VAL
8	R	66	LEU
8	R	76	SER
8	R	78	LEU
8	R	85	LEU
8	R	112	GLU
8	R	127	ASP
8	R	131	SER
8	R	140	SER
8	R	153	LEU
8	R	154	LEU
8	R	157	LEU
8	R	165	LEU
8	R	166	VAL
8	R	188	SER
8	R	192	LEU
8	R	195	LEU
8	R	205	LEU
8	R	206	ASP
8	R	208	THR
8	R	217	ARG
8	R	222	ASN
8	R	233	SER
8	R	259	SER
8	R	265	ARG
8	R	276	LEU
8	R	288	THR
8	R	290	VAL
8	R	293	VAL
8	R	294	MET
8	R	296	ARG
8	R	304	MET

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Mol	Chain	Res	Type
8	R	316	CYS
8	R	333	VAL
8	R	339	ARG
8	R	341	ARG
8	R	347	ASN
8	R	362	ARG
8	R	369	SER
8	R	373	VAL
8	R	380	ASN
8	R	385	SER
8	R	392	CYS
8	R	410	LYS
8	S	17	ILE
8	S	24	GLN
8	S	31	ILE
8	S	50	VAL
8	S	66	LEU
8	S	76	SER
8	S	78	LEU
8	S	85	LEU
8	S	112	GLU
8	S	127	ASP
8	S	131	SER
8	S	140	SER
8	S	153	LEU
8	S	154	LEU
8	S	157	LEU
8	S	165	LEU
8	S	166	VAL
8	S	188	SER
8	S	192	LEU
8	S	195	LEU
8	S	205	LEU
8	S	206	ASP
8	S	208	THR
8	S	217	ARG
8	S	222	ASN
8	S	233	SER
8	S	259	SER
8	S	265	ARG
8	S	276	LEU
8	S	288	THR

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Mol	Chain	Res	Type
8	S	290	VAL
8	S	293	VAL
8	S	294	MET
8	S	296	ARG
8	S	304	MET
8	S	316	CYS
8	S	333	VAL
8	S	339	ARG
8	S	341	ARG
8	S	347	ASN
8	S	362	ARG
8	S	369	SER
8	S	373	VAL
8	S	380	ASN
8	S	385	SER
8	S	392	CYS
8	S	410	LYS
8	T	17	ILE
8	T	24	GLN
8	T	31	ILE
8	T	50	VAL
8	T	66	LEU
8	T	76	SER
8	T	78	LEU
8	T	85	LEU
8	T	112	GLU
8	T	127	ASP
8	T	131	SER
8	T	140	SER
8	T	153	LEU
8	T	154	LEU
8	T	157	LEU
8	T	165	LEU
8	T	166	VAL
8	T	188	SER
8	T	192	LEU
8	T	195	LEU
8	T	205	LEU
8	T	206	ASP
8	T	208	THR
8	T	217	ARG
8	T	222	ASN

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Mol	Chain	Res	Type
8	T	233	SER
8	T	259	SER
8	T	265	ARG
8	T	276	LEU
8	T	288	THR
8	T	290	VAL
8	T	293	VAL
8	T	294	MET
8	T	296	ARG
8	T	304	MET
8	T	316	CYS
8	T	333	VAL
8	T	339	ARG
8	T	341	ARG
8	T	347	ASN
8	T	362	ARG
8	T	369	SER
8	T	373	VAL
8	T	380	ASN
8	T	385	SER
8	T	392	CYS
8	T	410	LYS
8	U	17	ILE
8	U	24	GLN
8	U	31	ILE
8	U	50	VAL
8	U	66	LEU
8	U	76	SER
8	U	78	LEU
8	U	85	LEU
8	U	112	GLU
8	U	127	ASP
8	U	131	SER
8	U	140	SER
8	U	153	LEU
8	U	154	LEU
8	U	157	LEU
8	U	165	LEU
8	U	166	VAL
8	U	188	SER
8	U	192	LEU
8	U	195	LEU

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Mol	Chain	Res	Type
8	U	205	LEU
8	U	206	ASP
8	U	208	THR
8	U	217	ARG
8	U	222	ASN
8	U	233	SER
8	U	259	SER
8	U	265	ARG
8	U	276	LEU
8	U	288	THR
8	U	290	VAL
8	U	293	VAL
8	U	294	MET
8	U	296	ARG
8	U	304	MET
8	U	316	CYS
8	U	333	VAL
8	U	339	ARG
8	U	341	ARG
8	U	347	ASN
8	U	362	ARG
8	U	369	SER
8	U	373	VAL
8	U	380	ASN
8	U	385	SER
8	U	392	CYS
8	U	410	LYS
8	V	17	ILE
8	V	24	GLN
8	V	31	ILE
8	V	50	VAL
8	V	66	LEU
8	V	76	SER
8	V	78	LEU
8	V	85	LEU
8	V	112	GLU
8	V	127	ASP
8	V	131	SER
8	V	140	SER
8	V	153	LEU
8	V	154	LEU
8	V	157	LEU

