Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:58 AM UTC

PDB ID	:	8RX1 / pdb_00008rx1
EMDB ID	:	EMD-19570
Title	:	CryoEM structure of the gTuRC-CM1dim complex
Authors	:	Llorca, O.; Serna, M.; Gonzalez-Rodriguez, N.
Deposited on	:	2024-02-06
Resolution	:	3.57 Å(reported)
Based on initial models	:	6X0V, 7AS4

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

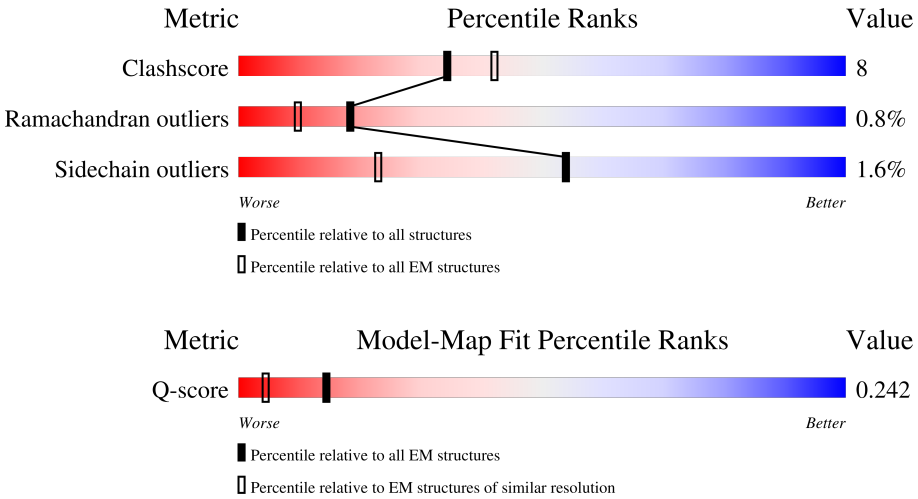
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.57 Å.

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



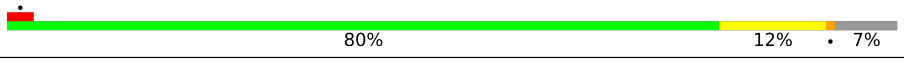
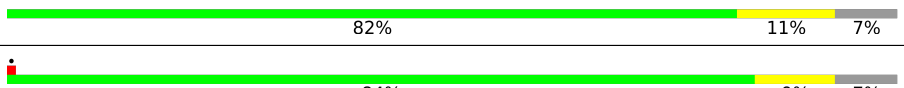
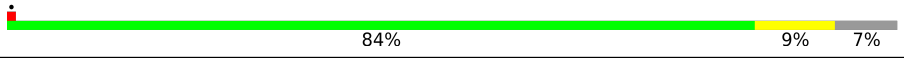
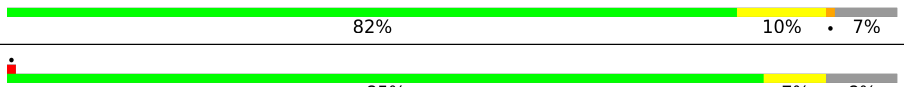
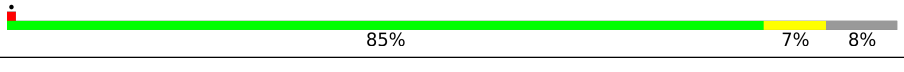
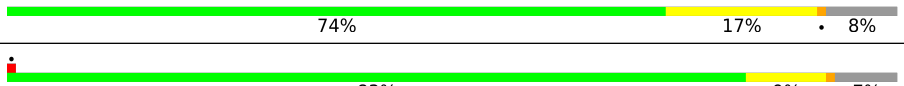
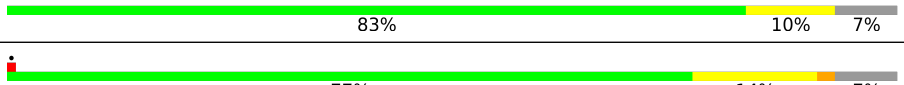
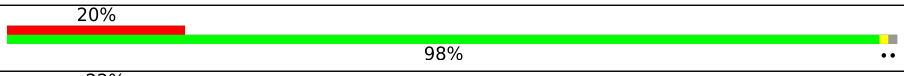
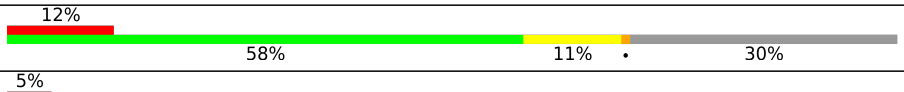
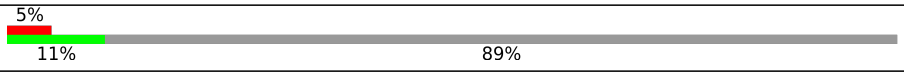
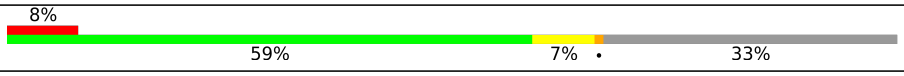
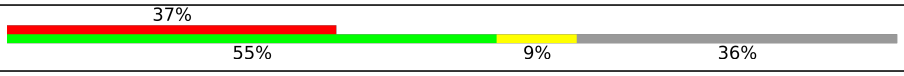
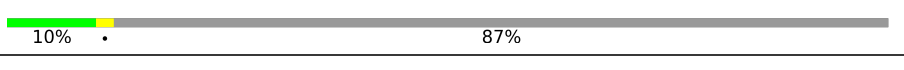
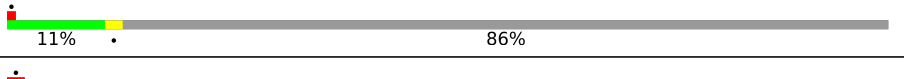
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12682 (3.07 - 4.07)

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

Mol	Chain	Length	Quality of chain
1	1	451	27% 81% 11% • 7%
1	2	451	61% 76% 13% • 8%
1	O	451	41% 72% 19% • 7%
1	P	451	26% 78% 14% • 7%

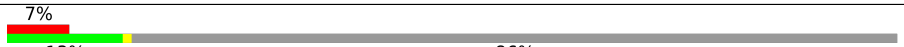
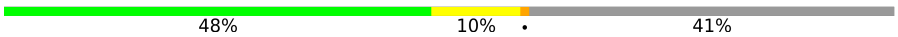
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Mol	Chain	Length	Quality of chain
1	Q	451	
1	R	451	
1	S	451	
1	T	451	
1	U	451	
1	V	451	
1	W	451	
1	X	451	
1	Y	451	
1	Z	451	
2	7	364	
3	A	902	
3	C	902	
3	E	902	
3	M	902	
3	f	902	
3	k	902	
4	B	907	
4	D	907	
4	F	907	
4	N	907	
4	b	907	
4	n	907	
5	G	229	
5	H	229	

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Mol	Chain	Length	Quality of chain
5	g	229	
5	h	229	
5	i	229	
5	j	229	
5	s	229	
5	t	229	
5	u	229	
5	v	229	
6	I	667	
6	K	667	
7	J	1024	
8	L	1819	
8	d	1819	
9	a	82	
9	c	82	
10	e	158	

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 123860 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	420	Total	C	N	O	S	0	0
			3365	2130	583	637	15		
1	2	415	Total	C	N	O	S	0	0
			3311	2095	574	627	15		
1	O	420	Total	C	N	O	S	0	0
			3365	2130	583	637	15		
1	P	420	Total	C	N	O	S	0	0
			3359	2127	580	637	15		
1	Q	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		
1	R	420	Total	C	N	O	S	0	0
			3365	2130	583	637	15		
1	S	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		
1	T	420	Total	C	N	O	S	0	0
			3359	2127	580	637	15		
1	U	420	Total	C	N	O	S	0	0
			3365	2130	583	637	15		
1	V	417	Total	C	N	O	S	0	0
			3325	2109	571	630	15		
1	W	417	Total	C	N	O	S	0	0
			3342	2114	579	634	15		
1	X	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		
1	Y	419	Total	C	N	O	S	0	0
			3363	2129	585	634	15		
1	Z	420	Total	C	N	O	S	0	0
			3365	2130	583	637	15		

- Molecule 2 is a protein called Actin b.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	7	360	Total	C	N	O	0	0
			1812	1091	360	361		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	599	Total	C	N	O	S	0	0
			4846	3135	802	877	32		
3	C	614	Total	C	N	O	S	0	0
			4973	3216	824	901	32		
3	E	638	Total	C	N	O	S	0	0
			5196	3351	870	942	33		
3	M	633	Total	C	N	O	S	0	0
			5158	3325	865	935	33		
3	f	95	Total	C	N	O		0	0
			481	291	95	95			
3	k	636	Total	C	N	O	S	0	0
			5180	3339	868	940	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
			5015	3195	885	910	25		
4	D	581	Total	C	N	O	S	0	0
			4790	3058	839	868	25		
4	F	599	Total	C	N	O	S	0	0
			4921	3140	865	891	25		
4	N	583	Total	C	N	O	S	0	0
			4810	3072	848	865	25		
4	b	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
4	n	594	Total	C	N	O	S	0	0
			4875	3113	852	885	25		

- Molecule 5 is a protein called CM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	31	Total	C	N	O	S	0	0
			270	173	46	50	1		
5	H	35	Total	C	N	O	S	0	0
			317	202	55	58	2		
5	g	35	Total	C	N	O	S	0	0
			303	192	54	55	2		
5	h	35	Total	C	N	O	S	0	0
			317	202	55	58	2		
5	i	31	Total	C	N	O	S	0	0
			274	176	46	50	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	32	Total	C	N	O	S	0	0
			290	187	48	54	1		
5	s	35	Total	C	N	O	S	0	0
			303	192	54	55	2		
5	t	35	Total	C	N	O	S	0	0
			303	192	54	55	2		
5	u	35	Total	C	N	O	S	0	0
			317	202	55	58	2		
5	v	35	Total	C	N	O	S	0	0
			317	202	55	58	2		

- 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
			4203	2722	714	749	18		
6	K	562	Total	C	N	O	S	0	0
			4573	2961	778	816	18		

- Molecule 7 is a protein called Gamma-tubulin complex component 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	601	Total	C	N	O	S	0	0
			4837	3127	811	872	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	617	Total	C	N	O	S	0	0
			4928	3217	830	855	26		
8	d	147	Total	C	N	O	S	0	0
			1152	727	198	219	8		

- Molecule 9 is a protein called Mitotic-spindle organizing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
9	c	59	Total	C	N	O	S	0	0
			454	281	79	90	4		

- Molecule 10 is a protein called Mitotic-spindle organizing protein 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	e	46	Total	C	N	O	0	0
			231	139	46	46		

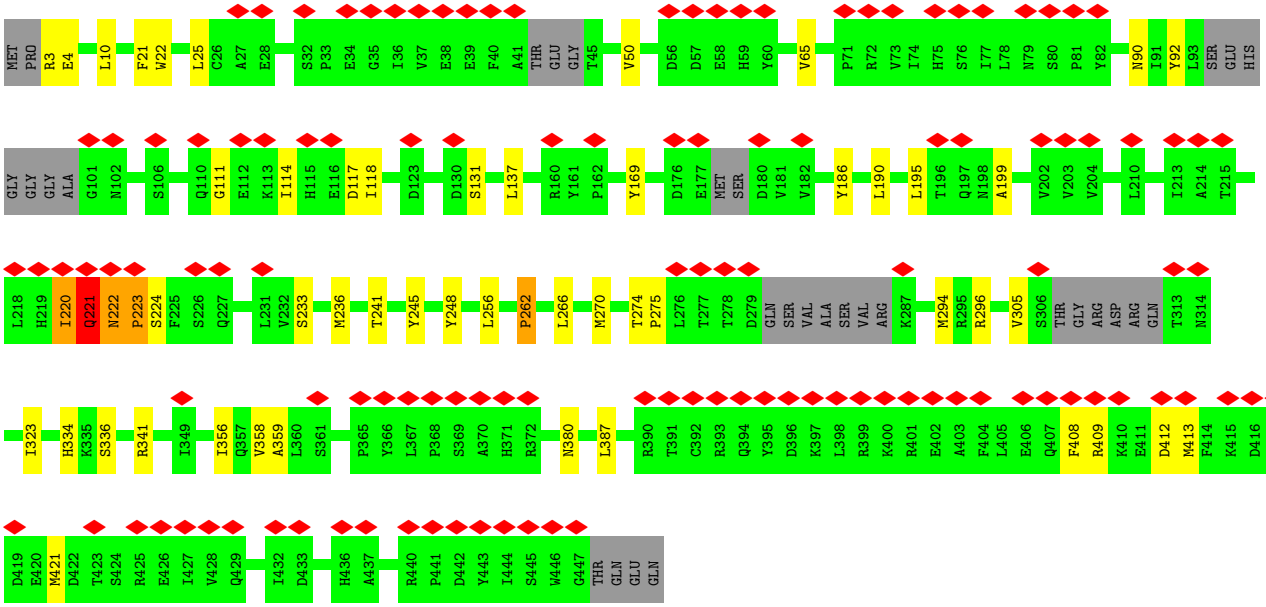
3 Residue-property plots (i)

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

• Molecule 1: Tubulin gamma-1 chain

Chain 1:

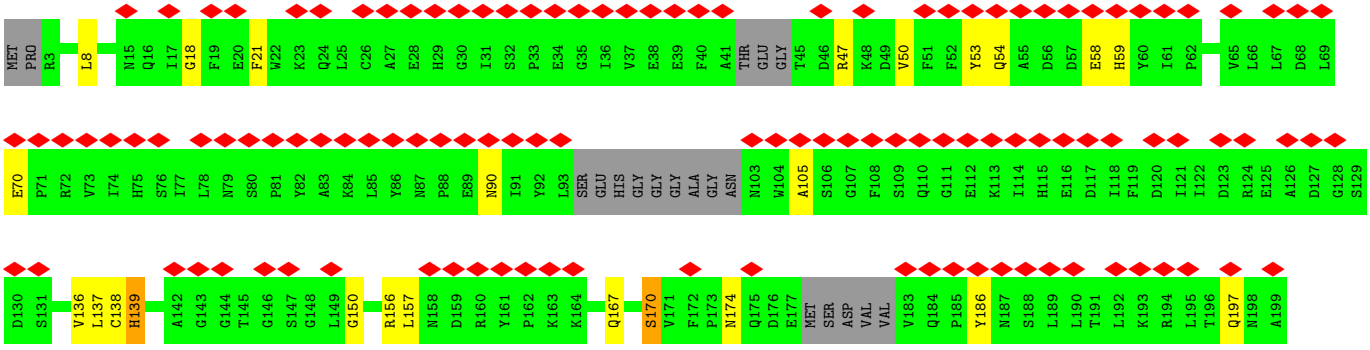


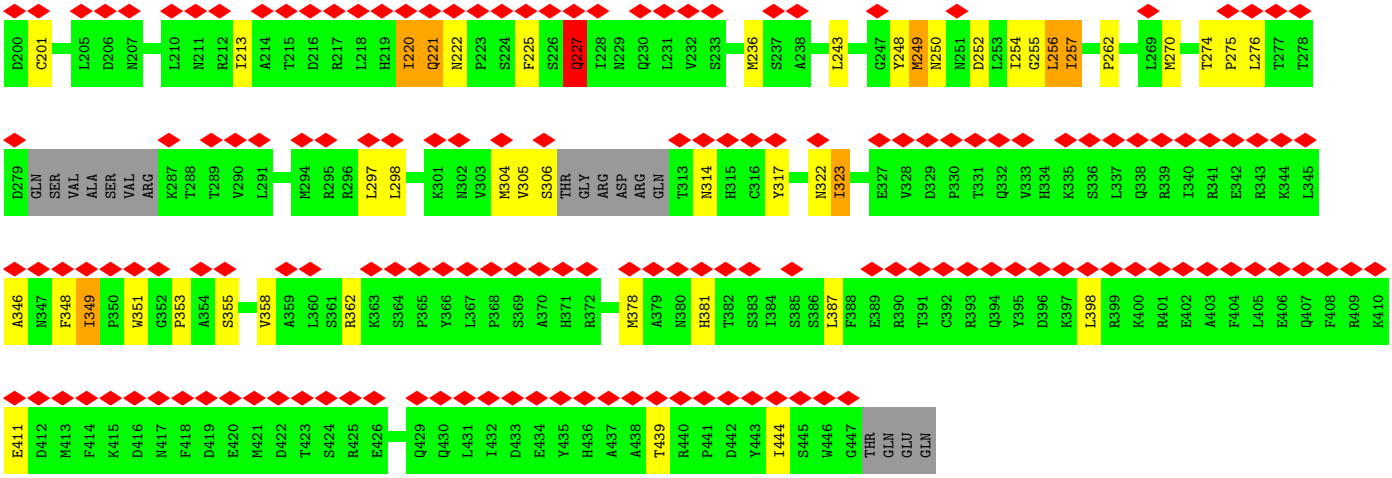


• Molecule 1: Tubulin gamma-1 chain

Chain 2:



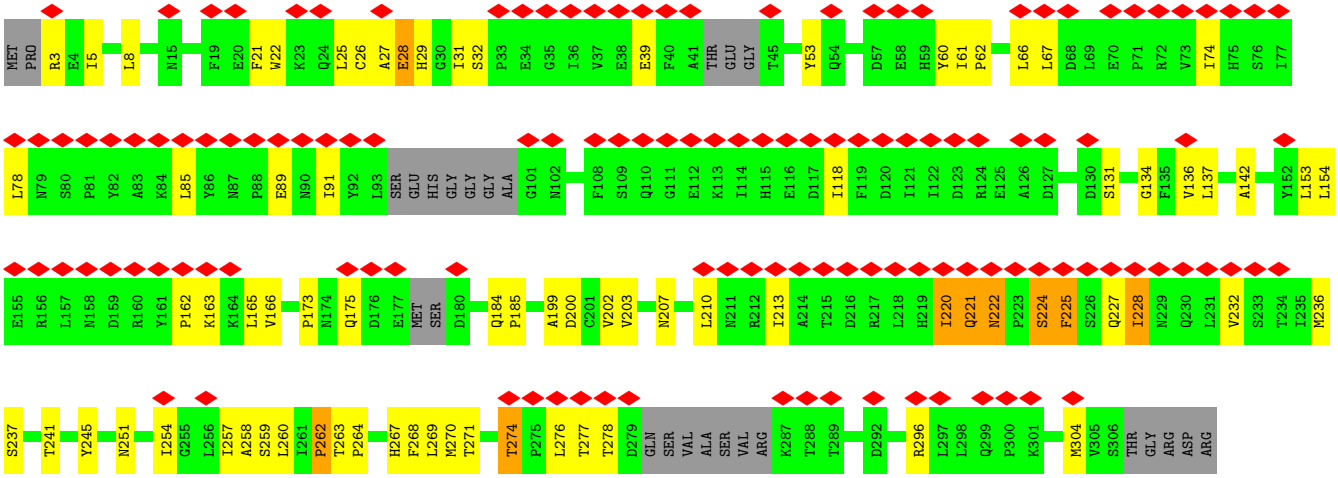




• Molecule 1: Tubulin gamma-1 chain

Chain O:

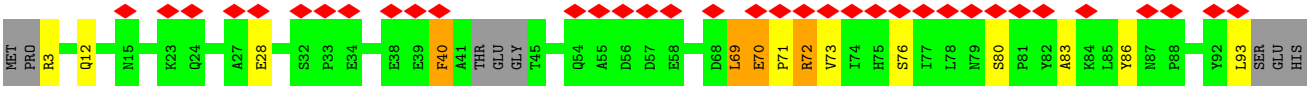


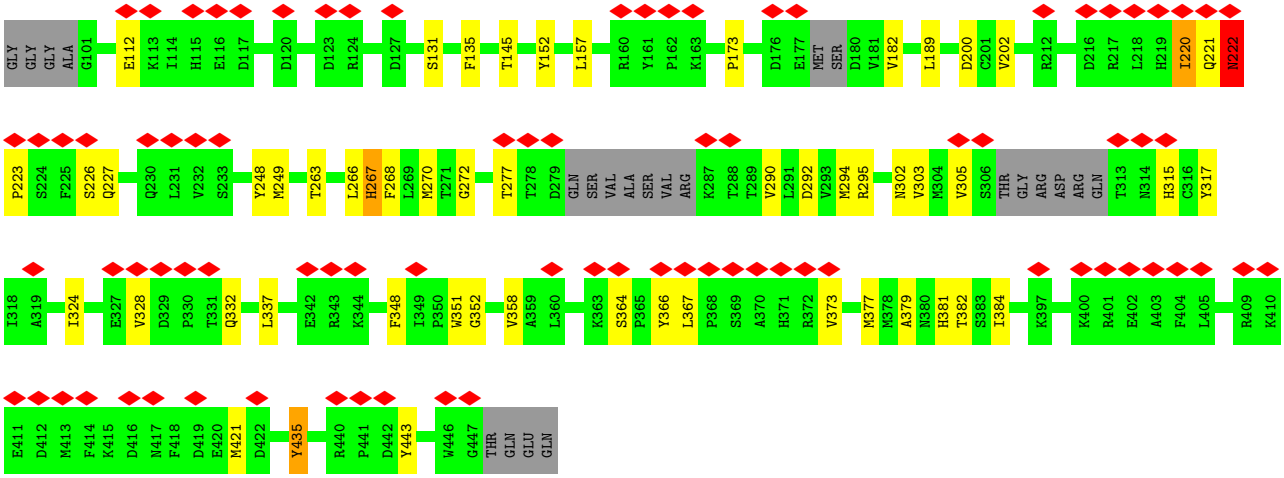


• Molecule 1: Tubulin gamma-1 chain

Chain P:



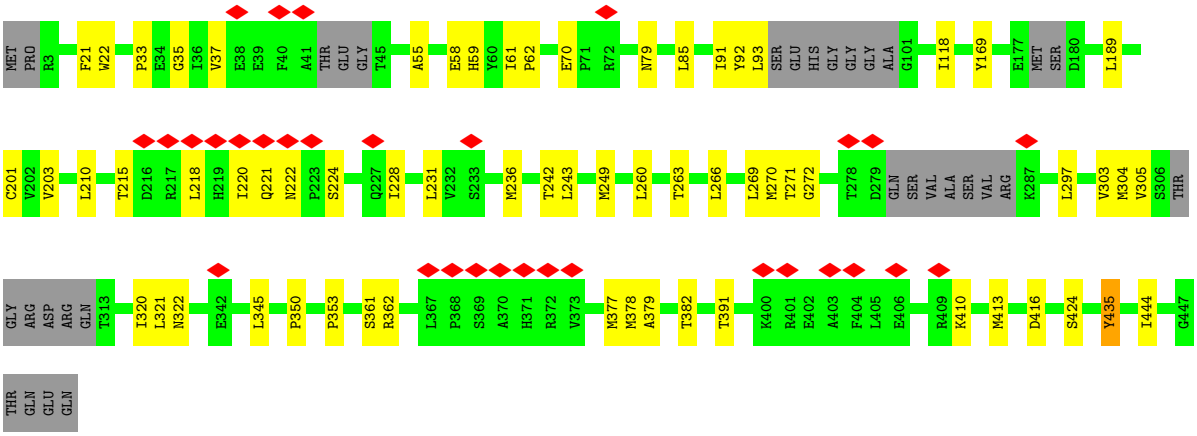




• Molecule 1: Tubulin gamma-1 chain

Chain Q:

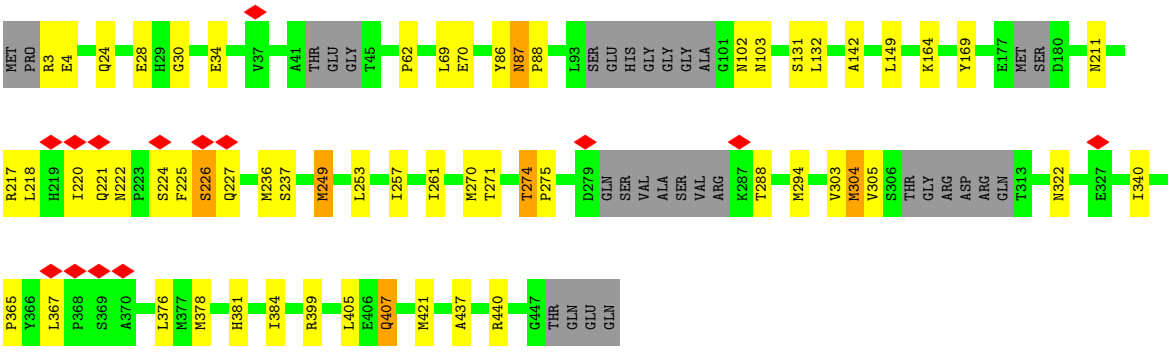




• Molecule 1: Tubulin gamma-1 chain

Chain R:

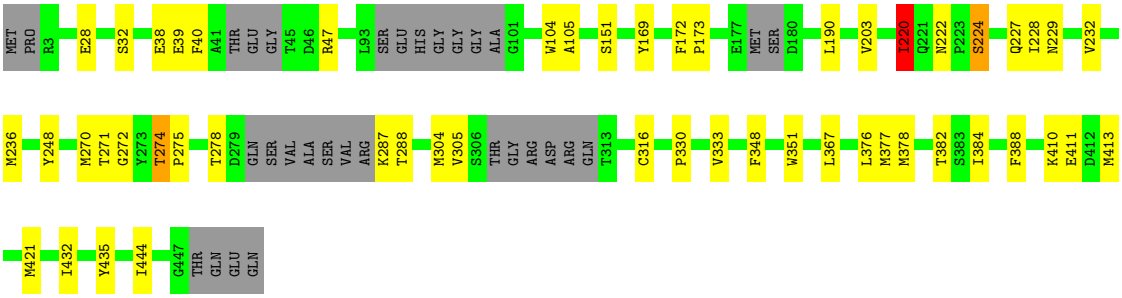




• Molecule 1: Tubulin gamma-1 chain

Chain S:

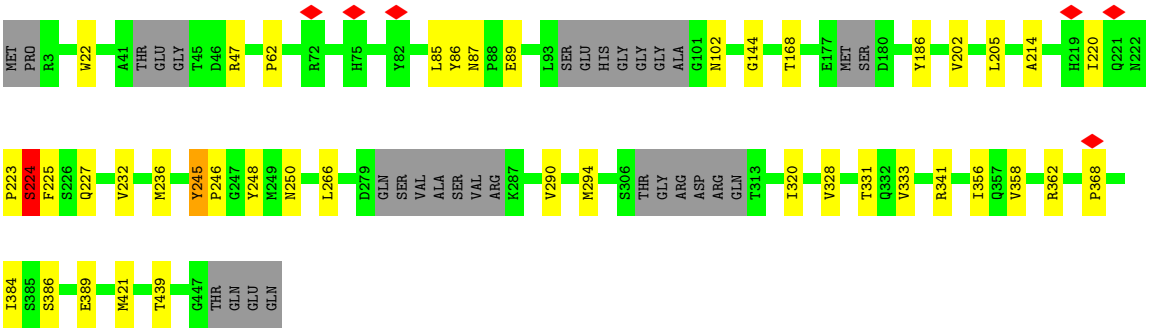




• Molecule 1: Tubulin gamma-1 chain

Chain T:

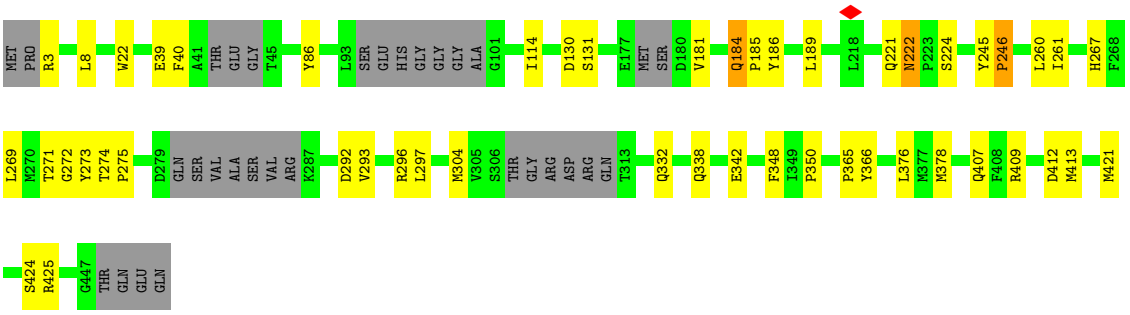




• Molecule 1: Tubulin gamma-1 chain

Chain U:

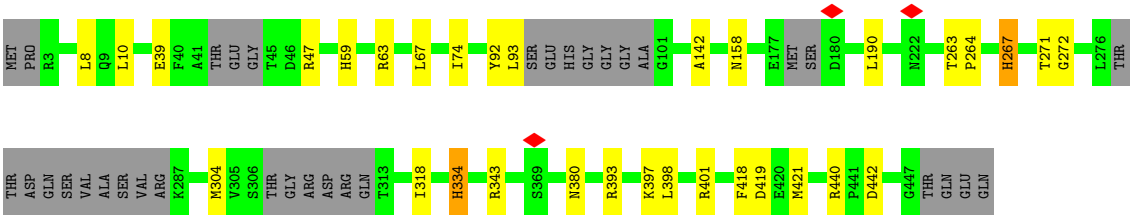




• Molecule 1: Tubulin gamma-1 chain

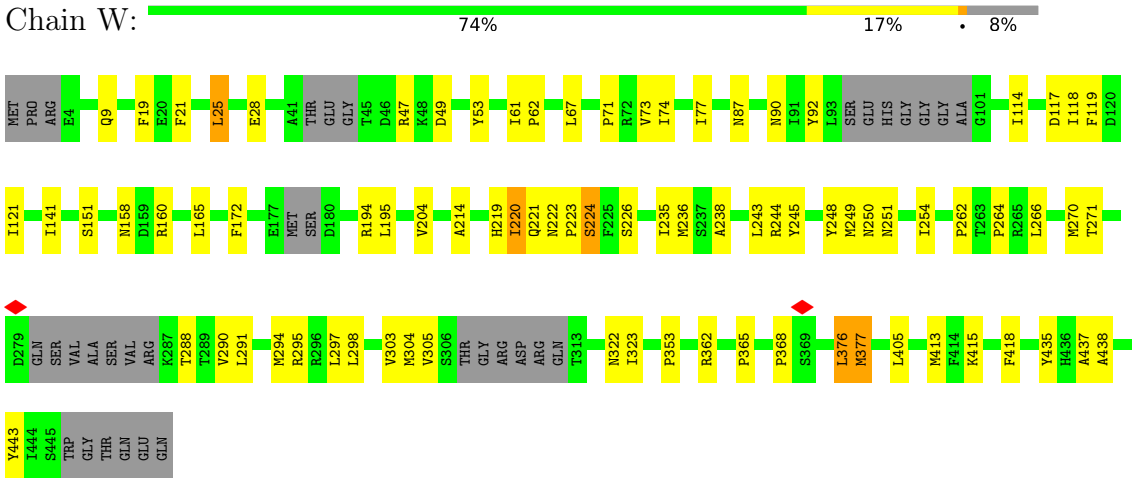
Chain V:





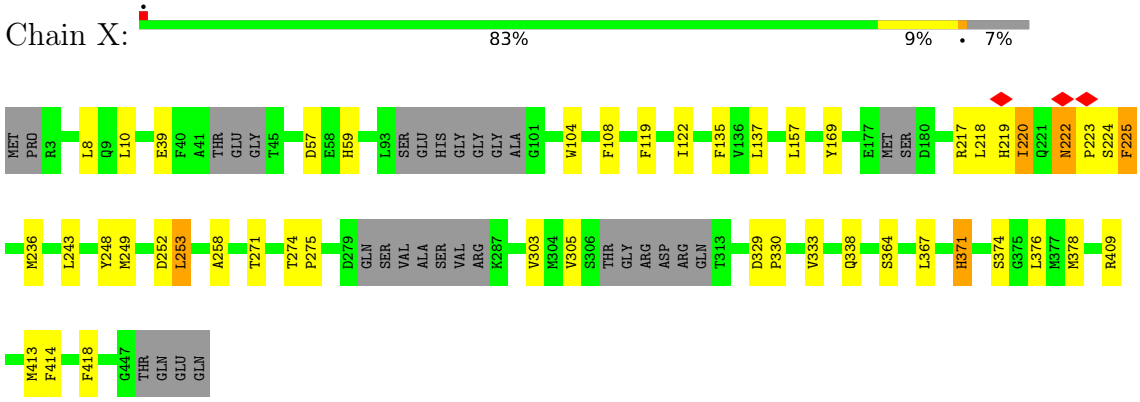
• Molecule 1: Tubulin gamma-1 chain

Chain W:



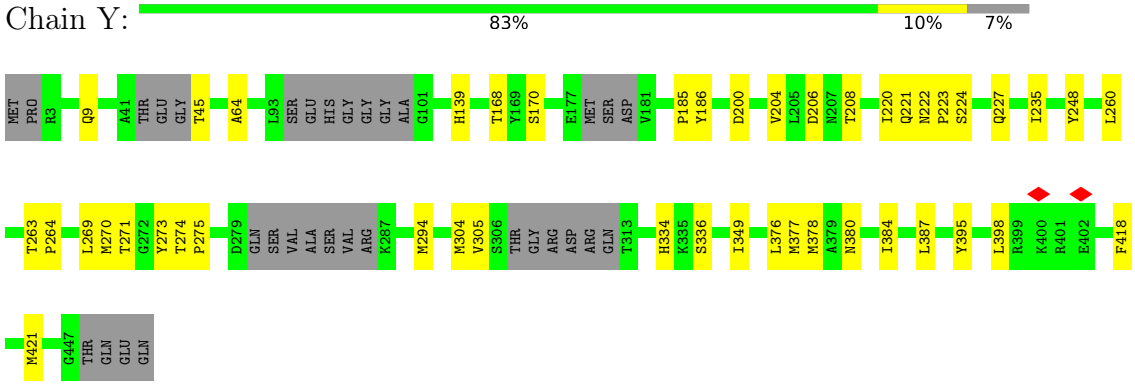
• Molecule 1: Tubulin gamma-1 chain

Chain X:



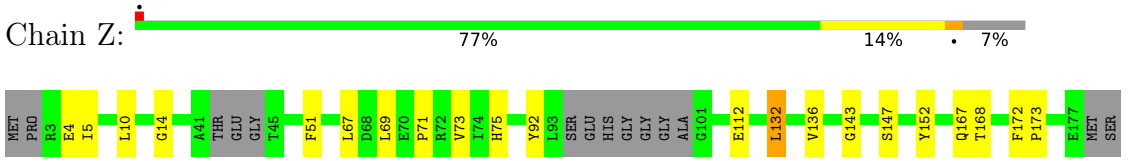
• Molecule 1: Tubulin gamma-1 chain

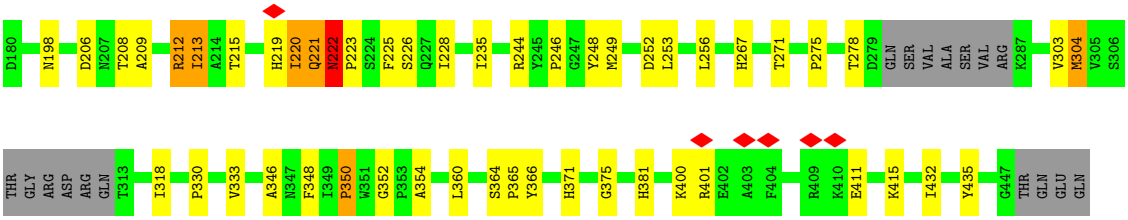
Chain Y:



• Molecule 1: Tubulin gamma-1 chain

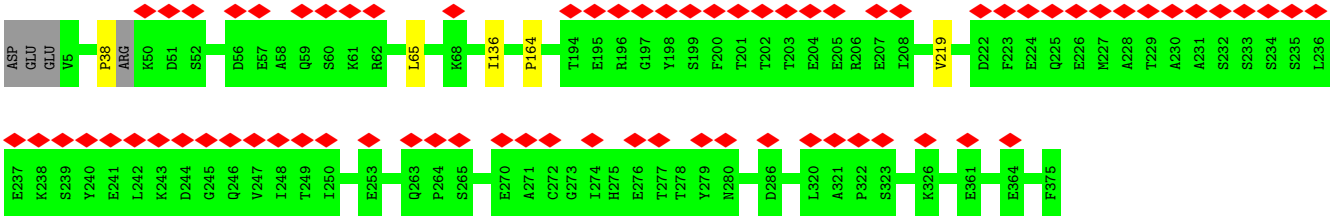
Chain Z:





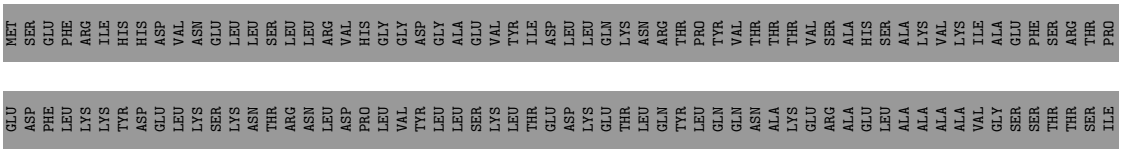
• Molecule 2: Actin b

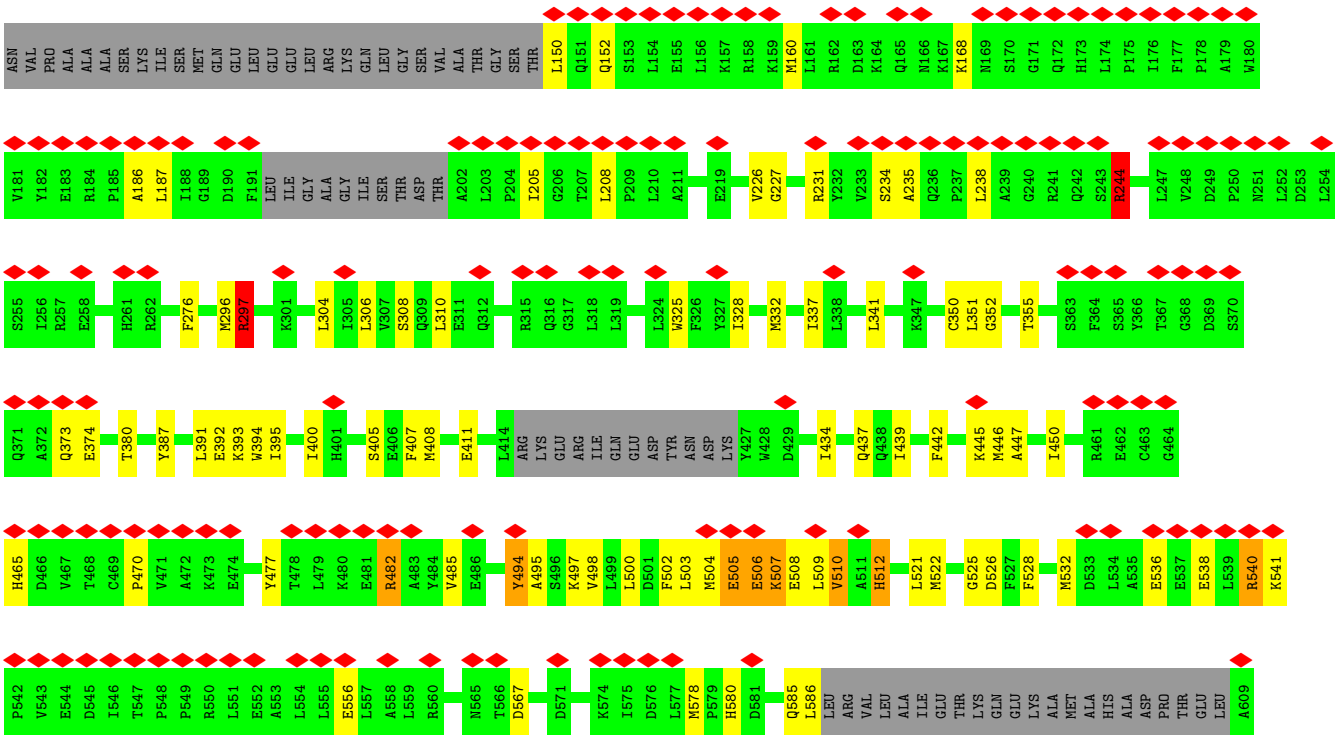


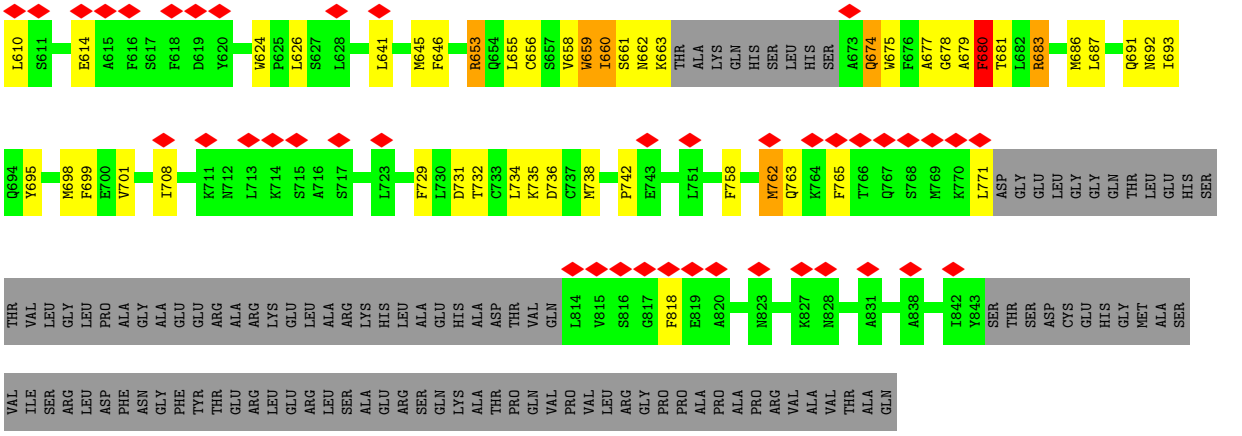


• Molecule 3: Gamma-tubulin complex component 2





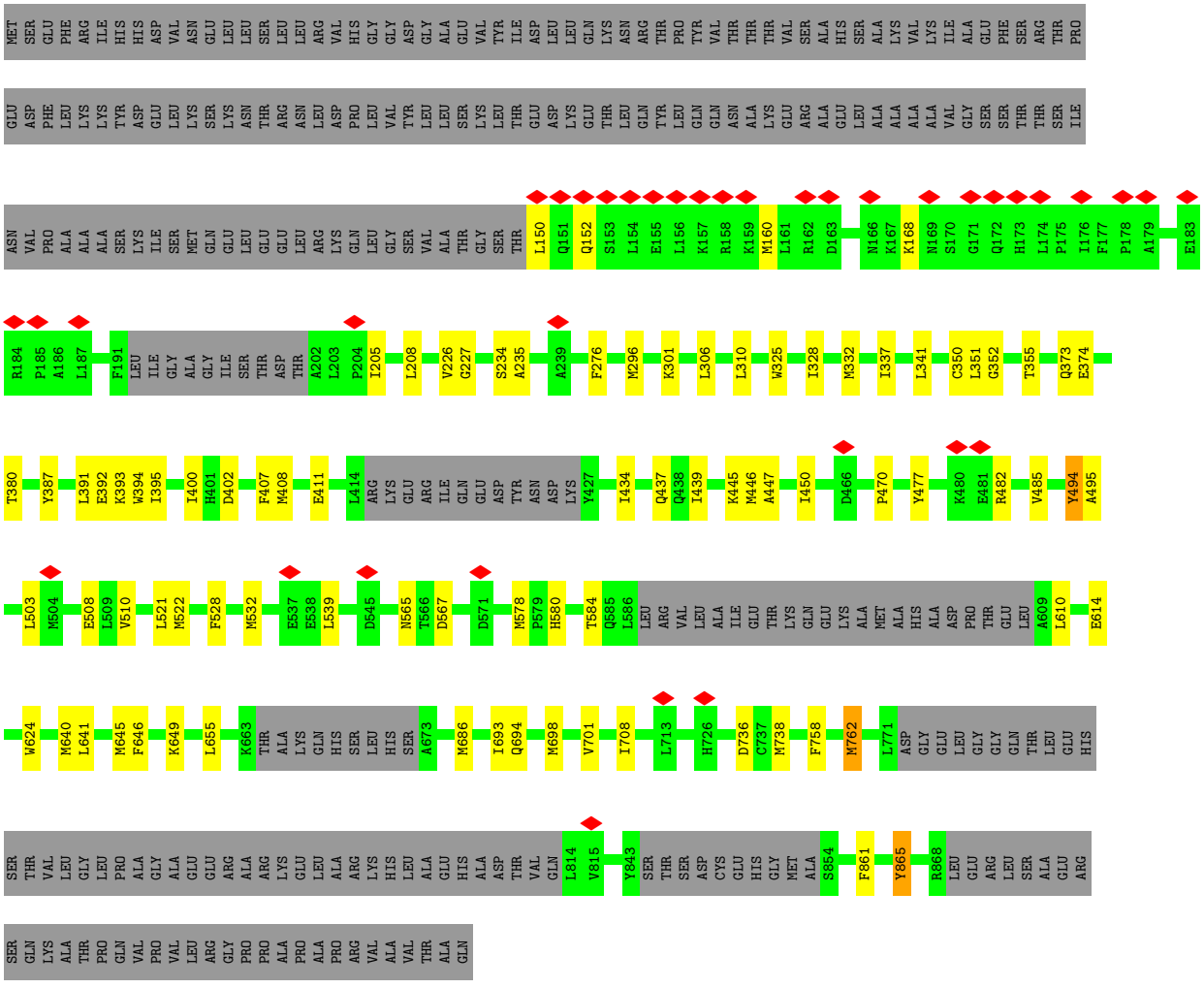




• Molecule 3: Gamma-tubulin complex component 2

Chain C:

