Full wwPDB EM Validation Report

Jan 29, 2022 – 06:16 am GMT

PDB ID	:	7QJ7
EMDB ID	:	EMD-14012
Title	:	Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 1-12 substoichiometric spokes 13-14)
Authors	:	Zupa, E.; Pfeffer, S.
Deposited on	:	2021-12-16
Resolution	:	8.70 Å(reported)
Based on initial models	:	7AS4, 6V6S, 6X0U, 6L81

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:

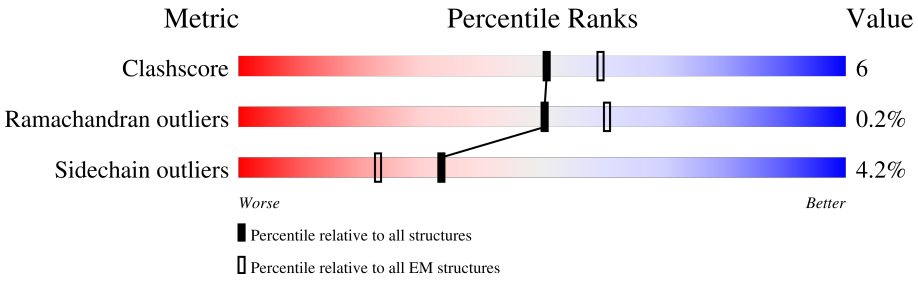
EMDB validation analysis	:	0.0.0.dev97
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 8.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	J	1024	46% 5% 48%
1	l	1024	10% 89%
2	e	375	30% 95%
3	A	902	62% 6% 32%
3	C	902	62% 7% 31%
3	E	902	63% 8% 29%
3	G	902	65% 6% 29%
4	B	907	58% 9% 33%

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Mol	Chain	Length	Quality of chain
4	D	907	56% 8% 36%
4	F	907	58% 7% 34%
4	H	907	59% 6% 35%
4	a	907	13% 87%
4	f	907	11% 89%
4	h	907	11% 89%
4	j	907	12% 88%
5	b	82	77% 21%
5	d	82	5% 72% 28%
5	g	82	13% 79% 21%
5	i	82	13% 79% 21%
5	k	82	6% 79% 21%
5	m	82	79% 21%
6	I	667	70% 7% 22%
6	K	667	72% 11% 16%
7	L	1819	28% 69%
7	c	1819	9% 91%
8	O	451	63% 27% 7%
8	P	451	62% 27% 7%
8	Q	451	5% 63% 26% 7%
8	R	451	62% 27% 7%
8	S	451	64% 26% 7%
8	T	451	62% 27% 7%
8	U	451	63% 26% 7%
8	V	451	63% 26% 7%

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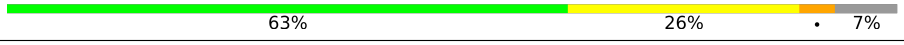
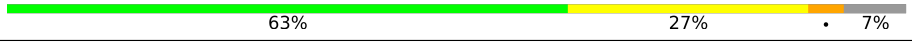
Mol	Chain	Length	Quality of chain
8	W	451	
8	X	451	
8	Y	451	
8	Z	451	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 109579 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 Gamma-tubulin complex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	613	Total	C	N	O	S	0	0
			4978	3212	831	903	32		
3	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
3	G	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		
3	E	640	Total	C	N	O	S	0	0
			5206	3354	875	944	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	610	Total	C	N	O	S	0	0
			5029	3203	888	913	25		
4	D	581	Total	C	N	O	S	0	0
			4796	3061	842	868	25		
4	F	599	Total	C	N	O	S	0	0
			4941	3151	871	894	25		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
4	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
4	f	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
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 Mitotic-spindle organizing protein 1.

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

- 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	O	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	P	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	Q	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	R	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	S	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	T	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	U	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	V	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	W	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	X	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	Y	420	Total 3373	C 2134	N 586	O 638	S 15	0	0
8	Z	420	Total 3373	C 2134	N 586	O 638	S 15	0	0

- Molecule 9 is water.

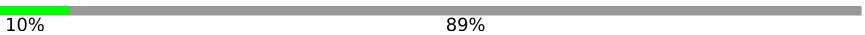
Mol	Chain	Residues	Atoms		AltConf
9	l	6	Total 6	O 6	0

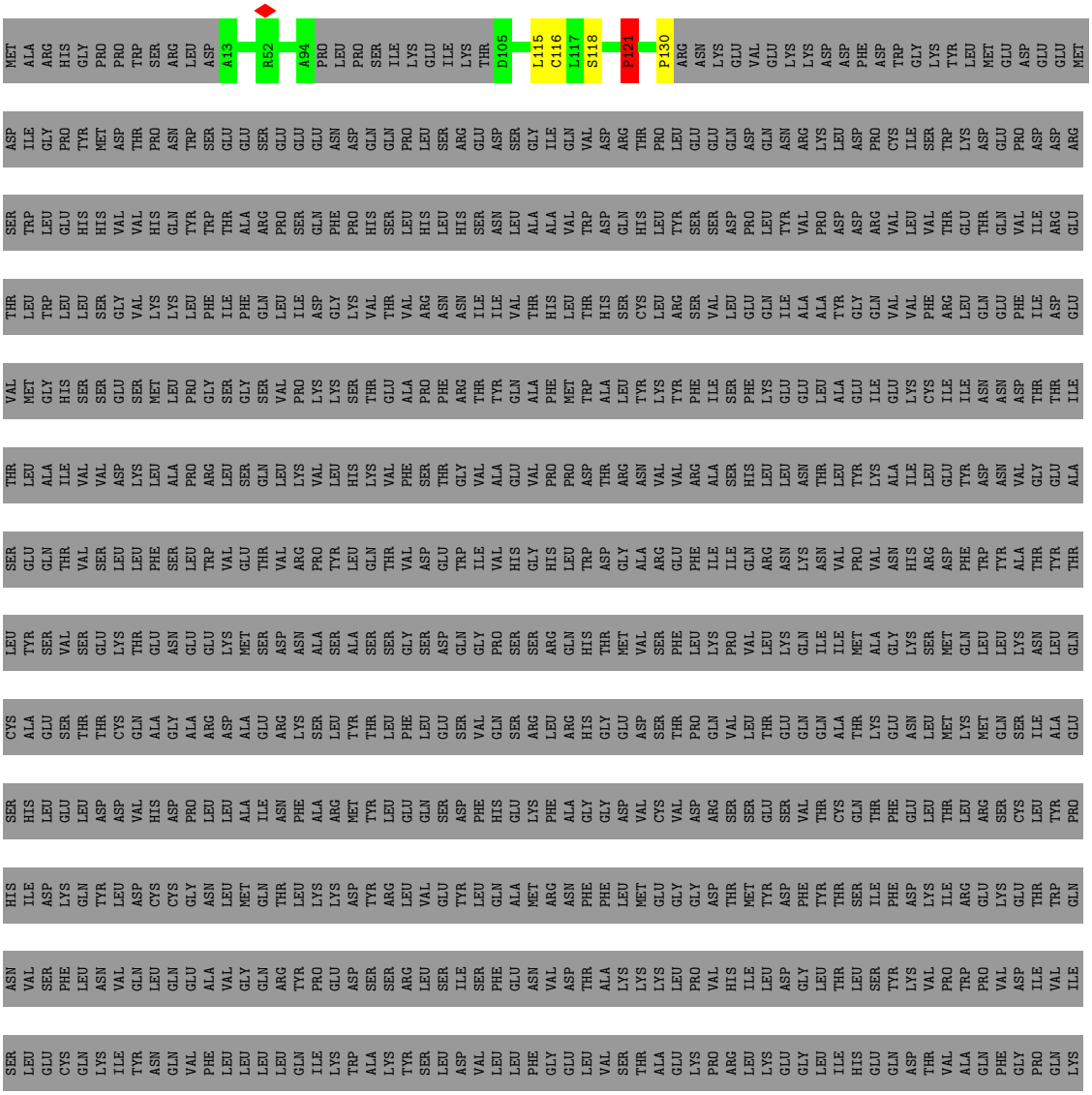
3 Residue-property plots (i)

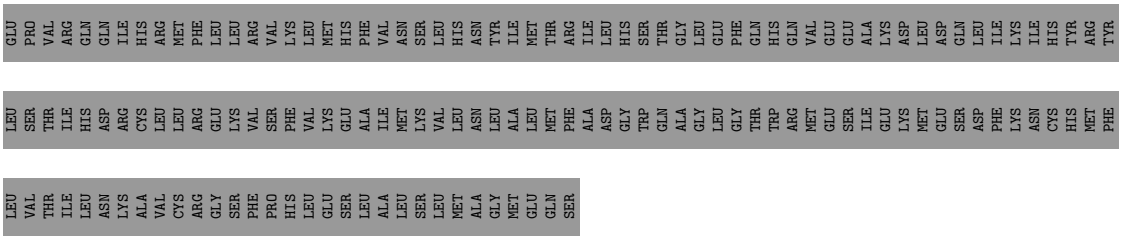
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Gamma-tubulin complex component 5

Chain l:

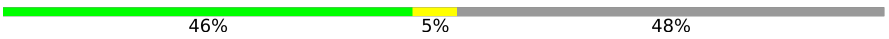


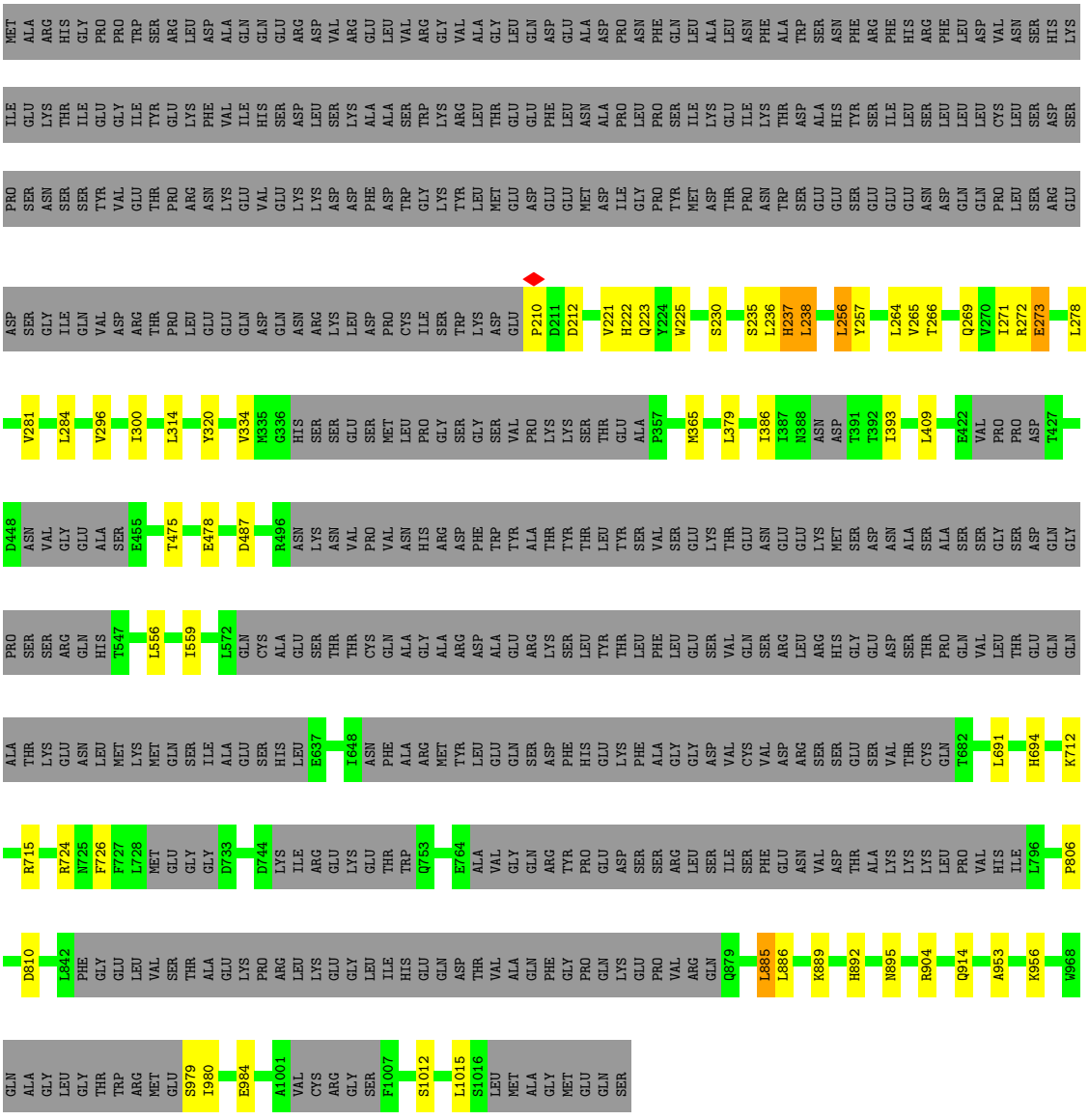




• Molecule 1: Gamma-tubulin complex component 5

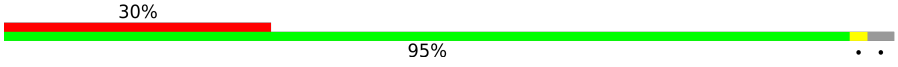
Chain J:

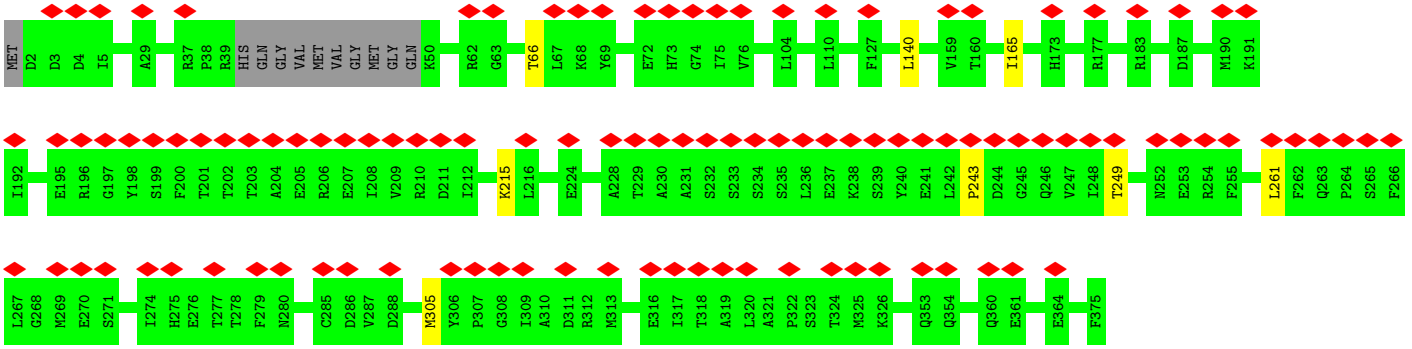




• Molecule 2: actin, cytoplasmic 1

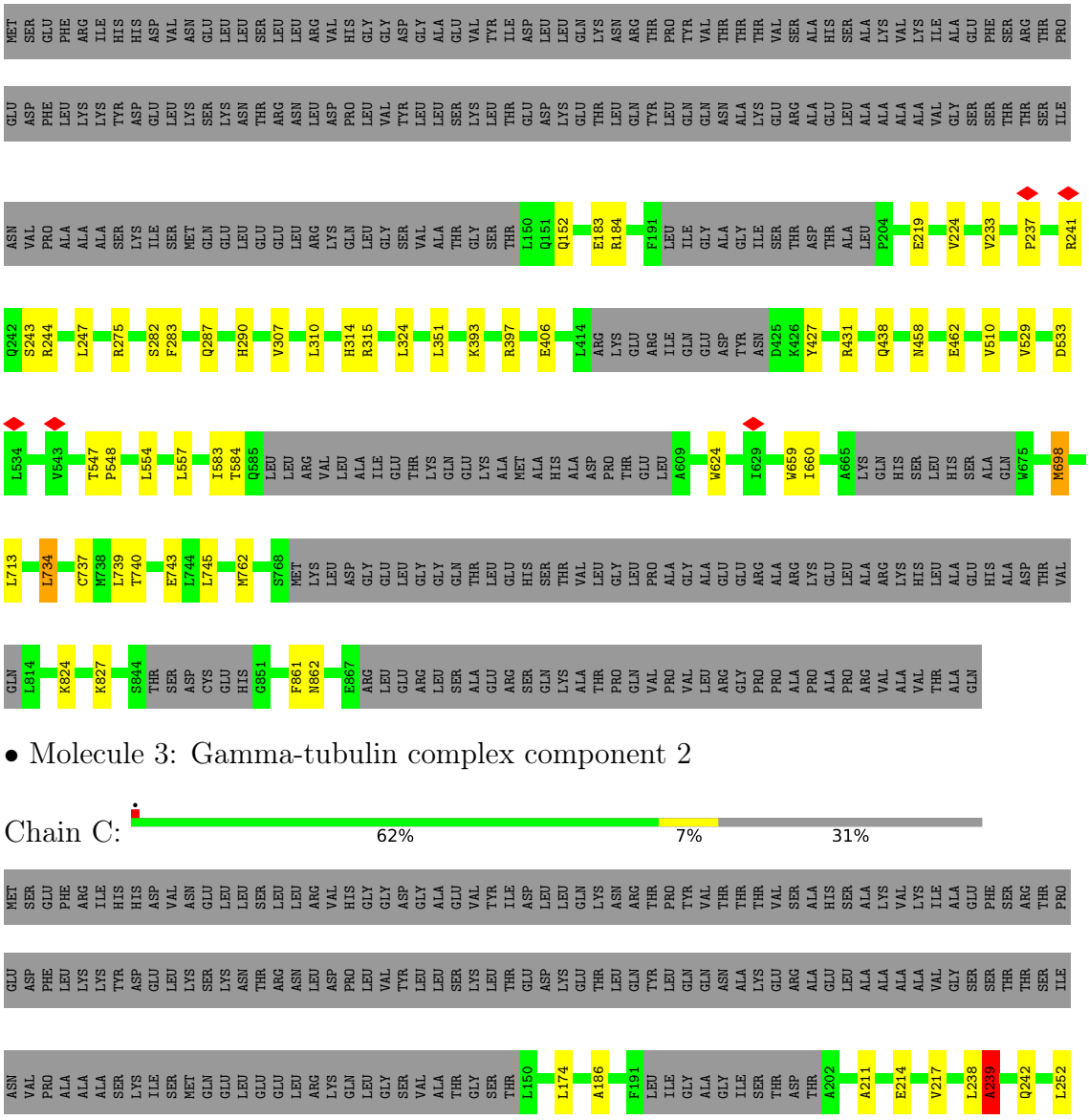
Chain e:





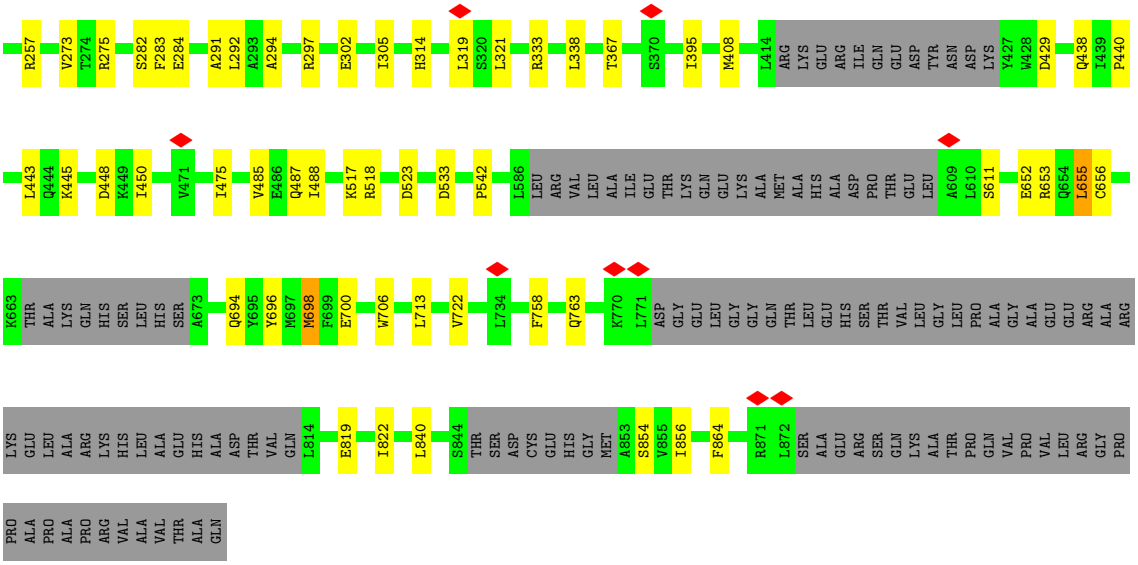
• Molecule 3: Gamma-tubulin complex component 2

Chain A:



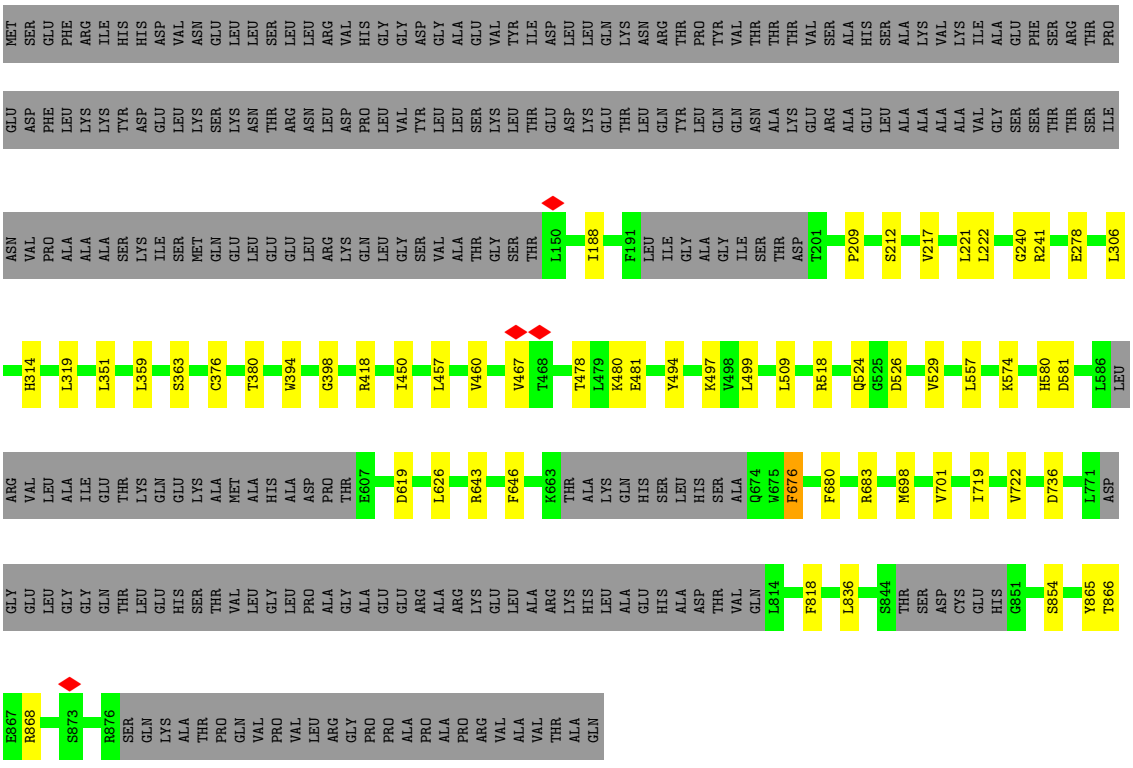
• Molecule 3: Gamma-tubulin complex component 2

Chain C:



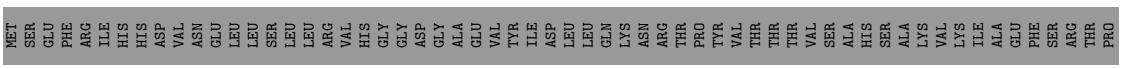
• Molecule 3: Gamma-tubulin complex component 2

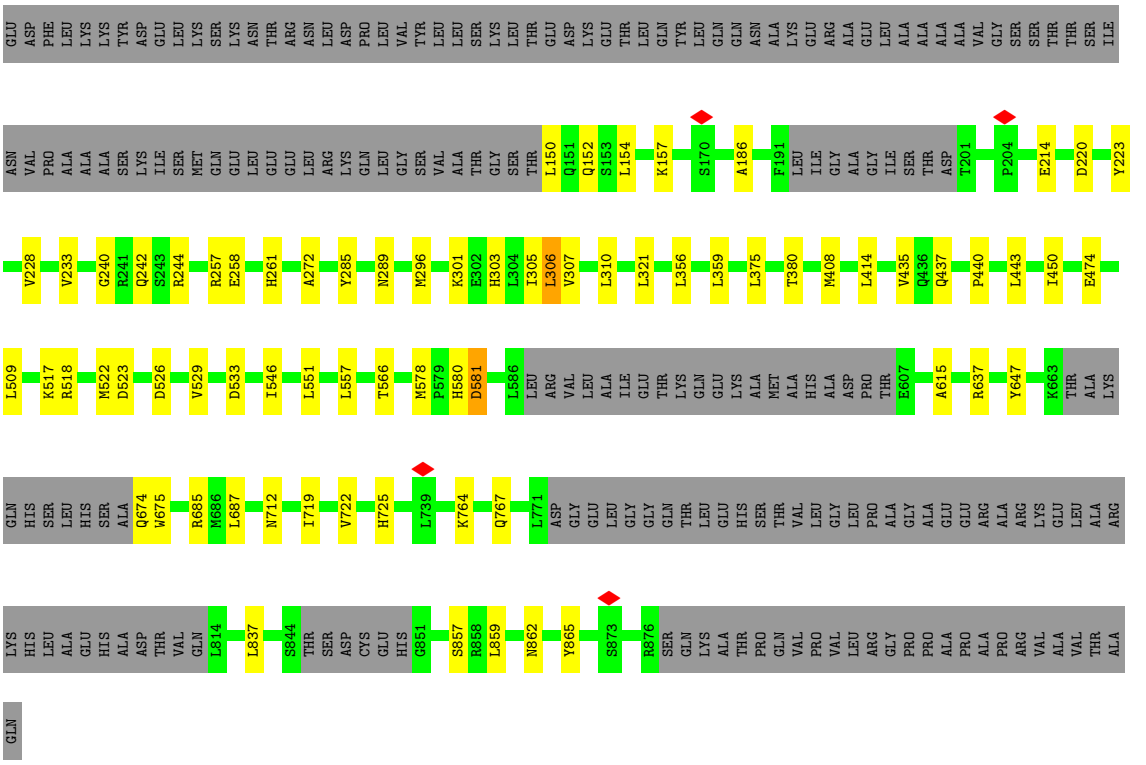
Chain G:



• Molecule 3: Gamma-tubulin complex component 2

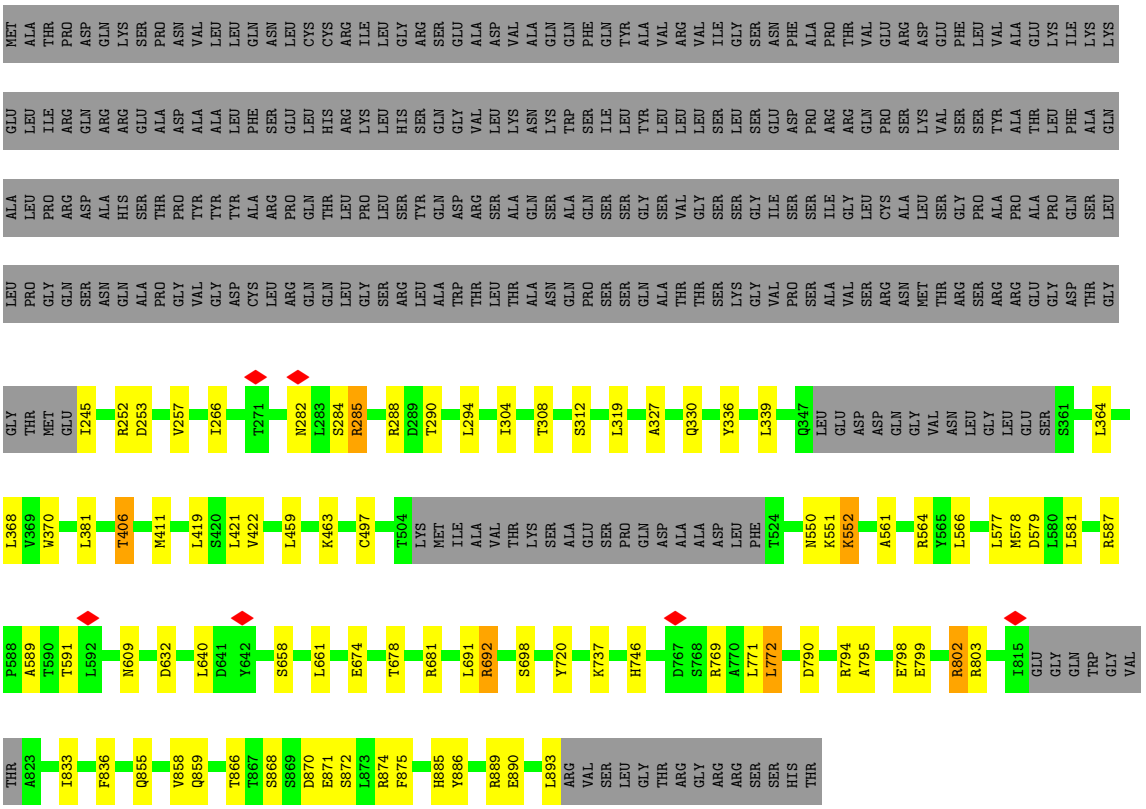
Chain E:





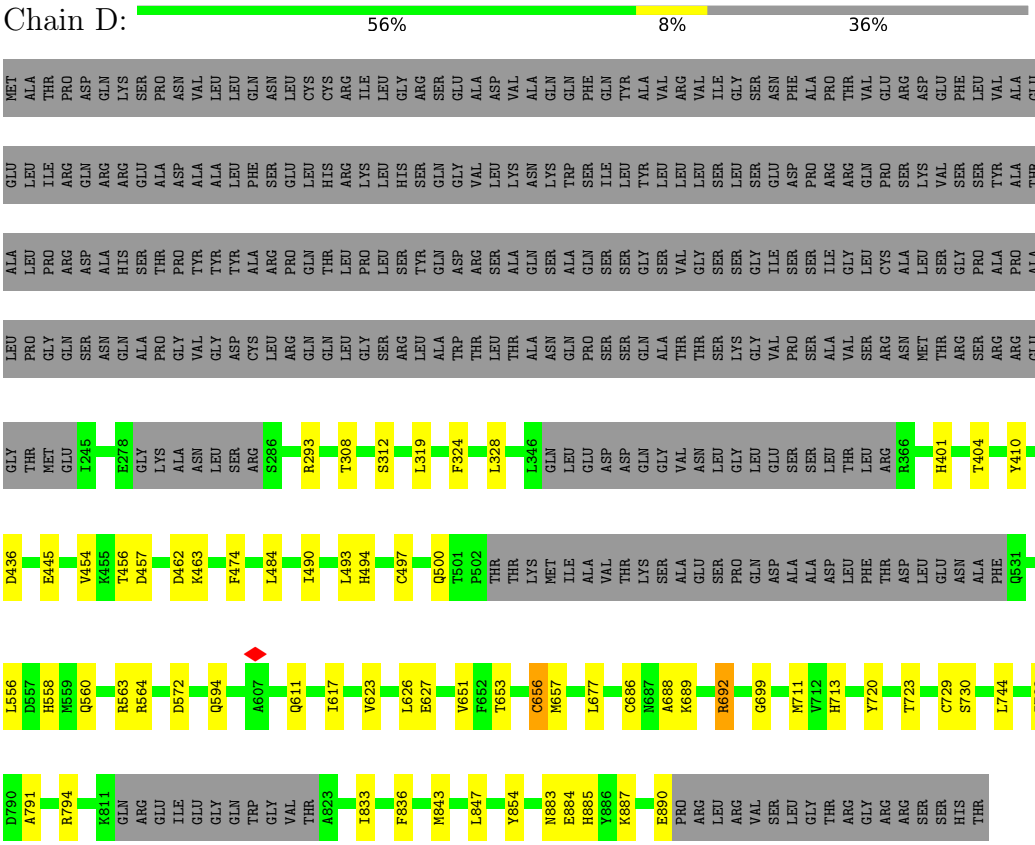
• Molecule 4: Gamma-tubulin complex component 3

Chain B:



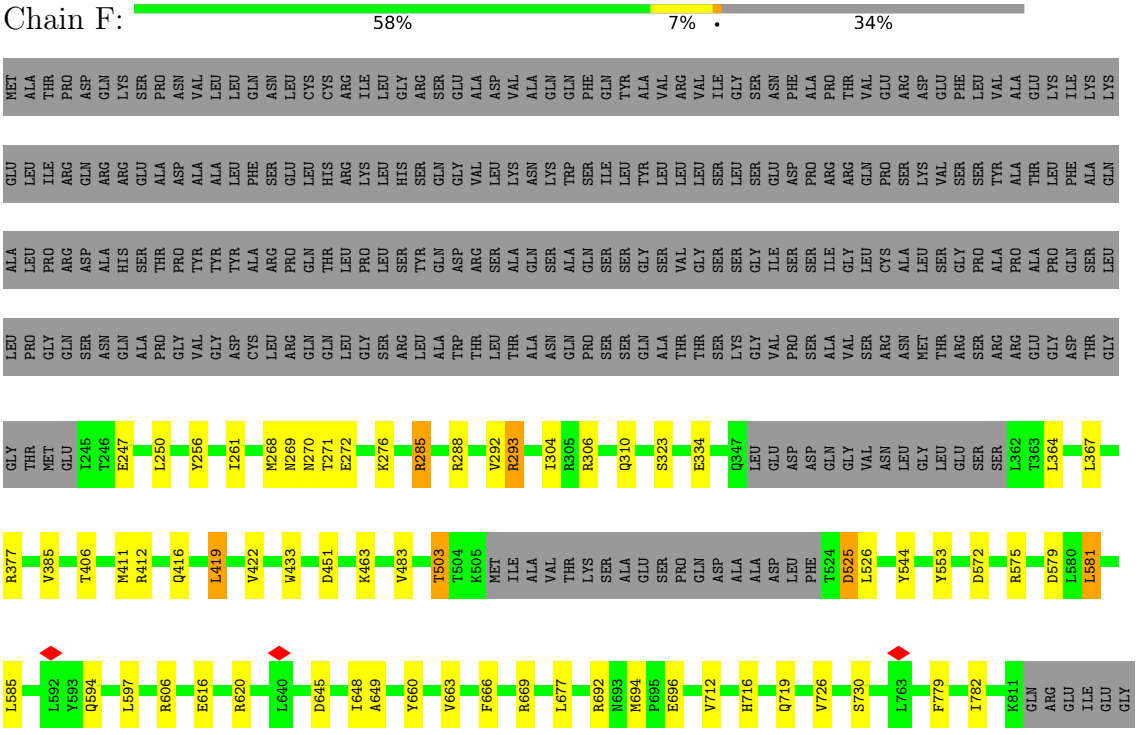
• Molecule 4: Gamma-tubulin complex component 3

Chain D:



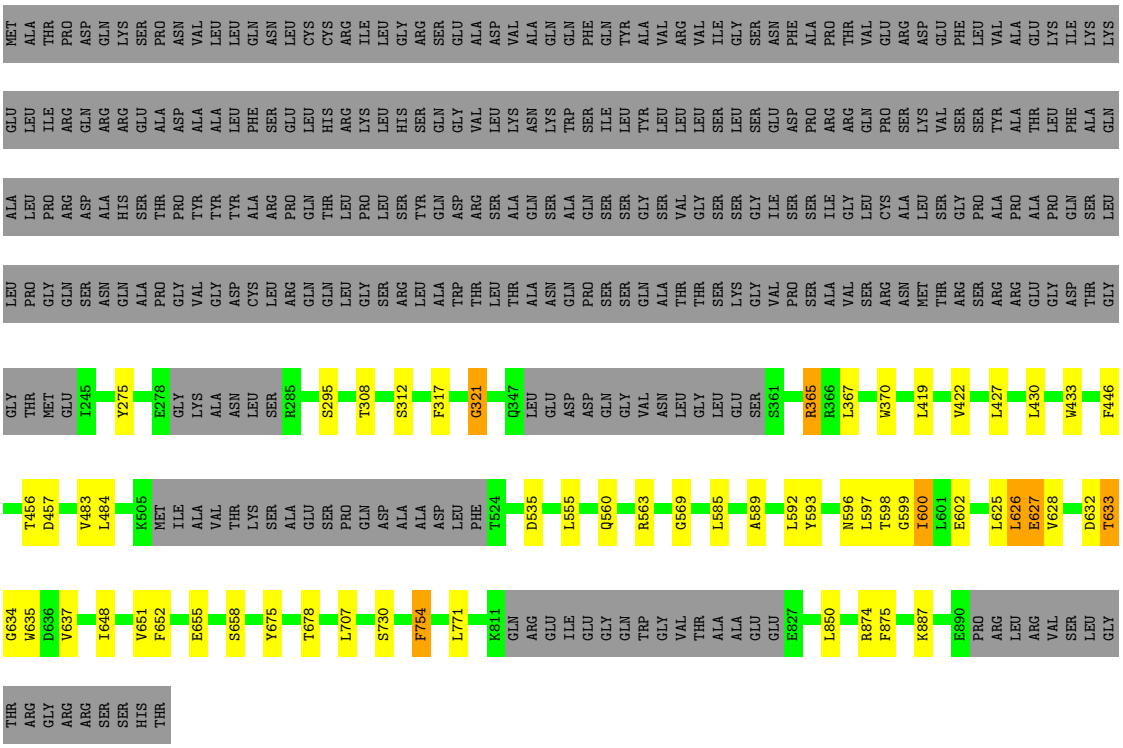
• Molecule 4: Gamma-tubulin complex component 3

Chain F:



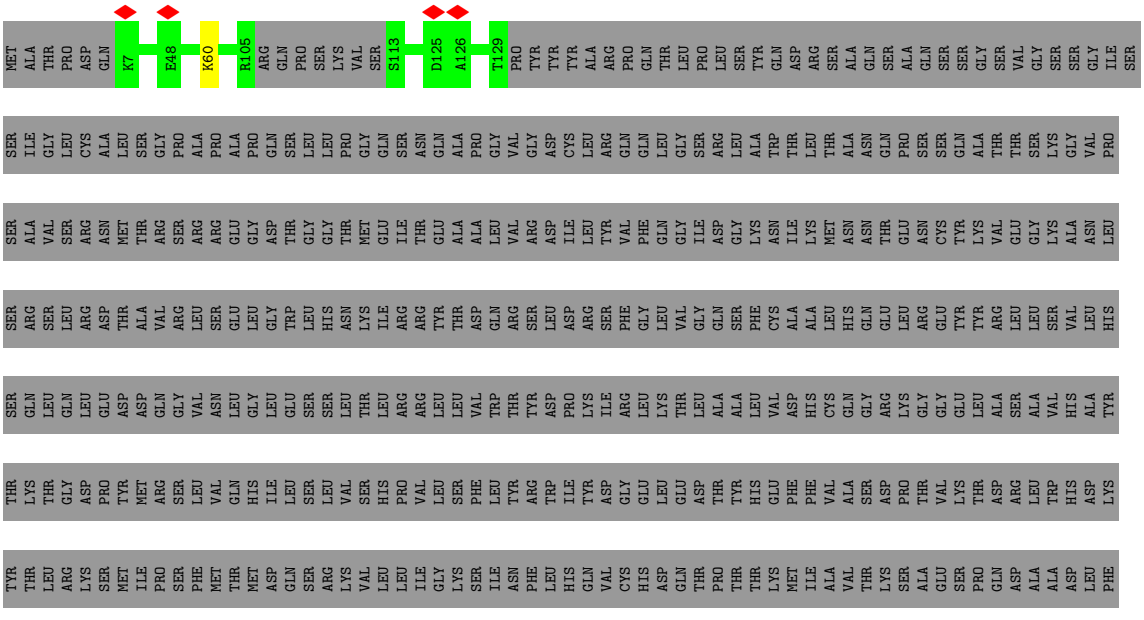
• Molecule 4: Gamma-tubulin complex component 3

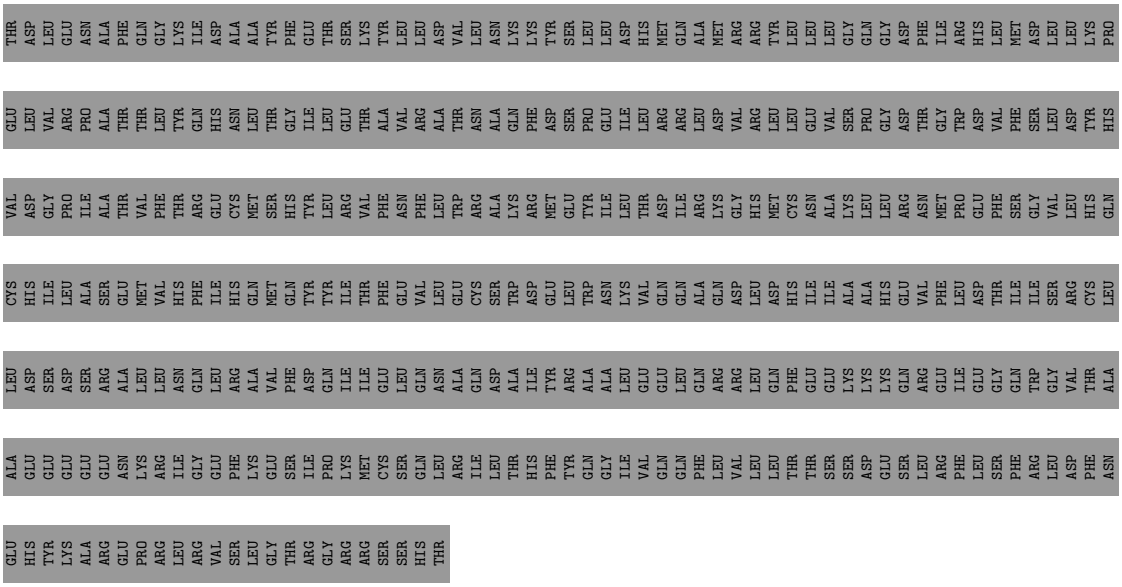
Chain H:



• Molecule 4: Gamma-tubulin complex component 3

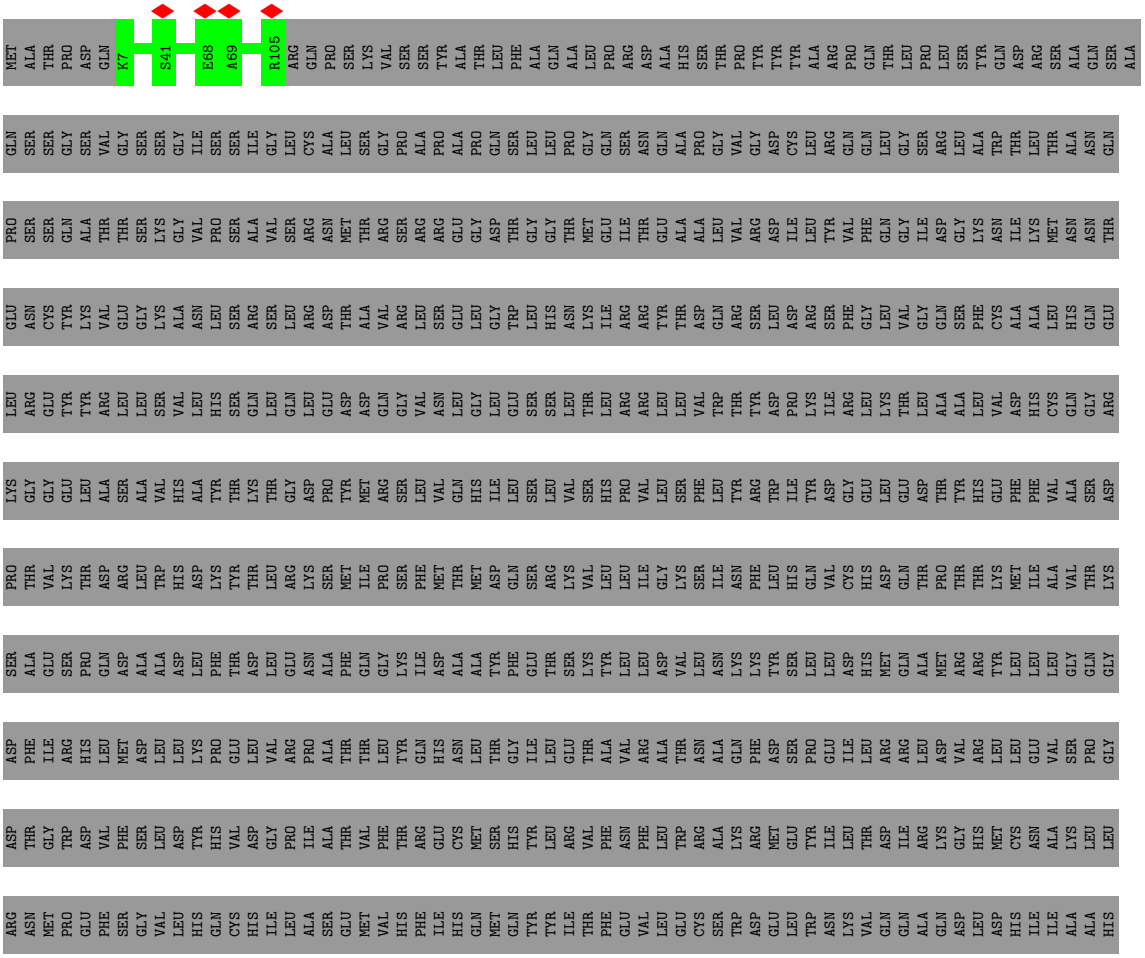
Chain a:

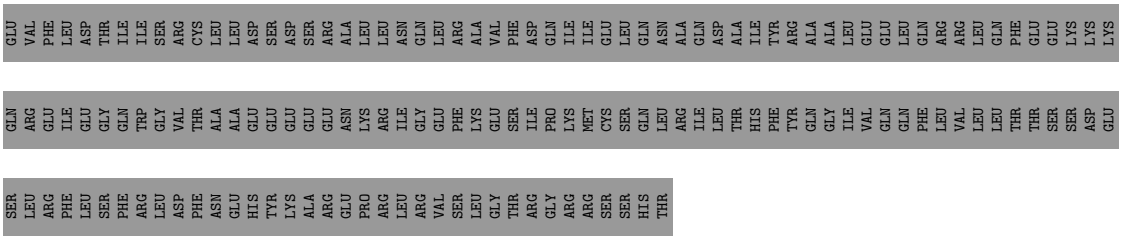




• Molecule 4: Gamma-tubulin complex component 3

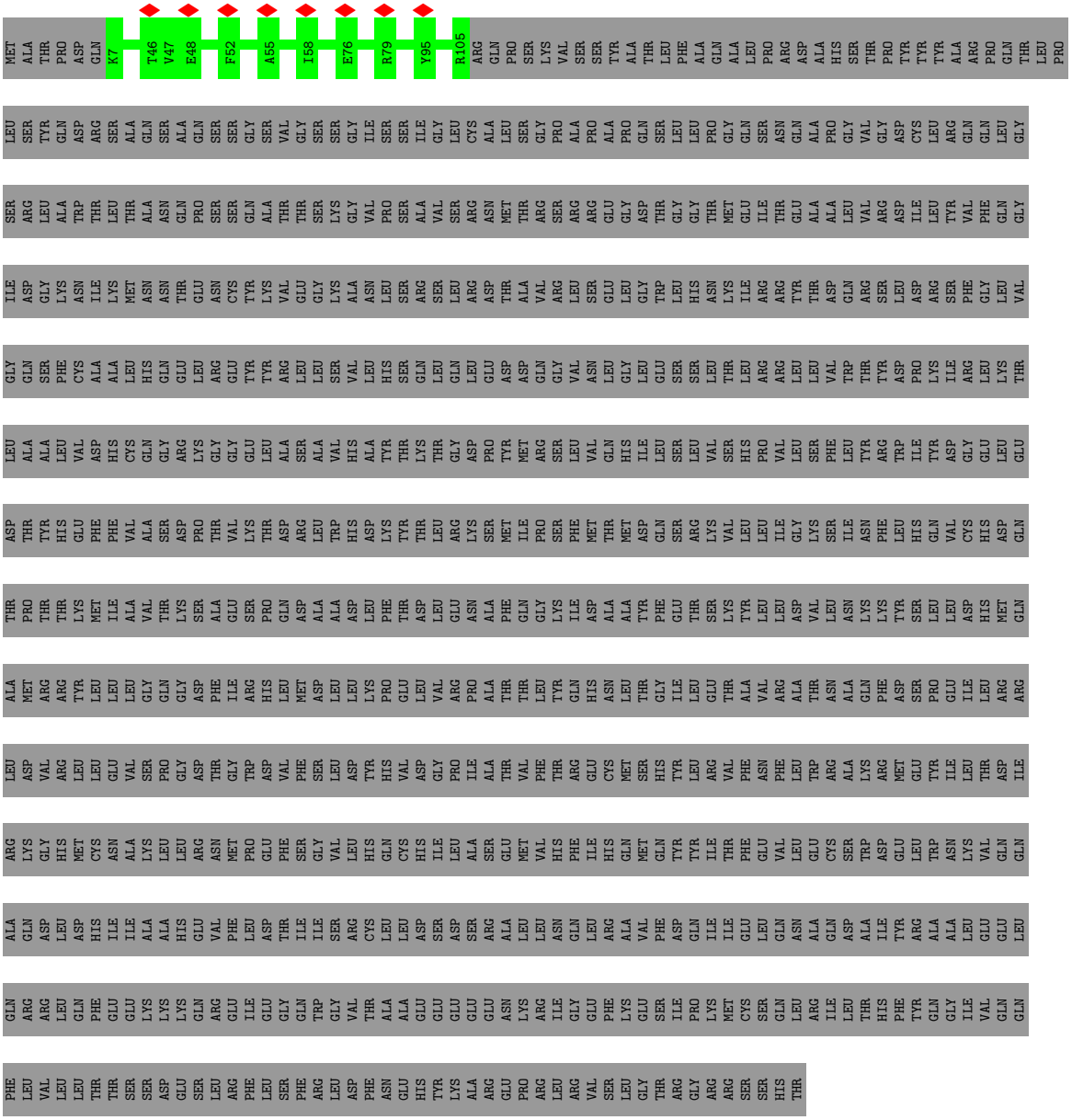
Chain f:





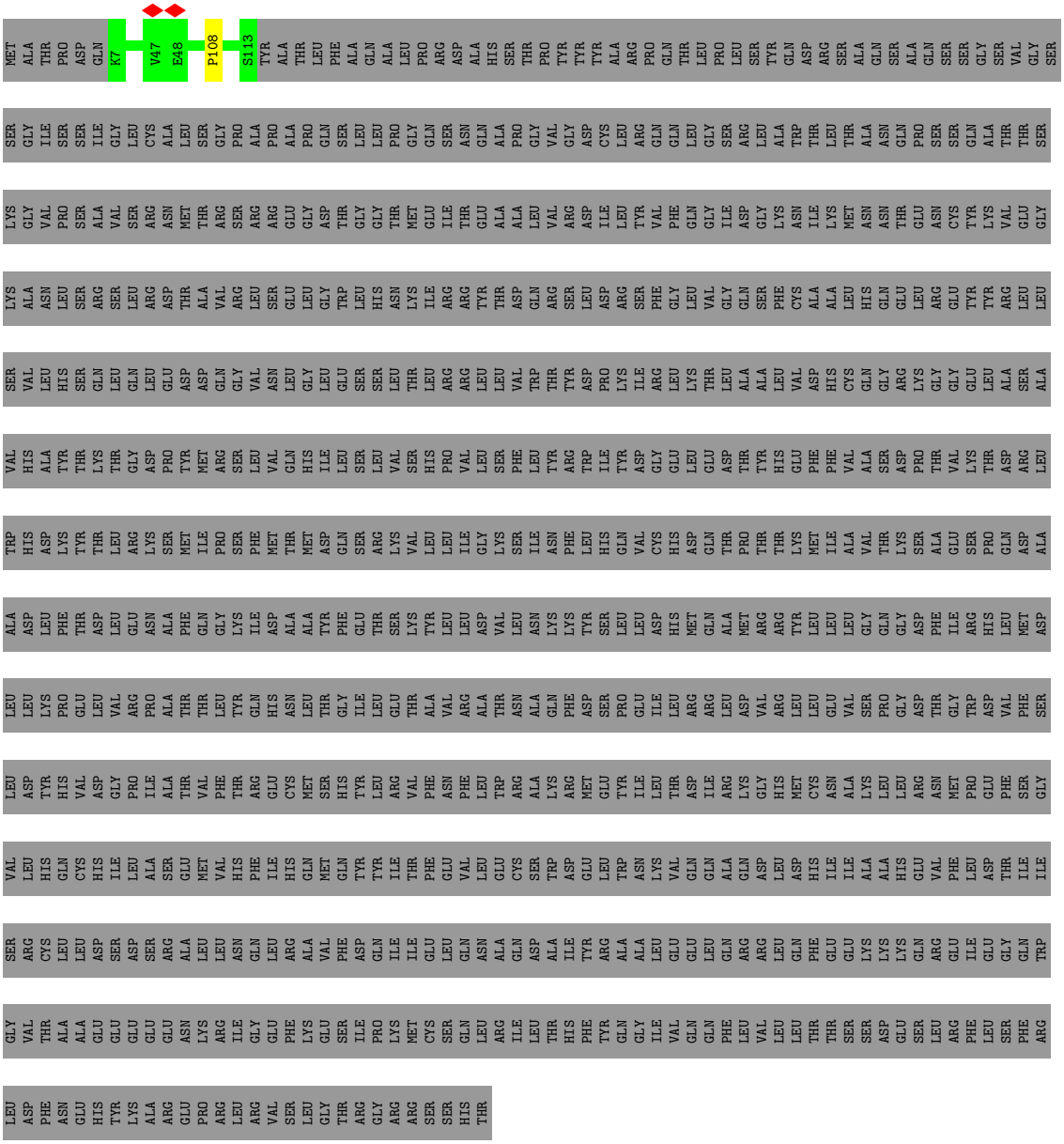
• Molecule 4: Gamma-tubulin complex component 3

Chain h:



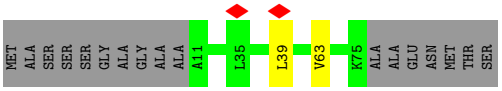
• Molecule 4: Gamma-tubulin complex component 3

Chain j:



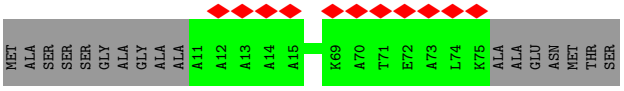
• Molecule 5: Mitotic-spindle organizing protein 1

Chain b:



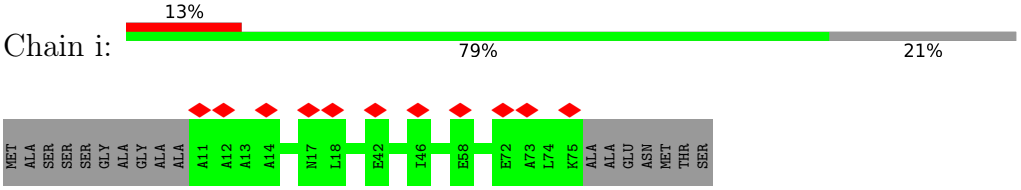
• Molecule 5: Mitotic-spindle organizing protein 1

Chain g:



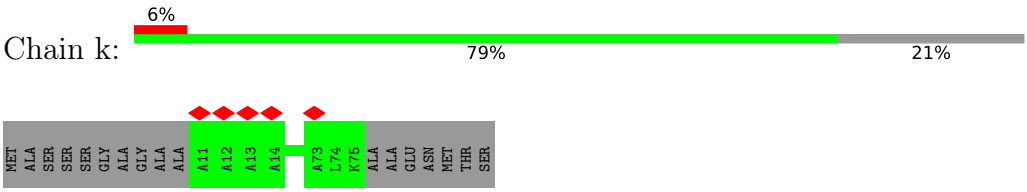
• Molecule 5: Mitotic-spindle organizing protein 1

Chain i:



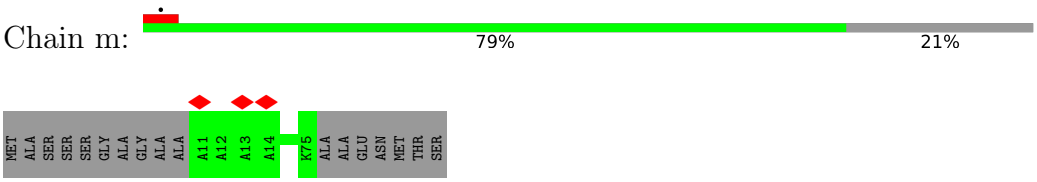
• Molecule 5: Mitotic-spindle organizing protein 1

Chain k:



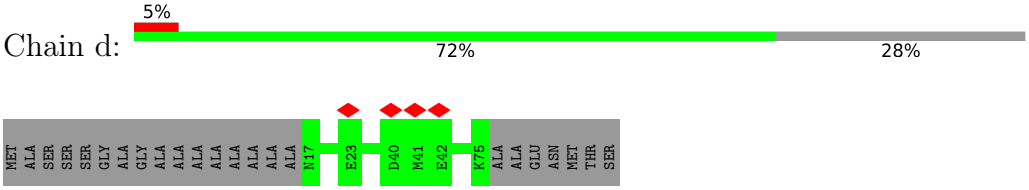
• Molecule 5: Mitotic-spindle organizing protein 1

Chain m:



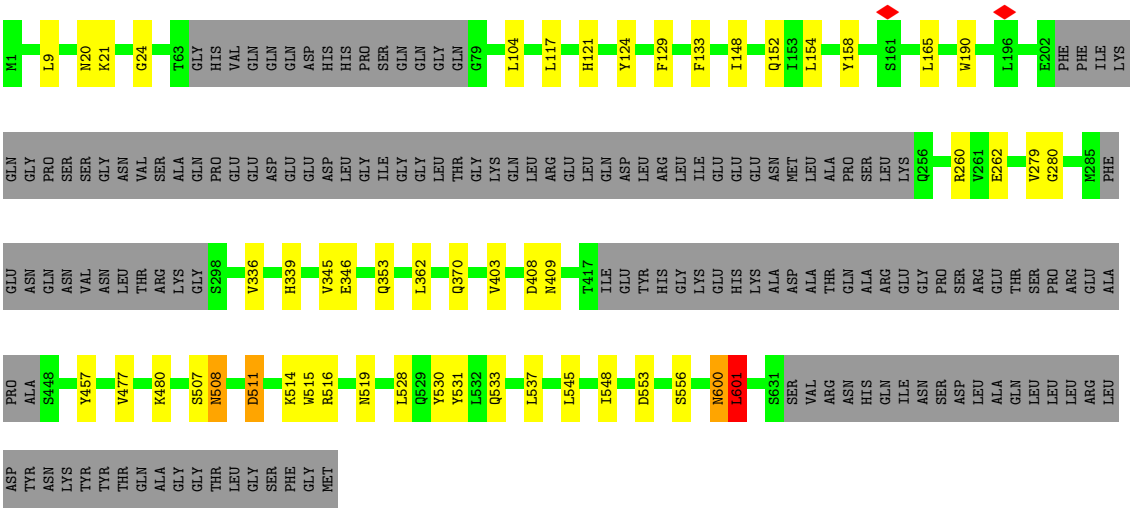
• Molecule 5: Mitotic-spindle organizing protein 1

Chain d:



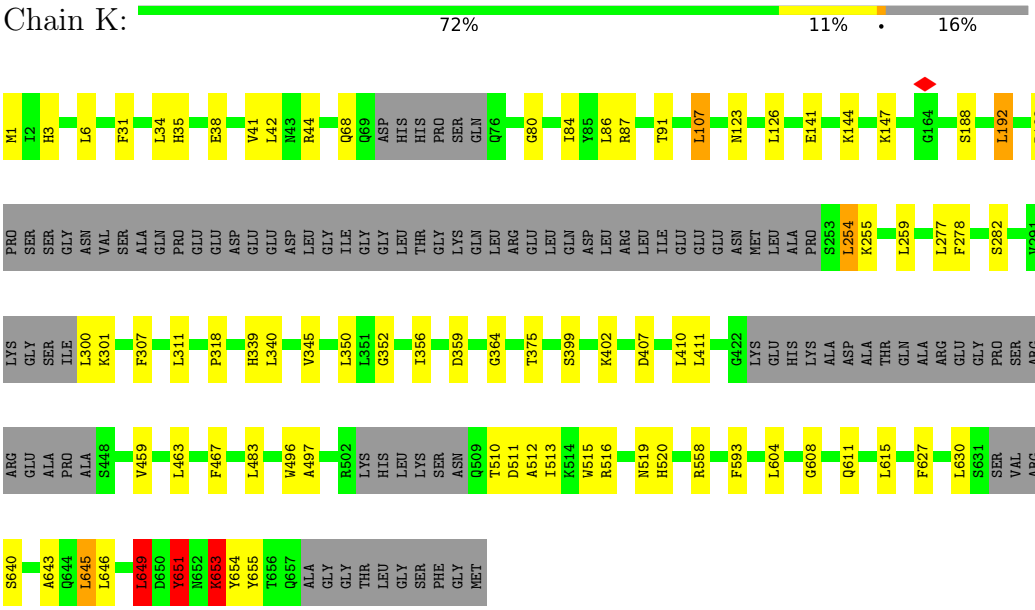
• Molecule 6: Gamma-tubulin complex component 4

Chain I:



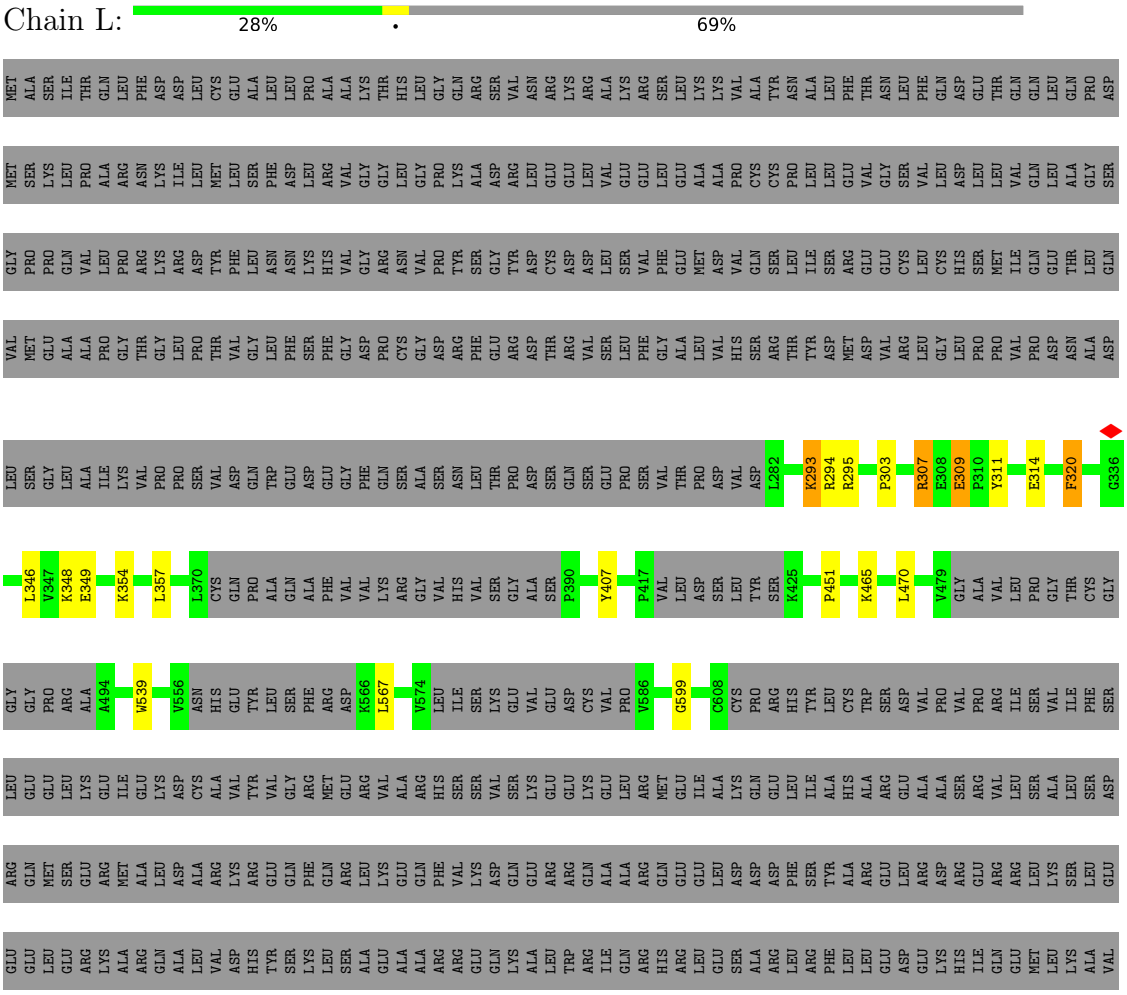
• Molecule 6: Gamma-tubulin complex component 4