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Mol	Chain	Res	Type
8	V	165	LEU
8	V	166	VAL
8	V	188	SER
8	V	192	LEU
8	V	195	LEU
8	V	205	LEU
8	V	206	ASP
8	V	208	THR
8	V	217	ARG
8	V	222	ASN
8	V	233	SER
8	V	259	SER
8	V	265	ARG
8	V	276	LEU
8	V	288	THR
8	V	290	VAL
8	V	293	VAL
8	V	294	MET
8	V	296	ARG
8	V	304	MET
8	V	316	CYS
8	V	333	VAL
8	V	339	ARG
8	V	341	ARG
8	V	347	ASN
8	V	362	ARG
8	V	369	SER
8	V	373	VAL
8	V	380	ASN
8	V	385	SER
8	V	392	CYS
8	V	410	LYS
8	W	17	ILE
8	W	24	GLN
8	W	31	ILE
8	W	50	VAL
8	W	66	LEU
8	W	76	SER
8	W	78	LEU
8	W	85	LEU
8	W	112	GLU
8	W	127	ASP

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Mol	Chain	Res	Type
8	W	131	SER
8	W	140	SER
8	W	153	LEU
8	W	154	LEU
8	W	157	LEU
8	W	165	LEU
8	W	166	VAL
8	W	188	SER
8	W	192	LEU
8	W	195	LEU
8	W	205	LEU
8	W	206	ASP
8	W	208	THR
8	W	217	ARG
8	W	222	ASN
8	W	233	SER
8	W	259	SER
8	W	265	ARG
8	W	276	LEU
8	W	288	THR
8	W	290	VAL
8	W	293	VAL
8	W	294	MET
8	W	296	ARG
8	W	304	MET
8	W	316	CYS
8	W	333	VAL
8	W	339	ARG
8	W	341	ARG
8	W	347	ASN
8	W	362	ARG
8	W	369	SER
8	W	373	VAL
8	W	380	ASN
8	W	385	SER
8	W	392	CYS
8	W	410	LYS
8	X	17	ILE
8	X	24	GLN
8	X	31	ILE
8	X	50	VAL
8	X	66	LEU

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Mol	Chain	Res	Type
8	X	76	SER
8	X	78	LEU
8	X	85	LEU
8	X	112	GLU
8	X	127	ASP
8	X	131	SER
8	X	140	SER
8	X	153	LEU
8	X	154	LEU
8	X	157	LEU
8	X	165	LEU
8	X	166	VAL
8	X	188	SER
8	X	192	LEU
8	X	195	LEU
8	X	205	LEU
8	X	206	ASP
8	X	208	THR
8	X	217	ARG
8	X	222	ASN
8	X	233	SER
8	X	259	SER
8	X	265	ARG
8	X	276	LEU
8	X	288	THR
8	X	290	VAL
8	X	293	VAL
8	X	294	MET
8	X	296	ARG
8	X	304	MET
8	X	316	CYS
8	X	333	VAL
8	X	339	ARG
8	X	341	ARG
8	X	347	ASN
8	X	362	ARG
8	X	369	SER
8	X	373	VAL
8	X	380	ASN
8	X	385	SER
8	X	392	CYS
8	X	410	LYS

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Mol	Chain	Res	Type
8	Y	17	ILE
8	Y	24	GLN
8	Y	31	ILE
8	Y	50	VAL
8	Y	66	LEU
8	Y	76	SER
8	Y	78	LEU
8	Y	85	LEU
8	Y	112	GLU
8	Y	127	ASP
8	Y	131	SER
8	Y	140	SER
8	Y	153	LEU
8	Y	154	LEU
8	Y	157	LEU
8	Y	165	LEU
8	Y	166	VAL
8	Y	188	SER
8	Y	192	LEU
8	Y	195	LEU
8	Y	205	LEU
8	Y	206	ASP
8	Y	208	THR
8	Y	217	ARG
8	Y	222	ASN
8	Y	233	SER
8	Y	259	SER
8	Y	265	ARG
8	Y	276	LEU
8	Y	288	THR
8	Y	290	VAL
8	Y	293	VAL
8	Y	294	MET
8	Y	296	ARG
8	Y	304	MET
8	Y	316	CYS
8	Y	333	VAL
8	Y	339	ARG
8	Y	341	ARG
8	Y	347	ASN
8	Y	362	ARG
8	Y	369	SER