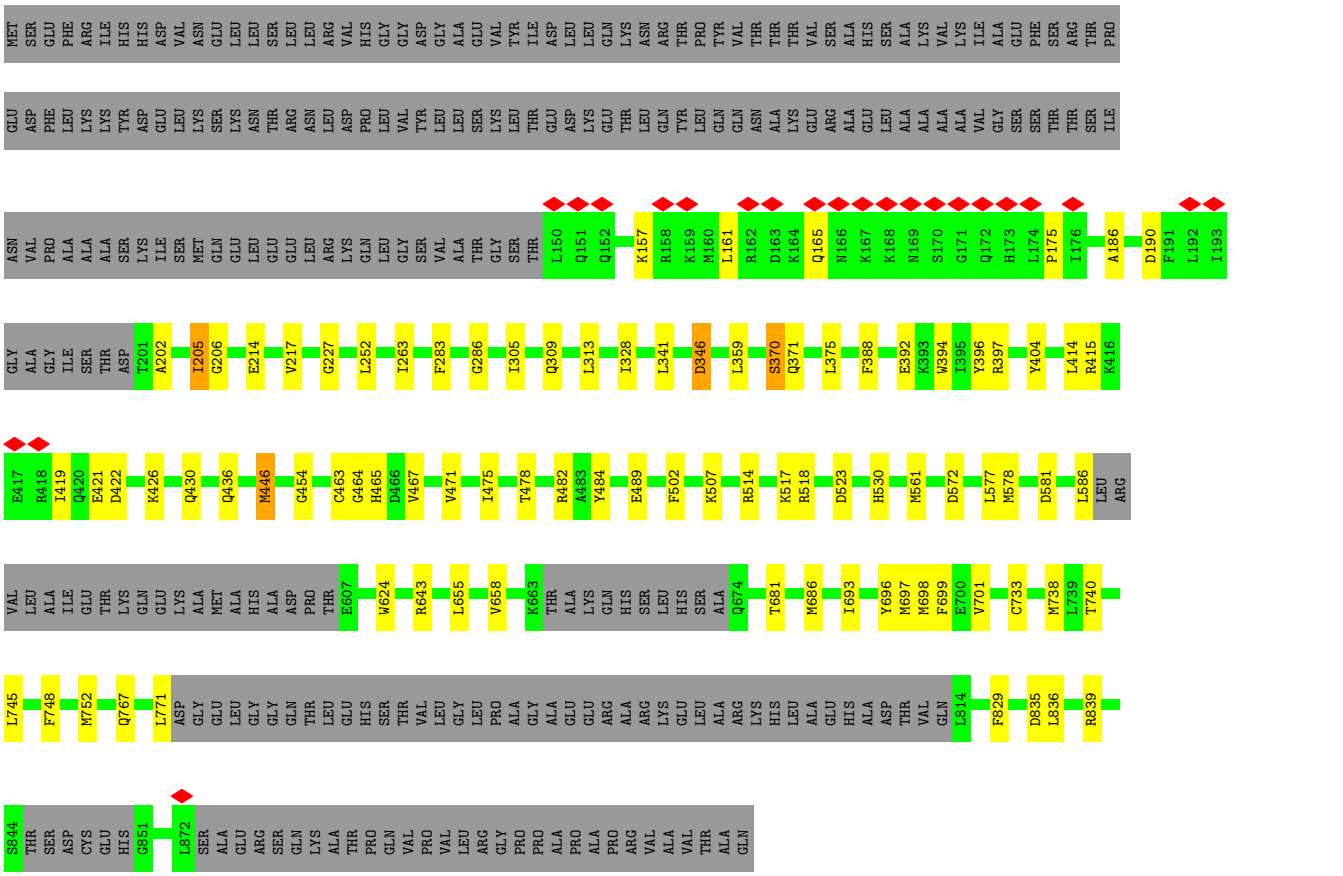




• Molecule 3: Gamma-tubulin complex component 2

Chain E:

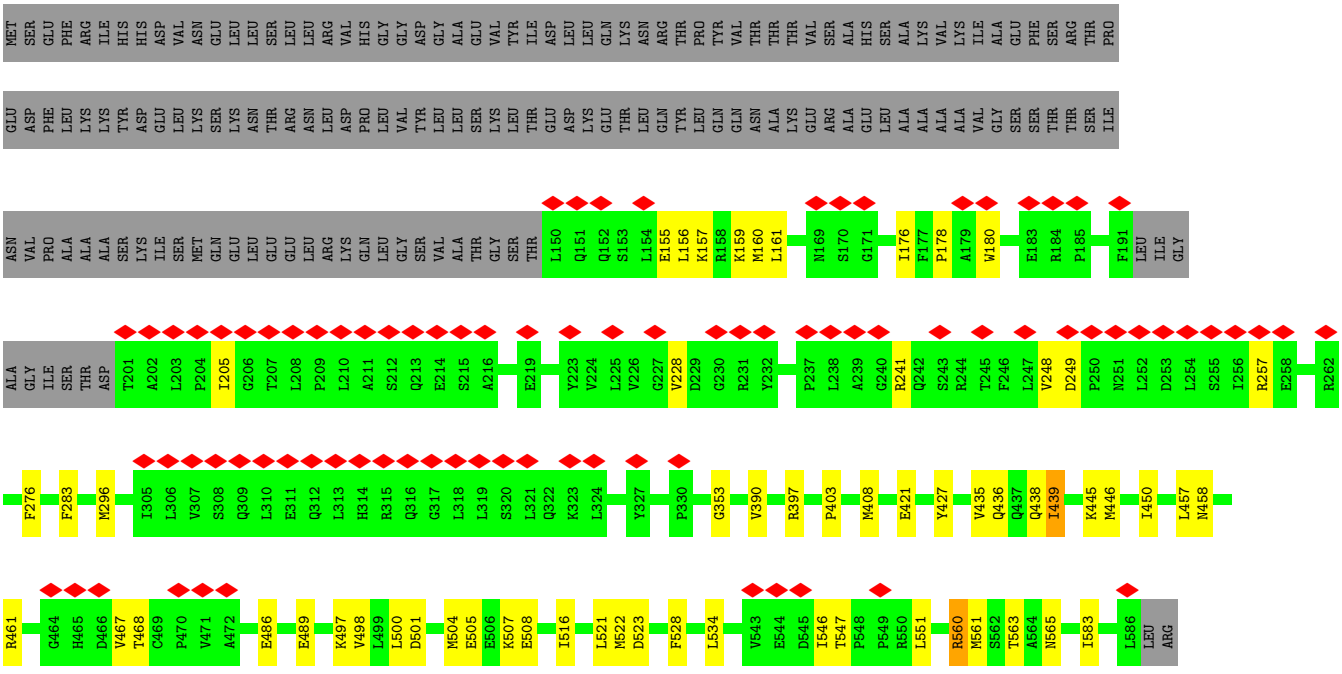


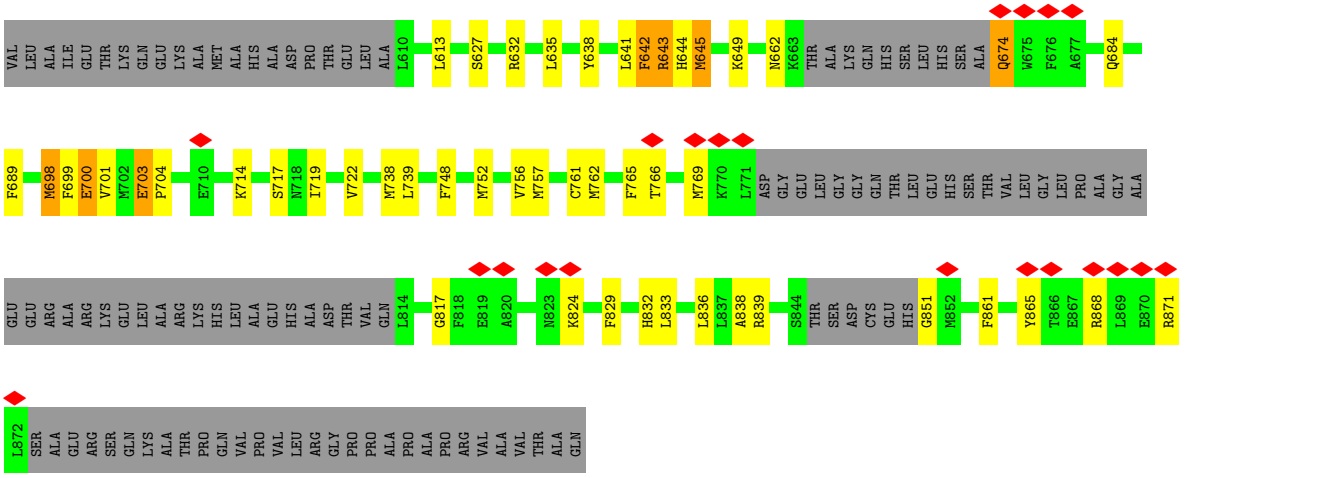


• Molecule 3: Gamma-tubulin complex component 2

Chain M:



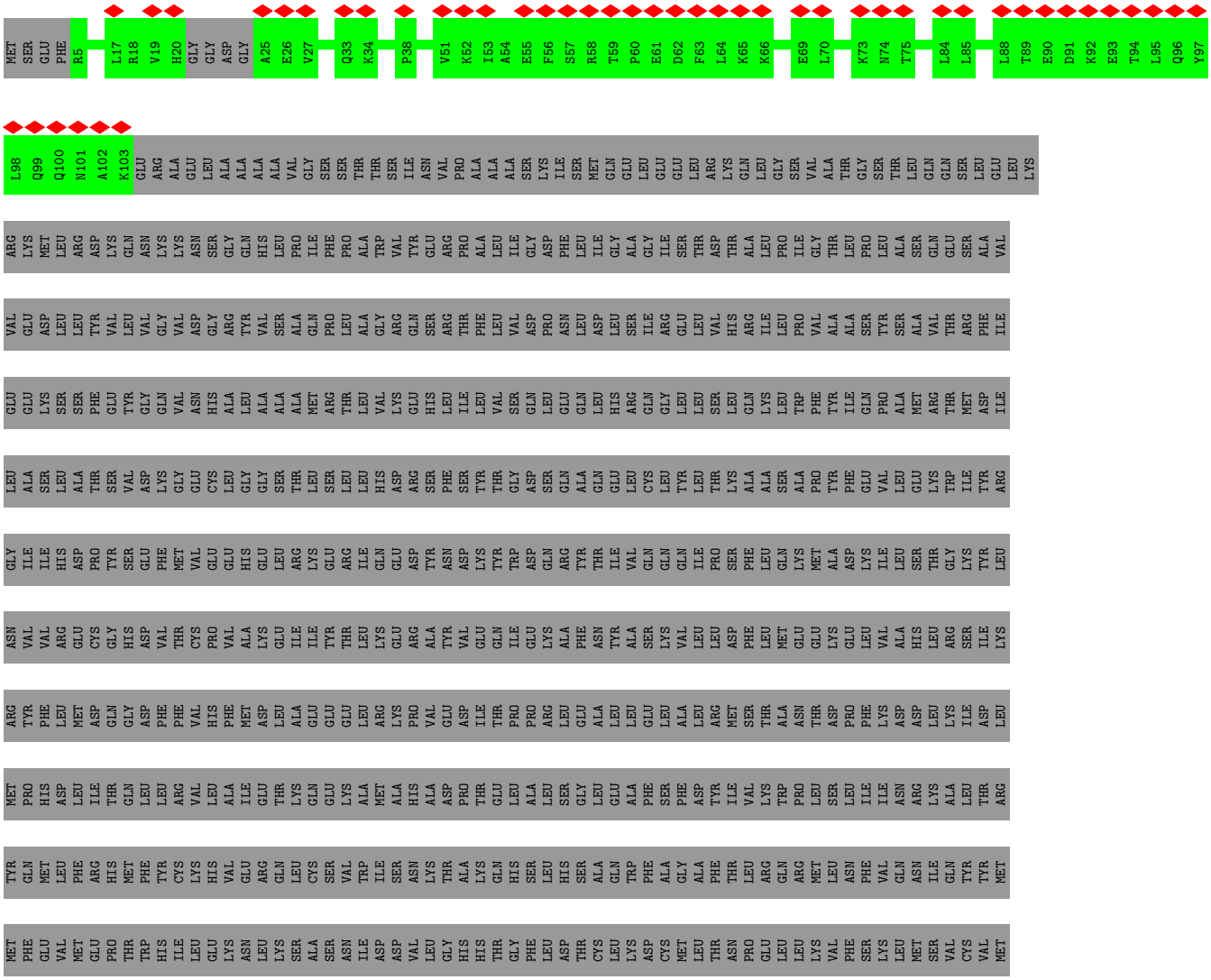


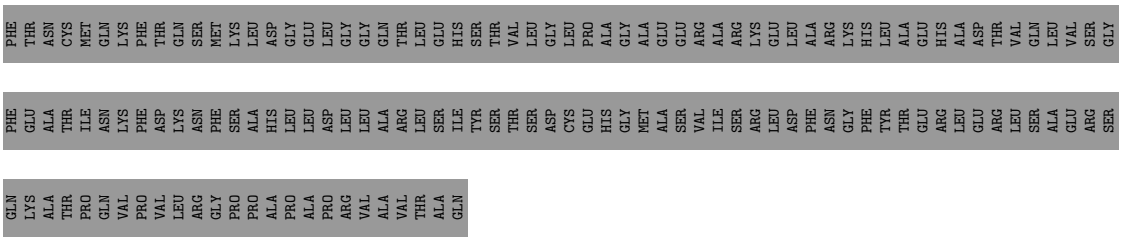


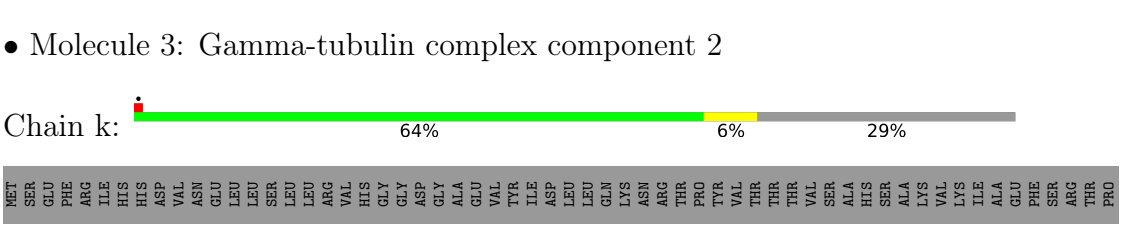
• Molecule 3: Gamma-tubulin complex component 2

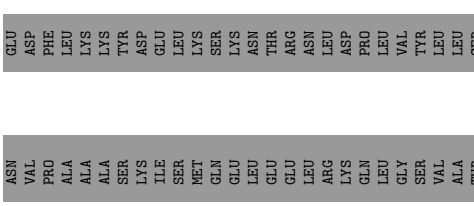
Chain f:









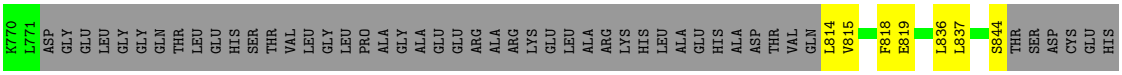


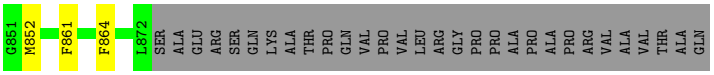
• Molecule 3: Gamma-tubulin complex component 2

Chain k:









• Molecule 4: Gamma-tubulin complex component 3

Chain B:

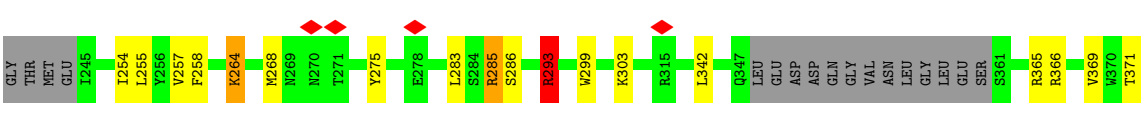


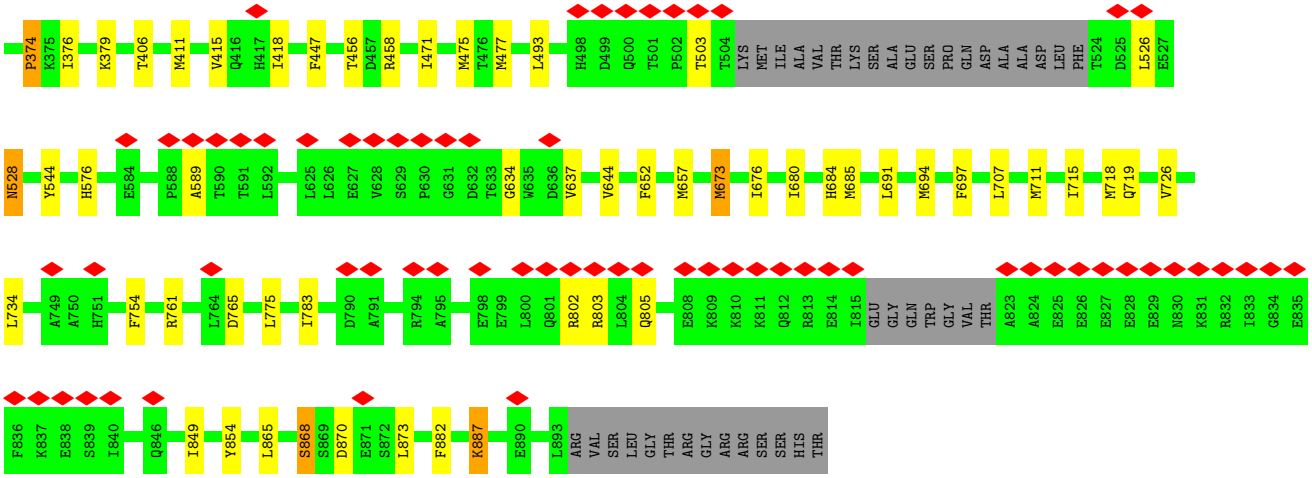








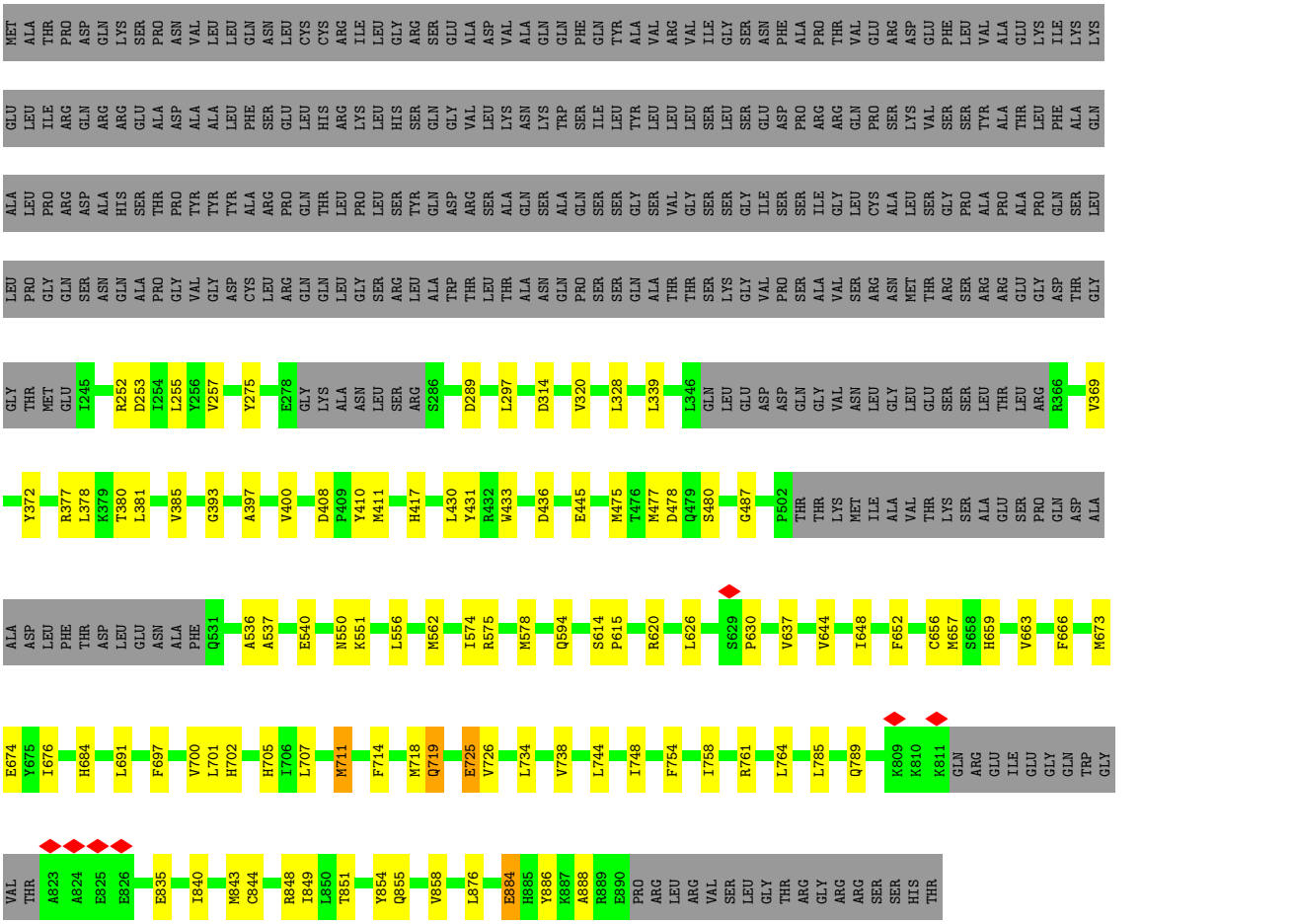




• Molecule 4: Gamma-tubulin complex component 3

Chain D:

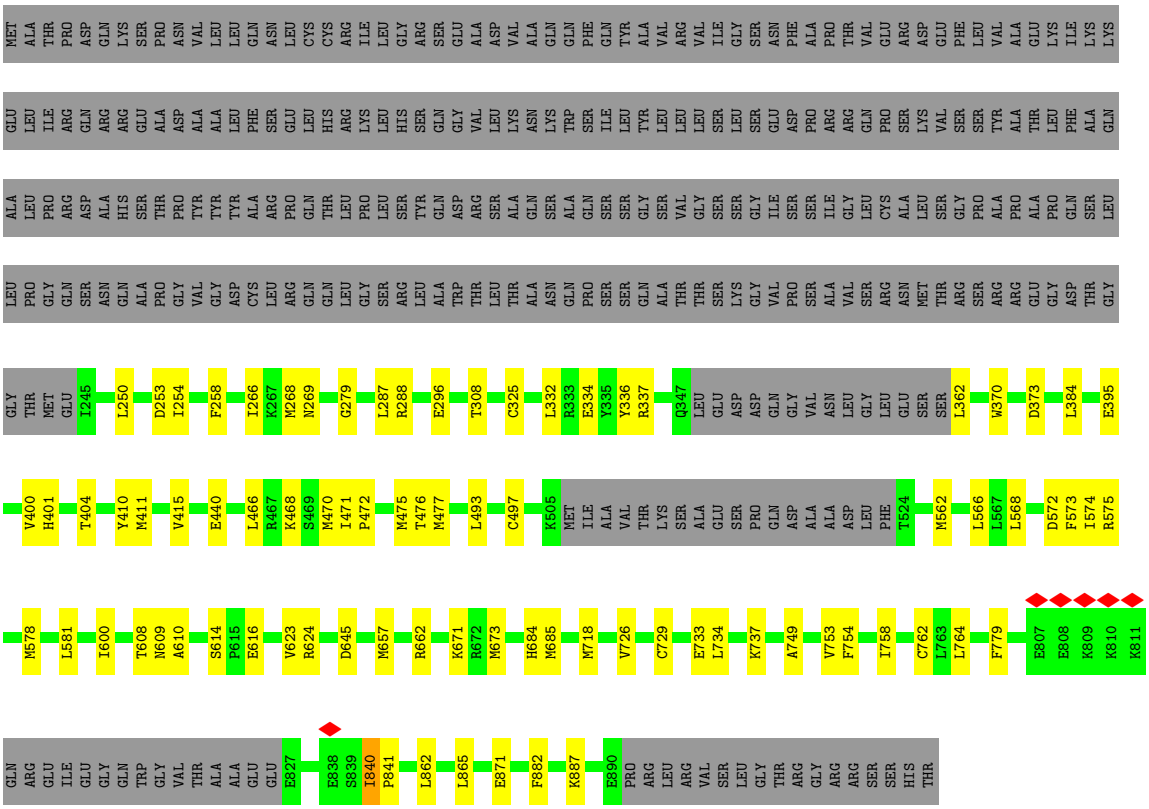




• Molecule 4: Gamma-tubulin complex component 3

Chain F:

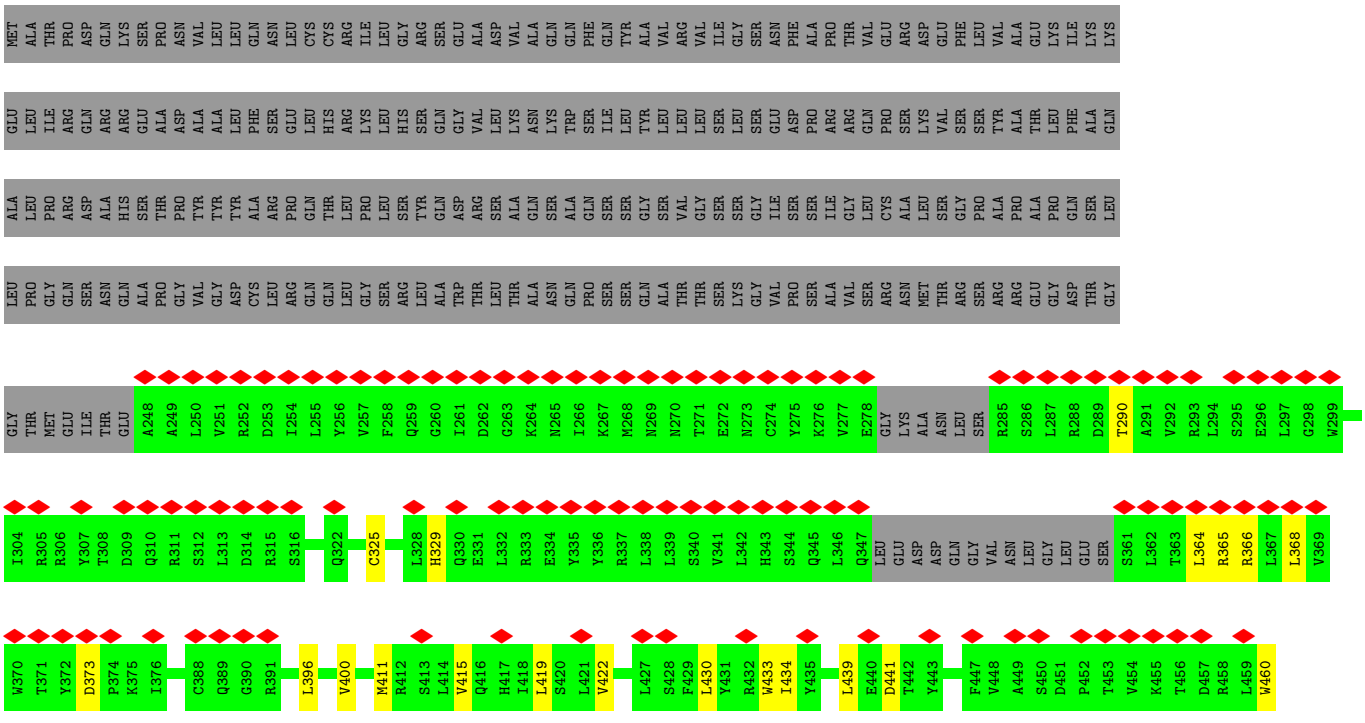


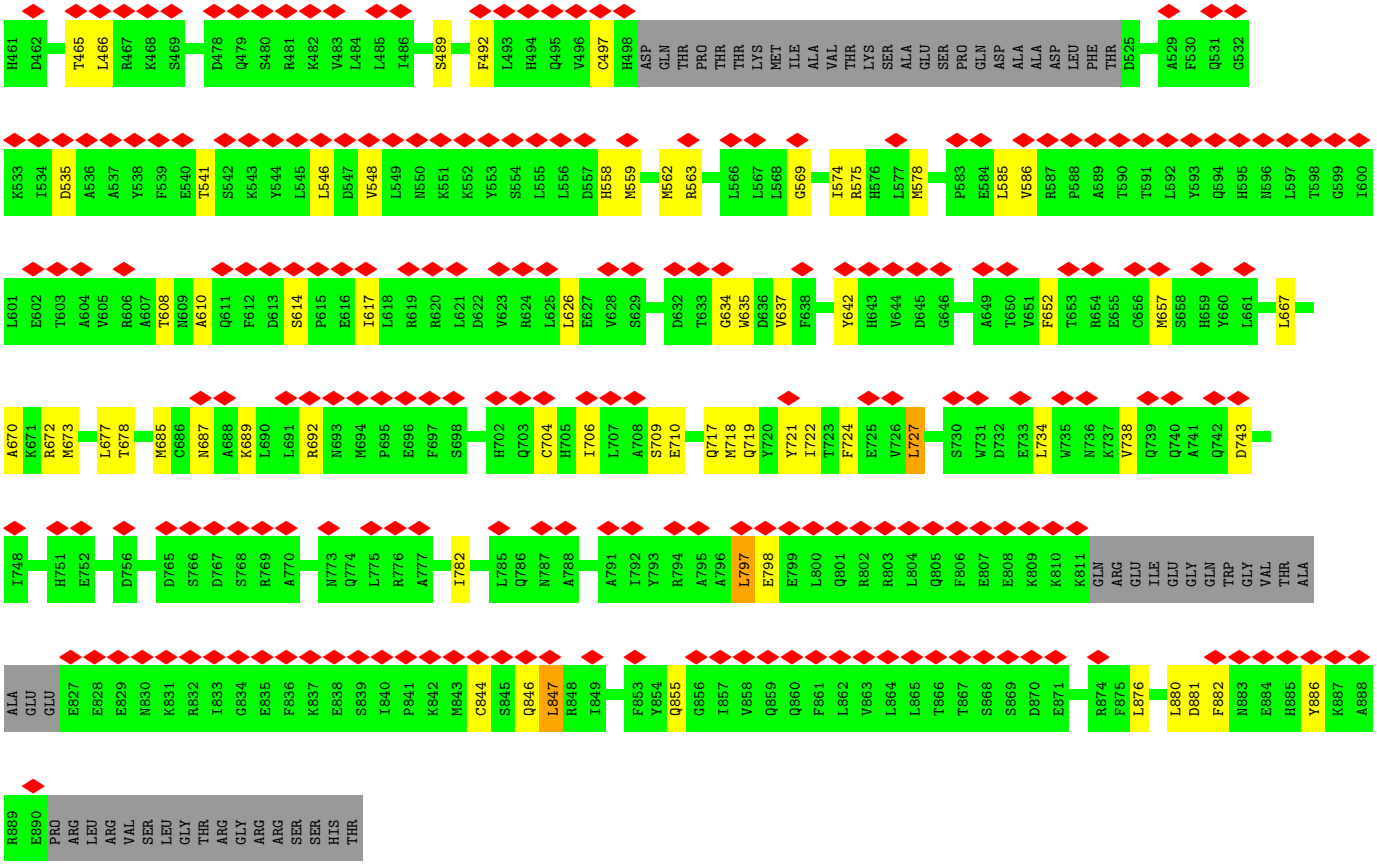


• Molecule 4: Gamma-tubulin complex component 3

Chain N:

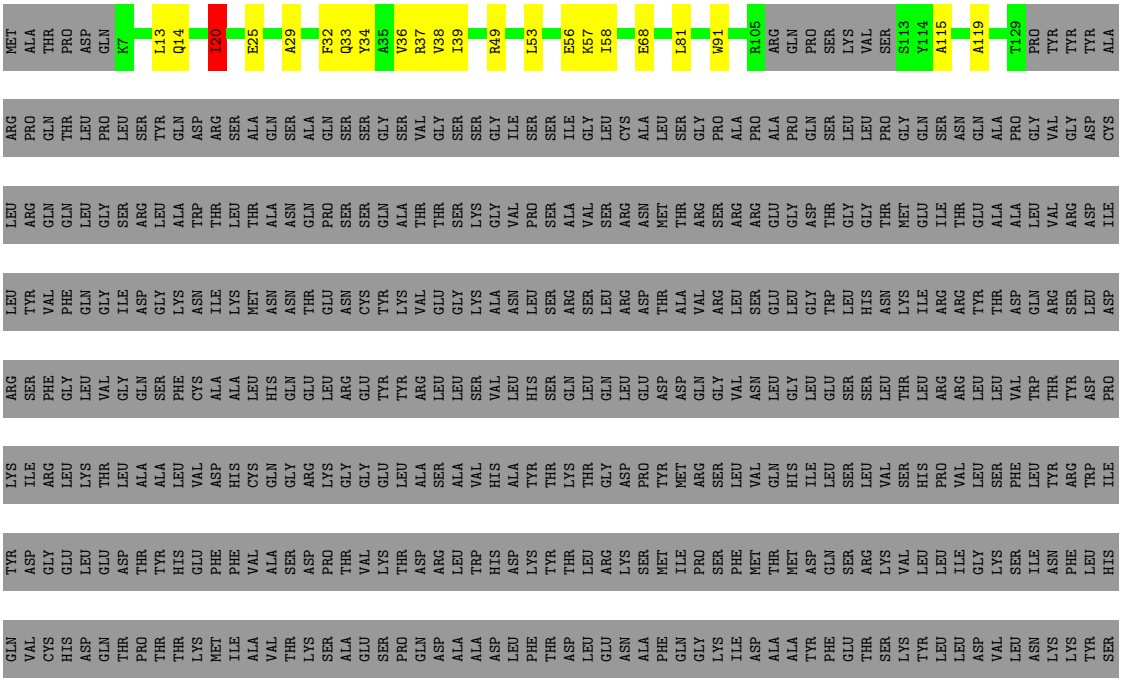


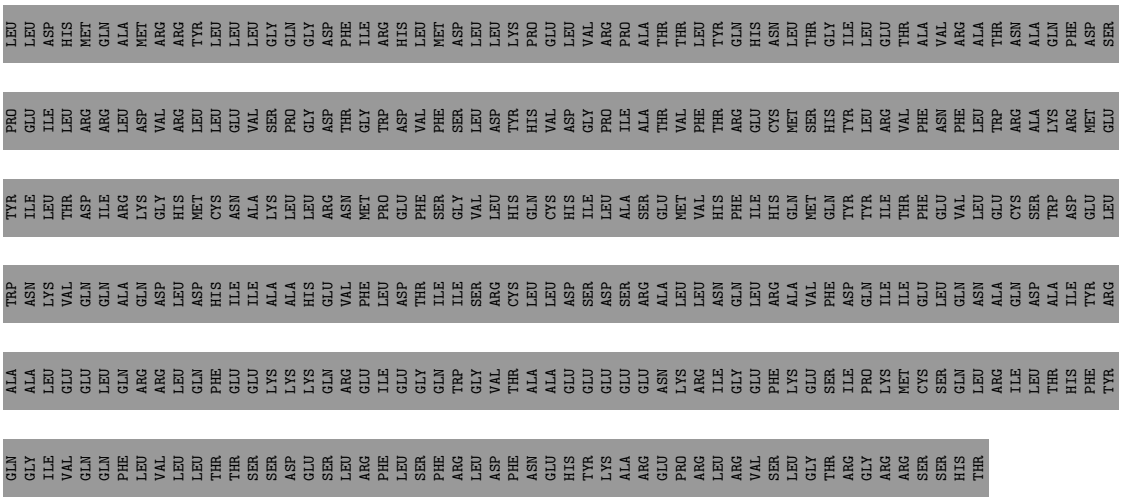




• Molecule 4: Gamma-tubulin complex component 3

Chain b:

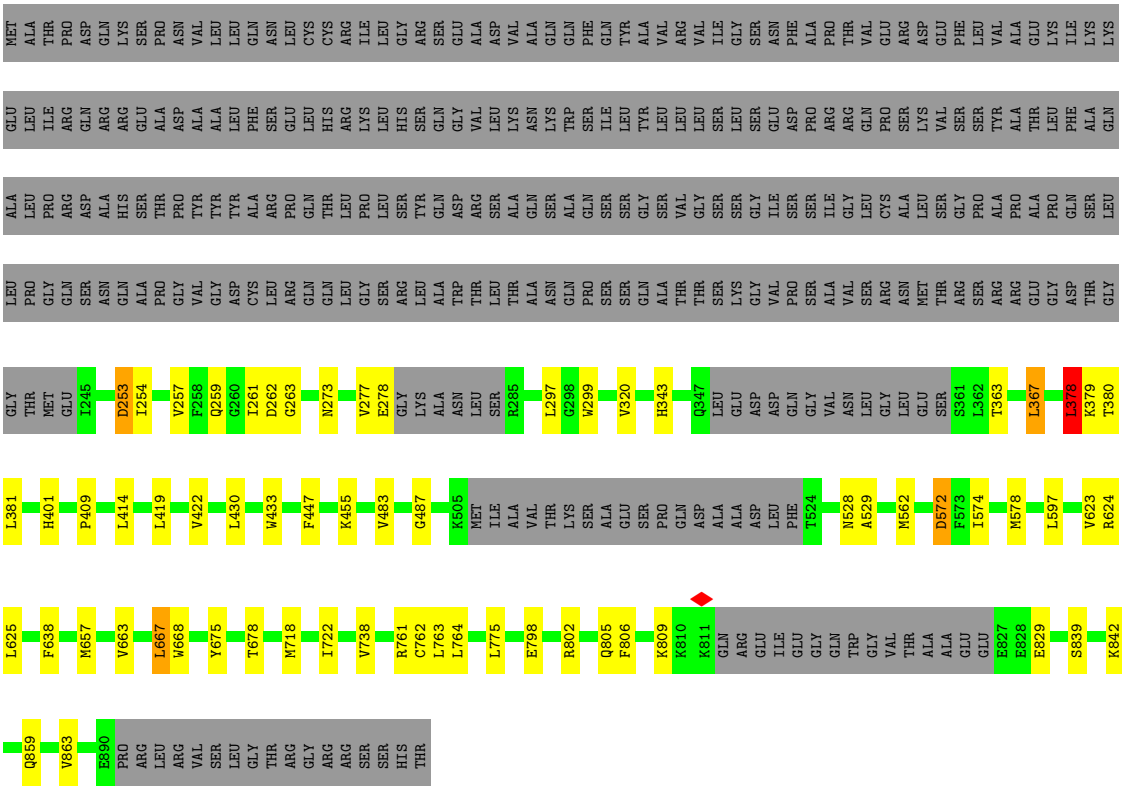




• Molecule 4: Gamma-tubulin complex component 3

Chain n:

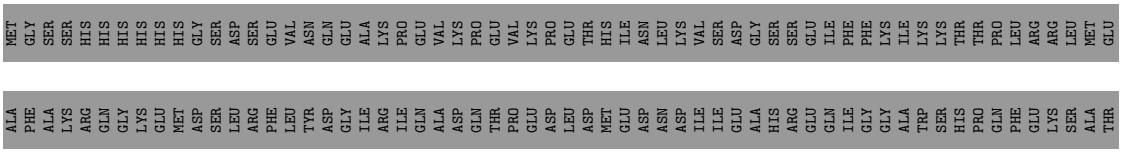


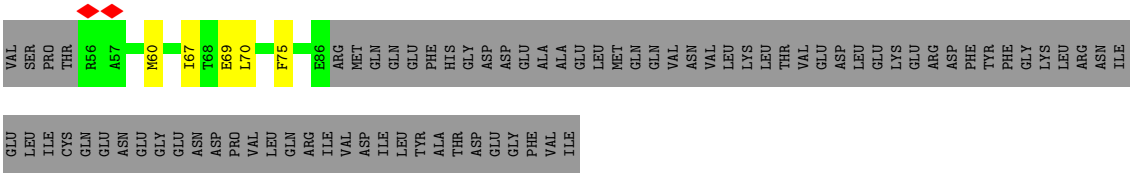


• Molecule 5: CM1

Chain G:



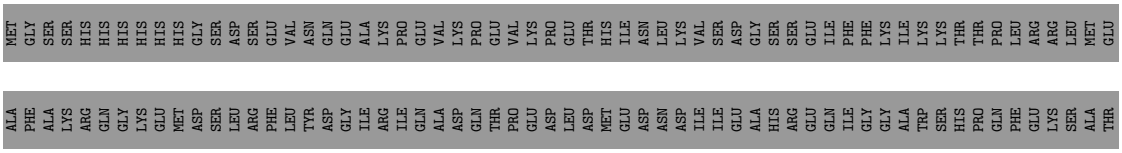


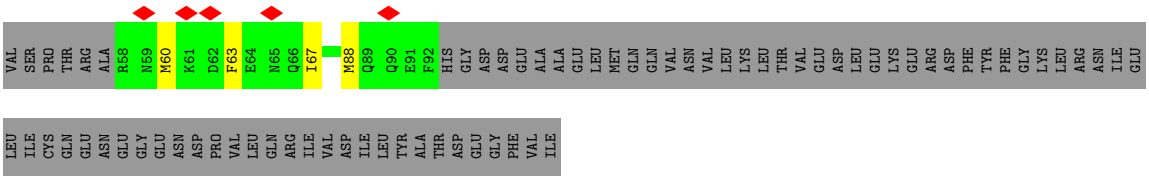


• Molecule 5: CM1

Chain H:



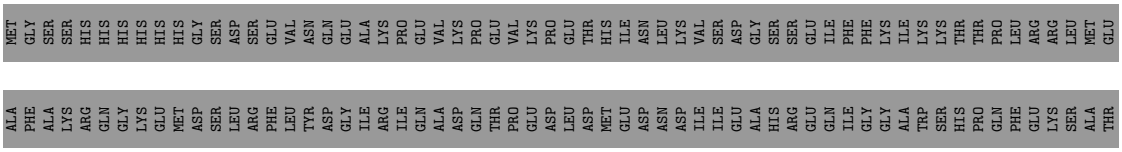


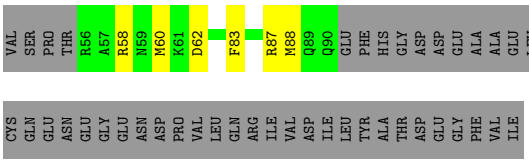


• Molecule 5: CM1

Chain g:



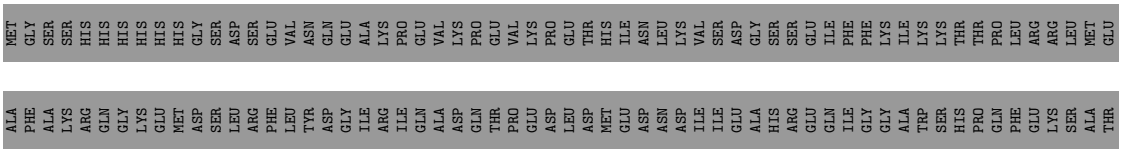


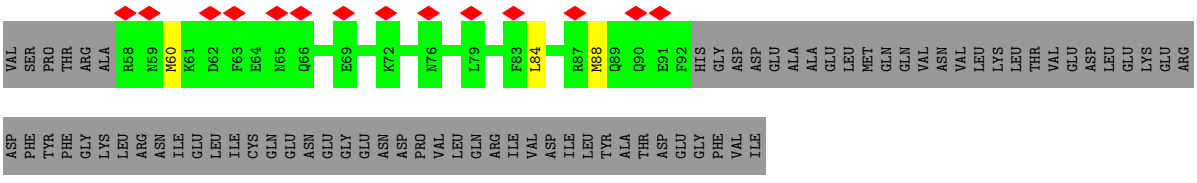


• Molecule 5: CM1

Chain h:

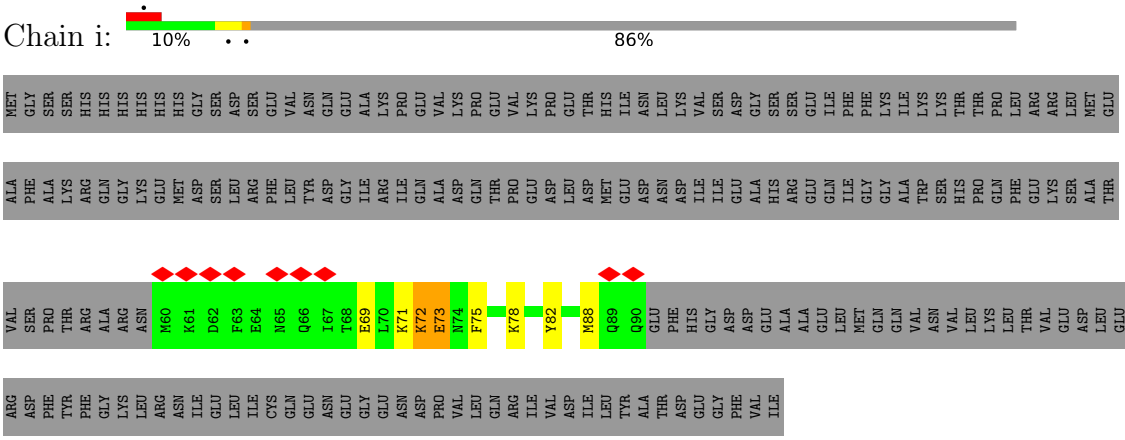






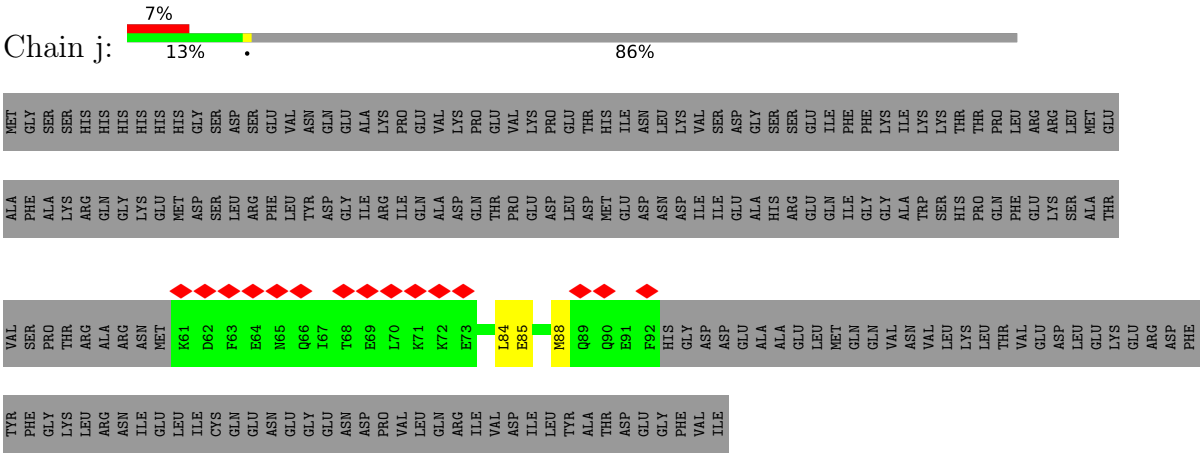
• Molecule 5: CM1

Chain i:



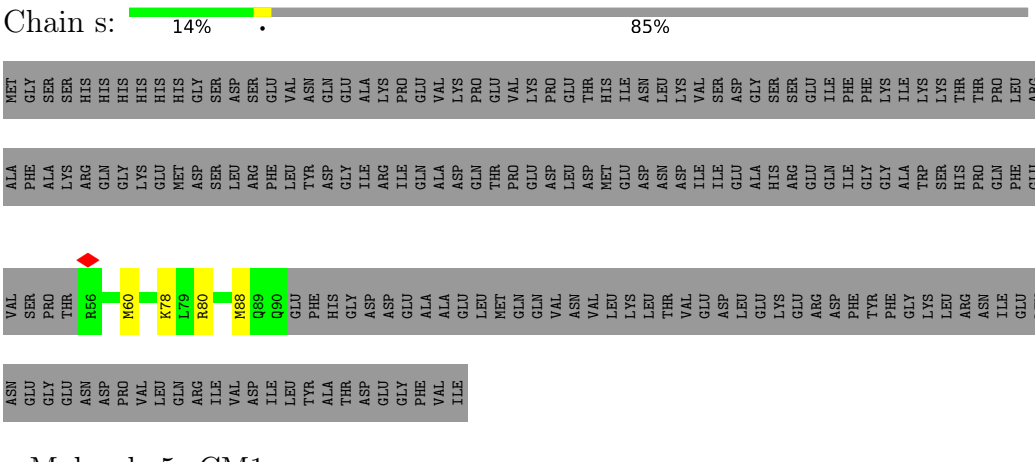
• Molecule 5: CM1

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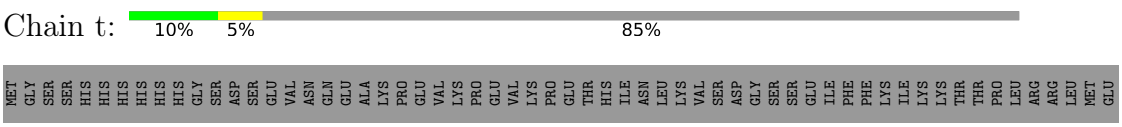
• Molecule 5: CM1

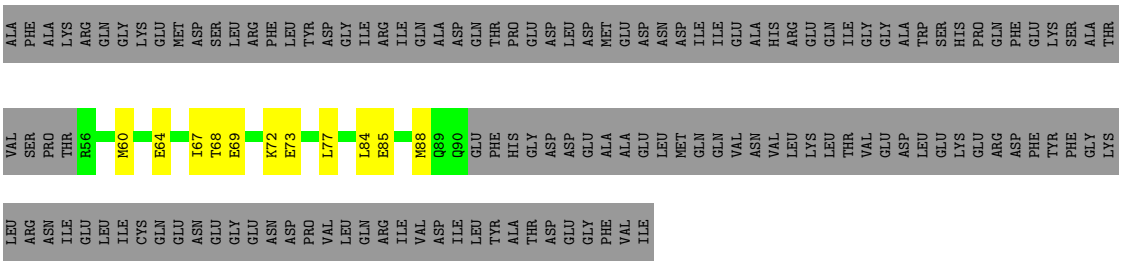
Chain s:



• Molecule 5: CM1

Chain t:

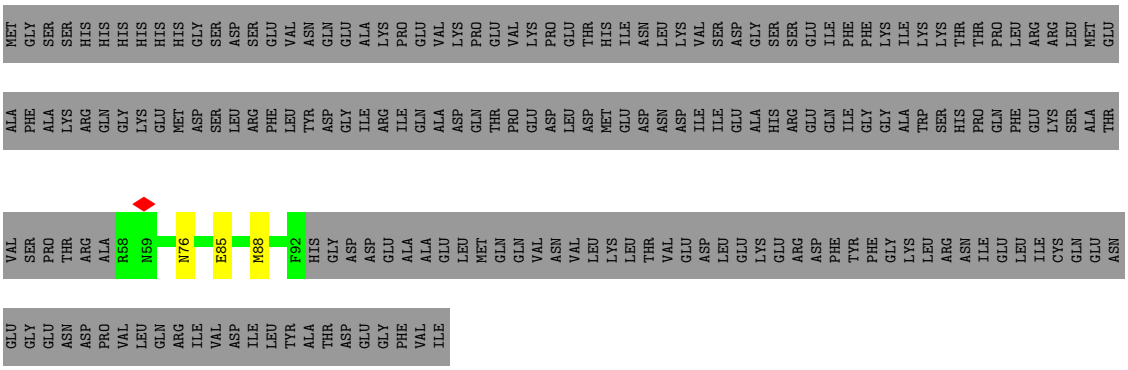




• Molecule 5: CM1

Chain u:

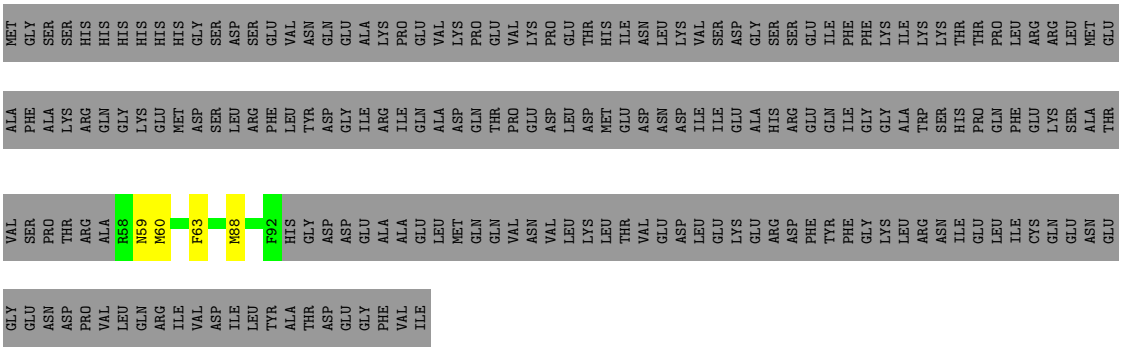




• Molecule 5: CM1

Chain v:

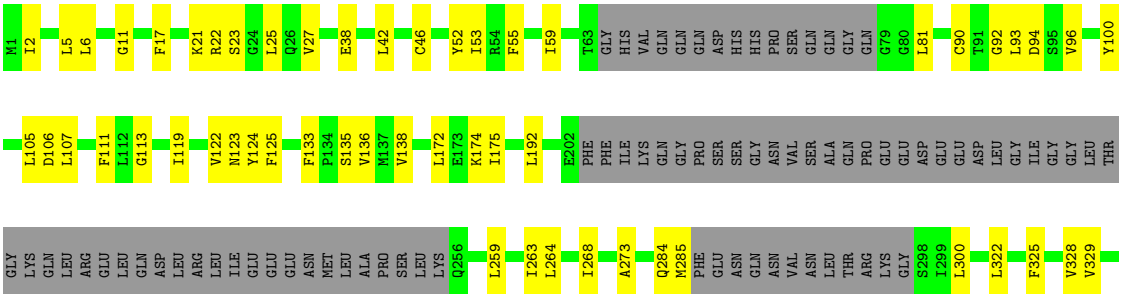


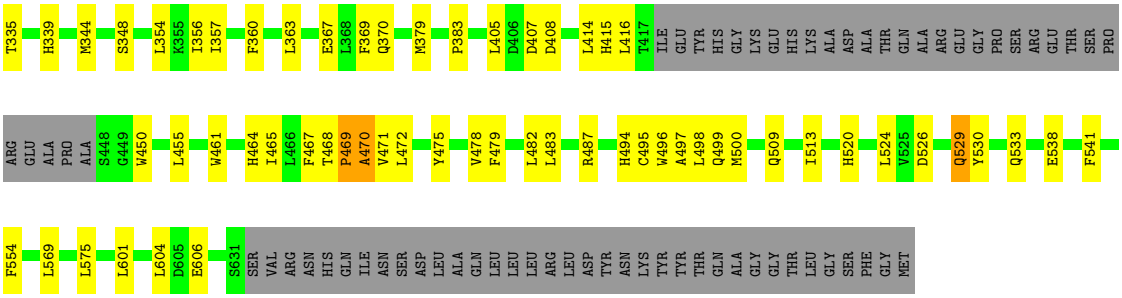


• Molecule 6: Gamma-tubulin complex component 4

Chain I:



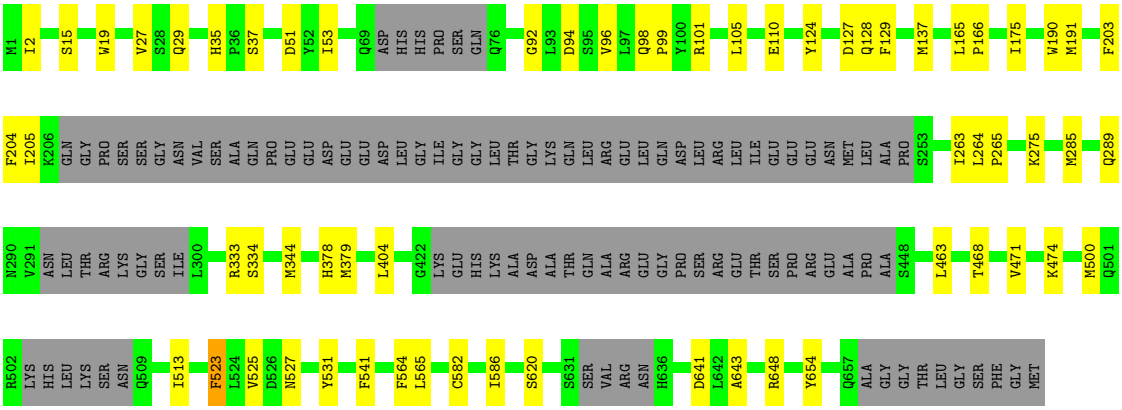




• Molecule 6: Gamma-tubulin complex component 4

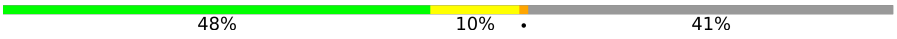
Chain K:

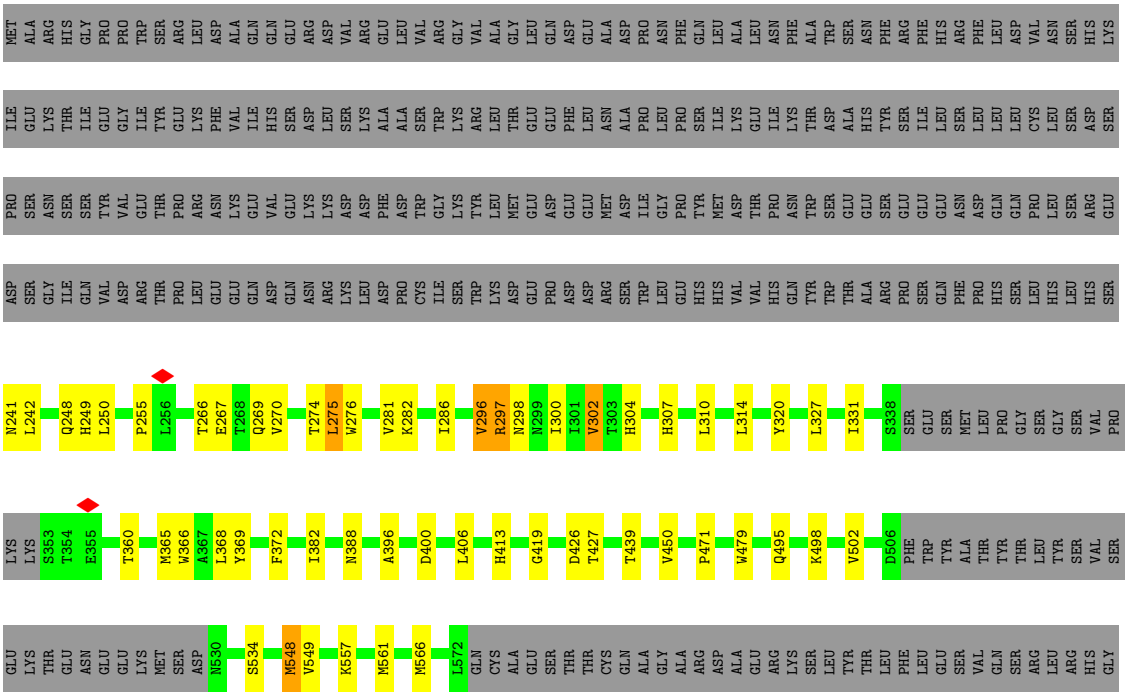


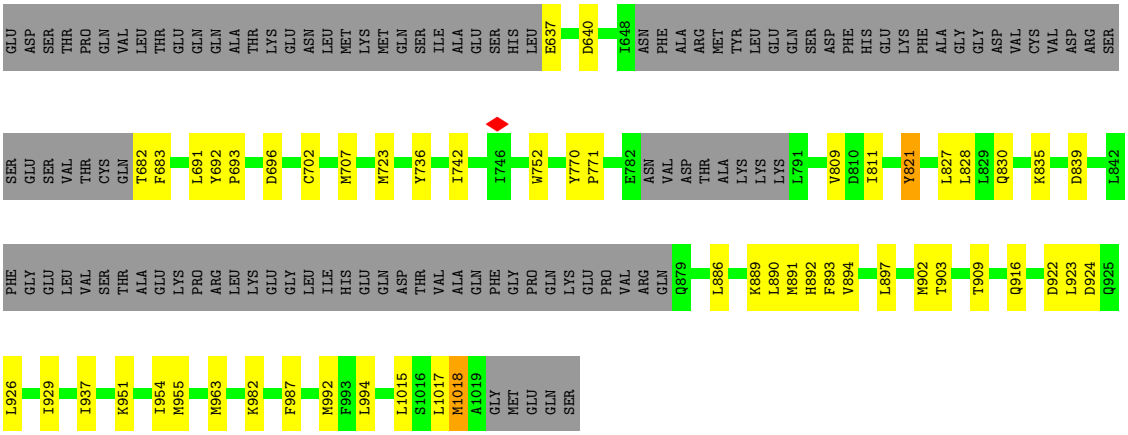


• Molecule 7: Gamma-tubulin complex component 5

Chain J:



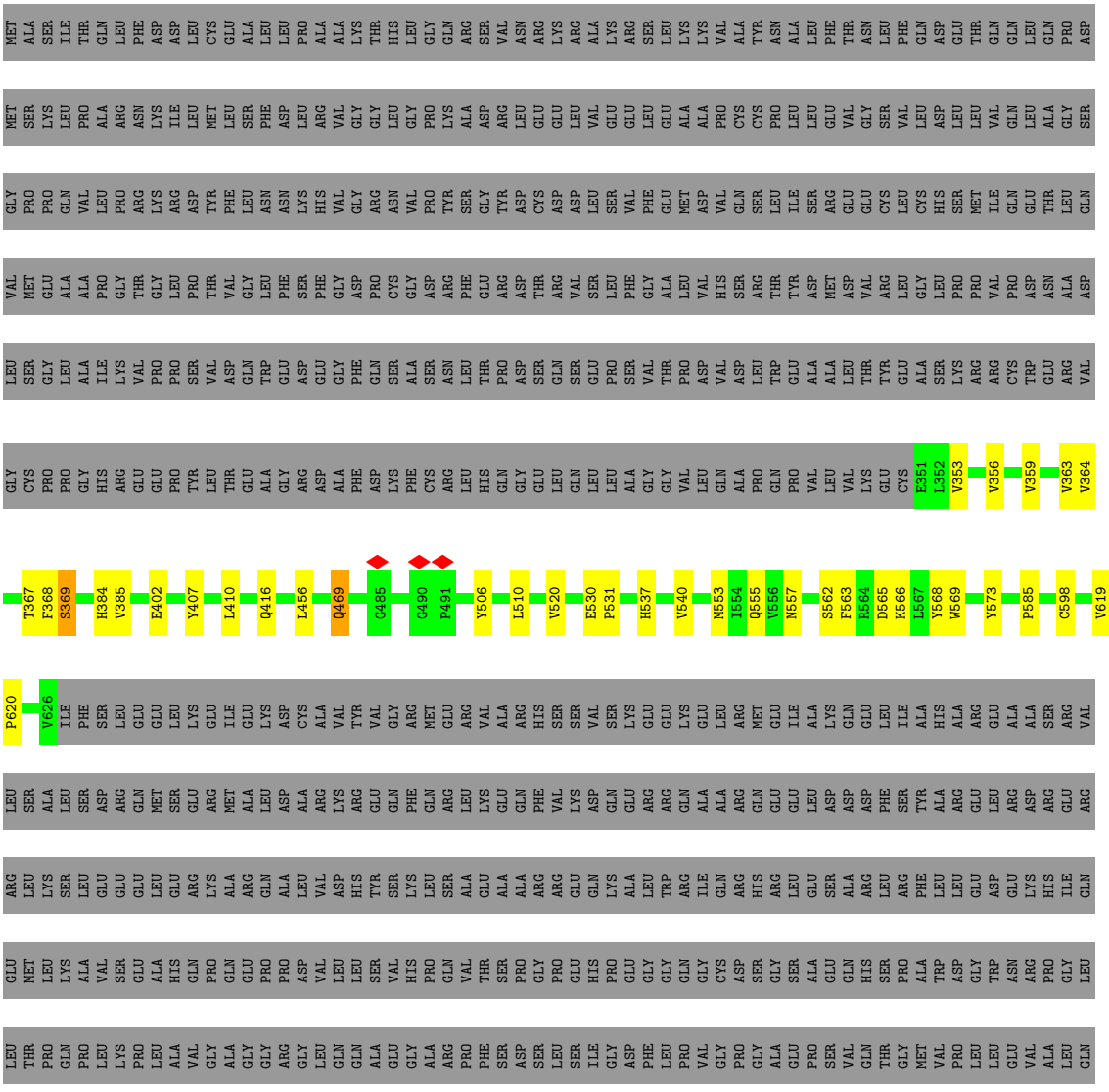


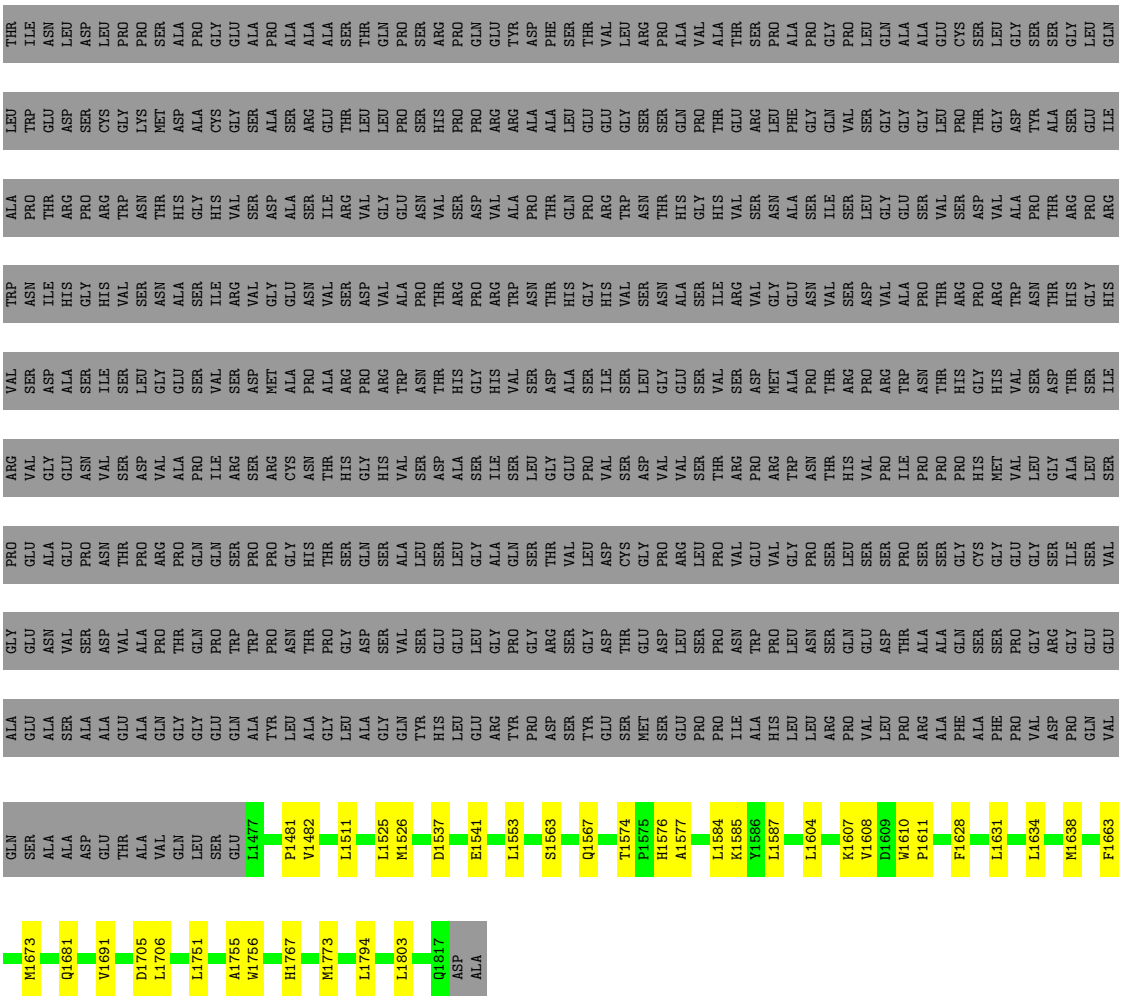


• Molecule 8: Gamma-tubulin complex component 6

Chain L:

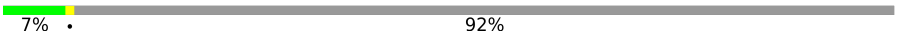


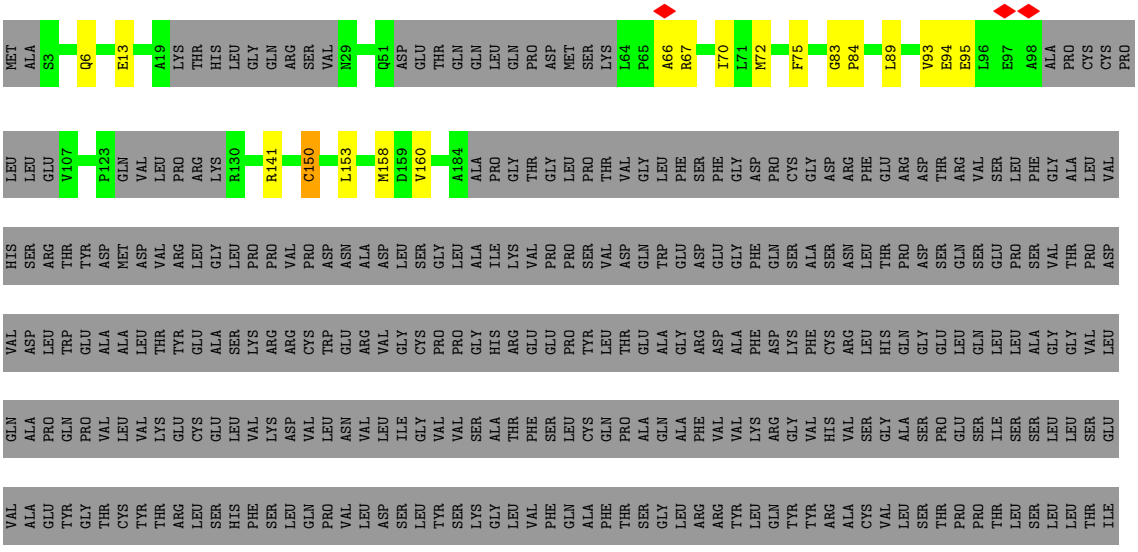


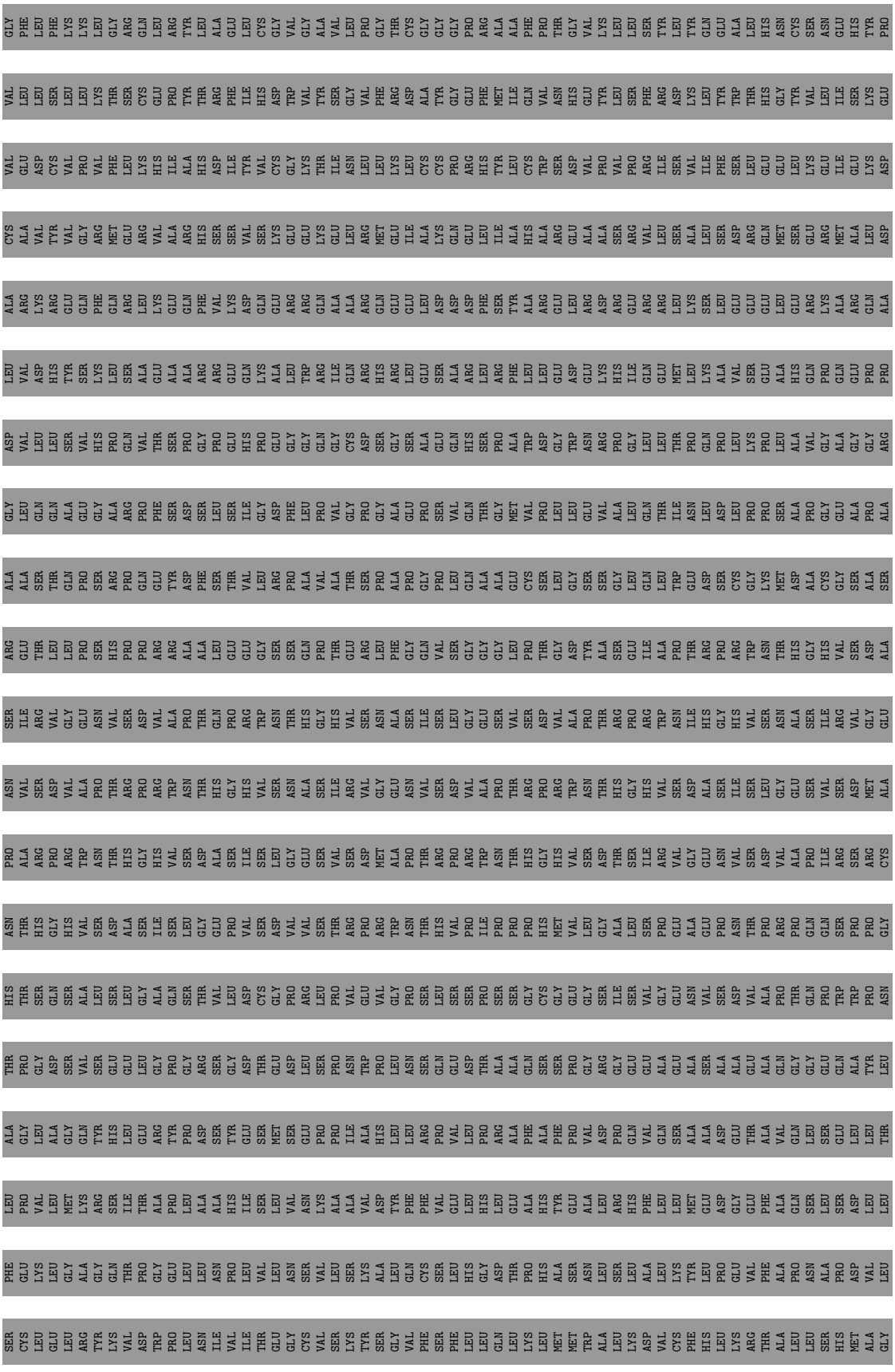


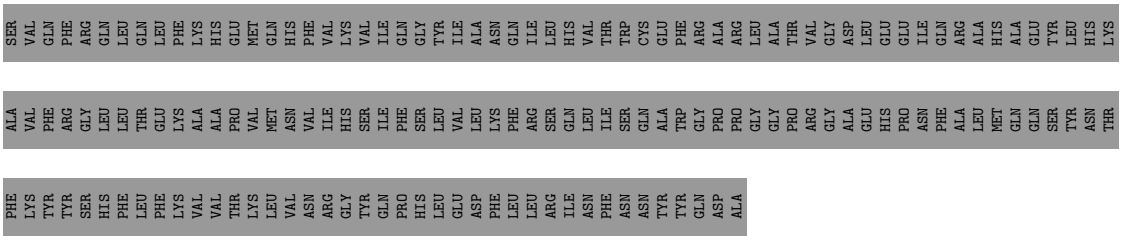
• Molecule 8: Gamma-tubulin complex component 6

Chain d:

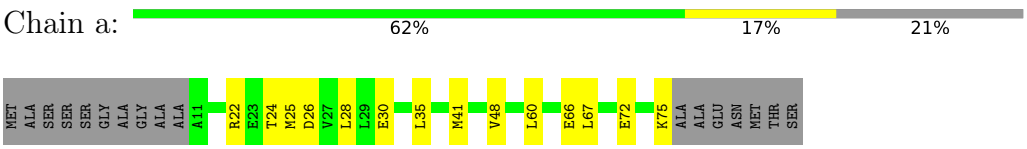




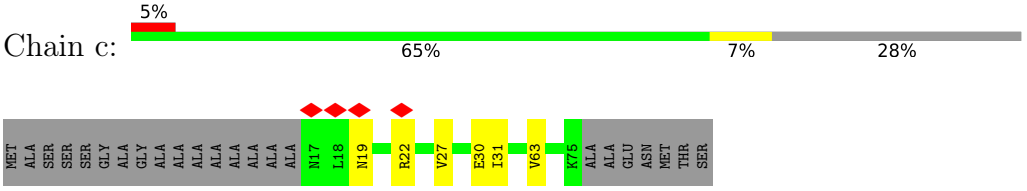

GLY PHE LEU PHE LYS LYS LEU GLY ARG GLN LEU ARG TYR LEU ALA GLU LEU CYS GLY VAL GLY ALA VAL LEU PRO GLY THR CYS GLY GLY GLY PRO ARG ALA ALA PHE PRO THR GLY VAL LYS LEU LEU SER TYR LEU TYR GLN GLU ALA LEU HIS ASN CYS SER ASN GLU HIS TYR PRO
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GLY LEU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



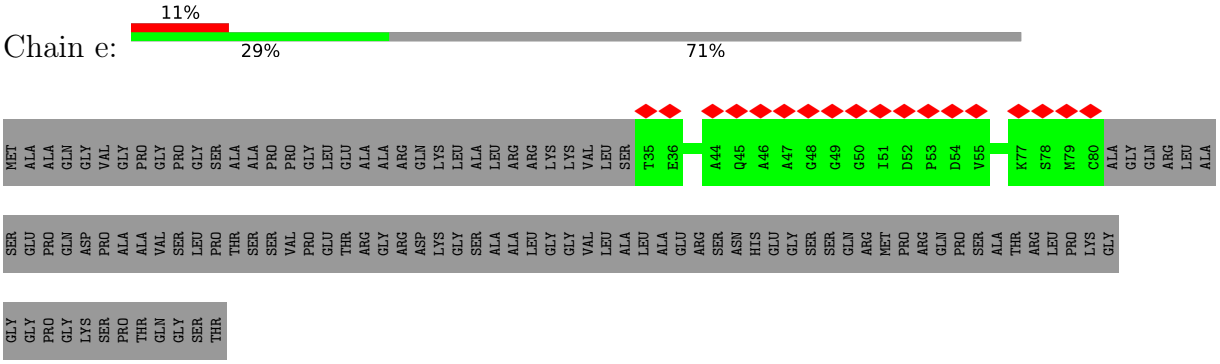
• Molecule 9: Mitotic-spindle organizing protein 1



• Molecule 9: Mitotic-spindle organizing protein 1



• Molecule 10: Mitotic-spindle organizing protein 2A



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	579078	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 ($e^-/Å^2$)	55.4	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	601.2, 601.2, 601.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6700001, 1.6700001, 1.6700001	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	1	0.50	0/3433	0.86	0/4651
1	2	0.64	2/3377 (0.1%)	1.02	6/4575 (0.1%)
1	O	0.63	0/3433	0.95	1/4651 (0.0%)
1	P	0.57	0/3427	0.89	0/4644
1	Q	0.48	0/3439	0.85	0/4658
1	R	0.53	2/3433 (0.1%)	0.86	0/4651
1	S	0.49	0/3439	0.88	0/4658
1	T	0.53	0/3427	0.92	0/4644
1	U	0.51	0/3433	0.96	1/4651 (0.0%)
1	V	0.51	0/3393	0.91	1/4599 (0.0%)
1	W	0.51	0/3408	0.95	2/4616 (0.0%)
1	X	0.46	0/3439	0.86	0/4658
1	Y	0.52	0/3431	0.90	2/4647 (0.0%)
1	Z	0.57	0/3433	0.99	2/4651 (0.0%)
2	7	0.34	0/1828	0.68	0/2554
3	A	0.54	0/4951	0.92	2/6692 (0.0%)
3	C	0.46	0/5080	0.87	0/6864
3	E	0.41	0/5305	0.83	0/7162
3	M	0.55	1/5267 (0.0%)	0.90	3/7110 (0.0%)
3	f	0.17	0/482	0.52	0/674
3	k	0.50	0/5289	0.94	4/7140 (0.1%)
4	B	0.45	0/5119	0.82	2/6912 (0.0%)
4	D	0.41	0/4891	0.81	4/6603 (0.1%)
4	F	0.47	1/5024 (0.0%)	0.88	1/6784 (0.0%)
4	N	0.51	0/4911	0.88	0/6627
4	b	0.44	1/948 (0.1%)	0.89	0/1277
4	n	0.46	0/4977	0.89	7/6722 (0.1%)
5	G	0.56	0/273	0.98	1/362 (0.3%)
5	H	0.44	0/321	0.80	0/424
5	g	0.40	0/306	0.82	0/405
5	h	0.36	0/321	0.65	0/424
5	i	0.55	0/277	0.83	0/366
5	j	0.39	0/294	0.68	0/389
5	s	0.43	0/306	0.87	0/405

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	t	0.44	0/306	0.80	0/405
5	u	0.43	0/321	0.84	0/424
5	v	0.44	0/321	0.85	0/424
6	I	0.54	1/4299 (0.0%)	1.00	4/5824 (0.1%)
6	K	0.39	0/4677	0.81	5/6331 (0.1%)
7	J	0.52	0/4939	0.98	3/6693 (0.0%)
8	L	0.42	0/5062	0.84	0/6877
8	d	0.47	0/1165	0.93	0/1566
9	a	0.37	0/484	0.81	0/653
9	c	0.61	0/454	1.04	0/611
10	e	0.22	0/232	0.42	0/323
All	All	0.50	8/126375 (0.0%)	0.89	51/170981 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	4
4	B	0	2
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	840	ILE	CA-CB	-11.46	1.48	1.54
1	2	70	GLU	C-O	6.73	1.27	1.23
1	2	323	ILE	CG1-CD1	-6.29	1.27	1.51
1	R	70	GLU	C-O	-5.97	1.21	1.23
6	I	529	GLN	C-N	-5.50	1.26	1.34
3	M	703	GLU	N-CA	5.11	1.50	1.46
1	R	249	MET	SD-CE	-5.08	1.66	1.79
4	b	20	ILE	CG1-CD1	-5.01	1.32	1.51

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	496	TRP	N-CA-C	-11.10	98.71	112.47
3	k	567	ASP	CA-CB-CG	7.38	119.98	112.60
4	D	719	GLN	CA-C-O	-7.27	113.37	121.00
1	2	139	HIS	CA-CB-CG	7.01	120.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	n	378	LEU	N-CA-C	-6.76	103.71	112.23
3	M	507	LYS	N-CA-C	-6.67	102.02	111.56
4	n	379	LYS	N-CA-C	-6.57	99.54	109.79
7	J	296	VAL	CA-C-O	-6.50	114.28	121.17
3	k	864	PHE	CA-CB-CG	6.27	120.07	113.80
1	Z	198	ASN	CA-CB-CG	6.17	118.77	112.60
3	M	458	ASN	CA-CB-CG	6.16	118.76	112.60
3	M	645	MET	N-CA-C	-6.15	106.41	114.04
4	B	887	LYS	N-CA-C	-6.10	107.67	114.62
4	n	379	LYS	CA-C-O	-6.09	114.00	121.67
1	Y	349	ILE	N-CA-C	6.09	122.03	108.88
4	B	447	PHE	CA-CB-CG	6.05	119.85	113.80
4	F	684	HIS	CA-CB-CG	5.92	119.72	113.80
6	I	469	PRO	CA-C-O	-5.87	114.72	121.36
4	n	572	ASP	CB-CA-C	-5.86	101.69	110.88
4	n	343	HIS	N-CA-C	-5.86	104.85	112.23
1	2	70	GLU	O-C-N	-5.85	118.84	121.53
4	D	369	VAL	O-C-N	5.81	127.77	121.90
4	D	719	GLN	N-CA-CB	5.79	118.37	109.91
6	K	2	ILE	CA-C-N	5.78	132.58	121.54
6	K	2	ILE	C-N-CA	5.78	132.58	121.54
3	A	674	GLN	N-CA-C	-5.68	101.70	109.71
1	W	226	SER	N-CA-C	-5.64	105.23	111.71
1	V	334	HIS	CB-CG-CD2	-5.53	124.02	131.20
4	n	761	ARG	N-CA-C	-5.49	104.99	110.97
3	k	861	PHE	CA-CB-CG	5.48	119.28	113.80
1	Y	248	TYR	CA-CB-CG	-5.40	104.18	113.90
3	A	297	ARG	N-CA-C	-5.38	106.22	112.89
1	2	254	ILE	CA-C-N	5.38	126.90	120.13
1	2	254	ILE	C-N-CA	5.38	126.90	120.13
6	I	55	PHE	CA-CB-CG	5.33	119.13	113.80
7	J	548	MET	O-C-N	-5.29	116.82	123.27
4	D	719	GLN	N-CA-C	-5.23	105.27	110.97
1	2	227	GLN	N-CA-C	-5.21	107.06	113.41
7	J	1018	MET	CB-CA-C	-5.18	110.58	116.54
4	n	455	LYS	N-CA-C	5.18	116.38	108.30
5	G	75	PHE	CA-CB-CG	5.17	118.97	113.80
6	K	35	HIS	CA-CB-CG	-5.17	108.63	113.80
1	O	28	GLU	N-CA-C	5.17	116.91	111.28
6	K	523	PHE	CA-CB-CG	5.14	118.94	113.80
1	W	87	ASN	N-CA-C	5.14	121.17	109.81
3	k	401	HIS	CA-CB-CG	5.12	118.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	381	HIS	CA-CB-CG	5.12	118.92	113.80
6	K	166	PRO	N-CA-C	5.11	116.93	110.70
1	2	90	ASN	N-CA-C	5.08	117.55	111.71
6	I	530	TYR	N-CA-CB	-5.08	102.40	110.22
1	U	332	GLN	OE1-CD-NE2	-5.02	117.58	122.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	244	ARG	Sidechain
3	A	540	ARG	Sidechain
3	A	653	ARG	Sidechain
3	A	683	ARG	Sidechain
4	B	285	ARG	Sidechain
4	B	293	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3365	0	3309	50	0
1	2	3311	0	3253	66	0
1	O	3365	0	3309	155	0
1	P	3359	0	3298	57	0
1	Q	3371	0	3320	62	0
1	R	3365	0	3309	44	0
1	S	3371	0	3320	45	0
1	T	3359	0	3298	43	0
1	U	3365	0	3309	40	0
1	V	3325	0	3258	26	0
1	W	3342	0	3294	77	0
1	X	3371	0	3320	43	0
1	Y	3363	0	3316	46	0
1	Z	3365	0	3309	54	0
2	7	1812	0	920	1	0
3	A	4846	0	4867	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	4973	0	4986	79	0
3	E	5196	0	5230	87	0
3	M	5158	0	5186	92	0
3	f	481	0	218	0	0
3	k	5180	0	5208	49	0
4	B	5015	0	4991	100	0
4	D	4790	0	4764	101	0
4	F	4921	0	4897	69	0
4	N	4810	0	4790	80	0
4	b	933	0	953	36	0
4	n	4875	0	4836	56	0
5	G	270	0	268	4	0
5	H	317	0	314	5	0
5	g	303	0	300	5	0
5	h	317	0	314	5	0
5	i	274	0	274	30	0
5	j	290	0	286	2	0
5	s	303	0	300	11	0
5	t	303	0	300	20	0
5	u	317	0	314	5	0
5	v	317	0	314	8	0
6	I	4203	0	4221	123	0
6	K	4573	0	4575	63	0
7	J	4837	0	4822	118	0
8	L	4928	0	4971	71	0
8	d	1152	0	1158	26	0
9	a	484	0	512	22	0
9	c	454	0	482	5	0
10	e	231	0	119	0	0
All	All	123860	0	121912	1996	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 8.

