



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:31 AM UTC

PDB ID : 7QJ8 / pdb_00007qj8
EMDB ID : EMD-14013
Title : Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 3-14, substoichiometric spokes 1-2)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 8.70 Å (reported)
Based on initial models : 6X0U, 6V6S, 6L81, 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 EMD 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

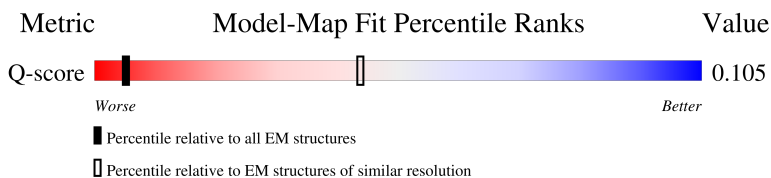
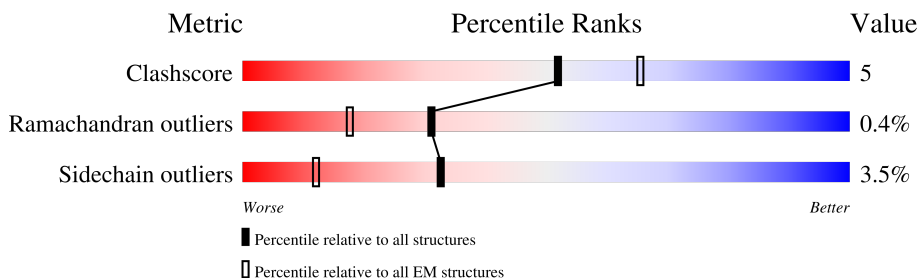
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 Å.

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



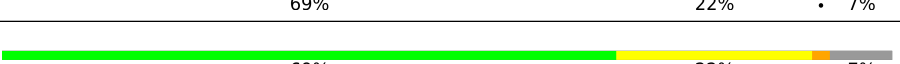
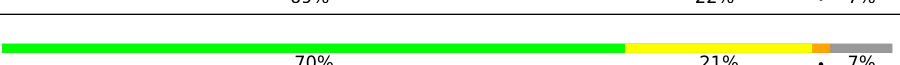
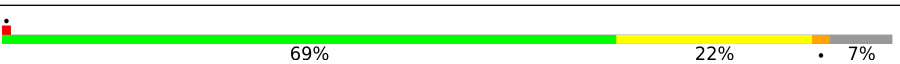
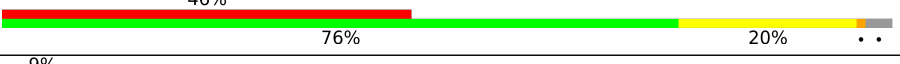
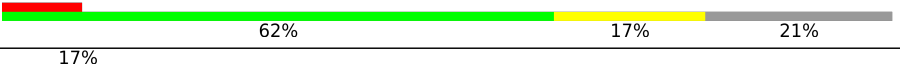
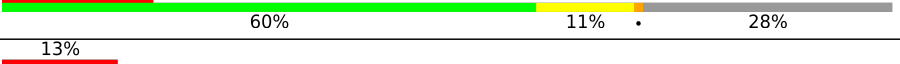
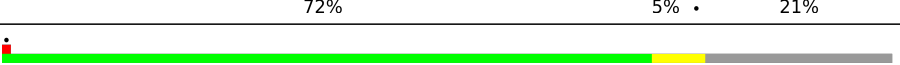
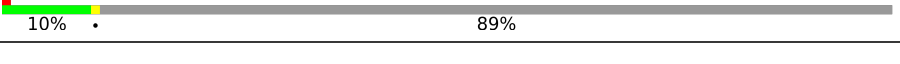
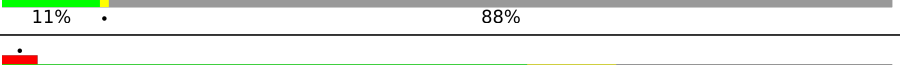
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	282 (8.20 - 9.20)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	J	1024	
1	1	1024	
2	1	451	
2	2	451	

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Mol	Chain	Length	Quality of chain
2	Q	451	
2	R	451	
2	S	451	
2	T	451	
2	U	451	
2	V	451	
2	W	451	
2	X	451	
2	Y	451	
2	Z	451	
3	e	375	
4	b	82	
4	d	82	
4	i	82	
4	k	82	
4	m	82	
5	D	907	
5	F	907	
5	H	907	
5	N	907	
5	a	907	
5	h	907	
5	j	907	
6	C	902	
6	E	902	

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Mol	Chain	Length	Quality of chain
6	G	902	
6	M	902	
7	I	667	
7	K	667	
8	L	1819	
8	c	1819	

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

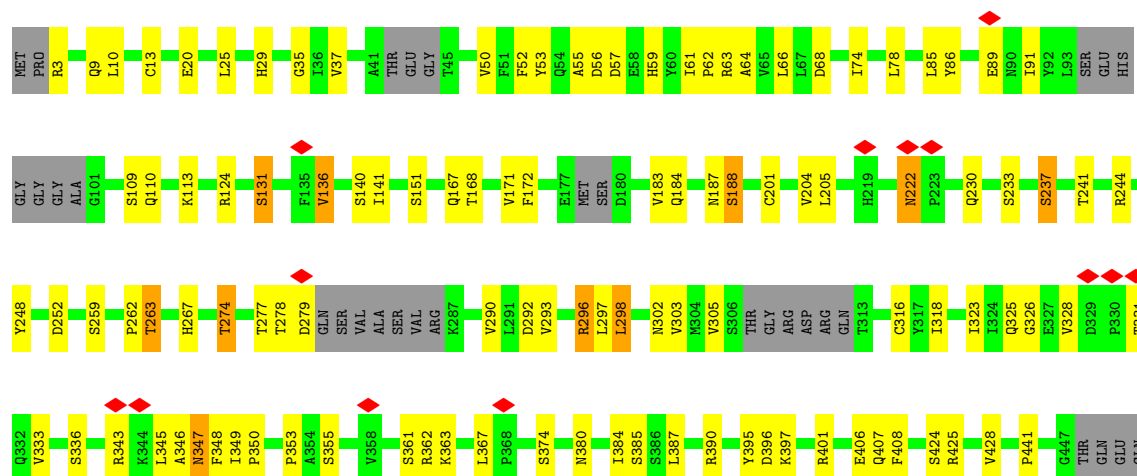
- Molecule 8 is a protein called Gamma-tubulin complex component 6.

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

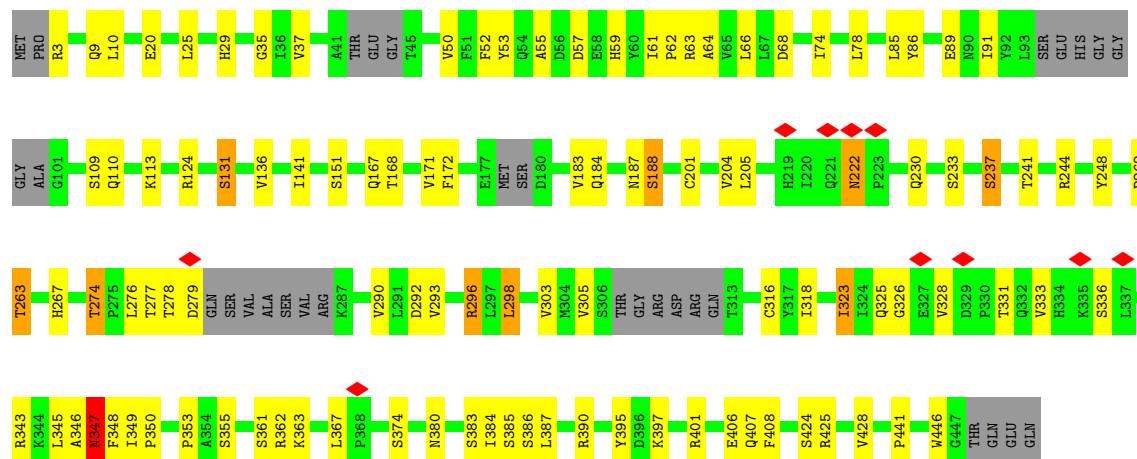
- Molecule 9 is water.