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Mol	Chain	Res	Type
8	Y	373	VAL
8	Y	380	ASN
8	Y	385	SER
8	Y	392	CYS
8	Y	410	LYS
8	Z	17	ILE
8	Z	24	GLN
8	Z	31	ILE
8	Z	50	VAL
8	Z	66	LEU
8	Z	76	SER
8	Z	78	LEU
8	Z	85	LEU
8	Z	112	GLU
8	Z	127	ASP
8	Z	131	SER
8	Z	140	SER
8	Z	153	LEU
8	Z	154	LEU
8	Z	157	LEU
8	Z	165	LEU
8	Z	166	VAL
8	Z	188	SER
8	Z	192	LEU
8	Z	195	LEU
8	Z	205	LEU
8	Z	206	ASP
8	Z	208	THR
8	Z	217	ARG
8	Z	222	ASN
8	Z	233	SER
8	Z	259	SER
8	Z	265	ARG
8	Z	276	LEU
8	Z	288	THR
8	Z	290	VAL
8	Z	293	VAL
8	Z	294	MET
8	Z	296	ARG
8	Z	304	MET
8	Z	316	CYS
8	Z	333	VAL

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Mol	Chain	Res	Type
8	Z	339	ARG
8	Z	341	ARG
8	Z	347	ASN
8	Z	362	ARG
8	Z	369	SER
8	Z	373	VAL
8	Z	380	ASN
8	Z	385	SER
8	Z	392	CYS
8	Z	410	LYS
3	k	39	LEU
3	k	63	VAL
7	c	34	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such sidechains are listed below:

Mol	Chain	Res	Type
2	e	263	GLN
4	a	82	HIS
4	a	120	GLN
5	C	169	ASN
5	C	172	GLN
5	C	312	GLN
5	C	493	ASN
5	C	524	GLN
5	C	644	HIS
5	C	823	ASN
4	D	269	ASN
4	D	416	GLN
4	D	560	GLN
4	D	609	ASN
4	D	705	HIS
4	D	773	ASN
4	D	801	GLN
5	E	261	HIS
5	E	420	GLN
5	E	430	GLN
5	E	458	ASN
5	E	654	GLN
5	E	662	ASN
5	E	691	GLN
5	E	741	ASN

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Mol	Chain	Res	Type
4	F	343	HIS
4	F	558	HIS
4	F	684	HIS
4	F	705	HIS
4	F	719	GLN
4	F	773	ASN
4	F	774	GLN
4	F	801	GLN
4	F	852	HIS
4	F	860	GLN
5	G	287	GLN
5	G	312	GLN
5	G	444	GLN
5	G	512	HIS
5	G	585	GLN
5	G	631	ASN
5	G	688	ASN
5	G	694	GLN
5	G	707	HIS
5	G	767	GLN
4	H	401	HIS
4	H	461	HIS
4	H	550	ASN
4	H	703	GLN
4	H	713	HIS
4	H	801	GLN
4	H	883	ASN
6	I	43	ASN
6	I	102	GLN
6	I	109	GLN
6	I	116	HIS
6	I	130	GLN
6	I	142	GLN
6	I	378	HIS
6	I	397	GLN
6	I	504	HIS
6	I	571	GLN
6	I	622	GLN
1	J	237	HIS
1	J	642	HIS
1	J	892	HIS
6	K	26	GLN

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Mol	Chain	Res	Type
6	K	35	HIS
6	K	61	GLN
6	K	78	GLN
6	K	142	GLN
6	K	160	HIS
6	K	377	GLN
6	K	409	ASN
6	K	489	GLN
6	K	501	GLN
6	K	529	GLN
6	K	543	GLN
6	K	591	HIS
6	K	657	GLN
7	L	517	HIS
7	L	603	ASN
7	L	1514	HIS
7	L	1625	GLN
7	L	1770	ASN
7	L	1803	ASN
8	Q	24	GLN
8	Q	167	GLN
8	Q	187	ASN
8	Q	299	GLN
8	Q	322	ASN
8	R	24	GLN
8	R	167	GLN
8	R	187	ASN
8	R	299	GLN
8	R	322	ASN
8	S	24	GLN
8	S	167	GLN
8	S	187	ASN
8	S	299	GLN
8	S	322	ASN
8	T	24	GLN
8	T	167	GLN
8	T	187	ASN
8	T	299	GLN
8	T	322	ASN
8	U	24	GLN
8	U	167	GLN
8	U	187	ASN