All (1996) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:220:ILE:CG2	1:O:224:SER:HB2	1.52	1.40
3:A:771:LEU:CD2	1:O:162:PRO:HG3	1.54	1.35
3:A:677:ALA:HB1	1:O:263:THR:CG2	1.73	1.17
3:A:765:PHE:CZ	1:O:163:LYS:HD3	1.78	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:505:GLU:CA	3:M:508:GLU:HG2	1.75	1.16
1:O:220:ILE:HG21	1:O:224:SER:CB	1.75	1.15
3:A:663:LYS:C	1:O:200:ASP:HB3	1.72	1.15
3:A:771:LEU:HD21	1:O:162:PRO:CG	1.75	1.14
3:A:663:LYS:HE3	1:O:200:ASP:HA	1.27	1.14
3:A:586:LEU:CD1	5:i:78:LYS:HD3	1.80	1.12
3:A:677:ALA:CB	1:O:263:THR:HB	1.84	1.07
3:A:659:TRP:HZ2	1:O:165:LEU:HD13	1.19	1.07
3:A:692:ASN:OD1	1:O:357:GLN:HG2	1.54	1.06
3:A:765:PHE:CZ	1:O:163:LYS:CD	2.40	1.04
3:M:505:GLU:HA	3:M:508:GLU:CG	1.88	1.02
3:A:586:LEU:HD11	5:i:78:LYS:HD3	1.36	1.01
3:A:677:ALA:HB2	1:O:263:THR:HB	1.39	1.00
3:A:765:PHE:HZ	1:O:163:LYS:HD3	1.17	1.00
3:A:304:LEU:HB3	4:B:369:VAL:CG1	1.93	0.99
3:M:505:GLU:HA	3:M:508:GLU:HG2	1.01	0.98
3:A:586:LEU:CD1	5:i:82:TYR:CD1	2.48	0.97
1:Z:219:HIS:CE1	1:Z:220:ILE:HD13	1.99	0.97
3:A:765:PHE:HZ	1:O:163:LYS:CD	1.76	0.96
3:A:771:LEU:CD2	1:O:162:PRO:CG	2.37	0.96
3:k:537:GLU:OE1	3:k:537:GLU:N	2.00	0.95
3:A:677:ALA:HB1	1:O:263:THR:HG22	1.45	0.94
3:A:304:LEU:CB	4:B:369:VAL:CG1	2.46	0.94
5:t:69:GLU:OE1	5:t:69:GLU:N	2.01	0.93
1:Y:270:MET:HE1	1:Y:377:MET:HE1	1.49	0.93
1:Q:269:LEU:HB3	1:Q:378:MET:SD	2.10	0.92
1:O:118:ILE:HD12	1:O:153:LEU:HD13	1.50	0.92
1:2:276:LEU:HD22	1:2:304:MET:HE3	1.53	0.91
3:A:525:GLY:C	1:O:251:ASN:ND2	2.28	0.91
6:K:500:MET:SD	1:Y:200:ASP:HA	2.11	0.91
3:A:586:LEU:CG	5:i:78:LYS:HD3	2.02	0.90
3:A:677:ALA:HB2	1:O:264:PRO:HD2	1.53	0.90
1:O:220:ILE:CB	1:O:224:SER:HB2	2.01	0.89
1:V:271:THR:HG23	1:V:304:MET:HE2	1.52	0.89
1:Q:382:THR:HG22	1:Q:435:TYR:CE1	2.08	0.89
7:J:267:GLU:OE1	7:J:267:GLU:N	2.06	0.88
1:V:67:LEU:HD23	1:V:67:LEU:O	1.73	0.88
3:A:677:ALA:HA	1:O:264:PRO:HD3	1.53	0.88
4:B:268:MET:HA	4:B:268:MET:HE3	1.53	0.88
3:A:663:LYS:HE3	1:O:200:ASP:CA	2.04	0.87
1:U:260:LEU:HD13	1:U:269:LEU:HD21	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:586:LEU:HD11	5:i:78:LYS:CD	2.05	0.86
1:Z:219:HIS:CE1	1:Z:220:ILE:CD1	2.58	0.86
3:A:525:GLY:C	1:O:251:ASN:HD22	1.84	0.86
3:A:677:ALA:HB1	1:O:263:THR:CB	2.05	0.86
6:I:497:ALA:HA	6:I:500:MET:SD	2.15	0.86
1:R:303:VAL:C	1:R:304:MET:HE2	2.01	0.86
3:E:693:ILE:O	3:E:697:MET:SD	2.33	0.85
7:J:248:GLN:OE1	7:J:248:GLN:N	2.08	0.85
3:E:518:ARG:HA	3:E:523:ASP:OD1	1.77	0.85
1:S:220:ILE:HB	1:S:224:SER:HB3	1.59	0.84
1:O:220:ILE:HG22	1:O:224:SER:H	1.41	0.84
6:I:461:TRP:CZ2	6:I:465:ILE:HD12	2.13	0.84
1:O:220:ILE:CG2	1:O:224:SER:CB	2.46	0.83
1:Z:136:VAL:HG22	1:Z:167:GLN:OE1	1.78	0.83
3:A:187:LEU:HD21	4:B:379:LYS:HD2	1.61	0.83
1:2:323:ILE:HD11	1:2:378:MET:HE3	1.59	0.83
1:O:220:ILE:HG21	1:O:224:SER:HB2	0.85	0.83
3:A:771:LEU:HD22	1:O:162:PRO:CB	2.09	0.83
1:S:190:LEU:HD11	1:S:421:MET:HE2	1.61	0.82
3:A:578:MET:HE2	3:A:580:HIS:O	1.80	0.82
3:A:586:LEU:HD13	5:i:82:TYR:CG	2.15	0.81
3:A:765:PHE:CE2	1:O:163:LYS:NZ	2.46	0.81
6:I:21:LYS:C	6:I:21:LYS:HD3	2.05	0.81
6:I:461:TRP:CE3	6:I:464:HIS:O	2.33	0.81
1:R:34:GLU:N	1:R:34:GLU:OE1	2.13	0.81
1:W:47:ARG:HG3	1:W:47:ARG:O	1.77	0.81
1:Y:235:ILE:HD11	1:Y:304:MET:SD	2.20	0.81
3:A:659:TRP:CZ2	1:O:165:LEU:HD13	2.12	0.81
3:A:663:LYS:C	1:O:200:ASP:CB	2.54	0.81
3:C:578:MET:HE2	3:C:580:HIS:O	1.80	0.81
3:M:228:VAL:HB	4:N:365:ARG:NH1	1.96	0.81
4:n:419:LEU:HD23	4:n:419:LEU:O	1.79	0.81
3:A:695:TYR:HE2	1:O:357:GLN:HB3	1.46	0.81
4:B:715:ILE:HG23	4:B:718:MET:CE	2.11	0.81
6:I:21:LYS:HD3	6:I:21:LYS:O	1.82	0.80
3:k:697:MET:HE2	3:k:737:CYS:SG	2.21	0.80
4:B:406:THR:HG22	4:B:411:MET:HE3	1.65	0.79
3:A:771:LEU:HD21	1:O:162:PRO:HG3	0.81	0.79
7:J:281:VAL:HG12	7:J:282:LYS:H	1.48	0.79
4:N:710:GLU:OE1	4:N:855:GLN:CG	2.30	0.79
1:1:22:TRP:CZ3	1:1:25:LEU:HD23	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:128:GLN:OE1	6:K:129:PHE:CD2	2.36	0.78
4:N:574:ILE:C	4:N:578:MET:SD	2.67	0.78
1:W:297:LEU:HD23	1:W:322:ASN:OD1	1.83	0.78
3:A:771:LEU:HD22	1:O:162:PRO:HB3	1.66	0.78
8:L:1587:LEU:HB3	5:h:60:MET:SD	2.24	0.78
1:R:376:LEU:HB3	1:R:378:MET:SD	2.24	0.78
3:A:586:LEU:HD11	5:i:82:TYR:CD1	2.18	0.78
4:N:710:GLU:OE1	4:N:855:GLN:HG3	1.85	0.77
4:B:685:MET:HE3	1:P:200:ASP:HB2	1.66	0.77
1:X:223:PRO:HA	1:X:225:PHE:CZ	2.19	0.77
4:B:715:ILE:HG23	4:B:718:MET:HE2	1.67	0.77
1:Q:382:THR:HA	1:Q:435:TYR:CZ	2.20	0.77
1:R:271:THR:OG1	1:R:378:MET:HE1	1.85	0.77
4:F:718:MET:HE3	4:F:718:MET:O	1.85	0.77
6:K:378:HIS:CE1	6:K:379:MET:HE1	2.20	0.77
3:A:677:ALA:CB	1:O:263:THR:CB	2.59	0.76
4:F:471:ILE:HG21	4:F:477:MET:HE1	1.68	0.76
8:L:1638:MET:HG3	1:Z:249:MET:HE2	1.66	0.76
3:A:660:ILE:HD13	1:O:165:LEU:HB3	1.67	0.76
4:b:14:GLN:OE1	8:d:72:MET:HE1	1.86	0.76
1:2:314:ASN:HB3	1:2:439:THR:HG21	1.68	0.76
6:I:367:GLU:HB2	1:W:47:ARG:NH2	1.99	0.76
3:M:674:GLN:N	3:M:674:GLN:HE21	1.82	0.76
3:A:659:TRP:CD1	1:O:254:ILE:HG13	2.21	0.75
1:R:407:GLN:NE2	1:R:407:GLN:O	2.19	0.75
3:A:304:LEU:CD1	4:B:369:VAL:HG12	2.17	0.75
1:2:351:TRP:CH2	4:N:706:ILE:HD12	2.22	0.74
3:A:677:ALA:CA	1:O:264:PRO:HD3	2.17	0.74
3:A:692:ASN:OD1	1:O:357:GLN:CG	2.36	0.74
3:M:155:GLU:O	3:M:160:MET:HE1	1.88	0.74
1:W:67:LEU:HD11	1:W:118:ILE:HD12	1.69	0.74
4:D:714:PHE:CE1	4:D:718:MET:SD	2.80	0.74
4:F:609:ASN:H	1:T:47:ARG:HD2	1.53	0.74
4:D:562:MET:HE1	4:D:652:PHE:CE1	2.22	0.74
3:E:698:MET:HE1	3:E:699:PHE:CG	2.21	0.74
1:O:260:LEU:HD22	1:O:378:MET:HG3	1.68	0.74
3:A:304:LEU:CB	4:B:369:VAL:HG12	2.17	0.73
3:E:165:GLN:OE1	3:E:165:GLN:O	2.06	0.73
3:A:187:LEU:CD2	4:B:379:LYS:HD2	2.18	0.73
6:I:96:VAL:HG12	6:I:174:LYS:HE3	1.71	0.73
8:L:1638:MET:HG3	1:Z:249:MET:CE	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:334:HIS:HD1	3:M:851:GLY:N	1.86	0.73
3:A:695:TYR:CE2	1:O:357:GLN:HB3	2.24	0.73
3:A:470:PRO:CD	3:A:494:TYR:CE2	2.71	0.73
3:C:470:PRO:CD	3:C:494:TYR:CE2	2.71	0.73
1:R:378:MET:SD	1:R:378:MET:N	2.61	0.73
1:X:169:TYR:CG	1:X:236:MET:HE1	2.24	0.73
1:O:118:ILE:CD1	1:O:153:LEU:HD13	2.18	0.73
4:B:299:TRP:CH2	4:B:303:LYS:HD2	2.24	0.73
6:I:136:VAL:HG22	6:I:172:LEU:HD11	1.69	0.73
7:J:1018:MET:N	7:J:1018:MET:SD	2.61	0.72
3:A:699:PHE:HD2	1:O:334:HIS:CD2	2.07	0.72
3:E:577:LEU:HD12	3:E:577:LEU:O	1.88	0.72
7:J:331:ILE:HA	7:J:365:MET:CE	2.18	0.72
3:A:659:TRP:NE1	1:O:254:ILE:HG13	2.05	0.72
6:K:285:MET:O	6:K:285:MET:SD	2.47	0.72
3:M:757:MET:HG2	3:M:761:CYS:SG	2.29	0.72
1:X:271:THR:HG22	1:X:378:MET:SD	2.29	0.72
3:M:644:HIS:HB3	3:M:739:LEU:HG	1.72	0.72
4:N:574:ILE:O	4:N:578:MET:SD	2.48	0.72
3:C:306:LEU:HD23	3:C:310:LEU:HD23	1.72	0.72
6:I:264:LEU:HD11	6:I:268:ILE:CG2	2.20	0.72
8:L:1681:GLN:CD	1:Z:249:MET:SD	2.73	0.72
1:U:292:ASP:O	1:U:296:ARG:HG3	1.90	0.72
3:k:392:GLU:OE2	3:k:474:GLU:HA	1.89	0.72
3:A:306:LEU:HD23	3:A:310:LEU:HD23	1.72	0.72
6:K:500:MET:HE3	1:Y:200:ASP:O	1.89	0.72
3:A:231:ARG:NH2	4:B:283:LEU:HD22	2.06	0.71
3:A:659:TRP:CH2	1:O:257:ILE:HG21	2.25	0.71
6:I:356:ILE:HG23	6:I:360:PHE:HE2	1.55	0.71
6:K:500:MET:SD	6:K:500:MET:O	2.48	0.71
1:U:376:LEU:HD21	1:U:378:MET:HE2	1.72	0.71
3:M:738:MET:HA	3:M:738:MET:HE3	1.72	0.71
1:T:232:VAL:O	1:T:236:MET:SD	2.49	0.71
1:W:235:ILE:HA	1:W:376:LEU:HD21	1.71	0.71
4:D:477:MET:SD	4:D:477:MET:C	2.74	0.71
6:I:367:GLU:HB2	1:W:47:ARG:CZ	2.19	0.71
4:N:400:VAL:HG21	4:N:422:VAL:HG11	1.72	0.71
1:W:270:MET:HG2	1:W:305:VAL:HG21	1.72	0.71
3:A:731:ASP:HB3	5:i:72:LYS:HG3	1.71	0.71
3:E:698:MET:HE1	3:E:699:PHE:CD2	2.26	0.71
4:F:250:LEU:O	4:F:254:ILE:HD12	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:264:LEU:HD11	6:I:268:ILE:HG22	1.73	0.71
1:U:271:THR:HG22	1:U:378:MET:HE1	1.71	0.71
3:A:586:LEU:CG	5:i:78:LYS:CD	2.68	0.71
3:A:765:PHE:CZ	1:O:163:LYS:HD2	2.24	0.71
1:Q:58:GLU:OE2	1:R:288:THR:HG22	1.91	0.71
4:D:411:MET:H	4:D:411:MET:HE2	1.55	0.71
1:V:272:GLY:HA2	1:V:304:MET:SD	2.30	0.71
3:C:482:ARG:NH1	3:C:485:VAL:HG11	2.06	0.71
1:T:232:VAL:HG13	1:T:236:MET:HE1	1.72	0.70
1:V:10:LEU:HD22	1:V:67:LEU:HD22	1.73	0.70
3:A:586:LEU:HG	5:i:78:LYS:HD3	1.72	0.70
3:A:732:THR:HA	5:i:72:LYS:HE2	1.71	0.70
3:A:304:LEU:HB3	4:B:369:VAL:HG13	1.73	0.70
3:A:304:LEU:HB2	4:B:369:VAL:CG1	2.21	0.70
6:I:461:TRP:CZ3	6:I:464:HIS:O	2.45	0.70
4:D:725:GLU:OE1	4:D:726:VAL:HG23	1.92	0.70
3:k:738:MET:HE1	3:k:748:PHE:CG	2.27	0.70
4:D:475:MET:HE1	4:D:480:SER:N	2.07	0.70
4:D:714:PHE:O	4:D:718:MET:HG3	1.92	0.70
3:E:426:LYS:O	3:E:430:GLN:CD	2.35	0.70
3:A:659:TRP:HB2	3:A:683:ARG:HH22	1.56	0.70
1:O:220:ILE:CG2	1:O:224:SER:H	2.03	0.70
3:A:205:ILE:HD12	3:A:208:LEU:HD12	1.74	0.69
1:P:223:PRO:HB2	1:P:227:GLN:HG2	1.75	0.69
1:U:271:THR:HG22	1:U:378:MET:SD	2.32	0.69
1:W:73:VAL:HG13	1:W:74:ILE:HD13	1.74	0.69
6:I:105:LEU:HD11	7:J:400:ASP:HB3	1.74	0.69
1:2:213:ILE:CD1	1:2:304:MET:HG2	2.22	0.69
3:E:738:MET:HE3	3:E:748:PHE:CE1	2.27	0.69
1:R:270:MET:HE2	1:R:381:HIS:O	1.92	0.69
1:W:25:LEU:HD21	1:W:244:ARG:CZ	2.22	0.69
3:A:525:GLY:O	1:O:251:ASN:ND2	2.21	0.69
4:D:320:VAL:HG22	4:D:445:GLU:OE2	1.92	0.69
3:M:228:VAL:HB	4:N:365:ARG:HH11	1.58	0.69
7:J:909:THR:OG1	7:J:937:ILE:HD11	1.91	0.69
1:Q:260:LEU:HD21	1:Q:321:LEU:HB2	1.75	0.69
1:1:169:TYR:CD1	1:1:236:MET:HE2	2.28	0.69
6:I:369:PHE:CE1	6:I:483:LEU:HD12	2.27	0.69
3:E:530:HIS:CD2	1:S:47:ARG:HH12	2.10	0.69
3:k:757:MET:HA	3:k:757:MET:HE3	1.74	0.68
1:Y:273:TYR:HB2	1:Y:304:MET:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:253:LEU:O	1:Z:256:LEU:HD12	1.93	0.68
3:C:205:ILE:HD12	3:C:208:LEU:HD12	1.74	0.68
3:C:701:VAL:HG22	3:C:736:ASP:O	1.94	0.68
3:A:308:SER:HB2	4:B:365:ARG:HG3	1.76	0.68
3:A:663:LYS:HZ3	1:O:267:HIS:CD2	2.11	0.68
1:2:276:LEU:CD2	1:2:304:MET:HE3	2.22	0.68
9:a:67:LEU:HD13	4:b:20:ILE:HD11	1.74	0.68
3:A:186:ALA:HB1	4:B:293:ARG:HA	1.76	0.68
4:F:477:MET:N	4:F:477:MET:HE2	2.08	0.68
3:E:217:VAL:HG11	3:E:252:LEU:HD21	1.76	0.68
1:W:290:VAL:O	1:W:294:MET:HG2	1.94	0.68
9:a:67:LEU:HB3	4:b:20:ILE:HD12	1.76	0.68
4:B:711:MET:HE2	4:B:854:TYR:CD1	2.28	0.68
3:A:699:PHE:CD2	1:O:334:HIS:HD2	2.12	0.67
1:2:248:TYR:OH	4:N:667:LEU:HG	1.93	0.67
3:A:586:LEU:HD11	5:i:78:LYS:CG	2.23	0.67
3:A:701:VAL:HG22	3:A:736:ASP:O	1.94	0.67
4:B:865:LEU:HD13	4:B:873:LEU:HD11	1.75	0.67
6:I:414:LEU:CD1	6:I:455:LEU:HD21	2.24	0.67
7:J:830:GLN:OE1	7:J:955:MET:HE1	1.93	0.67
6:I:2:ILE:HG12	7:J:242:LEU:HD11	1.76	0.67
4:D:666:PHE:CE2	4:D:764:LEU:HD22	2.29	0.67
4:D:697:PHE:O	4:D:701:LEU:HB2	1.95	0.67
7:J:320:TYR:CE2	7:J:406:LEU:HD13	2.30	0.67
7:J:691:LEU:C	7:J:693:PRO:HD2	2.20	0.67
3:A:677:ALA:HB1	1:O:263:THR:HB	1.64	0.67
1:O:220:ILE:CB	1:O:224:SER:CB	2.72	0.67
4:n:859:GLN:O	4:n:863:VAL:HG13	1.95	0.67
3:C:494:TYR:CD1	3:C:494:TYR:C	2.73	0.67
4:D:854:TYR:CE1	4:D:858:VAL:HG11	2.30	0.67
3:M:160:MET:N	3:M:160:MET:HE3	2.09	0.67
4:N:673:MET:HG3	4:N:782:ILE:HG21	1.76	0.67
3:A:663:LYS:HE2	1:O:200:ASP:O	1.95	0.67
7:J:886:LEU:O	7:J:890:LEU:HD23	1.94	0.67
6:K:500:MET:HG3	1:Y:200:ASP:OD2	1.95	0.67
1:Q:270:MET:C	1:Q:378:MET:HE1	2.19	0.67
1:S:382:THR:HG22	1:S:435:TYR:CD1	2.30	0.67
6:K:128:GLN:C	6:K:128:GLN:CD	2.62	0.67
3:C:701:VAL:HG13	3:C:736:ASP:HB3	1.77	0.67
9:a:67:LEU:CD1	4:b:20:ILE:HD11	2.24	0.66
4:B:694:MET:HE3	4:B:803:ARG:CZ	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:594:GLN:HB3	5:s:60:MET:HE3	1.77	0.66
3:E:686:MET:HE3	3:E:829:PHE:CD1	2.30	0.66
4:F:562:MET:CE	4:F:657:MET:HE1	2.25	0.66
4:F:749:ALA:O	4:F:753:VAL:HG13	1.94	0.66
6:K:110:GLU:HA	6:K:110:GLU:OE1	1.94	0.66
1:Q:382:THR:HA	1:Q:435:TYR:CE2	2.31	0.66
3:M:613:LEU:HD22	3:M:752:MET:HE1	1.76	0.66
1:T:205:LEU:HD22	1:T:236:MET:HE1	1.78	0.66
1:T:386:SER:HA	1:T:389:GLU:HG2	1.75	0.66
1:W:61:ILE:HG23	1:W:62:PRO:HD2	1.78	0.66
3:A:494:TYR:CD1	3:A:494:TYR:C	2.73	0.66
3:A:701:VAL:HG13	3:A:736:ASP:HB3	1.77	0.66
6:I:370:GLN:NE2	1:W:251:ASN:ND2	2.43	0.66
8:L:1681:GLN:NE2	1:Z:249:MET:HE1	2.11	0.66
1:T:236:MET:SD	1:T:236:MET:N	2.68	0.66
5:i:69:GLU:HA	5:i:72:LYS:HD2	1.78	0.66
3:k:536:GLU:CD	3:k:537:GLU:OE1	2.38	0.66
4:B:691:LEU:HD23	4:B:694:MET:SD	2.36	0.66
3:E:681:THR:HG21	1:S:351:TRP:HE1	1.60	0.66
6:K:128:GLN:OE1	6:K:129:PHE:CG	2.49	0.66
1:W:291:LEU:CD2	1:W:295:ARG:HH21	2.09	0.66
3:C:301:LYS:HG2	4:D:372:TYR:CD2	2.31	0.66
4:F:609:ASN:CG	1:T:47:ARG:HG2	2.21	0.66
4:N:670:ALA:HA	4:N:673:MET:HE2	1.77	0.66
7:J:331:ILE:HG12	7:J:365:MET:HE1	1.77	0.66
1:1:341:ARG:HD3	3:M:861:PHE:CD2	2.31	0.66
6:I:135:SER:O	6:I:138:VAL:HG22	1.96	0.66
1:O:270:MET:SD	1:O:379:ALA:HB3	2.36	0.66
1:S:330:PRO:O	1:S:333:VAL:HG22	1.96	0.66
3:A:586:LEU:HD13	5:i:82:TYR:CD1	2.31	0.65
3:A:663:LYS:HB3	1:O:200:ASP:O	1.96	0.65
4:B:255:LEU:HD21	4:B:342:LEU:HB3	1.79	0.65
7:J:742:ILE:HD11	7:J:752:TRP:HA	1.78	0.65
3:A:771:LEU:CD2	1:O:162:PRO:CB	2.73	0.65
6:K:582:CYS:O	6:K:586:ILE:HG12	1.95	0.65
1:O:118:ILE:HD12	1:O:153:LEU:CD1	2.24	0.65
1:1:266:LEU:HD23	1:1:266:LEU:O	1.96	0.65
3:A:497:LYS:HD3	3:A:500:LEU:HD12	1.78	0.65
4:D:652:PHE:C	4:D:657:MET:HE3	2.21	0.65
1:V:47:ARG:HD2	4:n:572:ASP:OD2	1.96	0.65
1:W:245:TYR:CG	1:W:362:ARG:HD3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:663:LYS:HG2	3:A:680:PHE:HE2	1.62	0.65
3:k:356:LEU:HD12	3:k:356:LEU:O	1.95	0.65
3:M:505:GLU:C	3:M:508:GLU:CG	2.70	0.65
1:R:253:LEU:HG	1:R:257:ILE:HD13	1.78	0.65
4:n:574:ILE:HG23	4:n:578:MET:HE1	1.79	0.65
3:A:586:LEU:HG	5:i:78:LYS:CD	2.26	0.65
3:A:663:LYS:CE	1:O:200:ASP:O	2.45	0.65
4:D:255:LEU:HD13	4:D:339:LEU:HD11	1.79	0.65
4:F:401:HIS:O	4:F:404:THR:HG22	1.96	0.65
1:P:377:MET:HE2	1:P:379:ALA:CB	2.27	0.65
4:D:253:ASP:O	4:D:257:VAL:HG23	1.97	0.65
4:F:762:CYS:HB3	4:F:764:LEU:HD13	1.79	0.65
1:Q:271:THR:O	1:Q:304:MET:SD	2.55	0.65
3:A:765:PHE:CE2	1:O:163:LYS:CD	2.80	0.65
6:K:525:VAL:HG11	6:K:586:ILE:HD12	1.78	0.65
3:M:522:MET:HE1	3:M:649:LYS:CB	2.27	0.65
1:O:22:TRP:CE3	1:O:62:PRO:HB3	2.31	0.65
1:Q:55:ALA:HB3	1:Q:59:HIS:HB2	1.79	0.65
1:R:270:MET:HE1	1:R:305:VAL:HG11	1.78	0.65
1:V:343:ARG:HH12	3:k:561:MET:HE2	1.62	0.65
3:C:528:PHE:CD1	3:C:646:PHE:CZ	2.85	0.64
4:D:475:MET:CE	4:D:480:SER:N	2.60	0.64
4:F:395:GLU:HG3	4:F:470:MET:SD	2.37	0.64
6:I:379:MET:HE2	6:I:379:MET:HA	1.78	0.64
3:A:659:TRP:HE1	1:O:254:ILE:HG13	1.63	0.64
6:I:379:MET:O	6:I:379:MET:SD	2.54	0.64
1:Q:270:MET:HE2	1:Q:305:VAL:HG23	1.79	0.64
1:Q:271:THR:HG23	1:Q:304:MET:HE2	1.79	0.64
5:t:60:MET:CE	5:v:59:ASN:O	2.45	0.64
3:A:528:PHE:CD1	3:A:646:PHE:CZ	2.85	0.64
3:E:426:LYS:NZ	5:u:85:GLU:OE1	2.30	0.64
3:E:752:MET:HA	3:E:752:MET:HE3	1.79	0.64
1:O:62:PRO:HG2	1:O:85:LEU:O	1.98	0.64
1:2:323:ILE:CD1	1:2:378:MET:CE	2.75	0.64
4:F:608:THR:HA	1:T:47:ARG:HE	1.62	0.64
6:I:495:CYS:C	6:I:497:ALA:N	2.49	0.64
1:U:189:LEU:HD21	1:U:424:SER:C	2.23	0.64
6:I:354:LEU:HA	6:I:357:ILE:HG22	1.80	0.64
1:Q:271:THR:N	1:Q:378:MET:HE1	2.12	0.64
1:2:248:TYR:HE2	4:N:722:ILE:HG22	1.63	0.64
1:Z:4:GLU:O	1:Z:132:LEU:HD13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:802:ARG:HA	4:B:805:GLN:HG2	1.80	0.64
3:M:505:GLU:C	3:M:508:GLU:HG2	2.23	0.63
1:V:398:LEU:HD23	1:V:401:ARG:NH2	2.13	0.63
3:A:304:LEU:HB2	4:B:369:VAL:HG12	1.78	0.63
8:L:456:LEU:H	8:L:456:LEU:HD12	1.63	0.63
1:X:376:LEU:HD21	1:X:378:MET:SD	2.38	0.63
9:c:27:VAL:HG11	8:d:95:GLU:OE2	1.98	0.63
3:A:507:LYS:HB3	3:A:626:LEU:HD13	1.80	0.63
4:B:873:LEU:HD12	4:B:873:LEU:O	1.97	0.63
4:D:377:ARG:O	4:D:381:LEU:HD23	1.98	0.63
4:D:410:TYR:HD1	4:D:411:MET:SD	2.21	0.63
7:J:365:MET:CA	7:J:365:MET:HE3	2.27	0.63
7:J:331:ILE:HA	7:J:365:MET:HE1	1.80	0.63
8:L:1537:ASP:O	8:L:1541:GLU:HB3	1.97	0.63
1:W:438:ALA:HB2	1:W:443:TYR:CE2	2.33	0.63
1:2:323:ILE:HD11	1:2:378:MET:CE	2.28	0.63
4:D:537:ALA:HA	4:D:540:GLU:CD	2.24	0.63
6:I:357:ILE:HD11	6:I:475:TYR:CE2	2.33	0.63
3:M:516:ILE:HG21	3:M:638:TYR:CE1	2.33	0.63
4:b:36:VAL:HA	8:d:75:PHE:HE2	1.63	0.63
1:2:351:TRP:HE1	1:2:444:ILE:HA	1.64	0.63
8:L:1553:LEU:HB2	8:L:1587:LEU:HD21	1.81	0.63
4:N:652:PHE:O	4:N:657:MET:HE3	1.98	0.63
1:Q:377:MET:CE	1:Q:379:ALA:HB2	2.29	0.63
1:2:197:GLN:HB3	4:N:692:ARG:HA	1.81	0.62
1:Z:67:LEU:HB3	1:Z:69:LEU:HD13	1.81	0.62
1:Y:273:TYR:HB2	1:Y:304:MET:HE3	1.79	0.62
4:b:33:GLN:O	4:b:37:ARG:HG3	1.99	0.62
3:A:186:ALA:CB	4:B:293:ARG:HA	2.30	0.62
1:Y:378:MET:HG3	1:Y:378:MET:O	1.99	0.62
1:2:351:TRP:HH2	4:N:706:ILE:HD12	1.64	0.62
7:J:302:VAL:HG23	7:J:310:LEU:HD11	1.82	0.62
3:M:505:GLU:CA	3:M:508:GLU:CG	2.62	0.62
8:L:1681:GLN:HE21	1:Z:249:MET:HE1	1.65	0.62
1:O:21:PHE:CD2	1:O:236:MET:HE2	2.34	0.62
1:S:270:MET:HE1	1:S:384:ILE:HD13	1.81	0.62
1:W:238:ALA:HB1	1:W:323:ILE:HD11	1.80	0.62
3:A:699:PHE:CD2	1:O:334:HIS:CD2	2.87	0.62
4:D:562:MET:HE1	4:D:652:PHE:CZ	2.35	0.62
1:1:21:PHE:CG	1:1:236:MET:SD	2.93	0.62
7:J:365:MET:HE3	7:J:365:MET:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:729:CYS:SG	1:T:331:THR:HA	2.40	0.61
1:W:238:ALA:CB	1:W:376:LEU:HD13	2.29	0.61
6:I:379:MET:HG3	6:I:450:TRP:CD2	2.34	0.61
3:A:304:LEU:CB	4:B:369:VAL:HG11	2.29	0.61
7:J:320:TYR:CZ	7:J:406:LEU:HD13	2.36	0.61
4:B:254:ILE:O	4:B:258:PHE:CD1	2.53	0.61
6:I:107:LEU:HD21	6:I:125:PHE:CD2	2.35	0.61
1:P:270:MET:SD	1:P:381:HIS:HB3	2.39	0.61
1:U:413:MET:HA	1:U:413:MET:HE2	1.83	0.61
4:b:56:GLU:OE1	4:b:56:GLU:HA	1.98	0.61
4:B:503:THR:HG21	4:B:544:TYR:CD2	2.35	0.61
3:E:426:LYS:HB3	3:E:430:GLN:NE2	2.15	0.61
8:L:1634:LEU:HD21	8:L:1681:GLN:NE2	2.16	0.61
1:O:203:VAL:CG2	1:O:378:MET:HE1	2.31	0.61
1:2:270:MET:HE2	1:2:381:HIS:HB3	1.82	0.61
1:2:323:ILE:CD1	1:2:378:MET:HE3	2.31	0.61
3:C:387:TYR:CE2	3:C:407:PHE:CE1	2.89	0.61
6:K:541:PHE:CD1	6:K:564:PHE:CZ	2.89	0.61
1:P:277:THR:O	1:P:277:THR:HG22	2.00	0.61
3:k:732:THR:HG22	5:t:72:LYS:NZ	2.15	0.61
3:A:308:SER:CB	4:B:365:ARG:HG3	2.30	0.61
4:B:718:MET:HE1	4:B:775:LEU:HD11	1.81	0.61
4:D:257:VAL:HG13	4:D:275:TYR:CD2	2.35	0.61
4:F:729:CYS:SG	1:T:331:THR:HG22	2.40	0.61
4:N:396:LEU:O	4:N:400:VAL:HG23	2.00	0.61
4:N:574:ILE:HG22	4:N:578:MET:SD	2.40	0.61
1:R:270:MET:HE1	1:R:384:ILE:N	2.15	0.61
1:R:304:MET:HE2	1:R:304:MET:N	2.16	0.61
1:S:169:TYR:CD1	1:S:236:MET:HE1	2.34	0.61
1:W:249:MET:HA	1:W:249:MET:HE3	1.83	0.61
1:X:57:ASP:CG	1:X:59:HIS:CE1	2.78	0.61
4:D:328:LEU:HD21	4:D:385:VAL:HG11	1.83	0.61
1:Q:33:PRO:O	1:Q:85:LEU:HG	2.01	0.61
1:U:130:ASP:OD2	3:k:561:MET:HE3	2.00	0.61
6:I:357:ILE:HD11	6:I:475:TYR:CZ	2.36	0.61
6:K:513:ILE:HD13	1:Y:263:THR:HG23	1.83	0.61
9:a:67:LEU:CB	4:b:20:ILE:HD12	2.31	0.61
7:J:566:MET:HE2	7:J:702:CYS:HB2	1.83	0.61
1:P:377:MET:CE	1:P:379:ALA:HB3	2.31	0.61
1:W:151:SER:HB2	1:W:194:ARG:HD2	1.82	0.61
3:A:434:ILE:HG23	3:A:439:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:388:PHE:C	3:E:392:GLU:OE2	2.43	0.60
5:t:64:GLU:HA	5:t:67:ILE:HG22	1.83	0.60
4:D:659:HIS:O	4:D:663:VAL:HG23	2.02	0.60
6:I:367:GLU:N	1:W:47:ARG:HH12	1.99	0.60
7:J:331:ILE:CG1	7:J:365:MET:HE1	2.31	0.60
3:M:283:PHE:CZ	4:N:411:MET:HE2	2.36	0.60
3:k:226:VAL:CG1	3:k:307:VAL:HG11	2.31	0.60
3:A:387:TYR:CE2	3:A:407:PHE:CE1	2.89	0.60
3:A:699:PHE:HD2	1:O:334:HIS:HD2	1.47	0.60
7:J:286:ILE:HG12	7:J:300:ILE:CD1	2.31	0.60
1:T:214:ALA:HB1	1:T:220:ILE:HB	1.83	0.60
4:n:562:MET:HE1	4:n:657:MET:SD	2.40	0.60
3:A:528:PHE:CE1	3:A:646:PHE:CE2	2.89	0.60
3:C:528:PHE:CE1	3:C:646:PHE:CE2	2.89	0.60
3:M:836:LEU:HB2	3:M:839:ARG:HH11	1.67	0.60
1:1:305:VAL:HG13	1:1:387:LEU:HD22	1.83	0.60
1:2:362:ARG:HH12	4:N:563:ARG:NH2	1.99	0.60
8:L:1681:GLN:CG	1:Z:249:MET:SD	2.90	0.60
1:V:271:THR:HG23	1:V:304:MET:CE	2.31	0.60
3:E:414:LEU:HD23	3:E:415:ARG:N	2.16	0.60
1:U:271:THR:HG22	1:U:378:MET:CE	2.30	0.60
1:T:62:PRO:CG	1:T:85:LEU:CD2	2.80	0.60
1:U:272:GLY:HA2	1:U:304:MET:HE2	1.83	0.60
3:E:655:LEU:O	3:E:658:VAL:HG22	2.02	0.60
8:L:1584:LEU:HD21	8:L:1587:LEU:HD12	1.84	0.60
3:C:434:ILE:HG23	3:C:439:ILE:HD11	1.83	0.60
3:C:470:PRO:HD3	3:C:494:TYR:CE2	2.37	0.60
7:J:327:LEU:HD22	7:J:368:LEU:HD21	1.83	0.60
1:O:74:ILE:O	1:O:78:LEU:HD23	2.02	0.60
1:1:21:PHE:CD1	1:1:236:MET:SD	2.95	0.59
1:1:117:ASP:OD1	1:1:118:ILE:N	2.35	0.59
3:A:586:LEU:CD1	5:i:82:TYR:CG	2.81	0.59
4:N:430:LEU:O	4:N:434:ILE:HG22	2.02	0.59
1:O:5:ILE:HG21	1:O:136:VAL:HG23	1.84	0.59
1:Y:305:VAL:HG11	1:Y:384:ILE:HG13	1.84	0.59
1:O:213:ILE:HG23	1:O:276:LEU:HD13	1.83	0.59
1:Y:395:TYR:CE1	1:Y:421:MET:HE3	2.37	0.59
6:I:414:LEU:HD12	6:I:455:LEU:HD21	1.83	0.59
6:I:509:GLN:HB3	6:I:513:ILE:HG22	1.85	0.59
4:N:710:GLU:CD	4:N:855:GLN:HG3	2.28	0.59
9:a:24:THR:O	9:a:28:LEU:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:150:LEU:HD12	3:A:152:GLN:OE1	2.01	0.59
3:A:693:ILE:CD1	3:A:738:MET:SD	2.91	0.59
3:C:693:ILE:CD1	3:C:738:MET:SD	2.91	0.59
3:M:865:TYR:CZ	3:M:868:ARG:NH2	2.70	0.59
4:n:297:LEU:CD1	4:n:378:LEU:HD22	2.32	0.59
4:B:268:MET:HA	4:B:268:MET:CE	2.30	0.59
4:F:562:MET:HE2	4:F:657:MET:HE1	1.84	0.59
4:n:718:MET:HE3	4:n:775:LEU:HD21	1.85	0.59
4:B:734:LEU:HD12	4:B:754:PHE:CG	2.38	0.59
7:J:368:LEU:O	7:J:372:PHE:CD1	2.56	0.59
4:N:559:MET:HE1	4:N:734:LEU:HD21	1.85	0.59
1:X:39:GLU:H	1:X:39:GLU:CD	2.11	0.59
3:C:150:LEU:HD12	3:C:152:GLN:OE1	2.01	0.59
1:O:271:THR:C	1:O:304:MET:HE2	2.28	0.59
1:Q:377:MET:CE	1:Q:379:ALA:CB	2.81	0.59
4:b:36:VAL:HG22	8:d:75:PHE:CD2	2.37	0.59
7:J:331:ILE:HG23	7:J:365:MET:HE1	1.85	0.59
9:a:28:LEU:HG	4:b:81:LEU:CD1	2.33	0.59
3:A:470:PRO:HD3	3:A:494:TYR:CE2	2.37	0.59
3:E:681:THR:CG2	1:S:351:TRP:HE1	2.16	0.59
4:F:733:GLU:OE2	4:F:737:LYS:HD3	2.02	0.59
4:N:558:HIS:HB3	4:N:562:MET:CE	2.32	0.59
1:W:25:LEU:CD2	1:W:244:ARG:NH2	2.66	0.59
4:b:36:VAL:HG22	8:d:75:PHE:HD2	1.67	0.59
4:B:685:MET:CE	1:P:200:ASP:HB2	2.31	0.58
3:E:475:ILE:O	3:E:475:ILE:HG22	2.03	0.58
6:I:354:LEU:HA	6:I:357:ILE:CG2	2.32	0.58
4:N:614:SER:HB3	4:N:617:ILE:HD12	1.85	0.58
1:1:21:PHE:CD2	1:1:236:MET:SD	2.96	0.58
4:B:719:GLN:OE1	1:P:249:MET:HE3	2.02	0.58
6:I:96:VAL:HG21	6:I:175:ILE:HG13	1.85	0.58
6:I:325:PHE:O	6:I:328:VAL:HG22	2.02	0.58
3:M:762:MET:HE2	3:M:762:MET:HA	1.83	0.58
3:A:304:LEU:HB3	4:B:369:VAL:HG11	1.83	0.58
3:A:677:ALA:HB1	1:O:263:THR:HG21	1.79	0.58
6:I:106:ASP:O	6:I:106:ASP:OD1	2.22	0.58
4:b:36:VAL:HA	8:d:75:PHE:CE2	2.38	0.58
3:k:658:VAL:HG13	3:k:762:MET:HE2	1.84	0.58
4:D:575:ARG:HD2	4:D:575:ARG:O	2.04	0.58
6:I:356:ILE:HG23	6:I:360:PHE:CE2	2.38	0.58
6:K:541:PHE:HD1	6:K:564:PHE:CZ	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:272:GLY:O	1:S:376:LEU:HD12	2.03	0.58
1:U:409:ARG:NH1	1:U:413:MET:HE3	2.18	0.58
6:I:513:ILE:HG22	6:I:513:ILE:O	2.02	0.58
6:K:127:ASP:C	6:K:127:ASP:OD1	2.46	0.58
3:M:446:MET:SD	3:M:446:MET:N	2.76	0.58
8:d:94:GLU:O	8:d:94:GLU:CD	2.46	0.58
5:g:88:MET:HE1	5:h:88:MET:HE1	1.84	0.58
4:F:477:MET:HE2	4:F:477:MET:CA	2.33	0.58
4:N:710:GLU:OE1	4:N:855:GLN:HG2	2.04	0.58
9:a:22:ARG:O	9:a:26:ASP:OD1	2.22	0.58
3:k:184:ARG:NH2	4:n:273:ASN:O	2.36	0.58
4:B:865:LEU:HD22	4:B:873:LEU:HD11	1.86	0.58
6:I:27:VAL:HG11	6:I:42:LEU:HB2	1.85	0.58
6:I:497:ALA:HA	6:I:500:MET:CE	2.34	0.58
1:Q:210:LEU:HD22	1:Q:231:LEU:HD13	1.85	0.58
1:Y:223:PRO:HD2	1:Y:227:GLN:HG3	1.85	0.58
8:d:89:LEU:C	8:d:89:LEU:HD23	2.29	0.58
5:G:60:MET:SD	5:G:60:MET:C	2.87	0.58
6:I:478:VAL:HG22	6:I:482:LEU:HD12	1.86	0.58
7:J:388:ASN:CG	7:J:388:ASN:O	2.45	0.58
6:K:523:PHE:CE1	6:K:527:ASN:ND2	2.72	0.58
1:Y:186:TYR:OH	1:Y:418:PHE:CE2	2.56	0.58
4:n:574:ILE:CG2	4:n:578:MET:CE	2.81	0.58
4:D:666:PHE:CD2	4:D:764:LEU:HD22	2.39	0.58
3:E:835:ASP:OD1	3:E:839:ARG:HG2	2.03	0.58
1:O:61:ILE:HG23	1:O:62:PRO:HD2	1.86	0.58
5:t:84:LEU:O	5:t:88:MET:SD	2.61	0.58
3:A:765:PHE:CE2	1:O:163:LYS:HD2	2.39	0.58
4:B:865:LEU:HD22	4:B:873:LEU:HD21	1.86	0.58
4:D:725:GLU:OE2	4:D:761:ARG:HB3	2.03	0.58
7:J:281:VAL:HG12	7:J:282:LYS:N	2.18	0.58
1:Y:263:THR:HG23	1:Y:264:PRO:HD2	1.85	0.58
3:k:697:MET:HG2	3:k:737:CYS:SG	2.44	0.58
3:E:686:MET:HE3	3:E:829:PHE:CG	2.39	0.57
7:J:903:THR:HG22	1:X:248:TYR:CZ	2.39	0.57
1:P:189:LEU:HD23	1:P:421:MET:HE2	1.85	0.57
1:2:50:VAL:HG21	1:2:243:LEU:CD1	2.34	0.57
4:D:550:ASN:OD1	4:D:556:LEU:CD2	2.52	0.57
8:d:6:GLN:H	8:d:6:GLN:CD	2.04	0.57
3:A:677:ALA:CA	1:O:264:PRO:CD	2.82	0.57
6:K:263:ILE:HG22	6:K:263:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:541:THR:CG2	4:N:743:ASP:OD1	2.52	0.57
1:Q:218:LEU:HD23	1:Q:220:ILE:HD11	1.87	0.57
4:b:25:GLU:OE1	4:b:25:GLU:N	2.23	0.57
3:k:190:ASP:OD1	3:k:227:GLY:HA2	2.03	0.57
3:E:346:ASP:C	3:E:346:ASP:OD1	2.46	0.57
6:I:569:LEU:HB3	6:I:575:LEU:HG	1.86	0.57
8:L:1673:MET:C	8:L:1673:MET:SD	2.88	0.57
1:R:376:LEU:CB	1:R:378:MET:SD	2.92	0.57
1:T:290:VAL:HG12	1:T:328:VAL:HG21	1.86	0.57
1:U:261:ILE:HD12	1:U:267:HIS:HA	1.85	0.57
4:D:380:THR:HG21	4:D:411:MET:HG3	1.87	0.57
8:L:1681:GLN:HG2	1:Z:249:MET:SD	2.44	0.57
1:O:260:LEU:HD22	1:O:378:MET:CG	2.35	0.57
1:T:362:ARG:O	1:T:362:ARG:HG2	2.05	0.57
1:W:298:LEU:C	1:W:298:LEU:HD23	2.29	0.57
3:k:738:MET:HE1	3:k:748:PHE:CB	2.34	0.57
5:i:88:MET:HE1	5:j:84:LEU:HG	1.87	0.57
1:O:142:ALA:CB	1:O:173:PRO:HG3	2.35	0.57
1:V:440:ARG:HG3	1:V:442:ASP:H	1.69	0.57
1:X:223:PRO:HA	1:X:225:PHE:CE2	2.39	0.57
3:A:536:GLU:HG2	3:A:540:ARG:HH11	1.69	0.57
3:A:538:GLU:C	3:A:540:ARG:H	2.13	0.57
6:I:533:GLN:OE1	6:I:533:GLN:HA	2.05	0.57
6:K:96:VAL:HG21	6:K:175:ILE:HG13	1.87	0.57
3:M:613:LEU:HD22	3:M:752:MET:CE	2.35	0.57
1:O:21:PHE:CD1	1:O:236:MET:HG2	2.39	0.57
1:U:274:THR:HB	1:U:275:PRO:HD3	1.87	0.57
8:L:1553:LEU:CB	8:L:1587:LEU:HD21	2.35	0.57
1:Q:169:TYR:CE2	1:Q:236:MET:HE1	2.40	0.57
1:2:358:VAL:HG23	4:N:724:PHE:CE2	2.40	0.56
4:N:558:HIS:O	4:N:562:MET:HG2	2.04	0.56
1:R:399:ARG:NH2	1:R:421:MET:SD	2.78	0.56
1:X:217:ARG:O	1:X:218:LEU:HD23	2.05	0.56
1:Z:275:PRO:O	1:Z:278:THR:HG22	2.05	0.56
4:D:835:GLU:OE2	4:D:843:MET:HE1	2.05	0.56
4:F:384:LEU:O	4:F:384:LEU:HD23	2.05	0.56
1:O:142:ALA:HB3	1:O:173:PRO:HG3	1.87	0.56
9:a:28:LEU:HG	4:b:81:LEU:HD11	1.87	0.56
6:K:541:PHE:HD1	6:K:564:PHE:CE1	2.23	0.56
1:P:3:ARG:N	1:P:131:SER:HG	2.03	0.56
1:Q:272:GLY:HA2	1:Q:304:MET:SD	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:245:TYR:CD1	1:W:362:ARG:HD3	2.39	0.56
1:Z:219:HIS:CE1	1:Z:220:ILE:HD11	2.36	0.56
4:n:574:ILE:CG2	4:n:578:MET:HE1	2.34	0.56
7:J:266:THR:HG23	7:J:269:GLN:OE1	2.04	0.56
1:P:303:VAL:HG12	1:P:305:VAL:HG22	1.87	0.56
1:R:24:GLN:O	1:R:28:GLU:HG2	2.06	0.56
1:T:62:PRO:HG2	1:T:85:LEU:CD2	2.36	0.56
1:2:50:VAL:HG11	1:2:243:LEU:HG	1.86	0.56
3:A:699:PHE:HE2	1:O:358:VAL:HG23	1.70	0.56
4:N:290:THR:HG21	4:N:366:ARG:CZ	2.35	0.56
1:Q:210:LEU:CD1	1:Q:228:ILE:HG23	2.36	0.56
1:Y:271:THR:HG22	1:Y:378:MET:SD	2.44	0.56
1:W:67:LEU:HD12	1:W:118:ILE:HB	1.87	0.56
3:A:663:LYS:HE3	1:O:200:ASP:C	2.31	0.56
4:B:254:ILE:HB	4:B:258:PHE:CZ	2.40	0.56
3:M:516:ILE:HD13	3:M:638:TYR:CE2	2.40	0.56
4:N:433:TRP:HB2	4:N:439:LEU:HD23	1.87	0.56
1:X:271:THR:CG2	1:X:378:MET:SD	2.94	0.56
3:C:694:GLN:OE1	1:Q:249:MET:HE3	2.06	0.56
3:E:686:MET:CE	3:E:829:PHE:CG	2.89	0.56
4:F:466:LEU:HD12	4:F:468:LYS:HE2	1.87	0.56
4:F:608:THR:HG23	4:F:610:ALA:H	1.71	0.56
1:P:377:MET:HE2	1:P:379:ALA:HB2	1.86	0.56
1:Q:304:MET:SD	1:Q:304:MET:N	2.79	0.56
4:n:574:ILE:HG22	4:n:578:MET:CE	2.36	0.56
1:2:243:LEU:HD21	4:N:575:ARG:NH2	2.20	0.56
4:B:471:ILE:HD12	4:B:475:MET:HE2	1.87	0.56
4:B:685:MET:HE3	1:P:200:ASP:CB	2.35	0.56
3:A:325:TRP:CZ3	3:A:332:MET:HE1	2.41	0.56
4:D:536:ALA:C	4:D:540:GLU:OE2	2.49	0.56
8:L:1607:LYS:HD3	8:L:1608:VAL:N	2.21	0.56
1:O:74:ILE:HG22	1:O:78:LEU:HD23	1.88	0.56
1:Q:320:ILE:HG23	1:Q:377:MET:HE2	1.88	0.56
1:V:39:GLU:N	1:V:39:GLU:OE1	2.39	0.56
9:a:60:LEU:HD23	9:a:60:LEU:H	1.70	0.56
1:1:248:TYR:CE1	3:M:698:MET:SD	2.99	0.55
7:J:963:MET:HA	7:J:963:MET:HE3	1.88	0.55
4:N:667:LEU:HD21	4:N:727:LEU:HD21	1.87	0.55
3:A:663:LYS:HZ3	1:O:267:HIS:CE1	2.24	0.55
3:E:578:MET:HE3	3:E:643:ARG:HD2	1.87	0.55
1:R:169:TYR:CD1	1:R:236:MET:HE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:290:VAL:CG1	1:T:328:VAL:HG21	2.35	0.55
3:A:586:LEU:CD1	5:i:82:TYR:CE1	2.89	0.55
3:A:731:ASP:HB3	5:i:72:LYS:CG	2.35	0.55
4:B:719:GLN:OE1	1:P:249:MET:CE	2.55	0.55
6:I:369:PHE:HE1	6:I:483:LEU:CD1	2.20	0.55
8:L:1634:LEU:CD2	8:L:1681:GLN:NE2	2.70	0.55
8:L:1751:LEU:HA	8:L:1773:MET:HE1	1.89	0.55
1:O:154:LEU:HD11	1:O:166:VAL:HG21	1.89	0.55
1:U:130:ASP:OD2	3:k:561:MET:CE	2.54	0.55
1:V:272:GLY:CA	1:V:304:MET:SD	2.94	0.55
1:Y:269:LEU:CD2	1:Y:380:ASN:HD21	2.19	0.55
4:n:419:LEU:O	4:n:419:LEU:CD2	2.51	0.55
4:n:623:VAL:HG12	4:n:624:ARG:N	2.21	0.55
1:1:323:ILE:HG22	1:1:359:ALA:HB3	1.88	0.55
6:I:25:LEU:HD21	6:I:53:ILE:CD1	2.37	0.55
1:O:262:PRO:HB2	1:O:263:THR:HG23	1.89	0.55
4:b:36:VAL:HG13	8:d:75:PHE:CD2	2.41	0.55
6:I:192:LEU:HA	6:I:300:LEU:HD11	1.88	0.55
6:I:370:GLN:HE21	1:W:251:ASN:ND2	2.03	0.55
3:M:500:LEU:HD22	3:M:717:SER:HA	1.89	0.55
1:S:270:MET:HE1	1:S:305:VAL:HG11	1.87	0.55
4:B:715:ILE:HD12	4:B:718:MET:HE2	1.89	0.55
3:C:325:TRP:CZ3	3:C:332:MET:HE1	2.40	0.55
6:I:367:GLU:H	1:W:47:ARG:HH12	1.52	0.55
1:Q:35:GLY:HA2	1:Q:85:LEU:HD23	1.88	0.55
1:Y:235:ILE:CD1	1:Y:304:MET:SD	2.94	0.55
3:M:157:LYS:C	3:M:160:MET:SD	2.90	0.55
3:M:766:THR:HA	3:M:769:MET:HE3	1.89	0.55
4:B:471:ILE:CD1	4:B:475:MET:HE2	2.36	0.55
4:B:715:ILE:HG23	4:B:718:MET:HE3	1.88	0.55
6:I:357:ILE:CD1	6:I:475:TYR:CZ	2.89	0.55
6:K:190:TRP:CE3	6:K:191:MET:SD	3.00	0.55
1:O:21:PHE:CE2	1:O:236:MET:HE2	2.41	0.55
4:D:430:LEU:C	4:D:430:LEU:HD23	2.31	0.55
4:D:594:GLN:HB2	5:s:60:MET:CE	2.37	0.55
4:F:254:ILE:CG2	4:F:258:PHE:CE1	2.90	0.55
4:F:477:MET:HE2	4:F:477:MET:HA	1.87	0.55
6:I:27:VAL:HG11	6:I:42:LEU:CB	2.37	0.55
7:J:366:TRP:CG	6:K:165:LEU:HD23	2.42	0.55
1:2:186:TYR:CZ	1:2:398:LEU:HD22	2.42	0.55
3:C:439:ILE:HD13	3:C:447:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:578:MET:HE1	4:F:671:LYS:C	2.32	0.55
8:L:1587:LEU:HB3	5:h:60:MET:CE	2.37	0.55
1:Q:377:MET:HE1	1:Q:379:ALA:HB3	1.89	0.55
1:X:413:MET:SD	1:X:414:PHE:N	2.80	0.55
1:2:349:ILE:HG13	1:2:351:TRP:O	2.07	0.54
3:A:693:ILE:HD13	3:A:738:MET:SD	2.47	0.54
4:D:707:LEU:HG	4:D:711:MET:HE3	1.89	0.54
4:D:718:MET:HG2	4:D:876:LEU:HD11	1.89	0.54
3:E:426:LYS:NZ	5:u:85:GLU:CD	2.65	0.54
7:J:557:LYS:HD2	7:J:561:MET:HE3	1.89	0.54
3:M:632:ARG:C	3:M:632:ARG:HD3	2.32	0.54
1:O:67:LEU:HD11	1:O:153:LEU:CD2	2.37	0.54
4:B:865:LEU:HD13	4:B:873:LEU:CD1	2.37	0.54
4:D:620:ARG:CZ	4:D:644:VAL:HG13	2.37	0.54
1:Q:35:GLY:HA2	1:Q:85:LEU:CD2	2.37	0.54
1:T:232:VAL:HG13	1:T:236:MET:CE	2.36	0.54
1:Y:186:TYR:OH	1:Y:418:PHE:HE2	1.90	0.54
5:t:85:GLU:O	5:t:88:MET:HG2	2.06	0.54
3:A:439:ILE:HD13	3:A:447:ALA:HB2	1.88	0.54
4:N:558:HIS:O	4:N:562:MET:HE2	2.06	0.54
1:O:319:ALA:HA	1:O:354:ALA:HB3	1.88	0.54
5:t:60:MET:HE3	5:v:60:MET:CB	2.38	0.54
5:t:60:MET:HE2	5:v:63:PHE:CZ	2.43	0.54
3:A:238:LEU:HD13	3:A:244:ARG:HH21	1.72	0.54
3:A:439:ILE:HD13	3:A:447:ALA:CB	2.38	0.54
4:D:744:LEU:HD11	4:D:748:ILE:HD11	1.90	0.54
3:E:370:SER:OG	3:E:371:GLN:N	2.40	0.54
4:F:370:TRP:CZ3	8:d:153:LEU:HD22	2.43	0.54
7:J:388:ASN:O	7:J:388:ASN:OD1	2.25	0.54
7:J:723:MET:CE	7:J:821:TYR:CD2	2.91	0.54
7:J:992:MET:HA	7:J:992:MET:HE2	1.89	0.54
6:K:344:MET:HE1	6:K:463:LEU:HA	1.89	0.54
1:T:290:VAL:HG23	1:T:294:MET:HE3	1.90	0.54
1:W:67:LEU:HD11	1:W:118:ILE:CD1	2.37	0.54
4:D:257:VAL:HG13	4:D:275:TYR:CE2	2.42	0.54
4:D:594:GLN:CB	5:s:60:MET:HE3	2.36	0.54
4:D:726:VAL:CG1	4:D:758:ILE:HG23	2.36	0.54
1:Q:169:TYR:CZ	1:Q:236:MET:HE1	2.42	0.54
4:n:433:TRP:CE2	4:n:487:GLY:HA3	2.42	0.54
4:n:447:PHE:CZ	4:n:483:VAL:HG21	2.41	0.54
7:J:331:ILE:CB	7:J:365:MET:HE1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:523:PHE:CD1	6:K:527:ASN:ND2	2.75	0.54
8:L:402:GLU:OE1	8:L:402:GLU:N	2.41	0.54
3:M:445:LYS:HB3	3:M:446:MET:HE1	1.89	0.54
1:S:274:THR:HB	1:S:275:PRO:CD	2.38	0.54
1:2:248:TYR:CE2	4:N:722:ILE:HG22	2.42	0.54
4:F:562:MET:HE2	4:F:566:LEU:HD23	1.88	0.54
6:K:379:MET:SD	6:K:379:MET:N	2.66	0.54
1:Y:305:VAL:HG12	1:Y:387:LEU:HD23	1.88	0.54
3:A:758:PHE:CD1	3:A:762:MET:HE3	2.43	0.54
3:E:396:TYR:OH	3:E:475:ILE:HD11	2.08	0.54
6:I:105:LEU:HD11	7:J:400:ASP:CB	2.37	0.54
4:b:25:GLU:H	4:b:25:GLU:CD	2.15	0.54
3:k:579:PRO:HA	3:k:608:LEU:HD13	1.88	0.54
3:k:734:LEU:HD23	3:k:740:THR:OG1	2.07	0.54
4:n:623:VAL:HG13	4:n:638:PHE:CE1	2.42	0.54
3:C:693:ILE:HD13	3:C:738:MET:SD	2.48	0.54
4:D:884:GLU:OE2	4:D:886:TYR:O	2.26	0.54
3:E:186:ALA:HB3	4:F:296:GLU:HG2	1.88	0.54
1:W:19:PHE:CD2	1:W:77:ILE:HG23	2.43	0.54
4:n:762:CYS:HB2	4:n:764:LEU:HD12	1.90	0.54
1:1:305:VAL:HG13	1:1:387:LEU:CD2	2.37	0.54
3:A:526:ASP:OD1	3:A:526:ASP:O	2.25	0.54
3:C:470:PRO:HD2	3:C:494:TYR:CE2	2.43	0.54
6:I:363:LEU:HG	6:I:369:PHE:CD2	2.42	0.54
7:J:723:MET:CE	7:J:821:TYR:CE2	2.90	0.54
4:N:365:ARG:O	4:N:366:ARG:HD2	2.08	0.54
1:P:328:VAL:HG23	1:P:373:VAL:HG13	1.88	0.54
1:Y:305:VAL:HG12	1:Y:384:ILE:HA	1.90	0.54
1:Z:69:LEU:O	1:Z:75:HIS:HE1	1.91	0.54
5:t:60:MET:HE2	5:v:59:ASN:O	2.08	0.54
1:1:190:LEU:HG	1:1:421:MET:SD	2.48	0.53
3:C:439:ILE:HD13	3:C:447:ALA:CB	2.38	0.53
3:C:445:LYS:CG	3:C:446:MET:SD	2.96	0.53
3:C:758:PHE:CD1	3:C:762:MET:HE3	2.43	0.53
7:J:369:TYR:O	7:J:372:PHE:HB2	2.08	0.53
1:Q:210:LEU:HD13	1:Q:228:ILE:HG23	1.88	0.53
1:W:245:TYR:HB3	1:W:362:ARG:CD	2.37	0.53
4:B:868:SER:HB2	4:B:873:LEU:HD23	1.89	0.53
4:D:252:ARG:C	4:D:252:ARG:HD3	2.33	0.53
4:D:550:ASN:OD1	4:D:556:LEU:HD23	2.07	0.53
4:N:546:LEU:HD21	4:N:738:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:71:PRO:O	1:P:72:ARG:C	2.50	0.53
1:Y:294:MET:HG3	1:Y:336:SER:HB2	1.90	0.53
1:2:8:LEU:HB2	1:2:137:LEU:HG	1.89	0.53
3:A:659:TRP:CZ3	1:O:257:ILE:HG21	2.43	0.53
4:F:573:PHE:HB2	4:F:608:THR:HG21	1.90	0.53
6:I:497:ALA:HA	6:I:500:MET:HE1	1.90	0.53
1:O:269:LEU:HB3	1:O:378:MET:SD	2.48	0.53
1:Z:346:ALA:O	1:Z:348:PHE:HD2	1.90	0.53
8:d:67:ARG:HB3	8:d:67:ARG:CZ	2.39	0.53
3:C:387:TYR:CE2	3:C:407:PHE:CZ	2.96	0.53
4:D:475:MET:HE1	4:D:480:SER:CA	2.38	0.53
7:J:897:LEU:HD22	7:J:954:ILE:HD11	1.89	0.53
1:U:260:LEU:CD1	1:U:269:LEU:HD21	2.33	0.53
3:A:308:SER:CB	4:B:365:ARG:CG	2.85	0.53
3:A:387:TYR:CE2	3:A:407:PHE:CZ	2.96	0.53
3:A:445:LYS:CG	3:A:446:MET:SD	2.97	0.53
3:A:691:GLN:HB3	1:O:357:GLN:NE2	2.23	0.53
3:C:482:ARG:HH12	3:C:485:VAL:HG11	1.72	0.53
4:D:297:LEU:HD12	4:D:378:LEU:HD23	1.89	0.53
4:F:476:THR:C	4:F:477:MET:HE2	2.32	0.53
4:F:572:ASP:OD2	1:T:47:ARG:NH2	2.42	0.53
6:I:369:PHE:HE1	6:I:483:LEU:HD12	1.72	0.53
7:J:406:LEU:C	7:J:406:LEU:HD12	2.34	0.53
7:J:835:LYS:HE3	1:X:249:MET:HE2	1.90	0.53
8:L:367:THR:HG22	8:L:369:SER:N	2.24	0.53
3:M:228:VAL:CB	4:N:365:ARG:NH1	2.71	0.53
4:n:806:PHE:CD1	4:n:806:PHE:C	2.87	0.53
1:2:249:MET:HB3	4:N:719:GLN:HB3	1.89	0.53
7:J:365:MET:HE3	7:J:365:MET:HA	1.90	0.53
1:O:210:LEU:HB3	1:O:228:ILE:CD1	2.39	0.53
1:S:272:GLY:HA2	1:S:304:MET:SD	2.49	0.53
3:k:408:MET:HE3	3:k:439:ILE:HG13	1.91	0.53
4:D:255:LEU:HD13	4:D:339:LEU:CD1	2.38	0.53
4:D:436:ASP:OD1	4:D:436:ASP:O	2.26	0.53
3:E:475:ILE:HG23	3:E:484:TYR:HB3	1.88	0.53
7:J:275:LEU:HD21	7:J:382:ILE:HG22	1.91	0.53
7:J:828:LEU:HD11	7:J:902:MET:SD	2.49	0.53
3:M:505:GLU:C	3:M:508:GLU:HG3	2.33	0.53
1:U:189:LEU:HD11	1:U:425:ARG:HA	1.90	0.53
3:A:470:PRO:HD2	3:A:494:TYR:CE2	2.43	0.53
3:A:660:ILE:CG2	1:O:254:ILE:HD11	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:400:VAL:HG13	4:N:419:LEU:HG	1.91	0.53
4:N:718:MET:HE3	4:N:876:LEU:HD11	1.89	0.53
1:P:70:GLU:HB3	1:P:72:ARG:HG3	1.91	0.53
5:t:60:MET:HE1	5:v:59:ASN:O	2.09	0.53
3:A:659:TRP:HA	3:A:680:PHE:CE1	2.44	0.53
3:E:681:THR:HG21	1:S:351:TRP:NE1	2.24	0.53
6:I:450:TRP:CD2	6:I:487:ARG:HD3	2.44	0.53
7:J:498:LYS:O	7:J:502:VAL:HG22	2.09	0.53
1:O:220:ILE:HB	1:O:224:SER:CB	2.38	0.53
1:R:274:THR:HB	1:R:275:PRO:HD3	1.91	0.53
4:B:673:MET:HE2	4:B:676:ILE:CD1	2.39	0.52
6:K:203:PHE:CD1	6:K:203:PHE:O	2.62	0.52
4:N:585:LEU:HB3	4:N:634:GLY:HA3	1.92	0.52
3:A:758:PHE:HD1	3:A:762:MET:HE3	1.74	0.52
4:B:711:MET:HE2	4:B:854:TYR:CG	2.43	0.52
7:J:1017:LEU:C	7:J:1018:MET:HE2	2.33	0.52
4:N:364:LEU:O	4:N:365:ARG:HG3	2.09	0.52
4:N:439:LEU:HD13	4:N:441:ASP:CG	2.33	0.52
1:T:290:VAL:C	1:T:294:MET:HE3	2.34	0.52
1:U:184:GLN:O	1:U:185:PRO:C	2.49	0.52
3:A:231:ARG:HH22	4:B:283:LEU:HD22	1.74	0.52
3:C:445:LYS:HG2	3:C:446:MET:SD	2.49	0.52
4:D:684:HIS:CD2	4:D:789:GLN:HE21	2.27	0.52
3:E:436:GLN:OE1	3:E:436:GLN:HA	2.08	0.52
5:G:69:GLU:C	5:G:69:GLU:OE1	2.53	0.52
8:L:1604:LEU:CB	8:L:1628:PHE:CE2	2.92	0.52
1:O:8:LEU:O	1:O:137:LEU:HD12	2.09	0.52
1:O:210:LEU:HB3	1:O:228:ILE:HD11	1.91	0.52
1:U:22:TRP:CD1	1:U:86:TYR:HH	2.28	0.52
3:E:586:LEU:HD12	3:E:586:LEU:O	2.09	0.52
1:O:21:PHE:CG	1:O:236:MET:HE2	2.44	0.52
1:Z:5:ILE:HD11	1:Z:136:VAL:CG2	2.39	0.52
1:1:21:PHE:CE1	1:1:236:MET:HG2	2.43	0.52
4:B:652:PHE:CD1	4:B:657:MET:HE2	2.44	0.52
4:F:384:LEU:HD21	4:F:400:VAL:CG1	2.39	0.52
5:G:69:GLU:OE2	5:G:70:LEU:HG	2.09	0.52
7:J:839:ASP:OD1	1:X:258:ALA:HB2	2.09	0.52
7:J:902:MET:SD	1:X:248:TYR:HB2	2.50	0.52
6:K:127:ASP:OD1	6:K:128:GLN:N	2.42	0.52
1:S:413:MET:SD	1:S:413:MET:C	2.92	0.52
3:A:445:LYS:HG2	3:A:446:MET:SD	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:683:ARG:HH11	3:A:683:ARG:HG3	1.75	0.52
1:T:223:PRO:O	1:T:224:SER:C	2.52	0.52
1:Z:271:THR:HB	1:Z:304:MET:HE2	1.90	0.52
3:k:697:MET:HE2	3:k:737:CYS:HB3	1.92	0.52
3:E:397:ARG:HG2	3:E:467:VAL:HG22	1.92	0.52
4:F:266:ILE:N	4:F:266:ILE:HD12	2.24	0.52
6:I:38:GLU:OE2	6:I:119:ILE:HD11	2.10	0.52
6:K:500:MET:CE	1:Y:200:ASP:O	2.56	0.52
1:P:328:VAL:CG2	1:P:373:VAL:HG13	2.40	0.52
1:W:117:ASP:C	1:W:117:ASP:OD1	2.52	0.52
1:Y:270:MET:CE	1:Y:377:MET:HE1	2.31	0.52
4:n:762:CYS:C	4:n:764:LEU:H	2.17	0.52
3:A:586:LEU:HD21	5:i:78:LYS:CD	2.40	0.52
3:E:426:LYS:NZ	5:s:80:ARG:NH1	2.58	0.52
1:Y:273:TYR:H	1:Y:304:MET:HE3	1.75	0.52
6:I:509:GLN:CB	6:I:513:ILE:HG22	2.40	0.52
7:J:365:MET:SD	7:J:368:LEU:HD23	2.50	0.52
7:J:889:LYS:HZ3	7:J:890:LEU:HD22	1.75	0.52
1:P:270:MET:HE3	1:P:384:ILE:HB	1.92	0.52
1:X:57:ASP:OD1	1:X:59:HIS:NE2	2.43	0.52
1:X:274:THR:HB	1:X:275:PRO:CD	2.40	0.52
3:A:677:ALA:CB	1:O:264:PRO:HD2	2.33	0.52
3:A:765:PHE:HE2	1:O:163:LYS:HZ2	1.39	0.52
6:I:123:ASN:OD1	6:I:124:TYR:N	2.42	0.52
6:I:370:GLN:HB2	1:W:251:ASN:HD21	1.74	0.52
1:O:21:PHE:CE1	1:O:236:MET:HG2	2.45	0.52
1:O:263:THR:HG21	1:O:351:TRP:CZ3	2.45	0.52
4:b:53:LEU:HD21	4:b:57:LYS:HZ2	1.75	0.52
1:1:117:ASP:OD1	1:1:118:ILE:HG23	2.10	0.51
3:A:482:ARG:NH1	3:A:485:VAL:HG21	2.25	0.51
3:A:659:TRP:CZ2	1:O:257:ILE:HG21	2.45	0.51
3:E:767:GLN:O	3:E:771:LEU:HB2	2.10	0.51
3:M:276:PHE:CD2	3:M:296:MET:HE3	2.46	0.51
1:W:92:TYR:CE2	1:W:117:ASP:OD2	2.63	0.51
1:X:274:THR:HB	1:X:275:PRO:HD3	1.91	0.51
1:2:355:SER:HB3	4:N:882:PHE:HB3	1.91	0.51
3:A:512:HIS:H	3:A:512:HIS:CD2	2.27	0.51
4:F:568:LEU:HD23	4:F:574:ILE:HG21	1.93	0.51
4:F:572:ASP:OD2	1:T:47:ARG:CZ	2.57	0.51
1:Q:22:TRP:CE3	1:Q:62:PRO:HB3	2.46	0.51
1:W:437:ALA:C	1:W:443:TYR:CE1	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:8:LEU:O	1:X:10:LEU:HD23	2.10	0.51
7:J:248:GLN:C	7:J:250:LEU:H	2.18	0.51
7:J:419:GLY:HA3	7:J:439:THR:HG21	1.93	0.51
1:Q:444:ILE:H	1:Q:444:ILE:HD12	1.75	0.51
3:C:758:PHE:HD1	3:C:762:MET:HE3	1.74	0.51
3:E:396:TYR:OH	3:E:475:ILE:CD1	2.58	0.51
7:J:286:ILE:CG1	7:J:300:ILE:HD11	2.41	0.51
3:M:156:LEU:HA	3:M:160:MET:HE1	1.92	0.51
4:N:586:VAL:HA	4:N:635:TRP:HE1	1.75	0.51
4:N:608:THR:HG23	4:N:610:ALA:H	1.74	0.51
1:O:203:VAL:HG22	1:O:378:MET:HE1	1.92	0.51
1:Q:321:LEU:HD23	1:Q:322:ASN:N	2.25	0.51
1:T:62:PRO:HG3	1:T:85:LEU:CD2	2.41	0.51
1:X:8:LEU:O	1:X:10:LEU:CD2	2.59	0.51
3:k:701:VAL:HG13	3:k:736:ASP:HB3	1.92	0.51
3:A:465:HIS:CE1	3:A:502:PHE:HB2	2.46	0.51
3:C:160:MET:HE1	3:C:351:LEU:HB2	1.92	0.51
4:D:840:ILE:HA	4:D:844:CYS:HB3	1.92	0.51
4:F:279:GLY:O	4:F:288:ARG:NH1	2.44	0.51
8:L:469:GLN:HE21	8:L:520:VAL:HG21	1.74	0.51
8:L:1607:LYS:HE2	8:L:1607:LYS:HA	1.91	0.51
1:Q:270:MET:HE2	1:Q:305:VAL:CG2	2.40	0.51
1:X:252:ASP:OD1	1:X:252:ASP:N	2.43	0.51
1:2:47:ARG:NH2	1:2:243:LEU:HD11	2.26	0.51
6:I:38:GLU:OE1	6:I:38:GLU:HA	2.10	0.51
1:P:377:MET:HE2	1:P:379:ALA:HB3	1.91	0.51
3:k:732:THR:HG22	5:t:72:LYS:HZ3	1.75	0.51
4:n:297:LEU:HD12	4:n:378:LEU:HD22	1.92	0.51
1:2:274:THR:HB	1:2:275:PRO:CD	2.41	0.51
5:H:88:MET:SD	5:H:88:MET:C	2.93	0.51
6:I:472:LEU:HA	6:I:475:TYR:HB2	1.92	0.51
1:O:439:THR:O	1:O:439:THR:HG22	2.11	0.51
3:k:697:MET:HE2	3:k:737:CYS:CB	2.41	0.51
4:n:363:THR:O	4:n:367:LEU:N	2.43	0.51
1:2:54:GLN:OE1	1:2:59:HIS:O	2.29	0.51
3:A:304:LEU:HD13	4:B:369:VAL:HG12	1.90	0.51
3:A:677:ALA:HB2	1:O:264:PRO:CD	2.34	0.51
4:B:493:LEU:CD2	4:B:544:TYR:CE2	2.94	0.51
6:I:604:LEU:HG	6:I:606:GLU:HG3	1.93	0.51
4:N:704:CYS:HB2	4:N:847:LEU:HD13	1.93	0.51
1:P:367:LEU:HD23	1:P:367:LEU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:21:PHE:CE1	1:W:236:MET:HG3	2.46	0.51
1:W:28:GLU:HG3	1:W:245:TYR:OH	2.11	0.51
1:Z:248:TYR:CZ	1:Z:249:MET:SD	3.04	0.51
5:t:73:GLU:OE2	5:t:77:LEU:HD22	2.10	0.51
4:B:371:THR:C	4:B:374:PRO:HD2	2.36	0.51
3:E:698:MET:C	3:E:698:MET:HE2	2.36	0.51
1:W:73:VAL:HG13	1:W:74:ILE:CD1	2.40	0.51
1:1:190:LEU:HD23	1:1:421:MET:HG3	1.93	0.51
3:A:656:CYS:SG	1:O:254:ILE:HG12	2.51	0.51
3:C:434:ILE:CG2	3:C:439:ILE:HD11	2.41	0.51
7:J:707:MET:HE2	7:J:922:ASP:C	2.36	0.51
1:O:21:PHE:CD1	1:O:236:MET:SD	3.04	0.51
1:O:61:ILE:CG2	1:O:62:PRO:HD2	2.41	0.51
1:R:303:VAL:CA	1:R:304:MET:HE2	2.40	0.51
1:U:272:GLY:CA	1:U:304:MET:HE2	2.40	0.51
1:S:220:ILE:CB	1:S:224:SER:HB3	2.38	0.50
1:1:248:TYR:CD1	3:M:523:ASP:HB2	2.46	0.50
3:A:658:VAL:O	3:A:659:TRP:C	2.53	0.50
3:C:392:GLU:HB2	3:C:393:LYS:HD2	1.94	0.50
3:E:157:LYS:O	3:E:161:LEU:HD23	2.10	0.50
3:M:522:MET:HE1	3:M:649:LYS:HB2	1.93	0.50
3:A:392:GLU:HB2	3:A:393:LYS:HD2	1.94	0.50
3:E:523:ASP:HB3	1:S:248:TYR:CZ	2.46	0.50
4:F:726:VAL:HG12	4:F:758:ILE:HD12	1.92	0.50
6:K:124:TYR:CD1	6:K:124:TYR:C	2.87	0.50
8:L:1604:LEU:HB2	8:L:1628:PHE:CE2	2.46	0.50
1:S:304:MET:SD	1:S:304:MET:N	2.79	0.50
3:A:659:TRP:CZ3	3:A:663:LYS:HB3	2.46	0.50
4:D:537:ALA:N	4:D:540:GLU:OE2	2.45	0.50
4:D:556:LEU:HD23	4:D:556:LEU:H	1.77	0.50
7:J:413:HIS:ND1	7:J:413:HIS:C	2.69	0.50
7:J:951:LYS:HA	7:J:954:ILE:HG22	1.92	0.50
1:Q:242:THR:HG23	1:Q:243:LEU:HD22	1.92	0.50
1:X:169:TYR:CD2	1:X:236:MET:HE1	2.47	0.50
4:B:493:LEU:HD22	4:B:544:TYR:CE2	2.47	0.50
3:E:740:THR:O	3:E:740:THR:HG22	2.11	0.50
6:K:92:GLY:O	6:K:96:VAL:HG23	2.11	0.50
6:K:203:PHE:O	6:K:203:PHE:CG	2.64	0.50
1:R:270:MET:CE	1:R:305:VAL:HG11	2.41	0.50
9:a:66:GLU:OE2	4:b:34:TYR:CE2	2.65	0.50
3:A:663:LYS:C	1:O:200:ASP:CG	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:522:MET:SD	3:C:698:MET:CE	3.00	0.50
4:F:332:LEU:O	4:F:336:TYR:CD2	2.65	0.50
7:J:302:VAL:HG23	7:J:310:LEU:CD1	2.41	0.50
7:J:366:TRP:CD1	6:K:165:LEU:CD2	2.94	0.50
6:K:128:GLN:OE1	6:K:129:PHE:N	2.44	0.50
4:N:575:ARG:HA	4:N:578:MET:SD	2.52	0.50
1:X:409:ARG:O	1:X:413:MET:HG3	2.12	0.50
1:2:18:GLY:HA2	1:2:21:PHE:CE2	2.46	0.50
3:E:697:MET:SD	3:E:697:MET:N	2.84	0.50
6:I:356:ILE:CG2	6:I:360:PHE:HE2	2.23	0.50
1:R:169:TYR:CE1	1:R:236:MET:HE1	2.47	0.50
1:V:318:ILE:HB	1:V:380:ASN:HB3	1.93	0.50
1:W:214:ALA:HB1	1:W:220:ILE:HG13	1.94	0.50
1:Y:270:MET:HE1	1:Y:377:MET:CE	2.33	0.50
3:A:160:MET:HE1	3:A:351:LEU:HB2	1.92	0.50
3:A:337:ILE:O	3:A:341:LEU:HD12	2.12	0.50
3:E:586:LEU:HD13	5:s:78:LYS:HE2	1.94	0.50
3:M:547:THR:HG23	3:M:547:THR:O	2.12	0.50
4:N:559:MET:CE	4:N:734:LEU:HD21	2.42	0.50
1:T:62:PRO:HG2	1:T:85:LEU:HD22	1.93	0.50
3:k:844:SER:C	3:k:852:MET:CE	2.85	0.50
1:2:349:ILE:C	1:2:351:TRP:H	2.20	0.50
3:A:434:ILE:CG2	3:A:439:ILE:HD11	2.41	0.50
3:A:522:MET:SD	3:A:698:MET:CE	3.00	0.50
3:A:586:LEU:HD12	5:i:82:TYR:CE1	2.46	0.50
3:A:677:ALA:HB3	1:O:443:TYR:CE2	2.47	0.50
4:D:714:PHE:CZ	4:D:718:MET:SD	3.05	0.50
6:I:348:SER:OG	6:I:464:HIS:CE1	2.65	0.50
6:I:414:LEU:HD12	6:I:455:LEU:CD2	2.42	0.50
6:I:455:LEU:HD12	6:I:479:PHE:CE1	2.47	0.50
8:L:1681:GLN:OE1	1:Z:248:TYR:HE2	1.95	0.50
1:R:211:ASN:OD1	1:R:222:ASN:HA	2.12	0.50
1:U:412:ASP:O	1:U:413:MET:HE2	2.11	0.50
1:X:329:ASP:HB2	1:X:330:PRO:HD2	1.94	0.50
1:Z:71:PRO:HA	1:Z:75:HIS:ND1	2.27	0.50
5:j:85:GLU:OE1	5:j:88:MET:HE1	2.12	0.50
1:1:190:LEU:CD2	1:1:421:MET:HG3	2.42	0.49
3:A:663:LYS:HE3	1:O:200:ASP:O	2.13	0.49
4:B:268:MET:HE3	4:B:268:MET:CA	2.33	0.49
3:E:463:CYS:HG	3:E:624:TRP:CD1	2.30	0.49
4:F:623:VAL:HG12	4:F:624:ARG:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:553:MET:HE3	8:L:553:MET:H	1.76	0.49
1:Z:248:TYR:CE2	1:Z:249:MET:SD	3.05	0.49
4:B:526:LEU:C	4:B:528:ASN:H	2.20	0.49
6:I:357:ILE:CD1	6:I:475:TYR:CE2	2.95	0.49
7:J:286:ILE:HG12	7:J:300:ILE:HD13	1.93	0.49
4:N:558:HIS:HB3	4:N:562:MET:HE3	1.94	0.49
4:N:574:ILE:HG22	4:N:578:MET:CE	2.42	0.49
1:Q:270:MET:HE1	1:Q:303:VAL:HB	1.94	0.49
1:Y:204:VAL:CG1	1:Y:384:ILE:HD11	2.42	0.49
3:k:394:TRP:CZ2	3:k:454:GLY:HA3	2.47	0.49
3:k:844:SER:N	3:k:852:MET:HE2	2.26	0.49
4:D:430:LEU:HD22	4:D:431:TYR:CD1	2.47	0.49
4:D:711:MET:HE3	4:D:785:LEU:HD22	1.93	0.49
7:J:281:VAL:CG1	7:J:282:LYS:H	2.21	0.49
1:S:39:GLU:O	1:S:40:PHE:C	2.55	0.49
1:T:290:VAL:HG23	1:T:294:MET:CE	2.43	0.49
1:Z:71:PRO:HA	1:Z:75:HIS:CG	2.48	0.49
3:C:584:THR:HG21	3:C:640:MET:HE2	1.94	0.49
4:F:862:LEU:HD23	4:F:865:LEU:HD23	1.94	0.49
7:J:723:MET:HE2	7:J:821:TYR:CD2	2.47	0.49
8:L:1587:LEU:HB3	5:h:60:MET:HE1	1.93	0.49
4:N:489:SER:HB2	4:N:743:ASP:OD2	2.13	0.49
1:O:237:SER:O	1:O:241:THR:N	2.44	0.49
1:Q:263:THR:HG21	1:Q:266:LEU:HB2	1.94	0.49
1:R:69:LEU:HD22	1:R:149:LEU:CD1	2.42	0.49
1:W:74:ILE:HD12	1:W:77:ILE:HD12	1.93	0.49
3:C:865:TYR:CE2	1:Q:353:PRO:HD3	2.47	0.49
6:I:468:THR:HG22	6:I:469:PRO:HD2	1.94	0.49
6:I:494:HIS:O	6:I:494:HIS:CD2	2.65	0.49
7:J:809:VAL:O	7:J:809:VAL:HG12	2.12	0.49
3:M:497:LYS:O	3:M:501:ASP:HB2	2.12	0.49
1:Y:45:THR:O	1:Y:45:THR:HG22	2.13	0.49