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

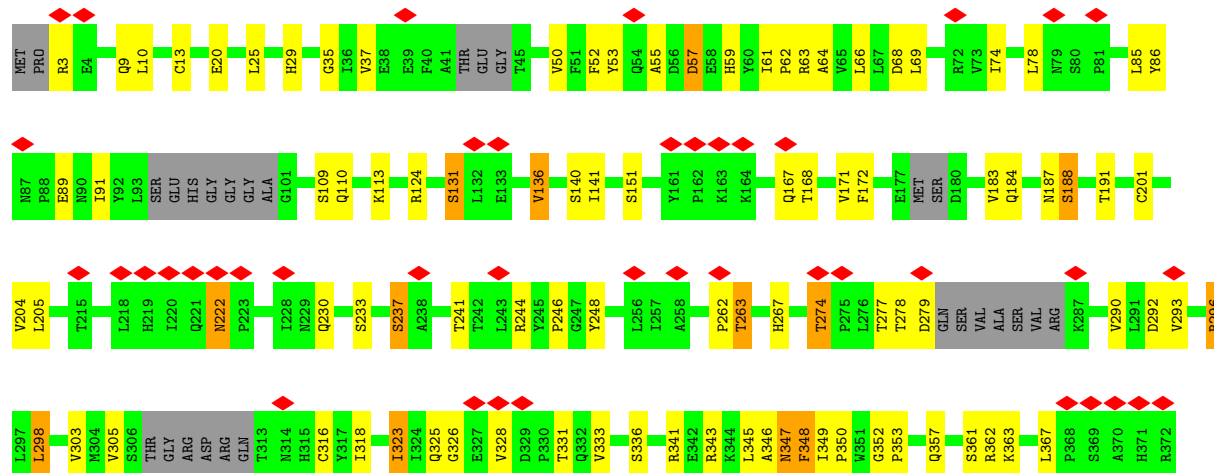


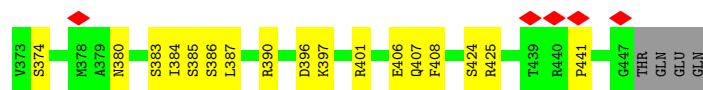


• Molecule 2: Tubulin gamma-1 chain

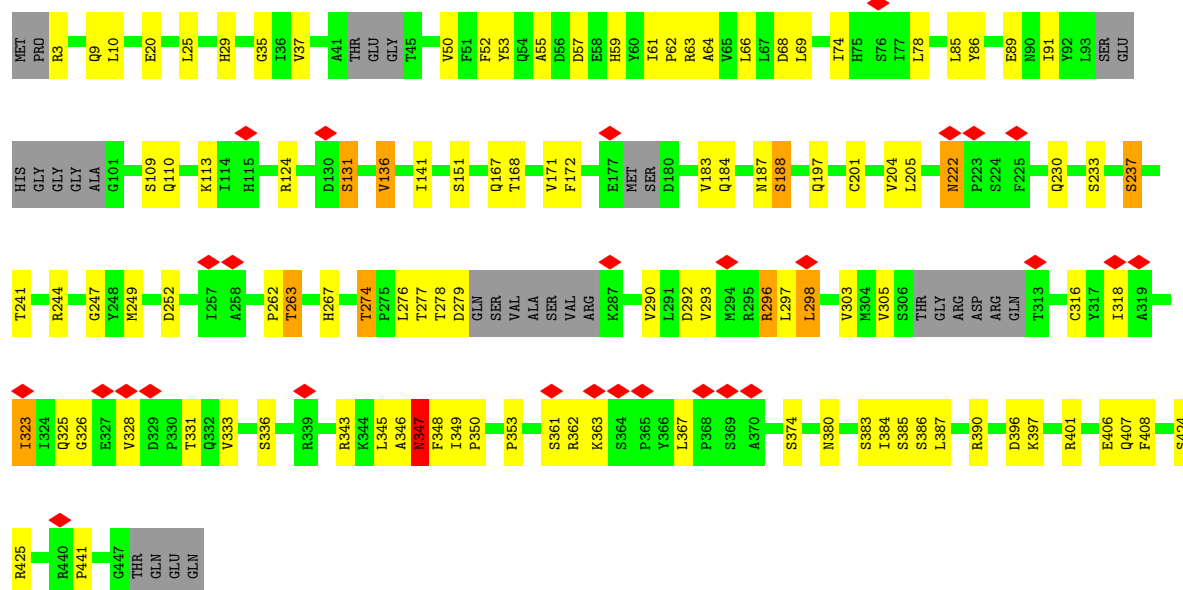


• Molecule 2: Tubulin gamma-1 chain

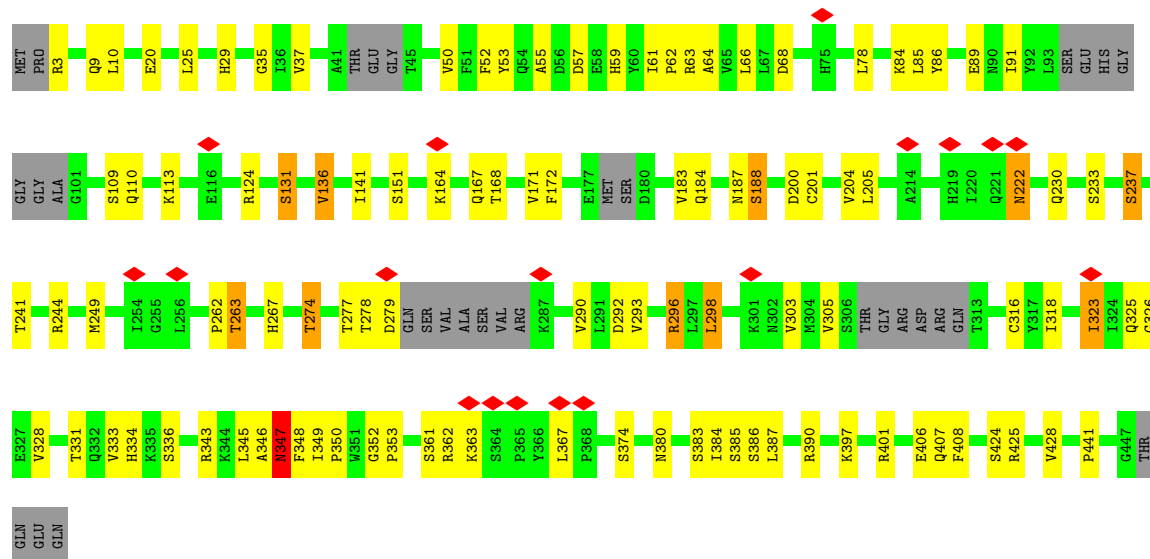




• Molecule 2: Tubulin gamma-1 chain

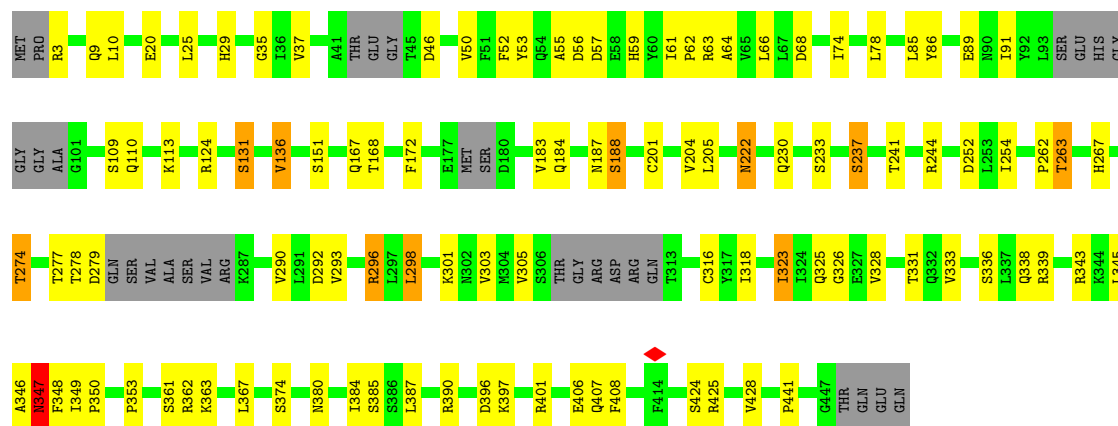


• Molecule 2: Tubulin gamma-1 chain



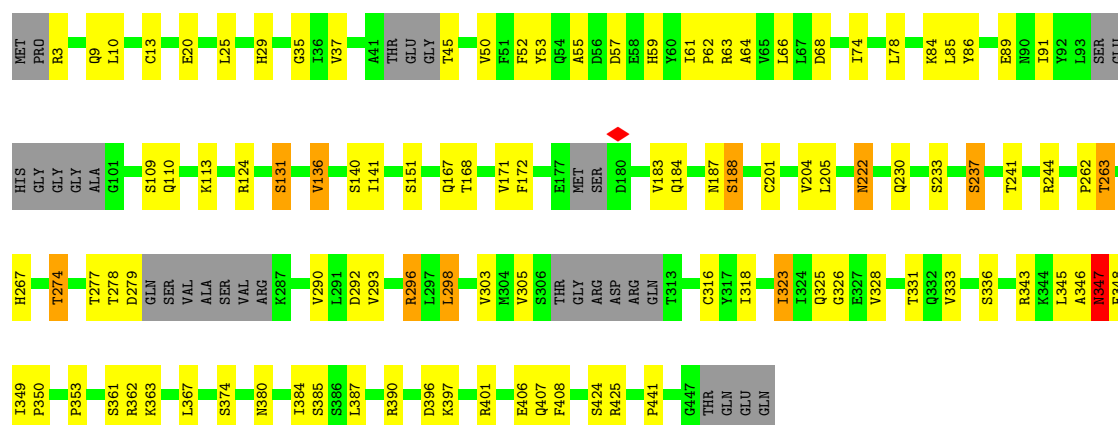
• Molecule 2: Tubulin gamma-1 chain





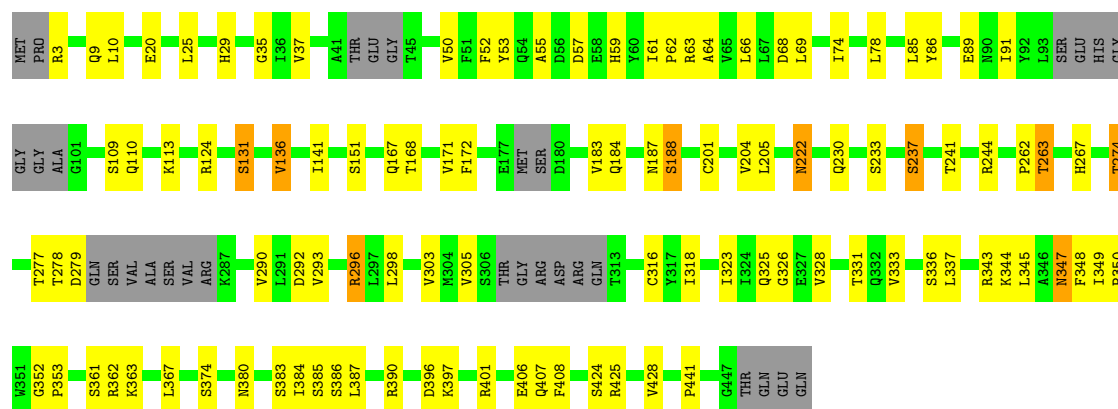
• Molecule 2: Tubulin gamma-1 chain

Chain U: 70% 21% 7%



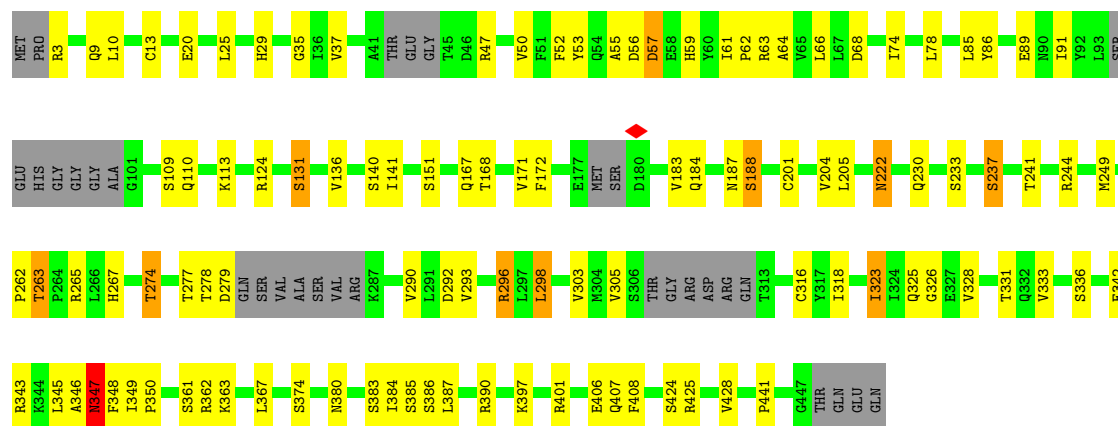
• Molecule 2: Tubulin gamma-1 chain

Chain V: 69% 22% 7%



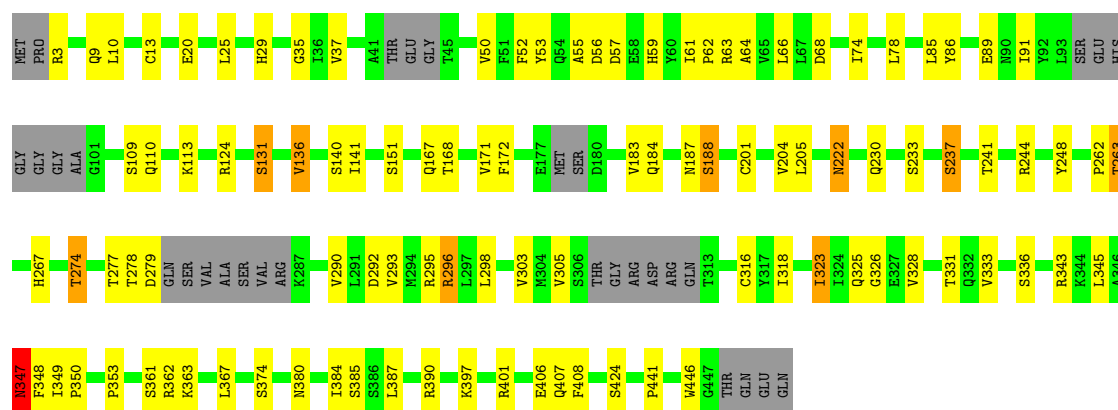
• Molecule 2: Tubulin gamma-1 chain

Chain W: 69% 22% 7%



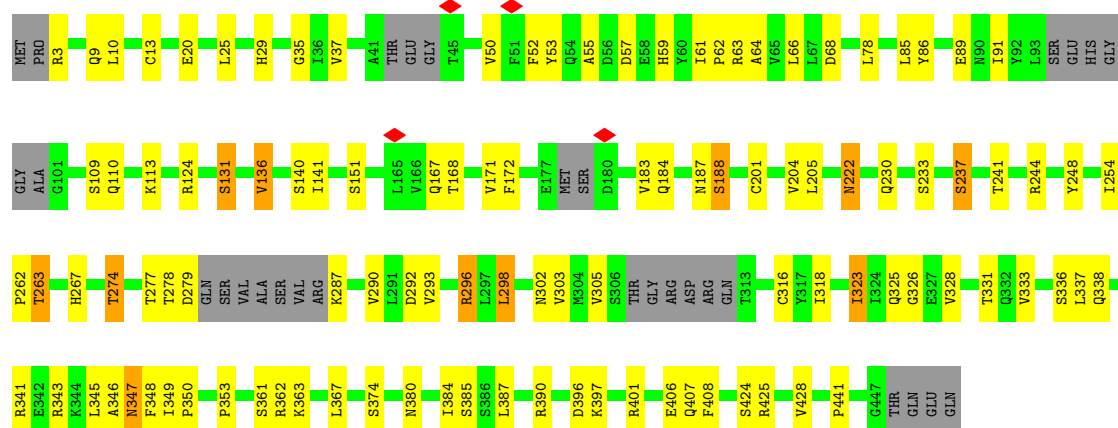
• Molecule 2: Tubulin gamma-1 chain

Chain X: 70% 21% 7%



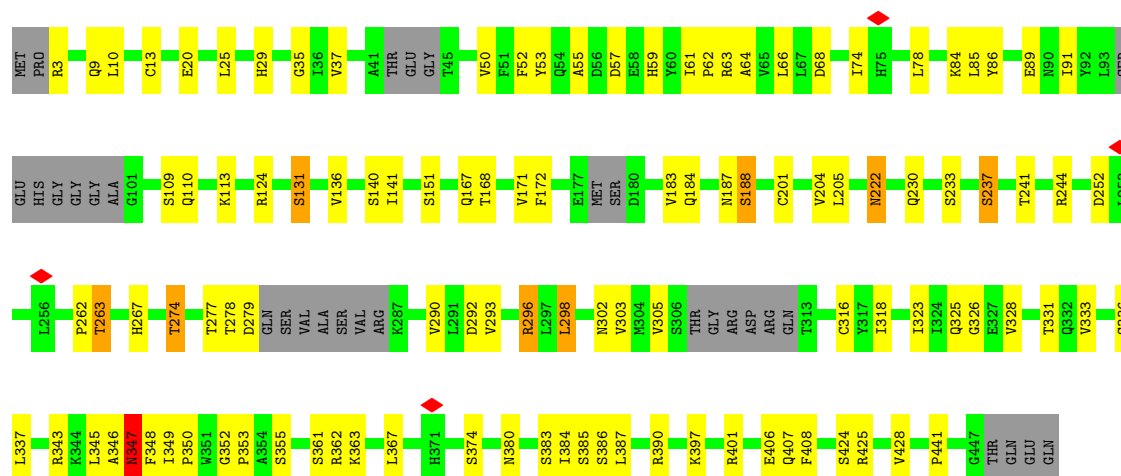
• Molecule 2: Tubulin gamma-1 chain

Chain Y: 69% 22% 7%

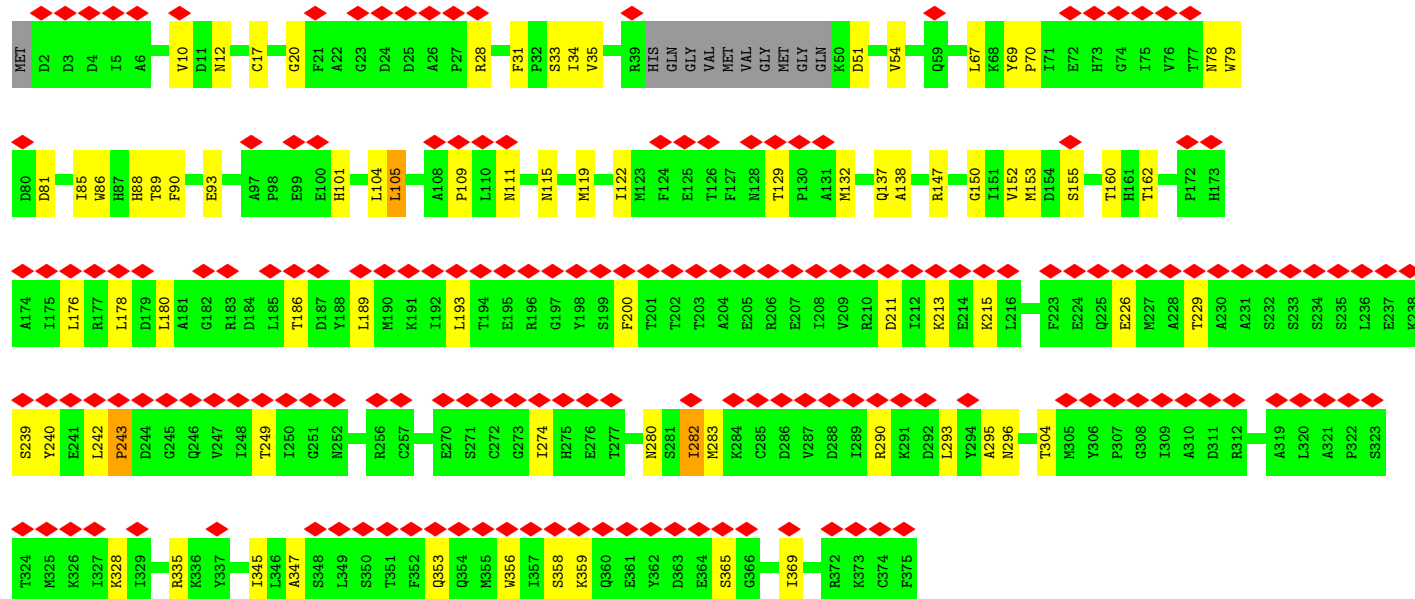
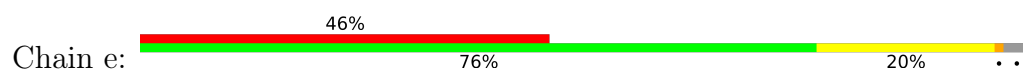


• Molecule 2: Tubulin gamma-1 chain

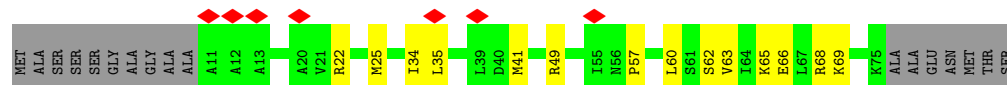
Chain Z: 69% 23% 7%



• Molecule 3: actin, cytoplasmic 1

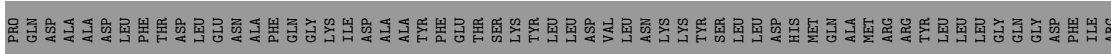


• Molecule 4: Mitotic-spindle organizing protein 1



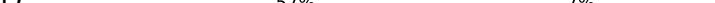
• Molecule 4: Mitotic-spindle organizing protein 1





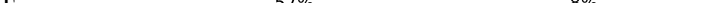
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THR	GLY	THR	THR	THR	PHE	VAL	LEU
THR	GLN	ILE	ILE	ILE	SER	PHE	LEU
THR	TRP	ILE	GLY	GLY	LEU	ASP	ASP
THR	VAL	ARG	GLY	ASP	LEU	ASP	LEU
THR	THR	CYS	THR	CYS	HIS	TYR	LYS
THR	ALA	LEU	LEU	GLN	GLN	HIS	PRO
THR	ALA	LEU	ALA	LEU	VAL	VAL	GLU
THR	GLU	ASP	ASP	ASP	CYS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

- Molecule 5: Gamma-tubulin complex component 3

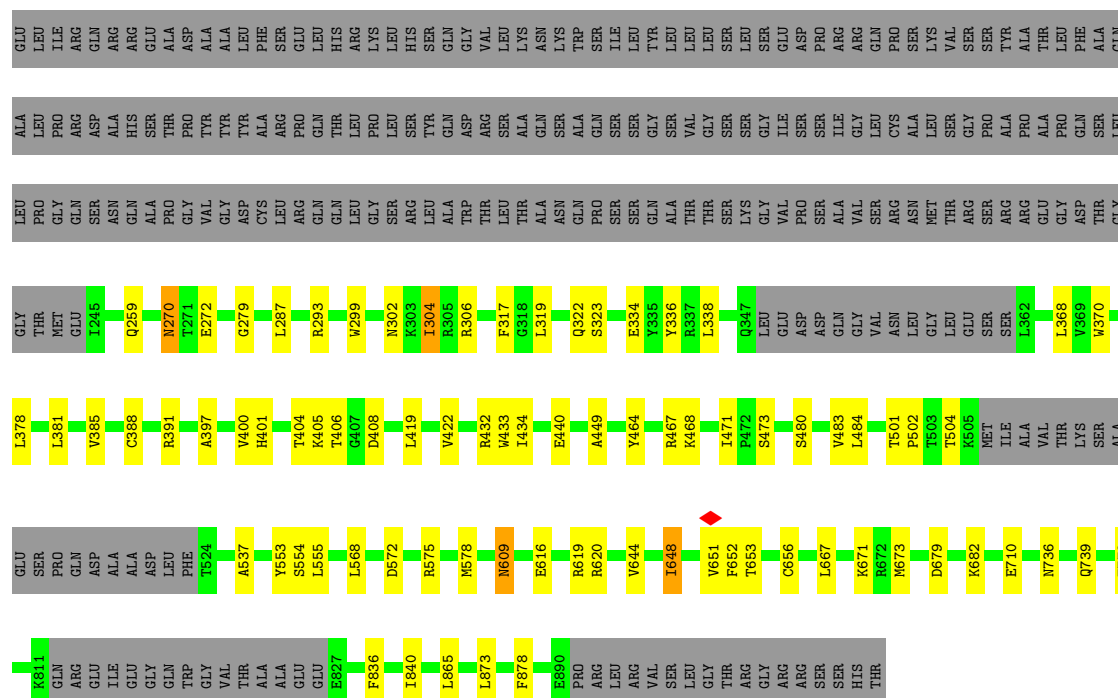
Chain D:  57% 7% 36%

Y720	THR	V369	GLY	LEU	ALA	GLU	MET
ASP	W370	THR	THR	PRO	ALA	LEU	ALA
LEU		MET	GLU	GLY	PRO	ILE	THR
GLU	K379	THR	GLU	GLN	ARG	GLN	PRO
ASN	T380	ASN	1245	SER	ASP	GLN	ASP
ALA	L381	ALA	1254	GLN	ALA	ARG	GLN
PHE				ASN	HIS	ARG	LYS
Q531	R391	R391	1261	ALA	SER	GLU	SER
T541	A399	A399	1266	PRO	THR	ALA	PRO
M550	A402	A402	1273	VAL	PRO	ASN	ASN
L556	T406	T406		GLY	TVR	ALA	VAL
Q570	P409	P409		ASP	TVR	LEU	LEU
L581	T410	T410		CYS	ALA	PHE	GLN
L587	M411	M411		ARG	ARG	SER	ASN
P588	R412	R412		GLN	PRO	LEU	LEU
A589				THR	GLN	HIS	CYS
T590	L418	L418		GLY	PRO	LYS	ILE
L591	P425	P425		ARG	LEU	ARG	ARG
L592	T426	T426		SER	SER	HIS	LEU
L593	L427	L427		LEU	TVR	SER	GLY
	L428	L428		ASN	GLN	GLN	SER
	S428	S428		ARG	ASP	GLY	GLU
	F429	F429		THR	ARG	VAL	ALA
	L430	L430		THR	ALA	LYS	VAL
				ALA	GLN	ASN	ALA
L597	R481	R481		ASN	SER	LYS	GLN
L601	K482	K482		GLN	ALA	TRP	GLN
N609				PRO	GLN	SER	PHE
D613	L486	L486		SER	SER	ILE	GLN
				SER	SER	LEU	TYR
T617	Q495	Q495		GLN	GLY	TYR	ALA
				ALA	SER	LEU	VAL
				THR	VAL	LEU	ARG
				THR	GLY	LEU	VAL
	Q500	Q500		THR	GLY	SER	VAL
	T501	T501		GLN	SER	LEU	GLY
	P502	P502		LYS	SER	SER	GLY
	THR	THR		LEU	ILE	GLU	ASN
	THR	THR		GLY	GLY	GLU	ASN
	LYS	LYS		VAL	ILE	VAL	PRO
	MET	MET		SER	SER	ARG	THR
	ILE	ILE		GLN	ALA	GLY	VAL
	T653	T653		VAL	GLY	LEU	VAL
	R654	R654		ASN	SER	PRO	GLU
	E655	E655		THR	ASN	CYS	ARG
	THR	THR		LYS	LEU	ALA	ARG
	F666	F666		SER	ASN	SER	ARG
	ALA	ALA		ALA	LEU	LYS	ASP
	GLU	GLU		GLY	THR	VAL	GLU
	R669	R669		LEU	THR	GLY	PHE
				SER	SER	SER	LEU
	R681	R681		PRO	PRO	TYR	VAL
				GLN	ALA	ALA	ALA
	A688	A688		ASP	PRO	THR	GLU
	R699	R699		ALA	ALA	GLY	LYS
				ALA	ALA	PHE	ILE
	R692	R692		ASP	GLN	THR	LYS
				LEU	SER	GLN	ASN
				LEU	THR	GLY	LYS

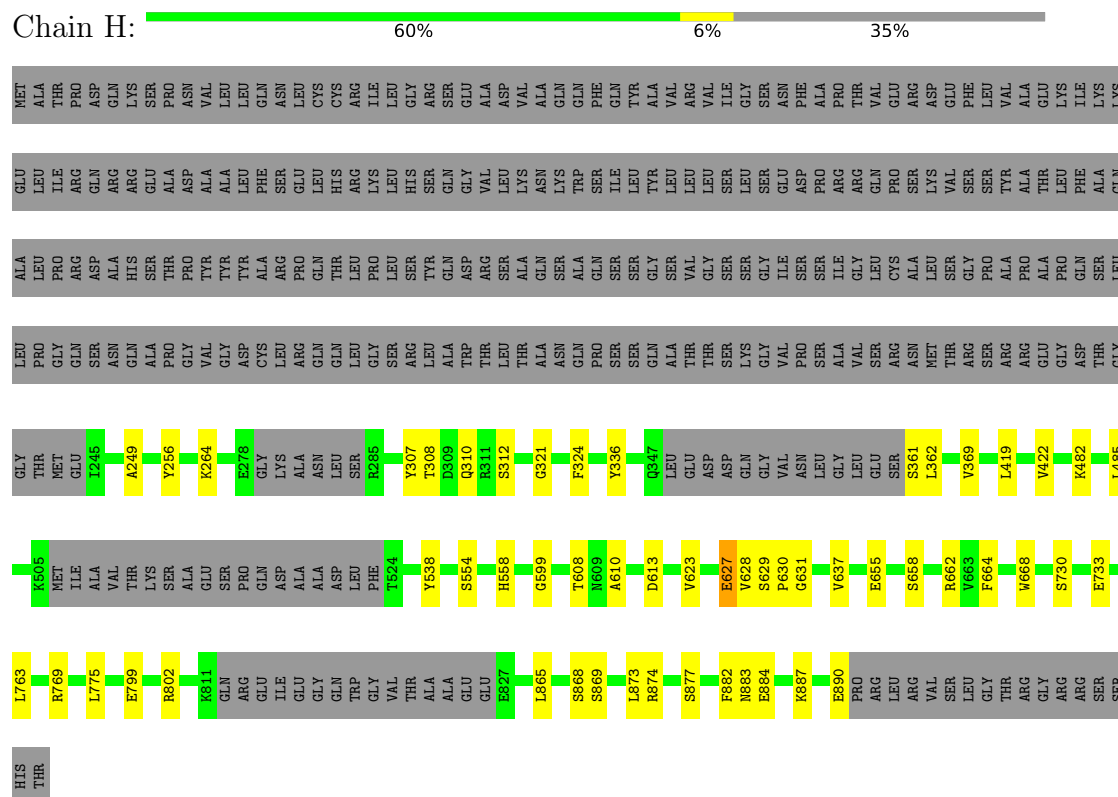
- Molecule 5: Gamma-tubulin complex component 3