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Mol	Chain	Res	Type
8	U	299	GLN
8	U	322	ASN
8	V	24	GLN
8	V	167	GLN
8	V	187	ASN
8	V	299	GLN
8	V	322	ASN
8	W	24	GLN
8	W	167	GLN
8	W	187	ASN
8	W	299	GLN
8	W	322	ASN
8	X	24	GLN
8	X	167	GLN
8	X	187	ASN
8	X	251	ASN
8	X	299	GLN
8	X	322	ASN
8	Y	24	GLN
8	Y	167	GLN
8	Y	187	ASN
8	Y	299	GLN
8	Y	322	ASN
8	Z	24	GLN
8	Z	167	GLN
8	Z	187	ASN
8	Z	299	GLN
8	Z	322	ASN
8	Z	357	GLN
3	d	19	ASN
7	c	43	ASN
7	c	48	ASN
7	c	116	GLN
7	c	161	GLN
4	j	78	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

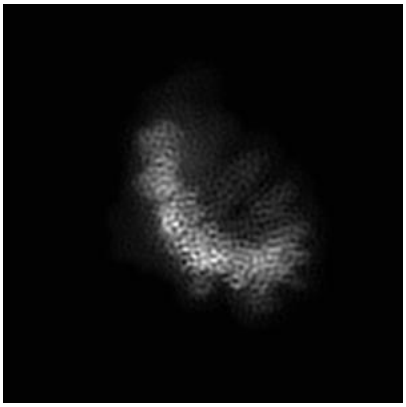
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14014. These allow visual inspection of the internal detail of the map and identification of artifacts.

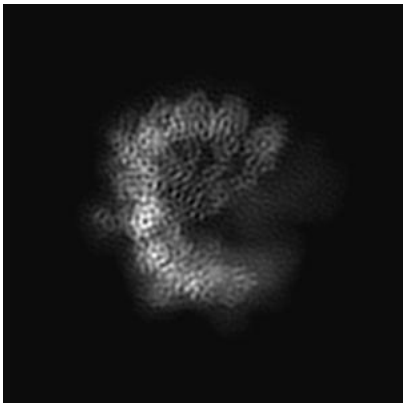
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

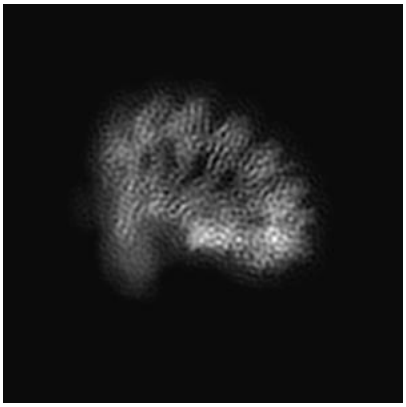
6.1.1 Primary map



X



Y



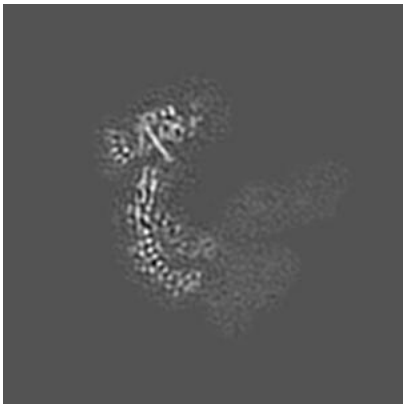
Z

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

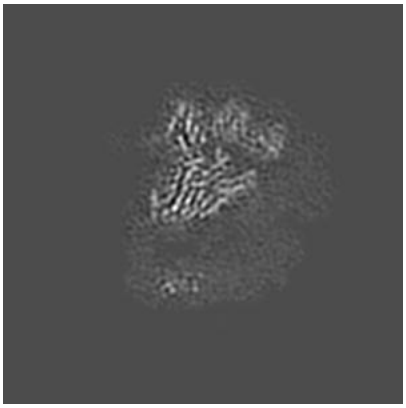
Z Index: 100

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

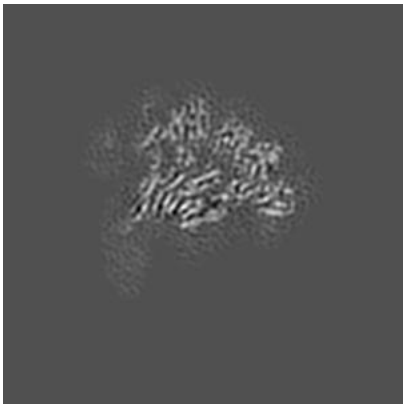
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 134