3:k:697:MET:CE	3:k:737:CYS:HB3	2.42	0.49
4:D:702:HIS:HA	4:D:705:HIS:HB2	1.95	0.49
8:L:367:THR:HG22	8:L:368:PHE:N	2.27	0.49
1:U:412:ASP:C	1:U:413:MET:HE2	2.38	0.49
1:W:438:ALA:N	1:W:443:TYR:CE1	2.80	0.49
3:A:663:LYS:NZ	1:O:199:ALA:O	2.30	0.49
4:F:268:MET:HG2	4:F:269:ASN:O	2.13	0.49
4:F:581:LEU:HD21	4:F:600:ILE:HG21	1.94	0.49
6:K:98:GLN:HA	6:K:98:GLN:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:262:ASP:OD1	4:n:263:GLY:N	2.45	0.49
1:1:294:MET:HE3	1:1:336:SER:HB2	1.94	0.49
1:2:298:LEU:HD22	1:2:346:ALA:HB2	1.95	0.49
3:A:308:SER:HB3	4:B:365:ARG:HG2	1.95	0.49
4:F:562:MET:HE2	4:F:566:LEU:CD2	2.43	0.49
7:J:992:MET:C	7:J:994:LEU:N	2.71	0.49
1:Q:382:THR:HG22	1:Q:435:TYR:HE1	1.70	0.49
1:W:141:ILE:HD11	1:W:195:LEU:HD22	1.95	0.49
1:Z:364:SER:O	1:Z:366:TYR:N	2.45	0.49
3:k:448:ASP:N	3:k:448:ASP:OD1	2.44	0.49
1:1:262:PRO:HD2	1:1:266:LEU:HD22	1.94	0.49
4:D:594:GLN:CB	5:s:60:MET:CE	2.91	0.49
3:E:392:GLU:OE1	8:d:141:ARG:NH2	2.42	0.49
3:M:824:LYS:O	3:M:824:LYS:HD3	2.13	0.49
1:O:21:PHE:CG	1:O:236:MET:SD	3.06	0.49
1:S:410:LYS:NZ	1:S:413:MET:HE1	2.27	0.49
1:U:114:ILE:HG22	1:U:114:ILE:O	2.13	0.49
3:A:701:VAL:CG2	3:A:736:ASP:O	2.60	0.49
3:C:337:ILE:O	3:C:341:LEU:HD12	2.12	0.49
8:L:1638:MET:CG	1:Z:249:MET:CE	2.88	0.49
3:M:161:LEU:HD11	3:M:176:ILE:HG22	1.94	0.49
3:M:516:ILE:HD13	3:M:638:TYR:CZ	2.48	0.49
3:M:824:LYS:HD3	3:M:824:LYS:C	2.37	0.49
1:O:220:ILE:CG2	1:O:224:SER:N	2.75	0.49
1:P:381:HIS:N	1:P:435:TYR:OH	2.46	0.49
1:W:90:ASN:OD1	1:W:121:ILE:HD12	2.13	0.49
1:Y:273:TYR:CE2	1:Y:376:LEU:HD12	2.48	0.49
1:Z:5:ILE:HG22	1:Z:51:PHE:HA	1.94	0.49
5:t:60:MET:HE3	5:v:60:MET:HB2	1.95	0.49
3:A:408:MET:HE2	3:A:450:ILE:CG2	2.43	0.48
4:D:754:PHE:CZ	4:D:758:ILE:HD11	2.48	0.48
3:E:446:MET:HE1	3:E:489:GLU:HG2	1.93	0.48
5:G:67:ILE:HD13	5:H:67:ILE:HD13	1.95	0.48
6:I:478:VAL:CG2	6:I:482:LEU:HD12	2.43	0.48
6:I:498:LEU:HD13	1:W:264:PRO:HB3	1.95	0.48
7:J:320:TYR:OH	7:J:406:LEU:HD12	2.13	0.48
6:K:527:ASN:HB2	6:K:531:TYR:CE1	2.47	0.48
3:M:522:MET:HA	3:M:528:PHE:CD2	2.48	0.48
4:b:13:LEU:HD11	4:b:39:ILE:HD13	1.94	0.48
4:b:68:GLU:OE1	4:b:68:GLU:C	2.56	0.48
1:O:21:PHE:CG	1:O:236:MET:CE	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:228:ILE:HG22	1:O:232:VAL:HG23	1.95	0.48
1:P:317:TYR:HE2	1:P:377:MET:HE1	1.77	0.48
1:Q:169:TYR:CD2	1:Q:236:MET:HE1	2.47	0.48
1:Q:377:MET:SD	1:Q:379:ALA:HB2	2.54	0.48
4:n:597:LEU:CD1	4:n:625:LEU:HD21	2.43	0.48
3:A:585:GLN:OE1	5:i:75:PHE:CE1	2.67	0.48
3:A:660:ILE:C	3:A:662:ASN:N	2.71	0.48
4:F:673:MET:HE3	4:F:779:PHE:CG	2.49	0.48
7:J:241:ASN:O	7:J:242:LEU:HB3	2.13	0.48
7:J:770:TYR:N	7:J:771:PRO:CD	2.77	0.48
8:L:1681:GLN:OE1	1:Z:248:TYR:CE2	2.66	0.48
1:U:189:LEU:C	1:U:189:LEU:HD23	2.37	0.48
1:X:243:LEU:HD22	1:X:253:LEU:HD13	1.95	0.48
4:B:477:MET:HE2	4:B:477:MET:HA	1.95	0.48
4:B:873:LEU:HD12	4:B:873:LEU:C	2.39	0.48
4:F:662:ARG:HB3	4:F:764:LEU:HD23	1.95	0.48
8:L:1604:LEU:N	8:L:1628:PHE:HE2	2.11	0.48
3:M:248:VAL:HG22	3:M:257:ARG:HB2	1.96	0.48
1:U:272:GLY:C	1:U:297:LEU:HD11	2.39	0.48
3:k:413:GLU:OE1	3:k:413:GLU:N	2.44	0.48
4:D:410:TYR:CD1	4:D:411:MET:SD	3.05	0.48
4:F:887:LYS:HA	4:F:887:LYS:CE	2.44	0.48
4:F:887:LYS:HA	4:F:887:LYS:HE3	1.95	0.48
6:I:2:ILE:CG1	7:J:242:LEU:HD11	2.42	0.48
6:I:498:LEU:HD12	6:I:499:GLN:N	2.29	0.48
1:T:87:ASN:C	1:T:89:GLU:H	2.21	0.48
1:X:135:PHE:CD2	1:X:157:LEU:HD12	2.48	0.48
4:b:36:VAL:HG13	8:d:75:PHE:HD2	1.77	0.48
1:2:274:THR:HB	1:2:275:PRO:HD3	1.95	0.48
3:C:387:TYR:CZ	3:C:407:PHE:CD1	3.01	0.48
4:D:477:MET:SD	4:D:478:ASP:N	2.87	0.48
3:E:388:PHE:O	3:E:392:GLU:OE2	2.31	0.48
6:I:405:LEU:HD11	6:I:407:ASP:HB3	1.95	0.48
7:J:366:TRP:CG	6:K:165:LEU:CD2	2.97	0.48
7:J:548:MET:SD	7:J:549:VAL:N	2.86	0.48
7:J:890:LEU:HD13	7:J:987:PHE:CE2	2.49	0.48
3:M:160:MET:HE3	3:M:160:MET:H	1.79	0.48
3:M:435:VAL:HB	3:M:438:GLN:OE1	2.13	0.48
1:1:222:ASN:O	1:1:223:PRO:C	2.56	0.48
3:C:408:MET:HE2	3:C:450:ILE:CG2	2.43	0.48
6:I:495:CYS:C	6:I:497:ALA:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:22:TRP:CZ3	1:O:62:PRO:HB3	2.49	0.48
1:X:303:VAL:HG12	1:X:305:VAL:H	1.77	0.48
1:Y:223:PRO:O	1:Y:224:SER:C	2.56	0.48
9:a:66:GLU:CD	4:b:34:TYR:CZ	2.92	0.48
5:v:88:MET:HA	5:v:88:MET:HE2	1.96	0.48
1:1:248:TYR:HA	3:M:523:ASP:HA	1.96	0.48
1:1:409:ARG:NH1	1:1:413:MET:SD	2.86	0.48
1:2:248:TYR:CD1	1:2:248:TYR:C	2.92	0.48
4:D:626:LEU:HD12	4:D:637:VAL:HA	1.96	0.48
4:D:697:PHE:HA	4:D:700:VAL:HG22	1.94	0.48
6:I:328:VAL:HG23	6:I:329:VAL:N	2.27	0.48
8:L:1526:MET:CE	8:L:1631:LEU:HB3	2.43	0.48
1:O:351:TRP:CZ2	1:O:438:ALA:HA	2.48	0.48
1:Q:361:SER:OG	1:Q:362:ARG:N	2.42	0.48
4:F:266:ILE:O	4:F:266:ILE:HG22	2.13	0.48
7:J:320:TYR:CZ	7:J:406:LEU:CD1	2.96	0.48
1:O:203:VAL:CG1	1:O:378:MET:HE1	2.43	0.48
1:W:172:PHE:CD1	1:W:204:VAL:HG13	2.49	0.48
1:Y:222:ASN:HB3	1:Y:223:PRO:HD3	1.95	0.48
4:D:855:GLN:HA	4:D:858:VAL:HG22	1.96	0.48
5:H:60:MET:HA	5:H:63:PHE:CD2	2.49	0.48
6:K:541:PHE:CD1	6:K:564:PHE:CE1	3.02	0.48
4:N:677:LEU:HD21	4:N:782:ILE:HG23	1.94	0.48
4:n:798:GLU:OE2	4:n:802:ARG:NH1	2.47	0.48
5:t:88:MET:HE3	5:t:88:MET:HA	1.94	0.48
4:B:715:ILE:CD1	4:B:718:MET:HE2	2.44	0.47
8:L:540:VAL:HG13	8:L:598:CYS:SG	2.54	0.47
3:A:387:TYR:CZ	3:A:407:PHE:CD1	3.01	0.47
3:A:699:PHE:CE2	1:O:358:VAL:HG23	2.49	0.47
4:N:365:ARG:HD3	4:N:368:LEU:HD11	1.96	0.47
1:R:69:LEU:HD22	1:R:149:LEU:HD12	1.96	0.47
6:I:344:MET:HE3	6:I:554:PHE:CE2	2.48	0.47
1:O:5:ILE:CG2	1:O:136:VAL:HG23	2.44	0.47
1:P:263:THR:HG21	1:P:443:TYR:CZ	2.49	0.47
1:U:186:TYR:CD2	1:U:421:MET:HE1	2.48	0.47
1:V:74:ILE:HD12	1:V:74:ILE:H	1.79	0.47
9:c:30:GLU:OE1	9:c:30:GLU:HA	2.14	0.47
3:k:814:LEU:O	3:k:814:LEU:HD23	2.14	0.47
3:A:525:GLY:O	1:O:251:ASN:HB2	2.14	0.47
7:J:992:MET:HE2	7:J:992:MET:CA	2.44	0.47
1:R:270:MET:HE1	1:R:384:ILE:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:206:ASP:OD2	1:Y:208:THR:HG22	2.14	0.47
4:b:29:ALA:HB3	8:d:67:ARG:HE	1.80	0.47
4:n:839:SER:HA	4:n:842:LYS:HE3	1.96	0.47
3:A:538:GLU:C	3:A:540:ARG:N	2.73	0.47
3:C:701:VAL:CG2	3:C:736:ASP:O	2.60	0.47
1:P:290:VAL:HG11	1:P:332:GLN:CG	2.45	0.47
9:a:35:LEU:HD21	4:b:58:ILE:CD1	2.44	0.47
1:2:262:PRO:O	4:N:709:SER:HB2	2.15	0.47
1:2:305:VAL:O	1:2:306:SER:C	2.57	0.47
3:C:522:MET:SD	3:C:698:MET:HE2	2.55	0.47
1:P:71:PRO:HB3	1:P:93:LEU:HD22	1.96	0.47
1:Q:169:TYR:CE1	1:Q:236:MET:HE1	2.50	0.47
1:Q:377:MET:HE1	1:Q:379:ALA:CB	2.44	0.47
1:R:294:MET:HE1	1:R:322:ASN:HB3	1.96	0.47
3:k:765:PHE:CE2	3:k:769:MET:HE3	2.50	0.47
1:1:92:TYR:CE2	1:1:117:ASP:CG	2.93	0.47
1:2:256:LEU:HD23	1:2:257:ILE:HD12	1.97	0.47
3:A:160:MET:HE1	3:A:351:LEU:CA	2.45	0.47
3:A:387:TYR:CD2	3:A:407:PHE:CE2	3.03	0.47
3:A:442:PHE:HD2	3:A:482:ARG:NH2	2.12	0.47
3:A:494:TYR:CD1	3:A:495:ALA:N	2.83	0.47
3:A:522:MET:SD	3:A:698:MET:HE2	2.55	0.47
3:A:677:ALA:HB3	1:O:443:TYR:HE2	1.80	0.47
4:B:673:MET:CE	4:B:676:ILE:HD13	2.45	0.47
4:B:765:ASP:OD1	4:B:765:ASP:N	2.46	0.47
4:D:289:ASP:OD1	4:D:289:ASP:N	2.46	0.47
4:D:674:GLU:OE1	1:R:249:MET:SD	2.73	0.47
3:E:414:LEU:HD12	3:E:430:GLN:OE1	2.15	0.47
7:J:286:ILE:CG1	7:J:300:ILE:CD1	2.92	0.47
6:K:500:MET:CE	1:Y:200:ASP:HA	2.44	0.47
3:M:865:TYR:OH	3:M:868:ARG:NH2	2.48	0.47
1:Q:215:THR:HG21	1:Q:221:GLN:HB2	1.96	0.47
1:R:28:GLU:OE1	1:R:367:LEU:CD1	2.63	0.47
1:W:25:LEU:HD21	1:W:244:ARG:NH2	2.30	0.47
1:Z:220:ILE:H	1:Z:220:ILE:HG12	1.48	0.47
9:a:66:GLU:CD	4:b:34:TYR:CE2	2.93	0.47
8:d:13:GLU:OE1	8:d:13:GLU:HA	2.13	0.47
4:n:762:CYS:O	4:n:764:LEU:N	2.43	0.47
1:2:351:TRP:CZ2	4:N:706:ILE:HD12	2.49	0.47
3:A:610:LEU:O	3:A:614:GLU:OE2	2.33	0.47
6:K:264:LEU:HD12	6:K:265:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:410:LEU:HD23	8:L:410:LEU:O	2.15	0.47
3:M:504:MET:CE	3:M:714:LYS:HA	2.44	0.47
1:Q:35:GLY:CA	1:Q:85:LEU:HD23	2.45	0.47
1:R:3:ARG:HA	1:R:131:SER:O	2.15	0.47
4:n:259:GLN:OE1	4:n:261:ILE:CD1	2.62	0.47
1:2:243:LEU:HD12	1:2:243:LEU:O	2.15	0.47
4:D:711:MET:CE	4:D:785:LEU:HD22	2.44	0.47
7:J:360:THR:HA	7:J:471:PRO:HG3	1.96	0.47
3:M:467:VAL:HG12	3:M:498:VAL:HG12	1.96	0.47
4:N:497:CYS:HB3	4:N:548:VAL:HG11	1.97	0.47
1:W:235:ILE:HD11	1:W:304:MET:HE3	1.96	0.47
1:W:270:MET:HE3	1:W:303:VAL:HG11	1.97	0.47
3:A:508:GLU:HG3	3:A:510:VAL:HG23	1.96	0.47
3:A:659:TRP:CE3	3:A:663:LYS:HB2	2.50	0.47
3:C:160:MET:HE1	3:C:351:LEU:CA	2.45	0.47
7:J:276:TRP:CE3	6:K:37:SER:HB3	2.49	0.47
7:J:682:THR:O	7:J:683:PHE:CD1	2.67	0.47
3:M:157:LYS:O	3:M:160:MET:SD	2.73	0.47
1:R:437:ALA:HA	1:R:440:ARG:HG2	1.97	0.47
1:V:92:TYR:CG	1:V:93:LEU:N	2.83	0.47
1:W:245:TYR:HB3	1:W:362:ARG:HD2	1.95	0.47
1:X:104:TRP:CH2	1:X:108:PHE:CD1	3.03	0.47
1:Y:273:TYR:CD2	1:Y:376:LEU:HD12	2.50	0.47
1:2:252:ASP:HB3	1:2:255:GLY:HA3	1.96	0.46
3:A:373:GLN:CD	3:A:374:GLU:N	2.73	0.46
3:A:494:TYR:HD1	3:A:495:ALA:N	2.13	0.46
3:C:610:LEU:O	3:C:614:GLU:OE2	2.33	0.46
6:I:100:TYR:CD1	6:I:133:PHE:CZ	3.03	0.46
6:I:106:ASP:OD1	6:I:106:ASP:C	2.58	0.46
7:J:286:ILE:HG12	7:J:300:ILE:HD11	1.97	0.46
8:L:356:VAL:HA	8:L:359:VAL:HB	1.97	0.46
1:P:377:MET:HE1	1:P:379:ALA:HB3	1.97	0.46
1:T:62:PRO:CG	1:T:85:LEU:HD23	2.45	0.46
1:W:291:LEU:CD2	1:W:295:ARG:NH2	2.77	0.46
1:X:223:PRO:O	1:X:224:SER:C	2.58	0.46
3:k:408:MET:HE3	3:k:439:ILE:CD1	2.45	0.46
1:1:92:TYR:CE2	1:1:117:ASP:OD2	2.69	0.46
1:1:186:TYR:O	1:1:421:MET:SD	2.73	0.46
3:C:373:GLN:CD	3:C:374:GLU:N	2.73	0.46
6:I:6:LEU:HD23	6:I:6:LEU:HA	1.83	0.46
8:L:1526:MET:HE1	8:L:1631:LEU:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:1587:LEU:CB	5:h:60:MET:SD	3.02	0.46
1:V:267:HIS:H	1:V:267:HIS:CD2	2.33	0.46
1:Y:186:TYR:CD1	1:Y:421:MET:HE2	2.49	0.46
9:c:27:VAL:HG21	8:d:95:GLU:OE2	2.15	0.46
4:n:578:MET:SD	4:n:668:TRP:CZ3	3.08	0.46
3:A:304:LEU:HD12	4:B:369:VAL:HG12	1.94	0.46
4:B:634:GLY:HA2	4:B:637:VAL:HG12	1.97	0.46
3:C:408:MET:HE1	3:C:447:ALA:HA	1.98	0.46
4:D:725:GLU:OE2	4:D:761:ARG:O	2.33	0.46
6:I:524:LEU:HD13	1:W:353:PRO:HG2	1.96	0.46
8:L:1638:MET:CG	1:Z:249:MET:HE2	2.41	0.46
1:U:260:LEU:HD13	1:U:269:LEU:CD2	2.36	0.46
1:W:405:LEU:HD11	1:W:418:PHE:CE1	2.50	0.46
4:n:663:VAL:O	4:n:667:LEU:HD12	2.15	0.46
3:A:308:SER:HB3	4:B:365:ARG:CG	2.45	0.46
3:A:678:GLY:HA2	3:A:681:THR:HG22	1.97	0.46
3:A:687:LEU:HD21	1:O:259:SER:HA	1.98	0.46
4:B:685:MET:CE	1:P:200:ASP:CG	2.88	0.46
3:C:301:LYS:CG	4:D:372:TYR:CD2	2.96	0.46
6:I:461:TRP:CH2	6:I:465:ILE:HD12	2.49	0.46
7:J:368:LEU:O	7:J:368:LEU:HG	2.16	0.46
3:M:353:GLY:HA3	3:M:438:GLN:O	2.16	0.46
1:O:276:LEU:O	1:O:278:THR:N	2.48	0.46
1:W:297:LEU:HG	1:W:377:MET:CB	2.46	0.46
5:u:76:ASN:O	5:u:76:ASN:OD1	2.32	0.46
4:B:694:MET:HE2	4:B:697:PHE:CD1	2.51	0.46
3:C:445:LYS:HG3	3:C:446:MET:SD	2.55	0.46
4:D:562:MET:CE	4:D:652:PHE:CZ	2.98	0.46
6:I:322:LEU:HD23	6:I:322:LEU:O	2.15	0.46
7:J:365:MET:HE3	7:J:365:MET:C	2.41	0.46
1:S:270:MET:CE	1:S:384:ILE:HD13	2.44	0.46
1:X:371:HIS:HB3	1:X:374:SER:HB3	1.98	0.46
4:b:49:ARG:HB2	4:b:91:TRP:CD2	2.51	0.46
4:n:253:ASP:OD1	4:n:253:ASP:N	2.49	0.46
4:n:574:ILE:O	4:n:578:MET:HE2	2.16	0.46
1:1:266:LEU:HD23	1:1:380:ASN:ND2	2.31	0.46
3:C:387:TYR:CD2	3:C:407:PHE:CE2	3.03	0.46
4:F:472:PRO:HG2	4:F:475:MET:HE3	1.96	0.46
4:F:609:ASN:OD1	1:T:47:ARG:HG2	2.15	0.46
8:L:1511:LEU:HD21	8:L:1611:PRO:HB2	1.96	0.46
8:L:1755:ALA:C	8:L:1767:HIS:HD1	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:364:SER:O	1:P:367:LEU:CD2	2.64	0.46
1:U:273:TYR:N	1:U:304:MET:HE2	2.30	0.46
1:X:57:ASP:OD1	1:X:59:HIS:CE1	2.69	0.46
1:Y:9:GLN:NE2	1:Y:64:ALA:HB1	2.31	0.46
4:b:119:ALA:H	3:k:302:GLU:CG	2.29	0.46
3:k:844:SER:C	3:k:852:MET:SD	2.99	0.46
4:B:685:MET:CE	1:P:200:ASP:CB	2.94	0.46
3:C:701:VAL:HA	3:C:736:ASP:OD2	2.16	0.46
3:E:305:ILE:HG22	8:d:160:VAL:HG11	1.98	0.46
3:E:375:LEU:HD23	3:E:375:LEU:C	2.40	0.46
8:L:555:GLN:OE1	8:L:557:ASN:OD1	2.33	0.46
3:M:205:ILE:HG21	3:M:249:ASP:HB2	1.97	0.46
1:X:217:ARG:C	1:X:218:LEU:HG	2.40	0.46
1:2:139:HIS:NE2	1:2:150:GLY:HA3	2.30	0.46
1:2:353:PRO:HB2	4:N:717:GLN:HE22	1.81	0.46
3:C:494:TYR:CD1	3:C:495:ALA:N	2.83	0.46
3:C:494:TYR:HD1	3:C:495:ALA:N	2.13	0.46
4:D:536:ALA:O	4:D:540:GLU:HG3	2.14	0.46
4:D:550:ASN:CG	4:D:556:LEU:HD22	2.41	0.46
4:D:574:ILE:HB	4:D:578:MET:HE1	1.96	0.46
6:I:379:MET:HE1	6:I:383:PRO:HD2	1.98	0.46
6:I:461:TRP:CZ3	6:I:465:ILE:HA	2.51	0.46
6:I:472:LEU:HD23	6:I:475:TYR:HD2	1.81	0.46
8:L:1553:LEU:HD13	8:L:1587:LEU:HG	1.96	0.46
3:M:765:PHE:CE1	3:M:817:GLY:HA3	2.51	0.46
1:O:134:GLY:HA3	1:O:165:LEU:O	2.16	0.46
4:n:675:TYR:HA	4:n:678:THR:HG22	1.98	0.46
1:2:317:TYR:O	1:2:348:PHE:HA	2.16	0.46
3:A:445:LYS:HG3	3:A:446:MET:SD	2.55	0.46
3:E:309:GLN:OE1	8:d:160:VAL:HG12	2.16	0.46
4:F:334:GLU:OE1	4:F:337:ARG:NH1	2.47	0.46
4:F:411:MET:O	4:F:415:VAL:HG23	2.16	0.46
3:M:522:MET:HA	3:M:528:PHE:CE2	2.51	0.46
4:N:574:ILE:HG22	4:N:578:MET:HE1	1.97	0.46
9:a:66:GLU:OE2	4:b:34:TYR:CZ	2.69	0.46
4:n:574:ILE:HG23	4:n:578:MET:CE	2.45	0.46
4:D:408:ASP:OD2	4:D:411:MET:CE	2.64	0.46
4:D:884:GLU:OE2	4:D:888:ALA:CB	2.64	0.46
7:J:298:ASN:O	7:J:307:HIS:HE1	1.99	0.46
6:K:27:VAL:O	6:K:29:GLN:OE1	2.34	0.46
1:R:261:ILE:HG23	1:R:261:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:305:VAL:CG1	1:Y:384:ILE:HA	2.46	0.46
3:A:641:LEU:HB3	3:A:645:MET:HE2	1.99	0.45
3:A:701:VAL:HA	3:A:736:ASP:OD2	2.16	0.45
4:B:673:MET:HE2	4:B:676:ILE:HD12	1.98	0.45
4:B:673:MET:HE1	4:B:783:ILE:HG13	1.98	0.45
4:D:674:GLU:HG3	1:R:249:MET:CE	2.46	0.45
7:J:891:MET:SD	7:J:891:MET:N	2.89	0.45
8:L:1587:LEU:HD23	8:L:1587:LEU:C	2.41	0.45
1:X:364:SER:HB3	1:X:367:LEU:HD21	1.98	0.45
3:A:742:PRO:HD3	5:i:71:LYS:HE2	1.97	0.45
3:E:286:GLY:HA2	3:E:404:TYR:CD2	2.51	0.45
4:F:308:THR:HG1	4:F:325:CYS:HG	1.62	0.45
7:J:331:ILE:CG2	7:J:365:MET:HE1	2.46	0.45
1:W:266:LEU:HG	1:W:435:TYR:CE1	2.51	0.45
1:W:438:ALA:HA	1:W:443:TYR:CD1	2.51	0.45
1:Y:186:TYR:O	1:Y:421:MET:HE1	2.17	0.45
1:1:220:ILE:HD12	1:1:220:ILE:HA	1.80	0.45
4:B:707:LEU:HD11	4:B:711:MET:HE3	1.99	0.45
4:D:656:CYS:SG	4:D:657:MET:HE2	2.56	0.45
3:E:394:TRP:CE2	3:E:454:GLY:HA3	2.52	0.45
3:E:577:LEU:O	3:E:577:LEU:CD1	2.60	0.45
7:J:723:MET:HE2	7:J:821:TYR:CE2	2.51	0.45
1:P:222:ASN:HB2	1:P:223:PRO:HD3	1.97	0.45
1:P:294:MET:HE1	1:P:337:LEU:HB2	1.98	0.45
1:R:87:ASN:N	1:R:88:PRO:HD3	2.31	0.45
1:Z:172:PHE:CG	1:Z:173:PRO:HD2	2.52	0.45
4:b:34:TYR:CZ	4:b:38:VAL:HG21	2.51	0.45
4:n:414:LEU:C	4:n:414:LEU:HD23	2.40	0.45
4:D:648:ILE:O	4:D:648:ILE:HG22	2.16	0.45
6:I:25:LEU:HB2	6:I:46:CYS:HB3	1.97	0.45
7:J:637:GLU:O	7:J:640:ASP:N	2.47	0.45
6:K:500:MET:SD	6:K:500:MET:C	2.97	0.45
1:P:351:TRP:CE3	1:P:352:GLY:HA3	2.51	0.45
1:Q:210:LEU:HD23	1:Q:210:LEU:HA	1.84	0.45
1:W:248:TYR:O	1:W:249:MET:C	2.60	0.45
1:W:291:LEU:HD21	1:W:295:ARG:HH21	1.80	0.45
1:2:351:TRP:CD1	1:2:444:ILE:HG13	2.51	0.45
4:D:397:ALA:O	4:D:400:VAL:HG13	2.16	0.45
8:L:1526:MET:HE1	8:L:1631:LEU:HB3	1.99	0.45
4:N:569:GLY:HA2	4:N:727:LEU:HD13	1.98	0.45
1:O:225:PHE:O	1:O:228:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:409:ARG:O	1:O:413:MET:HG3	2.17	0.45
1:Q:92:TYR:CG	1:Q:93:LEU:N	2.85	0.45
1:W:297:LEU:HD11	1:W:376:LEU:HA	1.99	0.45
1:W:362:ARG:HH22	1:W:365:PRO:HD3	1.82	0.45
4:n:401:HIS:ND1	4:n:419:LEU:HD11	2.31	0.45
4:B:493:LEU:HD22	4:B:544:TYR:CZ	2.52	0.45
6:K:643:ALA:HB2	1:Y:334:HIS:CE1	2.51	0.45
1:O:184:GLN:N	1:O:185:PRO:HD2	2.31	0.45
1:R:405:LEU:HD12	1:R:421:MET:HE1	1.98	0.45
1:U:245:TYR:O	1:U:246:PRO:C	2.60	0.45
1:W:413:MET:C	1:W:413:MET:SD	3.00	0.45
1:Z:221:GLN:HE21	1:Z:221:GLN:HB3	1.50	0.45
1:1:241:THR:HG23	1:1:245:TYR:CD2	2.51	0.45
3:A:408:MET:HE1	3:A:447:ALA:HA	1.98	0.45
4:F:762:CYS:HB3	4:F:764:LEU:CD1	2.45	0.45
6:I:520:HIS:CE1	1:W:262:PRO:HA	2.51	0.45
7:J:561:MET:CE	7:J:924:ASP:HB3	2.47	0.45
7:J:992:MET:C	7:J:994:LEU:H	2.25	0.45
6:K:105:LEU:HD23	6:K:105:LEU:C	2.41	0.45
8:L:1604:LEU:N	8:L:1628:PHE:CE2	2.84	0.45
1:T:186:TYR:HB3	1:T:421:MET:HE3	1.99	0.45
1:Z:167:GLN:HG2	1:Z:168:THR:H	1.82	0.45
9:a:28:LEU:CG	4:b:81:LEU:HD11	2.47	0.45
4:F:440:GLU:OE1	4:F:440:GLU:O	2.35	0.45
6:K:19:TRP:CH2	6:K:53:ILE:HG21	2.52	0.45
8:L:1525:LEU:C	8:L:1526:MET:HG3	2.41	0.45
4:N:373:ASP:C	4:N:373:ASP:OD1	2.60	0.45
4:N:635:TRP:CE3	4:N:672:ARG:HD3	2.51	0.45
1:O:27:ALA:HA	1:O:39:GLU:HG3	1.98	0.45
1:S:287:LYS:HD3	1:S:288:THR:H	1.81	0.45
1:V:271:THR:OG1	1:V:304:MET:HE1	2.16	0.45
1:Z:167:GLN:HG2	1:Z:168:THR:N	2.32	0.45
4:b:32:PHE:CD1	4:b:36:VAL:HG23	2.51	0.45
1:1:21:PHE:CE2	1:1:236:MET:SD	3.10	0.45
1:2:351:TRP:HE1	1:2:444:ILE:CA	2.28	0.45
4:D:320:VAL:HG21	4:D:393:GLY:N	2.32	0.45
4:D:707:LEU:HD13	4:D:851:THR:HG22	1.98	0.45
6:I:2:ILE:HG21	6:I:111:PHE:CD2	2.51	0.45
6:I:172:LEU:H	6:I:172:LEU:HD12	1.82	0.45
8:L:1691:VAL:HG22	1:Z:330:PRO:HB2	1.98	0.45
1:R:224:SER:C	1:R:226:SER:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:263:THR:OG1	1:V:264:PRO:HD2	2.16	0.45
1:Z:350:PRO:CG	1:Z:354:ALA:HB2	2.47	0.45
4:n:430:LEU:HD11	4:n:483:VAL:HG11	1.98	0.45
4:n:578:MET:SD	4:n:668:TRP:CH2	3.10	0.45
3:A:586:LEU:HD11	5:i:78:LYS:HG2	1.98	0.45
3:C:641:LEU:HB3	3:C:645:MET:HE2	1.99	0.45
4:D:707:LEU:HG	4:D:711:MET:CE	2.46	0.45
7:J:479:TRP:HE1	7:J:534:SER:CB	2.30	0.45
7:J:693:PRO:HA	7:J:696:ASP:HB3	1.99	0.45
7:J:902:MET:HE3	1:X:248:TYR:O	2.17	0.45
1:P:40:PHE:CE2	1:P:366:TYR:HB2	2.52	0.45
1:P:248:TYR:CD1	1:P:249:MET:HE2	2.51	0.45
1:Q:169:TYR:CE2	1:Q:203:VAL:HG21	2.52	0.45
1:T:168:THR:HB	1:T:202:VAL:HG22	1.99	0.45
3:k:734:LEU:HD23	3:k:734:LEU:C	2.42	0.45
1:1:190:LEU:HG	1:1:421:MET:HG3	1.99	0.44
3:A:680:PHE:HB3	1:O:262:PRO:O	2.17	0.44
3:A:731:ASP:HB3	5:i:72:LYS:HD3	1.99	0.44
3:E:578:MET:SD	3:E:643:ARG:HD3	2.57	0.44
4:F:253:ASP:HB3	4:F:266:ILE:HD13	1.99	0.44
4:F:370:TRP:CZ3	8:d:150:CYS:SG	3.10	0.44
7:J:248:GLN:C	7:J:250:LEU:N	2.74	0.44
7:J:331:ILE:CA	7:J:365:MET:HE1	2.44	0.44
8:L:1673:MET:SD	8:L:1673:MET:O	2.75	0.44
3:M:632:ARG:HA	3:M:635:LEU:HG	1.98	0.44
4:N:626:LEU:HD23	4:N:637:VAL:HA	1.98	0.44
1:Q:378:MET:SD	1:Q:379:ALA:N	2.91	0.44
1:Z:4:GLU:C	1:Z:132:LEU:HD13	2.40	0.44
5:g:87:ARG:NH1	5:g:88:MET:HE3	2.32	0.44
5:t:68:THR:C	5:t:69:GLU:OE1	2.59	0.44
3:A:521:LEU:HD23	3:A:645:MET:HE1	1.99	0.44
4:B:868:SER:CB	4:B:873:LEU:HD23	2.46	0.44
3:E:341:LEU:HD11	3:E:359:LEU:HD13	1.99	0.44
4:F:254:ILE:HG23	4:F:258:PHE:CE1	2.53	0.44
6:I:22:ARG:HG2	6:I:23:SER:N	2.32	0.44
6:I:52:TYR:CD1	6:I:100:TYR:CE2	3.05	0.44
6:I:123:ASN:OD1	6:I:123:ASN:C	2.60	0.44
8:L:416:GLN:CD	8:L:416:GLN:H	2.25	0.44
8:L:1526:MET:CE	8:L:1631:LEU:CB	2.96	0.44
3:M:563:THR:C	3:M:565:ASN:N	2.75	0.44
1:O:89:GLU:C	1:O:91:ILE:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:315:HIS:HA	1:P:382:THR:HB	1.98	0.44
1:R:4:GLU:H	1:R:132:LEU:HA	1.82	0.44
1:S:274:THR:HB	1:S:275:PRO:HD3	1.99	0.44
8:d:94:GLU:O	8:d:94:GLU:OE1	2.34	0.44
3:E:217:VAL:CG1	3:E:252:LEU:HD21	2.46	0.44
3:E:578:MET:HE3	3:E:643:ARG:CD	2.47	0.44
4:F:623:VAL:CG1	4:F:624:ARG:N	2.81	0.44
6:I:354:LEU:HD21	6:I:467:PHE:CE1	2.52	0.44
7:J:270:VAL:HG22	7:J:286:ILE:HD13	2.00	0.44
1:V:271:THR:O	1:V:304:MET:SD	2.76	0.44
1:1:274:THR:HG23	1:1:296:ARG:HB3	1.99	0.44
4:D:328:LEU:HD21	4:D:385:VAL:CG1	2.48	0.44
3:E:572:ASP:N	3:E:572:ASP:OD1	2.50	0.44
1:O:25:LEU:O	1:O:26:CYS:HB3	2.17	0.44
1:O:66:LEU:HD23	1:O:78:LEU:CD1	2.46	0.44
1:P:290:VAL:HG11	1:P:332:GLN:HG3	2.00	0.44
1:Q:270:MET:C	1:Q:378:MET:CE	2.90	0.44
1:S:172:PHE:CG	1:S:173:PRO:HD2	2.53	0.44
1:Y:260:LEU:O	1:Y:380:ASN:ND2	2.50	0.44
9:a:67:LEU:CB	4:b:20:ILE:CD1	2.96	0.44
1:2:221:GLN:O	1:2:222:ASN:C	2.60	0.44
3:C:521:LEU:HD23	3:C:645:MET:HE1	1.99	0.44
4:F:373:ASP:OD1	4:F:410:TYR:OH	2.27	0.44
6:I:92:GLY:C	6:I:94:ASP:H	2.24	0.44
3:M:700:GLU:HB3	3:M:701:VAL:H	1.68	0.44
4:N:881:ASP:HB2	4:N:886:TYR:CD2	2.52	0.44
1:O:53:TYR:O	1:O:60:TYR:HA	2.17	0.44
1:T:290:VAL:O	1:T:294:MET:HE3	2.17	0.44
1:X:222:ASN:O	1:X:225:PHE:CE1	2.71	0.44
5:g:58:ARG:HD2	5:g:60:MET:H	1.82	0.44
5:g:62:ASP:OD1	5:g:62:ASP:N	2.50	0.44
4:n:663:VAL:HG12	4:n:667:LEU:HD12	1.99	0.44
3:A:350:CYS:HB3	3:A:355:THR:OG1	2.17	0.44
3:A:387:TYR:CE2	3:A:407:PHE:CD1	3.06	0.44
4:B:870:ASP:N	4:B:870:ASP:OD1	2.50	0.44
7:J:811:ILE:HG21	7:J:923:LEU:HD11	1.99	0.44
7:J:889:LYS:NZ	7:J:890:LEU:HD22	2.33	0.44
8:L:407:TYR:CD1	8:L:407:TYR:C	2.96	0.44
1:S:224:SER:HA	1:S:227:GLN:HG2	2.00	0.44
5:t:68:THR:HG23	5:t:69:GLU:OE2	2.17	0.44
3:A:659:TRP:CZ3	3:A:663:LYS:CB	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:350:CYS:HB3	3:C:355:THR:OG1	2.17	0.44
4:D:691:LEU:HD21	4:D:701:LEU:HD11	1.98	0.44
3:E:175:PRO:HG2	3:E:283:PHE:CD1	2.53	0.44
5:H:60:MET:HA	5:H:63:PHE:CE2	2.52	0.44
6:I:105:LEU:HD22	7:J:396:ALA:O	2.18	0.44
6:I:367:GLU:H	1:W:47:ARG:NH1	2.16	0.44
6:I:469:PRO:O	6:I:470:ALA:HB3	2.18	0.44
3:M:838:ALA:HB1	3:M:871:ARG:HB2	1.99	0.44
1:P:382:THR:HA	1:P:435:TYR:CE1	2.53	0.44
1:Q:271:THR:HB	1:Q:378:MET:CE	2.48	0.44
1:W:47:ARG:HD2	1:W:243:LEU:O	2.16	0.44
5:t:69:GLU:N	5:t:69:GLU:CD	2.75	0.44
1:2:54:GLN:OE1	1:2:58:GLU:C	2.61	0.44
3:A:380:THR:HG21	3:A:477:TYR:CE1	2.53	0.44
3:C:400:ILE:HG13	3:C:402:ASP:H	1.83	0.44
3:E:696:TYR:O	3:E:697:MET:C	2.61	0.44
3:E:701:VAL:CG1	3:E:733:CYS:HA	2.48	0.44
6:K:525:VAL:CG1	6:K:586:ILE:HD12	2.45	0.44
1:S:190:LEU:CD1	1:S:421:MET:HE2	2.41	0.44
1:S:316:CYS:HB3	1:S:348:PHE:HA	2.00	0.44
1:S:351:TRP:CZ3	1:S:444:ILE:HG22	2.53	0.44
1:T:62:PRO:HD2	1:T:86:TYR:HA	1.98	0.44
1:2:54:GLN:OE1	1:2:59:HIS:C	2.60	0.44
3:C:522:MET:CE	3:C:698:MET:CE	2.96	0.44
7:J:723:MET:HE3	7:J:821:TYR:CE2	2.53	0.44
6:K:474:LYS:HD3	6:K:565:LEU:HD22	2.00	0.44
4:N:465:THR:HG22	4:N:466:LEU:H	1.83	0.44
1:O:220:ILE:HB	1:O:224:SER:HB3	1.99	0.44
1:V:271:THR:C	1:V:304:MET:CE	2.91	0.44
1:Z:400:LYS:C	1:Z:401:ARG:HD3	2.43	0.44
9:a:25:MET:HE1	9:a:48:VAL:HG11	1.99	0.44
3:A:586:LEU:CD2	5:i:78:LYS:CD	2.96	0.43
4:B:264:LYS:HA	4:B:264:LYS:HD2	1.70	0.43
4:B:268:MET:SD	4:B:275:TYR:CZ	3.11	0.43
4:D:734:LEU:O	4:D:738:VAL:HG12	2.18	0.43
6:K:333:ARG:NH1	6:K:334:SER:OG	2.50	0.43
3:M:546:ILE:HD11	3:M:551:LEU:HD21	1.99	0.43
1:S:169:TYR:CD2	1:S:236:MET:SD	3.11	0.43
1:V:67:LEU:O	1:V:67:LEU:CD2	2.56	0.43
1:X:224:SER:O	1:X:225:PHE:C	2.61	0.43
9:c:19:ASN:OD1	9:c:22:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:543:VAL:HG13	3:k:544:GLU:HG2	2.00	0.43
3:k:683:ARG:HG2	3:k:683:ARG:HH21	1.82	0.43
4:n:254:ILE:HA	4:n:257:VAL:HG22	2.00	0.43
4:n:433:TRP:CZ2	4:n:487:GLY:HA3	2.53	0.43
1:2:362:ARG:HH12	4:N:563:ARG:HH22	1.64	0.43
3:A:586:LEU:HD21	5:i:78:LYS:HD2	1.99	0.43
3:C:380:THR:HG21	3:C:477:TYR:CE1	2.53	0.43
6:I:284:GLN:O	6:I:285:MET:SD	2.76	0.43
6:I:415:HIS:CE1	6:I:416:LEU:O	2.71	0.43
1:S:413:MET:SD	1:S:413:MET:O	2.76	0.43
1:V:271:THR:C	1:V:304:MET:HE1	2.44	0.43
4:n:663:VAL:HG12	4:n:667:LEU:CD1	2.48	0.43
1:1:4:GLU:HG3	1:1:50:VAL:HG22	2.00	0.43
3:C:387:TYR:CE2	3:C:407:PHE:CD1	3.06	0.43
4:D:711:MET:HE3	4:D:785:LEU:CD2	2.48	0.43
4:F:614:SER:OG	4:F:616:GLU:OE1	2.32	0.43
4:F:762:CYS:CB	4:F:764:LEU:HD13	2.45	0.43
6:I:263:ILE:HG22	6:I:263:ILE:O	2.18	0.43
1:O:28:GLU:OE1	1:O:367:LEU:HD12	2.18	0.43
1:P:292:ASP:OD2	1:P:295:ARG:NH2	2.48	0.43
1:W:25:LEU:HD22	1:W:244:ARG:NH2	2.34	0.43
1:Z:10:LEU:O	1:Z:14:GLY:HA3	2.18	0.43
9:c:31:ILE:HG21	8:d:93:VAL:CG1	2.48	0.43
3:k:815:VAL:HA	3:k:819:GLU:HB2	1.99	0.43
3:A:276:PHE:CD1	3:A:296:MET:HE2	2.53	0.43
3:A:522:MET:CE	3:A:698:MET:CE	2.96	0.43
3:E:186:ALA:CB	4:F:296:GLU:CD	2.92	0.43
3:E:502:PHE:CZ	3:E:507:LYS:HE3	2.53	0.43
7:J:811:ILE:CG2	7:J:923:LEU:HD11	2.47	0.43
6:K:541:PHE:CE1	6:K:564:PHE:CZ	3.06	0.43
1:O:274:THR:HG21	1:O:296:ARG:HB2	2.01	0.43
1:Z:252:ASP:OD1	1:Z:252:ASP:N	2.47	0.43
5:i:72:LYS:HB3	5:i:72:LYS:HE3	1.82	0.43
4:n:805:GLN:O	4:n:809:LYS:HB3	2.19	0.43
3:A:505:GLU:H	3:A:505:GLU:HG3	1.67	0.43
4:B:544:TYR:CD1	4:B:544:TYR:C	2.96	0.43
4:B:680:ILE:HG23	4:B:684:HIS:CE1	2.53	0.43
3:C:276:PHE:CD1	3:C:296:MET:HE2	2.53	0.43
4:D:674:GLU:CD	1:R:249:MET:SD	3.01	0.43
4:D:744:LEU:HD12	4:D:744:LEU:O	2.18	0.43
4:D:854:TYR:O	4:D:858:VAL:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:586:LEU:HD11	5:s:78:LYS:HG2	2.01	0.43
4:F:384:LEU:HD23	4:F:384:LEU:C	2.44	0.43
7:J:366:TRP:HB2	6:K:165:LEU:HD21	1.99	0.43
3:M:445:LYS:HB3	3:M:446:MET:CE	2.48	0.43
3:M:461:ARG:NH1	3:M:467:VAL:O	2.52	0.43
1:O:207:ASN:HB3	1:O:225:PHE:HE1	1.83	0.43
1:U:184:GLN:HG3	1:U:185:PRO:HD3	2.01	0.43
1:X:217:ARG:HG2	1:X:220:ILE:HD11	2.01	0.43
1:Z:69:LEU:CD1	1:Z:92:TYR:HD2	2.31	0.43
4:b:32:PHE:CE1	4:b:36:VAL:HG23	2.54	0.43
3:A:407:PHE:CD1	3:A:408:MET:HB2	2.53	0.43
3:A:503:LEU:HA	3:A:506:GLU:O	2.17	0.43
3:A:660:ILE:O	3:A:662:ASN:N	2.52	0.43
4:D:550:ASN:CG	4:D:556:LEU:CD2	2.92	0.43
3:E:414:LEU:HD23	3:E:414:LEU:C	2.43	0.43
3:E:414:LEU:HD12	3:E:430:GLN:HB2	2.00	0.43
3:E:698:MET:SD	3:E:699:PHE:N	2.92	0.43
5:H:60:MET:HG3	5:H:63:PHE:CD2	2.54	0.43
6:I:468:THR:HG22	6:I:469:PRO:CD	2.48	0.43
6:K:582:CYS:O	6:K:586:ILE:HG23	2.18	0.43
1:P:272:GLY:HA3	1:P:377:MET:SD	2.58	0.43
1:S:388:PHE:HB2	1:S:432:ILE:HD11	2.00	0.43
3:k:814:LEU:HD23	3:k:818:PHE:HD2	1.84	0.43
3:A:306:LEU:HD23	3:A:306:LEU:C	2.44	0.43
3:A:470:PRO:HD2	3:A:494:TYR:CD2	2.53	0.43
3:A:679:ALA:HB2	3:A:818:PHE:HZ	1.84	0.43
6:I:363:LEU:HG	6:I:369:PHE:CE2	2.53	0.43
1:O:3:ARG:HA	1:O:131:SER:O	2.18	0.43
1:O:66:LEU:HD23	1:O:78:LEU:HD11	2.00	0.43
1:P:112:GLU:HB2	1:P:152:TYR:CE2	2.54	0.43
1:R:28:GLU:OE2	1:R:237:SER:OG	2.33	0.43
1:U:293:VAL:HA	1:U:296:ARG:HG3	2.01	0.43
3:E:482:ARG:HA	3:E:482:ARG:HE	1.83	0.43
3:M:486:GLU:O	3:M:489:GLU:HG3	2.18	0.43
1:O:74:ILE:HG22	1:O:78:LEU:CD2	2.49	0.43
1:P:76:SER:O	1:P:80:SER:HB3	2.19	0.43
1:U:338:GLN:HB3	1:U:342:GLU:OE2	2.19	0.43
1:Z:215:THR:N	1:Z:221:GLN:HE22	2.17	0.43
9:a:41:MET:SD	9:a:41:MET:O	2.77	0.43
8:d:66:ALA:O	8:d:70:ILE:HG12	2.18	0.43
4:n:806:PHE:CD2	4:n:829:GLU:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:65:VAL:HA	1:1:90:ASN:HB2	2.01	0.43
3:A:586:LEU:HD21	5:i:78:LYS:HG2	2.00	0.43
3:A:659:TRP:HA	3:A:680:PHE:HE1	1.81	0.43
4:B:415:VAL:HA	4:B:418:ILE:HG22	2.01	0.43
4:B:456:THR:C	4:B:458:ARG:H	2.26	0.43
4:B:865:LEU:CD1	4:B:873:LEU:HD11	2.45	0.43
4:D:433:TRP:CE2	4:D:487:GLY:HA3	2.54	0.43
4:D:537:ALA:HA	4:D:540:GLU:OE2	2.19	0.43
6:I:468:THR:CG2	6:I:469:PRO:HD2	2.48	0.43
6:K:94:ASP:OD1	6:K:101:ARG:NH2	2.46	0.43
3:M:583:ILE:HB	5:g:83:PHE:CE1	2.54	0.43
3:M:703:GLU:O	3:M:704:PRO:C	2.61	0.43
1:P:324:ILE:HG21	1:P:328:VAL:HG11	2.01	0.43
1:P:351:TRP:CD2	1:P:352:GLY:N	2.87	0.43
1:U:413:MET:HE2	1:U:413:MET:CA	2.49	0.43
1:1:10:LEU:HD12	1:1:137:LEU:HD23	2.01	0.43
3:A:304:LEU:HD13	4:B:369:VAL:CG1	2.48	0.43
4:B:365:ARG:HB3	4:B:369:VAL:HG22	2.00	0.43
3:E:426:LYS:O	3:E:430:GLN:OE1	2.37	0.43
3:E:464:GLY:C	3:E:465:HIS:CG	2.96	0.43
6:I:354:LEU:HD21	6:I:467:PHE:HE1	1.84	0.43
7:J:479:TRP:HE1	7:J:534:SER:HB2	1.84	0.43
8:L:469:GLN:NE2	8:L:520:VAL:HG21	2.34	0.43
8:L:1576:HIS:ND1	8:L:1576:HIS:N	2.67	0.43
8:L:1610:TRP:CD2	8:L:1610:TRP:C	2.96	0.43
3:M:719:ILE:HA	3:M:722:VAL:HB	2.01	0.43
3:M:761:CYS:O	3:M:762:MET:HE2	2.18	0.43
4:N:411:MET:O	4:N:415:VAL:HG12	2.19	0.43
4:N:460:TRP:CZ3	4:N:492:PHE:HB2	2.54	0.43
1:U:365:PRO:O	1:U:366:TYR:CG	2.72	0.43
1:W:25:LEU:HD23	1:W:25:LEU:HA	1.69	0.43
1:2:248:TYR:CD2	4:N:727:LEU:HD12	2.54	0.42
3:A:226:VAL:HG12	3:A:227:GLY:N	2.34	0.42
3:A:659:TRP:CD1	1:O:254:ILE:CG1	2.98	0.42
4:D:666:PHE:CD2	4:D:764:LEU:CD2	3.01	0.42
8:L:1663:PHE:CD2	8:L:1756:TRP:CZ2	3.06	0.42
1:S:28:GLU:HA	1:S:367:LEU:HD22	2.01	0.42
1:S:32:SER:OG	1:S:38:GLU:HA	2.18	0.42
1:S:190:LEU:HD21	1:S:421:MET:HG2	2.00	0.42
1:S:377:MET:C	1:S:377:MET:SD	3.02	0.42
1:Z:112:GLU:HA	1:Z:152:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:k:307:VAL:O	3:k:307:VAL:HG22	2.19	0.42
1:1:270:MET:SD	1:1:305:VAL:HB	2.59	0.42
1:2:220:ILE:HD12	1:2:220:ILE:HA	1.79	0.42
3:C:407:PHE:CD1	3:C:408:MET:HB2	2.53	0.42
3:C:470:PRO:HD2	3:C:494:TYR:CD2	2.53	0.42
3:E:748:PHE:O	3:E:752:MET:HG2	2.19	0.42
6:K:289:GLN:OE1	6:K:289:GLN:HA	2.19	0.42
8:L:568:TYR:CD2	8:L:569:TRP:CD1	3.07	0.42
3:M:521:LEU:HD23	3:M:642:PHE:HB2	2.00	0.42
4:N:562:MET:HE1	4:N:642:TYR:HD2	1.83	0.42
1:Q:377:MET:HE2	1:Q:379:ALA:HB2	1.99	0.42
1:S:203:VAL:HG11	1:S:378:MET:CE	2.49	0.42
1:V:393:ARG:HG2	1:V:397:LYS:HZ2	1.84	0.42
1:X:8:LEU:HD22	1:X:122:ILE:HD12	2.01	0.42
3:C:328:ILE:HD12	3:C:332:MET:HE2	2.01	0.42
6:K:474:LYS:HD3	6:K:565:LEU:CD2	2.49	0.42
8:L:1681:GLN:NE2	1:Z:249:MET:CE	2.82	0.42
4:N:325:CYS:O	4:N:329:HIS:ND1	2.52	0.42
4:N:717:GLN:HG3	4:N:880:LEU:HA	2.01	0.42
1:X:39:GLU:CD	1:X:39:GLU:N	2.77	0.42
1:Z:333:VAL:HG11	1:Z:360:LEU:HD11	2.01	0.42
1:Z:411:GLU:OE2	1:Z:415:LYS:NZ	2.49	0.42
4:n:562:MET:CE	4:n:657:MET:HE1	2.48	0.42
1:2:21:PHE:HE2	1:2:138:CYS:SG	2.42	0.42
1:2:139:HIS:HB3	1:2:170:SER:HB3	2.00	0.42
3:A:328:ILE:HD12	3:A:332:MET:HE2	2.01	0.42
3:C:306:LEU:HD23	3:C:306:LEU:C	2.44	0.42
3:C:482:ARG:HH22	3:C:485:VAL:HG21	1.85	0.42
3:E:263:ILE:CD1	3:E:328:ILE:HG21	2.50	0.42
4:F:887:LYS:HE3	4:F:887:LYS:CA	2.49	0.42
6:I:468:THR:O	6:I:469:PRO:C	2.62	0.42
7:J:886:LEU:HD12	7:J:890:LEU:HD23	2.02	0.42
7:J:893:PHE:CD2	7:J:894:VAL:N	2.87	0.42
8:L:1585:LYS:HE2	8:L:1585:LYS:HA	2.00	0.42
3:M:408:MET:HE2	3:M:450:ILE:HG22	2.02	0.42
3:M:421:GLU:HA	3:M:627:SER:HB3	2.01	0.42
3:M:701:VAL:HG22	3:M:851:GLY:HA2	2.01	0.42
9:a:30:GLU:OE1	9:a:30:GLU:HA	2.18	0.42
3:k:647:TYR:HD1	3:k:647:TYR:HA	1.74	0.42
4:n:806:PHE:C	4:n:806:PHE:HD1	2.28	0.42
1:2:227:GLN:H	1:2:227:GLN:HG2	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:258:PHE:CD1	4:B:258:PHE:N	2.86	0.42
4:B:726:VAL:HG22	4:B:761:ARG:HB3	2.01	0.42
3:C:408:MET:HE2	3:C:450:ILE:HG21	2.02	0.42
3:C:446:MET:HA	3:C:446:MET:HE3	2.02	0.42
3:E:530:HIS:CD2	1:S:47:ARG:NH1	2.82	0.42
7:J:296:VAL:HG12	7:J:314:LEU:HB2	2.00	0.42
7:J:426:ASP:O	7:J:427:THR:HG23	2.19	0.42
7:J:736:TYR:CZ	1:X:252:ASP:HB3	2.55	0.42
8:L:1574:THR:H	8:L:1577:ALA:HB3	1.83	0.42
3:M:662:ASN:ND2	3:M:769:MET:HE1	2.34	0.42
4:N:797:LEU:HD22	4:N:797:LEU:HA	1.68	0.42
1:O:270:MET:HE2	1:O:379:ALA:HB3	2.02	0.42
1:R:62:PRO:HD2	1:R:86:TYR:HA	2.01	0.42
1:W:297:LEU:HD21	1:W:376:LEU:C	2.44	0.42
3:k:536:GLU:OE2	3:k:537:GLU:OE1	2.37	0.42
1:2:53:TYR:CG	1:2:54:GLN:N	2.88	0.42
3:A:408:MET:HE2	3:A:450:ILE:HG21	2.02	0.42
4:B:493:LEU:HD21	4:B:544:TYR:CE2	2.54	0.42
3:E:190:ASP:H	3:E:227:GLY:HA3	1.85	0.42
7:J:296:VAL:O	7:J:297:ARG:CB	2.67	0.42
7:J:963:MET:HE3	7:J:963:MET:CA	2.48	0.42
6:K:275:LYS:HD2	6:K:333:ARG:HD3	2.02	0.42
3:M:752:MET:HE3	3:M:756:VAL:CG2	2.50	0.42
1:T:384:ILE:O	1:T:384:ILE:HG22	2.20	0.42
9:a:72:GLU:OE2	9:a:75:LYS:NZ	2.50	0.42
4:n:277:VAL:HG12	4:n:278:GLU:N	2.35	0.42
1:1:270:MET:CE	1:1:305:VAL:HB	2.50	0.42
1:1:356:ILE:HG22	1:1:358:VAL:HG13	2.01	0.42
3:A:677:ALA:CB	1:O:264:PRO:CD	2.97	0.42
4:B:673:MET:HE2	4:B:676:ILE:HD13	2.01	0.42
6:I:38:GLU:OE1	6:I:38:GLU:CA	2.68	0.42
3:M:833:LEU:HA	3:M:836:LEU:CD2	2.50	0.42
4:N:489:SER:CB	4:N:743:ASP:OD2	2.67	0.42
1:P:40:PHE:CZ	1:P:366:TYR:HB2	2.54	0.42
1:T:220:ILE:HG23	1:T:223:PRO:HB2	2.01	0.42
5:t:60:MET:CE	5:v:60:MET:HA	2.49	0.42
1:2:105:ALA:HB3	1:2:411:GLU:CD	2.45	0.42
3:A:408:MET:HE2	3:A:450:ILE:HB	2.02	0.42
3:A:661:SER:CB	3:A:763:GLN:HE21	2.32	0.42
6:I:5:LEU:HA	6:I:17:PHE:CZ	2.54	0.42
6:I:192:LEU:O	6:I:300:LEU:HD21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:379:MET:HE1	6:I:383:PRO:CD	2.49	0.42
6:I:471:VAL:HG12	6:I:471:VAL:O	2.20	0.42
6:K:468:THR:O	6:K:471:VAL:HG22	2.20	0.42
3:M:689:PHE:CZ	3:M:748:PHE:CE2	3.08	0.42
4:N:710:GLU:CD	4:N:855:GLN:CG	2.89	0.42
1:O:175:GLN:HG3	1:O:225:PHE:HZ	1.84	0.42
1:O:409:ARG:HH21	1:O:409:ARG:HG3	1.84	0.42
1:R:225:PHE:C	1:R:227:GLN:N	2.78	0.42
1:S:203:VAL:HG11	1:S:378:MET:HE1	2.00	0.42
1:U:3:ARG:HA	1:U:131:SER:O	2.19	0.42
8:d:83:GLY:N	8:d:84:PRO:HD2	2.34	0.42
4:n:528:ASN:O	4:n:529:ALA:HB3	2.20	0.42
4:n:597:LEU:HB3	4:n:623:VAL:HG11	2.01	0.42
1:2:256:LEU:O	1:2:256:LEU:HG	2.18	0.42
4:B:286:SER:O	4:B:366:ARG:NH2	2.52	0.42
3:C:226:VAL:HG12	3:C:227:GLY:N	2.34	0.42
4:D:475:MET:HE3	4:D:475:MET:HB2	1.88	0.42
8:L:1563:SER:O	8:L:1567:GLN:HG2	2.20	0.42
3:M:390:VAL:HG11	3:M:403:PRO:HD3	2.01	0.42
3:M:436:GLN:O	3:M:439:ILE:HG13	2.20	0.42
1:P:135:PHE:CE1	1:P:157:LEU:HD12	2.55	0.42
1:S:224:SER:O	1:S:228:ILE:HG13	2.20	0.42
1:U:271:THR:CG2	1:U:378:MET:HE1	2.45	0.42
1:X:10:LEU:HD21	1:X:137:LEU:HG	2.02	0.42
1:Z:212:ARG:O	1:Z:213:ILE:C	2.63	0.42
1:1:3:ARG:HG2	1:1:131:SER:HB2	2.02	0.42
3:A:234:SER:OG	3:A:235:ALA:N	2.53	0.42
3:C:522:MET:SD	3:C:698:MET:HE1	2.60	0.42
3:E:341:LEU:HD11	3:E:359:LEU:CD1	2.50	0.42
3:E:426:LYS:HZ1	5:s:80:ARG:HH11	1.67	0.42
3:E:561:MET:O	1:S:47:ARG:NE	2.52	0.42
6:I:38:GLU:CD	6:I:119:ILE:HD11	2.44	0.42
6:I:524:LEU:HD13	1:W:353:PRO:HB2	2.02	0.42
7:J:419:GLY:CA	7:J:439:THR:HG21	2.49	0.42
6:K:98:GLN:HB3	6:K:99:PRO:HD3	2.02	0.42
3:M:643:ARG:H	3:M:643:ARG:HG3	1.47	0.42
1:R:217:ARG:O	1:R:218:LEU:HD22	2.20	0.42
1:S:203:VAL:CG1	1:S:378:MET:HE2	2.50	0.42
1:T:320:ILE:HB	1:T:356:ILE:HD13	2.01	0.42
1:Y:9:GLN:HE22	1:Y:64:ALA:HB1	1.85	0.42
1:Y:139:HIS:CE1	1:Y:168:THR:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:190:LEU:CG	1:1:421:MET:HG3	2.50	0.41
1:1:262:PRO:HB3	3:M:684:GLN:CB	2.50	0.41
3:C:394:TRP:CE3	3:C:400:ILE:HD13	2.55	0.41
6:I:259:LEU:HD11	6:I:273:ALA:HB1	2.02	0.41
6:I:367:GLU:CB	1:W:47:ARG:NH1	2.83	0.41
8:L:506:TYR:CD1	8:L:585:PRO:HG3	2.55	0.41
1:P:382:THR:HA	1:P:435:TYR:CD1	2.55	0.41
1:Q:21:PHE:CG	1:Q:236:MET:HG2	2.55	0.41
1:Q:263:THR:HG23	1:Q:266:LEU:H	1.84	0.41
1:S:229:ASN:HA	1:S:232:VAL:HG12	2.02	0.41
1:W:271:THR:O	1:W:303:VAL:HG13	2.19	0.41
4:n:320:VAL:HG13	4:n:422:VAL:HG13	2.02	0.41
1:2:297:LEU:CD2	1:2:322:ASN:HD22	2.33	0.41
2:7:38:PRO:HA	2:7:65:LEU:HA	2.01	0.41
4:B:376:ILE:HD12	4:B:376:ILE:H	1.85	0.41
4:B:526:LEU:C	4:B:528:ASN:N	2.78	0.41
4:D:575:ARG:O	4:D:575:ARG:NH2	2.29	0.41
6:I:541:PHE:CD1	6:I:541:PHE:C	2.98	0.41
7:J:566:MET:HE2	7:J:702:CYS:CB	2.49	0.41
6:K:275:LYS:HB3	6:K:333:ARG:HD3	2.02	0.41
8:L:619:VAL:O	8:L:620:PRO:C	2.63	0.41
3:M:560:ARG:HA	3:M:560:ARG:HD3	1.72	0.41
3:M:674:GLN:N	3:M:674:GLN:NE2	2.60	0.41
1:P:83:ALA:HA	1:P:86:TYR:CE1	2.55	0.41
1:Q:210:LEU:CD2	1:Q:231:LEU:HD13	2.50	0.41
1:R:217:ARG:C	1:R:218:LEU:HD22	2.45	0.41
1:W:28:GLU:CD	1:W:244:ARG:HH22	2.28	0.41
1:W:165:LEU:HD22	1:W:254:ILE:HD12	2.02	0.41
1:Z:206:ASP:HB2	1:Z:209:ALA:HB3	2.02	0.41
4:b:32:PHE:CE1	4:b:36:VAL:CG2	3.03	0.41
8:d:158:MET:HE2	8:d:158:MET:HA	2.02	0.41
1:1:21:PHE:CE1	1:1:236:MET:SD	3.14	0.41
1:2:398:LEU:O	1:2:398:LEU:HD23	2.19	0.41
3:E:745:LEU:HD22	3:E:836:LEU:HD13	2.01	0.41
7:J:891:MET:O	7:J:892:HIS:C	2.63	0.41
3:M:641:LEU:HA	3:M:641:LEU:HD23	1.70	0.41
4:N:465:THR:HG22	4:N:466:LEU:N	2.34	0.41
1:Q:410:LYS:NZ	1:Q:413:MET:HE1	2.35	0.41
1:Z:225:PHE:O	1:Z:226:SER:C	2.63	0.41
3:k:184:ARG:NH1	4:n:299:TRP:CG	2.88	0.41
4:n:623:VAL:CG1	4:n:624:ARG:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:137:LEU:HB2	1:2:167:GLN:O	2.20	0.41
1:2:174:ASN:ND2	1:2:387:LEU:CD1	2.83	0.41
1:2:250:ASN:O	1:2:256:LEU:HB2	2.20	0.41
1:2:255:GLY:HA2	4:N:678:THR:HG21	2.02	0.41
4:B:254:ILE:HA	4:B:257:VAL:HG22	2.03	0.41
4:B:685:MET:HE3	1:P:200:ASP:C	2.46	0.41
3:E:426:LYS:CE	5:s:80:ARG:NH1	2.83	0.41
4:F:493:LEU:HA	4:F:497:CYS:HB3	2.01	0.41
6:I:335:THR:O	6:I:339:HIS:N	2.50	0.41
7:J:926:LEU:HA	7:J:929:ILE:HG22	2.00	0.41
6:K:203:PHE:O	6:K:205:ILE:N	2.48	0.41
6:K:620:SER:HB3	6:K:654:TYR:CE1	2.54	0.41
3:M:159:LYS:HB2	3:M:160:MET:HE3	2.03	0.41
1:V:418:PHE:HB3	1:V:421:MET:HE1	2.01	0.41
1:Y:170:SER:HB2	1:Y:204:VAL:HA	2.02	0.41
1:Z:143:GLY:O	1:Z:147:SER:OG	2.31	0.41
1:1:111:GLY:HA2	1:1:114:ILE:HG22	2.03	0.41
1:1:221:GLN:O	1:1:222:ASN:C	2.63	0.41
1:2:156:ARG:O	1:2:157:LEU:C	2.63	0.41
1:2:248:TYR:CD1	1:2:248:TYR:O	2.73	0.41
3:C:655:LEU:HD13	3:C:686:MET:SD	2.61	0.41
7:J:916:GLN:HG2	7:J:929:ILE:HD12	2.03	0.41
8:L:1705:ASP:OD1	8:L:1706:LEU:N	2.53	0.41
1:P:220:ILE:H	1:P:220:ILE:HG13	1.57	0.41
1:T:245:TYR:CZ	1:T:362:ARG:HB3	2.55	0.41
1:W:119:PHE:CZ	1:W:160:ARG:HG3	2.56	0.41
1:W:291:LEU:CD2	1:W:295:ARG:HD3	2.51	0.41
4:n:806:PHE:CD2	4:n:829:GLU:CG	3.03	0.41
3:C:234:SER:OG	3:C:235:ALA:N	2.53	0.41
3:C:391:LEU:O	3:C:395:ILE:HG22	2.21	0.41
7:J:692:TYR:N	7:J:693:PRO:CD	2.83	0.41
7:J:770:TYR:N	7:J:771:PRO:HD3	2.35	0.41
1:Q:189:LEU:O	1:Q:424:SER:OG	2.35	0.41
1:T:102:ASN:C	1:T:144:GLY:HA3	2.46	0.41
1:U:8:LEU:HD23	1:U:8:LEU:H	1.85	0.41
4:b:13:LEU:O	4:b:13:LEU:HD23	2.20	0.41
3:k:241:ARG:HD3	3:k:241:ARG:N	2.35	0.41
4:n:297:LEU:HD11	4:n:378:LEU:HD22	2.03	0.41
3:A:373:GLN:NE2	3:A:374:GLU:CA	2.84	0.41
3:A:701:VAL:HA	3:A:736:ASP:CG	2.46	0.41
4:B:882:PHE:CD1	1:P:348:PHE:CD2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:408:MET:HE2	3:C:450:ILE:HB	2.02	0.41
6:I:414:LEU:HD11	6:I:455:LEU:HD21	2.01	0.41
6:K:51:ASP:OD1	6:K:137:MET:HE2	2.21	0.41
1:P:202:VAL:HG23	1:P:267:HIS:CE1	2.55	0.41
1:P:266:LEU:C	1:P:268:PHE:H	2.29	0.41
1:W:323:ILE:O	1:W:323:ILE:HG13	2.20	0.41
1:Z:51:PHE:CG	1:Z:244:ARG:HD3	2.56	0.41
3:A:655:LEU:HD13	3:A:686:MET:SD	2.61	0.41
4:B:477:MET:HE2	4:B:477:MET:CA	2.50	0.41
3:C:301:LYS:CG	4:D:372:TYR:CE2	3.04	0.41
3:E:517:LYS:HG2	3:E:523:ASP:OD2	2.21	0.41
4:F:882:PHE:CE2	1:T:341:ARG:HD3	2.56	0.41
7:J:365:MET:HE2	7:J:365:MET:HB3	1.89	0.41
6:K:648:ARG:HG2	6:K:648:ARG:HH21	1.86	0.41
1:O:21:PHE:CD2	1:O:236:MET:CE	3.02	0.41
1:O:31:ILE:HG22	1:O:32:SER:N	2.36	0.41
1:O:319:ALA:O	1:O:379:ALA:HB1	2.21	0.41
1:Q:201:CYS:SG	1:Q:269:LEU:HD12	2.61	0.41
1:S:105:ALA:HB3	1:S:411:GLU:HA	2.02	0.41
1:S:271:THR:HG22	1:S:378:MET:HE3	2.02	0.41
1:T:232:VAL:CG1	1:T:236:MET:CE	2.99	0.41
1:X:217:ARG:O	1:X:218:LEU:CD2	2.68	0.41
1:Z:73:VAL:O	1:Z:73:VAL:HG12	2.21	0.41
8:d:67:ARG:NH2	8:d:67:ARG:CB	2.83	0.41
3:k:184:ARG:NH1	4:n:299:TRP:CD1	2.88	0.41
4:n:718:MET:HE3	4:n:775:LEU:CD2	2.48	0.41
3:A:394:TRP:CE3	3:A:400:ILE:HD13	2.55	0.41
3:A:437:GLN:C	3:A:439:ILE:H	2.29	0.41
3:A:446:MET:HA	3:A:446:MET:HE3	2.02	0.41
3:A:663:LYS:HG2	3:A:680:PHE:CE2	2.49	0.41
3:A:679:ALA:HB2	3:A:818:PHE:CZ	2.55	0.41
3:A:687:LEU:CD2	1:O:258:ALA:O	2.69	0.41
3:C:160:MET:HE1	3:C:351:LEU:CB	2.50	0.41
3:C:437:GLN:C	3:C:439:ILE:H	2.29	0.41
4:D:550:ASN:C	4:D:551:LYS:HZ3	2.29	0.41
3:E:419:ILE:CG2	3:E:422:ASP:HA	2.51	0.41
4:F:308:THR:HA	4:F:325:CYS:SG	2.61	0.41
6:I:461:TRP:CZ2	6:I:465:ILE:CD1	2.95	0.41
7:J:982:LYS:HA	7:J:982:LYS:HE2	2.03	0.41
7:J:1017:LEU:C	7:J:1018:MET:CE	2.94	0.41
6:K:565:LEU:HD23	6:K:565:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:565:ASP:CG	8:L:566:LYS:H	2.29	0.41
8:L:619:VAL:HG22	8:L:620:PRO:HD2	2.02	0.41
3:M:457:LEU:HD23	3:M:468:THR:HA	2.03	0.41
3:M:500:LEU:HD23	3:M:504:MET:HE2	2.03	0.41
1:P:290:VAL:HG11	1:P:332:GLN:CD	2.46	0.41
1:R:249:MET:HB2	1:R:249:MET:HE2	1.70	0.41
1:T:333:VAL:CG1	1:T:358:VAL:HG11	2.51	0.41
1:T:439:THR:O	1:T:439:THR:HG22	2.21	0.41
1:U:260:LEU:C	1:U:261:ILE:HD13	2.46	0.41
1:U:274:THR:CB	1:U:275:PRO:HD3	2.51	0.41
1:W:114:ILE:O	1:W:114:ILE:CG2	2.69	0.41
1:Y:274:THR:N	1:Y:275:PRO:HD2	2.36	0.41
5:i:72:LYS:HG2	5:i:73:GLU:N	2.33	0.41
3:k:836:LEU:HD23	3:k:837:LEU:N	2.36	0.41
4:n:381:LEU:HD21	4:n:414:LEU:HD21	2.02	0.41
1:1:21:PHE:HA	1:1:233:SER:HB3	2.03	0.41
3:A:297:ARG:HH12	4:B:411:MET:HB3	1.86	0.41
3:A:391:LEU:O	3:A:395:ILE:HG22	2.21	0.41
4:B:644:VAL:HG11	4:B:657:MET:HE3	2.03	0.41
4:B:849:ILE:HD13	4:B:849:ILE:HA	1.96	0.41
4:D:408:ASP:OD2	4:D:411:MET:HE1	2.20	0.41
4:D:614:SER:HA	4:D:615:PRO:HD3	1.89	0.41
4:D:754:PHE:CE1	4:D:758:ILE:HD11	2.56	0.41
4:F:575:ARG:HG3	4:F:575:ARG:HH21	1.85	0.41
6:I:59:ILE:HA	6:I:90:CYS:SG	2.61	0.41
6:I:469:PRO:O	6:I:470:ALA:CB	2.69	0.41
6:I:575:LEU:HD23	6:I:575:LEU:HA	1.97	0.41
3:M:521:LEU:H	3:M:642:PHE:HB2	1.86	0.41
1:Y:273:TYR:N	1:Y:304:MET:HE3	2.36	0.41
1:Z:222:ASN:O	1:Z:223:PRO:C	2.65	0.41
9:a:26:ASP:OD1	9:a:26:ASP:N	2.45	0.41
1:1:274:THR:HB	1:1:275:PRO:HD3	2.03	0.40
1:1:408:PHE:O	1:1:412:ASP:HB2	2.22	0.40
3:A:526:ASP:N	1:O:251:ASN:ND2	2.68	0.40
3:E:426:LYS:HZ1	5:u:85:GLU:CD	2.20	0.40
6:I:526:ASP:O	6:I:529:GLN:HB3	2.22	0.40
4:N:400:VAL:CG1	4:N:419:LEU:HG	2.51	0.40
1:P:351:TRP:CE3	1:P:352:GLY:N	2.89	0.40
1:Q:59:HIS:HB3	1:Q:61:ILE:HG13	2.04	0.40
1:Q:297:LEU:HD21	1:Q:377:MET:HB2	2.03	0.40
1:R:28:GLU:OE1	1:R:367:LEU:HD11	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:39:GLU:O	1:U:40:PHE:CG	2.74	0.40
1:V:398:LEU:HD23	1:V:401:ARG:HH21	1.85	0.40
1:V:419:ASP:OD1	1:V:419:ASP:N	2.55	0.40
1:Z:235:ILE:HG21	1:Z:304:MET:HE3	2.03	0.40
3:k:732:THR:HG22	5:t:72:LYS:HZ1	1.83	0.40
5:t:88:MET:SD	5:t:88:MET:N	2.95	0.40
3:A:641:LEU:C	3:A:645:MET:HE2	2.46	0.40
4:B:673:MET:HE1	4:B:676:ILE:HG21	2.02	0.40
3:C:351:LEU:O	3:C:352:GLY:C	2.64	0.40
3:C:373:GLN:NE2	3:C:374:GLU:CA	2.84	0.40
3:C:701:VAL:HA	3:C:736:ASP:CG	2.46	0.40
4:D:673:MET:HA	4:D:676:ILE:HG22	2.03	0.40
3:E:426:LYS:HZ1	5:s:80:ARG:NH1	2.19	0.40
3:M:178:PRO:HB3	3:M:180:TRP:CH2	2.56	0.40
3:M:836:LEU:HA	3:M:839:ARG:HE	1.85	0.40
4:N:844:CYS:C	4:N:846:GLN:H	2.29	0.40
1:P:358:VAL:O	1:P:358:VAL:HG13	2.22	0.40
1:S:104:TRP:CG	1:S:190:LEU:HD13	2.56	0.40
1:T:22:TRP:CH2	1:T:62:PRO:HB3	2.56	0.40
1:T:223:PRO:HB2	1:T:227:GLN:HG3	2.03	0.40
1:W:92:TYR:CE1	1:W:114:ILE:HG23	2.56	0.40
1:W:223:PRO:O	1:W:224:SER:C	2.62	0.40
1:W:323:ILE:O	1:W:323:ILE:CG1	2.69	0.40
1:Y:260:LEU:HD13	1:Y:378:MET:HE2	2.03	0.40
3:k:318:LEU:O	3:k:318:LEU:HD23	2.21	0.40
5:s:88:MET:HG3	5:u:88:MET:SD	2.62	0.40
1:2:213:ILE:HD13	1:2:304:MET:HG2	2.00	0.40
3:A:160:MET:HE1	3:A:351:LEU:CB	2.50	0.40
3:A:522:MET:SD	3:A:698:MET:HE1	2.60	0.40
3:C:649:LYS:HB2	1:Q:249:MET:HE1	2.02	0.40
3:E:205:ILE:O	3:E:206:GLY:C	2.62	0.40
3:E:686:MET:HE1	3:E:829:PHE:CB	2.51	0.40
4:F:734:LEU:HD22	4:F:754:PHE:CG	2.56	0.40
4:F:840:ILE:HB	4:F:841:PRO:HD3	2.03	0.40
7:J:1015:LEU:HD13	1:X:338:GLN:HG2	2.03	0.40
8:L:510:LEU:HD21	8:L:1482:VAL:CG2	2.51	0.40
8:L:1794:LEU:HD23	8:L:1803:LEU:CD1	2.52	0.40
3:M:157:LYS:CA	3:M:160:MET:SD	3.09	0.40
3:M:832:HIS:O	3:M:836:LEU:HD22	2.21	0.40
1:Q:416:ASP:OD1	1:Q:416:ASP:N	2.54	0.40
1:U:181:VAL:O	1:U:184:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:185:PRO:HD2	1:Y:398:LEU:CD1	2.51	0.40
1:1:117:ASP:OD1	1:1:117:ASP:C	2.64	0.40
1:1:195:LEU:HA	1:1:199:ALA:HB3	2.04	0.40
3:A:351:LEU:O	3:A:352:GLY:C	2.64	0.40
3:A:678:GLY:C	3:A:680:PHE:H	2.29	0.40
3:A:771:LEU:CD2	1:O:162:PRO:HB3	2.41	0.40
3:C:641:LEU:C	3:C:645:MET:HE2	2.46	0.40
4:D:848:ARG:HD2	4:D:848:ARG:HA	1.92	0.40
3:E:586:LEU:O	3:E:586:LEU:CD1	2.69	0.40
6:I:407:ASP:O	6:I:408:ASP:C	2.64	0.40
6:I:472:LEU:HD23	6:I:475:TYR:CD2	2.56	0.40
8:L:367:THR:HG22	8:L:369:SER:H	1.84	0.40
1:P:69:LEU:H	1:P:145:THR:HB	1.87	0.40
1:Q:189:LEU:HD13	1:Q:391:THR:HG23	2.03	0.40
1:V:190:LEU:HD11	1:V:421:MET:HG2	2.04	0.40
1:W:245:TYR:CB	1:W:362:ARG:HD3	2.51	0.40
4:D:849:ILE:HD12	4:D:849:ILE:HA	1.97	0.40
8:L:530:GLU:HB3	8:L:531:PRO:HD3	2.03	0.40
8:L:562:SER:C	8:L:563:PHE:CD1	2.99	0.40
4:N:721:TYR:CZ	4:N:876:LEU:HB2	2.57	0.40
1:O:202:VAL:HG21	1:O:268:PHE:CZ	2.57	0.40
1:R:87:ASN:N	1:R:88:PRO:CD	2.85	0.40
1:X:169:TYR:CD1	1:X:236:MET:SD	3.15	0.40
9:a:35:LEU:HD21	4:b:58:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	408/451 (90%)	373 (91%)	32 (8%)	3 (1%)	18 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	403/451 (89%)	363 (90%)	40 (10%)	0	100	100
1	O	408/451 (90%)	357 (88%)	43 (10%)	8 (2%)	6	32
1	P	408/451 (90%)	359 (88%)	43 (10%)	6 (2%)	8	37
1	Q	408/451 (90%)	370 (91%)	32 (8%)	6 (2%)	8	37
1	R	408/451 (90%)	363 (89%)	40 (10%)	5 (1%)	10	41
1	S	408/451 (90%)	356 (87%)	49 (12%)	3 (1%)	18	51
1	T	408/451 (90%)	362 (89%)	42 (10%)	4 (1%)	12	44
1	U	408/451 (90%)	365 (90%)	39 (10%)	4 (1%)	12	44
1	V	405/451 (90%)	356 (88%)	46 (11%)	3 (1%)	18	51
1	W	405/451 (90%)	363 (90%)	35 (9%)	7 (2%)	7	35
1	X	408/451 (90%)	360 (88%)	47 (12%)	1 (0%)	43	72
1	Y	407/451 (90%)	353 (87%)	53 (13%)	1 (0%)	43	72
1	Z	408/451 (90%)	355 (87%)	44 (11%)	9 (2%)	5	30
2	7	356/364 (98%)	305 (86%)	48 (14%)	3 (1%)	16	49
3	A	587/902 (65%)	542 (92%)	43 (7%)	2 (0%)	36	65
3	C	600/902 (66%)	549 (92%)	45 (8%)	6 (1%)	12	44
3	E	626/902 (69%)	558 (89%)	64 (10%)	4 (1%)	21	54
3	M	621/902 (69%)	555 (89%)	65 (10%)	1 (0%)	43	72
3	f	91/902 (10%)	81 (89%)	10 (11%)	0	100	100
3	k	624/902 (69%)	564 (90%)	55 (9%)	5 (1%)	16	49
4	B	602/907 (66%)	544 (90%)	57 (10%)	1 (0%)	43	72
4	D	571/907 (63%)	529 (93%)	40 (7%)	2 (0%)	30	60
4	F	591/907 (65%)	535 (90%)	55 (9%)	1 (0%)	43	72
4	N	573/907 (63%)	521 (91%)	51 (9%)	1 (0%)	43	72
4	b	112/907 (12%)	104 (93%)	7 (6%)	1 (1%)	14	46
4	n	584/907 (64%)	526 (90%)	54 (9%)	4 (1%)	18	51
5	G	29/229 (13%)	25 (86%)	4 (14%)	0	100	100
5	H	33/229 (14%)	32 (97%)	1 (3%)	0	100	100
5	g	33/229 (14%)	31 (94%)	2 (6%)	0	100	100
5	h	33/229 (14%)	30 (91%)	3 (9%)	0	100	100
5	i	29/229 (13%)	26 (90%)	3 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	j	30/229 (13%)	30 (100%)	0	0	100	100
5	s	33/229 (14%)	31 (94%)	2 (6%)	0	100	100
5	t	33/229 (14%)	30 (91%)	3 (9%)	0	100	100
5	u	33/229 (14%)	33 (100%)	0	0	100	100
5	v	33/229 (14%)	31 (94%)	2 (6%)	0	100	100
6	I	511/667 (77%)	436 (85%)	69 (14%)	6 (1%)	10	41
6	K	548/667 (82%)	504 (92%)	41 (8%)	3 (0%)	24	57
7	J	587/1024 (57%)	499 (85%)	82 (14%)	6 (1%)	12	44
8	L	613/1819 (34%)	537 (88%)	69 (11%)	7 (1%)	11	43
8	d	137/1819 (8%)	128 (93%)	8 (6%)	1 (1%)	18	51
9	a	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
9	c	57/82 (70%)	54 (95%)	3 (5%)	0	100	100
10	e	44/158 (28%)	40 (91%)	4 (9%)	0	100	100
All	All	15117/26140 (58%)	13525 (90%)	1478 (10%)	114 (1%)	18	49