Chain F:  57% 8% 34%

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

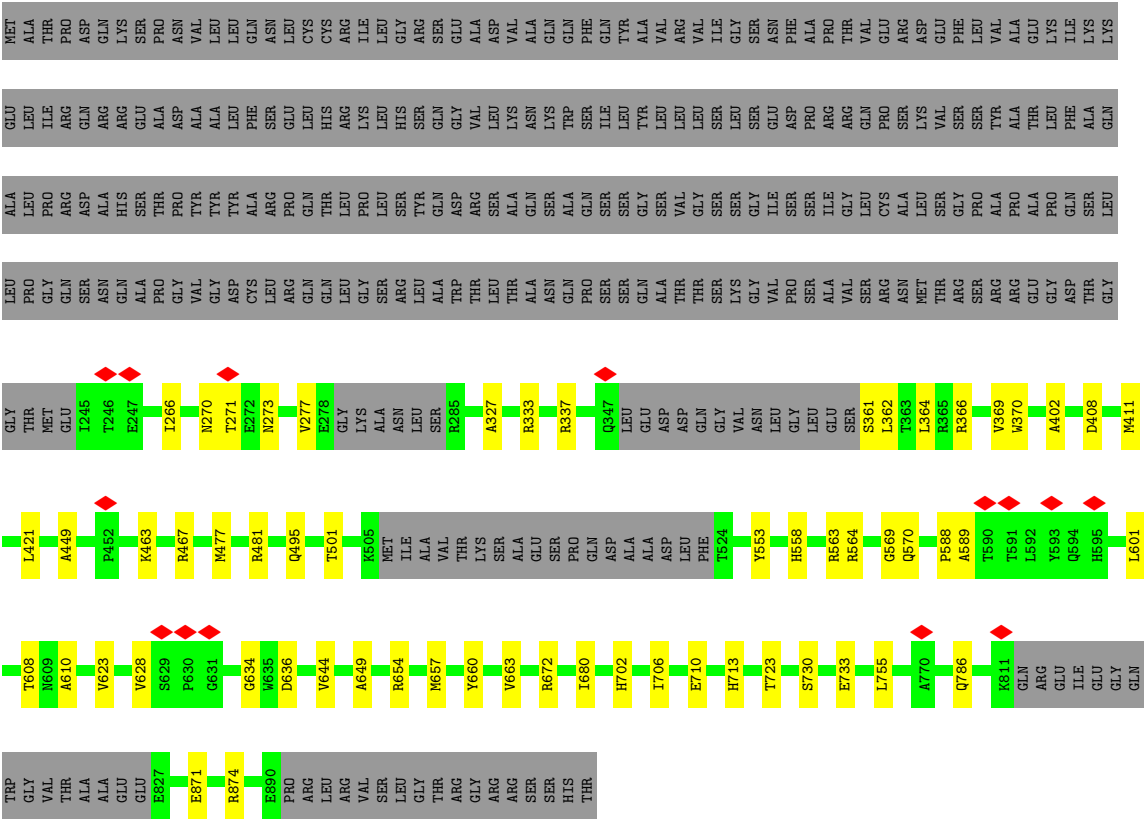


• Molecule 5: Gamma-tubulin complex component 3

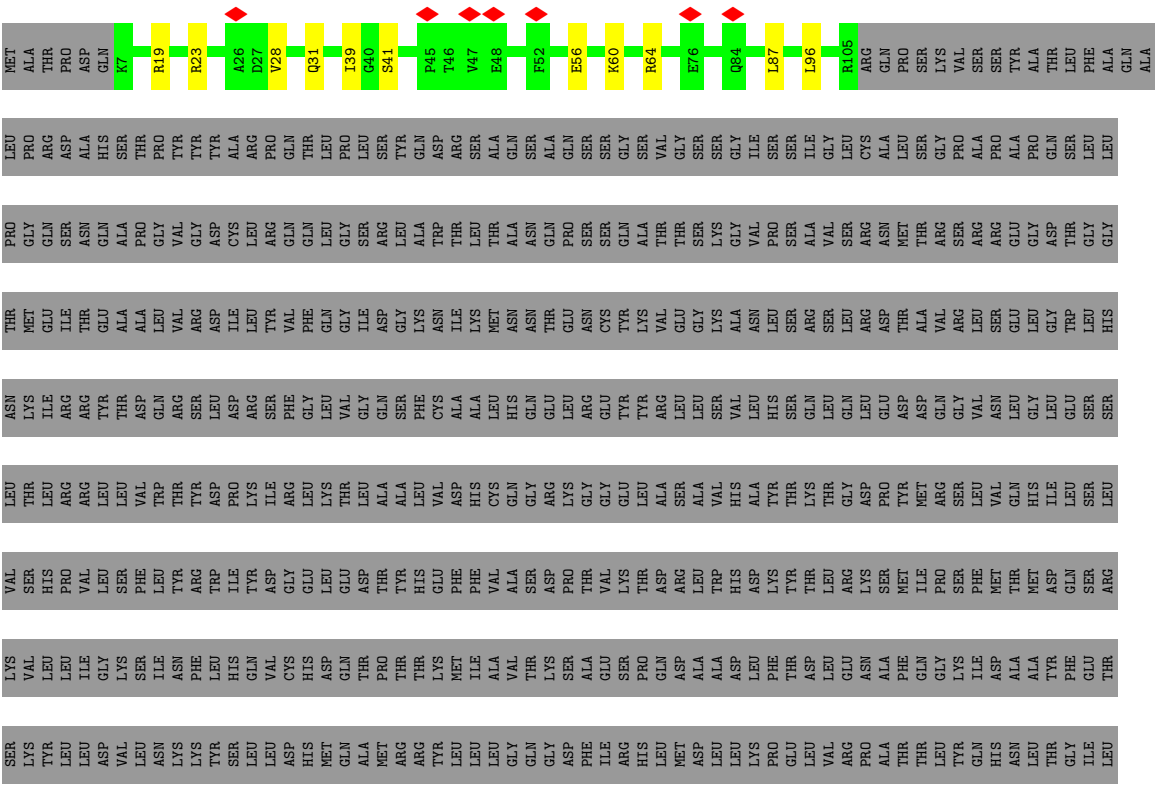


• Molecule 5: Gamma-tubulin complex component 3





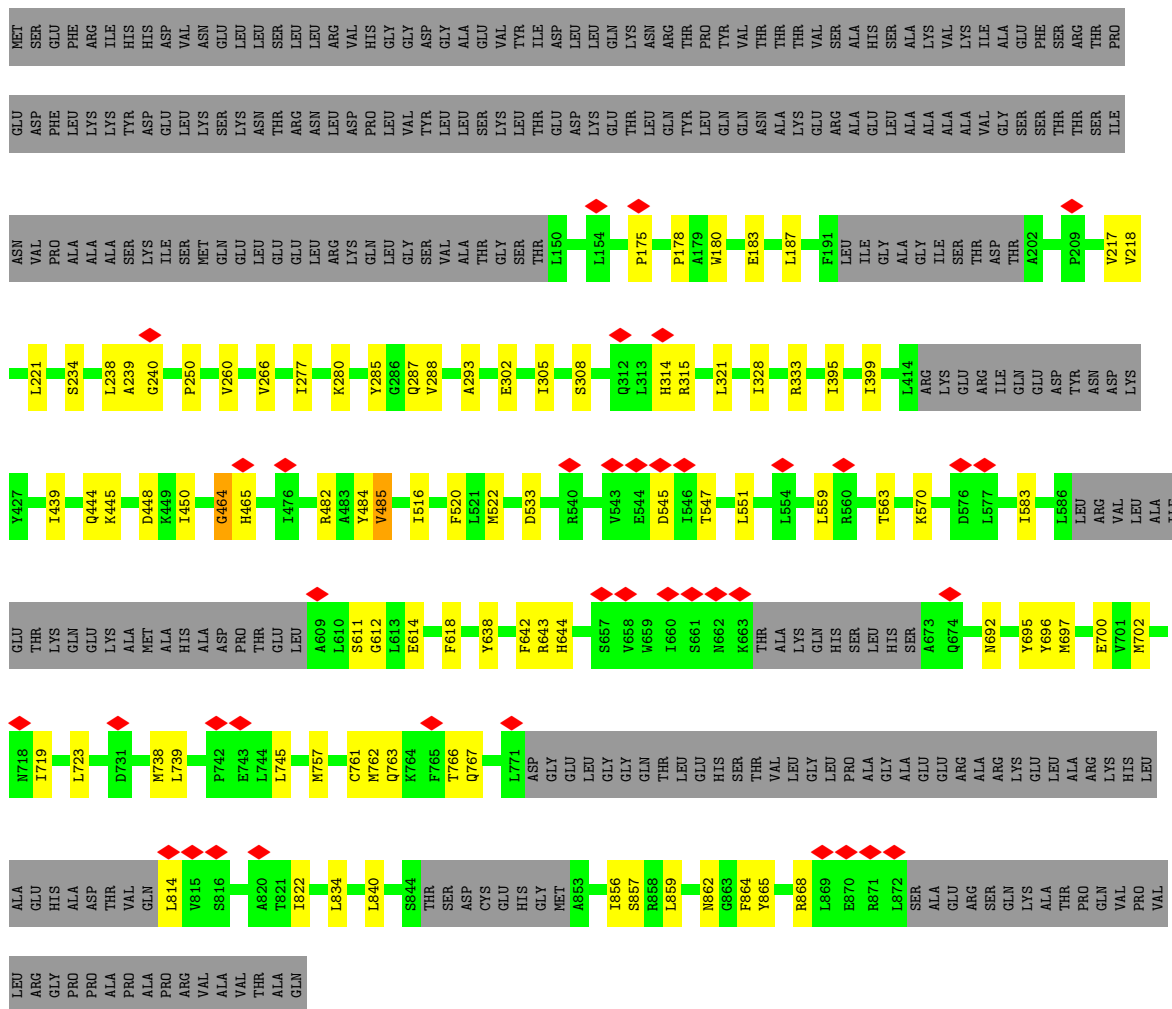
● Molecule 5: Gamma-tubulin complex component 3



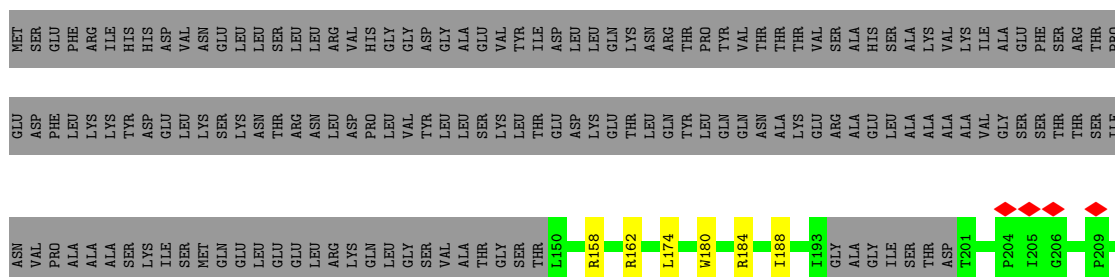
- Molecule 5: Gamma-tubulin complex component 3

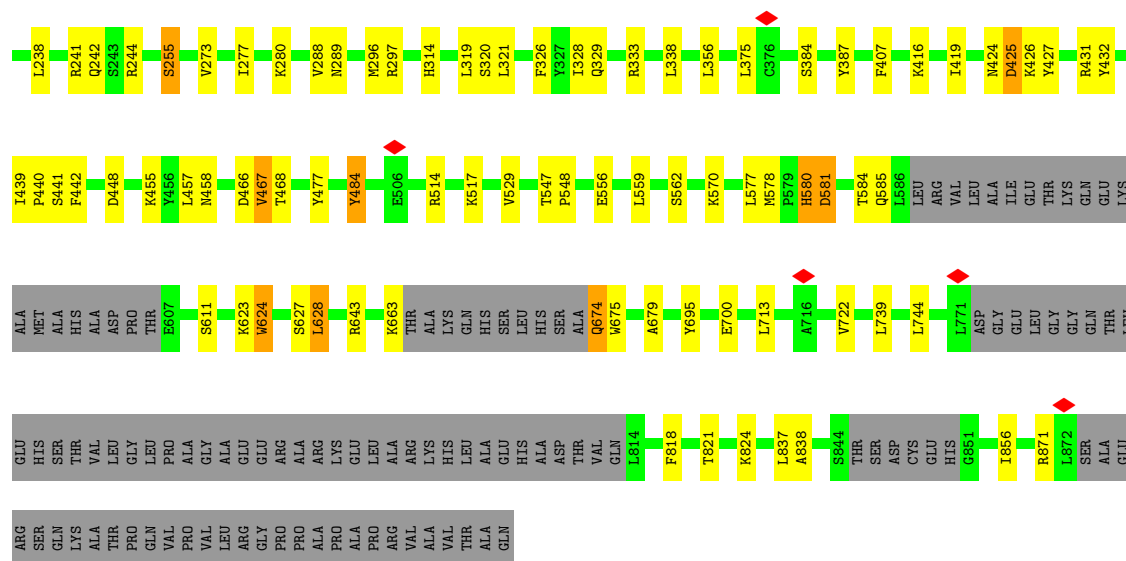
[illegible]

- Molecule 6: Gamma-tubulin complex component 2



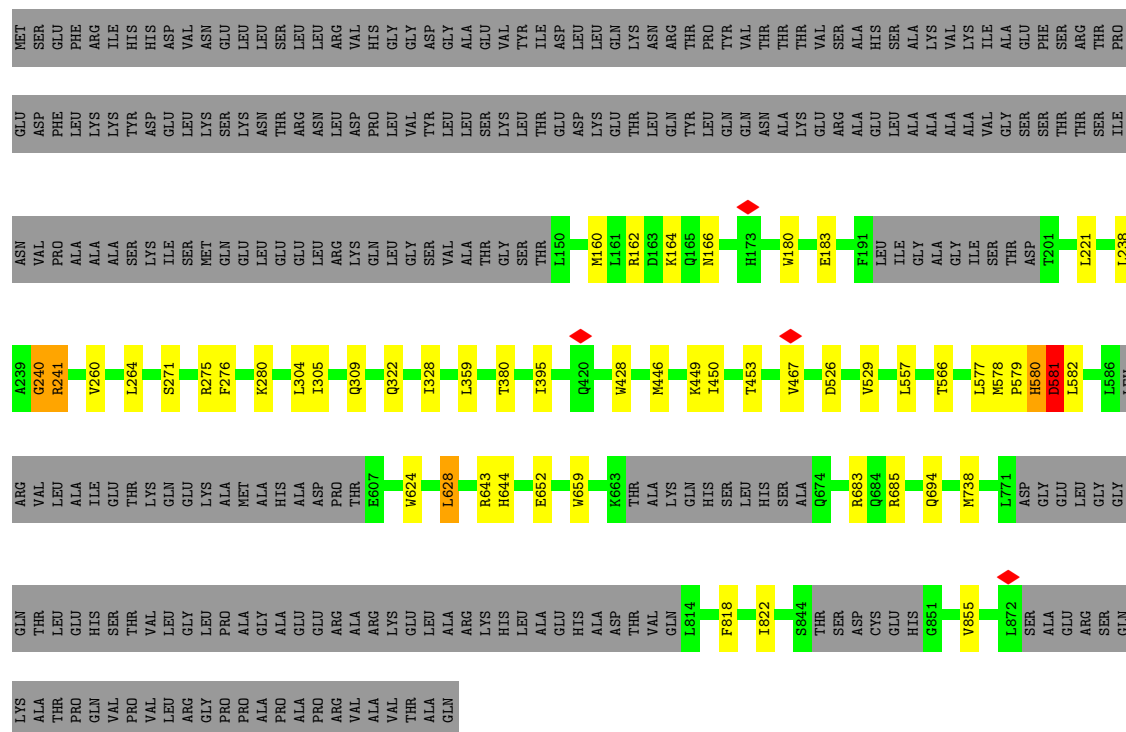
- Molecule 6: Gamma-tubulin complex component 2





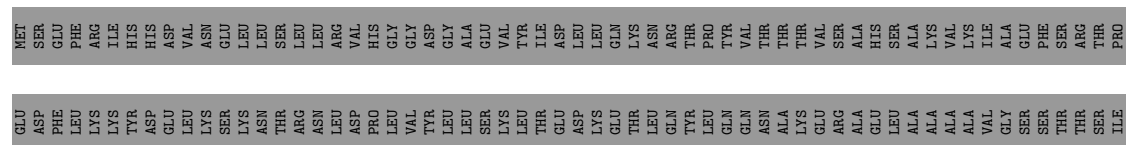
• Molecule 6: Gamma-tubulin complex component 2