Y Index: 84



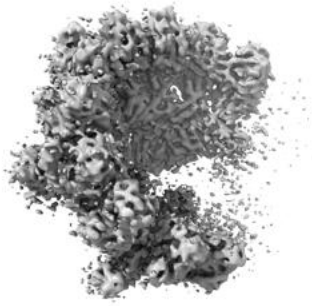
Z Index: 72

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 0.0299. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

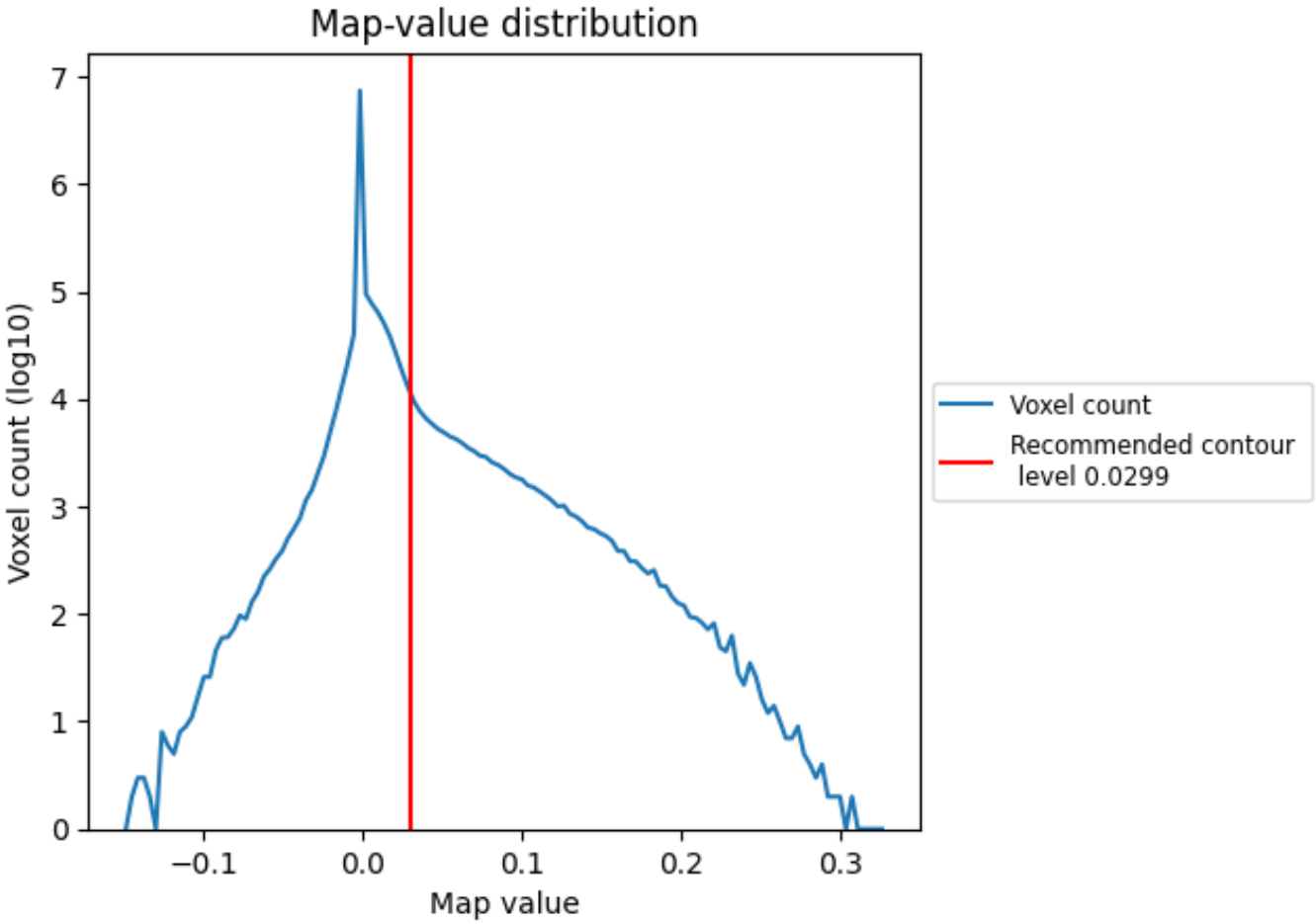
6.5 Mask visualisation (i)