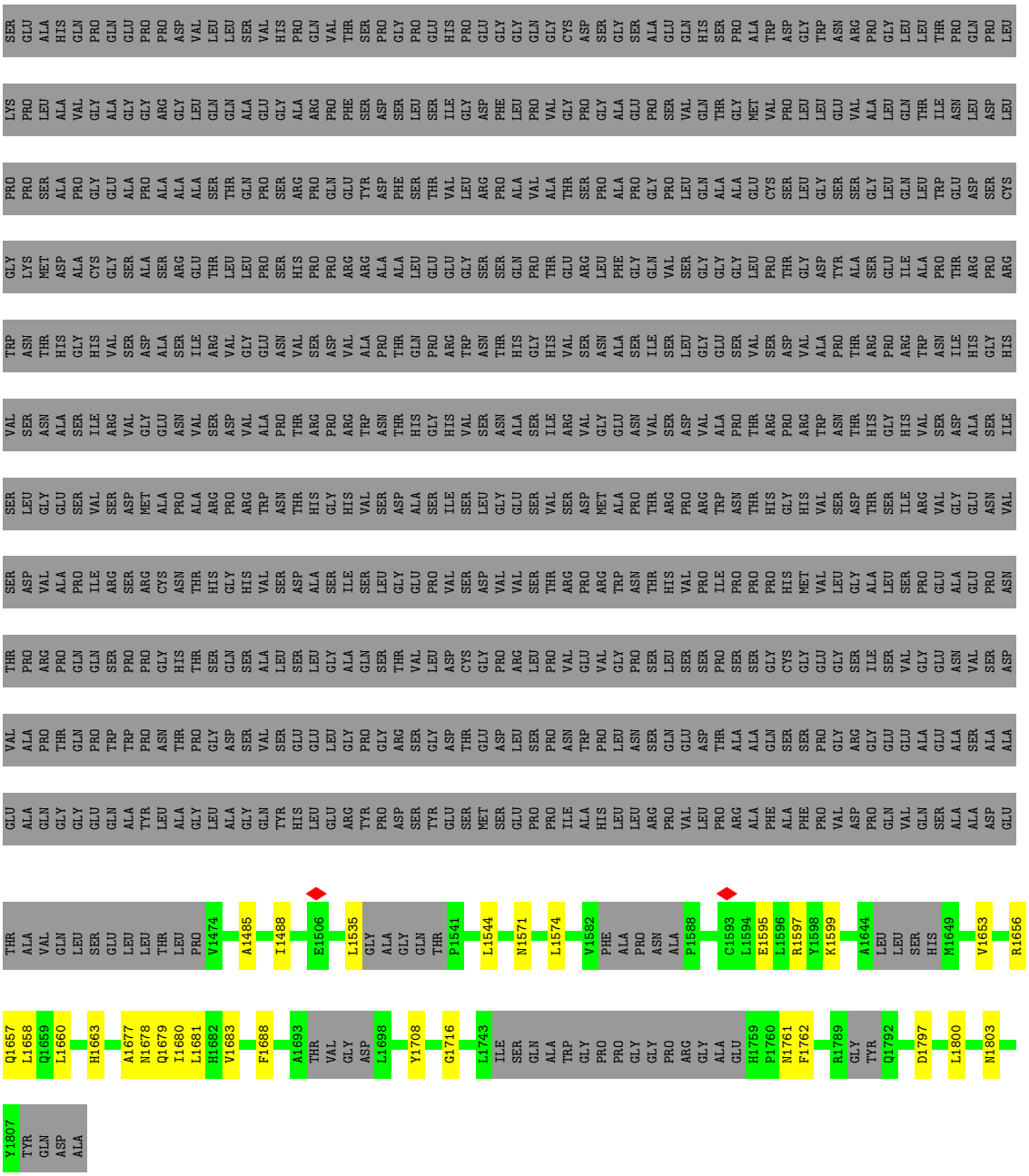
Chain K:



• Molecule 7: Gamma-tubulin complex component 6

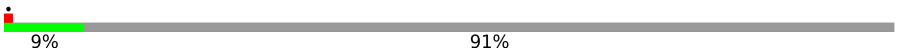
Chain L:

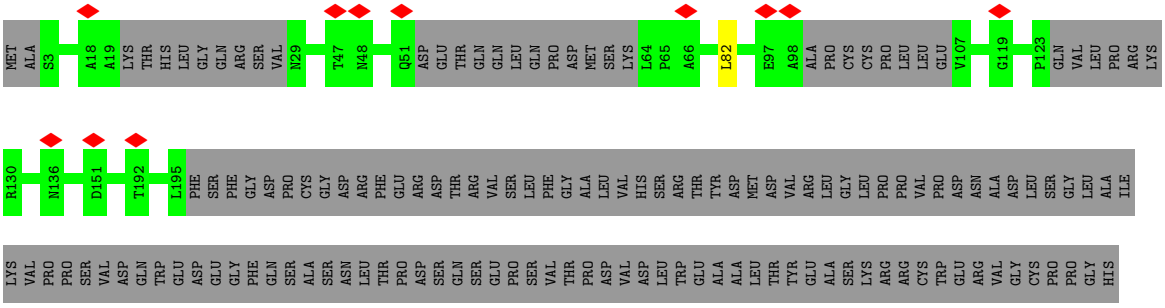




• Molecule 7: Gamma-tubulin complex component 6

Chain c:





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

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

LEU VAL PHE GLN ALA PHE THR SER GLY LEU ARG ARG TYR LEU GLN TYR TYR ARG ALA CYS VAL LEU SER THR PRO PRO THR LEU SER LEU LEU THR ILE GLY PHE LEU PHE LYS LYS LEU GLY ARG GLN LEU ARG TYR LEU ALA GLU LEU CYS GLY VAL GLY ALA VAL LEU PRO GLY THR

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

ILE ALA LYS GLN GLU LEU ILE ALA HIS ALA ARG GLU 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

GLU LEU ASP ASP PHE SER TYR ALA ARG GLU LEU ARG ASP ARG GLU ARG ARG LEU LYS SER LEU GLU GLU GLU LEU GLU ARG LYS ALA ARG GLN ALA LEU VAL ASP HIS TYR SER LYS LEU SER ALA GLU ALA ALA ARG ARG GLU GLN LYS ALA LEU TRP ARG ILE GLN ARG HIS ARG

LEU GLU SER ALA ARG LEU ARG PHE LEU LEU GLU ASP GLU LYS HIS ILE GLN GLU 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 GLY GLN GLY CYS ASP SER GLY

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

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

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

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

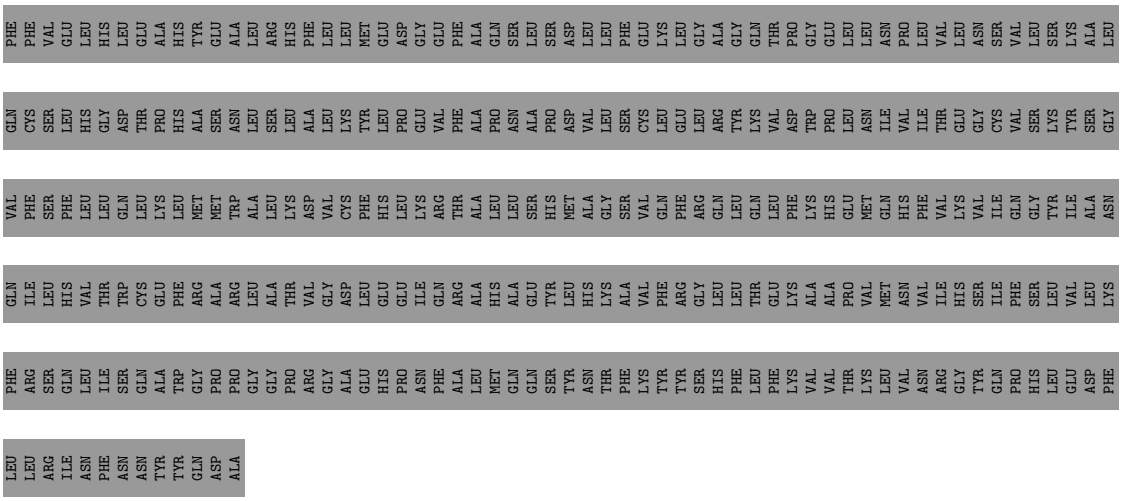
PRO THR ARG PRO ARG TRP ASN THR HIS GLY HIS VAL SER ASP THR SER ILE ARG VAL GLY GLU ASN VAL SER ASP VAL ALA PRO ILE ARG SER ARG CYS ASN THR HIS GLY HIS VAL SER ASP ALA SER ILE SER LEU GLY GLU PRO VAL SER ASP VAL VAL SER THR ARG PRO ARG TRP

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

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

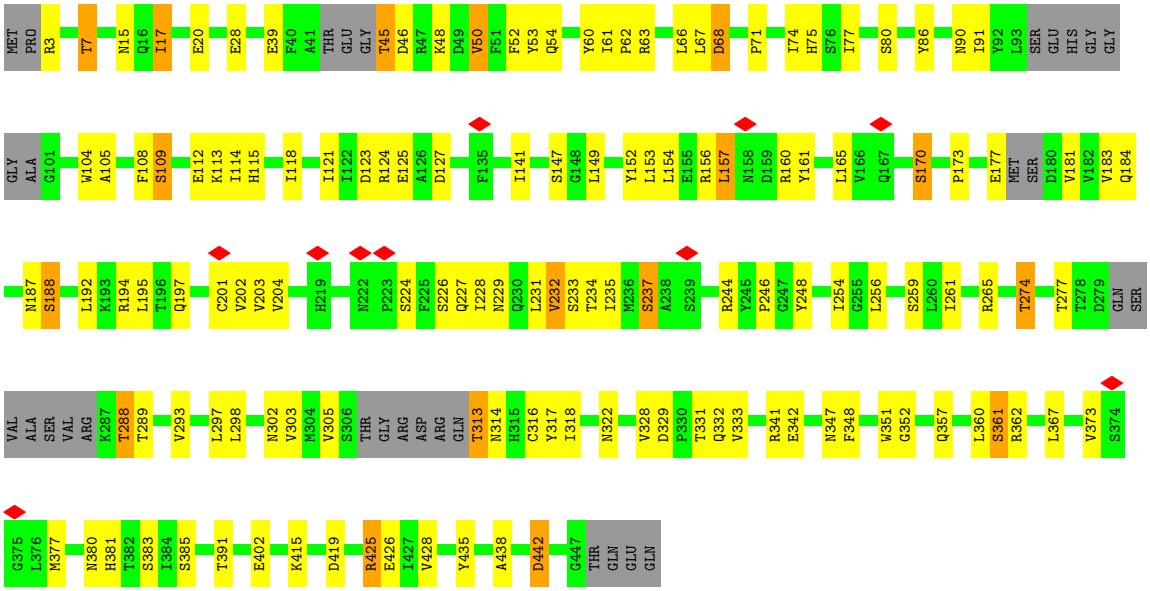
ASN SER GLN GLU ASP THR ALA ALA GLN SER SER PRO GLY ARG GLY GLU GLU ALA GLU ALA SER ALA ALA GLU ALA GLN GLY GLY GLU GLN ALA TYR LEU ALA GLY LEU ALA GLY GLN TYR HIS LEU GLU ARG TYR PRO ASP SER TYR GLU SER MET SER GLU PRO PRO ILE ALA HIS LEU

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



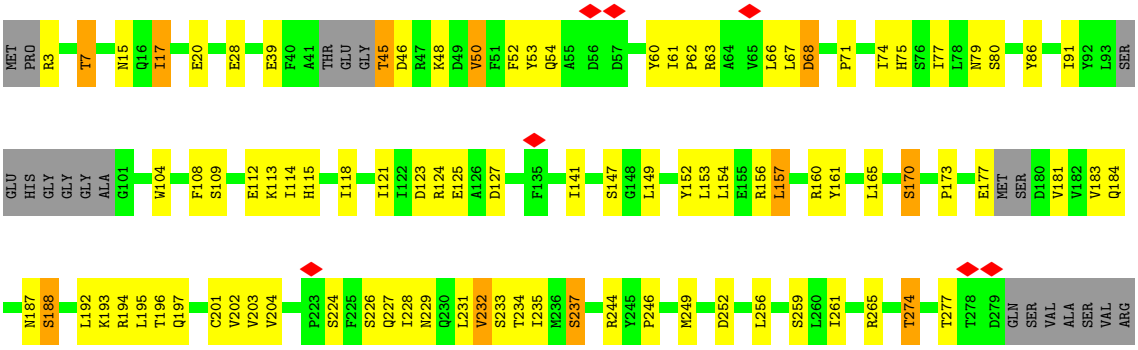
• Molecule 8: Tubulin gamma-1 chain

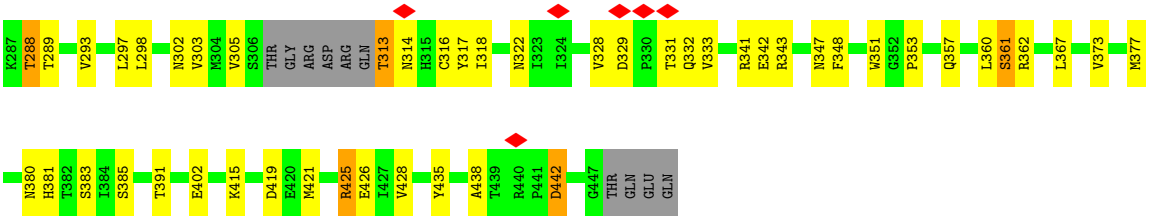
Chain O:



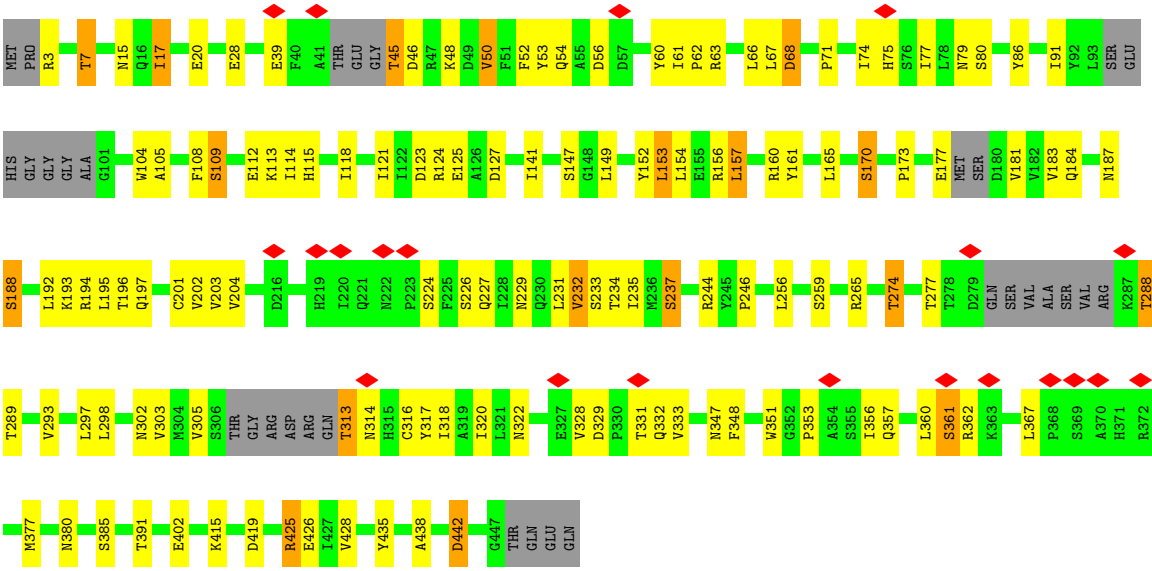
• Molecule 8: Tubulin gamma-1 chain

Chain P:

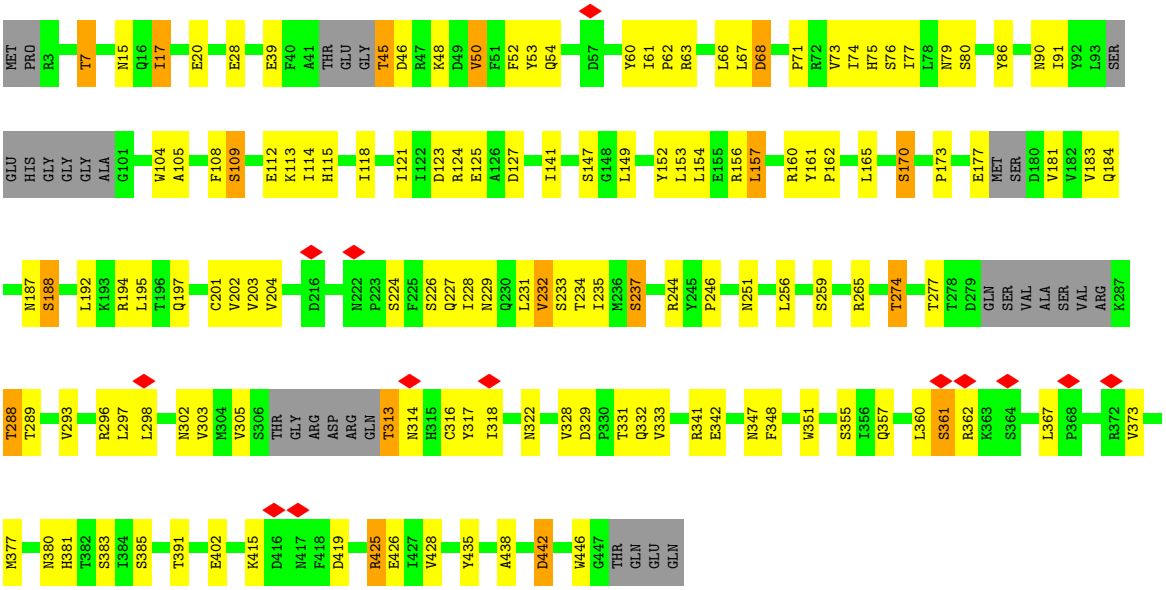




• Molecule 8: Tubulin gamma-1 chain

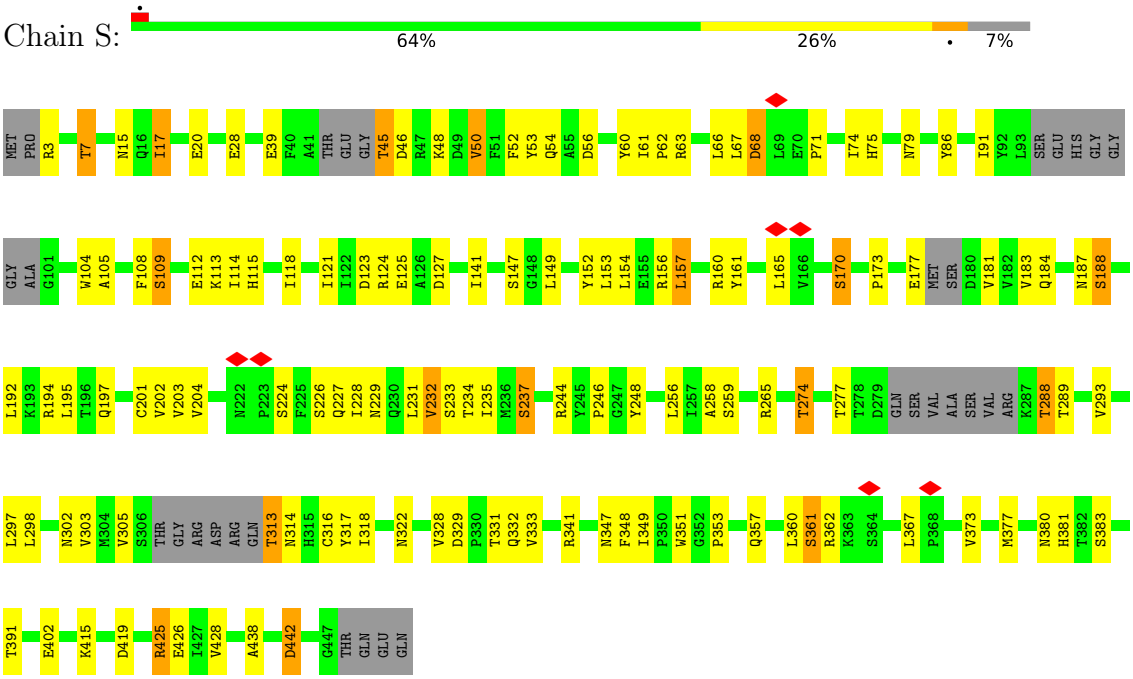


• Molecule 8: Tubulin gamma-1 chain



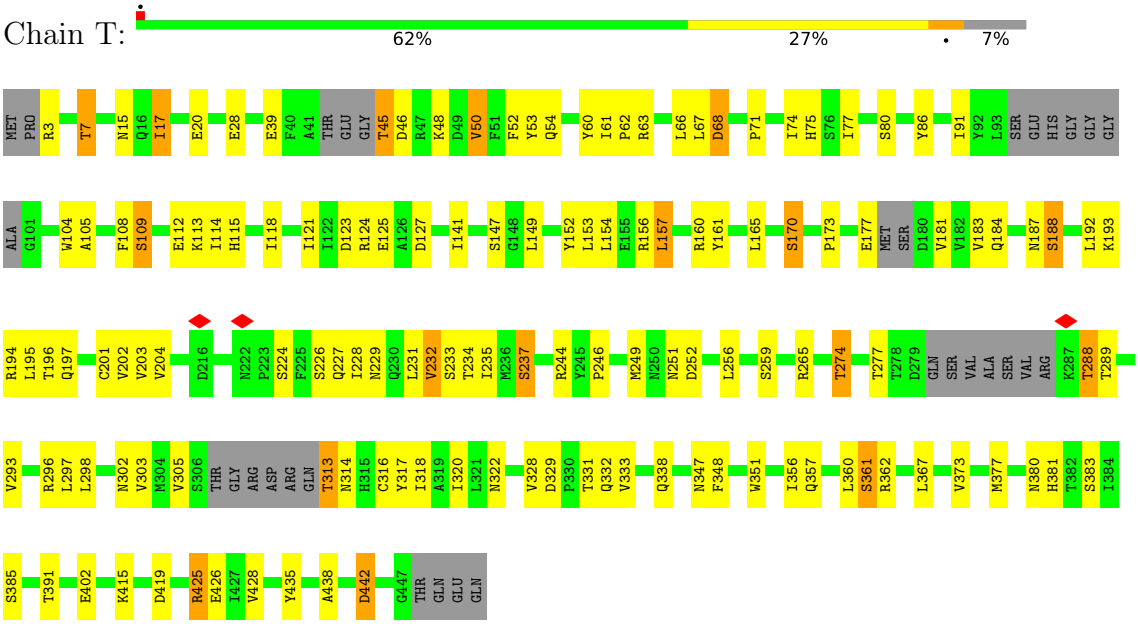
• Molecule 8: Tubulin gamma-1 chain

Chain S:



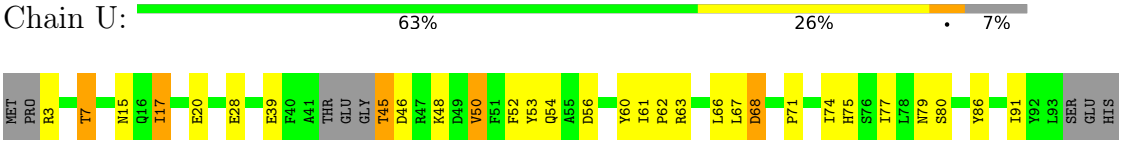
• Molecule 8: Tubulin gamma-1 chain

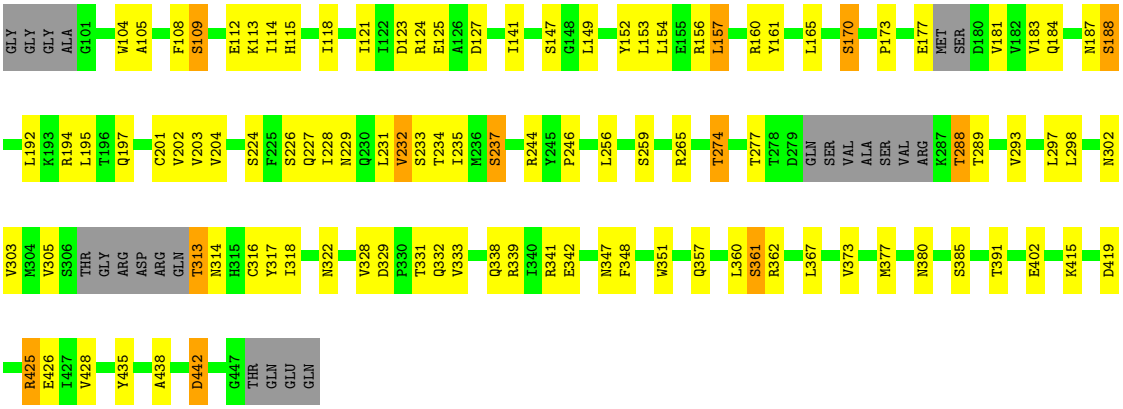
Chain T:



• Molecule 8: Tubulin gamma-1 chain

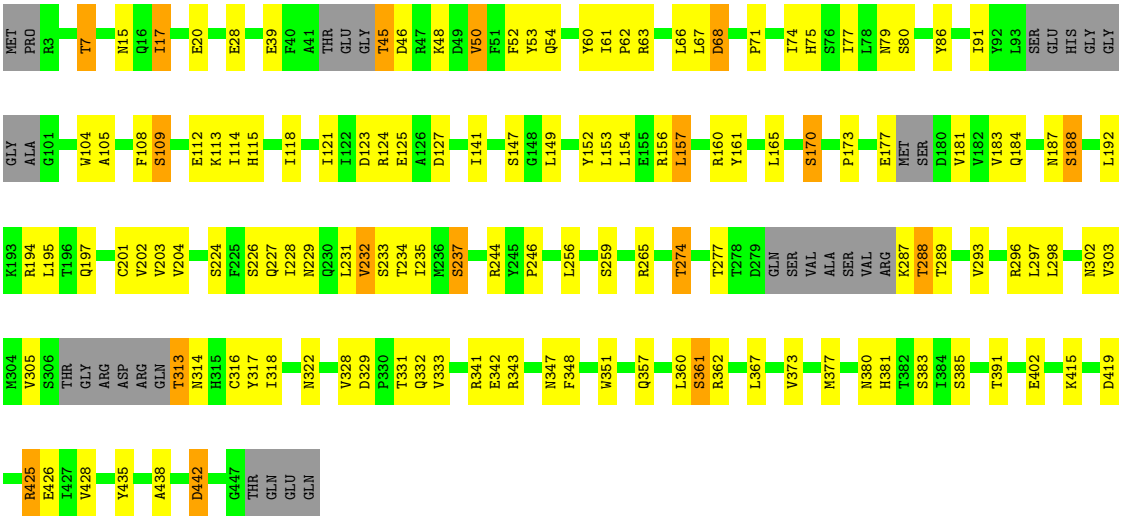
Chain U:





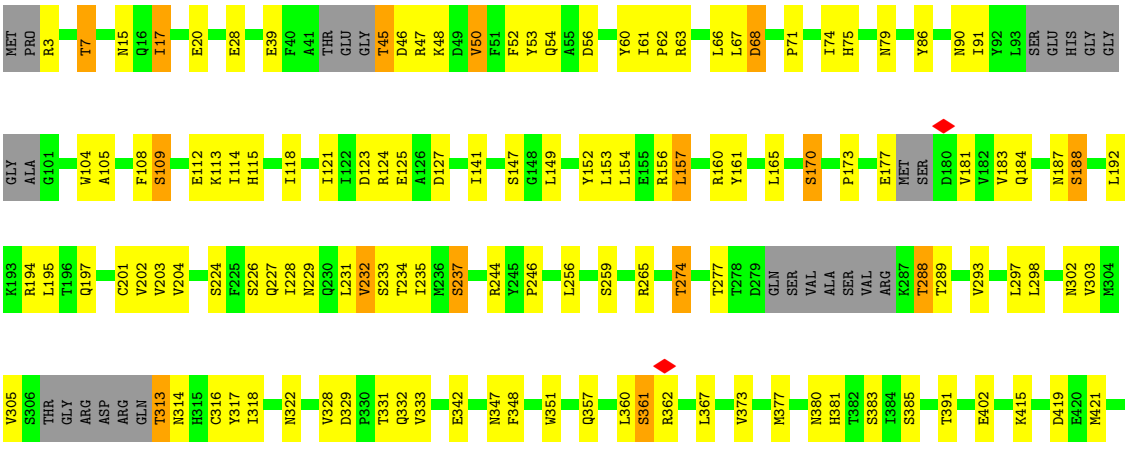
• Molecule 8: Tubulin gamma-1 chain

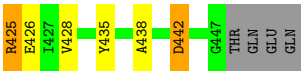
Chain V:



• Molecule 8: Tubulin gamma-1 chain

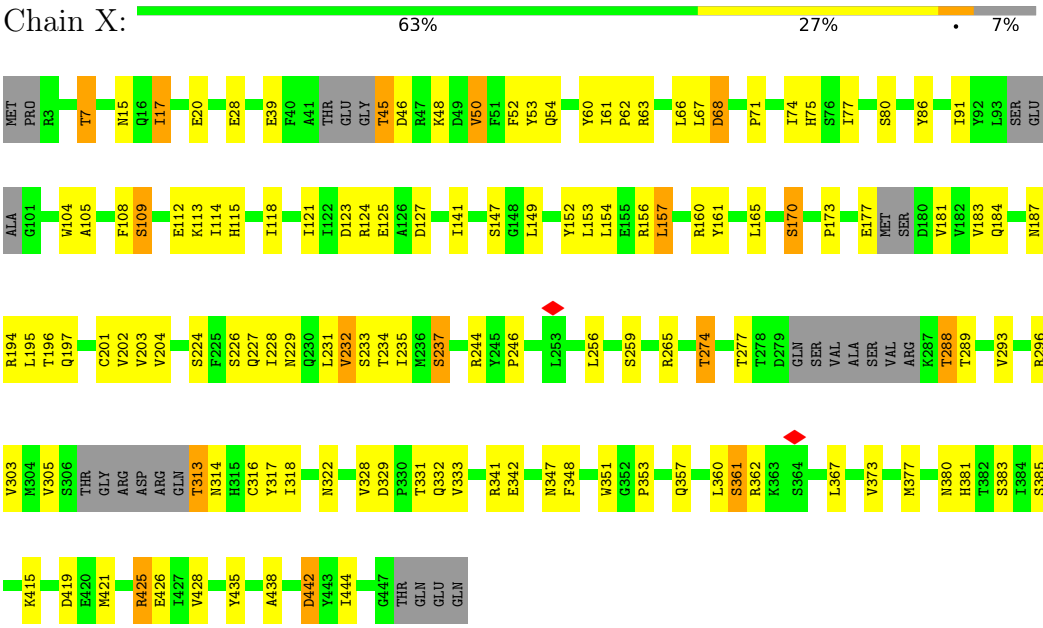
Chain W:





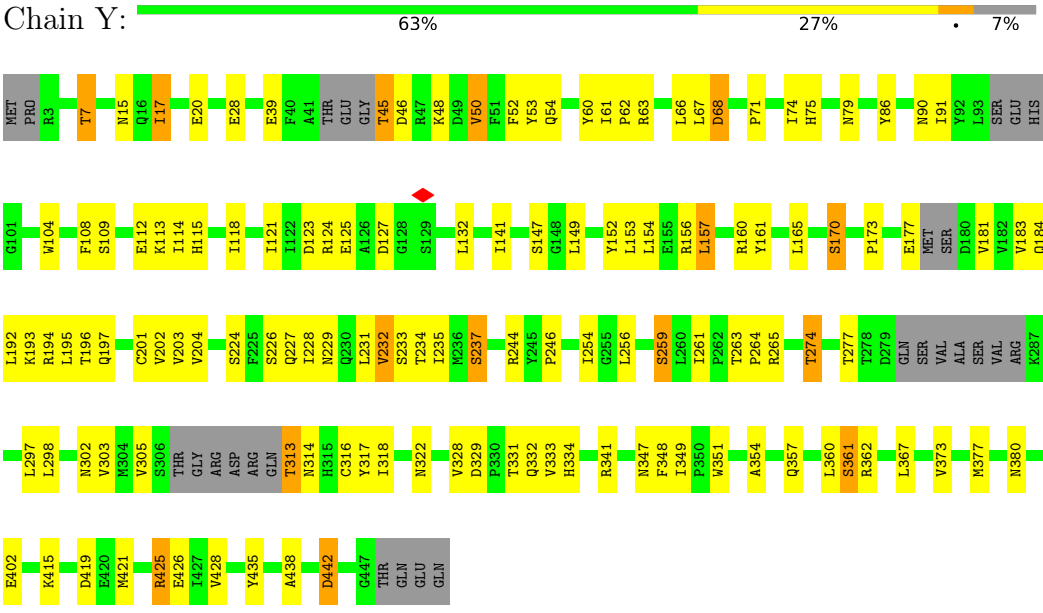
• Molecule 8: Tubulin gamma-1 chain

Chain X:



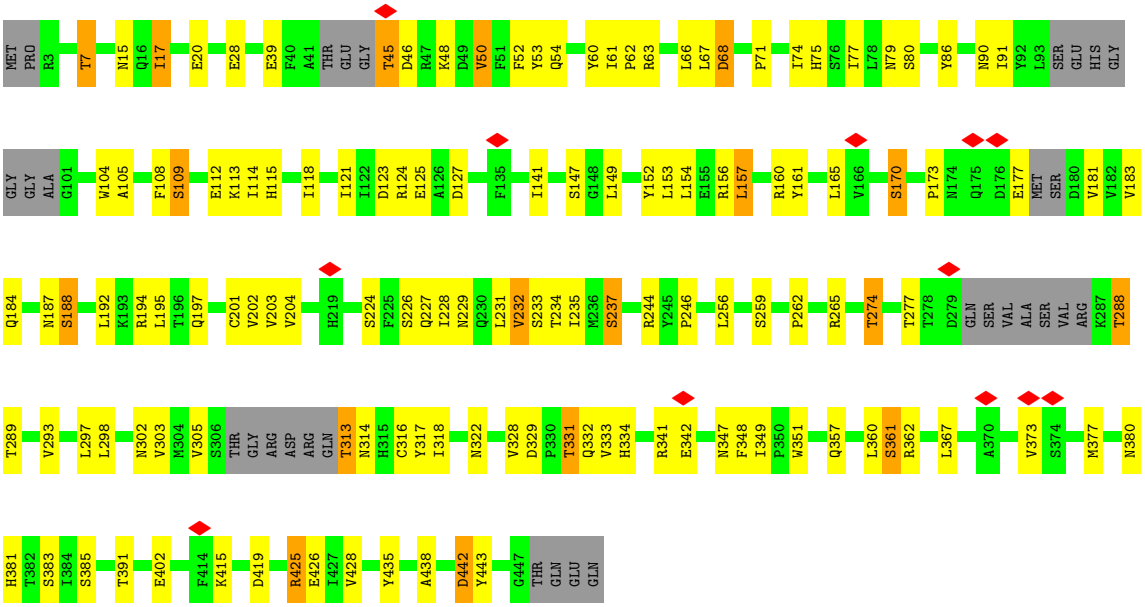
• Molecule 8: Tubulin gamma-1 chain

Chain Y:



• Molecule 8: Tubulin gamma-1 chain

Chain Z:


MET PRO R3 T7 N15 Q16 I17 E20 E28 E39 F40 A41 THR GLU GLY T45 D46 R47 K48 D49 V50 F51 F52 Y53 Q54 Y60 I61 P62 R63 L66 L67 D68 P71 I74 H75 S76 I77 L78 N79 S80 Y86 N90 I91 Y92 L93 SER GLU HIS GLY
GLY GLY ALA G101 W104 A105 F108 S109 E112 K113 I114 H115 I118 I121 I122 D123 R124 E125 A126 D127 F135 I141 S147 G148 L149 Y152 L153 L154 E155 R156 L157 R160 Y161 L165 V166 S170 P173 N174 Q175 D176 E177 MET SER D180 V181 V182 V183
Q184 N187 S188 L192 K193 R194 L195 T196 Q197 C201 V202 V203 V204 H219 S224 P225 S226 Q227 I228 N229 Q230 L231 V232 S233 T234 I235 M236 S237 R244 Y245 P246 L256 S259 P262 R265 T274 T277 T278 D279 GLN SER VAL ALA SER VAL ARG K287 T288
T289 V293 L297 L298 N302 V303 M304 V305 S306 THR GLY ARG ASP ARG GLN T313 N314 H315 C316 Y317 I318 N322 V328 D329 P330 T331 Q332 V333 H334 R341 E342 N347 F348 I349 P350 W351 Q357 L360 S361 R362 L367 A370 V373 S374 M377 N380
H381 T382 S383 I384 S385 T391 E402 F414 K415 D419 R425 E426 I427 V428 Y435 A438 D442 Y443 G447 THR GLN GLU GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8270	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	0.184	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0368	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	0.38	0/4525	0.71	6/6119 (0.1%)
1	l	0.35	0/863	0.67	2/1166 (0.2%)
2	e	0.54	1/2908 (0.0%)	0.67	1/3938 (0.0%)
3	A	0.38	0/5085	0.61	4/6866 (0.1%)
3	C	0.35	0/5151	0.63	2/6955 (0.0%)
3	E	0.38	0/5315	0.66	5/7175 (0.1%)
3	G	0.37	0/5315	0.64	4/7175 (0.1%)
4	B	0.38	0/5133	0.67	6/6930 (0.1%)
4	D	0.38	1/4897 (0.0%)	0.62	3/6610 (0.0%)
4	F	0.36	0/5044	0.62	2/6809 (0.0%)
4	H	0.41	1/5009 (0.0%)	0.66	4/6761 (0.1%)
4	a	0.38	0/948	0.60	0/1277
4	f	0.30	0/815	0.50	0/1096
4	h	0.31	0/815	0.56	0/1096
4	j	0.37	0/855	0.64	1/1152 (0.1%)
5	b	0.34	0/484	0.70	1/653 (0.2%)
5	d	0.33	0/454	0.63	0/611
5	g	0.30	0/484	0.59	0/653
5	i	0.33	0/484	0.62	0/653
5	k	0.35	0/484	0.67	0/653
5	m	0.33	0/484	0.59	0/653
6	I	0.41	1/4322 (0.0%)	0.65	0/5853
6	K	0.46	3/4683 (0.1%)	0.70	10/6338 (0.2%)
7	L	0.38	2/4697 (0.0%)	0.65	8/6348 (0.1%)
7	c	0.30	0/1235	0.57	1/1664 (0.1%)
8	O	0.32	0/3441	0.56	1/4661 (0.0%)
8	P	0.32	0/3441	0.56	1/4661 (0.0%)
8	Q	0.32	0/3441	0.56	1/4661 (0.0%)
8	R	0.32	0/3441	0.56	1/4661 (0.0%)
8	S	0.32	0/3441	0.56	1/4661 (0.0%)
8	T	0.32	0/3441	0.56	1/4661 (0.0%)
8	U	0.32	0/3441	0.56	1/4661 (0.0%)
8	V	0.32	0/3441	0.56	1/4661 (0.0%)
8	W	0.32	0/3441	0.57	1/4661 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
8	X	0.32	0/3441	0.56	1/4661 (0.0%)
8	Y	0.32	0/3441	0.56	1/4661 (0.0%)
8	Z	0.32	0/3441	0.56	1/4661 (0.0%)
All	All	0.37	9/111781 (0.0%)	0.62	72/151136 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	5
1	l	0	1
2	e	0	1
3	A	0	1
3	C	0	2
3	E	0	4
3	G	0	2
4	B	0	2
4	D	0	1
4	F	0	1
4	H	0	3
6	I	0	6
6	K	0	3
7	L	0	3
8	O	0	1
8	P	0	1
8	Q	0	1
8	R	0	1
8	S	0	1
8	T	0	1
8	U	0	1
8	V	0	1
8	W	0	1
8	X	0	1
8	Y	0	1
8	Z	0	1
All	All	0	47

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	243	PRO	N-CD	19.87	1.75	1.47
6	K	653	LYS	CD-CE	-8.02	1.31	1.51
7	L	1708	TYR	CD1-CE1	-6.35	1.29	1.39
7	L	1653	VAL	CB-CG1	-6.20	1.39	1.52
4	D	692	ARG	CB-CG	-5.95	1.36	1.52
4	H	754	PHE	CD1-CE1	-5.82	1.27	1.39
6	K	651	TYR	CG-CD1	-5.42	1.32	1.39
6	K	651	TYR	CD1-CE1	-5.19	1.31	1.39
6	I	530	TYR	CE1-CZ	5.06	1.45	1.38

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	238	LEU	CA-CB-CG	11.06	140.73	115.30
6	K	649	LEU	CA-CB-CG	10.51	139.47	115.30
1	J	238	LEU	CB-CG-CD1	-9.70	94.51	111.00
4	H	365	ARG	NE-CZ-NH1	-8.32	116.14	120.30
6	K	651	TYR	CB-CG-CD1	-7.91	116.26	121.00
4	B	790	ASP	CB-CG-OD1	7.53	125.08	118.30
1	J	885	LEU	CB-CG-CD1	-7.43	98.37	111.00
4	F	581	LEU	CA-CB-CG	7.39	132.30	115.30
1	l	121	PRO	N-CA-CB	7.29	112.05	103.30
2	e	140	LEU	CA-CB-CG	7.02	131.45	115.30
7	L	567	LEU	CA-CB-CG	6.99	131.39	115.30
4	D	692	ARG	NE-CZ-NH1	-6.91	116.85	120.30
6	K	86	LEU	CB-CG-CD1	-6.73	99.55	111.00
1	J	237	HIS	C-N-CA	6.60	138.20	121.70
7	c	82	LEU	CA-CB-CG	6.56	130.40	115.30
6	K	107	LEU	CB-CG-CD1	-6.42	100.08	111.00
6	K	651	TYR	CB-CG-CD2	6.39	124.84	121.00
7	L	1800	LEU	CA-CB-CG	6.38	129.96	115.30
4	B	581	LEU	CA-CB-CG	6.32	129.83	115.30
3	G	698	MET	CA-CB-CG	6.25	123.92	113.30
8	S	157	LEU	CA-CB-CG	6.23	129.63	115.30
8	V	157	LEU	CA-CB-CG	6.22	129.61	115.30
8	O	157	LEU	CA-CB-CG	6.22	129.60	115.30
8	Y	157	LEU	CA-CB-CG	6.22	129.60	115.30
8	Z	157	LEU	CA-CB-CG	6.22	129.60	115.30
8	U	157	LEU	CA-CB-CG	6.21	129.59	115.30
8	X	157	LEU	CA-CB-CG	6.21	129.59	115.30
8	T	157	LEU	CA-CB-CG	6.21	129.58	115.30
8	W	157	LEU	CA-CB-CG	6.21	129.57	115.30
8	Q	157	LEU	CA-CB-CG	6.21	129.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	157	LEU	CA-CB-CG	6.20	129.56	115.30
7	L	1708	TYR	CB-CG-CD1	-6.20	117.28	121.00
8	R	157	LEU	CA-CB-CG	6.19	129.54	115.30
3	E	375	LEU	CA-CB-CG	6.18	129.52	115.30
3	G	351	LEU	CA-CB-CG	6.12	129.37	115.30
1	l	130	PRO	N-CA-CB	6.01	110.52	103.30
7	L	1535	LEU	CA-CB-CG	5.93	128.95	115.30
3	E	509	LEU	CA-CB-CG	5.93	128.93	115.30
7	L	320	PHE	CB-CG-CD1	-5.92	116.65	120.80
4	H	365	ARG	CG-CD-NE	-5.84	99.54	111.80
6	K	192	LEU	CB-CG-CD2	-5.79	101.16	111.00
7	L	1800	LEU	CB-CG-CD2	-5.69	101.33	111.00
4	D	692	ARG	NE-CZ-NH2	5.62	123.11	120.30
3	C	239	ALA	N-CA-CB	5.61	117.95	110.10
3	E	414	LEU	CA-CB-CG	5.58	128.13	115.30
4	B	692	ARG	NE-CZ-NH2	-5.57	117.52	120.30
6	K	411	LEU	CB-CG-CD2	-5.54	101.58	111.00
4	F	419	LEU	CA-CB-CG	5.54	128.04	115.30
7	L	1544	LEU	CA-CB-CG	5.52	128.00	115.30
7	L	307	ARG	NE-CZ-NH1	-5.45	117.57	120.30
6	K	254	LEU	CA-CB-CG	5.43	127.79	115.30
6	K	645	LEU	CB-CG-CD2	-5.42	101.78	111.00
4	D	556	LEU	CA-CB-CG	5.37	127.66	115.30
6	K	407	ASP	CB-CG-OD1	5.36	123.12	118.30
1	J	256	LEU	CA-CB-CG	5.33	127.57	115.30
1	J	273	GLU	OE1-CD-OE2	5.22	129.57	123.30
3	E	557	LEU	CA-CB-CG	5.20	127.27	115.30
4	H	625	LEU	CA-CB-CG	5.14	127.12	115.30
3	A	734	LEU	CA-CB-CG	5.12	127.08	115.30
4	H	771	LEU	CA-CB-CG	5.11	127.06	115.30
3	C	655	LEU	CA-CB-CG	5.11	127.04	115.30
3	G	306	LEU	CA-CB-CG	5.10	127.03	115.30
3	A	247	LEU	CA-CB-CG	5.10	127.03	115.30
4	j	108	PRO	N-CA-CB	5.06	109.38	103.30
4	B	771	LEU	CA-CB-CG	5.04	126.89	115.30
3	A	698	MET	CB-CG-SD	5.03	127.48	112.40
4	B	691	LEU	CA-CB-CG	5.02	126.85	115.30
3	G	836	LEU	CA-CB-CG	5.02	126.84	115.30
3	A	698	MET	CA-CB-CG	-5.01	104.78	113.30
4	B	772	LEU	CA-CB-CG	5.01	126.83	115.30
5	b	39	LEU	CA-CB-CG	5.01	126.83	115.30
3	E	306	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	583	ILE	Peptide
4	B	868	SER	Peptide
4	B	889	ARG	Peptide
3	C	238	LEU	Peptide
3	C	239	ALA	Peptide
4	D	626	LEU	Peptide
3	E	240	GLY	Peptide
3	E	474	GLU	Peptide
3	E	580	HIS	Peptide
3	E	674	GLN	Peptide
4	F	525	ASP	Peptide
3	G	240	GLY	Peptide
3	G	580	HIS	Peptide
4	H	321	GLY	Peptide
4	H	626	LEU	Peptide
4	H	632	ASP	Peptide
6	I	507	SER	Peptide
6	I	508	ASN	Mainchain
6	I	511	ASP	Peptide
6	I	516	ARG	Peptide
6	I	600	ASN	Peptide
6	I	601	LEU	Peptide
1	J	210	PRO	Peptide
1	J	235	SER	Peptide
1	J	237	HIS	Peptide
1	J	256	LEU	Peptide
1	J	726	PHE	Peptide
6	K	254	LEU	Peptide
6	K	318	PRO	Peptide
6	K	410	LEU	Peptide
7	L	1688	PHE	Peptide
7	L	293	LYS	Peptide
7	L	346	LEU	Peptide
8	O	347	ASN	Peptide
8	P	347	ASN	Peptide
8	Q	347	ASN	Peptide
8	R	347	ASN	Peptide
8	S	347	ASN	Peptide
8	T	347	ASN	Peptide
8	U	347	ASN	Peptide