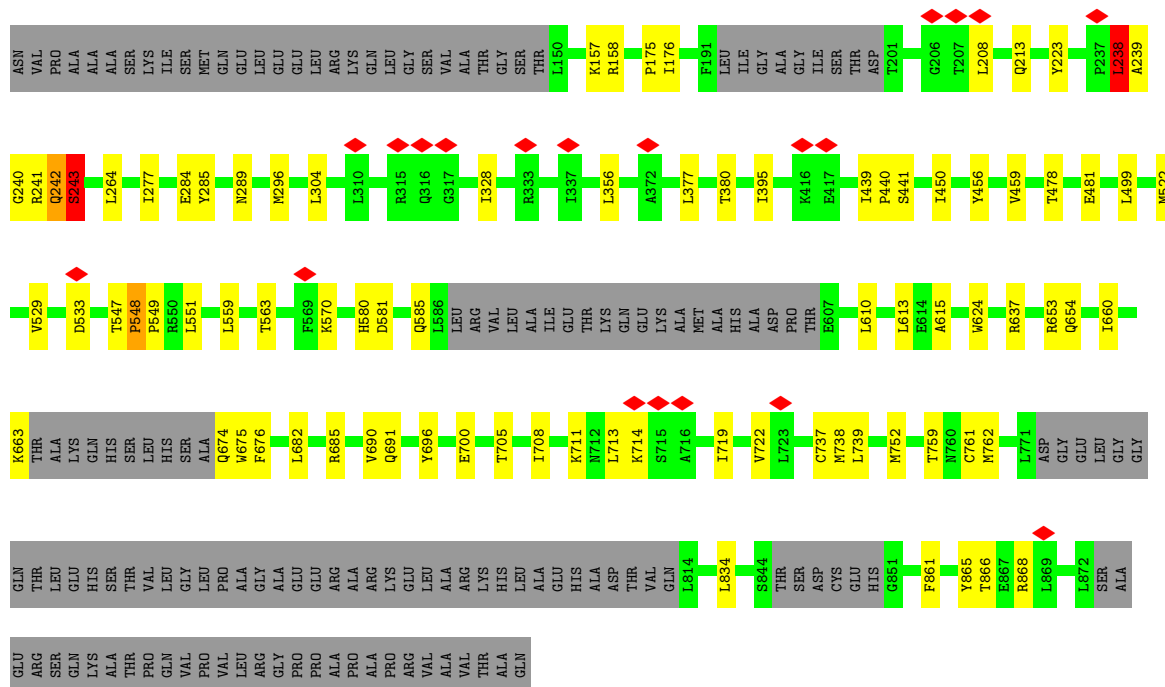
Chain G: 65% 5% 29%



• Molecule 6: Gamma-tubulin complex component 2

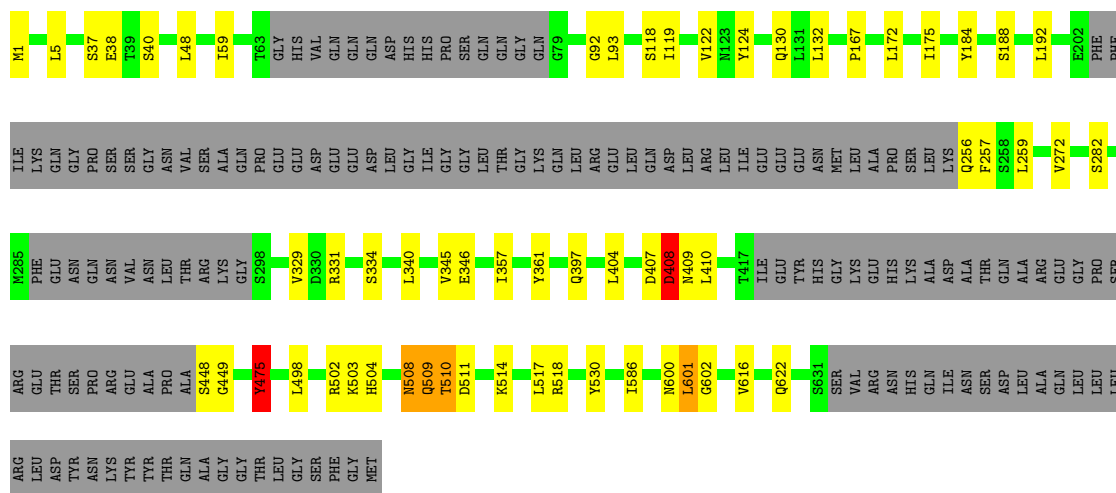
Chain M: 61% 9% 29%





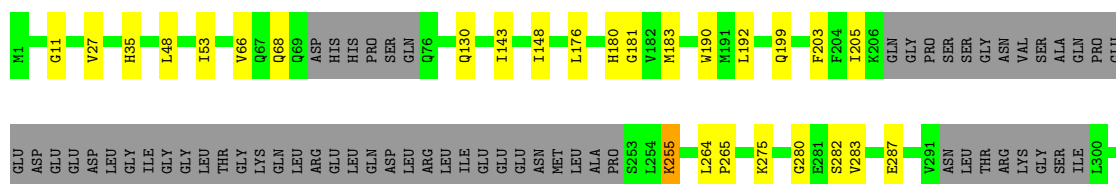
• Molecule 7: Gamma-tubulin complex component 4

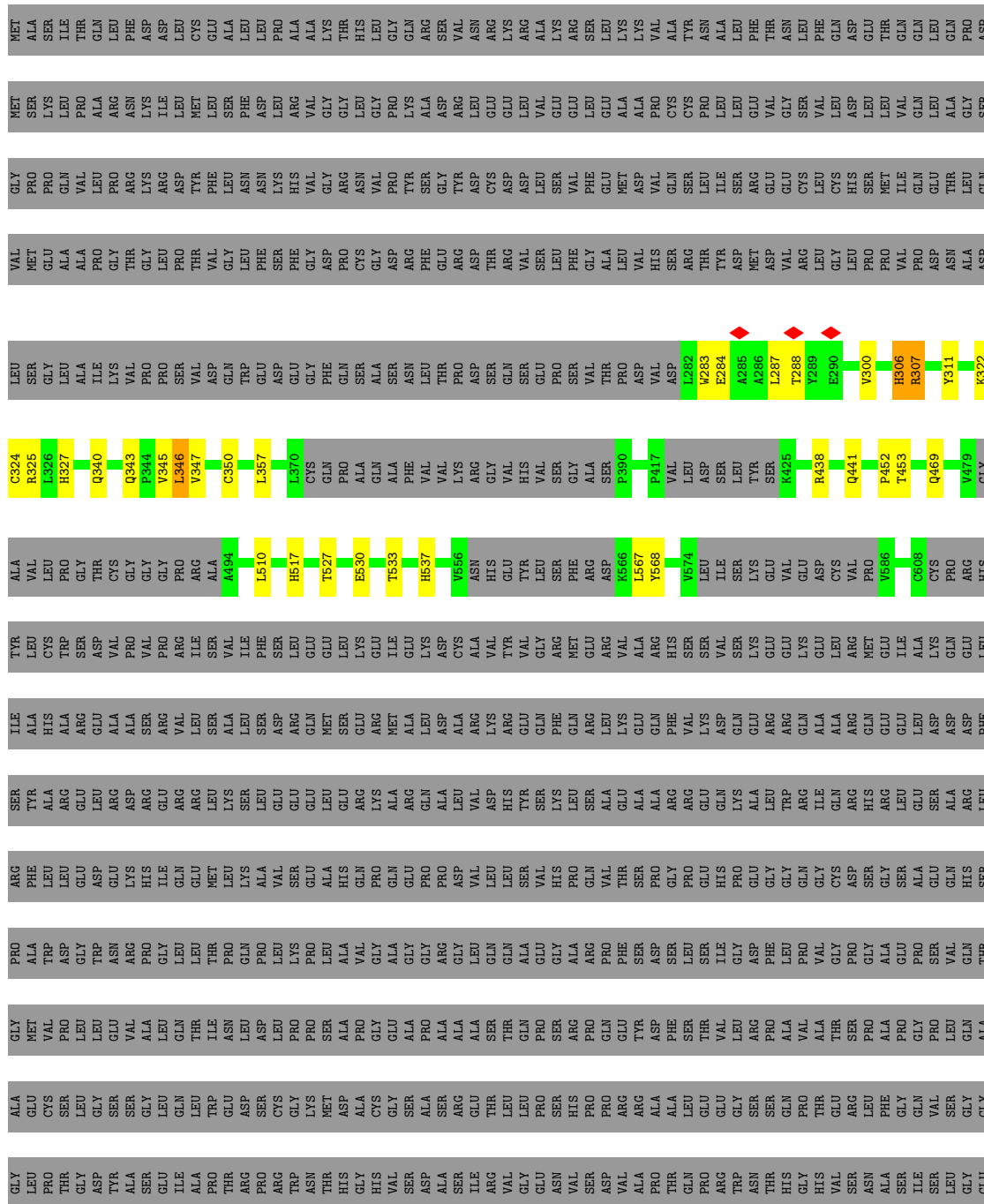
Chain I: 69% 8% 22%



• Molecule 7: Gamma-tubulin complex component 4

Chain K: 75% 9% 16%







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

4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	J	0.36	0/4525	0.80	7/6119 (0.1%)
1	l	0.28	0/863	0.75	2/1166 (0.2%)
2	1	0.24	0/3441	0.60	0/4661
2	2	0.24	0/3441	0.60	0/4661
2	Q	0.24	0/3441	0.60	0/4661
2	R	0.24	0/3441	0.60	0/4661
2	S	0.24	0/3441	0.60	0/4661
2	T	0.24	0/3441	0.60	0/4661
2	U	0.24	0/3441	0.60	0/4661
2	V	0.24	0/3441	0.60	0/4661
2	W	0.24	0/3441	0.60	0/4661
2	X	0.24	0/3441	0.60	0/4661
2	Y	0.24	0/3441	0.60	0/4661
2	Z	0.24	0/3441	0.60	0/4661
3	e	0.51	1/2908 (0.0%)	0.80	2/3938 (0.1%)
4	b	0.32	0/484	0.73	0/653
4	d	0.33	0/454	0.77	0/611
4	i	0.26	0/484	0.62	0/653
4	k	0.25	0/484	0.61	0/653
4	m	0.28	0/484	0.65	0/653
5	D	0.35	0/4897	0.72	4/6610 (0.1%)
5	F	0.33	0/5044	0.73	1/6809 (0.0%)
5	H	0.31	0/5009	0.69	4/6761 (0.1%)
5	N	0.32	0/5009	0.73	2/6761 (0.0%)
5	a	0.28	0/948	0.70	0/1277
5	h	0.28	0/815	0.64	1/1096 (0.1%)
5	j	0.26	0/855	0.87	7/1152 (0.6%)
6	C	0.37	0/5151	0.82	9/6955 (0.1%)
6	E	0.43	2/5311 (0.0%)	0.79	8/7169 (0.1%)
6	G	0.33	1/5295 (0.0%)	0.72	6/7147 (0.1%)
6	M	0.37	1/5295 (0.0%)	0.80	11/7147 (0.2%)
7	I	0.35	0/4322	0.75	5/5853 (0.1%)
7	K	0.37	1/4683 (0.0%)	0.77	9/6338 (0.1%)
8	L	0.36	0/4697	0.78	9/6348 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	c	0.32	0/1235	0.76	4/1664 (0.2%)
All	All	0.32	6/110544 (0.0%)	0.70	91/149465 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	2
1	l	0	1
2	1	0	4
2	2	0	4
2	Q	0	4
2	R	0	4
2	S	0	4
2	T	0	4
2	U	0	4
2	V	0	4
2	W	0	4
2	X	0	4
2	Y	0	4
2	Z	0	4
5	D	0	2
5	F	0	2
5	N	0	1
5	j	0	1
6	C	0	2
6	E	0	4
6	G	0	3
6	M	0	4
7	I	0	4
7	K	0	1
8	L	0	1
8	c	0	1
All	All	0	77

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	243	PRO	N-CD	17.64	1.72	1.47
6	E	624	TRP	CZ2-CH2	-6.60	1.24	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	624	TRP	CD1-NE1	-6.45	1.24	1.37
6	M	624	TRP	C-N	5.95	1.39	1.33
6	G	624	TRP	C-N	5.66	1.38	1.33
7	K	35	HIS	CE1-NE2	5.07	1.37	1.32

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	j	107	GLN	CA-C-N	9.44	131.63	119.84
5	j	107	GLN	C-N-CA	9.44	131.63	119.84
8	L	300	VAL	N-CA-C	-9.32	102.52	113.42
6	E	624	TRP	CE3-CZ3-CH2	8.37	131.97	121.10
6	C	583	ILE	N-CA-C	-8.06	105.63	113.53
5	j	41	SER	N-CA-C	-8.03	104.63	114.75
1	J	235	SER	CA-C-N	7.98	136.79	121.54
1	J	235	SER	C-N-CA	7.98	136.79	121.54
1	l	121	PRO	N-CA-CB	7.97	111.62	103.25
5	F	434	ILE	N-CA-C	-7.96	105.43	112.12
6	C	464	GLY	CA-C-N	7.52	135.90	121.54
6	C	464	GLY	C-N-CA	7.52	135.90	121.54
6	C	485	VAL	N-CA-C	-7.25	104.31	113.22
1	l	130	PRO	N-CA-CB	6.96	110.66	103.00
5	H	882	PHE	N-CA-C	-6.96	105.41	114.04
6	M	674	GLN	CA-C-N	6.96	134.83	121.54
6	M	674	GLN	C-N-CA	6.96	134.83	121.54
5	D	482	LYS	N-CA-C	-6.86	106.10	114.75
7	K	409	ASN	CA-C-N	6.60	134.15	121.54
7	K	409	ASN	C-N-CA	6.60	134.15	121.54
6	G	580	HIS	CA-C-N	6.53	134.01	121.54
6	G	580	HIS	C-N-CA	6.53	134.01	121.54
5	D	418	ILE	N-CA-C	-6.51	106.65	112.12
6	G	264	LEU	N-CA-C	6.51	124.19	109.81
6	E	624	TRP	CG-CD2-CE3	6.50	140.40	133.90
7	K	203	PHE	CA-C-N	6.29	133.56	121.54
7	K	203	PHE	C-N-CA	6.29	133.56	121.54
8	L	1804	PHE	CA-CB-CG	-6.28	107.52	113.80
6	M	548	PRO	N-CA-C	6.27	118.35	110.70
7	K	574	ILE	N-CA-C	-6.19	107.83	113.71
6	E	624	TRP	CB-CG-CD2	6.18	135.45	126.80
6	E	580	HIS	CA-C-N	6.10	129.97	120.82
6	E	580	HIS	C-N-CA	6.10	129.97	120.82
5	D	886	TYR	N-CA-C	-6.05	100.22	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	509	GLN	CA-C-N	6.05	133.09	121.54
7	I	509	GLN	C-N-CA	6.05	133.09	121.54
8	L	306	HIS	CA-C-N	6.05	133.09	121.54
8	L	306	HIS	C-N-CA	6.05	133.09	121.54
7	I	475	TYR	CA-CB-CG	6.00	124.70	113.90
7	K	651	TYR	CA-CB-CG	5.96	124.63	113.90
3	e	51	ASP	N-CA-C	-5.95	107.01	114.56
8	c	82	LEU	CA-CB-CG	5.93	137.05	116.30
5	H	613	ASP	CA-C-N	5.88	129.04	120.51
5	H	613	ASP	C-N-CA	5.88	129.04	120.51
7	K	651	TYR	N-CA-CB	5.81	118.58	110.56
6	M	675	TRP	CA-C-N	5.75	132.51	121.54
6	M	675	TRP	C-N-CA	5.75	132.51	121.54
7	K	651	TYR	CB-CA-C	-5.74	100.88	110.81
8	c	141	ARG	N-CA-C	-5.67	107.36	114.56
7	I	503	LYS	N-CA-C	-5.66	107.61	114.75
7	K	35	HIS	N-CA-C	5.66	114.81	108.25
6	C	333	ARG	N-CA-C	-5.65	107.63	114.75
6	G	240	GLY	CA-C-N	5.62	132.28	121.54
6	G	240	GLY	C-N-CA	5.62	132.28	121.54
6	C	545	ASP	N-CA-C	-5.60	104.21	111.71
6	M	243	SER	N-CA-C	5.59	122.71	110.80
8	L	1689	ARG	N-CA-C	-5.57	107.73	114.75
1	J	236	LEU	CA-CB-CG	5.50	135.53	116.30
6	C	250	PRO	CA-C-N	5.40	132.25	123.93
6	C	250	PRO	C-N-CA	5.40	132.25	123.93
6	C	484	TYR	N-CA-C	-5.33	106.27	114.16
3	e	243	PRO	CA-N-CD	-5.32	104.56	112.00
8	c	149	ASP	CA-C-N	5.29	130.36	122.74
8	c	149	ASP	C-N-CA	5.29	130.36	122.74
1	J	236	LEU	N-CA-C	5.29	122.06	110.80
8	L	340	GLN	N-CA-C	5.27	117.08	110.91
6	E	581	ASP	N-CA-C	5.26	120.05	111.37
1	J	488	GLY	CA-C-N	5.24	130.28	122.74
1	J	488	GLY	C-N-CA	5.24	130.28	122.74
5	h	41	SER	N-CA-C	-5.23	108.16	114.75
6	M	264	LEU	N-CA-C	5.23	121.36	109.81
7	I	408	ASP	N-CA-C	5.22	121.92	110.80
6	M	238	LEU	CA-C-N	5.21	131.49	121.54
6	M	238	LEU	C-N-CA	5.21	131.49	121.54
5	j	104	PRO	CA-C-N	5.17	131.42	121.54
5	j	104	PRO	C-N-CA	5.17	131.42	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	440	PRO	CA-C-N	5.12	131.30	123.47
6	E	440	PRO	C-N-CA	5.12	131.30	123.47
5	N	271	THR	CA-C-N	5.11	131.30	121.54
5	N	271	THR	C-N-CA	5.11	131.30	121.54
6	G	581	ASP	O-C-N	-5.10	115.81	122.59
5	H	627	GLU	CA-CB-CG	5.09	124.28	114.10
8	L	452	PRO	CA-C-O	-5.09	117.46	121.38
1	J	238	LEU	N-CA-C	5.08	121.62	110.80
5	j	41	SER	CA-C-N	5.08	131.23	121.54
5	j	41	SER	C-N-CA	5.08	131.23	121.54
8	L	567	LEU	CA-C-N	5.07	129.81	122.36
8	L	567	LEU	C-N-CA	5.07	129.81	122.36
5	D	368	LEU	CA-CB-CG	5.03	133.92	116.30
6	M	580	HIS	CA-C-N	5.01	131.11	121.54
6	M	580	HIS	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (77) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
7	I	600	ASN	Peptide
7	I	601	LEU	Mainchain
7	I	602	GLY	Peptide
1	J	210	PRO	Peptide
1	J	255	PRO	Peptide
7	K	410	LEU	Peptide
8	L	306	HIS	Peptide
6	M	239	ALA	Peptide
6	M	240	GLY	Peptide
6	M	242	GLN	Peptide
6	M	866	THR	Peptide
5	N	501	THR	Peptide
2	Q	347	ASN	Peptide
2	Q	406	GLU	Peptide
2	Q	55	ALA	Peptide
2	Q	86	TYR	Peptide
2	R	347	ASN	Peptide
2	R	406	GLU	Peptide
2	R	55	ALA	Peptide
2	R	86	TYR	Peptide
2	S	347	ASN	Peptide
2	S	406	GLU	Peptide
2	S	55	ALA	Peptide
2	S	86	TYR	Peptide
2	T	347	ASN	Peptide
2	T	406	GLU	Peptide
2	T	55	ALA	Peptide
2	T	86	TYR	Peptide
2	U	347	ASN	Peptide
2	U	406	GLU	Peptide
2	U	55	ALA	Peptide
2	U	86	TYR	Peptide
2	V	347	ASN	Peptide
2	V	406	GLU	Peptide
2	V	55	ALA	Peptide
2	V	86	TYR	Peptide
2	W	347	ASN	Peptide
2	W	406	GLU	Peptide
2	W	55	ALA	Peptide
2	W	86	TYR	Peptide
2	X	347	ASN	Peptide
2	X	406	GLU	Peptide