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	589	ALA
4	D	314	ASP
3	E	370	SER
4	F	287	LEU
6	I	470	ALA
7	J	297	ARG
6	K	15	SER
8	L	363	VAL
1	W	49	ASP
1	W	368	PRO
1	Z	246	PRO
1	1	221	GLN
6	I	11	GLY
8	L	385	VAL
1	O	221	GLN
1	O	274	THR
1	P	267	HIS
1	T	224	SER
1	T	250	ASN

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Mol	Chain	Res	Type
1	W	250	ASN
1	Z	303	VAL
1	Z	318	ILE
1	Z	371	HIS
3	k	483	ALA
4	n	763	LEU
3	C	503	LEU
3	C	565	ASN
3	E	421	GLU
6	I	93	LEU
6	I	113	GLY
7	J	249	HIS
8	L	369	SER
1	O	262	PRO
1	O	277	THR
1	O	354	ALA
1	Q	118	ILE
1	R	226	SER
1	U	222	ASN
1	V	8	LEU
1	W	288	THR
2	7	164	PRO
3	A	680	PHE
3	C	539	LEU
7	J	302	VAL
6	K	404	LEU
8	L	384	HIS
3	M	241	ARG
4	N	687	ASN
1	P	40	PHE
1	P	222	ASN
1	Q	345	LEU
1	R	142	ALA
1	S	220	ILE
1	S	222	ASN
1	U	246	PRO
1	U	350	PRO
1	W	415	LYS
1	X	371	HIS
3	k	186	ALA
3	k	427	TYR
4	n	367	LEU