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

7 Map analysis

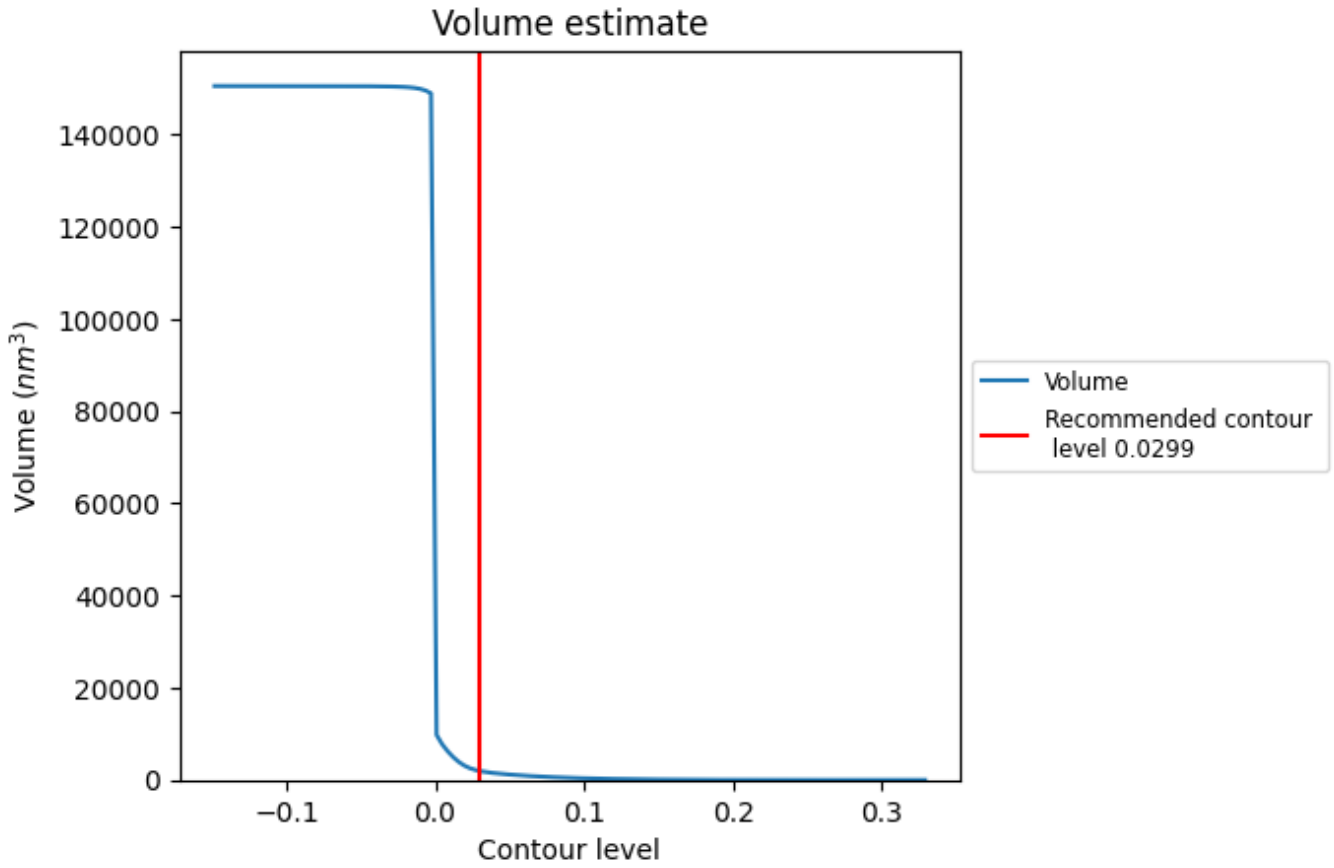
This section contains the results of statistical analysis of the map.

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.