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	4429	0	4482	27	0
1	l	847	0	789	12	0
2	1	3373	0	3325	60	0
2	2	3373	0	3325	55	0
2	Q	3373	0	3325	61	0
2	R	3373	0	3325	57	0
2	S	3373	0	3325	56	0
2	T	3373	0	3325	57	0
2	U	3373	0	3325	55	0
2	V	3373	0	3325	54	0
2	W	3373	0	3325	59	0
2	X	3373	0	3325	55	0
2	Y	3373	0	3325	56	0
2	Z	3373	0	3325	58	0
3	e	2847	0	2810	50	0
4	b	484	0	512	12	0
4	d	454	0	482	7	0
4	i	484	0	512	6	0
4	k	484	0	512	4	0
4	m	484	0	512	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	4796	0	4775	44	0
5	F	4941	0	4935	50	0
5	H	4907	0	4896	32	0
5	N	4907	0	4896	33	0
5	a	933	0	953	4	0
5	h	803	0	831	8	0
5	j	843	0	846	4	0
6	C	5044	0	5081	49	0
6	E	5202	0	5241	59	0
6	G	5186	0	5219	28	0
6	M	5186	0	5219	42	0
7	I	4225	0	4259	37	0
7	K	4579	0	4586	36	0
8	L	4587	0	4636	30	0
8	c	1220	0	1231	19	0
9	l	5	0	0	2	0
9	m	1	0	0	0	0
All	All	108354	0	108115	1166	0