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Mol	Chain	Res	Type
4	n	380	THR
1	1	224	SER
3	C	865	TYR
3	E	202	ALA
6	I	81	LEU
6	I	601	LEU
7	J	255	PRO
7	J	450	VAL
7	J	495	GLN
6	K	204	PHE
8	L	1481	PRO
1	O	222	ASN
1	Q	350	PRO
1	R	365	PRO
1	S	274	THR
1	U	407	GLN
1	V	142	ALA
1	W	71	PRO
1	Y	220	ILE
1	Z	365	PRO
8	d	150	CYS
1	1	262	PRO
3	C	510	VAL
3	C	861	PHE
8	L	353	VAL
8	L	364	VAL
1	P	72	ARG
1	R	87	ASN
1	V	63	ARG
1	W	224	SER
4	b	115	ALA
2	7	136	ILE
4	D	630	PRO
1	Q	37	VAL
1	Q	70	GLU
1	T	368	PRO
1	Z	222	ASN
3	E	471	VAL
1	O	228	ILE
1	Z	375	GLY
3	k	204	PRO
3	k	265	PRO

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Mol	Chain	Res	Type
4	n	409	PRO
2	7	219	VAL
3	A	510	VAL
1	P	173	PRO
1	Z	352	GLY
1	O	368	PRO
1	P	182	VAL
1	Q	91	ILE
1	R	30	GLY
1	T	246	PRO
1	Z	350	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	374/400 (94%)	369 (99%)	5 (1%)	61	72
1	2	367/400 (92%)	355 (97%)	12 (3%)	33	58
1	O	374/400 (94%)	362 (97%)	12 (3%)	34	58
1	P	373/400 (93%)	362 (97%)	11 (3%)	37	60
1	Q	375/400 (94%)	371 (99%)	4 (1%)	65	74
1	R	374/400 (94%)	365 (98%)	9 (2%)	43	63
1	S	375/400 (94%)	371 (99%)	4 (1%)	65	74
1	T	373/400 (93%)	368 (99%)	5 (1%)	61	72
1	U	374/400 (94%)	369 (99%)	5 (1%)	61	72
1	V	368/400 (92%)	364 (99%)	4 (1%)	65	74
1	W	373/400 (93%)	363 (97%)	10 (3%)	39	61
1	X	375/400 (94%)	367 (98%)	8 (2%)	47	65
1	Y	374/400 (94%)	373 (100%)	1 (0%)	86	83
1	Z	374/400 (94%)	362 (97%)	12 (3%)	34	58
2	7	18/310 (6%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	533/791 (67%)	503 (94%)	30 (6%)	19	46
3	C	547/791 (69%)	538 (98%)	9 (2%)	55	69
3	E	573/791 (72%)	565 (99%)	8 (1%)	59	71
3	M	569/791 (72%)	555 (98%)	14 (2%)	42	63
3	f	3/791 (0%)	3 (100%)	0	100	100
3	k	571/791 (72%)	565 (99%)	6 (1%)	65	74
4	B	547/798 (68%)	538 (98%)	9 (2%)	55	69
4	D	524/798 (66%)	519 (99%)	5 (1%)	68	75
4	F	537/798 (67%)	533 (99%)	4 (1%)	76	78
4	N	525/798 (66%)	518 (99%)	7 (1%)	61	72
4	b	101/798 (13%)	100 (99%)	1 (1%)	68	75
4	n	532/798 (67%)	527 (99%)	5 (1%)	70	76
5	G	29/207 (14%)	29 (100%)	0	100	100
5	H	35/207 (17%)	35 (100%)	0	100	100
5	g	32/207 (16%)	32 (100%)	0	100	100
5	h	35/207 (17%)	34 (97%)	1 (3%)	37	60
5	i	30/207 (14%)	28 (93%)	2 (7%)	15	42
5	j	32/207 (16%)	32 (100%)	0	100	100
5	s	32/207 (16%)	32 (100%)	0	100	100
5	t	32/207 (16%)	32 (100%)	0	100	100
5	u	35/207 (17%)	35 (100%)	0	100	100
5	v	35/207 (17%)	35 (100%)	0	100	100
6	I	468/594 (79%)	466 (100%)	2 (0%)	84	81
6	K	508/594 (86%)	507 (100%)	1 (0%)	87	85
7	J	531/933 (57%)	526 (99%)	5 (1%)	70	76
8	L	540/1546 (35%)	537 (99%)	3 (1%)	78	79
8	d	128/1546 (8%)	128 (100%)	0	100	100
9	a	53/62 (86%)	53 (100%)	0	100	100
9	c	53/62 (86%)	52 (98%)	1 (2%)	50	67
10	e	2/118 (2%)	2 (100%)	0	100	100
All	All	13413/22969 (58%)	13198 (98%)	215 (2%)	54	69

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	220	ILE
1	1	221	GLN
1	1	222	ASN
1	1	223	PRO
1	1	256	LEU
1	2	136	VAL
1	2	170	SER
1	2	201	CYS
1	2	220	ILE
1	2	221	GLN
1	2	225	PHE
1	2	227	GLN
1	2	236	MET
1	2	249	MET
1	2	256	LEU
1	2	257	ILE
1	2	349	ILE
3	A	168	LYS
3	A	244	ARG
3	A	297	ARG
3	A	405	SER
3	A	411	GLU
3	A	482	ARG
3	A	494	TYR
3	A	498	VAL
3	A	504	MET
3	A	505	GLU
3	A	506	GLU
3	A	507	LYS
3	A	509	LEU
3	A	512	HIS
3	A	532	MET
3	A	541	LYS
3	A	556	GLU
3	A	567	ASP
3	A	624	TRP
3	A	653	ARG
3	A	659	TRP
3	A	660	ILE
3	A	674	GLN
3	A	675	TRP
3	A	680	PHE

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Mol	Chain	Res	Type
3	A	708	ILE
3	A	729	PHE
3	A	734	LEU
3	A	735	LYS
3	A	762	MET
4	B	264	LYS
4	B	285	ARG
4	B	293	ARG
4	B	374	PRO
4	B	528	ASN
4	B	576	HIS
4	B	673	MET
4	B	868	SER
4	B	887	LYS
3	C	168	LYS
3	C	411	GLU
3	C	494	TYR
3	C	508	GLU
3	C	532	MET
3	C	567	ASP
3	C	624	TRP
3	C	708	ILE
3	C	762	MET
4	D	417	HIS
4	D	711	MET
4	D	719	GLN
4	D	725	GLU
4	D	884	GLU
3	E	205	ILE
3	E	214	GLU
3	E	313	LEU
3	E	346	ASP
3	E	446	MET
3	E	478	THR
3	E	514	ARG
3	E	581	ASP
4	F	362	LEU
4	F	645	ASP
4	F	685	MET
4	F	871	GLU
6	I	122	VAL
6	I	538	GLU

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Mol	Chain	Res	Type
7	J	274	THR
7	J	275	LEU
7	J	304	HIS
7	J	821	TYR
7	J	827	LEU
6	K	641	ASP
8	L	469	GLN
8	L	537	HIS
8	L	573	TYR
3	M	397	ARG
3	M	427	TYR
3	M	439	ILE
3	M	534	LEU
3	M	560	ARG
3	M	561	MET
3	M	642	PHE
3	M	643	ARG
3	M	645	MET
3	M	674	GLN
3	M	698	MET
3	M	699	PHE
3	M	700	GLU
3	M	829	PHE
4	N	535	ASP
4	N	685	MET
4	N	689	LYS
4	N	727	LEU
4	N	797	LEU
4	N	798	GLU
4	N	847	LEU
1	O	29	HIS
1	O	220	ILE
1	O	221	GLN
1	O	222	ASN
1	O	224	SER
1	O	225	PHE
1	O	227	GLN
1	O	245	TYR
1	O	349	ILE
1	O	353	PRO
1	O	358	VAL
1	O	367	LEU

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Mol	Chain	Res	Type
1	P	12	GLN
1	P	28	GLU
1	P	69	LEU
1	P	70	GLU
1	P	73	VAL
1	P	220	ILE
1	P	221	GLN
1	P	222	ASN
1	P	226	SER
1	P	302	ASN
1	P	435	TYR
1	Q	79	ASN
1	Q	222	ASN
1	Q	224	SER
1	Q	435	TYR
1	R	102	ASN
1	R	103	ASN
1	R	164	LYS
1	R	220	ILE
1	R	221	GLN
1	R	274	THR
1	R	304	MET
1	R	340	ILE
1	R	407	GLN
1	S	151	SER
1	S	220	ILE
1	S	224	SER
1	S	278	THR
1	T	224	SER
1	T	225	PHE
1	T	245	TYR
1	T	248	TYR
1	T	266	LEU
1	U	184	GLN
1	U	221	GLN
1	U	222	ASN
1	U	224	SER
1	U	348	PHE
1	V	59	HIS
1	V	158	ASN
1	V	267	HIS
1	V	334	HIS

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Mol	Chain	Res	Type
1	W	9	GLN
1	W	25	LEU
1	W	53	TYR
1	W	158	ASN
1	W	219	HIS
1	W	220	ILE
1	W	221	GLN
1	W	222	ASN
1	W	376	LEU
1	W	377	MET
1	X	119	PHE
1	X	219	HIS
1	X	220	ILE
1	X	222	ASN
1	X	225	PHE
1	X	253	LEU
1	X	333	VAL
1	X	418	PHE
1	Y	221	GLN
1	Z	132	LEU
1	Z	208	THR
1	Z	212	ARG
1	Z	213	ILE
1	Z	220	ILE
1	Z	221	GLN
1	Z	222	ASN
1	Z	228	ILE
1	Z	267	HIS
1	Z	304	MET
1	Z	432	ILE
1	Z	435	TYR
4	b	20	ILE
9	c	63	VAL
5	h	84	LEU
5	i	72	LYS
5	i	73	GLU
3	k	405	SER
3	k	413	GLU
3	k	537	GLU
3	k	567	ASP
3	k	645	MET
3	k	647	TYR

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Mol	Chain	Res	Type
4	n	253	ASP
4	n	378	LEU
4	n	667	LEU
4	n	722	ILE
4	n	738	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	24	GLN
1	1	167	GLN
1	1	315	HIS
1	1	407	GLN
1	2	12	GLN
1	2	29	HIS
1	2	59	HIS
1	2	75	HIS
1	2	174	ASN
1	2	198	ASN
1	2	250	ASN
1	2	315	HIS
1	2	357	GLN
1	2	436	HIS
3	A	373	GLN
3	A	430	GLN
3	A	465	HIS
3	A	684	GLN
4	B	330	GLN
4	B	417	HIS
4	B	528	ASN
4	B	742	GLN
4	B	789	GLN
3	C	169	ASN
3	C	312	GLN
3	C	373	GLN
4	D	259	GLN
4	D	387	HIS
4	D	595	HIS
4	D	789	GLN
3	E	165	GLN
3	E	287	GLN
3	E	322	GLN

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Mol	Chain	Res	Type
3	E	360	HIS
3	E	487	GLN
3	E	524	GLN
3	E	580	HIS
3	E	707	HIS
4	F	273	ASN
4	F	491	ASN
4	F	494	HIS
4	F	716	HIS
4	F	781	GLN
4	F	786	GLN
6	I	43	ASN
6	I	142	GLN
6	I	302	ASN
6	I	303	GLN
6	I	370	GLN
6	I	415	HIS
6	I	464	HIS
6	I	494	HIS
7	J	307	HIS
7	J	456	GLN
7	J	495	GLN
7	J	504	HIS
7	J	642	HIS
7	J	698	GLN
7	J	991	HIS
6	K	26	GLN
6	K	29	GLN
6	K	121	HIS
6	K	186	GLN
6	K	353	GLN
6	K	370	GLN
6	K	415	HIS
6	K	499	GLN
6	K	540	GLN
6	K	543	GLN
6	K	591	HIS
6	K	599	GLN
6	K	600	ASN
8	L	507	GLN
8	L	1571	HIS
8	L	1633	GLN

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Mol	Chain	Res	Type
8	L	1656	HIS
8	L	1681	GLN
8	L	1750	GLN
8	L	1754	GLN
8	L	1785	HIS
8	L	1796	ASN
3	M	213	GLN
3	M	289	ASN
3	M	401	HIS
3	M	694	GLN
3	M	707	HIS
3	M	763	GLN
3	M	862	ASN
4	N	301	HIS
4	N	716	HIS
4	N	742	GLN
4	N	855	GLN
4	N	885	HIS
1	O	24	GLN
1	O	175	GLN
1	O	207	ASN
1	O	219	HIS
1	O	229	ASN
1	O	334	HIS
1	O	357	GLN
1	O	407	GLN
1	O	429	GLN
1	P	24	GLN
1	P	79	ASN
1	P	230	GLN
1	P	250	ASN
1	P	302	ASN
1	P	325	GLN
1	Q	24	GLN
1	Q	198	ASN
1	Q	267	HIS
1	Q	299	GLN
1	Q	429	GLN
1	R	16	GLN
1	R	24	GLN
1	R	222	ASN
1	R	314	ASN

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Mol	Chain	Res	Type
1	R	322	ASN
1	R	357	GLN
1	S	24	GLN
1	S	251	ASN
1	T	87	ASN
1	T	115	HIS
1	T	167	GLN
1	T	175	GLN
1	T	219	HIS
1	T	322	ASN
1	T	325	GLN
1	T	338	GLN
1	T	394	GLN
1	T	429	GLN
1	U	12	GLN
1	U	16	GLN
1	U	87	ASN
1	U	110	GLN
1	U	184	GLN
1	U	221	GLN
1	U	230	GLN
1	U	251	ASN
1	U	302	ASN
1	U	334	HIS
1	V	24	GLN
1	V	158	ASN
1	V	167	GLN
1	V	198	ASN
1	V	250	ASN
1	V	347	ASN
1	V	380	ASN
1	V	430	GLN
1	W	110	GLN
1	W	207	ASN
1	W	227	GLN
1	W	251	ASN
1	W	315	HIS
1	W	407	GLN
1	W	430	GLN
1	X	315	HIS
1	X	322	ASN
1	Y	103	ASN

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Mol	Chain	Res	Type
1	Y	158	ASN
1	Y	184	GLN
1	Y	187	ASN
1	Y	222	ASN
1	Z	15	ASN
1	Z	54	GLN
1	Z	158	ASN
1	Z	219	HIS
1	Z	221	GLN
4	b	33	GLN
4	b	42	ASN
4	b	82	HIS
8	d	116	GLN
5	h	89	GLN
5	h	90	GLN
3	k	524	GLN
3	k	725	HIS
3	k	832	HIS
3	k	862	ASN
4	n	417	HIS
4	n	461	HIS
4	n	558	HIS
4	n	596	ASN
4	n	830	ASN
5	u	74	ASN
5	u	76	ASN
5	v	65	ASN
5	v	74	ASN
5	v	76	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

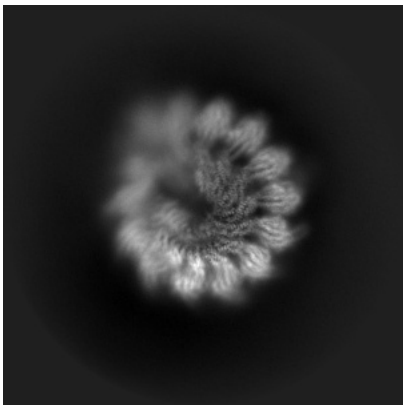
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-19570. These allow visual inspection of the internal detail of the map and identification of artifacts.