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Mol	Chain	Res	Type	Group
8	V	347	ASN	Peptide
8	W	347	ASN	Peptide
8	X	347	ASN	Peptide
8	Y	347	ASN	Peptide
8	Z	347	ASN	Peptide
2	e	249	THR	Peptide
1	l	121	PRO	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	34	0
1	l	847	0	789	0	0
2	e	2847	0	2810	0	0
3	A	4978	0	4996	32	0
3	C	5044	0	5081	40	0
3	E	5206	0	5230	40	0
3	G	5206	0	5230	29	0
4	B	5029	0	5018	47	0
4	D	4796	0	4775	42	0
4	F	4941	0	4935	45	0
4	H	4907	0	4896	34	0
4	a	933	0	953	0	0
4	f	803	0	831	0	0
4	h	803	0	831	0	0
4	j	843	0	846	0	0
5	b	484	0	512	0	0
5	d	454	0	482	0	0
5	g	484	0	512	0	0
5	i	484	0	512	0	0
5	k	484	0	512	0	0
5	m	484	0	512	0	0
6	I	4225	0	4259	28	0
6	K	4579	0	4586	60	0
7	L	4587	0	4636	26	0
7	c	1220	0	1231	0	0
8	O	3373	0	3325	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	P	3373	0	3325	74	0
8	Q	3373	0	3325	66	0
8	R	3373	0	3325	71	0
8	S	3373	0	3325	69	0
8	T	3373	0	3325	71	0
8	U	3373	0	3325	68	0
8	V	3373	0	3325	69	0
8	W	3373	0	3325	69	0
8	X	3373	0	3325	71	0
8	Y	3373	0	3325	80	0
8	Z	3373	0	3325	70	0
9	l	6	0	0	0	0
All	All	109579	0	109357	1214	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1214) 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)
6:K:653:LYS:NZ	8:Y:349:ILE:O	2.13	0.80
3:G:222:LEU:HG	4:H:365:ARG:HH12	1.46	0.80
3:C:696:TYR:O	3:C:700:GLU:HB2	1.85	0.76
6:K:497:ALA:HB2	8:Y:254:ILE:HD11	1.68	0.76
4:F:572:ASP:OD1	8:T:251:ASN:ND2	2.21	0.74
4:B:799:GLU:OE2	4:B:803:ARG:NH1	2.22	0.73
8:S:3:ARG:HH12	3:E:533:ASP:HB3	1.55	0.72
4:F:692:ARG:HD3	8:T:265:ARG:HD2	1.72	0.72
8:O:328:VAL:HG21	8:O:360:LEU:HD11	1.74	0.70
8:Z:328:VAL:HG21	8:Z:360:LEU:HD11	1.74	0.70
8:U:328:VAL:HG21	8:U:360:LEU:HD11	1.74	0.70
8:S:328:VAL:HG21	8:S:360:LEU:HD11	1.74	0.70
8:W:328:VAL:HG21	8:W:360:LEU:HD11	1.74	0.70
8:R:328:VAL:HG21	8:R:360:LEU:HD11	1.74	0.69
8:V:328:VAL:HG21	8:V:360:LEU:HD11	1.74	0.69
8:Q:328:VAL:HG21	8:Q:360:LEU:HD11	1.74	0.69
4:B:364:LEU:H	4:B:370:TRP:HE1	1.39	0.69
8:P:328:VAL:HG21	8:P:360:LEU:HD11	1.74	0.69
6:I:154:LEU:O	6:I:158:TYR:HB2	1.93	0.68
3:A:529:VAL:HG22	8:O:3:ARG:HH11	1.57	0.68
8:X:328:VAL:HG21	8:X:360:LEU:HD11	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:328:VAL:HG21	8:Y:360:LEU:HD11	1.74	0.68
3:A:698:MET:SD	8:O:248:TYR:OH	2.47	0.68
6:K:375:THR:OG1	6:K:402:LYS:NZ	2.26	0.68
6:K:646:LEU:HB3	8:Y:341:ARG:HD2	1.75	0.68
8:T:328:VAL:HG21	8:T:360:LEU:HD11	1.74	0.67
6:I:362:LEU:HB3	6:I:537:LEU:HD13	1.76	0.67
6:K:651:TYR:CZ	8:Y:354:ALA:HB3	2.30	0.67
3:C:533:ASP:OD2	8:Q:3:ARG:NH1	2.26	0.66
4:B:579:ASP:OD2	8:P:3:ARG:NH1	2.30	0.65
8:Q:48:LYS:O	8:Q:54:GLN:NE2	2.30	0.65
3:E:578:MET:H	3:E:615:ALA:HB1	1.61	0.65
4:H:560:GLN:OE1	4:H:563:ARG:NH1	2.30	0.65
8:Z:48:LYS:O	8:Z:54:GLN:NE2	2.30	0.65
4:B:609:ASN:ND2	8:P:46:ASP:O	2.30	0.64
3:G:854:SER:OG	8:U:338:GLN:NE2	2.29	0.64
8:S:48:LYS:O	8:S:54:GLN:NE2	2.30	0.64
8:P:48:LYS:O	8:P:54:GLN:NE2	2.30	0.64
8:U:48:LYS:O	8:U:54:GLN:NE2	2.30	0.64
4:B:319:LEU:HD21	3:C:367:THR:HB	1.80	0.64
6:I:345:VAL:HG13	6:I:346:GLU:HG3	1.80	0.64
8:W:48:LYS:O	8:W:54:GLN:NE2	2.30	0.64
8:T:48:LYS:O	8:T:54:GLN:NE2	2.30	0.64
8:X:48:LYS:O	8:X:54:GLN:NE2	2.30	0.64
4:F:306:ARG:HH11	4:F:310:GLN:HE22	1.46	0.64
8:V:48:LYS:O	8:V:54:GLN:NE2	2.30	0.64
3:E:685:ARG:HE	3:E:865:TYR:HE2	1.46	0.64
6:K:649:LEU:HB3	6:K:655:TYR:HB2	1.80	0.63
6:K:649:LEU:HB2	8:Y:341:ARG:HH21	1.63	0.63
8:Y:48:LYS:O	8:Y:54:GLN:NE2	2.30	0.63
4:H:599:GLY:HA3	8:W:342:GLU:HG3	1.80	0.63
8:R:48:LYS:O	8:R:54:GLN:NE2	2.30	0.63
8:O:66:LEU:HD21	8:O:74:ILE:HG12	1.81	0.63
8:O:48:LYS:O	8:O:54:GLN:NE2	2.30	0.63
8:Z:66:LEU:HD21	8:Z:74:ILE:HG12	1.81	0.63
8:S:45:THR:HG23	3:E:566:THR:HG21	1.81	0.63
1:J:266:THR:OG1	1:J:269:GLN:NE2	2.32	0.63
6:K:516:ARG:HD2	8:Y:264:PRO:HD3	1.81	0.63
8:P:66:LEU:HD21	8:P:74:ILE:HG12	1.81	0.63
8:T:442:ASP:OD1	8:T:442:ASP:N	2.32	0.63
8:V:66:LEU:HD21	8:V:74:ILE:HG12	1.81	0.63
4:D:454:VAL:H	4:D:463:LYS:HE3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:66:LEU:HD21	8:W:74:ILE:HG12	1.81	0.62
4:D:686:CYS:O	4:D:689:LYS:NZ	2.31	0.62
8:W:442:ASP:OD1	8:W:442:ASP:N	2.32	0.62
8:Z:442:ASP:OD1	8:Z:442:ASP:N	2.32	0.62
8:Q:442:ASP:N	8:Q:442:ASP:OD1	2.32	0.62
8:S:233:SER:O	8:S:237:SER:OG	2.18	0.62
8:X:442:ASP:N	8:X:442:ASP:OD1	2.32	0.62
8:Y:66:LEU:HD21	8:Y:74:ILE:HG12	1.81	0.62
8:R:442:ASP:OD1	8:R:442:ASP:N	2.32	0.62
8:U:66:LEU:HD21	8:U:74:ILE:HG12	1.81	0.62
8:U:233:SER:O	8:U:237:SER:OG	2.18	0.62
8:W:233:SER:O	8:W:237:SER:OG	2.18	0.62
8:X:66:LEU:HD21	8:X:74:ILE:HG12	1.81	0.62
8:Y:233:SER:O	8:Y:237:SER:OG	2.18	0.62
3:E:359:LEU:HB3	3:E:380:THR:HG22	1.82	0.62
8:P:442:ASP:OD1	8:P:442:ASP:N	2.32	0.62
8:S:442:ASP:OD1	8:S:442:ASP:N	2.32	0.62
8:Z:233:SER:O	8:Z:237:SER:OG	2.18	0.62
4:B:681:ARG:NH1	8:P:261:ILE:O	2.33	0.61
3:G:529:VAL:O	8:U:3:ARG:NH1	2.33	0.61
6:I:148:ILE:HG23	6:I:152:GLN:HG2	1.81	0.61
8:Q:66:LEU:HD21	8:Q:74:ILE:HG12	1.81	0.61
6:K:649:LEU:HB2	8:Y:341:ARG:NH2	2.16	0.61
8:T:66:LEU:HD21	8:T:74:ILE:HG12	1.81	0.61
4:H:593:TYR:H	4:H:596:ASN:HD22	1.48	0.61
8:Q:313:THR:OG1	8:Q:314:ASN:N	2.34	0.61
8:Y:442:ASP:OD1	8:Y:442:ASP:N	2.32	0.61
8:Q:233:SER:O	8:Q:237:SER:OG	2.18	0.61
8:R:66:LEU:HD21	8:R:74:ILE:HG12	1.81	0.61
8:X:233:SER:O	8:X:237:SER:OG	2.18	0.61
8:S:66:LEU:HD21	8:S:74:ILE:HG12	1.81	0.61
8:V:351:TRP:NE1	8:V:438:ALA:O	2.31	0.61
8:P:351:TRP:NE1	8:P:438:ALA:O	2.31	0.61
8:R:351:TRP:NE1	8:R:438:ALA:O	2.31	0.61
8:V:233:SER:O	8:V:237:SER:OG	2.18	0.61
8:V:442:ASP:N	8:V:442:ASP:OD1	2.32	0.61
6:K:259:LEU:HG	6:K:277:LEU:HD22	1.81	0.60
8:P:233:SER:O	8:P:237:SER:OG	2.18	0.60
8:Z:313:THR:OG1	8:Z:314:ASN:N	2.34	0.60
4:H:430:LEU:HD23	4:H:446:PHE:HE1	1.66	0.60
8:T:313:THR:OG1	8:T:314:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:313:THR:OG1	8:V:314:ASN:N	2.34	0.60
3:C:475:ILE:HG12	3:C:487:GLN:HE21	1.67	0.60
8:O:351:TRP:NE1	8:O:438:ALA:O	2.31	0.60
8:U:313:THR:OG1	8:U:314:ASN:N	2.34	0.60
8:W:313:THR:OG1	8:W:314:ASN:N	2.34	0.60
8:T:233:SER:O	8:T:237:SER:OG	2.18	0.60
8:P:313:THR:OG1	8:P:314:ASN:N	2.34	0.60
8:Y:313:THR:OG1	8:Y:314:ASN:N	2.34	0.60
8:S:313:THR:OG1	8:S:314:ASN:N	2.34	0.60
3:A:554:LEU:HA	3:A:557:LEU:HD12	1.84	0.60
3:C:314:HIS:HB2	3:C:319:LEU:HD12	1.84	0.59
4:D:319:LEU:N	4:D:445:GLU:OE2	2.35	0.59
7:L:1683:VAL:HG12	8:Z:331:THR:HA	1.84	0.59
8:O:233:SER:O	8:O:237:SER:OG	2.18	0.59
8:U:442:ASP:OD1	8:U:442:ASP:N	2.32	0.59
8:R:313:THR:OG1	8:R:314:ASN:N	2.34	0.59
4:B:561:ALA:HA	4:B:564:ARG:HE	1.68	0.59
6:K:31:PHE:HB2	6:K:34:LEU:HG	1.84	0.59
6:K:399:SER:HA	6:K:402:LYS:HE2	1.83	0.59
6:K:646:LEU:O	8:Y:341:ARG:NE	2.35	0.59
8:O:442:ASP:N	8:O:442:ASP:OD1	2.32	0.59
8:X:351:TRP:NE1	8:X:438:ALA:O	2.31	0.59
8:Y:351:TRP:NE1	8:Y:438:ALA:O	2.31	0.59
4:F:406:THR:HG21	4:F:411:MET:HB2	1.85	0.58
8:X:313:THR:OG1	8:X:314:ASN:N	2.34	0.58
3:E:719:ILE:HA	3:E:722:VAL:HG22	1.85	0.58
4:D:572:ASP:OD1	8:R:251:ASN:ND2	2.36	0.58
6:I:511:ASP:H	6:I:514:LYS:HD2	1.67	0.58
3:A:533:ASP:HB2	8:O:3:ARG:HH12	1.69	0.58
6:K:188:SER:HA	6:K:311:LEU:HD13	1.85	0.58
8:O:141:ILE:HB	8:O:173:PRO:HD3	1.86	0.58
8:O:303:VAL:HG12	8:O:305:VAL:H	1.69	0.58
8:S:303:VAL:HG12	8:S:305:VAL:H	1.69	0.58
8:Y:226:SER:OG	8:Y:227:GLN:NE2	2.37	0.58
8:Z:303:VAL:HG12	8:Z:305:VAL:H	1.69	0.58
4:B:737:LYS:HE3	4:B:746:HIS:HB3	1.85	0.58
8:Q:226:SER:OG	8:Q:227:GLN:NE2	2.37	0.58
8:V:141:ILE:HB	8:V:173:PRO:HD3	1.86	0.58
8:O:226:SER:OG	8:O:227:GLN:NE2	2.37	0.58
8:R:141:ILE:HB	8:R:173:PRO:HD3	1.86	0.58
4:H:589:ALA:HA	4:H:592:LEU:HG	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:226:SER:OG	8:P:227:GLN:NE2	2.37	0.58
8:S:141:ILE:HB	8:S:173:PRO:HD3	1.86	0.58
8:T:303:VAL:HG12	8:T:305:VAL:H	1.69	0.58
8:U:351:TRP:NE1	8:U:438:ALA:O	2.31	0.58
8:W:303:VAL:HG12	8:W:305:VAL:H	1.69	0.58
8:Y:303:VAL:HG12	8:Y:305:VAL:H	1.69	0.58
4:B:886:TYR:CE2	8:P:353:PRO:HG3	2.39	0.58
8:W:226:SER:OG	8:W:227:GLN:NE2	2.37	0.58
4:F:419:LEU:HA	4:F:422:VAL:HG22	1.86	0.57
1:J:724:ARG:HH12	1:J:914:GLN:HB3	1.69	0.57
8:R:226:SER:OG	8:R:227:GLN:NE2	2.37	0.57
8:S:226:SER:OG	8:S:227:GLN:NE2	2.37	0.57
8:U:303:VAL:HG12	8:U:305:VAL:H	1.69	0.57
8:X:141:ILE:HB	8:X:173:PRO:HD3	1.86	0.57
4:H:599:GLY:HA2	4:H:602:GLU:HG3	1.85	0.57
8:R:233:SER:O	8:R:237:SER:OG	2.18	0.57
8:R:303:VAL:HG12	8:R:305:VAL:H	1.69	0.57
8:X:303:VAL:HG12	8:X:305:VAL:H	1.69	0.57
8:O:313:THR:OG1	8:O:314:ASN:N	2.34	0.57
3:E:154:LEU:HA	3:E:157:LYS:HD2	1.87	0.57
8:V:226:SER:OG	8:V:227:GLN:NE2	2.37	0.57
8:Z:141:ILE:HB	8:Z:173:PRO:HD3	1.86	0.57
4:B:284:SER:OG	4:B:285:ARG:NH2	2.36	0.57
4:D:494:HIS:HD2	4:D:500:GLN:HG3	1.70	0.57
1:J:885:LEU:HD11	8:X:444:ILE:HA	1.86	0.57
8:T:141:ILE:HB	8:T:173:PRO:HD3	1.86	0.57
6:I:353:GLN:NE2	6:I:457:TYR:OH	2.37	0.57
8:Z:226:SER:OG	8:Z:227:GLN:NE2	2.37	0.57
8:Q:303:VAL:HG12	8:Q:305:VAL:H	1.69	0.57
8:Y:141:ILE:HB	8:Y:173:PRO:HD3	1.86	0.57
4:F:645:ASP:HA	4:F:649:ALA:HB2	1.87	0.57
7:L:1677:ALA:HA	7:L:1681:LEU:HD12	1.86	0.57
8:T:226:SER:OG	8:T:227:GLN:NE2	2.37	0.57
8:W:141:ILE:HB	8:W:173:PRO:HD3	1.86	0.57
8:X:226:SER:OG	8:X:227:GLN:NE2	2.37	0.57
3:E:518:ARG:HA	3:E:523:ASP:H	1.69	0.57
8:S:258:ALA:HB1	3:E:687:LEU:HD21	1.87	0.57
8:U:141:ILE:HB	8:U:173:PRO:HD3	1.86	0.57
8:U:226:SER:OG	8:U:227:GLN:NE2	2.37	0.57
3:C:297:ARG:HH12	4:D:410:TYR:HB2	1.70	0.57
8:V:303:VAL:HG12	8:V:305:VAL:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:303:VAL:HG12	8:P:305:VAL:H	1.69	0.56
3:C:864:PHE:HB3	8:Q:353:PRO:HA	1.88	0.56
8:T:351:TRP:NE1	8:T:438:ALA:O	2.31	0.56
4:D:560:GLN:HE21	4:D:564:ARG:HE	1.54	0.56
4:D:594:GLN:NE2	4:D:623:VAL:O	2.39	0.56
4:H:563:ARG:HH21	4:H:569:GLY:HA3	1.71	0.56
8:U:177:GLU:OE2	8:U:184:GLN:NE2	2.39	0.56
8:X:177:GLU:OE2	8:X:184:GLN:NE2	2.39	0.56
8:P:141:ILE:HB	8:P:173:PRO:HD3	1.86	0.56
8:Q:351:TRP:NE1	8:Q:438:ALA:O	2.31	0.56
3:A:237:PRO:HA	3:A:244:ARG:HE	1.71	0.56
8:Q:141:ILE:HB	8:Q:173:PRO:HD3	1.86	0.56
8:R:177:GLU:OE2	8:R:184:GLN:NE2	2.39	0.56
8:W:177:GLU:OE2	8:W:184:GLN:NE2	2.39	0.56
8:S:112:GLU:O	8:S:115:HIS:ND1	2.39	0.56
8:S:177:GLU:OE2	8:S:184:GLN:NE2	2.39	0.56
8:Y:177:GLU:OE2	8:Y:184:GLN:NE2	2.39	0.56
1:J:1015:LEU:HD13	8:X:341:ARG:HG3	1.89	0.55
8:R:112:GLU:O	8:R:115:HIS:ND1	2.39	0.55
8:T:177:GLU:OE2	8:T:184:GLN:NE2	2.39	0.55
8:Z:177:GLU:OE2	8:Z:184:GLN:NE2	2.39	0.55
3:C:518:ARG:HA	3:C:523:ASP:HB3	1.87	0.55
8:O:177:GLU:OE2	8:O:184:GLN:NE2	2.39	0.55
8:P:177:GLU:OE2	8:P:184:GLN:NE2	2.39	0.55
4:B:308:THR:O	4:B:312:SER:OG	2.23	0.55
8:Z:124:ARG:NH1	8:Z:125:GLU:OE2	2.40	0.55
1:J:278:LEU:HD23	1:J:379:LEU:HD11	1.89	0.55
8:X:121:ILE:HG23	8:X:124:ARG:HH21	1.72	0.55
8:Y:112:GLU:O	8:Y:115:HIS:ND1	2.39	0.55
8:Z:351:TRP:NE1	8:Z:438:ALA:O	2.31	0.55
8:O:124:ARG:NH1	8:O:125:GLU:OE2	2.40	0.55
8:W:124:ARG:NH1	8:W:125:GLU:OE2	2.40	0.55
8:O:62:PRO:HD2	8:O:86:TYR:HB3	1.89	0.55
4:H:633:THR:OG1	4:H:634:GLY:N	2.40	0.55
6:I:528:LEU:HD13	6:I:531:TYR:HD2	1.70	0.55
8:O:112:GLU:O	8:O:115:HIS:ND1	2.39	0.55
8:Q:112:GLU:O	8:Q:115:HIS:ND1	2.39	0.55
8:R:62:PRO:HD2	8:R:86:TYR:HB3	1.89	0.55
8:S:121:ILE:HG23	8:S:124:ARG:HH21	1.72	0.55
8:Y:62:PRO:HD2	8:Y:86:TYR:HB3	1.89	0.55
8:Y:121:ILE:HG23	8:Y:124:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:124:ARG:NH1	8:Q:125:GLU:OE2	2.40	0.55
8:Q:177:GLU:OE2	8:Q:184:GLN:NE2	2.39	0.55
8:V:62:PRO:HD2	8:V:86:TYR:HB3	1.89	0.55
8:V:177:GLU:OE2	8:V:184:GLN:NE2	2.39	0.55
8:X:62:PRO:HD2	8:X:86:TYR:HB3	1.89	0.55
7:L:311:TYR:HD2	7:L:314:GLU:HG3	1.71	0.55
8:P:112:GLU:O	8:P:115:HIS:ND1	2.39	0.55
8:R:124:ARG:NH1	8:R:125:GLU:OE2	2.40	0.55
8:S:351:TRP:NE1	8:S:438:ALA:O	2.31	0.55
8:V:121:ILE:HG23	8:V:124:ARG:HH21	1.72	0.55
8:X:124:ARG:NH1	8:X:125:GLU:OE2	2.40	0.55
3:C:696:TYR:HE1	3:C:854:SER:HB2	1.71	0.55
3:G:359:LEU:HB3	3:G:380:THR:HG22	1.89	0.55
8:W:62:PRO:HD2	8:W:86:TYR:HB3	1.89	0.55
8:R:121:ILE:HG23	8:R:124:ARG:HH21	1.72	0.54
8:U:124:ARG:NH1	8:U:125:GLU:OE2	2.40	0.54
8:V:112:GLU:O	8:V:115:HIS:ND1	2.39	0.54
8:V:124:ARG:NH1	8:V:125:GLU:OE2	2.40	0.54
8:W:112:GLU:O	8:W:115:HIS:ND1	2.39	0.54
8:W:121:ILE:HG23	8:W:124:ARG:HH21	1.72	0.54
8:O:121:ILE:HG23	8:O:124:ARG:HH21	1.72	0.54
8:S:124:ARG:NH1	8:S:125:GLU:OE2	2.40	0.54
4:B:550:ASN:HB3	4:B:551:LYS:HZ3	1.71	0.54
4:D:699:GLY:HA2	8:R:446:TRP:HE1	1.73	0.54
4:F:451:ASP:H	4:F:463:LYS:HA	1.72	0.54
8:T:121:ILE:HG23	8:T:124:ARG:HH21	1.72	0.54
8:W:351:TRP:NE1	8:W:438:ALA:O	2.31	0.54
8:Z:62:PRO:HD2	8:Z:86:TYR:HB3	1.89	0.54
3:C:440:PRO:HD2	3:C:443:LEU:HD11	1.90	0.54
6:K:68:GLN:NE2	6:K:198:ASP:OD2	2.40	0.54
8:W:184:GLN:O	8:W:188:SER:OG	2.26	0.54
8:Z:121:ILE:HG23	8:Z:124:ARG:HH21	1.72	0.54
8:Z:184:GLN:O	8:Z:188:SER:OG	2.26	0.54
8:R:184:GLN:O	8:R:188:SER:OG	2.26	0.54
8:T:112:GLU:O	8:T:115:HIS:ND1	2.39	0.54
8:Y:124:ARG:NH1	8:Y:125:GLU:OE2	2.40	0.54
8:Z:112:GLU:O	8:Z:115:HIS:ND1	2.39	0.54
4:B:566:LEU:HG	4:B:640:LEU:HD21	1.89	0.54
8:Q:62:PRO:HD2	8:Q:86:TYR:HB3	1.89	0.54
8:T:124:ARG:NH1	8:T:125:GLU:OE2	2.40	0.54
8:U:62:PRO:HD2	8:U:86:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:361:SER:OG	8:W:362:ARG:N	2.41	0.54
8:X:184:GLN:O	8:X:188:SER:OG	2.26	0.54
8:Z:20:GLU:HG2	8:Z:229:ASN:HB3	1.90	0.54
8:U:112:GLU:O	8:U:115:HIS:ND1	2.39	0.54
8:X:112:GLU:O	8:X:115:HIS:ND1	2.39	0.54
8:Z:361:SER:OG	8:Z:362:ARG:N	2.41	0.54
8:V:20:GLU:HG2	8:V:229:ASN:HB3	1.90	0.54
3:E:356:LEU:HG	3:E:440:PRO:HB3	1.89	0.54
4:H:627:GLU:HG2	4:H:628:VAL:H	1.73	0.54
8:P:121:ILE:HG23	8:P:124:ARG:HH21	1.72	0.54
8:Q:121:ILE:HG23	8:Q:124:ARG:HH21	1.72	0.54
8:U:20:GLU:HG2	8:U:229:ASN:HB3	1.90	0.54
8:U:361:SER:OG	8:U:362:ARG:N	2.41	0.54
8:Y:184:GLN:O	8:Y:188:SER:OG	2.26	0.54
4:B:866:THR:HA	4:B:874:ARG:HE	1.71	0.53
8:R:20:GLU:HG2	8:R:229:ASN:HB3	1.90	0.53
8:T:62:PRO:HD2	8:T:86:TYR:HB3	1.89	0.53
8:Z:231:LEU:O	8:Z:234:THR:OG1	2.24	0.53
6:I:515:TRP:HE1	6:I:519:ASN:H	1.55	0.53
8:O:20:GLU:HG2	8:O:229:ASN:HB3	1.90	0.53
8:S:62:PRO:HD2	8:S:86:TYR:HB3	1.89	0.53
8:V:184:GLN:O	8:V:188:SER:OG	2.26	0.53
8:Y:20:GLU:HG2	8:Y:229:ASN:HB3	1.90	0.53
8:P:62:PRO:HD2	8:P:86:TYR:HB3	1.89	0.53
8:S:20:GLU:HG2	8:S:229:ASN:HB3	1.90	0.53
8:T:184:GLN:O	8:T:188:SER:OG	2.26	0.53
3:E:764:LYS:HG2	3:E:767:GLN:HE21	1.73	0.53
8:O:184:GLN:O	8:O:188:SER:OG	2.26	0.53
8:P:124:ARG:NH1	8:P:125:GLU:OE2	2.40	0.53
8:Q:361:SER:OG	8:Q:362:ARG:N	2.41	0.53
3:E:242:GLN:NE2	3:E:272:ALA:O	2.42	0.53
4:H:433:TRP:HD1	4:H:483:VAL:HG22	1.74	0.53
3:C:485:VAL:HA	3:C:488:ILE:HD12	1.89	0.53
6:I:370:GLN:HE22	8:W:3:ARG:NH1	2.07	0.53
8:P:361:SER:OG	8:P:362:ARG:N	2.40	0.53
8:Q:184:GLN:O	8:Q:188:SER:OG	2.26	0.53
8:S:67:LEU:HD13	8:S:118:ILE:HB	1.91	0.53
8:W:67:LEU:HD13	8:W:118:ILE:HB	1.91	0.53
8:Y:231:LEU:O	8:Y:234:THR:OG1	2.24	0.53
8:S:53:TYR:HB3	8:S:61:ILE:HB	1.91	0.53
8:Q:20:GLU:HG2	8:Q:229:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:184:GLN:O	8:S:188:SER:OG	2.26	0.53
3:E:223:TYR:HB3	3:E:228:VAL:HG13	1.89	0.53
8:S:353:PRO:HG3	3:E:865:TYR:CD2	2.44	0.53
8:U:184:GLN:O	8:U:188:SER:OG	2.26	0.53
8:U:231:LEU:O	8:U:234:THR:OG1	2.24	0.53
4:D:885:HIS:NE2	4:D:890:GLU:HG3	2.24	0.53
8:O:53:TYR:HB3	8:O:61:ILE:HB	1.91	0.53
8:Q:67:LEU:HD13	8:Q:118:ILE:HB	1.91	0.53
8:S:231:LEU:O	8:S:234:THR:OG1	2.24	0.53
8:S:361:SER:OG	8:S:362:ARG:N	2.41	0.53
8:T:67:LEU:HD13	8:T:118:ILE:HB	1.91	0.53
8:U:52:PHE:HB3	8:U:60:TYR:HB3	1.92	0.53
8:U:121:ILE:HG23	8:U:124:ARG:HH21	1.72	0.53
8:W:20:GLU:HG2	8:W:229:ASN:HB3	1.90	0.53
8:W:52:PHE:HB3	8:W:60:TYR:HB3	1.92	0.53
3:G:529:VAL:HG22	8:U:3:ARG:HH11	1.73	0.52
8:P:20:GLU:HG2	8:P:229:ASN:HB3	1.90	0.52
8:Q:53:TYR:HB3	8:Q:61:ILE:HB	1.91	0.52
8:R:67:LEU:HD13	8:R:118:ILE:HB	1.91	0.52
8:T:361:SER:OG	8:T:362:ARG:N	2.41	0.52
8:X:53:TYR:HB3	8:X:61:ILE:HB	1.91	0.52
8:T:20:GLU:HG2	8:T:229:ASN:HB3	1.90	0.52
8:U:46:ASP:OD1	8:U:46:ASP:N	2.42	0.52
8:X:46:ASP:OD1	8:X:46:ASP:N	2.42	0.52
8:X:67:LEU:HD13	8:X:118:ILE:HB	1.91	0.52
4:H:427:LEU:HD12	4:H:430:LEU:HD12	1.90	0.52
8:O:46:ASP:OD1	8:O:46:ASP:N	2.42	0.52
8:P:53:TYR:HB3	8:P:61:ILE:HB	1.91	0.52
8:O:67:LEU:HD13	8:O:118:ILE:HB	1.91	0.52
8:P:184:GLN:O	8:P:188:SER:OG	2.26	0.52
8:S:353:PRO:HA	3:E:862:ASN:ND2	2.24	0.52
8:X:20:GLU:HG2	8:X:229:ASN:HB3	1.90	0.52
8:X:231:LEU:O	8:X:234:THR:OG1	2.24	0.52
4:B:336:TYR:HA	4:B:339:LEU:HD12	1.92	0.52
8:V:361:SER:OG	8:V:362:ARG:N	2.41	0.52
8:X:52:PHE:HB3	8:X:60:TYR:HB3	1.91	0.52
3:C:217:VAL:HG23	3:C:321:LEU:HD21	1.91	0.52
6:K:520:HIS:NE2	8:Y:259:SER:O	2.39	0.52
8:P:46:ASP:OD1	8:P:46:ASP:N	2.42	0.52
8:T:52:PHE:HB3	8:T:60:TYR:HB3	1.91	0.52
8:Z:67:LEU:HD13	8:Z:118:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:546:ILE:HD11	3:E:551:LEU:HD21	1.92	0.52
6:K:651:TYR:HB3	6:K:653:LYS:NZ	2.25	0.52
8:P:67:LEU:HD13	8:P:118:ILE:HB	1.91	0.52
8:R:46:ASP:N	8:R:46:ASP:OD1	2.42	0.52
8:U:67:LEU:HD13	8:U:118:ILE:HB	1.91	0.52
4:H:626:LEU:HG	4:H:637:VAL:HA	1.92	0.52
8:Q:52:PHE:HB3	8:Q:60:TYR:HB3	1.92	0.52
8:T:53:TYR:HB3	8:T:61:ILE:HB	1.91	0.52
8:R:52:PHE:HB3	8:R:60:TYR:HB3	1.91	0.52
8:Y:67:LEU:HD13	8:Y:118:ILE:HB	1.91	0.52
8:Y:361:SER:OG	8:Y:362:ARG:N	2.41	0.52
3:C:395:ILE:HD11	3:C:450:ILE:HG23	1.91	0.52
6:I:117:LEU:HD22	6:I:121:HIS:HB2	1.92	0.52
1:J:273:GLU:OE2	1:J:284:LEU:HB3	2.10	0.52
8:Y:46:ASP:N	8:Y:46:ASP:OD1	2.42	0.52
8:Y:53:TYR:HB3	8:Y:61:ILE:HB	1.91	0.52
8:P:52:PHE:HB3	8:P:60:TYR:HB3	1.92	0.51
8:Q:46:ASP:OD1	8:Q:46:ASP:N	2.42	0.51
8:R:361:SER:OG	8:R:362:ARG:N	2.41	0.51
8:T:46:ASP:N	8:T:46:ASP:OD1	2.42	0.51
8:W:46:ASP:N	8:W:46:ASP:OD1	2.42	0.51
8:Z:46:ASP:OD1	8:Z:46:ASP:N	2.42	0.51
4:H:874:ARG:HH21	4:H:875:PHE:HB2	1.74	0.51
8:O:231:LEU:O	8:O:234:THR:OG1	2.24	0.51
8:T:231:LEU:O	8:T:234:THR:OG1	2.24	0.51
8:V:53:TYR:HB3	8:V:61:ILE:HB	1.91	0.51
3:C:186:ALA:HB1	4:D:293:ARG:HA	1.92	0.51
1:J:320:TYR:HD1	1:J:409:LEU:HD23	1.75	0.51
8:O:317:TYR:HB2	8:O:348:PHE:HE1	1.76	0.51
8:P:231:LEU:O	8:P:234:THR:OG1	2.24	0.51
8:Q:231:LEU:O	8:Q:234:THR:OG1	2.24	0.51
8:V:67:LEU:HD13	8:V:118:ILE:HB	1.91	0.51
8:V:317:TYR:HB2	8:V:348:PHE:HE1	1.76	0.51
8:Z:53:TYR:HB3	8:Z:61:ILE:HB	1.91	0.51
8:Z:317:TYR:HB2	8:Z:348:PHE:HE1	1.76	0.51
4:F:694:MET:HG3	4:F:696:GLU:HG2	1.92	0.51
4:H:707:LEU:HD21	4:H:850:LEU:HD22	1.92	0.51
8:V:46:ASP:OD1	8:V:46:ASP:N	2.42	0.51
3:G:314:HIS:HB2	3:G:319:LEU:HD12	1.93	0.51
8:O:52:PHE:HB3	8:O:60:TYR:HB3	1.91	0.51
8:T:229:ASN:O	8:T:233:SER:OG	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:15:ASN:ND2	8:X:68:ASP:OD1	2.40	0.51
4:D:729:CYS:SG	4:D:730:SER:N	2.83	0.51
6:K:649:LEU:HD22	8:Y:341:ARG:HH22	1.74	0.51
8:O:361:SER:OG	8:O:362:ARG:N	2.40	0.51
8:P:317:TYR:HB2	8:P:348:PHE:HE1	1.76	0.51
8:S:52:PHE:HB3	8:S:60:TYR:HB3	1.92	0.51
8:T:317:TYR:HB2	8:T:348:PHE:HE1	1.76	0.51
8:U:317:TYR:HB2	8:U:348:PHE:HE1	1.76	0.51
8:W:53:TYR:HB3	8:W:61:ILE:HB	1.91	0.51
8:W:231:LEU:O	8:W:234:THR:OG1	2.24	0.51
8:W:274:THR:HA	8:W:302:ASN:HD22	1.76	0.51
3:A:427:TYR:OH	3:A:462:GLU:OE1	2.29	0.51
8:P:156:ARG:O	8:P:160:ARG:HB2	2.11	0.51
8:R:53:TYR:HB3	8:R:61:ILE:HB	1.91	0.51
8:U:156:ARG:O	8:U:160:ARG:HB2	2.11	0.51
8:Y:156:ARG:O	8:Y:160:ARG:HB2	2.11	0.51
8:U:274:THR:HA	8:U:302:ASN:HD22	1.76	0.51
8:Z:52:PHE:HB3	8:Z:60:TYR:HB3	1.92	0.51
8:Z:156:ARG:O	8:Z:160:ARG:HB2	2.11	0.51
3:C:273:VAL:HG22	3:C:338:LEU:HD22	1.93	0.51
3:G:557:LEU:HD13	8:V:343:ARG:HB2	1.92	0.51
8:P:15:ASN:ND2	8:P:68:ASP:OD1	2.40	0.51
8:S:46:ASP:OD1	8:S:46:ASP:N	2.42	0.51
8:S:274:THR:HA	8:S:302:ASN:HD22	1.76	0.51
8:U:53:TYR:HB3	8:U:61:ILE:HB	1.91	0.51
8:V:52:PHE:HB3	8:V:60:TYR:HB3	1.92	0.51
8:V:274:THR:HA	8:V:302:ASN:HD22	1.76	0.51
8:X:274:THR:HA	8:X:302:ASN:HD22	1.76	0.51
8:Y:274:THR:HA	8:Y:302:ASN:HD22	1.76	0.51
8:T:156:ARG:O	8:T:160:ARG:HB2	2.11	0.50
8:V:156:ARG:O	8:V:160:ARG:HB2	2.11	0.50
3:A:290:HIS:ND1	4:B:406:THR:O	2.39	0.50
3:A:862:ASN:ND2	8:O:352:GLY:O	2.39	0.50
4:H:317:PHE:HE2	4:H:321:GLY:HA3	1.75	0.50
8:R:231:LEU:O	8:R:234:THR:OG1	2.24	0.50
8:R:274:THR:HA	8:R:302:ASN:HD22	1.76	0.50
8:X:361:SER:OG	8:X:362:ARG:N	2.41	0.50
8:Y:317:TYR:HB2	8:Y:348:PHE:HE1	1.76	0.50
8:Q:274:THR:HA	8:Q:302:ASN:HD22	1.76	0.50
8:W:317:TYR:HB2	8:W:348:PHE:HE1	1.76	0.50
8:Y:15:ASN:ND2	8:Y:68:ASP:OD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:214:GLU:OE2	3:E:321:LEU:N	2.45	0.50
4:H:367:LEU:HA	4:H:370:TRP:HD1	1.77	0.50
6:K:630:LEU:HD13	6:K:645:LEU:HD21	1.93	0.50
8:P:160:ARG:O	8:P:160:ARG:NH1	2.45	0.50
8:Q:317:TYR:HB2	8:Q:348:PHE:HE1	1.76	0.50
8:S:317:TYR:HB2	8:S:348:PHE:HE1	1.76	0.50
8:W:156:ARG:O	8:W:160:ARG:HB2	2.11	0.50
8:X:317:TYR:HB2	8:X:348:PHE:HE1	1.76	0.50
8:Y:52:PHE:HB3	8:Y:60:TYR:HB3	1.92	0.50
8:Z:274:THR:HA	8:Z:302:ASN:HD22	1.76	0.50
3:C:302:GLU:HA	3:C:305:ILE:HD12	1.93	0.50
4:F:247:GLU:HA	4:F:250:LEU:HD12	1.93	0.50
4:H:597:LEU:HD12	4:H:600:ILE:HD11	1.94	0.50
6:K:510:THR:OG1	6:K:511:ASP:N	2.45	0.50
8:P:274:THR:HA	8:P:302:ASN:HD22	1.76	0.50
8:Q:160:ARG:O	8:Q:160:ARG:NH1	2.45	0.50
8:R:317:TYR:HB2	8:R:348:PHE:HE1	1.76	0.50
8:S:156:ARG:O	8:S:160:ARG:HB2	2.11	0.50
8:X:156:ARG:O	8:X:160:ARG:HB2	2.11	0.50
3:C:542:PRO:HA	3:C:611:SER:HA	1.92	0.50
4:F:606:ARG:HE	8:U:339:ARG:NE	2.10	0.50
8:O:160:ARG:NH1	8:O:160:ARG:O	2.45	0.50
8:T:160:ARG:O	8:T:160:ARG:NH1	2.45	0.50
8:Z:160:ARG:O	8:Z:160:ARG:NH1	2.45	0.50
4:H:585:LEU:HD22	4:H:635:TRP:HA	1.92	0.50
8:Q:156:ARG:O	8:Q:160:ARG:HB2	2.11	0.50
8:R:156:ARG:O	8:R:160:ARG:HB2	2.11	0.50
4:D:462:ASP:OD2	4:D:462:ASP:N	2.43	0.50
7:L:1761:ASN:OD1	7:L:1761:ASN:N	2.44	0.50
8:R:160:ARG:O	8:R:160:ARG:NH1	2.45	0.50
3:A:152:GLN:HE22	3:A:241:ARG:HB2	1.76	0.50
8:Q:183:VAL:HG13	8:Q:187:ASN:HD21	1.77	0.50
8:S:160:ARG:O	8:S:160:ARG:NH1	2.45	0.50
8:U:160:ARG:O	8:U:160:ARG:NH1	2.45	0.50
8:V:183:VAL:HG13	8:V:187:ASN:HD21	1.77	0.49
8:W:160:ARG:O	8:W:160:ARG:NH1	2.45	0.49
8:W:195:LEU:HB3	8:W:202:VAL:HG21	1.94	0.49
6:I:553:ASP:O	6:I:556:SER:OG	2.30	0.49
1:J:556:LEU:HA	1:J:559:ILE:HD12	1.93	0.49
8:Q:195:LEU:HB3	8:Q:202:VAL:HG21	1.94	0.49
8:T:195:LEU:HB3	8:T:202:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:183:VAL:HG13	8:Y:187:ASN:HD21	1.77	0.49
4:F:553:TYR:HB3	4:F:648:ILE:HD11	1.94	0.49
8:S:183:VAL:HG13	8:S:187:ASN:HD21	1.77	0.49
8:T:274:THR:HA	8:T:302:ASN:HD22	1.76	0.49
8:U:113:LYS:HG3	8:U:114:ILE:HG23	1.95	0.49
8:W:229:ASN:O	8:W:233:SER:OG	2.22	0.49
4:B:319:LEU:HD11	3:C:367:THR:H	1.77	0.49
4:D:651:VAL:HG22	4:D:744:LEU:HD11	1.94	0.49
1:J:487:ASP:OD1	1:J:487:ASP:N	2.44	0.49
8:O:156:ARG:O	8:O:160:ARG:HB2	2.11	0.49
8:T:183:VAL:HG13	8:T:187:ASN:HD21	1.77	0.49
8:T:415:LYS:HZ2	8:T:419:ASP:H	1.60	0.49
8:V:113:LYS:HG3	8:V:114:ILE:HG23	1.95	0.49
8:W:183:VAL:HG13	8:W:187:ASN:HD21	1.77	0.49
8:X:183:VAL:HG13	8:X:187:ASN:HD21	1.77	0.49
8:Y:160:ARG:O	8:Y:160:ARG:NH1	2.45	0.49
3:A:224:VAL:HG21	3:A:233:VAL:HG13	1.92	0.49
4:D:490:ILE:HG13	4:D:494:HIS:CE1	2.48	0.49
4:F:433:TRP:HD1	4:F:483:VAL:HG22	1.77	0.49
8:O:183:VAL:HG13	8:O:187:ASN:HD21	1.77	0.49
8:O:274:THR:HA	8:O:302:ASN:HD22	1.76	0.49
8:P:79:ASN:OD1	8:P:79:ASN:N	2.46	0.49
8:S:56:ASP:HA	8:T:296:ARG:HH21	1.78	0.49
8:T:113:LYS:HG3	8:T:114:ILE:HG23	1.95	0.49
8:W:79:ASN:OD1	8:W:79:ASN:N	2.46	0.49
4:B:886:TYR:HE2	8:P:353:PRO:HG3	1.76	0.49
4:F:660:TYR:HA	4:F:663:VAL:HG12	1.94	0.49
6:I:260:ARG:HG2	6:I:262:GLU:H	1.77	0.49
8:S:188:SER:O	8:S:192:LEU:HB2	2.13	0.49
8:S:415:LYS:HZ2	8:S:419:ASP:H	1.61	0.49
8:U:79:ASN:OD1	8:U:79:ASN:N	2.46	0.49
8:W:113:LYS:HG3	8:W:114:ILE:HG23	1.95	0.49
8:X:160:ARG:O	8:X:160:ARG:NH1	2.45	0.49
8:X:188:SER:O	8:X:192:LEU:HB2	2.13	0.49
3:A:307:VAL:HA	3:A:310:LEU:HD12	1.95	0.49
4:H:308:THR:O	4:H:312:SER:OG	2.26	0.49
8:P:183:VAL:HG13	8:P:187:ASN:HD21	1.77	0.49
8:R:183:VAL:HG13	8:R:187:ASN:HD21	1.77	0.49
8:V:160:ARG:O	8:V:160:ARG:NH1	2.45	0.49
8:Z:79:ASN:OD1	8:Z:79:ASN:N	2.46	0.49
8:Z:188:SER:O	8:Z:192:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:188:SER:O	8:O:192:LEU:HB2	2.13	0.49
8:U:195:LEU:HB3	8:U:202:VAL:HG21	1.94	0.49
8:Y:195:LEU:HB3	8:Y:202:VAL:HG21	1.94	0.49
4:D:688:ALA:HB1	4:D:692:ARG:NH1	2.28	0.49
4:F:412:ARG:O	4:F:416:GLN:HB2	2.12	0.49
1:J:221:VAL:HG22	6:K:35:HIS:CE1	2.48	0.49
8:O:195:LEU:HB3	8:O:202:VAL:HG21	1.94	0.49
8:P:188:SER:O	8:P:192:LEU:HB2	2.13	0.49
8:R:79:ASN:OD1	8:R:79:ASN:N	2.46	0.49
8:R:188:SER:O	8:R:192:LEU:HB2	2.13	0.49
8:T:15:ASN:ND2	8:T:68:ASP:OD1	2.40	0.49
8:U:183:VAL:HG13	8:U:187:ASN:HD21	1.77	0.49
8:W:188:SER:O	8:W:192:LEU:HB2	2.13	0.49
8:X:113:LYS:HG3	8:X:114:ILE:HG23	1.95	0.49
8:Z:183:VAL:HG13	8:Z:187:ASN:HD21	1.77	0.49
4:B:330:GLN:HB2	3:C:333:ARG:HH12	1.78	0.49
4:F:712:VAL:O	4:F:716:HIS:HB2	2.12	0.49
1:J:886:LEU:HD21	1:J:984:GLU:HB3	1.95	0.49
8:S:7:THR:OG1	8:S:63:ARG:O	2.28	0.49
8:V:231:LEU:O	8:V:234:THR:OG1	2.24	0.49
8:Z:15:ASN:ND2	8:Z:68:ASP:OD1	2.40	0.49
8:Z:113:LYS:HG3	8:Z:114:ILE:HG23	1.95	0.49
8:Z:195:LEU:HB3	8:Z:202:VAL:HG21	1.94	0.49
6:K:627:PHE:CE1	6:K:645:LEU:HB3	2.48	0.48
8:P:113:LYS:HG3	8:P:114:ILE:HG23	1.95	0.48
8:S:195:LEU:HB3	8:S:202:VAL:HG21	1.94	0.48
8:U:188:SER:O	8:U:192:LEU:HB2	2.13	0.48
3:C:653:ARG:NH1	3:C:656:CYS:SG	2.86	0.48
8:Q:113:LYS:HG3	8:Q:114:ILE:HG23	1.95	0.48
8:R:195:LEU:HB3	8:R:202:VAL:HG21	1.94	0.48
8:S:113:LYS:HG3	8:S:114:ILE:HG23	1.95	0.48
8:T:17:ILE:HD13	8:T:232:VAL:HB	1.95	0.48
8:T:188:SER:O	8:T:192:LEU:HB2	2.13	0.48
7:L:1571:ASN:HB3	7:L:1599:LYS:HG2	1.95	0.48
8:P:195:LEU:HB3	8:P:202:VAL:HG21	1.95	0.48
8:S:17:ILE:HD13	8:S:232:VAL:HB	1.95	0.48
8:S:341:ARG:HD2	3:E:857:SER:HB2	1.95	0.48
8:T:237:SER:O	8:T:244:ARG:NH2	2.44	0.48
8:V:195:LEU:HB3	8:V:202:VAL:HG21	1.94	0.48
8:V:329:ASP:HB3	8:V:332:GLN:HB2	1.96	0.48
8:X:123:ASP:OD1	8:X:161:TYR:OH	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:364:LEU:HB2	4:F:367:LEU:HA	1.95	0.48
8:P:17:ILE:HD13	8:P:232:VAL:HB	1.95	0.48
8:Q:123:ASP:OD1	8:Q:161:TYR:OH	2.32	0.48
8:R:17:ILE:HD13	8:R:232:VAL:HB	1.95	0.48
8:U:56:ASP:HA	8:V:296:ARG:HH21	1.78	0.48
8:V:188:SER:O	8:V:192:LEU:HB2	2.13	0.48
3:G:557:LEU:HD22	8:V:343:ARG:HD3	1.94	0.48
8:Q:329:ASP:HB3	8:Q:332:GLN:HB2	1.96	0.48
8:X:229:ASN:O	8:X:233:SER:OG	2.22	0.48
8:Z:329:ASP:HB3	8:Z:332:GLN:HB2	1.96	0.48
4:B:795:ALA:O	4:B:799:GLU:HB2	2.13	0.48
3:G:188:ILE:HG22	3:G:278:GLU:HG3	1.94	0.48
6:I:370:GLN:HE22	8:W:3:ARG:HH11	1.60	0.48
7:L:1797:ASP:HB2	8:Z:334:HIS:CE1	2.48	0.48
8:R:329:ASP:HB3	8:R:332:GLN:HB2	1.96	0.48
8:T:329:ASP:HB3	8:T:332:GLN:HB2	1.96	0.48
8:X:17:ILE:HD13	8:X:232:VAL:HB	1.95	0.48
8:X:197:GLN:HA	8:X:265:ARG:HH22	1.79	0.48
8:Y:113:LYS:HG3	8:Y:114:ILE:HG23	1.95	0.48
8:Y:329:ASP:HB3	8:Y:332:GLN:HB2	1.96	0.48
3:E:435:VAL:HG12	3:E:437:GLN:H	1.79	0.48
4:B:794:ARG:HH11	4:B:798:GLU:HG2	1.78	0.48
4:D:436:ASP:HB2	4:D:490:ILE:HG23	1.96	0.48
4:H:555:LEU:HD11	4:H:651:VAL:HG21	1.96	0.48
8:O:7:THR:OG1	8:O:63:ARG:O	2.28	0.48
8:P:415:LYS:HZ2	8:P:419:ASP:H	1.61	0.48
8:Q:197:GLN:HA	8:Q:265:ARG:HH22	1.79	0.48
8:R:123:ASP:OD1	8:R:161:TYR:OH	2.32	0.48
8:V:17:ILE:HD13	8:V:232:VAL:HB	1.95	0.48
8:X:195:LEU:HB3	8:X:202:VAL:HG21	1.94	0.48
8:X:329:ASP:HB3	8:X:332:GLN:HB2	1.96	0.48
8:Y:188:SER:O	8:Y:192:LEU:HB2	2.13	0.48
8:Y:197:GLN:HA	8:Y:265:ARG:HH22	1.79	0.48
8:O:197:GLN:HA	8:O:265:ARG:HH22	1.79	0.48
8:Q:7:THR:OG1	8:Q:63:ARG:O	2.28	0.48
8:Q:17:ILE:HD13	8:Q:232:VAL:HB	1.95	0.48
8:W:197:GLN:HA	8:W:265:ARG:HH22	1.79	0.48
6:I:279:VAL:HG13	6:I:336:VAL:HG11	1.96	0.48
8:R:415:LYS:HZ2	8:R:419:ASP:H	1.62	0.48
8:T:197:GLN:HA	8:T:265:ARG:HH22	1.79	0.48
8:O:15:ASN:ND2	8:O:68:ASP:OD1	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:17:ILE:HD13	8:O:232:VAL:HB	1.95	0.48
8:S:123:ASP:OD1	8:S:161:TYR:OH	2.32	0.48
8:U:232:VAL:HA	8:U:235:ILE:HD12	1.96	0.48
8:X:141:ILE:HG12	8:X:170:SER:HB2	1.96	0.48
4:B:253:ASP:HB3	4:B:266:ILE:HG22	1.96	0.47
8:O:113:LYS:HG3	8:O:114:ILE:HG23	1.95	0.47
8:O:318:ILE:HB	8:O:380:ASN:HB3	1.96	0.47
8:P:197:GLN:HA	8:P:265:ARG:HH22	1.79	0.47
8:R:318:ILE:HB	8:R:380:ASN:HB3	1.96	0.47
8:S:232:VAL:HA	8:S:235:ILE:HD12	1.96	0.47
8:S:329:ASP:HB3	8:S:332:GLN:HB2	1.96	0.47
8:T:7:THR:OG1	8:T:63:ARG:O	2.28	0.47
8:T:123:ASP:OD1	8:T:161:TYR:OH	2.32	0.47
8:U:318:ILE:HB	8:U:380:ASN:HB3	1.96	0.47
8:V:197:GLN:HA	8:V:265:ARG:HH22	1.79	0.47
8:W:237:SER:O	8:W:244:ARG:NH2	2.43	0.47
8:W:329:ASP:HB3	8:W:332:GLN:HB2	1.96	0.47
8:Z:415:LYS:HZ2	8:Z:419:ASP:H	1.62	0.47
4:F:575:ARG:NH1	8:T:252:ASP:OD1	2.48	0.47
1:J:334:VAL:HG21	1:J:365:MET:HG2	1.95	0.47
6:K:107:LEU:HD11	6:K:126:LEU:HD21	1.95	0.47