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

All (1166) 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)
3:e:243:PRO:CD	3:e:243:PRO:N	1.72	1.44
3:e:160:THR:HG21	3:e:180:LEU:O	1.36	1.24
3:e:242:LEU:HD12	3:e:243:PRO:HD2	1.12	1.10
2:T:56:ASP:OD1	2:U:296:ARG:NH1	1.96	0.98
3:e:242:LEU:HD12	3:e:243:PRO:CD	1.96	0.95
3:e:160:THR:CG2	3:e:180:LEU:O	2.16	0.94
7:I:48:LEU:HD21	7:I:130:GLN:HG2	1.64	0.79
7:K:646:LEU:HG	2:Y:338:GLN:HE22	1.44	0.79
7:I:361:TYR:HE2	7:I:475:TYR:HB3	1.48	0.79
7:I:357:ILE:O	7:I:361:TYR:HB3	1.84	0.77
5:D:692:ARG:HH22	2:R:197:GLN:HA	1.51	0.76
3:e:242:LEU:CD1	3:e:243:PRO:HD2	2.06	0.75
3:e:160:THR:OG1	3:e:178:LEU:O	2.03	0.75
6:M:304:LEU:HB3	5:N:369:VAL:HG12	1.67	0.75
6:C:522:MET:SD	2:Q:248:TYR:OH	2.45	0.73
5:F:616:GLU:HG3	5:F:619:ARG:HH11	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:56:ASP:C	2:X:296:ARG:HH12	1.95	0.73
3:e:79:TRP:HE1	3:e:122:ILE:HG13	1.52	0.73
6:E:273:VAL:HG11	6:E:296:MET:HE2	1.71	0.72
1:J:684:GLU:H	1:J:687:LEU:HB3	1.56	0.71
2:W:56:ASP:O	2:X:295:ARG:NH1	2.24	0.71
7:K:649:LEU:HB3	2:Y:341:ARG:HH21	1.56	0.70
7:I:361:TYR:CE2	7:I:475:TYR:HB3	2.26	0.70
3:e:155:SER:HA	3:e:160:THR:HG22	1.73	0.69
5:F:553:TYR:HB3	5:F:648:ILE:HD11	1.74	0.69
2:2:136:VAL:HG23	2:2:167:GLN:HB3	1.75	0.69
2:Q:136:VAL:HG23	2:Q:167:GLN:HB3	1.75	0.69
2:W:136:VAL:HG23	2:W:167:GLN:HB3	1.75	0.69
6:C:696:TYR:O	6:C:700:GLU:HB2	1.93	0.69
2:T:136:VAL:HG23	2:T:167:GLN:HB3	1.75	0.69
8:c:64:LEU:HG	8:c:66:ALA:H	1.58	0.69
2:V:136:VAL:HG23	2:V:167:GLN:HB3	1.75	0.69
5:N:563:ARG:HH22	5:N:569:GLY:HA3	1.58	0.69
8:L:527:THR:HA	8:L:530:GLU:HG2	1.75	0.68
2:R:136:VAL:HG23	2:R:167:GLN:HB3	1.75	0.68
2:U:136:VAL:HG23	2:U:167:GLN:HB3	1.75	0.68
2:X:136:VAL:HG23	2:X:167:GLN:HB3	1.75	0.68
2:S:136:VAL:HG23	2:S:167:GLN:HB3	1.75	0.68
7:K:653:LYS:HZ2	2:Y:353:PRO:HG3	1.59	0.68
2:Z:136:VAL:HG23	2:Z:167:GLN:HB3	1.75	0.68
2:1:136:VAL:HG23	2:1:167:GLN:HB3	1.75	0.67
2:Y:136:VAL:HG23	2:Y:167:GLN:HB3	1.75	0.67
5:F:259:GLN:NE2	6:G:322:GLN:OE1	2.28	0.67
2:1:248:TYR:OH	6:M:522:MET:SD	2.51	0.67
3:e:282:ILE:HD13	3:e:293:LEU:HD22	1.78	0.66
5:D:322:GLN:HG2	6:E:333:ARG:HH22	1.61	0.66
4:b:49:ARG:NH2	8:L:284:GLU:OE1	2.28	0.66
2:W:56:ASP:O	2:X:296:ARG:NH1	2.20	0.66
6:E:581:ASP:O	6:E:643:ARG:NH1	2.29	0.65
5:N:601:LEU:HD22	5:N:623:VAL:HG13	1.78	0.65
5:H:307:TYR:HA	5:H:310:GLN:HE21	1.62	0.65
6:M:158:ARG:HH12	6:M:176:ILE:HG21	1.61	0.65
1:l:113:LEU:O	1:l:117:LEU:HB2	1.97	0.64
6:C:315:ARG:HH12	5:D:366:ARG:HB3	1.61	0.64
7:K:532:LEU:HD22	7:K:644:GLN:HG2	1.80	0.64
5:D:266:ILE:HG12	5:D:277:VAL:HB	1.79	0.64
6:C:395:ILE:HD11	6:C:450:ILE:HG23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:132:LEU:HG	7:I:167:PRO:HB3	1.81	0.63
5:F:878:PHE:HD2	2:T:338:GLN:HE22	1.47	0.63
5:h:28:VAL:HG13	5:h:31:GLN:HE21	1.64	0.63
5:F:620:ARG:HH21	5:F:644:VAL:HA	1.63	0.63
2:Z:3:ARG:N	2:Z:131:SER:HG	1.98	0.62
8:L:1663:HIS:CG	2:Z:262:PRO:HA	2.34	0.62
6:C:533:ASP:OD2	2:Q:3:ARG:NH2	2.32	0.62
7:I:1:MET:HE3	1:J:238:LEU:HD12	1.81	0.62
2:W:3:ARG:N	2:W:131:SER:HG	1.98	0.62
5:F:304:ILE:HD12	5:F:381:LEU:HD13	1.79	0.62
5:F:865:LEU:HD11	5:F:873:LEU:HD22	1.81	0.62
8:L:1797:ASP:HA	8:L:1800:LEU:HD23	1.81	0.62
6:C:644:HIS:HB2	6:C:739:LEU:HD21	1.82	0.62
5:F:736:ASN:HA	5:F:739:GLN:HE21	1.64	0.62
2:X:3:ARG:N	2:X:131:SER:HG	1.98	0.62
2:1:3:ARG:NH1	6:M:529:VAL:O	2.33	0.62
5:F:401:HIS:HD2	5:F:419:LEU:HD21	1.65	0.62
6:G:221:LEU:HD11	6:G:260:VAL:HG22	1.82	0.62
2:S:3:ARG:N	2:S:131:SER:HG	1.98	0.62
6:C:187:LEU:HD22	5:D:379:LYS:HE3	1.82	0.61
7:K:192:LEU:HD11	7:K:307:PHE:HB2	1.81	0.61
2:Y:3:ARG:N	2:Y:131:SER:HG	1.98	0.61
5:D:570:GLN:NE2	2:R:247:GLY:O	2.33	0.61
2:T:3:ARG:N	2:T:131:SER:HG	1.98	0.61
2:W:292:ASP:O	2:W:296:ARG:HB2	2.01	0.61
5:D:486:ILE:HG23	5:D:541:THR:HG21	1.82	0.61
2:Q:292:ASP:O	2:Q:296:ARG:HB2	2.01	0.61
2:1:292:ASP:O	2:1:296:ARG:HB2	2.01	0.61
8:L:283:TRP:O	8:L:287:LEU:HB2	1.99	0.61
2:2:3:ARG:N	2:2:131:SER:HG	1.98	0.61
2:Y:318:ILE:HB	2:Y:380:ASN:HB3	1.83	0.61
6:M:585:GLN:OE1	6:M:637:ARG:NH2	2.34	0.61
2:Z:318:ILE:HB	2:Z:380:ASN:HB3	1.83	0.61
2:R:292:ASP:O	2:R:296:ARG:HB2	2.01	0.60
2:1:3:ARG:N	2:1:131:SER:HG	1.98	0.60
2:R:3:ARG:N	2:R:131:SER:HG	1.98	0.60
2:S:292:ASP:O	2:S:296:ARG:HB2	2.01	0.60
2:2:292:ASP:O	2:2:296:ARG:HB2	2.01	0.60
8:L:1732:ILE:HG23	8:L:1772:PHE:HE1	1.64	0.60
2:Q:3:ARG:N	2:Q:131:SER:HG	1.98	0.60
2:U:3:ARG:N	2:U:131:SER:HG	1.98	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:3:ARG:N	2:V:131:SER:HG	1.98	0.60
2:X:292:ASP:O	2:X:296:ARG:HB2	2.01	0.60
2:T:292:ASP:O	2:T:296:ARG:HB2	2.01	0.60
2:V:292:ASP:O	2:V:296:ARG:HB2	2.01	0.60
2:Z:292:ASP:O	2:Z:296:ARG:HB2	2.01	0.60
2:W:318:ILE:HB	2:W:380:ASN:HB3	1.83	0.60
2:Y:292:ASP:O	2:Y:296:ARG:HB2	2.01	0.60
2:T:318:ILE:HB	2:T:380:ASN:HB3	1.83	0.60
5:N:477:MET:HG3	5:N:481:ARG:HE	1.65	0.60
7:K:397:GLN:HE22	7:K:411:LEU:HB3	1.66	0.60
2:U:318:ILE:HB	2:U:380:ASN:HB3	1.83	0.60
2:2:318:ILE:HB	2:2:380:ASN:HB3	1.83	0.60
5:F:304:ILE:HA	5:F:385:VAL:HG11	1.84	0.60
7:I:272:VAL:HG13	7:I:329:VAL:HG11	1.83	0.60
6:M:696:TYR:O	6:M:700:GLU:HB3	2.01	0.60
2:R:318:ILE:HB	2:R:380:ASN:HB3	1.83	0.59
2:U:292:ASP:O	2:U:296:ARG:HB2	2.01	0.59
2:Q:318:ILE:HB	2:Q:380:ASN:HB3	1.83	0.59
2:1:3:ARG:N	2:1:131:SER:OG	2.36	0.59
2:1:318:ILE:HB	2:1:380:ASN:HB3	1.83	0.59
7:I:404:LEU:HD11	2:W:47:ARG:HG3	1.85	0.59
2:S:3:ARG:N	2:S:131:SER:OG	2.36	0.59
2:2:3:ARG:N	2:2:131:SER:OG	2.36	0.59
2:S:318:ILE:HB	2:S:380:ASN:HB3	1.83	0.59
6:G:577:LEU:HG	6:G:579:PRO:HD3	1.84	0.59
2:T:3:ARG:N	2:T:131:SER:OG	2.36	0.59
2:V:318:ILE:HB	2:V:380:ASN:HB3	1.83	0.59
7:I:404:LEU:HD21	2:W:47:ARG:HA	1.85	0.59
6:M:547:THR:HG22	6:M:549:PRO:HD2	1.84	0.59
2:Y:3:ARG:N	2:Y:131:SER:OG	2.36	0.59
2:V:3:ARG:N	2:V:131:SER:OG	2.36	0.58
2:X:318:ILE:HB	2:X:380:ASN:HB3	1.83	0.58
1:l:74:ILE:HA	5:H:662:ARG:HG2	1.85	0.58
6:E:556:GLU:HG2	2:T:339:ARG:HE	1.68	0.58
5:F:504:THR:HG21	5:F:537:ALA:HA	1.85	0.58
2:Q:3:ARG:N	2:Q:131:SER:OG	2.36	0.58
2:V:326:GLY:HA2	2:V:363:LYS:HD3	1.85	0.58
2:W:3:ARG:N	2:W:131:SER:OG	2.36	0.58
2:Z:66:LEU:HB3	2:Z:91:ILE:HA	1.85	0.58
3:e:186:THR:HA	3:e:189:LEU:HD12	1.84	0.58
6:E:188:ILE:HG22	6:E:244:ARG:HH22	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:285:TYR:O	6:M:289:ASN:ND2	2.36	0.58
2:R:3:ARG:N	2:R:131:SER:OG	2.36	0.58
2:X:3:ARG:N	2:X:131:SER:OG	2.36	0.58
2:Z:3:ARG:N	2:Z:131:SER:OG	2.36	0.58
4:d:43:THR:HA	4:d:46:ILE:HG22	1.86	0.58
2:S:66:LEU:HB3	2:S:91:ILE:HA	1.85	0.58
1:J:255:PRO:HD2	1:J:257:TYR:H	1.68	0.58
2:T:66:LEU:HB3	2:T:91:ILE:HA	1.85	0.58
6:E:174:LEU:HD11	5:F:405:LYS:HD2	1.85	0.58
5:F:270:ASN:HD21	5:F:302:ASN:HD22	1.52	0.58
2:U:3:ARG:N	2:U:131:SER:OG	2.36	0.58
5:F:609:ASN:ND2	2:T:46:ASP:O	2.36	0.58
2:U:66:LEU:HB3	2:U:91:ILE:HA	1.85	0.58
6:E:314:HIS:HB2	6:E:319:LEU:HD23	1.85	0.58
5:F:682:LYS:HB2	2:T:254:ILE:HD11	1.85	0.58
8:L:438:ARG:NH1	8:L:441:GLN:OE1	2.37	0.58
2:R:326:GLY:HA2	2:R:363:LYS:HD3	1.85	0.58
2:W:66:LEU:HB3	2:W:91:ILE:HA	1.85	0.58
2:1:353:PRO:HG2	6:M:685:ARG:HG2	1.85	0.57
2:U:326:GLY:HA2	2:U:363:LYS:HD3	1.85	0.57
2:X:326:GLY:HA2	2:X:363:LYS:HD3	1.85	0.57
2:2:66:LEU:HB3	2:2:91:ILE:HA	1.85	0.57
4:b:49:ARG:HH22	8:L:283:TRP:H	1.51	0.57
6:C:614:GLU:HA	6:C:643:ARG:HH12	1.69	0.57
6:M:478:THR:OG1	6:M:481:GLU:O	2.22	0.57
2:Q:66:LEU:HB3	2:Q:91:ILE:HA	1.85	0.57
2:V:66:LEU:HB3	2:V:91:ILE:HA	1.85	0.57
2:Y:66:LEU:HB3	2:Y:91:ILE:HA	1.85	0.57
8:c:69:LYS:HB3	8:c:115:VAL:HG21	1.85	0.57
2:S:326:GLY:HA2	2:S:363:LYS:HD3	1.85	0.57
2:Y:326:GLY:HA2	2:Y:363:LYS:HD3	1.85	0.57
5:H:308:THR:O	5:H:312:SER:OG	2.21	0.57
2:T:326:GLY:HA2	2:T:363:LYS:HD3	1.85	0.57
2:X:66:LEU:HB3	2:X:91:ILE:HA	1.85	0.57
2:2:326:GLY:HA2	2:2:363:LYS:HD3	1.85	0.57
3:e:12:ASN:ND2	3:e:17:CYS:SG	2.77	0.57
3:e:54:VAL:HG22	3:e:88:HIS:HD2	1.70	0.57
2:Q:326:GLY:HA2	2:Q:363:LYS:HD3	1.85	0.57
7:I:92:GLY:HA3	7:I:175:ILE:HG12	1.86	0.57
7:K:48:LEU:HD21	7:K:130:GLN:HA	1.87	0.57
5:F:555:LEU:HD13	5:F:651:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:883:ASN:HD21	2:V:350:PRO:HA	1.68	0.57
8:L:324:CYS:HA	8:L:327:HIS:CE1	2.40	0.57
2:W:326:GLY:HA2	2:W:363:LYS:HD3	1.85	0.57
2:Z:326:GLY:HA2	2:Z:363:LYS:HD3	1.85	0.56
2:1:66:LEU:HB3	2:1:91:ILE:HA	1.85	0.56
5:F:578:MET:HE1	5:F:671:LYS:HB3	1.87	0.56
2:R:66:LEU:HB3	2:R:91:ILE:HA	1.85	0.56
2:1:233:SER:O	2:1:237:SER:OG	2.24	0.56
2:1:326:GLY:HA2	2:1:363:LYS:HD3	1.85	0.56
6:G:395:ILE:HD11	6:G:450:ILE:HG23	1.88	0.56
2:V:303:VAL:HG12	2:V:305:VAL:H	1.71	0.56
2:2:303:VAL:HG12	2:2:305:VAL:H	1.71	0.56
8:L:1589:ASP:H	8:L:1737:LEU:HD13	1.69	0.56
5:F:432:ARG:HH12	5:F:440:GLU:H	1.52	0.56
2:R:233:SER:O	2:R:237:SER:OG	2.24	0.56
2:S:233:SER:O	2:S:237:SER:OG	2.24	0.56
2:Y:233:SER:O	2:Y:237:SER:OG	2.24	0.56
2:2:233:SER:O	2:2:237:SER:OG	2.24	0.56
2:U:303:VAL:HG12	2:U:305:VAL:H	1.71	0.56
2:1:303:VAL:HG12	2:1:305:VAL:H	1.71	0.56
6:C:738:MET:HG3	6:C:745:LEU:HD13	1.88	0.56
5:F:464:TYR:HB3	5:F:484:LEU:HD11	1.88	0.56
6:E:439:ILE:HG22	6:E:441:SER:H	1.71	0.56
2:S:303:VAL:HG12	2:S:305:VAL:H	1.71	0.56
6:E:277:ILE:HD11	6:E:296:MET:HG3	1.87	0.55
2:R:303:VAL:HG12	2:R:305:VAL:H	1.71	0.55
2:X:303:VAL:HG12	2:X:305:VAL:H	1.71	0.55
2:Z:52:PHE:HA	2:Z:62:PRO:HA	1.88	0.55
6:M:696:TYR:O	6:M:700:GLU:CB	2.55	0.55
2:S:52:PHE:HA	2:S:62:PRO:HA	1.89	0.55
2:U:233:SER:O	2:U:237:SER:OG	2.24	0.55
2:X:52:PHE:HA	2:X:62:PRO:HA	1.89	0.55
2:Z:233:SER:O	2:Z:237:SER:OG	2.24	0.55
8:L:1592:SER:OG	8:L:1593:CYS:N	2.38	0.55
2:T:303:VAL:HG12	2:T:305:VAL:H	1.71	0.55
2:U:52:PHE:HA	2:U:62:PRO:HA	1.89	0.55
2:Z:303:VAL:HG12	2:Z:305:VAL:H	1.71	0.55
5:D:550:ASN:HD21	5:D:556:LEU:HD22	1.72	0.55
4:b:22:ARG:HB2	8:L:287:LEU:HD11	1.89	0.55
2:R:52:PHE:HA	2:R:62:PRO:HA	1.88	0.55
2:T:52:PHE:HA	2:T:62:PRO:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:52:PHE:HA	2:V:62:PRO:HA	1.88	0.55
2:2:446:TRP:HB3	5:N:702:HIS:CG	2.42	0.55
6:C:308:SER:HB3	8:c:182:MET:HE3	1.89	0.55
5:D:254:ILE:HG13	5:D:366:ARG:HH22	1.72	0.55
5:D:666:PHE:HA	5:D:669:ARG:HE	1.72	0.55
2:W:52:PHE:HA	2:W:62:PRO:HA	1.88	0.55
5:F:378:LEU:HD13	5:F:381:LEU:HD11	1.88	0.55
5:H:256:TYR:OH	7:I:38:GLU:OE1	2.25	0.55
1:J:881:HIS:CE1	2:X:446:TRP:HD1	2.25	0.55
2:Q:233:SER:O	2:Q:237:SER:OG	2.24	0.55
2:V:233:SER:O	2:V:237:SER:OG	2.24	0.55
6:G:644:HIS:HE1	6:G:738:MET:HE3	1.72	0.55
2:X:233:SER:O	2:X:237:SER:OG	2.24	0.55
8:L:1800:LEU:HD11	2:Z:337:LEU:HG	1.90	0.54
2:W:233:SER:O	2:W:237:SER:OG	2.24	0.54
6:C:520:PHE:HB3	6:C:642:PHE:HB2	1.89	0.54
6:M:682:LEU:HD13	6:M:685:ARG:HH11	1.72	0.54
2:Q:52:PHE:HA	2:Q:62:PRO:HA	1.88	0.54
2:Q:303:VAL:HG12	2:Q:305:VAL:H	1.71	0.54
2:T:233:SER:O	2:T:237:SER:OG	2.24	0.54
2:1:259:SER:HB3	6:M:691:GLN:HE22	1.72	0.54
5:D:427:LEU:HA	5:D:430:LEU:HD12	1.89	0.54
5:D:601:LEU:HD21	5:D:621:LEU:HD21	1.90	0.54
6:G:271:SER:OG	6:G:275:ARG:NH2	2.41	0.54
2:1:52:PHE:HA	2:1:62:PRO:HA	1.89	0.54
2:2:355:SER:HB2	5:N:713:HIS:NE2	2.23	0.54
5:N:266:ILE:HG12	5:N:277:VAL:HG22	1.89	0.54
2:Q:57:ASP:OD2	2:R:276:LEU:HB3	2.08	0.54
2:Y:303:VAL:HG12	2:Y:305:VAL:H	1.71	0.54
2:2:52:PHE:HA	2:2:62:PRO:HA	1.89	0.54
7:K:534:VAL:HG21	2:Y:248:TYR:HE2	1.71	0.54
2:Y:52:PHE:HA	2:Y:62:PRO:HA	1.88	0.54
6:C:445:LYS:HD3	6:C:482:ARG:HH12	1.73	0.54
7:I:188:SER:O	7:I:192:LEU:HB2	2.08	0.54
5:F:419:LEU:HA	5:F:422:VAL:HG22	1.90	0.54
2:1:222:ASN:OD1	2:1:222:ASN:N	2.41	0.54
6:C:834:LEU:HD13	6:C:868:ARG:HH11	1.73	0.54
5:H:608:THR:HG23	5:H:610:ALA:H	1.72	0.54
2:W:303:VAL:HG12	2:W:305:VAL:H	1.71	0.54
2:Y:222:ASN:N	2:Y:222:ASN:OD1	2.41	0.54
7:K:618:GLY:O	7:K:622:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:222:ASN:OD1	2:U:222:ASN:N	2.41	0.53
2:W:241:THR:HB	2:W:325:GLN:HE22	1.74	0.53
2:Z:222:ASN:OD1	2:Z:222:ASN:N	2.41	0.53
3:e:239:SER:HA	3:e:249:THR:HG21	1.90	0.53
5:N:636:ASP:OD1	5:N:672:ARG:NH1	2.42	0.53
2:U:241:THR:HB	2:U:325:GLN:HE22	1.74	0.53
2:W:66:LEU:HD22	2:W:91:ILE:HG23	1.91	0.53
2:1:241:THR:HB	2:1:325:GLN:HE22	1.73	0.53
7:I:508:ASN:C	7:I:510:THR:H	2.17	0.53
5:D:885:HIS:CG	2:R:353:PRO:HA	2.43	0.53
6:E:214:GLU:OE2	6:E:320:SER:OG	2.26	0.53
5:H:664:PHE:O	5:H:668:TRP:HB2	2.09	0.53
4:i:64:ILE:HD12	5:h:96:LEU:HD11	1.91	0.53
2:Q:241:THR:HB	2:Q:325:GLN:HE22	1.73	0.53
2:T:241:THR:HB	2:T:325:GLN:HE22	1.73	0.53
2:X:66:LEU:HD22	2:X:91:ILE:HG23	1.91	0.53
2:1:66:LEU:HD22	2:1:91:ILE:HG23	1.91	0.53
2:2:241:THR:HB	2:2:325:GLN:HE22	1.73	0.53
2:S:66:LEU:HD22	2:S:91:ILE:HG23	1.91	0.53
2:S:241:THR:HB	2:S:325:GLN:HE22	1.73	0.53
2:X:222:ASN:OD1	2:X:222:ASN:N	2.41	0.53
2:Z:241:THR:HB	2:Z:325:GLN:HE22	1.73	0.53
2:2:66:LEU:HD22	2:2:91:ILE:HG23	1.91	0.53
3:e:365:SER:HB3	3:e:369:ILE:HG13	1.89	0.53
6:E:297:ARG:HH11	8:c:138:HIS:HB3	1.72	0.53
7:I:5:LEU:HD11	7:I:122:VAL:HG21	1.90	0.53
2:Q:222:ASN:OD1	2:Q:222:ASN:N	2.41	0.53
2:T:66:LEU:HD22	2:T:91:ILE:HG23	1.91	0.53
2:Y:241:THR:HB	2:Y:325:GLN:HE22	1.73	0.53
2:Z:184:GLN:O	2:Z:188:SER:OG	2.27	0.53
2:1:237:SER:O	2:1:241:THR:OG1	2.25	0.53
2:2:222:ASN:N	2:2:222:ASN:OD1	2.41	0.53
3:e:150:GLY:HA3	3:e:296:ASN:HB3	1.90	0.53
6:G:160:MET:HE2	6:G:164:LYS:HE3	1.90	0.53
2:R:66:LEU:HD22	2:R:91:ILE:HG23	1.91	0.53
2:U:66:LEU:HD22	2:U:91:ILE:HG23	1.91	0.53
2:W:222:ASN:N	2:W:222:ASN:OD1	2.41	0.53
6:C:757:MET:HA	6:C:761:CYS:HB3	1.91	0.53