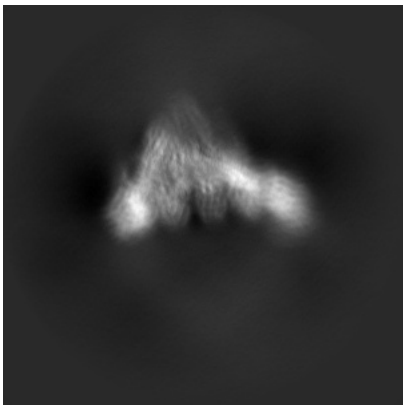
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

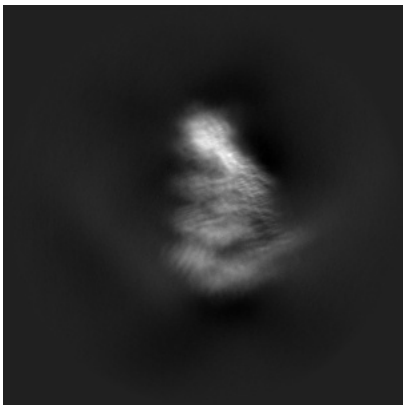
6.1.1 Primary map



X

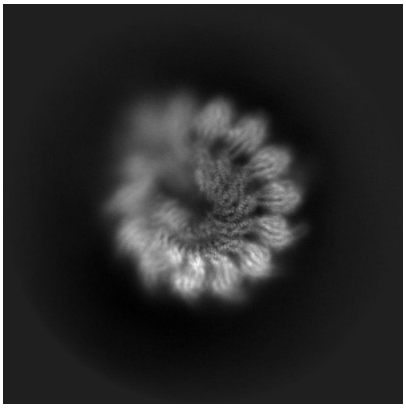


Y

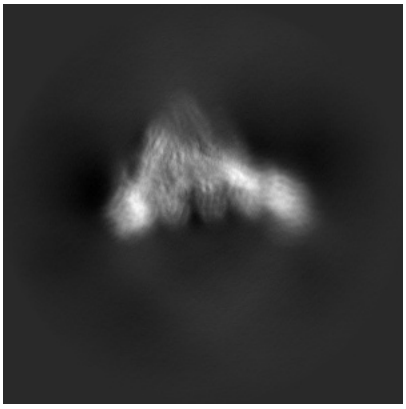


Z

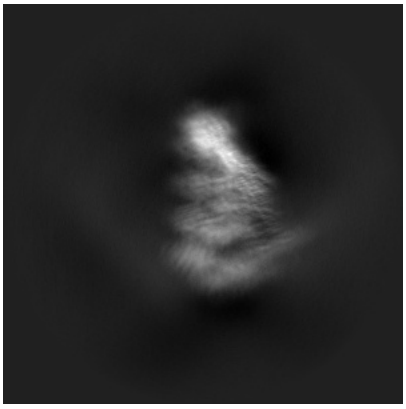
6.1.2 Raw map



X



Y

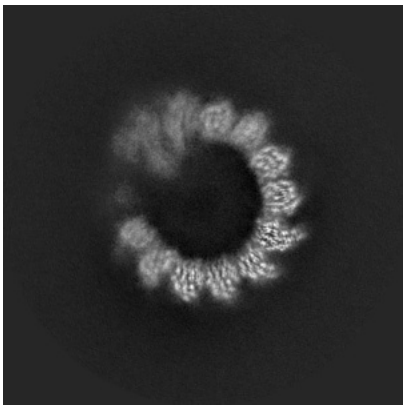


Z

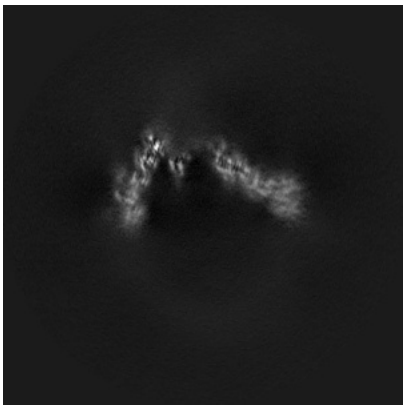
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

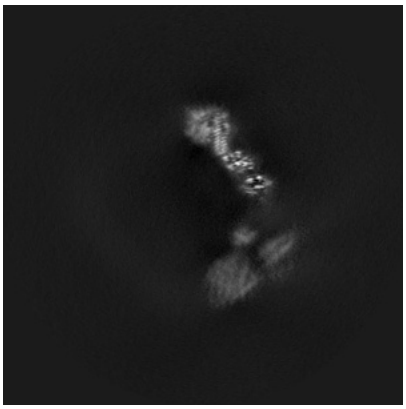
6.2.1 Primary map



X Index: 180

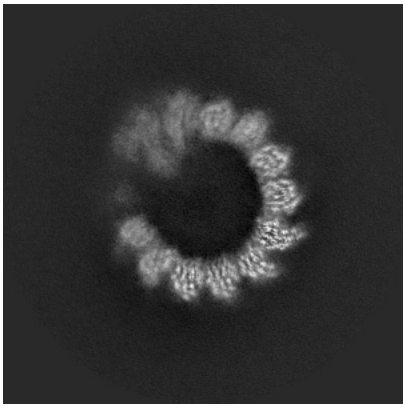


Y Index: 180

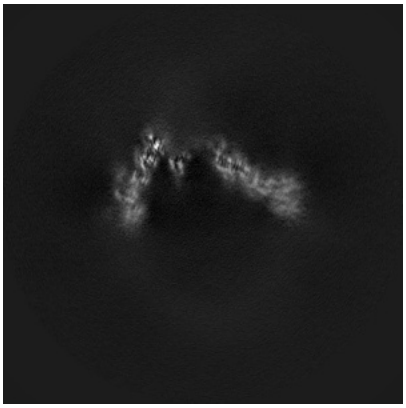


Z Index: 180

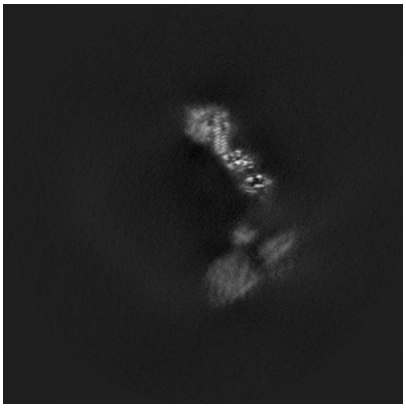
6.2.2 Raw map



X Index: 180



Y Index: 180

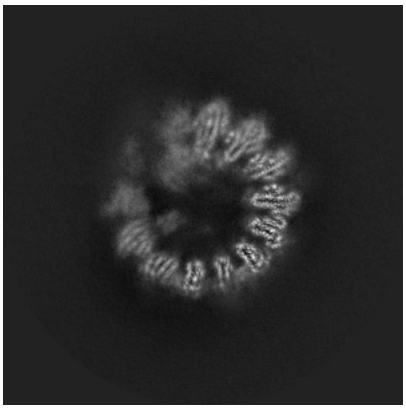


Z Index: 180

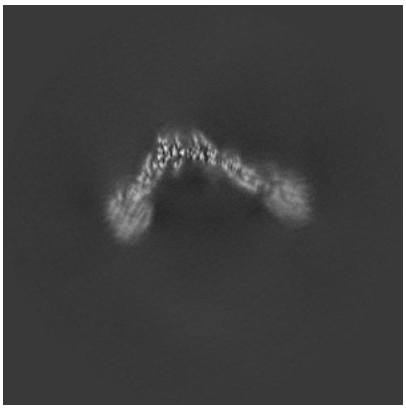
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

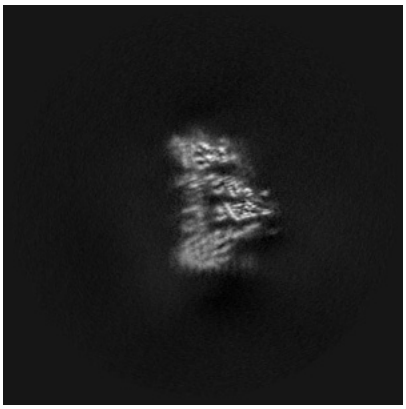
6.3.1 Primary map



X Index: 195

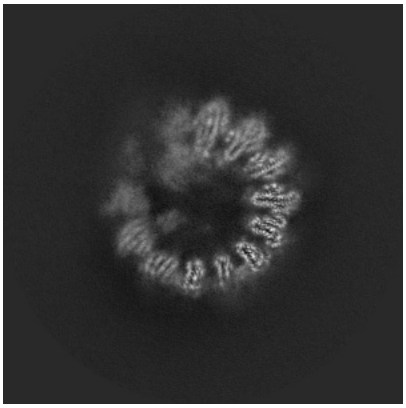


Y Index: 200

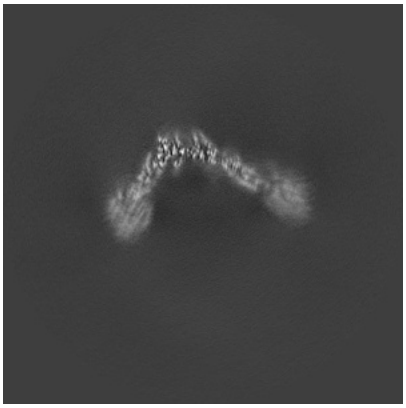


Z Index: 126

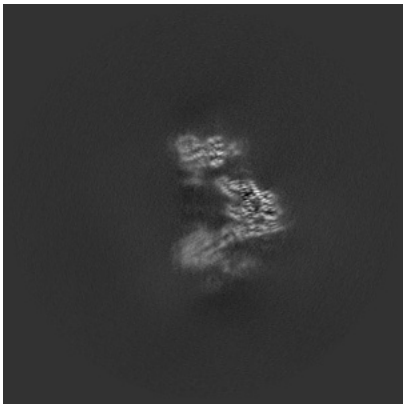
6.3.2 Raw map



X Index: 195



Y Index: 200

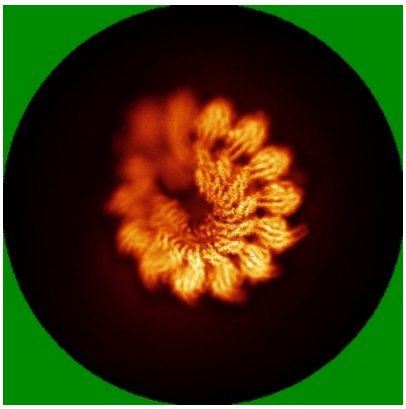


Z Index: 132

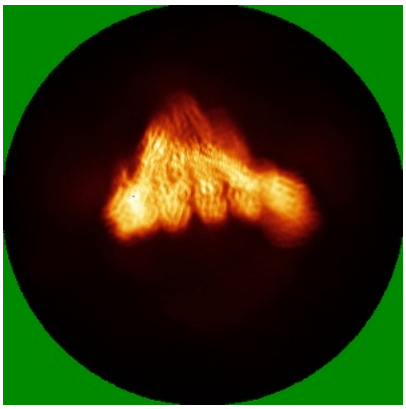
The images above show the largest variance slices of the map in three orthogonal directions.

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

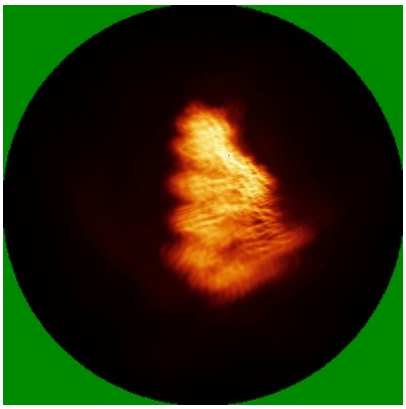
6.4.1 Primary map



X

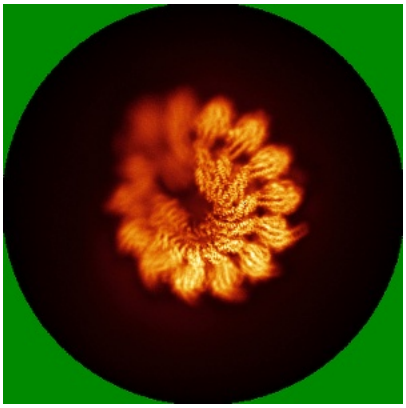


Y

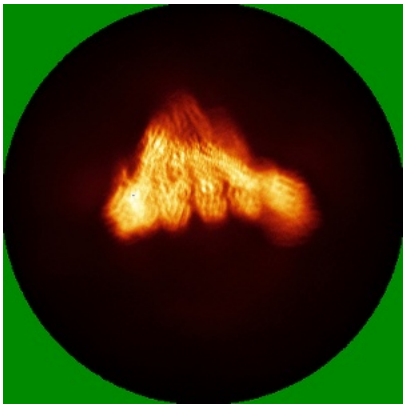


Z

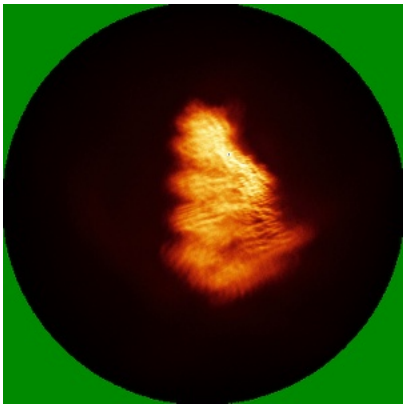
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

This section was not generated.

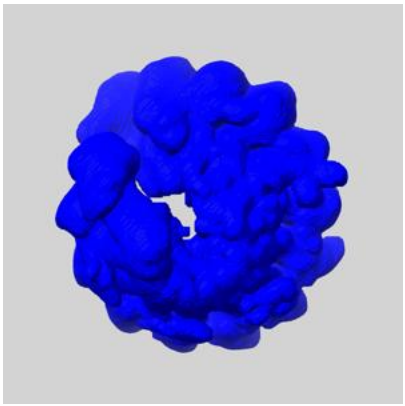
6.6 Mask visualisation (i)

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

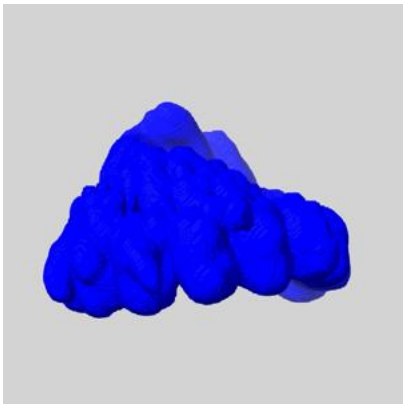
A mask typically either:

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

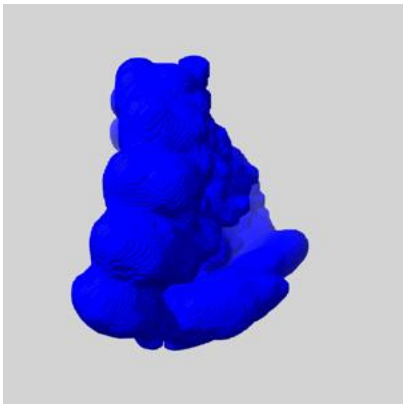
6.6.1 emd_19570_msk_1.map (i)



X



Y

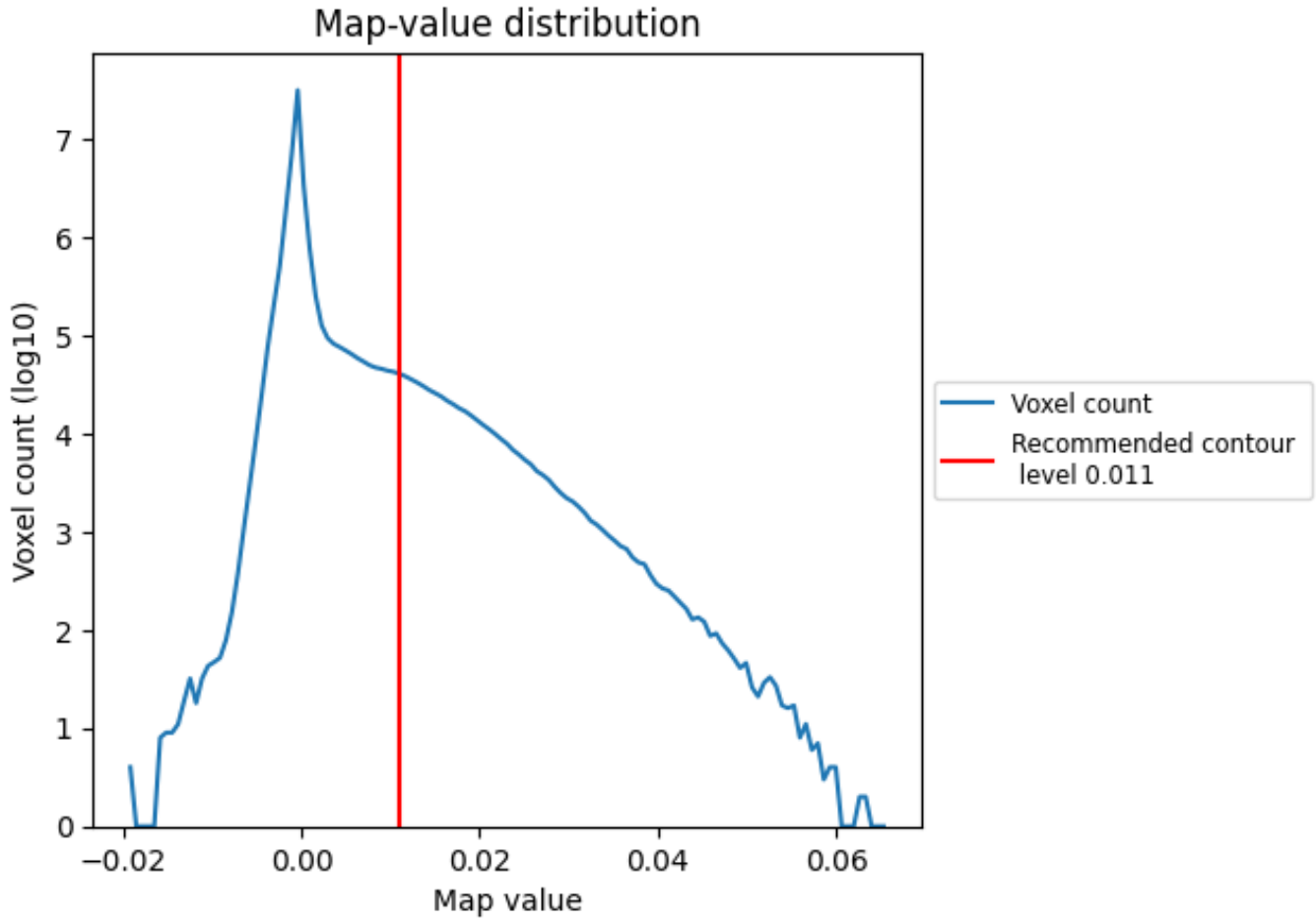


Z

7 Map analysis

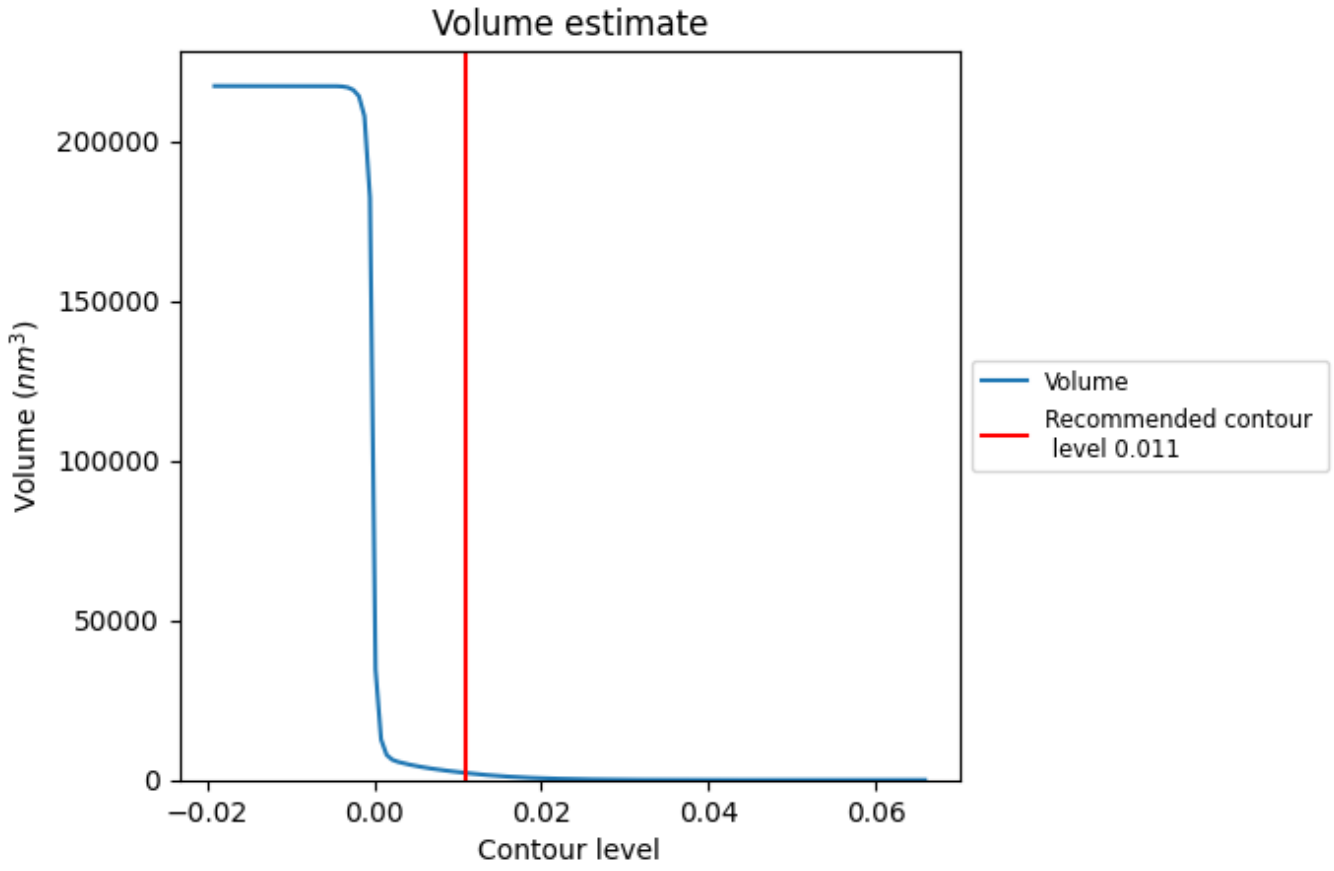
This section contains the results of statistical analysis of the map.

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.

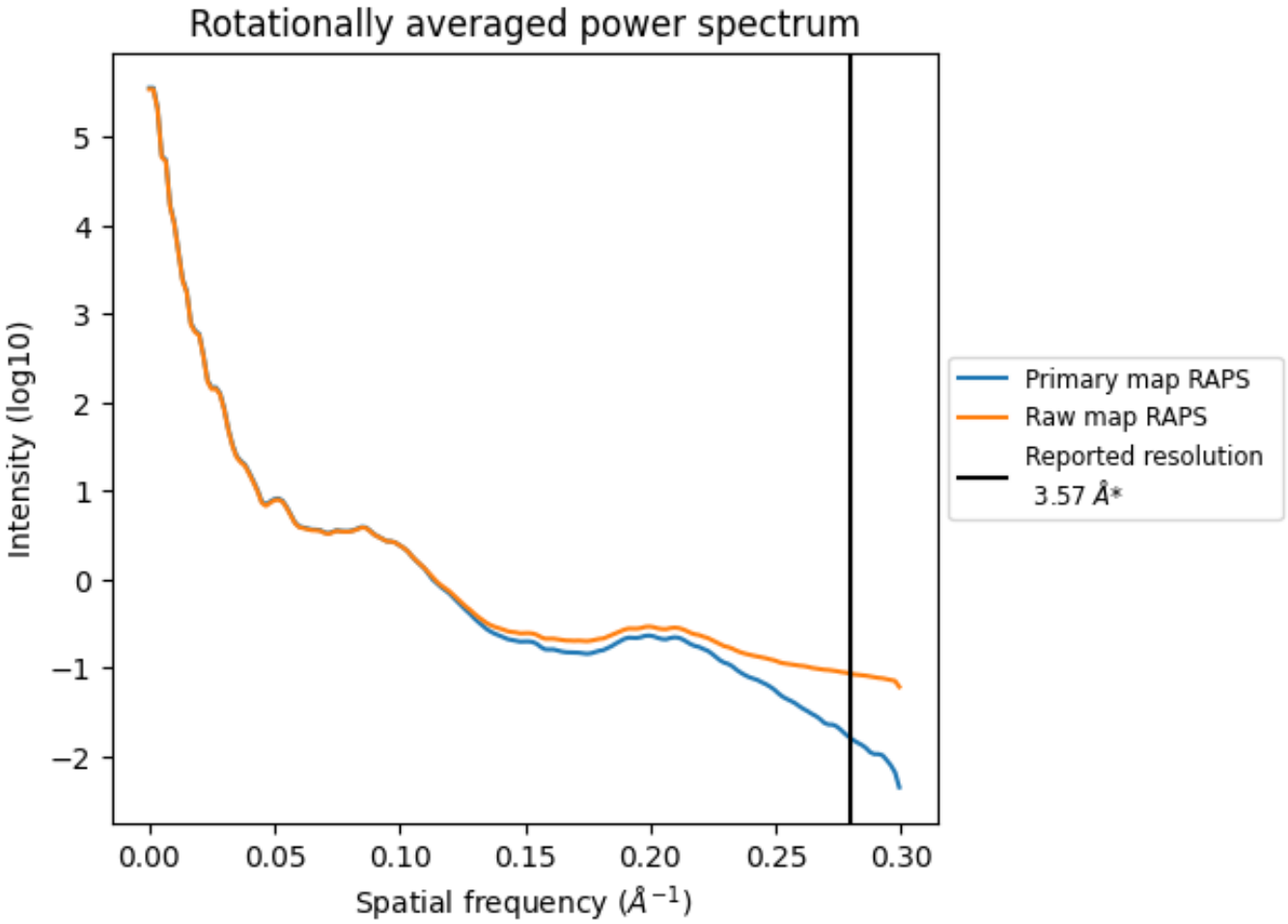
7.2 Volume estimate



The volume at the recommended contour level is 2186 nm^3; this corresponds to an approximate mass of 1974 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)

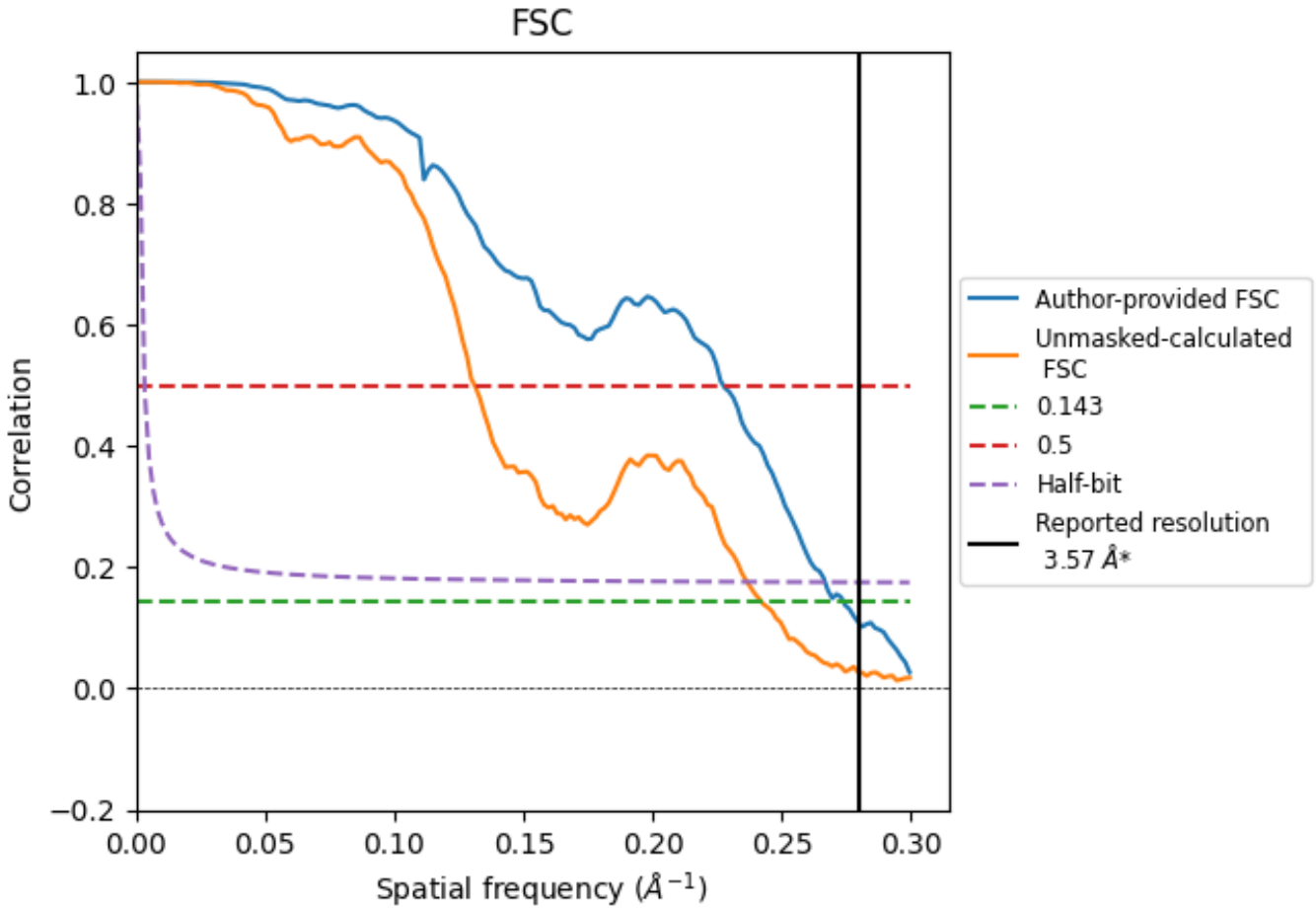


*Reported resolution corresponds to spatial frequency of 0.280 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.280 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.65	4.40	3.75
Unmasked-calculated*	4.13	7.63	4.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.57 by more than 10 %

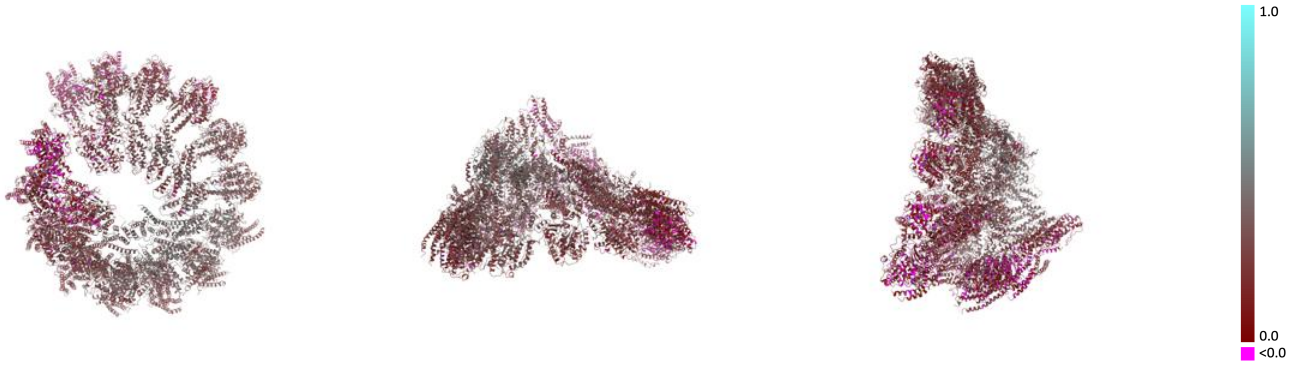
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19570 and PDB model 8RX1. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay

This section was not generated.

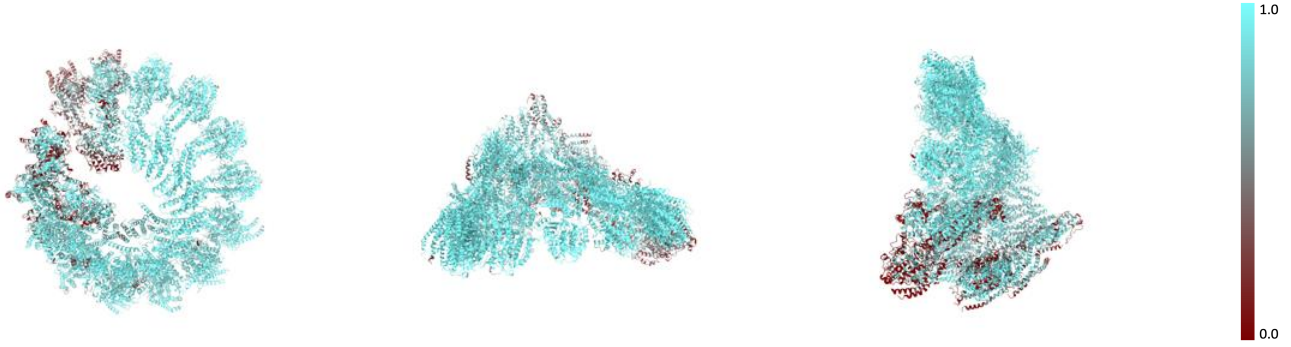
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

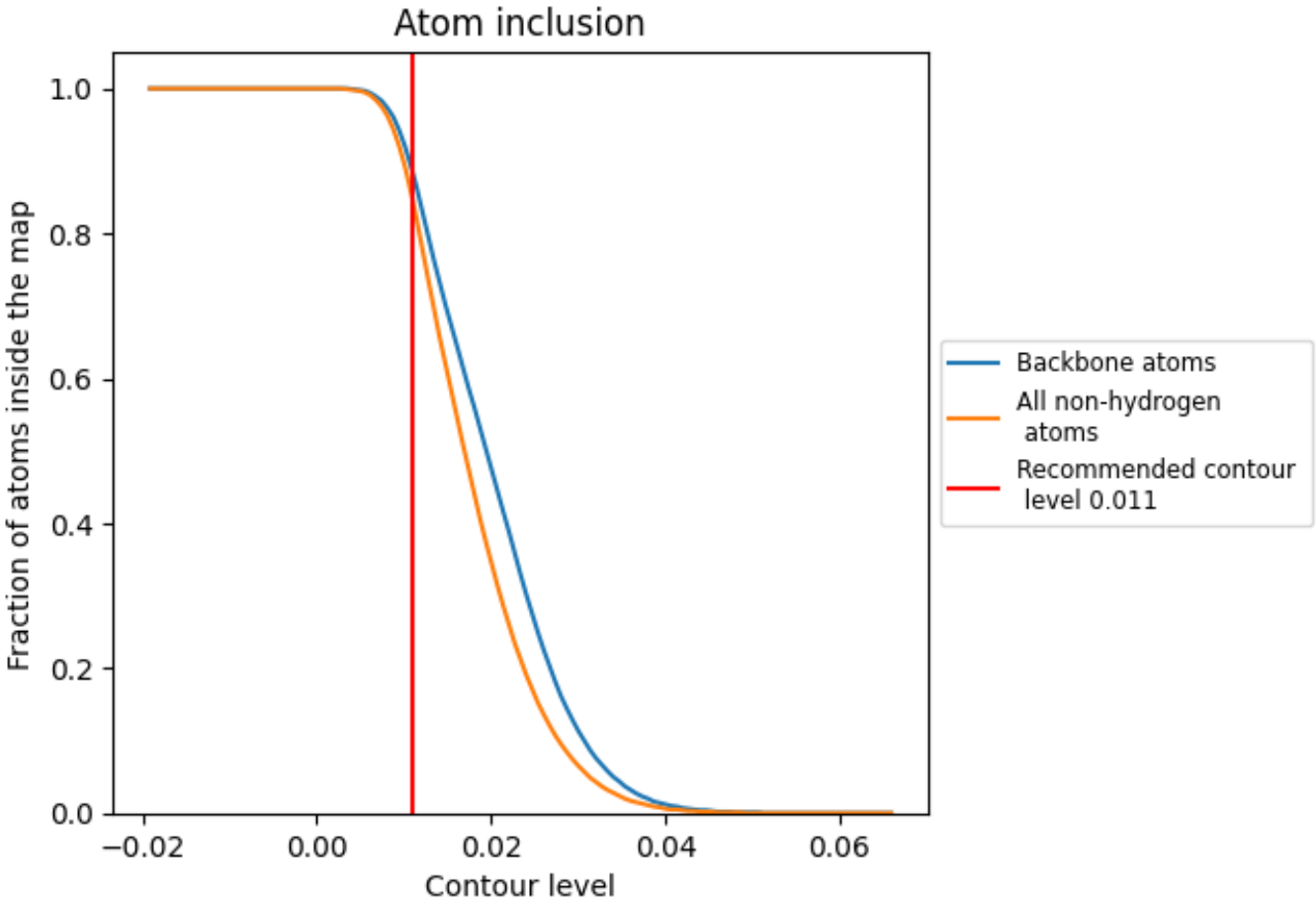
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.2420
1	0.6500	0.1390
2	0.2930	0.1280
7	0.7740	0.2890
A	0.5960	0.0970
B	0.7720	0.2080
C	0.8890	0.2370
D	0.9390	0.2560
E	0.9270	0.3150
F	0.9630	0.3150
G	0.8450	0.2400
H	0.7190	0.2450
I	0.9670	0.3310
J	0.9680	0.3030
K	0.9860	0.2860
L	0.9870	0.2510
M	0.7860	0.1870
N	0.3640	0.1570
O	0.5060	0.1430
P	0.6560	0.1500
Q	0.8800	0.1800
R	0.9380	0.1760
S	0.9840	0.2480
T	0.9640	0.2310
U	0.9760	0.2810
V	0.9640	0.3260
W	0.9760	0.2510
X	0.9800	0.2330
Y	0.9780	0.1470
Z	0.9680	0.1580
a	0.8470	0.3880
b	0.8690	0.4020
c	0.7440	0.2880
d	0.8240	0.3470
e	0.5630	0.3180



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.5280	0.2940
g	0.9560	0.2570
h	0.5900	0.2510
i	0.5990	0.2530
j	0.4390	0.2430
k	0.9510	0.3560
n	0.9730	0.3800
s	0.9260	0.2890
t	0.9830	0.3430
u	0.8680	0.2570
v	0.9520	0.2860