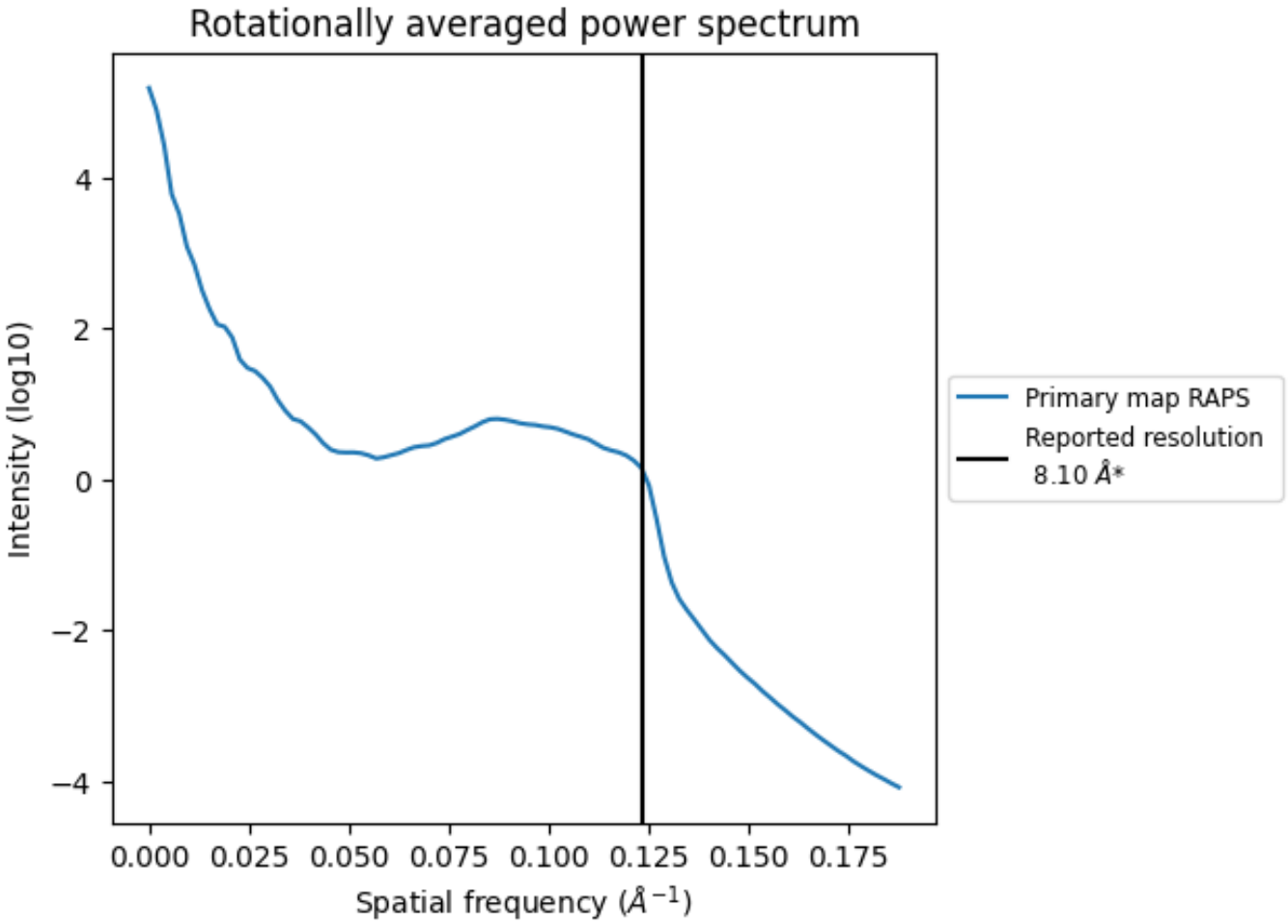
7.2 Volume estimate



The volume at the recommended contour level is 1956 nm^3; this corresponds to an approximate mass of 1767 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 0.123 Å^{-1}

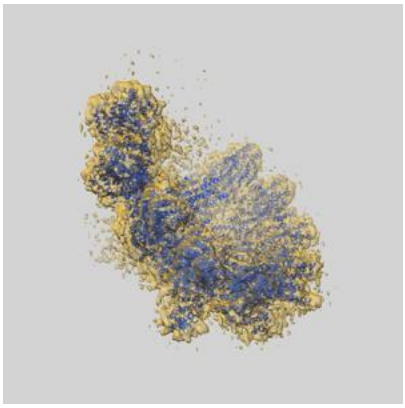
8 Fourier-Shell correlation (i)

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

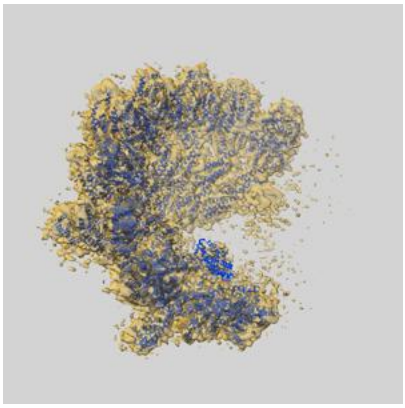
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14014 and PDB model 7QJ9. Per-residue inclusion information can be found in section 3 on page 7.