8:R:66:LEU:HD22	8:R:91:ILE:HG23	1.96	0.47
8:S:197:GLN:HA	8:S:265:ARG:HH22	1.79	0.47
8:S:318:ILE:HB	8:S:380:ASN:HB3	1.96	0.47
8:V:123:ASP:OD1	8:V:161:TYR:OH	2.32	0.47
8:Y:17:ILE:HD13	8:Y:232:VAL:HB	1.95	0.47
8:Z:7:THR:OG1	8:Z:63:ARG:O	2.28	0.47
8:Z:66:LEU:HD22	8:Z:91:ILE:HG23	1.96	0.47
4:B:327:ALA:HB2	4:B:421:LEU:HD12	1.96	0.47
3:C:291:ALA:HA	3:C:294:ALA:HB3	1.96	0.47
8:O:123:ASP:OD1	8:O:161:TYR:OH	2.32	0.47
8:R:113:LYS:HG3	8:R:114:ILE:HG23	1.95	0.47
8:U:197:GLN:HA	8:U:265:ARG:HH22	1.79	0.47
8:W:141:ILE:HG12	8:W:170:SER:HB2	1.96	0.47
8:Y:123:ASP:OD1	8:Y:161:TYR:OH	2.32	0.47
8:Z:17:ILE:HD13	8:Z:232:VAL:HB	1.95	0.47
8:T:66:LEU:HD22	8:T:91:ILE:HG23	1.96	0.47
8:W:15:ASN:ND2	8:W:68:ASP:OD1	2.40	0.47
8:W:232:VAL:HA	8:W:235:ILE:HD12	1.96	0.47
8:W:415:LYS:HZ2	8:W:419:ASP:H	1.62	0.47
8:X:66:LEU:HD22	8:X:91:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:66:LEU:HD22	8:Y:91:ILE:HG23	1.96	0.47
8:Y:232:VAL:HA	8:Y:235:ILE:HD12	1.96	0.47
3:A:533:ASP:CB	8:O:3:ARG:HH12	2.26	0.47
4:B:885:HIS:CD2	4:B:893:LEU:HB2	2.50	0.47
8:Q:188:SER:O	8:Q:192:LEU:HB2	2.13	0.47
8:T:232:VAL:HA	8:T:235:ILE:HD12	1.96	0.47
8:U:123:ASP:OD1	8:U:161:TYR:OH	2.32	0.47
8:Z:141:ILE:HG12	8:Z:170:SER:HB2	1.97	0.47
8:Z:232:VAL:HA	8:Z:235:ILE:HD12	1.96	0.47
4:B:674:GLU:O	4:B:678:THR:OG1	2.27	0.47
6:K:80:GLY:HA3	6:K:147:LYS:HA	1.97	0.47
8:O:329:ASP:HB3	8:O:332:GLN:HB2	1.96	0.47
8:P:232:VAL:HA	8:P:235:ILE:HD12	1.96	0.47
8:W:17:ILE:HD13	8:W:232:VAL:HB	1.95	0.47
8:W:66:LEU:HD22	8:W:91:ILE:HG23	1.96	0.47
4:D:656:CYS:SG	4:D:657:MET:N	2.87	0.47
4:D:711:MET:HG2	4:D:854:TYR:CZ	2.50	0.47
6:I:545:LEU:HD12	6:I:548:ILE:HD11	1.97	0.47
6:K:141:GLU:OE2	6:K:144:LYS:NZ	2.46	0.47
6:K:496:TRP:HZ2	8:Y:261:ILE:HB	1.79	0.47
8:O:66:LEU:HD22	8:O:91:ILE:HG23	1.96	0.47
8:O:141:ILE:HG12	8:O:170:SER:HB2	1.97	0.47
8:O:229:ASN:O	8:O:233:SER:OG	2.22	0.47
8:P:123:ASP:OD1	8:P:161:TYR:OH	2.32	0.47
8:R:15:ASN:ND2	8:R:68:ASP:OD1	2.40	0.47
8:R:232:VAL:HA	8:R:235:ILE:HD12	1.96	0.47
8:S:248:TYR:HE1	3:E:522:MET:HB3	1.80	0.47
8:T:318:ILE:HB	8:T:380:ASN:HB3	1.96	0.47
8:U:141:ILE:HG12	8:U:170:SER:HB2	1.96	0.47
8:V:415:LYS:HZ2	8:V:419:ASP:H	1.63	0.47
8:X:237:SER:O	8:X:244:ARG:NH2	2.44	0.47
8:Y:237:SER:O	8:Y:244:ARG:NH2	2.43	0.47
3:A:737:CYS:HB2	3:A:739:LEU:HD23	1.96	0.47
3:C:282:SER:OG	3:C:284:GLU:OE1	2.29	0.47
7:L:293:LYS:HA	7:L:295:ARG:HH11	1.80	0.47
8:Q:66:LEU:HD22	8:Q:91:ILE:HG23	1.96	0.47
8:S:15:ASN:ND2	8:S:68:ASP:OD1	2.40	0.47
8:Z:197:GLN:HA	8:Z:265:ARG:HH22	1.79	0.47
3:A:310:LEU:HD13	3:A:324:LEU:HD13	1.96	0.47
4:D:677:LEU:HD21	4:D:782:ILE:HD12	1.97	0.47
1:J:223:GLN:HB2	1:J:230:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:318:ILE:HB	8:Q:380:ASN:HB3	1.96	0.47
8:S:66:LEU:HD22	8:S:91:ILE:HG23	1.96	0.47
8:U:329:ASP:HB3	8:U:332:GLN:HB2	1.96	0.47
8:V:66:LEU:HD22	8:V:91:ILE:HG23	1.96	0.47
4:D:401:HIS:HA	4:D:404:THR:HG23	1.97	0.47
8:U:66:LEU:HD22	8:U:91:ILE:HG23	1.96	0.47
8:V:232:VAL:HA	8:V:235:ILE:HD12	1.96	0.47
3:E:581:ASP:OD2	3:E:647:TYR:OH	2.33	0.47
3:C:242:GLN:O	3:C:275:ARG:NH1	2.48	0.46
4:F:575:ARG:NH2	8:T:249:MET:HA	2.29	0.46
8:R:229:ASN:O	8:R:233:SER:OG	2.22	0.46
8:V:7:THR:OG1	8:V:63:ARG:O	2.28	0.46
8:Z:322:ASN:ND2	8:Z:357:GLN:O	2.49	0.46
4:D:885:HIS:CE1	4:D:890:GLU:HA	2.50	0.46
4:H:312:SER:HB3	6:I:165:LEU:HD11	1.97	0.46
8:Q:232:VAL:HA	8:Q:235:ILE:HD12	1.96	0.46
3:C:713:LEU:HD22	3:C:722:VAL:HG13	1.96	0.46
1:J:953:ALA:HA	1:J:956:LYS:HG2	1.97	0.46
8:P:318:ILE:HB	8:P:380:ASN:HB3	1.96	0.46
8:R:7:THR:OG1	8:R:63:ARG:O	2.28	0.46
8:T:141:ILE:HG12	8:T:170:SER:HB2	1.96	0.46
8:W:7:THR:OG1	8:W:63:ARG:O	2.28	0.46
8:X:232:VAL:HA	8:X:235:ILE:HD12	1.96	0.46
4:B:284:SER:HB2	4:B:288:ARG:HE	1.80	0.46
4:D:308:THR:O	4:D:312:SER:OG	2.24	0.46
8:P:141:ILE:HG12	8:P:170:SER:HB2	1.96	0.46
8:U:17:ILE:HD13	8:U:232:VAL:HB	1.95	0.46
8:U:322:ASN:ND2	8:U:357:GLN:O	2.49	0.46
8:V:322:ASN:ND2	8:V:357:GLN:O	2.49	0.46
8:X:322:ASN:ND2	8:X:357:GLN:O	2.49	0.46
3:A:287:GLN:N	3:A:406:GLU:OE2	2.49	0.46
6:K:3:HIS:HB2	7:L:320:PHE:CZ	2.51	0.46
7:L:354:LYS:HA	7:L:357:LEU:HD12	1.98	0.46
8:R:197:GLN:HA	8:R:265:ARG:HH22	1.79	0.46
8:Z:123:ASP:OD1	8:Z:161:TYR:OH	2.32	0.46
8:Z:318:ILE:HB	8:Z:380:ASN:HB3	1.96	0.46
3:G:581:ASP:OD1	3:G:643:ARG:NH2	2.48	0.46
6:K:627:PHE:HE1	6:K:645:LEU:HB3	1.81	0.46
8:P:66:LEU:HD22	8:P:91:ILE:HG23	1.96	0.46
8:P:329:ASP:HB3	8:P:332:GLN:HB2	1.96	0.46
8:Q:141:ILE:HG12	8:Q:170:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:322:ASN:ND2	8:R:357:GLN:O	2.49	0.46
8:S:141:ILE:HG12	8:S:170:SER:HB2	1.96	0.46
8:U:415:LYS:HZ2	8:U:419:ASP:H	1.63	0.46
8:V:237:SER:O	8:V:244:ARG:NH2	2.43	0.46
3:A:283:PHE:HA	3:A:290:HIS:CE1	2.51	0.46
3:G:457:LEU:HD21	3:G:467:VAL:HG23	1.97	0.46
4:H:648:ILE:HD12	4:H:652:PHE:HE2	1.79	0.46
8:Q:415:LYS:HZ2	8:Q:419:ASP:H	1.63	0.46
8:W:318:ILE:HB	8:W:380:ASN:HB3	1.96	0.46
8:Y:141:ILE:HG12	8:Y:170:SER:HB2	1.96	0.46
8:Y:322:ASN:ND2	8:Y:357:GLN:O	2.49	0.46
6:K:496:TRP:HB2	6:K:519:ASN:ND2	2.31	0.46
8:V:141:ILE:HG12	8:V:170:SER:HB2	1.97	0.46
3:E:517:LYS:HD2	3:E:523:ASP:HB2	1.97	0.46
8:P:322:ASN:ND2	8:P:357:GLN:O	2.49	0.46
8:R:141:ILE:HG12	8:R:170:SER:HB2	1.96	0.46
8:T:154:LEU:HD23	8:T:194:ARG:HB3	1.98	0.46
8:U:15:ASN:ND2	8:U:68:ASP:OD1	2.40	0.46
4:D:785:LEU:HD23	4:D:789:GLN:HB2	1.97	0.46
7:L:1656:ARG:NH2	8:Z:443:TYR:OH	2.49	0.46
8:Q:154:LEU:HD23	8:Q:194:ARG:HB3	1.98	0.46
8:V:79:ASN:OD1	8:V:79:ASN:N	2.46	0.46
8:X:318:ILE:HB	8:X:380:ASN:HB3	1.96	0.46
8:Y:318:ILE:HB	8:Y:380:ASN:HB3	1.96	0.46
8:Z:154:LEU:HD23	8:Z:194:ARG:HB3	1.98	0.46
3:A:734:LEU:HD13	3:A:740:THR:HG21	1.97	0.45
3:C:819:GLU:HA	3:C:822:ILE:HD12	1.97	0.45
4:D:493:LEU:O	4:D:497:CYS:HB3	2.17	0.45
1:J:712:LYS:HA	1:J:715:ARG:HE	1.80	0.45
8:O:415:LYS:HZ2	8:O:419:ASP:H	1.64	0.45
8:T:50:VAL:HG21	8:T:244:ARG:HG2	1.99	0.45
8:U:7:THR:OG1	8:U:63:ARG:O	2.28	0.45
8:W:123:ASP:OD1	8:W:161:TYR:OH	2.32	0.45
6:K:87:ARG:O	6:K:91:THR:HG23	2.16	0.45
6:K:611:GLN:O	6:K:615:LEU:HG	2.16	0.45
8:O:232:VAL:HA	8:O:235:ILE:HD12	1.96	0.45
8:Q:322:ASN:ND2	8:Q:357:GLN:O	2.49	0.45
8:Y:50:VAL:HG21	8:Y:244:ARG:HG2	1.98	0.45
8:O:322:ASN:ND2	8:O:357:GLN:O	2.49	0.45
8:R:237:SER:O	8:R:244:ARG:NH2	2.43	0.45
8:V:318:ILE:HB	8:V:380:ASN:HB3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:154:LEU:HD23	8:W:194:ARG:HB3	1.98	0.45
8:W:322:ASN:ND2	8:W:357:GLN:O	2.49	0.45
4:B:587:ARG:HD3	4:B:591:THR:OG1	2.16	0.45
4:D:490:ILE:HG13	4:D:494:HIS:HE1	1.82	0.45
8:P:50:VAL:HG21	8:P:244:ARG:HG2	1.98	0.45
8:Q:56:ASP:HA	8:R:296:ARG:HH21	1.82	0.45
8:Q:237:SER:O	8:Q:244:ARG:NH2	2.44	0.45
8:S:322:ASN:ND2	8:S:357:GLN:O	2.49	0.45
4:F:268:MET:HB2	4:F:276:LYS:H	1.81	0.45
1:J:895:ASN:OD1	8:X:357:GLN:NE2	2.49	0.45
6:K:646:LEU:HD22	8:Y:341:ARG:NH1	2.32	0.45
8:P:154:LEU:HD23	8:P:194:ARG:HB3	1.98	0.45
8:R:50:VAL:HG21	8:R:244:ARG:HG2	1.98	0.45
8:R:108:PHE:CD1	8:R:152:TYR:HB2	2.52	0.45
8:U:105:ALA:O	8:U:109:SER:OG	2.34	0.45
8:V:154:LEU:HD23	8:V:194:ARG:HB3	1.98	0.45
8:W:105:ALA:O	8:W:109:SER:OG	2.34	0.45
4:F:581:LEU:HG	4:F:585:LEU:HG	1.97	0.45
8:O:50:VAL:HG21	8:O:244:ARG:HG2	1.98	0.45
8:O:154:LEU:HD23	8:O:194:ARG:HB3	1.98	0.45
8:Q:108:PHE:CD1	8:Q:152:TYR:HB2	2.52	0.45
8:R:154:LEU:HD23	8:R:194:ARG:HB3	1.98	0.45
8:S:108:PHE:CD1	8:S:152:TYR:HB2	2.52	0.45
8:T:322:ASN:ND2	8:T:357:GLN:O	2.49	0.45
8:U:154:LEU:HD23	8:U:194:ARG:HB3	1.98	0.45
8:V:50:VAL:HG21	8:V:244:ARG:HG2	1.98	0.45
8:Y:415:LYS:HZ2	8:Y:419:ASP:H	1.63	0.45
8:U:50:VAL:HG21	8:U:244:ARG:HG2	1.99	0.45
8:V:229:ASN:O	8:V:233:SER:OG	2.22	0.45
1:J:265:VAL:HB	1:J:300:ILE:HD11	1.98	0.45
8:Q:50:VAL:HG21	8:Q:244:ARG:HG2	1.99	0.45
8:U:108:PHE:CD1	8:U:152:TYR:HB2	2.52	0.45
8:X:108:PHE:CD1	8:X:152:TYR:HB2	2.52	0.45
8:X:154:LEU:HD23	8:X:194:ARG:HB3	1.98	0.45
8:Z:50:VAL:HG21	8:Z:244:ARG:HG2	1.98	0.45
4:H:535:ASP:OD1	4:H:535:ASP:N	2.50	0.45
6:K:651:TYR:OH	8:Y:318:ILE:O	2.35	0.45
8:P:7:THR:OG1	8:P:63:ARG:O	2.28	0.45
8:W:50:VAL:HG21	8:W:244:ARG:HG2	1.98	0.45
8:Y:7:THR:OG1	8:Y:63:ARG:O	2.28	0.45
8:Y:108:PHE:CD1	8:Y:152:TYR:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:45:THR:OG1	8:Z:46:ASP:N	2.50	0.45
4:B:419:LEU:HA	4:B:422:VAL:HG22	1.99	0.45
3:G:526:ASP:HA	3:G:529:VAL:HG12	1.99	0.45
8:P:108:PHE:CD1	8:P:152:TYR:HB2	2.52	0.45
8:R:73:VAL:O	8:R:76:SER:OG	2.31	0.45
8:W:104:TRP:O	8:W:108:PHE:HB2	2.17	0.45
8:Z:381:HIS:CE1	8:Z:383:SER:HG	2.33	0.45
6:K:653:LYS:HD2	6:K:653:LYS:N	2.33	0.44
8:Q:105:ALA:O	8:Q:109:SER:OG	2.34	0.44
8:S:104:TRP:O	8:S:108:PHE:HB2	2.17	0.44
8:T:108:PHE:CD1	8:T:152:TYR:HB2	2.52	0.44
8:Y:154:LEU:HD23	8:Y:194:ARG:HB3	1.98	0.44
3:E:258:GLU:HA	3:E:261:HIS:CD2	2.52	0.44
4:D:833:ILE:HA	4:D:836:PHE:HD2	1.81	0.44
4:F:364:LEU:H	4:F:367:LEU:H	1.66	0.44
1:J:271:ILE:HD13	1:J:393:ILE:HG22	1.99	0.44
8:S:154:LEU:HD23	8:S:194:ARG:HB3	1.98	0.44
8:V:108:PHE:CD1	8:V:152:TYR:HB2	2.52	0.44
8:W:108:PHE:CD1	8:W:152:TYR:HB2	2.52	0.44
4:B:658:SER:HA	4:B:661:LEU:HD12	1.98	0.44
3:C:840:LEU:HB3	3:C:856:ILE:HD11	1.98	0.44
4:F:572:ASP:OD1	4:F:572:ASP:N	2.50	0.44
6:K:639:ASN:OD1	6:K:640:SER:N	2.51	0.44
6:K:643:ALA:HA	6:K:646:LEU:HD12	1.98	0.44
8:O:104:TRP:O	8:O:108:PHE:HB2	2.18	0.44
8:P:104:TRP:O	8:P:108:PHE:HB2	2.17	0.44
8:S:381:HIS:CE1	8:S:383:SER:HG	2.32	0.44
8:X:77:ILE:O	8:X:80:SER:OG	2.31	0.44
8:X:415:LYS:HZ2	8:X:419:ASP:H	1.65	0.44
3:E:285:TYR:HB3	3:E:289:ASN:HD22	1.82	0.44
4:F:666:PHE:HA	4:F:669:ARG:HE	1.82	0.44
1:J:806:PRO:O	1:J:810:ASP:N	2.50	0.44
1:J:892:HIS:HB2	8:X:353:PRO:O	2.18	0.44
8:Z:108:PHE:CD1	8:Z:152:TYR:HB2	2.52	0.44
8:V:45:THR:OG1	8:V:46:ASP:N	2.50	0.44
8:W:45:THR:OG1	8:W:46:ASP:N	2.50	0.44
8:W:381:HIS:CE1	8:W:383:SER:HG	2.33	0.44
3:A:427:TYR:H	3:A:624:TRP:HZ3	1.65	0.44
4:F:269:ASN:O	4:F:270:ASN:ND2	2.51	0.44
4:H:730:SER:HB3	4:H:754:PHE:HE1	1.82	0.44
8:S:45:THR:OG1	8:S:46:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:104:TRP:O	8:V:108:PHE:HB2	2.17	0.44
8:W:56:ASP:OD2	8:X:296:ARG:NE	2.51	0.44
8:X:50:VAL:HG21	8:X:244:ARG:HG2	1.99	0.44
6:I:20:ASN:H	6:I:24:GLY:HA3	1.82	0.44
8:Q:104:TRP:O	8:Q:108:PHE:HB2	2.17	0.44
3:E:517:LYS:O	3:E:522:MET:N	2.51	0.44
3:G:574:LYS:HB2	3:G:619:ASP:HB3	1.99	0.44
8:V:381:HIS:CE1	8:V:383:SER:HG	2.33	0.44
3:A:659:TRP:CZ2	8:O:261:ILE:HG21	2.53	0.44
4:B:257:VAL:HG21	4:B:266:ILE:HD13	1.99	0.44
4:F:433:TRP:CD1	4:F:483:VAL:HG22	2.53	0.44
4:H:275:TYR:CD2	4:H:295:SER:HB2	2.52	0.44
1:J:212:ASP:OD1	1:J:212:ASP:N	2.51	0.44
6:K:68:GLN:NE2	6:K:84:ILE:HB	2.32	0.44
6:K:192:LEU:HD21	6:K:307:PHE:HB2	2.00	0.44
8:R:104:TRP:O	8:R:108:PHE:HB2	2.17	0.44
8:S:237:SER:O	8:S:244:ARG:NH2	2.43	0.44
8:O:45:THR:OG1	8:O:46:ASP:N	2.50	0.43
8:O:77:ILE:O	8:O:80:SER:OG	2.31	0.43
8:O:108:PHE:CD1	8:O:152:TYR:HB2	2.52	0.43
8:U:104:TRP:O	8:U:108:PHE:HB2	2.17	0.43
3:C:696:TYR:CE1	3:C:854:SER:HB2	2.51	0.43
4:F:285:ARG:NH1	3:E:220:ASP:OD1	2.51	0.43
3:G:865:TYR:H	3:G:868:ARG:NH1	2.16	0.43
4:H:456:THR:OG1	4:H:457:ASP:N	2.50	0.43
6:K:459:VAL:HG21	6:K:467:PHE:HB2	1.99	0.43
8:P:77:ILE:O	8:P:80:SER:OG	2.31	0.43
8:P:229:ASN:O	8:P:233:SER:OG	2.22	0.43
8:U:77:ILE:O	8:U:80:SER:OG	2.31	0.43
8:X:104:TRP:O	8:X:108:PHE:HB2	2.17	0.43
6:I:121:HIS:HA	6:I:124:TYR:CE1	2.52	0.43
7:L:1657:GLN:HA	7:L:1660:LEU:HG	2.01	0.43
8:O:297:LEU:HD21	8:O:377:MET:HB3	2.01	0.43
8:Y:297:LEU:HD21	8:Y:377:MET:HB3	2.01	0.43
3:A:351:LEU:HG	3:A:438:GLN:HE22	1.83	0.43
6:K:300:LEU:HB3	6:K:301:LYS:H	1.67	0.43
8:R:297:LEU:HD21	8:R:377:MET:HB3	2.01	0.43
8:S:425:ARG:HA	8:S:428:VAL:HG12	2.01	0.43
8:T:104:TRP:O	8:T:108:PHE:HB2	2.17	0.43
8:T:193:LYS:O	8:T:196:THR:OG1	2.32	0.43
8:Z:105:ALA:O	8:Z:109:SER:OG	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:183:GLU:HG2	3:A:184:ARG:HD2	2.01	0.43
4:B:304:ILE:HD12	4:B:381:LEU:HB3	2.01	0.43
3:C:294:ALA:HA	3:C:297:ARG:HE	1.84	0.43
4:F:878:PHE:HE2	8:T:338:GLN:HE22	1.66	0.43
6:I:190:TRP:CE2	6:I:280:GLY:HA3	2.53	0.43
1:J:904:ARG:HH11	1:J:1012:SER:HB3	1.84	0.43
6:K:44:ARG:NE	6:K:123:ASN:HD21	2.16	0.43
8:R:45:THR:OG1	8:R:46:ASP:N	2.50	0.43
8:S:105:ALA:O	8:S:109:SER:OG	2.34	0.43
8:T:297:LEU:HD21	8:T:377:MET:HB3	2.01	0.43
8:X:297:LEU:HD21	8:X:377:MET:HB3	2.01	0.43
8:X:425:ARG:HA	8:X:428:VAL:HG12	2.01	0.43
8:Y:104:TRP:O	8:Y:108:PHE:HB2	2.17	0.43
8:Z:104:TRP:O	8:Z:108:PHE:HB2	2.17	0.43
3:E:303:HIS:O	3:E:307:VAL:HG22	2.18	0.43
4:B:803:ARG:HH12	4:B:833:ILE:HD11	1.84	0.43
8:P:341:ARG:NH1	8:P:342:GLU:OE2	2.46	0.43
8:U:425:ARG:HA	8:U:428:VAL:HG12	2.01	0.43
8:W:297:LEU:HD21	8:W:377:MET:HB3	2.01	0.43
3:E:306:LEU:O	3:E:310:LEU:HG	2.19	0.43
3:G:518:ARG:HG2	3:G:524:GLN:HG2	2.01	0.43
8:O:425:ARG:HA	8:O:428:VAL:HG12	2.01	0.43
8:Z:297:LEU:HD21	8:Z:377:MET:HB3	2.01	0.43
4:F:526:LEU:HA	4:F:526:LEU:HD12	1.80	0.43
8:P:425:ARG:HA	8:P:428:VAL:HG12	2.01	0.43
8:S:50:VAL:HG21	8:S:244:ARG:HG2	1.99	0.43
8:U:45:THR:OG1	8:U:46:ASP:N	2.50	0.43
8:Y:421:MET:H	8:Y:421:MET:HG3	1.69	0.43
4:B:855:GLN:HA	4:B:858:VAL:HG22	2.01	0.43
3:G:217:VAL:O	3:G:221:LEU:HG	2.19	0.43
6:I:403:VAL:HG11	8:W:47:ARG:NH1	2.34	0.43
8:O:425:ARG:HH21	8:O:426:GLU:HA	1.84	0.43
8:Q:45:THR:OG1	8:Q:46:ASP:N	2.50	0.43
8:V:297:LEU:HD21	8:V:377:MET:HB3	2.01	0.43
8:X:105:ALA:O	8:X:109:SER:OG	2.34	0.43
8:X:381:HIS:CE1	8:X:383:SER:HG	2.34	0.43
8:X:425:ARG:HH21	8:X:426:GLU:HA	1.84	0.43
8:Z:425:ARG:HA	8:Z:428:VAL:HG12	2.01	0.43
4:B:692:ARG:HH22	4:B:698:SER:HA	1.84	0.43
3:C:694:GLN:O	3:C:698:MET:HE3	2.19	0.43
1:J:889:LYS:HA	8:X:353:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:639:ASN:HB2	8:Y:334:HIS:NE2	2.34	0.43
8:P:45:THR:OG1	8:P:46:ASP:N	2.50	0.43
8:S:425:ARG:HH21	8:S:426:GLU:HA	1.84	0.43
8:U:297:LEU:HD21	8:U:377:MET:HB3	2.01	0.43
3:E:150:LEU:HB2	3:E:152:GLN:HE22	1.83	0.43
3:A:557:LEU:HD13	8:P:343:ARG:HD3	2.00	0.42
4:F:256:TYR:HB3	4:F:261:ILE:HB	2.00	0.42
3:G:494:TYR:HA	3:G:497:LYS:HE2	2.01	0.42
4:H:675:TYR:HA	4:H:678:THR:HG22	2.00	0.42
6:K:345:VAL:HG23	6:K:350:LEU:HB3	2.00	0.42
6:K:651:TYR:HB3	6:K:653:LYS:HZ2	1.83	0.42
8:R:425:ARG:HH21	8:R:426:GLU:HA	1.84	0.42
8:V:77:ILE:O	8:V:80:SER:OG	2.31	0.42
8:Y:45:THR:OG1	8:Y:46:ASP:N	2.50	0.42
3:C:758:PHE:O	3:C:763:GLN:HG2	2.19	0.42
4:F:616:GLU:O	4:F:620:ARG:HG2	2.18	0.42
6:K:282:SER:HB2	6:K:340:LEU:HD11	2.01	0.42
6:K:649:LEU:HG	6:K:654:TYR:C	2.39	0.42
8:Q:79:ASN:N	8:Q:79:ASN:OD1	2.46	0.42
8:V:105:ALA:O	8:V:109:SER:OG	2.34	0.42
8:V:425:ARG:HA	8:V:428:VAL:HG12	2.01	0.42
3:E:408:MET:O	3:E:435:VAL:N	2.49	0.42
3:A:510:VAL:HG12	3:A:713:LEU:HD13	2.02	0.42
4:B:459:LEU:HA	4:B:463:LYS:HB2	2.02	0.42
3:C:445:LYS:H	3:C:445:LYS:HG3	1.62	0.42
4:H:275:TYR:HD2	4:H:295:SER:HB2	1.84	0.42
4:H:655:GLU:O	4:H:658:SER:OG	2.31	0.42
1:J:230:SER:HB3	1:J:264:LEU:O	2.19	0.42
6:K:352:GLY:O	6:K:356:ILE:HG12	2.18	0.42
6:K:604:LEU:HD13	6:K:608:GLY:HA3	2.02	0.42
8:P:237:SER:O	8:P:244:ARG:NH2	2.43	0.42
8:R:105:ALA:O	8:R:109:SER:OG	2.34	0.42
8:W:90:ASN:OD1	8:W:90:ASN:N	2.53	0.42
3:E:837:LEU:HD21	3:E:859:LEU:HD23	2.01	0.42
4:B:294:LEU:HD11	4:B:368:LEU:HD22	2.01	0.42
4:D:611:GLN:H	4:D:611:GLN:HG2	1.63	0.42
6:I:477:VAL:HA	6:I:480:LYS:HE2	2.02	0.42
6:I:601:LEU:HD23	6:I:601:LEU:HA	1.67	0.42
7:L:348:LYS:HG3	7:L:349:GLU:H	1.85	0.42
8:T:381:HIS:CE1	8:T:383:SER:HG	2.34	0.42
8:W:425:ARG:HH21	8:W:426:GLU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:193:LYS:O	8:X:196:THR:OG1	2.32	0.42
8:Y:79:ASN:OD1	8:Y:79:ASN:N	2.46	0.42
8:Y:425:ARG:HH21	8:Y:426:GLU:HA	1.84	0.42
8:Z:90:ASN:OD1	8:Z:90:ASN:N	2.53	0.42
8:Z:341:ARG:NH1	8:Z:342:GLU:OE2	2.46	0.42
4:D:427:LEU:HD13	4:D:427:LEU:HA	1.94	0.42
3:G:363:SER:HA	3:G:376:CYS:SG	2.60	0.42
1:J:386:ILE:O	7:L:294:ARG:NH1	2.52	0.42
8:P:28:GLU:HG3	8:P:367:LEU:HD11	2.02	0.42
8:P:425:ARG:HH21	8:P:426:GLU:HA	1.84	0.42
8:Q:288:THR:OG1	8:Q:289:THR:N	2.53	0.42
8:R:425:ARG:HA	8:R:428:VAL:HG12	2.01	0.42
8:T:45:THR:OG1	8:T:46:ASP:N	2.50	0.42
4:B:769:ARG:O	4:B:772:LEU:HG	2.19	0.42
4:F:677:LEU:HD13	4:F:712:VAL:HG22	2.02	0.42
3:G:460:VAL:HB	3:G:499:LEU:HD13	2.02	0.42
3:G:680:PHE:HA	3:G:683:ARG:HG2	2.01	0.42
7:L:1663:HIS:CD2	8:Z:262:PRO:HB3	2.54	0.42
8:P:297:LEU:HD21	8:P:377:MET:HB3	2.01	0.42
8:P:421:MET:H	8:P:421:MET:HG3	1.69	0.42
8:R:90:ASN:OD1	8:R:90:ASN:N	2.53	0.42
8:R:381:HIS:CE1	8:R:383:SER:HG	2.32	0.42
8:U:425:ARG:HH21	8:U:426:GLU:HA	1.84	0.42
8:V:341:ARG:NH1	8:V:342:GLU:OE2	2.46	0.42
8:Y:288:THR:OG1	8:Y:289:THR:N	2.53	0.42
3:A:547:THR:HA	3:A:548:PRO:HD3	1.94	0.42
4:B:802:ARG:HH22	4:B:836:PHE:HE2	1.65	0.42
4:D:713:HIS:NE2	8:R:355:SER:OG	2.48	0.42
4:F:334:GLU:HB2	4:F:377:ARG:HH22	1.84	0.42
1:J:222:HIS:CG	1:J:225:TRP:HB2	2.55	0.42
8:Q:297:LEU:HD21	8:Q:377:MET:HB3	2.01	0.42
8:R:46:ASP:HA	8:R:246:PRO:HD3	2.02	0.42
8:R:288:THR:OG1	8:R:289:THR:N	2.53	0.42
8:W:425:ARG:HA	8:W:428:VAL:HG12	2.01	0.42
8:X:7:THR:OG1	8:X:63:ARG:O	2.28	0.42
4:F:726:VAL:O	4:F:730:SER:OG	2.30	0.42
3:G:701:VAL:HG13	3:G:736:ASP:HB3	2.01	0.42
3:G:719:ILE:HA	3:G:722:VAL:HG22	2.01	0.42
4:H:887:LYS:HA	4:H:887:LYS:HD3	1.80	0.42
7:L:1680:ILE:HD11	7:L:1716:GLY:HA3	2.02	0.42
8:O:90:ASN:OD1	8:O:90:ASN:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:288:THR:OG1	8:T:289:THR:N	2.53	0.42
8:V:425:ARG:HH21	8:V:426:GLU:HA	1.84	0.42
8:Y:425:ARG:HA	8:Y:428:VAL:HG12	2.01	0.42
8:Z:288:THR:OG1	8:Z:289:THR:N	2.53	0.42
3:A:219:GLU:HB2	3:A:314:HIS:CE1	2.55	0.42
4:B:589:ALA:HB3	4:B:632:ASP:HB3	2.02	0.42
4:F:848:ARG:HD2	4:F:848:ARG:HA	1.86	0.42
6:I:9:LEU:HD22	6:I:104:LEU:HD13	2.01	0.42
6:K:593:PHE:HB2	6:K:615:LEU:HD13	2.00	0.42
7:L:1803:ASN:HD22	8:Z:341:ARG:NH2	2.17	0.42
8:O:288:THR:OG1	8:O:289:THR:N	2.53	0.42
8:R:77:ILE:O	8:R:80:SER:OG	2.31	0.42
8:Y:90:ASN:OD1	8:Y:90:ASN:N	2.53	0.42
8:Z:46:ASP:HA	8:Z:246:PRO:HD3	2.02	0.42
8:Z:425:ARG:HH21	8:Z:426:GLU:HA	1.84	0.42
3:E:257:ARG:HG2	3:E:261:HIS:CE1	2.55	0.42
4:B:577:LEU:HD12	4:B:578:MET:HG3	2.02	0.42
4:F:293:ARG:HA	3:E:186:ALA:HB1	2.01	0.42
4:F:606:ARG:HH21	8:U:339:ARG:HE	1.68	0.42
6:K:278:PHE:O	6:K:282:SER:OG	2.31	0.42
8:O:105:ALA:O	8:O:109:SER:OG	2.34	0.42
8:Q:153:LEU:HD12	8:Q:153:LEU:HA	1.95	0.42
8:Q:425:ARG:HA	8:Q:428:VAL:HG12	2.01	0.42
8:Q:425:ARG:HH21	8:Q:426:GLU:HA	1.84	0.42
8:T:28:GLU:HG3	8:T:367:LEU:HD11	2.02	0.42
8:T:425:ARG:HA	8:T:428:VAL:HG12	2.01	0.42
8:T:425:ARG:HH21	8:T:426:GLU:HA	1.84	0.42
8:V:385:SER:HB2	8:V:435:TYR:CD2	2.55	0.42
8:W:46:ASP:HA	8:W:246:PRO:HD3	2.02	0.42
8:X:28:GLU:HG3	8:X:367:LEU:HD11	2.02	0.42
8:Z:28:GLU:HG3	8:Z:367:LEU:HD11	2.02	0.42
3:C:429:ASP:N	3:C:429:ASP:OD1	2.53	0.41
8:P:228:ILE:O	8:P:232:VAL:HG23	2.20	0.41
8:S:46:ASP:HA	8:S:246:PRO:HD3	2.02	0.41
8:Z:348:PHE:HB3	8:Z:349:ILE:H	1.76	0.41
4:B:497:CYS:SG	4:B:552:LYS:NZ	2.93	0.41
4:D:433:TRP:HZ2	4:D:484:LEU:HD12	1.85	0.41
6:I:515:TRP:HE1	6:I:519:ASN:N	2.18	0.41
6:I:533:GLN:O	6:I:537:LEU:HG	2.20	0.41
8:P:288:THR:OG1	8:P:289:THR:N	2.53	0.41
8:Q:28:GLU:HG3	8:Q:367:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:77:ILE:O	8:Q:80:SER:OG	2.31	0.41
8:Q:385:SER:HB2	8:Q:435:TYR:CD2	2.55	0.41
8:R:28:GLU:HG3	8:R:367:LEU:HD11	2.02	0.41
8:U:228:ILE:O	8:U:232:VAL:HG23	2.20	0.41
8:V:287:LYS:HB3	8:V:288:THR:H	1.74	0.41
8:W:385:SER:HB2	8:W:435:TYR:CD2	2.55	0.41
8:X:45:THR:OG1	8:X:46:ASP:N	2.50	0.41
8:Z:77:ILE:O	8:Z:80:SER:OG	2.31	0.41
8:Z:385:SER:HB2	8:Z:435:TYR:CD2	2.55	0.41
3:C:652:GLU:O	3:C:655:LEU:HG	2.21	0.41
4:F:594:GLN:HA	4:F:597:LEU:HD13	2.02	0.41
6:K:646:LEU:HB3	8:Y:341:ARG:CD	2.48	0.41
8:P:46:ASP:HA	8:P:246:PRO:HD3	2.02	0.41
8:P:381:HIS:CG	8:P:383:SER:HG	2.36	0.41
8:S:349:ILE:HD12	8:S:349:ILE:HA	1.98	0.41
8:T:228:ILE:O	8:T:232:VAL:HG23	2.21	0.41
8:T:385:SER:HB2	8:T:435:TYR:CD2	2.55	0.41
8:X:228:ILE:O	8:X:232:VAL:HG23	2.21	0.41
8:X:385:SER:HB2	8:X:435:TYR:CD2	2.55	0.41
8:Y:385:SER:HB2	8:Y:435:TYR:CD2	2.55	0.41
3:E:526:ASP:HA	3:E:529:VAL:HG12	2.02	0.41
3:C:408:MET:HA	3:C:438:GLN:HB2	2.03	0.41
3:C:448:ASP:OD1	3:C:448:ASP:N	2.54	0.41
4:F:288:ARG:O	4:F:292:VAL:HG22	2.20	0.41
1:J:272:ARG:HH12	7:L:311:TYR:HB2	1.86	0.41
1:J:691:LEU:HD12	1:J:694:HIS:HD2	1.85	0.41
7:L:1595:GLU:OE1	7:L:1597:ARG:NH2	2.53	0.41
8:S:288:THR:OG1	8:S:289:THR:N	2.53	0.41
8:U:46:ASP:HA	8:U:246:PRO:HD3	2.02	0.41
8:U:288:THR:OG1	8:U:289:THR:N	2.53	0.41
8:X:341:ARG:NH1	8:X:342:GLU:OE2	2.46	0.41
3:A:243:SER:HA	3:A:275:ARG:HH22	1.86	0.41
4:B:290:THR:HB	4:B:368:LEU:HD21	2.03	0.41
4:D:456:THR:OG1	4:D:457:ASP:N	2.53	0.41
1:J:475:THR:HA	1:J:478:GLU:HG3	2.02	0.41
8:X:71:PRO:O	8:X:75:HIS:NE2	2.54	0.41
8:Y:46:ASP:HA	8:Y:246:PRO:HD3	2.02	0.41
8:Y:71:PRO:O	8:Y:75:HIS:NE2	2.54	0.41
3:A:743:GLU:HG3	3:A:745:LEU:H	1.86	0.41
4:B:859:GLN:NE2	4:B:890:GLU:OE2	2.53	0.41
3:C:211:ALA:O	3:C:214:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:221:VAL:HG22	6:K:35:HIS:HE1	1.86	0.41
8:S:297:LEU:HD21	8:S:377:MET:HB3	2.01	0.41
8:U:385:SER:HB2	8:U:435:TYR:CD2	2.55	0.41
8:W:28:GLU:HG3	8:W:367:LEU:HD11	2.02	0.41
8:Y:132:LEU:HD12	8:Y:132:LEU:HA	1.95	0.41
3:E:443:LEU:HG	3:E:450:ILE:HD11	2.02	0.41
4:B:406:THR:HG21	4:B:411:MET:HB2	2.01	0.41
4:B:720:TYR:HA	8:P:249:MET:HE1	2.03	0.41
4:D:548:VAL:HA	4:D:552:LYS:HE2	2.02	0.41
4:D:887:LYS:HD2	4:D:887:LYS:HA	1.92	0.41
4:F:304:ILE:HG13	4:F:385:VAL:HG21	2.02	0.41
3:G:676:PHE:HB2	3:G:818:PHE:CE2	2.56	0.41
6:K:300:LEU:HD12	6:K:339:HIS:HE1	1.86	0.41
8:O:28:GLU:HG3	8:O:367:LEU:HD11	2.02	0.41
8:O:381:HIS:CE1	8:O:383:SER:HG	2.33	0.41
8:Q:15:ASN:ND2	8:Q:68:ASP:OD1	2.40	0.41
8:S:28:GLU:HG3	8:S:367:LEU:HD11	2.02	0.41
8:S:79:ASN:OD1	8:S:79:ASN:N	2.46	0.41
8:U:28:GLU:HG3	8:U:367:LEU:HD11	2.02	0.41
8:V:288:THR:OG1	8:V:289:THR:N	2.53	0.41
8:W:71:PRO:O	8:W:75:HIS:NE2	2.54	0.41
8:Y:193:LYS:O	8:Y:196:THR:OG1	2.32	0.41
4:D:843:MET:O	4:D:847:LEU:HG	2.21	0.41
4:F:779:PHE:HA	4:F:782:ILE:HD12	2.03	0.41
3:G:643:ARG:HA	3:G:646:PHE:HB3	2.03	0.41
1:J:221:VAL:HG12	7:L:309:GLU:HB3	2.02	0.41
1:J:979:SER:OG	1:J:980:ILE:N	2.53	0.41
8:O:228:ILE:O	8:O:232:VAL:HG23	2.20	0.41
8:O:385:SER:HB2	8:O:435:TYR:CD2	2.55	0.41
8:Q:71:PRO:O	8:Q:75:HIS:NE2	2.54	0.41
8:T:46:ASP:HA	8:T:246:PRO:HD3	2.02	0.41
8:U:71:PRO:O	8:U:75:HIS:NE2	2.54	0.41
8:Y:28:GLU:HG3	8:Y:367:LEU:HD11	2.02	0.41
8:Y:228:ILE:O	8:Y:232:VAL:HG23	2.20	0.41
3:A:393:LYS:HD2	3:A:397:ARG:HE	1.86	0.41
3:A:431:ARG:HH11	3:A:458:ASN:HD21	1.68	0.41
3:C:174:LEU:HD13	3:C:283:PHE:HB2	2.03	0.41
3:C:252:LEU:HB2	3:C:257:ARG:HE	1.85	0.41
4:D:558:HIS:CD2	4:D:617:ILE:HD11	2.56	0.41
4:D:653:THR:O	4:D:657:MET:HG2	2.20	0.41
4:F:268:MET:HG3	4:F:276:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:503:THR:HG21	4:F:544:TYR:CD2	2.56	0.41
4:H:433:TRP:HE1	4:H:484:LEU:HA	1.86	0.41
6:I:129:PHE:O	6:I:133:PHE:HB2	2.20	0.41
6:I:336:VAL:HA	6:I:339:HIS:HD1	1.86	0.41
6:K:359:ASP:HA	6:K:364:GLY:HA3	2.02	0.41
7:L:1658:LEU:HG	7:L:1762:PHE:HE1	1.84	0.41
7:L:1678:ASN:OD1	7:L:1679:GLN:NE2	2.54	0.41
8:P:385:SER:HB2	8:P:435:TYR:CD2	2.55	0.41
8:T:77:ILE:O	8:T:80:SER:OG	2.31	0.41
8:V:15:ASN:ND2	8:V:68:ASP:OD1	2.40	0.41
8:W:228:ILE:O	8:W:232:VAL:HG23	2.20	0.41
8:W:421:MET:H	8:W:421:MET:HG3	1.69	0.41
8:X:46:ASP:HA	8:X:246:PRO:HD3	2.02	0.41
8:X:288:THR:OG1	8:X:289:THR:N	2.53	0.41
3:E:244:ARG:HD3	3:E:244:ARG:HA	1.89	0.41
3:A:824:LYS:HA	3:A:827:LYS:HD2	2.03	0.41
3:C:517:LYS:HB2	3:C:706:TRP:CZ2	2.56	0.41
4:F:579:ASP:OD2	8:T:3:ARG:NH1	2.48	0.41
3:G:509:LEU:HD13	3:G:626:LEU:HD22	2.02	0.41
6:K:38:GLU:O	6:K:42:LEU:HG	2.20	0.41
8:O:71:PRO:O	8:O:75:HIS:NE2	2.54	0.41
1:J:296:VAL:HG23	1:J:314:LEU:HB2	2.04	0.40
7:L:1485:ALA:HA	7:L:1488:ILE:HD12	2.02	0.40
7:L:1574:LEU:HD23	7:L:1574:LEU:HA	1.91	0.40
8:P:289:THR:OG1	8:P:332:GLN:NE2	2.55	0.40
8:R:385:SER:HB2	8:R:435:TYR:CD2	2.55	0.40
8:S:228:ILE:O	8:S:232:VAL:HG23	2.20	0.40
3:E:296:MET:HE2	3:E:296:MET:HB2	1.71	0.40
3:A:282:SER:O	3:A:290:HIS:NE2	2.54	0.40
3:C:292:LEU:HD23	3:C:292:LEU:HA	1.93	0.40
3:G:209:PRO:O	3:G:212:SER:OG	2.36	0.40
3:G:319:LEU:HD23	3:G:319:LEU:HA	1.73	0.40
6:K:512:ALA:HA	6:K:515:TRP:CE3	2.55	0.40
6:K:513:ILE:HG13	8:Y:263:THR:HG23	2.02	0.40
8:P:252:ASP:OD1	8:P:252:ASP:N	2.51	0.40
8:R:71:PRO:O	8:R:75:HIS:NE2	2.54	0.40
8:T:71:PRO:O	8:T:75:HIS:NE2	2.54	0.40
8:V:228:ILE:O	8:V:232:VAL:HG23	2.20	0.40
8:V:289:THR:OG1	8:V:332:GLN:NE2	2.55	0.40
8:Z:71:PRO:O	8:Z:75:HIS:NE2	2.54	0.40
8:Z:228:ILE:O	8:Z:232:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:324:PHE:O	4:D:328:LEU:HG	2.21	0.40
1:J:281:VAL:HG11	6:K:41:VAL:HG22	2.03	0.40
8:O:289:THR:OG1	8:O:332:GLN:NE2	2.55	0.40
8:Q:320:ILE:HB	8:Q:356:ILE:HG13	2.04	0.40
8:S:71:PRO:O	8:S:75:HIS:NE2	2.54	0.40
8:T:105:ALA:O	8:T:109:SER:OG	2.34	0.40
8:T:320:ILE:HB	8:T:356:ILE:HG13	2.04	0.40
8:V:71:PRO:O	8:V:75:HIS:NE2	2.54	0.40
3:E:301:LYS:O	3:E:305:ILE:HG12	2.21	0.40
4:B:872:SER:HA	4:B:875:PHE:CE2	2.56	0.40
4:D:401:HIS:CE1	4:D:474:PHE:HB3	2.57	0.40
4:D:689:LYS:HE3	8:R:162:PRO:HB2	2.03	0.40
4:D:791:ALA:HA	4:D:794:ARG:HH21	1.86	0.40
4:F:889:ARG:HD3	4:F:889:ARG:HA	1.82	0.40
3:G:394:TRP:NE1	3:G:450:ILE:O	2.51	0.40
3:G:676:PHE:HB2	3:G:818:PHE:CZ	2.57	0.40
4:H:419:LEU:HA	4:H:422:VAL:HG22	2.04	0.40
6:K:1:MET:H2	7:L:320:PHE:HD1	1.69	0.40
6:K:483:LEU:HD12	6:K:483:LEU:HA	1.89	0.40
8:O:341:ARG:NH1	8:O:342:GLU:OE2	2.46	0.40
8:P:193:LYS:O	8:P:196:THR:OG1	2.32	0.40
8:Q:46:ASP:HA	8:Q:246:PRO:HD3	2.02	0.40
8:Q:193:LYS:O	8:Q:196:THR:OG1	2.32	0.40
8:R:228:ILE:O	8:R:232:VAL:HG23	2.20	0.40
8:U:237:SER:O	8:U:244:ARG:NH2	2.43	0.40
8:U:341:ARG:NH1	8:U:342:GLU:OE2	2.46	0.40
8:V:46:ASP:HA	8:V:246:PRO:HD3	2.02	0.40
8:W:288:THR:OG1	8:W:289:THR:N	2.53	0.40
8:Z:237:SER:O	8:Z:244:ARG:NH2	2.43	0.40
3:E:637:ARG:HA	3:E:637:ARG:HD3	1.88	0.40
3:E:712:ASN:HB3	3:E:725:HIS:CG	2.56	0.40
3:A:660:ILE:HD11	8:O:254:ILE:HD12	2.03	0.40
4:B:245:ILE:HG22	4:B:282:ASN:HB3	2.04	0.40
4:D:720:TYR:HA	4:D:723:THR:HG22	2.02	0.40
4:F:271:THR:OG1	4:F:272:GLU:N	2.55	0.40
4:H:433:TRP:CD1	4:H:483:VAL:HG22	2.54	0.40
6:I:148:ILE:HA	6:I:152:GLN:HE21	1.85	0.40
7:L:407:TYR:HB2	7:L:470:LEU:HD21	2.03	0.40
7:L:539:TRP:CE2	7:L:599:GLY:HA3	2.57	0.40
8:O:46:ASP:HA	8:O:246:PRO:HD3	2.02	0.40
8:P:71:PRO:O	8:P:75:HIS:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:341:ARG:NH1	8:R:342:GLU:OE2	2.46	0.40
8:V:28:GLU:HG3	8:V:367:LEU:HD11	2.02	0.40
8:X:421:MET:H	8:X:421:MET:HG3	1.69	0.40
8:Y:289:THR:OG1	8:Y:332:GLN:NE2	2.55	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%)	465 (92%)	38 (8%)	3 (1%)	25 66
1	l	104/1024 (10%)	96 (92%)	4 (4%)	4 (4%)	3 24
2	e	360/375 (96%)	339 (94%)	21 (6%)	0	100 100
3	A	599/902 (66%)	576 (96%)	22 (4%)	1 (0%)	47 81
3	C	606/902 (67%)	568 (94%)	37 (6%)	1 (0%)	47 81
3	E	628/902 (70%)	594 (95%)	32 (5%)	2 (0%)	41 77
3	G	628/902 (70%)	587 (94%)	37 (6%)	4 (1%)	25 66
4	B	602/907 (66%)	573 (95%)	27 (4%)	2 (0%)	41 77
4	D	571/907 (63%)	547 (96%)	21 (4%)	3 (0%)	29 69
4	F	591/907 (65%)	555 (94%)	35 (6%)	1 (0%)	47 81
4	H	584/907 (64%)	559 (96%)	23 (4%)	2 (0%)	41 77
4	a	112/907 (12%)	107 (96%)	5 (4%)	0	100 100
4	f	97/907 (11%)	92 (95%)	5 (5%)	0	100 100
4	h	97/907 (11%)	93 (96%)	4 (4%)	0	100 100
4	j	105/907 (12%)	98 (93%)	7 (7%)	0	100 100
5	b	63/82 (77%)	62 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
5	g	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	i	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
5	k	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
5	m	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
6	I	511/667 (77%)	482 (94%)	24 (5%)	5 (1%)	15	55
6	K	548/667 (82%)	528 (96%)	19 (4%)	1 (0%)	47	81
7	L	540/1819 (30%)	493 (91%)	43 (8%)	4 (1%)	22	63
7	c	148/1819 (8%)	142 (96%)	6 (4%)	0	100	100
8	O	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	P	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Q	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	R	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	S	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	T	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	U	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	V	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	W	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	X	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Y	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
8	Z	408/451 (90%)	390 (96%)	18 (4%)	0	100	100
All	All	13205/24163 (55%)	12536 (95%)	636 (5%)	33 (0%)	50	81