2:Q:184:GLN:O	2:Q:188:SER:OG	2.27	0.53
2:X:241:THR:HB	2:X:325:GLN:HE22	1.74	0.53
1:l:71:LYS:NZ	9:l:1102:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:554:SER:O	5:H:558:HIS:ND1	2.33	0.53
2:U:184:GLN:O	2:U:188:SER:OG	2.27	0.53
2:Y:37:VAL:HG12	2:Y:59:HIS:HD2	1.74	0.53
2:Y:66:LEU:HD22	2:Y:91:ILE:HG23	1.91	0.53
8:c:3:SER:OG	8:c:4:ILE:N	2.42	0.53
2:2:184:GLN:O	2:2:188:SER:OG	2.27	0.52
6:E:559:LEU:HD21	6:E:570:LYS:HD2	1.91	0.52
1:J:889:LYS:HA	2:X:353:PRO:HG2	1.91	0.52
8:L:568:TYR:HB3	8:L:1606:ILE:HD13	1.91	0.52
2:S:37:VAL:HG12	2:S:59:HIS:HD2	1.74	0.52
2:V:222:ASN:OD1	2:V:222:ASN:N	2.41	0.52
7:K:143:ILE:HA	7:K:148:ILE:HD12	1.91	0.52
4:k:24:THR:HA	4:k:27:VAL:HG12	1.91	0.52
2:V:184:GLN:O	2:V:188:SER:OG	2.27	0.52
2:2:37:VAL:HG12	2:2:59:HIS:HD2	1.74	0.52
5:D:261:ILE:HG21	6:E:255:SER:HB3	1.92	0.52
6:E:387:TYR:HE2	6:E:407:PHE:HD1	1.56	0.52
6:E:514:ARG:HG2	6:E:517:LYS:HZ3	1.73	0.52
7:K:66:VAL:HG13	7:K:68:GLN:H	1.74	0.52
5:D:286:SER:OG	5:D:287:LEU:N	2.39	0.52
2:R:222:ASN:N	2:R:222:ASN:OD1	2.41	0.52
2:T:361:SER:OG	2:T:362:ARG:N	2.43	0.52
6:E:585:GLN:HE21	6:E:744:LEU:HD21	1.74	0.52
2:Q:37:VAL:HG12	2:Q:59:HIS:HD2	1.74	0.52
2:V:37:VAL:HG12	2:V:59:HIS:HD2	1.74	0.52
2:1:184:GLN:O	2:1:188:SER:OG	2.27	0.52
5:H:419:LEU:HA	5:H:422:VAL:HG22	1.92	0.52
7:I:408:ASP:HB2	7:I:410:LEU:H	1.74	0.52
2:1:37:VAL:HG12	2:1:59:HIS:HD2	1.74	0.52
6:E:448:ASP:N	6:E:448:ASP:OD2	2.43	0.52
5:F:619:ARG:HH12	5:F:620:ARG:HH11	1.57	0.52
2:T:222:ASN:N	2:T:222:ASN:OD1	2.41	0.52
2:X:37:VAL:HG12	2:X:59:HIS:HD2	1.74	0.52
2:1:353:PRO:HG3	6:M:865:TYR:CD2	2.45	0.52
3:e:111:ASN:OD1	3:e:115:ASN:ND2	2.43	0.52
6:C:180:TRP:HA	6:C:183:GLU:HB2	1.92	0.52
2:R:184:GLN:O	2:R:188:SER:OG	2.27	0.52
2:R:241:THR:HB	2:R:325:GLN:HE22	1.74	0.52
2:W:361:SER:OG	2:W:362:ARG:N	2.43	0.52
2:2:361:SER:OG	2:2:362:ARG:N	2.43	0.52
7:K:199:GLN:NE2	8:L:510:LEU:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:222:ASN:OD1	2:S:222:ASN:N	2.41	0.52
2:U:37:VAL:HG12	2:U:59:HIS:HD2	1.74	0.52
2:W:237:SER:O	2:W:241:THR:OG1	2.25	0.52
2:X:361:SER:OG	2:X:362:ARG:N	2.43	0.52
2:Y:184:GLN:O	2:Y:188:SER:OG	2.27	0.52
2:2:290:VAL:HG23	2:2:336:SER:HB2	1.92	0.52
2:R:37:VAL:HG12	2:R:59:HIS:HD2	1.74	0.52
2:S:361:SER:OG	2:S:362:ARG:N	2.43	0.52
2:V:66:LEU:HD22	2:V:91:ILE:HG23	1.91	0.52
2:Y:290:VAL:HG23	2:Y:336:SER:HB2	1.92	0.52
2:Z:66:LEU:HD22	2:Z:91:ILE:HG23	1.91	0.52
2:Q:66:LEU:HD22	2:Q:91:ILE:HG23	1.91	0.51
2:S:290:VAL:HG23	2:S:336:SER:HB2	1.92	0.51
2:U:361:SER:OG	2:U:362:ARG:N	2.43	0.51
9:l:1101:HOH:O	5:H:769:ARG:NH1	2.44	0.51
7:K:192:LEU:HD22	7:K:304:GLU:HG2	1.92	0.51
2:R:290:VAL:HG23	2:R:336:SER:HB2	1.92	0.51
2:V:241:THR:HB	2:V:325:GLN:HE22	1.74	0.51
2:W:184:GLN:O	2:W:188:SER:OG	2.27	0.51
6:G:428:TRP:CD1	6:G:628:LEU:HB3	2.46	0.51
2:U:290:VAL:HG23	2:U:336:SER:HB2	1.92	0.51
2:X:184:GLN:O	2:X:188:SER:OG	2.27	0.51
3:e:153:MET:CE	3:e:274:ILE:HG23	2.40	0.51
5:F:433:TRP:HZ2	5:F:484:LEU:HD12	1.75	0.51
7:I:37:SER:O	7:I:40:SER:OG	2.29	0.51
7:K:353:GLN:HG3	7:K:463:LEU:HD13	1.93	0.51
2:T:37:VAL:HG12	2:T:59:HIS:HD2	1.74	0.51
2:W:53:TYR:HB2	2:W:63:ARG:HG2	1.93	0.51
4:d:60:LEU:HA	4:d:63:VAL:HG22	1.91	0.51
6:C:763:GLN:HG3	6:C:766:THR:H	1.75	0.51
2:T:53:TYR:HB2	2:T:63:ARG:HG2	1.93	0.51
2:V:361:SER:OG	2:V:362:ARG:N	2.43	0.51
2:X:290:VAL:HG23	2:X:336:SER:HB2	1.92	0.51
2:Z:290:VAL:HG23	2:Z:336:SER:HB2	1.92	0.51
3:e:147:ARG:HH11	8:c:49:LEU:HB3	1.75	0.51
8:L:1609:THR:HG22	8:L:1611:GLY:H	1.76	0.51
2:Y:53:TYR:HB2	2:Y:63:ARG:HG2	1.93	0.51
2:Z:361:SER:OG	2:Z:362:ARG:N	2.43	0.51
2:2:53:TYR:HB2	2:2:63:ARG:HG2	1.93	0.51
5:D:726:VAL:HG13	5:D:761:ARG:HB2	1.93	0.51
2:Q:361:SER:OG	2:Q:362:ARG:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:53:TYR:HB2	2:R:63:ARG:HG2	1.93	0.51
2:W:37:VAL:HG12	2:W:59:HIS:HD2	1.74	0.51
2:Z:37:VAL:HG12	2:Z:59:HIS:HD2	1.74	0.51
2:T:184:GLN:O	2:T:188:SER:OG	2.27	0.51
2:Z:53:TYR:HB2	2:Z:63:ARG:HG2	1.93	0.51
2:1:53:TYR:HB2	2:1:63:ARG:HG2	1.93	0.51
2:1:290:VAL:HG23	2:1:336:SER:HB2	1.92	0.51
2:1:361:SER:OG	2:1:362:ARG:N	2.43	0.51
6:C:439:ILE:HD12	6:C:444:GLN:HE22	1.76	0.51
5:F:449:ALA:HB2	5:F:467:ARG:HB2	1.92	0.51
6:M:690:VAL:HG12	6:M:752:MET:HE1	1.92	0.51
2:T:237:SER:O	2:T:241:THR:OG1	2.25	0.51
2:U:53:TYR:HB2	2:U:63:ARG:HG2	1.93	0.51
5:H:631:GLY:HA3	5:H:637:VAL:HG23	1.93	0.50
1:J:316:GLN:NE2	1:J:320:TYR:OH	2.31	0.50
1:J:899:ASN:O	1:J:903:THR:OG1	2.28	0.50
7:K:176:LEU:HG	7:K:180:HIS:CE1	2.46	0.50
2:S:184:GLN:O	2:S:188:SER:OG	2.27	0.50
2:X:35:GLY:HA2	2:X:85:LEU:HD12	1.94	0.50
4:d:48:VAL:HG23	8:c:110:VAL:HG21	1.93	0.50
2:R:383:SER:O	2:R:386:SER:OG	2.29	0.50
7:I:345:VAL:HG23	7:I:346:GLU:HG3	1.92	0.50
2:Q:290:VAL:HG23	2:Q:336:SER:HB2	1.92	0.50
2:Y:35:GLY:HA2	2:Y:85:LEU:HD12	1.94	0.50
6:C:266:VAL:HG21	6:C:328:ILE:HD12	1.93	0.50
5:F:370:TRP:O	8:c:148:TYR:OH	2.24	0.50
2:V:290:VAL:HG23	2:V:336:SER:HB2	1.92	0.50
2:Q:53:TYR:HB2	2:Q:63:ARG:HG2	1.93	0.50
2:V:53:TYR:HB2	2:V:63:ARG:HG2	1.93	0.50
2:R:361:SER:OG	2:R:362:ARG:N	2.43	0.50
2:W:35:GLY:HA2	2:W:85:LEU:HD12	1.93	0.50
2:T:35:GLY:HA2	2:T:85:LEU:HD12	1.94	0.50
2:T:290:VAL:HG23	2:T:336:SER:HB2	1.92	0.50
2:V:35:GLY:HA2	2:V:85:LEU:HD12	1.93	0.50
4:k:28:LEU:HD21	5:j:93:ILE:HG12	1.94	0.50
6:E:695:TYR:HE1	2:S:249:MET:HG3	1.76	0.49
7:I:397:GLN:HB3	7:I:409:ASN:HD22	1.75	0.49
6:M:377:LEU:O	6:M:380:THR:OG1	2.31	0.49
5:N:608:THR:HG23	5:N:610:ALA:H	1.77	0.49
2:S:53:TYR:HB2	2:S:63:ARG:HG2	1.93	0.49
2:U:35:GLY:HA2	2:U:85:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:290:VAL:HG23	2:W:336:SER:HB2	1.92	0.49
5:D:613:ASP:HB2	5:D:617:ILE:HD11	1.93	0.49
1:J:220:VAL:HG13	8:L:311:TYR:HA	1.94	0.49
2:Z:35:GLY:HA2	2:Z:85:LEU:HD12	1.94	0.49
1:l:114:LEU:HD22	4:m:37:THR:HG21	1.94	0.49
2:2:35:GLY:HA2	2:2:85:LEU:HD12	1.94	0.49
2:S:124:ARG:HG3	2:T:301:LYS:NZ	2.27	0.49
2:X:53:TYR:HB2	2:X:63:ARG:HG2	1.93	0.49
6:C:563:THR:HG21	2:Q:246:PRO:HG3	1.94	0.49
6:E:280:LYS:HD2	6:E:289:ASN:HD21	1.76	0.49
2:1:35:GLY:HA2	2:1:85:LEU:HD12	1.94	0.49
3:e:282:ILE:HD11	3:e:290:ARG:HG3	1.94	0.49
5:F:259:GLN:HG2	5:F:336:TYR:HE1	1.76	0.49
5:F:279:GLY:HA3	5:F:287:LEU:HD11	1.94	0.49
5:N:564:ARG:HB3	5:N:570:GLN:HB2	1.94	0.49
2:Q:35:GLY:HA2	2:Q:85:LEU:HD12	1.94	0.49
3:e:358:SER:OG	3:e:359:LYS:N	2.46	0.49
5:D:333:ARG:HG3	6:E:329:GLN:HG3	1.95	0.49
6:E:432:TYR:OH	6:E:458:ASN:ND2	2.36	0.49
5:F:653:THR:OG1	5:F:656:CYS:SG	2.71	0.49
5:H:884:GLU:OE2	2:V:344:LYS:NZ	2.45	0.49
5:N:270:ASN:HD22	5:N:273:ASN:HB2	1.78	0.49
5:F:710:GLU:HG2	2:T:353:PRO:HG2	1.94	0.49
7:K:192:LEU:HD21	7:K:307:PHE:HD2	1.77	0.49
7:K:540:GLN:HE21	7:K:564:PHE:HA	1.78	0.49
2:R:35:GLY:HA2	2:R:85:LEU:HD12	1.94	0.49
5:j:34:TYR:HA	5:j:37:ARG:HE	1.77	0.49
2:2:248:TYR:HD2	5:N:723:THR:HG23	1.78	0.49
5:D:720:TYR:HE1	2:R:249:MET:HG3	1.78	0.49
7:K:176:LEU:O	7:K:180:HIS:ND1	2.45	0.49
6:M:277:ILE:HD11	6:M:296:MET:HB3	1.95	0.49
2:S:383:SER:O	2:S:386:SER:OG	2.29	0.49
2:T:262:PRO:HG3	2:T:318:ILE:HG21	1.95	0.49
2:Y:361:SER:OG	2:Y:362:ARG:N	2.43	0.49
2:Z:383:SER:O	2:Z:386:SER:OG	2.29	0.49
6:E:837:LEU:HD22	6:E:856:ILE:HG12	1.94	0.49
5:F:432:ARG:NH1	5:F:440:GLU:OE1	2.45	0.49
7:I:282:SER:HB3	7:I:340:LEU:HD11	1.95	0.49
6:M:834:LEU:HD11	6:M:868:ARG:HB2	1.94	0.49
2:X:262:PRO:HG3	2:X:318:ILE:HG21	1.95	0.49
2:Z:262:PRO:HG3	2:Z:318:ILE:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:387:LEU:HA	2:Q:390:ARG:HD3	1.95	0.49
2:W:387:LEU:HA	2:W:390:ARG:HD3	1.95	0.49
4:b:22:ARG:HH11	4:b:25:MET:HB3	1.77	0.48
5:H:249:ALA:HB1	5:H:264:LYS:HZ1	1.78	0.48
6:C:221:LEU:HD11	6:C:260:VAL:HG22	1.95	0.48
6:G:526:ASP:HA	6:G:529:VAL:HG12	1.95	0.48
4:i:48:VAL:HG13	5:h:87:LEU:HD13	1.96	0.48
2:U:262:PRO:HG3	2:U:318:ILE:HG21	1.95	0.48
2:W:262:PRO:HG3	2:W:318:ILE:HG21	1.95	0.48
5:F:554:SER:O	5:F:554:SER:OG	2.31	0.48
6:G:578:MET:HG3	6:G:643:ARG:HD3	1.94	0.48
5:H:627:GLU:HB2	5:H:630:PRO:HG2	1.94	0.48
2:S:35:GLY:HA2	2:S:85:LEU:HD12	1.94	0.48
2:Y:387:LEU:HA	2:Y:390:ARG:HD3	1.95	0.48
2:1:56:ASP:HB3	2:2:276:LEU:HD22	1.94	0.48
3:e:153:MET:HE1	3:e:274:ILE:CG2	2.43	0.48
5:F:317:PHE:HB3	5:F:322:GLN:HE21	1.77	0.48
1:J:398:VAL:HA	1:J:401:LYS:HE2	1.94	0.48
2:Q:262:PRO:HG3	2:Q:318:ILE:HG21	1.95	0.48
2:V:262:PRO:HG3	2:V:318:ILE:HG21	1.95	0.48
2:Z:387:LEU:HA	2:Z:390:ARG:HD3	1.95	0.48
2:2:237:SER:O	2:2:241:THR:OG1	2.25	0.48
6:G:566:THR:HG22	2:U:45:THR:HG21	1.95	0.48
6:M:175:PRO:HG3	5:N:402:ALA:HB1	1.94	0.48
2:X:387:LEU:HA	2:X:390:ARG:HD3	1.95	0.48
2:Y:262:PRO:HG3	2:Y:318:ILE:HG21	1.95	0.48
5:D:370:TRP:CD1	8:c:182:MET:HE1	2.48	0.48
6:G:305:ILE:HG22	6:G:309:GLN:HE21	1.78	0.48
8:L:1572:LEU:HD22	8:L:1599:LYS:H	1.79	0.48
2:S:347:ASN:OD1	2:S:347:ASN:N	2.47	0.48
2:T:347:ASN:OD1	2:T:347:ASN:N	2.47	0.48
2:U:387:LEU:HA	2:U:390:ARG:HD3	1.95	0.48
5:H:874:ARG:O	5:H:877:SER:OG	2.29	0.48
5:H:887:LYS:HA	5:H:890:GLU:HB2	1.96	0.48
2:V:407:GLN:NE2	2:V:408:PHE:O	2.47	0.48
6:C:175:PRO:HB3	5:D:402:ALA:HB1	1.95	0.48
6:C:187:LEU:HA	5:D:379:LYS:HE2	1.96	0.48
5:D:406:THR:HG23	5:D:412:ARG:HG2	1.96	0.48
2:R:237:SER:O	2:R:241:THR:OG1	2.25	0.48
2:1:387:LEU:HA	2:1:390:ARG:HD3	1.95	0.48
6:M:737:CYS:SG	6:M:738:MET:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:237:SER:O	2:Z:241:THR:OG1	2.25	0.48
6:C:302:GLU:HA	6:C:305:ILE:HD12	1.96	0.47
5:F:568:LEU:HD22	5:F:667:LEU:HG	1.95	0.47
8:L:1667:HIS:CE1	2:Z:355:SER:H	2.32	0.47
2:U:347:ASN:OD1	2:U:347:ASN:N	2.47	0.47
2:W:383:SER:O	2:W:386:SER:OG	2.29	0.47
8:c:74:SER:HB3	8:c:89:LEU:HD23	1.96	0.47
1:l:24:ARG:NH1	1:l:32:GLU:OE2	2.46	0.47
2:1:262:PRO:HG3	2:1:318:ILE:HG21	1.95	0.47
2:2:407:GLN:NE2	2:2:408:PHE:O	2.47	0.47
3:e:78:ASN:OD1	3:e:81:ASP:HB3	2.14	0.47
5:H:865:LEU:O	5:H:868:SER:OG	2.27	0.47
7:K:283:VAL:O	7:K:287:GLU:HB2	2.14	0.47
4:k:56:ASN:OD1	4:k:56:ASN:N	2.41	0.47
2:1:237:SER:O	2:1:244:ARG:NH2	2.48	0.47
6:C:862:ASN:HB2	6:C:864:PHE:CZ	2.49	0.47
2:Z:237:SER:O	2:Z:244:ARG:NH2	2.48	0.47
2:1:407:GLN:NE2	2:1:408:PHE:O	2.47	0.47
2:2:387:LEU:HA	2:2:390:ARG:HD3	1.95	0.47
6:G:446:MET:SD	6:G:446:MET:N	2.87	0.47
2:V:237:SER:O	2:V:244:ARG:NH2	2.48	0.47
2:W:407:GLN:NE2	2:W:408:PHE:O	2.47	0.47
2:2:262:PRO:HG3	2:2:318:ILE:HG21	1.95	0.47
5:D:587:ARG:HH12	5:D:592:LEU:HB2	1.79	0.47
5:D:627:GLU:HG3	5:h:64:ARG:HB2	1.97	0.47
6:M:533:ASP:OD2	6:M:653:ARG:NH2	2.48	0.47
5:N:333:ARG:HE	5:N:337:ARG:HH11	1.62	0.47
2:Q:237:SER:O	2:Q:244:ARG:NH2	2.48	0.47
2:V:387:LEU:HA	2:V:390:ARG:HD3	1.95	0.47
2:Y:407:GLN:NE2	2:Y:408:PHE:O	2.47	0.47
2:Z:347:ASN:OD1	2:Z:347:ASN:N	2.47	0.47
1:l:64:THR:HG21	1:l:115:LEU:HD11	1.97	0.47
4:b:34:ILE:HG13	4:b:35:LEU:HD22	1.97	0.47
6:C:559:LEU:HD21	6:C:570:LYS:HB2	1.97	0.47
6:C:644:HIS:HE1	6:C:738:MET:HB2	1.79	0.47
6:E:416:LYS:H	6:E:419:ILE:HB	1.80	0.47
2:T:387:LEU:HA	2:T:390:ARG:HD3	1.95	0.47
2:T:407:GLN:NE2	2:T:408:PHE:O	2.47	0.47
8:c:64:LEU:HD12	8:c:65:PRO:HD2	1.97	0.47
3:e:138:ALA:HB1	3:e:152:VAL:HG11	1.95	0.47
4:b:25:MET:HG3	4:b:41:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:482:ARG:HD2	6:C:485:VAL:HG21	1.97	0.47
5:D:337:ARG:NH1	8:c:174:MET:SD	2.87	0.47
5:F:302:ASN:O	5:F:306:ARG:HB2	2.15	0.47
6:G:238:LEU:HD11	6:G:241:ARG:HH21	1.79	0.47
6:M:223:TYR:OH	5:N:366:ARG:NH2	2.47	0.47
6:M:713:LEU:HD22	6:M:722:VAL:HG13	1.96	0.47
4:k:25:MET:HE1	4:k:48:VAL:HG11	1.97	0.47
2:S:262:PRO:HG3	2:S:318:ILE:HG21	1.95	0.47
2:S:387:LEU:HA	2:S:390:ARG:HD3	1.95	0.47
2:U:237:SER:O	2:U:241:THR:OG1	2.25	0.47
2:U:407:GLN:NE2	2:U:408:PHE:O	2.47	0.47
2:2:347:ASN:OD1	2:2:347:ASN:N	2.47	0.47
7:I:184:TYR:O	7:I:188:SER:OG	2.30	0.47
2:R:387:LEU:HA	2:R:390:ARG:HD3	1.95	0.47
6:E:442:PHE:CE1	6:E:484:TYR:HE1	2.33	0.47
2:R:68:ASP:OD2	2:R:68:ASP:N	2.48	0.47
2:Y:384:ILE:HD12	2:Y:387:LEU:HD12	1.97	0.47
4:d:46:ILE:HD12	8:c:11:LEU:HB2	1.97	0.47
5:j:24:SER:OG	5:j:25:GLU:N	2.48	0.47
6:C:857:SER:O	2:Q:341:ARG:NE	2.48	0.47
2:R:237:SER:O	2:R:244:ARG:NH2	2.48	0.47
2:W:68:ASP:OD2	2:W:68:ASP:N	2.48	0.47
2:Z:407:GLN:NE2	2:Z:408:PHE:O	2.47	0.47
2:1:384:ILE:HD12	2:1:387:LEU:HD12	1.97	0.46
2:2:89:GLU:O	2:2:124:ARG:NH2	2.48	0.46
5:N:361:SER:OG	5:N:362:LEU:N	2.48	0.46
2:R:407:GLN:NE2	2:R:408:PHE:O	2.47	0.46
2:S:89:GLU:O	2:S:124:ARG:NH2	2.48	0.46
2:X:68:ASP:OD2	2:X:68:ASP:N	2.48	0.46
2:Y:89:GLU:O	2:Y:124:ARG:NH2	2.49	0.46
2:2:274:THR:HG21	2:2:293:VAL:HG12	1.97	0.46
6:M:559:LEU:HD11	6:M:570:LYS:HB2	1.97	0.46
2:Q:68:ASP:OD2	2:Q:68:ASP:N	2.48	0.46
2:R:262:PRO:HG3	2:R:318:ILE:HG21	1.95	0.46
2:W:237:SER:O	2:W:244:ARG:NH2	2.48	0.46
2:1:68:ASP:OD2	2:1:68:ASP:N	2.48	0.46
2:2:384:ILE:HD12	2:2:387:LEU:HD12	1.97	0.46
7:I:511:ASP:H	7:I:514:LYS:HG2	1.80	0.46
6:M:581:ASP:HB2	6:M:615:ALA:HB2	1.97	0.46
2:S:384:ILE:HD12	2:S:387:LEU:HD12	1.97	0.46
2:U:274:THR:HG21	2:U:293:VAL:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:292:ASP:HA	2:W:296:ARG:HH21	1.81	0.46
2:X:89:GLU:O	2:X:124:ARG:NH2	2.48	0.46
2:Y:68:ASP:OD2	2:Y:68:ASP:N	2.48	0.46
2:1:274:THR:HG21	2:1:293:VAL:HG12	1.97	0.46
3:e:353:GLN:HA	3:e:356:TRP:HB3	1.98	0.46
6:E:296:MET:HE1	6:E:338:LEU:HD13	1.97	0.46
7:K:647:LEU:HD22	2:Y:337:LEU:HD23	1.97	0.46
2:Q:89:GLU:O	2:Q:124:ARG:NH2	2.49	0.46
2:T:68:ASP:OD2	2:T:68:ASP:N	2.48	0.46
2:U:237:SER:O	2:U:244:ARG:NH2	2.48	0.46
2:W:274:THR:HG21	2:W:293:VAL:HG12	1.97	0.46