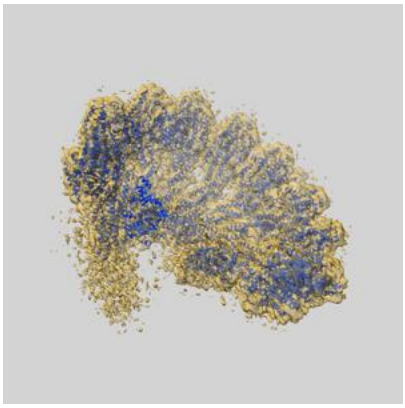
9.1 Map-model overlay



X



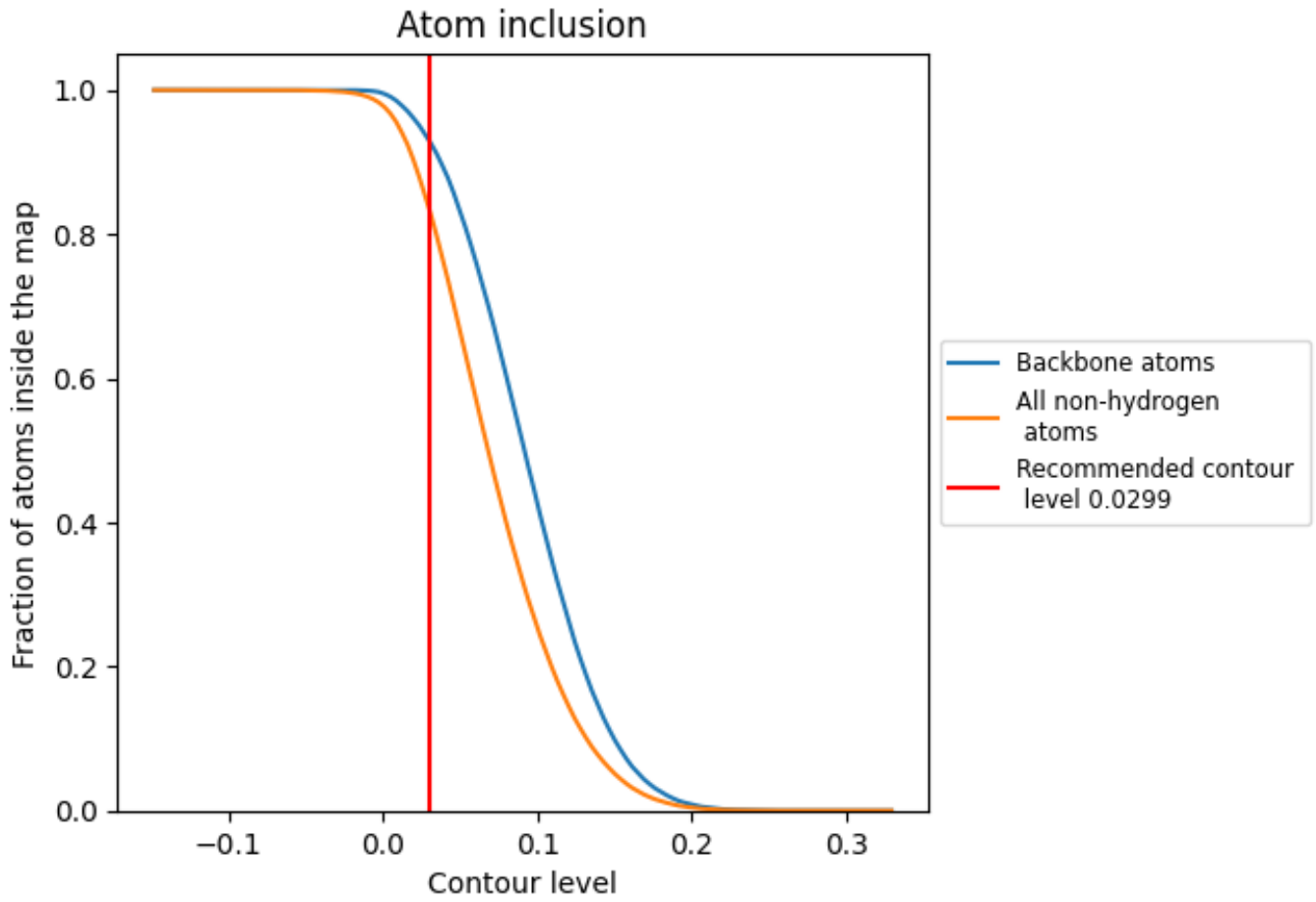
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0299 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, 93% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.