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	121	PRO
3	A	584	THR
3	C	239	ALA
4	D	627	GLU
4	D	884	GLU
3	G	241	ARG
6	I	508	ASN
6	I	601	LEU
1	J	236	LEU

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Mol	Chain	Res	Type
1	J	238	LEU
1	J	257	TYR
6	K	255	LYS
3	E	675	TRP
1	l	116	CYS
4	B	871	GLU
4	H	633	THR
6	I	600	ASN
3	E	581	ASP
3	G	481	GLU
7	L	451	PRO
1	l	115	LEU
1	l	118	SER
4	D	883	ASN
6	I	408	ASP
6	I	409	ASN
4	B	870	ASP
4	F	525	ASP
3	G	480	LYS
4	H	627	GLU
7	L	307	ARG
7	L	303	PRO
7	L	309	GLU
3	G	398	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%)	498 (100%)	0	100 100
1	l	84/933 (9%)	84 (100%)	0	100 100
2	e	310/318 (98%)	305 (98%)	5 (2%)	62 79
3	A	549/791 (69%)	546 (100%)	3 (0%)	88 93
3	C	556/791 (70%)	555 (100%)	1 (0%)	93 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	572/791 (72%)	571 (100%)	1 (0%)	93 96
3	G	572/791 (72%)	568 (99%)	4 (1%)	84 90
4	B	551/798 (69%)	546 (99%)	5 (1%)	78 87
4	D	525/798 (66%)	523 (100%)	2 (0%)	91 94
4	F	542/798 (68%)	537 (99%)	5 (1%)	78 87
4	H	539/798 (68%)	537 (100%)	2 (0%)	91 94
4	a	101/798 (13%)	100 (99%)	1 (1%)	76 86
4	f	88/798 (11%)	88 (100%)	0	100 100
4	h	88/798 (11%)	88 (100%)	0	100 100
4	j	88/798 (11%)	88 (100%)	0	100 100
5	b	53/62 (86%)	52 (98%)	1 (2%)	57 75
5	d	53/62 (86%)	53 (100%)	0	100 100
5	g	53/62 (86%)	53 (100%)	0	100 100
5	i	53/62 (86%)	53 (100%)	0	100 100
5	k	53/62 (86%)	53 (100%)	0	100 100
5	m	53/62 (86%)	53 (100%)	0	100 100
6	I	472/594 (80%)	471 (100%)	1 (0%)	93 96
6	K	509/594 (86%)	503 (99%)	6 (1%)	71 83
7	L	501/1546 (32%)	500 (100%)	1 (0%)	93 96
7	c	135/1546 (9%)	135 (100%)	0	100 100
8	O	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	P	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	Q	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	R	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	S	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	T	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	U	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	V	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	W	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	X	376/400 (94%)	337 (90%)	39 (10%)	7 24
8	Y	376/400 (94%)	337 (90%)	39 (10%)	7 24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	Z	376/400 (94%)	337 (90%)	39 (10%)	7 24
All	All	12110/21184 (57%)	11604 (96%)	506 (4%)	33 54

All (506) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	e	66	THR
2	e	165	ILE
2	e	215	LYS
2	e	261	LEU
2	e	305	MET
3	A	315	ARG
3	A	762	MET
3	A	861	PHE
4	B	252	ARG
4	B	285	ARG
4	B	406	THR
4	B	552	LYS
4	B	802	ARG
3	C	698	MET
4	D	563	ARG
4	D	656	CYS
5	b	63	VAL
4	F	285	ARG
4	F	293	ARG
4	F	323	SER
4	F	503	THR
4	F	719	GLN
3	G	418	ARG
3	G	478	THR
3	G	676	PHE
3	G	866	THR
4	H	598	THR
4	H	600	ILE
6	I	21	LYS
6	K	6	LEU
6	K	463	LEU
6	K	558	ARG
6	K	649	LEU
6	K	651	TYR
6	K	653	LYS
7	L	465	LYS

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Mol	Chain	Res	Type
8	O	7	THR
8	O	17	ILE
8	O	39	GLU
8	O	45	THR
8	O	50	VAL
8	O	68	ASP
8	O	109	SER
8	O	127	ASP
8	O	147	SER
8	O	149	LEU
8	O	153	LEU
8	O	157	LEU
8	O	165	LEU
8	O	170	SER
8	O	181	VAL
8	O	188	SER
8	O	201	CYS
8	O	203	VAL
8	O	204	VAL
8	O	224	SER
8	O	232	VAL
8	O	237	SER
8	O	256	LEU
8	O	259	SER
8	O	274	THR
8	O	277	THR
8	O	288	THR
8	O	293	VAL
8	O	298	LEU
8	O	313	THR
8	O	316	CYS
8	O	331	THR
8	O	333	VAL
8	O	361	SER
8	O	373	VAL
8	O	391	THR
8	O	402	GLU
8	O	425	ARG
8	O	442	ASP
8	P	7	THR
8	P	17	ILE
8	P	39	GLU

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Mol	Chain	Res	Type
8	P	45	THR
8	P	50	VAL
8	P	68	ASP
8	P	109	SER
8	P	127	ASP
8	P	147	SER
8	P	149	LEU
8	P	153	LEU
8	P	157	LEU
8	P	165	LEU
8	P	170	SER
8	P	181	VAL
8	P	188	SER
8	P	201	CYS
8	P	203	VAL
8	P	204	VAL
8	P	224	SER
8	P	232	VAL
8	P	237	SER
8	P	256	LEU
8	P	259	SER
8	P	274	THR
8	P	277	THR
8	P	288	THR
8	P	293	VAL
8	P	298	LEU
8	P	313	THR
8	P	316	CYS
8	P	331	THR
8	P	333	VAL
8	P	361	SER
8	P	373	VAL
8	P	391	THR
8	P	402	GLU
8	P	425	ARG
8	P	442	ASP
8	Q	7	THR
8	Q	17	ILE
8	Q	39	GLU
8	Q	45	THR
8	Q	50	VAL
8	Q	68	ASP

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Mol	Chain	Res	Type
8	Q	109	SER
8	Q	127	ASP
8	Q	147	SER
8	Q	149	LEU
8	Q	153	LEU
8	Q	157	LEU
8	Q	165	LEU
8	Q	170	SER
8	Q	181	VAL
8	Q	188	SER
8	Q	201	CYS
8	Q	203	VAL
8	Q	204	VAL
8	Q	224	SER
8	Q	232	VAL
8	Q	237	SER
8	Q	256	LEU
8	Q	259	SER
8	Q	274	THR
8	Q	277	THR
8	Q	288	THR
8	Q	293	VAL
8	Q	298	LEU
8	Q	313	THR
8	Q	316	CYS
8	Q	331	THR
8	Q	333	VAL
8	Q	361	SER
8	Q	373	VAL
8	Q	391	THR
8	Q	402	GLU
8	Q	425	ARG
8	Q	442	ASP
8	R	7	THR
8	R	17	ILE
8	R	39	GLU
8	R	45	THR
8	R	50	VAL
8	R	68	ASP
8	R	109	SER
8	R	127	ASP
8	R	147	SER

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Mol	Chain	Res	Type
8	R	149	LEU
8	R	153	LEU
8	R	157	LEU
8	R	165	LEU
8	R	170	SER
8	R	181	VAL
8	R	188	SER
8	R	201	CYS
8	R	203	VAL
8	R	204	VAL
8	R	224	SER
8	R	232	VAL
8	R	237	SER
8	R	256	LEU
8	R	259	SER
8	R	274	THR
8	R	277	THR
8	R	288	THR
8	R	293	VAL
8	R	298	LEU
8	R	313	THR
8	R	316	CYS
8	R	331	THR
8	R	333	VAL
8	R	361	SER
8	R	373	VAL
8	R	391	THR
8	R	402	GLU
8	R	425	ARG
8	R	442	ASP
8	S	7	THR
8	S	17	ILE
8	S	39	GLU
8	S	45	THR
8	S	50	VAL
8	S	68	ASP
8	S	109	SER
8	S	127	ASP
8	S	147	SER
8	S	149	LEU
8	S	153	LEU
8	S	157	LEU

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Mol	Chain	Res	Type
8	S	165	LEU
8	S	170	SER
8	S	181	VAL
8	S	188	SER
8	S	201	CYS
8	S	203	VAL
8	S	204	VAL
8	S	224	SER
8	S	232	VAL
8	S	237	SER
8	S	256	LEU
8	S	259	SER
8	S	274	THR
8	S	277	THR
8	S	288	THR
8	S	293	VAL
8	S	298	LEU
8	S	313	THR
8	S	316	CYS
8	S	331	THR
8	S	333	VAL
8	S	361	SER
8	S	373	VAL
8	S	391	THR
8	S	402	GLU
8	S	425	ARG
8	S	442	ASP
8	T	7	THR
8	T	17	ILE
8	T	39	GLU
8	T	45	THR
8	T	50	VAL
8	T	68	ASP
8	T	109	SER
8	T	127	ASP
8	T	147	SER
8	T	149	LEU
8	T	153	LEU
8	T	157	LEU
8	T	165	LEU
8	T	170	SER
8	T	181	VAL

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Mol	Chain	Res	Type
8	T	188	SER
8	T	201	CYS
8	T	203	VAL
8	T	204	VAL
8	T	224	SER
8	T	232	VAL
8	T	237	SER
8	T	256	LEU
8	T	259	SER
8	T	274	THR
8	T	277	THR
8	T	288	THR
8	T	293	VAL
8	T	298	LEU
8	T	313	THR
8	T	316	CYS
8	T	331	THR
8	T	333	VAL
8	T	361	SER
8	T	373	VAL
8	T	391	THR
8	T	402	GLU
8	T	425	ARG
8	T	442	ASP
8	U	7	THR
8	U	17	ILE
8	U	39	GLU
8	U	45	THR
8	U	50	VAL
8	U	68	ASP
8	U	109	SER
8	U	127	ASP
8	U	147	SER
8	U	149	LEU
8	U	153	LEU
8	U	157	LEU
8	U	165	LEU
8	U	170	SER
8	U	181	VAL
8	U	188	SER
8	U	201	CYS
8	U	203	VAL

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Mol	Chain	Res	Type
8	U	204	VAL
8	U	224	SER
8	U	232	VAL
8	U	237	SER
8	U	256	LEU
8	U	259	SER
8	U	274	THR
8	U	277	THR
8	U	288	THR
8	U	293	VAL
8	U	298	LEU
8	U	313	THR
8	U	316	CYS
8	U	331	THR
8	U	333	VAL
8	U	361	SER
8	U	373	VAL
8	U	391	THR
8	U	402	GLU
8	U	425	ARG
8	U	442	ASP
8	V	7	THR
8	V	17	ILE
8	V	39	GLU
8	V	45	THR
8	V	50	VAL
8	V	68	ASP
8	V	109	SER
8	V	127	ASP
8	V	147	SER
8	V	149	LEU
8	V	153	LEU
8	V	157	LEU
8	V	165	LEU
8	V	170	SER
8	V	181	VAL
8	V	188	SER
8	V	201	CYS
8	V	203	VAL
8	V	204	VAL
8	V	224	SER
8	V	232	VAL

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Mol	Chain	Res	Type
8	V	237	SER
8	V	256	LEU
8	V	259	SER
8	V	274	THR
8	V	277	THR
8	V	288	THR
8	V	293	VAL
8	V	298	LEU
8	V	313	THR
8	V	316	CYS
8	V	331	THR
8	V	333	VAL
8	V	361	SER
8	V	373	VAL
8	V	391	THR
8	V	402	GLU
8	V	425	ARG
8	V	442	ASP
8	W	7	THR
8	W	17	ILE
8	W	39	GLU
8	W	45	THR
8	W	50	VAL
8	W	68	ASP
8	W	109	SER
8	W	127	ASP
8	W	147	SER
8	W	149	LEU
8	W	153	LEU
8	W	157	LEU
8	W	165	LEU
8	W	170	SER
8	W	181	VAL
8	W	188	SER
8	W	201	CYS
8	W	203	VAL
8	W	204	VAL
8	W	224	SER
8	W	232	VAL
8	W	237	SER
8	W	256	LEU
8	W	259	SER

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Mol	Chain	Res	Type
8	W	274	THR
8	W	277	THR
8	W	288	THR
8	W	293	VAL
8	W	298	LEU
8	W	313	THR
8	W	316	CYS
8	W	331	THR
8	W	333	VAL
8	W	361	SER
8	W	373	VAL
8	W	391	THR
8	W	402	GLU
8	W	425	ARG
8	W	442	ASP
8	X	7	THR
8	X	17	ILE
8	X	39	GLU
8	X	45	THR
8	X	50	VAL
8	X	68	ASP
8	X	109	SER
8	X	127	ASP
8	X	147	SER
8	X	149	LEU
8	X	153	LEU
8	X	157	LEU
8	X	165	LEU
8	X	170	SER
8	X	181	VAL
8	X	188	SER
8	X	201	CYS
8	X	203	VAL
8	X	204	VAL
8	X	224	SER
8	X	232	VAL
8	X	237	SER
8	X	256	LEU
8	X	259	SER
8	X	274	THR
8	X	277	THR
8	X	288	THR

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Mol	Chain	Res	Type
8	X	293	VAL
8	X	298	LEU
8	X	313	THR
8	X	316	CYS
8	X	331	THR
8	X	333	VAL
8	X	361	SER
8	X	373	VAL
8	X	391	THR
8	X	402	GLU
8	X	425	ARG
8	X	442	ASP
8	Y	7	THR
8	Y	17	ILE
8	Y	39	GLU
8	Y	45	THR
8	Y	50	VAL
8	Y	68	ASP
8	Y	109	SER
8	Y	127	ASP
8	Y	147	SER
8	Y	149	LEU
8	Y	153	LEU
8	Y	157	LEU
8	Y	165	LEU
8	Y	170	SER
8	Y	181	VAL
8	Y	188	SER
8	Y	201	CYS
8	Y	203	VAL
8	Y	204	VAL
8	Y	224	SER
8	Y	232	VAL
8	Y	237	SER
8	Y	256	LEU
8	Y	259	SER
8	Y	274	THR
8	Y	277	THR
8	Y	288	THR
8	Y	293	VAL
8	Y	298	LEU
8	Y	313	THR

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Mol	Chain	Res	Type
8	Y	316	CYS
8	Y	331	THR
8	Y	333	VAL
8	Y	361	SER
8	Y	373	VAL
8	Y	391	THR
8	Y	402	GLU
8	Y	425	ARG
8	Y	442	ASP
8	Z	7	THR
8	Z	17	ILE
8	Z	39	GLU
8	Z	45	THR
8	Z	50	VAL
8	Z	68	ASP
8	Z	109	SER
8	Z	127	ASP
8	Z	147	SER
8	Z	149	LEU
8	Z	153	LEU
8	Z	157	LEU
8	Z	165	LEU
8	Z	170	SER
8	Z	181	VAL
8	Z	188	SER
8	Z	201	CYS
8	Z	203	VAL
8	Z	204	VAL
8	Z	224	SER
8	Z	232	VAL
8	Z	237	SER
8	Z	256	LEU
8	Z	259	SER
8	Z	274	THR
8	Z	277	THR
8	Z	288	THR
8	Z	293	VAL
8	Z	298	LEU
8	Z	313	THR
8	Z	316	CYS
8	Z	331	THR
8	Z	333	VAL

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Mol	Chain	Res	Type
8	Z	361	SER
8	Z	373	VAL
8	Z	391	THR
8	Z	402	GLU
8	Z	425	ARG
8	Z	442	ASP
4	a	60	LYS
3	E	233	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (223) such sidechains are listed below:

Mol	Chain	Res	Type
2	e	101	HIS
3	A	152	GLN
3	A	360	HIS
3	A	412	HIS
3	A	438	GLN
3	A	458	ASN
3	A	631	ASN
3	A	684	GLN
3	A	688	ASN
3	A	692	ASN
4	B	550	ASN
4	B	703	GLN
4	B	773	ASN
4	B	774	GLN
4	B	781	GLN
4	B	830	ASN
3	C	371	GLN
3	C	530	HIS
3	C	639	GLN
4	D	389	GLN
4	D	401	HIS
4	D	558	HIS
4	D	560	GLN
4	D	659	HIS
4	D	705	HIS
4	D	773	ASN
4	D	789	GLN
4	D	801	GLN
4	F	270	ASN
4	F	310	GLN

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Mol	Chain	Res	Type
4	F	329	HIS
4	F	416	GLN
4	F	461	HIS
4	F	713	HIS
4	F	742	GLN
4	F	773	ASN
3	G	309	GLN
3	G	438	GLN
3	G	662	ASN
3	G	684	GLN
3	G	726	HIS
3	G	828	ASN
3	G	832	HIS
4	H	273	ASN
4	H	387	HIS
4	H	416	GLN
4	H	479	GLN
4	H	570	GLN
4	H	596	ASN
4	H	687	ASN
4	H	703	GLN
6	I	116	HIS
6	I	303	GLN
6	I	353	GLN
6	I	370	GLN
6	I	504	HIS
6	I	533	GLN
6	I	547	GLN
6	I	599	GLN
1	J	269	GLN
1	J	298	ASN
1	J	456	GLN
1	J	694	HIS
1	J	721	GLN
1	J	822	ASN
1	J	892	HIS
1	J	895	ASN
1	J	925	GLN
1	J	938	HIS
6	K	35	HIS
6	K	61	GLN
6	K	123	ASN

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Mol	Chain	Res	Type
6	K	130	GLN
6	K	290	ASN
6	K	339	HIS
6	K	499	GLN
6	K	509	GLN
6	K	543	GLN
7	L	469	GLN
7	L	512	ASN
7	L	517	HIS
7	L	1492	ASN
7	L	1667	HIS
7	L	1679	GLN
7	L	1770	ASN
7	L	1792	GLN
8	O	54	GLN
8	O	187	ASN
8	O	207	ASN
8	O	227	GLN
8	O	229	ASN
8	O	302	ASN
8	O	314	ASN
8	O	332	GLN
8	O	357	GLN
8	O	430	GLN
8	P	54	GLN
8	P	187	ASN
8	P	207	ASN
8	P	227	GLN
8	P	229	ASN
8	P	302	ASN
8	P	314	ASN
8	P	332	GLN
8	P	430	GLN
8	Q	54	GLN
8	Q	187	ASN
8	Q	207	ASN
8	Q	227	GLN
8	Q	229	ASN
8	Q	302	ASN
8	Q	314	ASN
8	Q	332	GLN
8	Q	430	GLN

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Mol	Chain	Res	Type
8	R	54	GLN
8	R	187	ASN
8	R	207	ASN
8	R	227	GLN
8	R	229	ASN
8	R	251	ASN
8	R	302	ASN
8	R	314	ASN
8	R	332	GLN
8	R	430	GLN
8	S	54	GLN
8	S	187	ASN
8	S	207	ASN
8	S	227	GLN
8	S	229	ASN
8	S	302	ASN
8	S	314	ASN
8	S	332	GLN
8	S	430	GLN
8	T	54	GLN
8	T	175	GLN
8	T	187	ASN
8	T	207	ASN
8	T	227	GLN
8	T	229	ASN
8	T	251	ASN
8	T	302	ASN
8	T	314	ASN
8	T	332	GLN
8	T	334	HIS
8	T	430	GLN
8	U	54	GLN
8	U	175	GLN
8	U	187	ASN
8	U	207	ASN
8	U	227	GLN
8	U	229	ASN
8	U	302	ASN
8	U	314	ASN
8	U	332	GLN
8	U	334	HIS
8	U	338	GLN

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Mol	Chain	Res	Type
8	U	430	GLN
8	V	54	GLN
8	V	175	GLN
8	V	187	ASN
8	V	207	ASN
8	V	227	GLN
8	V	229	ASN
8	V	302	ASN
8	V	314	ASN
8	V	332	GLN
8	V	357	GLN
8	V	430	GLN
8	W	54	GLN
8	W	158	ASN
8	W	175	GLN
8	W	187	ASN
8	W	207	ASN
8	W	227	GLN
8	W	229	ASN
8	W	302	ASN
8	W	314	ASN
8	W	332	GLN
8	W	430	GLN
8	X	54	GLN
8	X	187	ASN
8	X	207	ASN
8	X	227	GLN
8	X	229	ASN
8	X	302	ASN
8	X	314	ASN
8	X	332	GLN
8	X	357	GLN
8	X	430	GLN
8	Y	54	GLN
8	Y	187	ASN
8	Y	207	ASN
8	Y	227	GLN
8	Y	229	ASN
8	Y	302	ASN
8	Y	314	ASN
8	Y	332	GLN
8	Y	430	GLN

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Mol	Chain	Res	Type
8	Z	54	GLN
8	Z	187	ASN
8	Z	207	ASN
8	Z	227	GLN
8	Z	229	ASN
8	Z	302	ASN
8	Z	314	ASN
8	Z	332	GLN
8	Z	430	GLN
4	a	33	GLN
4	f	78	HIS
7	c	29	ASN
7	c	48	ASN
7	c	176	GLN
3	E	152	GLN
3	E	261	HIS
3	E	309	GLN
3	E	316	GLN
3	E	420	GLN
3	E	438	GLN
3	E	580	HIS
3	E	725	HIS
3	E	741	ASN
3	E	763	GLN
3	E	767	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (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.

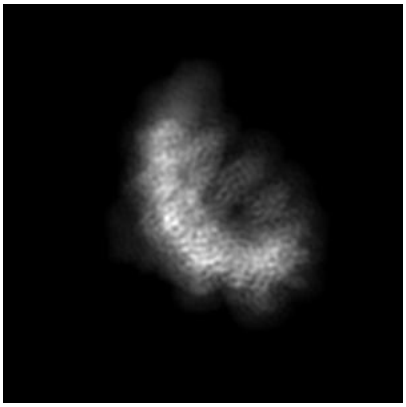
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14012. These allow visual inspection of the internal detail of the map and identification of artifacts.

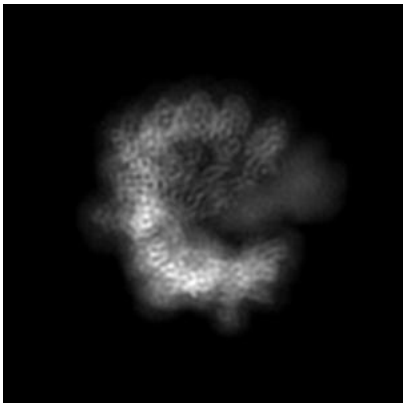
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

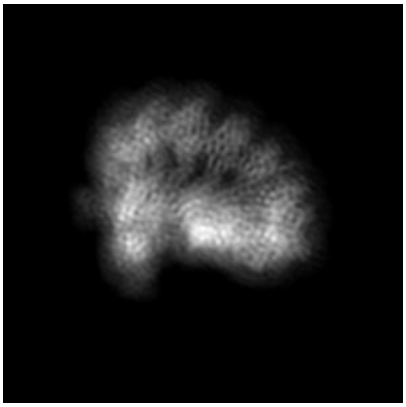
6.1.1 Primary map



X



Y

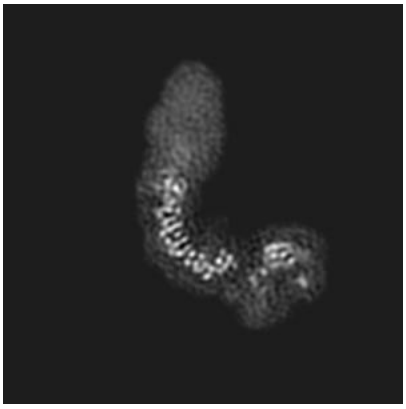


Z

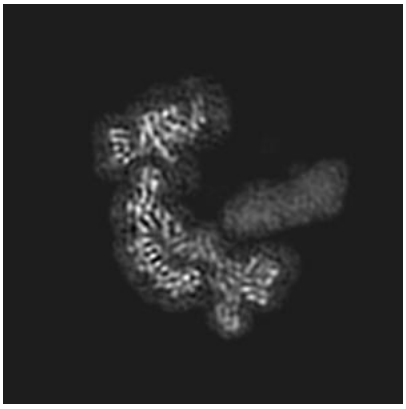
The images above show the map projected in three orthogonal directions.

6.2 Central slices

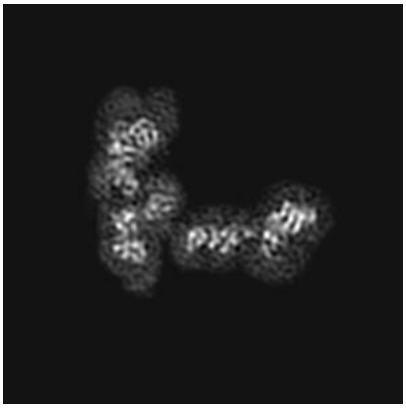
6.2.1 Primary map



X Index: 100



Y Index: 100

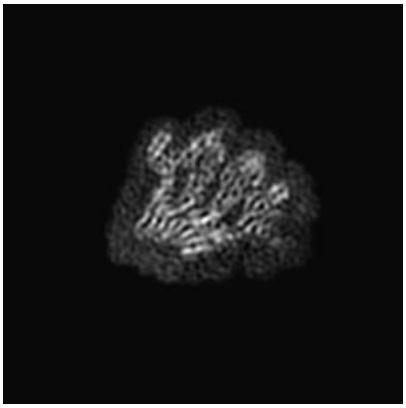


Z Index: 100

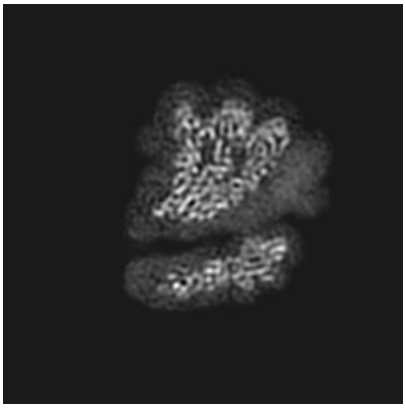
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

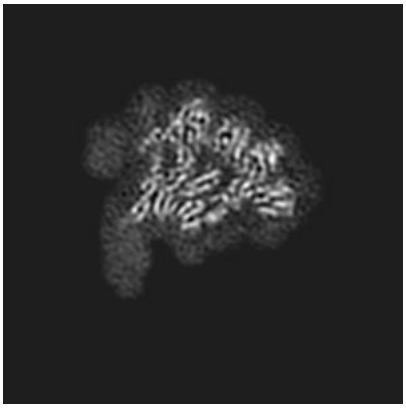
6.3.1 Primary map



X Index: 63



Y Index: 81

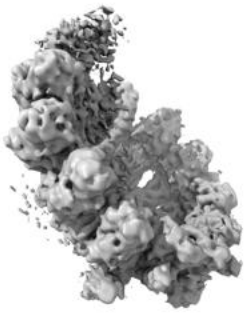


Z Index: 72

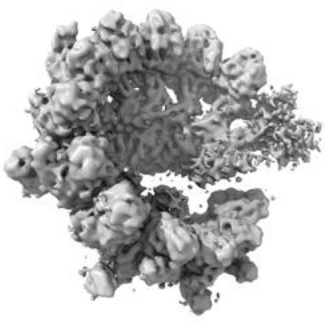
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

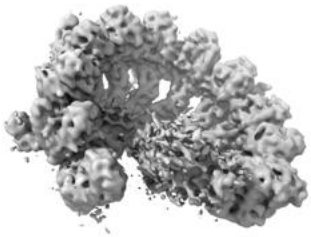
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0368. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

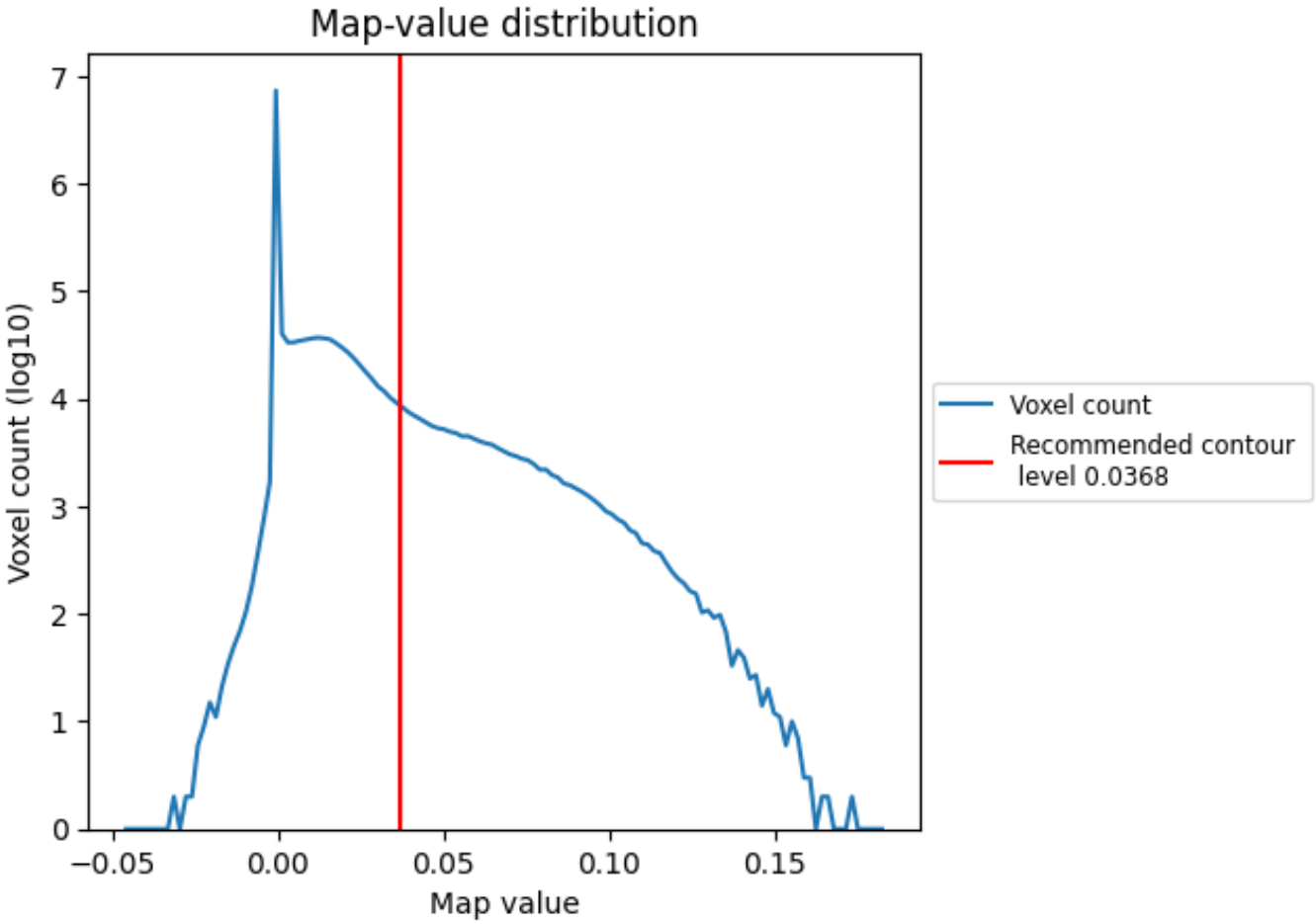
6.5 Mask visualisation (i)

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

7 Map analysis

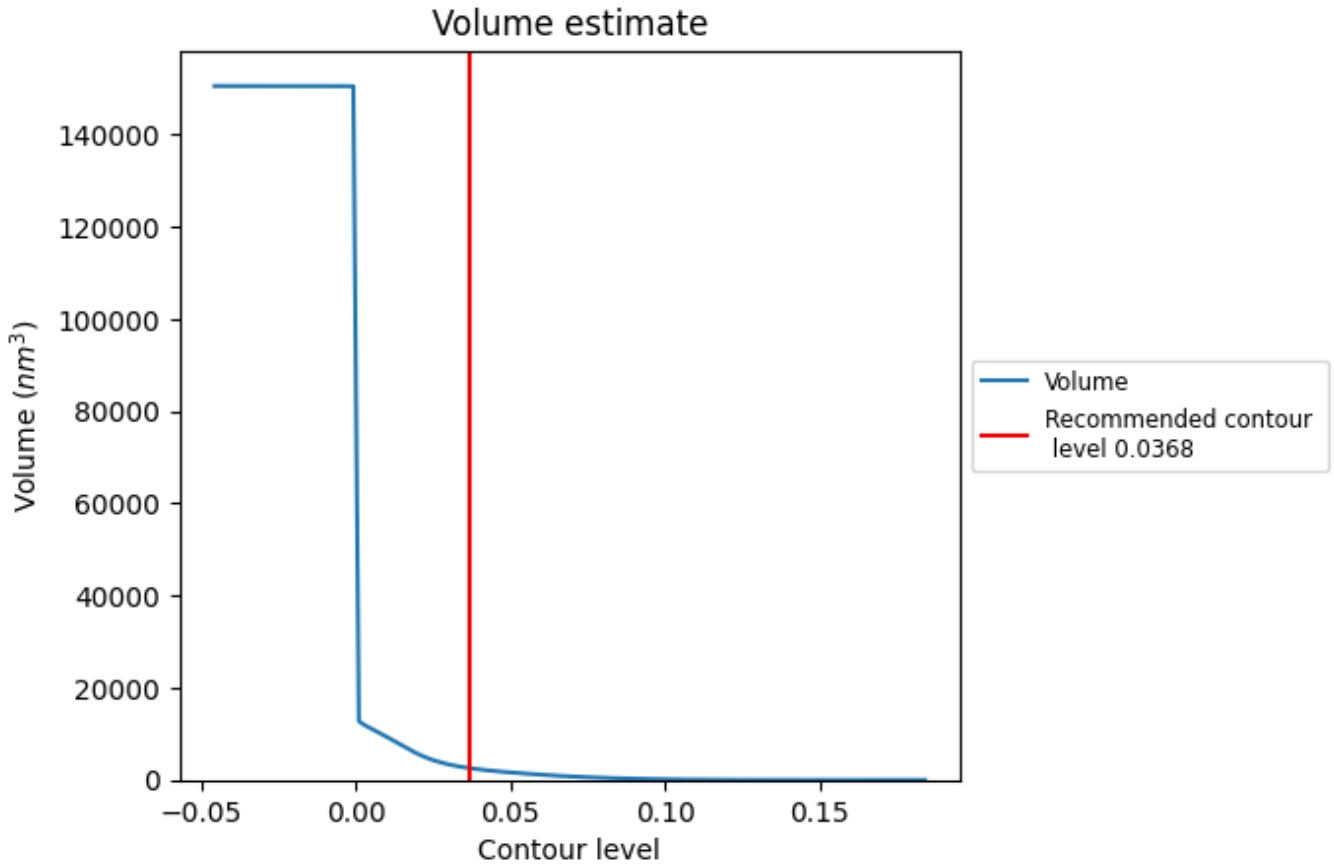
This section contains the results of statistical analysis of the map.

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.

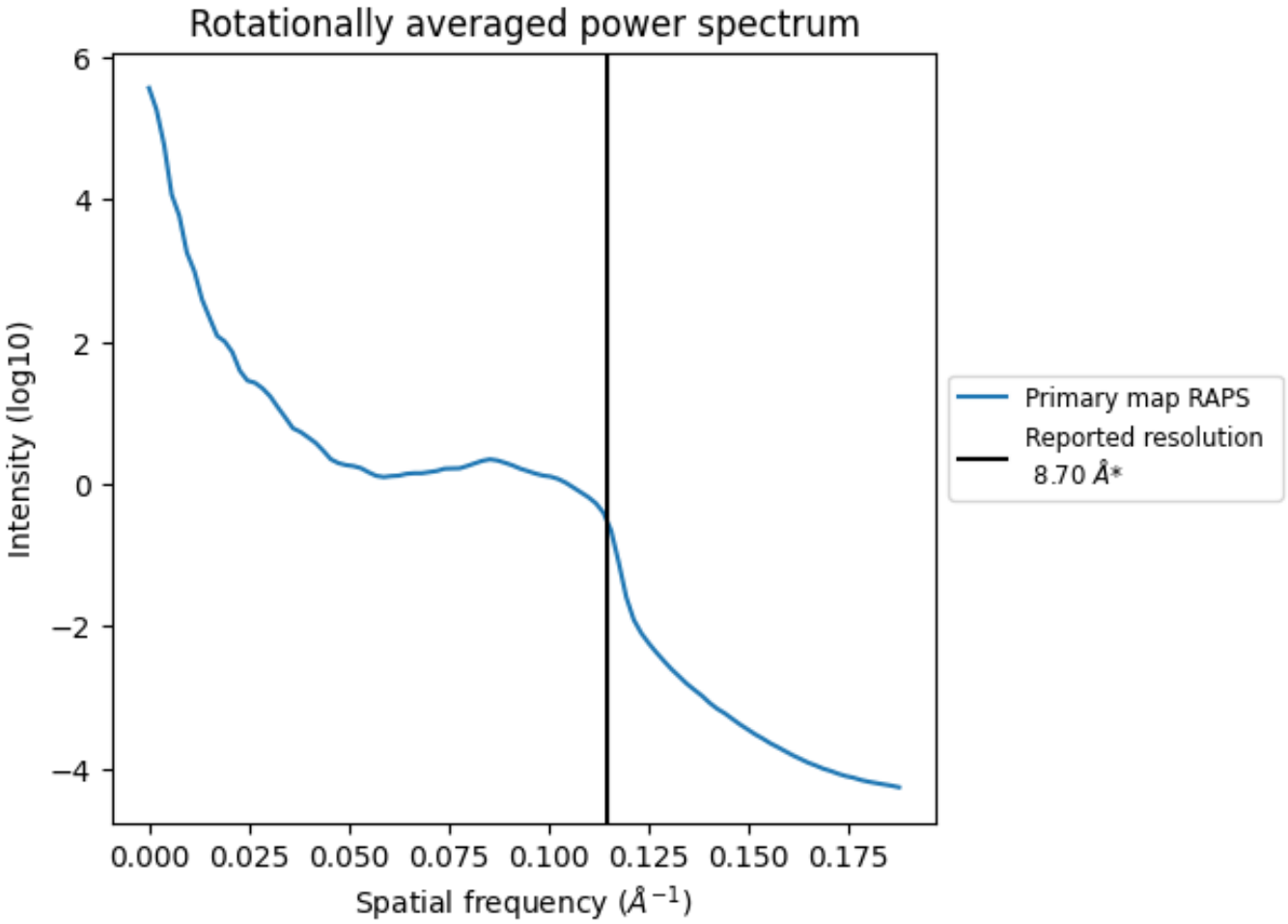
7.2 Volume estimate



The volume at the recommended contour level is 2556 nm^3; this corresponds to an approximate mass of 2308 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.115 Å^{-1}

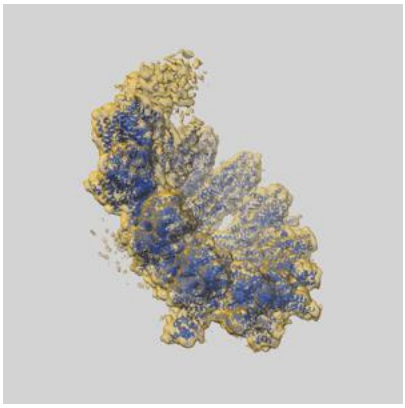
8 Fourier-Shell correlation

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

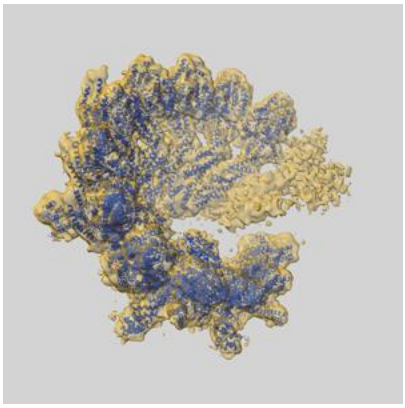
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14012 and PDB model 7QJ7. Per-residue inclusion information can be found in section 3 on page 8.

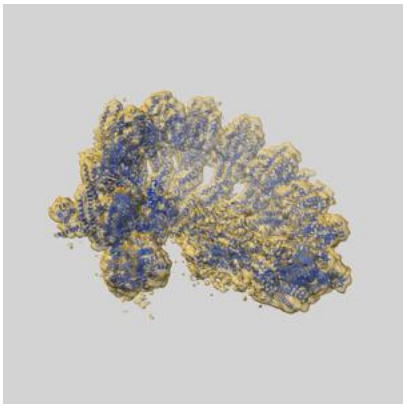
9.1 Map-model overlay



X



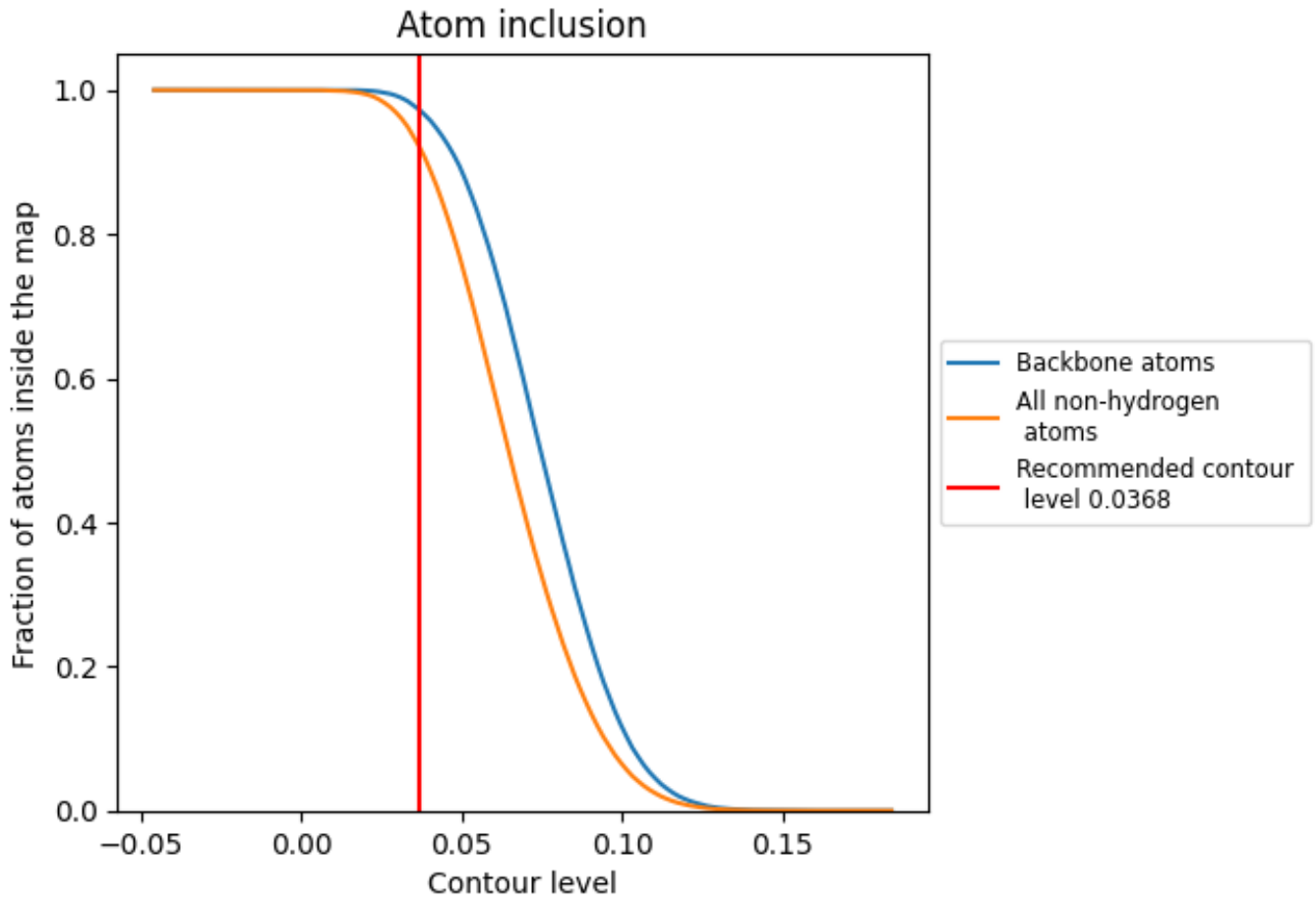
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0368 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, 97% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.