2:X:407:GLN:NE2	2:X:408:PHE:O	2.47	0.46
2:1:172:PHE:N	2:1:205:LEU:O	2.49	0.46
2:2:383:SER:O	2:2:386:SER:OG	2.29	0.46
5:D:689:LYS:HA	5:D:692:ARG:NE	2.31	0.46
6:E:427:TYR:OH	6:E:455:LYS:O	2.31	0.46
2:U:292:ASP:HA	2:U:296:ARG:HH21	1.81	0.46
2:V:89:GLU:O	2:V:124:ARG:NH2	2.49	0.46
2:W:89:GLU:O	2:W:124:ARG:NH2	2.49	0.46
2:X:384:ILE:HD12	2:X:387:LEU:HD12	1.97	0.46
2:Z:89:GLU:O	2:Z:124:ARG:NH2	2.48	0.46
2:1:89:GLU:O	2:1:124:ARG:NH2	2.49	0.46
6:G:162:ARG:O	6:G:166:ASN:ND2	2.48	0.46
1:J:902:MET:HG3	2:X:248:TYR:CE2	2.51	0.46
7:K:341:TRP:CE2	7:K:552:ARG:HA	2.51	0.46
8:L:533:THR:O	8:L:537:HIS:HB2	2.15	0.46
6:M:761:CYS:SG	6:M:762:MET:N	2.89	0.46
2:R:89:GLU:O	2:R:124:ARG:NH2	2.48	0.46
2:R:292:ASP:HA	2:R:296:ARG:HH21	1.81	0.46
2:T:323:ILE:HD12	2:T:323:ILE:HA	1.81	0.46
3:e:345:ILE:HG13	8:c:39:LYS:HG2	1.97	0.46
6:E:628:LEU:H	6:E:628:LEU:HG	1.56	0.46
1:J:548:MET:HE1	1:J:556:LEU:HD22	1.98	0.46
2:T:172:PHE:N	2:T:205:LEU:O	2.49	0.46
2:X:56:ASP:OD1	2:Y:287:LYS:HD2	2.16	0.46
2:Y:292:ASP:HA	2:Y:296:ARG:HH21	1.81	0.46
2:2:172:PHE:N	2:2:205:LEU:O	2.49	0.46
2:2:353:PRO:HD2	5:N:710:GLU:HG2	1.97	0.46
6:E:529:VAL:O	2:S:3:ARG:NH1	2.49	0.46
7:I:357:ILE:O	7:I:361:TYR:CB	2.62	0.46
7:I:498:LEU:HA	7:I:502:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:292:ASP:HA	2:Q:296:ARG:HH21	1.81	0.46
2:R:384:ILE:HD12	2:R:387:LEU:HD12	1.97	0.46
2:S:237:SER:O	2:S:241:THR:OG1	2.25	0.46
2:S:292:ASP:HA	2:S:296:ARG:HH21	1.81	0.46
2:T:237:SER:O	2:T:244:ARG:NH2	2.48	0.46
2:U:68:ASP:N	2:U:68:ASP:OD2	2.48	0.46
2:V:274:THR:HG21	2:V:293:VAL:HG12	1.97	0.46
2:X:292:ASP:HA	2:X:296:ARG:HH21	1.81	0.46
6:E:457:LEU:HD22	6:E:467:VAL:HG12	1.97	0.46
5:H:730:SER:HA	5:H:733:GLU:HG3	1.98	0.46
2:Q:383:SER:O	2:Q:386:SER:OG	2.29	0.46
2:Q:384:ILE:HD12	2:Q:387:LEU:HD12	1.97	0.46
2:S:274:THR:HG21	2:S:293:VAL:HG12	1.97	0.46
2:T:274:THR:HG21	2:T:293:VAL:HG12	1.97	0.46
2:U:89:GLU:O	2:U:124:ARG:NH2	2.48	0.46
2:V:68:ASP:OD2	2:V:68:ASP:N	2.48	0.46
2:Y:172:PHE:N	2:Y:205:LEU:O	2.49	0.46
2:Z:384:ILE:HD12	2:Z:387:LEU:HD12	1.97	0.46
6:E:238:LEU:HD23	6:E:244:ARG:H	1.80	0.46
2:U:172:PHE:N	2:U:205:LEU:O	2.49	0.46
2:U:323:ILE:HD12	2:U:323:ILE:HA	1.81	0.46
5:a:94:LEU:HA	5:a:97:LEU:HG	1.98	0.45
5:D:425:PRO:O	5:D:428:SER:OG	2.33	0.45
5:F:397:ALA:O	5:F:473:SER:OG	2.33	0.45
5:H:482:LYS:HD2	5:H:538:TYR:CZ	2.51	0.45
1:J:275:LEU:HA	1:J:379:LEU:HD12	1.97	0.45
1:J:879:GLN:HB3	1:J:880:ILE:HD12	1.98	0.45
2:T:89:GLU:O	2:T:124:ARG:NH2	2.48	0.45
2:X:237:SER:O	2:X:244:ARG:NH2	2.48	0.45
5:h:19:ARG:HD2	5:h:19:ARG:HA	1.82	0.45
2:2:237:SER:O	2:2:244:ARG:NH2	2.48	0.45
6:C:234:SER:HG	5:D:286:SER:N	2.14	0.45
6:E:338:LEU:HD11	6:E:375:LEU:HD21	1.97	0.45
7:K:176:LEU:HG	7:K:180:HIS:HE1	1.81	0.45
6:M:705:THR:HA	6:M:708:ILE:HG22	1.98	0.45
2:W:347:ASN:OD1	2:W:347:ASN:N	2.47	0.45
2:Y:237:SER:O	2:Y:244:ARG:NH2	2.48	0.45
2:Z:274:THR:HG21	2:Z:293:VAL:HG12	1.97	0.45
2:2:292:ASP:HA	2:2:296:ARG:HH21	1.81	0.45
5:D:254:ILE:HB	5:D:366:ARG:HH12	1.81	0.45
6:E:427:TYR:CD2	6:E:431:ARG:HD3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:364:LEU:HD13	5:N:370:TRP:HE1	1.81	0.45
2:T:292:ASP:HA	2:T:296:ARG:HH21	1.81	0.45
2:T:384:ILE:HD12	2:T:387:LEU:HD12	1.97	0.45
2:V:384:ILE:HD12	2:V:387:LEU:HD12	1.97	0.45
2:Y:274:THR:HG21	2:Y:293:VAL:HG12	1.97	0.45
6:E:241:ARG:HH21	6:E:242:GLN:NE2	2.15	0.45
1:J:879:GLN:N	1:J:879:GLN:OE1	2.48	0.45
1:J:882:ARG:NH2	1:J:984:GLU:OE2	2.50	0.45
7:K:577:LYS:O	7:K:581:HIS:HB2	2.15	0.45
2:Q:407:GLN:NE2	2:Q:408:PHE:O	2.47	0.45
2:S:323:ILE:HD12	2:S:323:ILE:HA	1.81	0.45
2:W:384:ILE:HD12	2:W:387:LEU:HD12	1.97	0.45
2:X:274:THR:HG21	2:X:293:VAL:HG12	1.97	0.45
2:Z:68:ASP:N	2:Z:68:ASP:OD2	2.48	0.45
3:e:104:LEU:HD13	3:e:347:ALA:HB2	1.98	0.45
6:E:427:TYR:HB3	6:E:624:TRP:HZ2	1.80	0.45
5:F:480:SER:HA	5:F:483:VAL:HG22	1.98	0.45
8:L:322:LYS:HG3	8:L:325:ARG:NH2	2.31	0.45
4:i:44:LEU:HA	4:i:47:CYS:HB3	1.99	0.45
2:S:68:ASP:OD2	2:S:68:ASP:N	2.48	0.45
4:d:33:ARG:NH1	4:d:37:THR:OG1	2.49	0.45
3:e:89:THR:O	3:e:93:GLU:HB3	2.17	0.45
3:e:153:MET:HE1	3:e:274:ILE:HG23	1.97	0.45
6:M:654:GLN:HB3	6:M:759:THR:HG21	1.98	0.45
2:Q:274:THR:HG21	2:Q:293:VAL:HG12	1.97	0.45
2:R:274:THR:HG21	2:R:293:VAL:HG12	1.97	0.45
2:U:384:ILE:HD12	2:U:387:LEU:HD12	1.97	0.45
8:c:16:LEU:HD11	8:c:34:LYS:HA	1.98	0.45
1:l:71:LYS:HG3	5:H:630:PRO:HG3	1.98	0.45
6:C:865:TYR:CD1	2:Q:353:PRO:HG3	2.52	0.45
5:D:718:MET:HE3	5:D:718:MET:HB3	1.83	0.45
5:H:321:GLY:HA2	5:H:324:PHE:HB3	1.99	0.45
8:L:1679:GLN:HB3	8:L:1715:ARG:HB3	1.99	0.45
6:M:499:LEU:HD23	6:M:719:ILE:HG13	1.98	0.45
2:S:237:SER:O	2:S:244:ARG:NH2	2.48	0.45
5:F:406:THR:HG22	5:F:408:ASP:H	1.81	0.45
7:I:256:GLN:HB3	7:I:257:PHE:H	1.67	0.45
7:I:397:GLN:HB3	7:I:409:ASN:ND2	2.32	0.45
2:U:343:ARG:HG3	2:U:345:LEU:HB2	1.99	0.45
2:V:172:PHE:N	2:V:205:LEU:O	2.49	0.45
2:W:29:HIS:HE1	2:W:244:ARG:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:296:ARG:HH11	2:1:296:ARG:HD3	1.59	0.45
2:1:343:ARG:HG3	2:1:345:LEU:HB2	1.99	0.45
7:I:504:HIS:HD2	2:W:265:ARG:HH12	1.65	0.45
6:M:157:LYS:HG2	6:M:284:GLU:HG3	1.99	0.45
5:N:680:ILE:HD11	5:N:786:GLN:HA	1.98	0.45
2:Z:292:ASP:HA	2:Z:296:ARG:HH21	1.81	0.45
2:1:292:ASP:HA	2:1:296:ARG:HH21	1.81	0.45
6:C:551:LEU:HA	6:C:551:LEU:HD12	1.80	0.45
6:E:241:ARG:HH21	6:E:242:GLN:HE22	1.63	0.45
2:R:343:ARG:HG3	2:R:345:LEU:HB2	1.99	0.45
2:W:343:ARG:HG3	2:W:345:LEU:HB2	1.99	0.45
8:c:64:LEU:HD23	8:c:67:ARG:HD2	1.99	0.45
3:e:33:SER:HB2	3:e:69:TYR:CD2	2.52	0.44
6:C:218:VAL:HG13	6:C:314:HIS:NE2	2.31	0.44
6:G:276:PHE:CE1	6:G:280:LYS:HG3	2.51	0.44
6:M:456:TYR:HA	6:M:459:VAL:HG22	1.98	0.44
2:S:262:PRO:HG2	2:S:263:THR:HG22	2.00	0.44
2:V:29:HIS:HE1	2:V:244:ARG:HD2	1.82	0.44
2:V:296:ARG:HH11	2:V:296:ARG:HD3	1.59	0.44
2:X:237:SER:O	2:X:241:THR:OG1	2.25	0.44
2:Y:343:ARG:HG3	2:Y:345:LEU:HB2	1.99	0.44
2:2:29:HIS:HE1	2:2:244:ARG:HD2	1.82	0.44
2:2:343:ARG:HG3	2:2:345:LEU:HB2	1.99	0.44
5:F:388:CYS:HA	5:F:391:ARG:HE	1.82	0.44
6:G:529:VAL:HG22	2:U:3:ARG:HH12	1.82	0.44
6:M:208:LEU:O	6:M:213:GLN:NE2	2.50	0.44
2:R:347:ASN:OD1	2:R:347:ASN:N	2.47	0.44
2:W:57:ASP:HA	2:X:296:ARG:NH1	2.32	0.44
2:X:183:VAL:HG13	2:X:187:ASN:HD21	1.83	0.44
2:X:343:ARG:HG3	2:X:345:LEU:HB2	1.99	0.44
2:Z:172:PHE:N	2:Z:205:LEU:O	2.49	0.44
1:J:391:THR:N	8:L:307:ARG:HH12	2.16	0.44
2:Q:29:HIS:HE1	2:Q:244:ARG:HD2	1.82	0.44
2:R:172:PHE:N	2:R:205:LEU:O	2.49	0.44
2:S:183:VAL:HG13	2:S:187:ASN:HD21	1.83	0.44
2:V:277:THR:HG22	2:V:279:ASP:H	1.83	0.44
2:W:277:THR:HG22	2:W:279:ASP:H	1.83	0.44
2:2:68:ASP:OD2	2:2:68:ASP:N	2.48	0.44
3:e:193:LEU:HD23	3:e:193:LEU:HA	1.89	0.44
6:C:719:ILE:HG22	6:C:723:LEU:HD23	1.99	0.44
5:D:277:VAL:HG13	5:D:288:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:328:VAL:HG23	7:K:331:ARG:HH21	1.81	0.44
4:i:55:ILE:HD11	5:h:39:ILE:HD12	1.99	0.44
2:Q:277:THR:HG22	2:Q:279:ASP:H	1.83	0.44
2:S:407:GLN:NE2	2:S:408:PHE:O	2.47	0.44
2:T:277:THR:HG22	2:T:279:ASP:H	1.83	0.44
2:V:292:ASP:HA	2:V:296:ARG:HH21	1.81	0.44
2:W:183:VAL:HG13	2:W:187:ASN:HD21	1.83	0.44
3:e:10:VAL:HB	3:e:86:TRP:CH2	2.53	0.44
6:C:611:SER:OG	6:C:612:GLY:N	2.50	0.44
2:Q:262:PRO:HG2	2:Q:263:THR:HG22	2.00	0.44
2:R:262:PRO:HG2	2:R:263:THR:HG22	2.00	0.44
2:1:277:THR:HG22	2:1:279:ASP:H	1.83	0.44
6:C:516:ILE:HG23	6:C:638:TYR:CE2	2.53	0.44
6:C:520:PHE:CZ	6:C:618:PHE:HB2	2.52	0.44
6:E:288:VAL:HG11	6:E:356:LEU:HD12	2.00	0.44
6:M:548:PRO:HA	6:M:551:LEU:HD12	1.99	0.44
2:Q:237:SER:H	2:Q:237:SER:HG	1.51	0.44
2:R:277:THR:HG22	2:R:279:ASP:H	1.83	0.44
2:U:396:ASP:OD2	2:U:425:ARG:NH2	2.47	0.44
2:Y:350:PRO:HG2	2:Y:441:PRO:HG3	2.00	0.44
4:b:68:ARG:HG2	5:a:20:ILE:HD11	1.98	0.44
6:E:158:ARG:HB3	6:E:162:ARG:HH21	1.82	0.44
5:N:327:ALA:HB2	5:N:421:LEU:HD23	1.99	0.44
2:Q:183:VAL:HG13	2:Q:187:ASN:HD21	1.83	0.44
2:T:262:PRO:HG2	2:T:263:THR:HG22	2.00	0.44
2:U:29:HIS:HE1	2:U:244:ARG:HD2	1.82	0.44
2:W:350:PRO:HG2	2:W:441:PRO:HG3	2.00	0.44
2:X:172:PHE:N	2:X:205:LEU:O	2.49	0.44
2:X:262:PRO:HG2	2:X:263:THR:HG22	2.00	0.44
8:L:1804:PHE:CD1	2:Z:355:SER:HB3	2.52	0.44
2:R:323:ILE:HD12	2:R:323:ILE:HA	1.81	0.44
2:T:343:ARG:HG3	2:T:345:LEU:HB2	1.99	0.44
2:U:262:PRO:HG2	2:U:263:THR:HG22	2.00	0.44
2:Z:29:HIS:HE1	2:Z:244:ARG:HD2	1.82	0.44
1:l:48:PHE:HD1	4:m:59:ALA:HB1	1.83	0.44
2:1:183:VAL:HG13	2:1:187:ASN:HD21	1.83	0.44
2:1:355:SER:OG	6:M:861:PHE:HB3	2.18	0.44
2:2:262:PRO:HG2	2:2:263:THR:HG22	1.99	0.44
3:e:162:THR:HB	3:e:176:LEU:HD13	1.99	0.44
6:E:663:LYS:NZ	2:S:164:LYS:O	2.40	0.44
6:E:663:LYS:NZ	2:S:200:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:361:SER:OG	5:H:362:LEU:N	2.50	0.44
7:I:530:TYR:CE2	2:W:249:MET:HE3	2.53	0.44
2:T:396:ASP:OD2	2:T:425:ARG:NH2	2.47	0.44
2:V:183:VAL:HG13	2:V:187:ASN:HD21	1.83	0.44
2:Z:262:PRO:HG2	2:Z:263:THR:HG22	2.00	0.44
2:1:29:HIS:HE1	2:1:244:ARG:HD2	1.82	0.43
2:1:350:PRO:HG2	2:1:441:PRO:HG3	2.00	0.43
2:2:323:ILE:HD12	2:2:323:ILE:HA	1.81	0.43
3:e:35:VAL:HG23	3:e:85:ILE:HD12	1.98	0.43
6:G:359:LEU:HB3	6:G:380:THR:HG22	2.00	0.43
2:R:183:VAL:HG13	2:R:187:ASN:HD21	1.83	0.43
2:S:29:HIS:HE1	2:S:244:ARG:HD2	1.82	0.43
2:T:29:HIS:HE1	2:T:244:ARG:HD2	1.82	0.43
5:D:337:ARG:HB2	6:E:326:PHE:CE1	2.53	0.43
5:D:581:LEU:HD21	5:D:597:LEU:HD23	2.00	0.43
6:G:529:VAL:O	2:U:3:ARG:NH1	2.51	0.43
7:K:275:LYS:HB3	7:K:333:ARG:HG3	2.00	0.43
7:K:497:ALA:HB2	2:Y:254:ILE:HD11	1.99	0.43
2:W:172:PHE:N	2:W:205:LEU:O	2.49	0.43
2:W:262:PRO:HG2	2:W:263:THR:HG22	2.00	0.43
2:X:347:ASN:OD1	2:X:347:ASN:N	2.47	0.43
2:2:183:VAL:HG13	2:2:187:ASN:HD21	1.83	0.43
7:I:448:SER:OG	7:I:449:GLY:N	2.50	0.43
1:J:283:LYS:HD2	1:J:283:LYS:HA	1.78	0.43
7:K:11:GLY:HA2	7:K:53:ILE:HG12	2.00	0.43
6:M:610:LEU:HB3	6:M:613:LEU:HD13	2.00	0.43
2:Q:343:ARG:HG3	2:Q:345:LEU:HB2	1.99	0.43
2:R:29:HIS:HE1	2:R:244:ARG:HD2	1.82	0.43
2:T:296:ARG:HH11	2:T:296:ARG:HD3	1.59	0.43
2:Y:277:THR:HG22	2:Y:279:ASP:H	1.83	0.43
2:Z:183:VAL:HG13	2:Z:187:ASN:HD21	1.83	0.43
2:Z:277:THR:HG22	2:Z:279:ASP:H	1.83	0.43
8:c:182:MET:HB3	8:c:182:MET:HE2	1.70	0.43
5:D:688:ALA:O	5:D:692:ARG:HG3	2.17	0.43
6:G:659:TRP:CD1	6:G:683:ARG:HE	2.37	0.43
5:N:654:ARG:HA	5:N:657:MET:HG2	2.00	0.43
2:R:20:GLU:OE1	2:R:230:GLN:NE2	2.52	0.43
2:R:69:LEU:HD12	2:R:69:LEU:HA	1.88	0.43
2:S:20:GLU:OE1	2:S:230:GLN:NE2	2.52	0.43
2:S:277:THR:HG22	2:S:279:ASP:H	1.83	0.43
2:T:183:VAL:HG13	2:T:187:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:396:ASP:OD2	2:V:425:ARG:NH2	2.47	0.43
2:W:20:GLU:OE1	2:W:230:GLN:NE2	2.52	0.43
2:Y:237:SER:O	2:Y:241:THR:OG1	2.25	0.43
2:1:297:LEU:HD12	2:1:297:LEU:HA	1.91	0.43
5:D:380:THR:HG23	5:D:411:MET:HE3	2.00	0.43
6:E:821:THR:HA	6:E:824:LYS:HG2	2.00	0.43
7:I:498:LEU:HD11	7:I:517:LEU:HD22	2.00	0.43
8:L:350:CYS:HB2	8:L:453:THR:HG21	1.99	0.43
2:U:183:VAL:HG13	2:U:187:ASN:HD21	1.83	0.43
2:V:343:ARG:HG3	2:V:345:LEU:HB2	1.99	0.43
4:d:46:ILE:HG12	4:d:50:LEU:HD13	1.99	0.43
2:1:262:PRO:HG2	2:1:263:THR:HG22	2.00	0.43
6:C:697:MET:HB3	6:C:702:MET:HE1	2.01	0.43
6:E:180:TRP:O	6:E:184:ARG:HG2	2.18	0.43
6:E:713:LEU:HD22	6:E:722:VAL:HG13	2.00	0.43
6:G:449:LYS:O	6:G:453:THR:OG1	2.30	0.43
5:H:599:GLY:C	2:W:342:GLU:HG3	2.44	0.43
2:Z:343:ARG:HG3	2:Z:345:LEU:HB2	1.99	0.43
2:1:110:GLN:HA	2:1:113:LYS:HE3	2.01	0.43
2:2:277:THR:HG22	2:2:279:ASP:H	1.83	0.43
6:C:692:ASN:HD22	6:C:859:LEU:HD23	1.82	0.43
5:D:409:PRO:HA	5:D:412:ARG:HB2	2.01	0.43
6:E:320:SER:OG	6:E:321:LEU:N	2.51	0.43
6:E:674:GLN:HB2	6:E:675:TRP:H	1.62	0.43
5:F:400:VAL:HG11	5:F:422:VAL:HG21	1.99	0.43
8:L:469:GLN:HA	8:L:517:HIS:CE1	2.53	0.43
2:Q:110:GLN:HA	2:Q:113:LYS:HE3	2.01	0.43
2:S:172:PHE:N	2:S:205:LEU:O	2.49	0.43
2:T:110:GLN:HA	2:T:113:LYS:HE3	2.01	0.43
2:U:110:GLN:HA	2:U:113:LYS:HE3	2.01	0.43
2:U:277:THR:HG22	2:U:279:ASP:H	1.83	0.43
2:X:29:HIS:HE1	2:X:244:ARG:HD2	1.82	0.43
2:Z:110:GLN:HA	2:Z:113:LYS:HE3	2.01	0.43
7:K:183:MET:HE3	7:K:183:MET:HB3	1.83	0.43
2:T:350:PRO:HG2	2:T:441:PRO:HG3	2.00	0.43
2:Y:29:HIS:HE1	2:Y:244:ARG:HD2	1.82	0.43
2:Y:262:PRO:HG2	2:Y:263:THR:HG22	1.99	0.43
2:Z:350:PRO:HG2	2:Z:441:PRO:HG3	2.00	0.43
2:2:350:PRO:HG2	2:2:441:PRO:HG3	2.00	0.43
5:a:19:ARG:HD2	5:a:19:ARG:HA	1.78	0.43
6:C:695:TYR:HE2	2:Q:357:GLN:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:578:MET:HG2	6:E:584:THR:HG21	2.00	0.43
5:N:408:ASP:HB3	5:N:411:MET:HB2	2.01	0.43
2:Q:350:PRO:HG2	2:Q:441:PRO:HG3	2.00	0.43
2:X:277:THR:HG22	2:X:279:ASP:H	1.83	0.43
3:e:304:THR:HG23	3:e:335:ARG:HD3	1.99	0.43
6:E:585:GLN:HB2	6:E:739:LEU:HD12	2.01	0.43
6:E:623:LYS:O	6:E:627:SER:N	2.52	0.43
5:H:658:SER:O	5:H:662:ARG:HG3	2.19	0.43
5:N:660:TYR:HA	5:N:663:VAL:HG22	2.01	0.43
2:Q:69:LEU:HD12	2:Q:69:LEU:HA	1.88	0.43
2:U:20:GLU:OE1	2:U:230:GLN:NE2	2.52	0.43
2:V:262:PRO:HG2	2:V:263:THR:HG22	2.00	0.43
4:m:55:ILE:HD12	4:m:55:ILE:HA	1.85	0.43
3:e:119:MET:HE3	3:e:119:MET:HB2	1.96	0.42
6:C:280:LYS:HD2	6:C:285:TYR:CE2	2.54	0.42
6:C:448:ASP:OD1	6:C:448:ASP:N	2.52	0.42
6:C:762:MET:HE1	6:C:822:ILE:HG13	2.00	0.42
6:E:427:TYR:HD1	6:E:628:LEU:HD22	1.84	0.42
6:E:679:ALA:HB2	6:E:818:PHE:CE2	2.53	0.42
1:J:311:ARG:O	1:J:315:GLU:HB2	2.19	0.42
7:K:282:SER:HB2	7:K:340:LEU:HD21	2.01	0.42
5:N:589:ALA:HB1	5:N:628:VAL:HG12	2.00	0.42
5:N:755:LEU:HA	5:N:755:LEU:HD13	1.86	0.42
2:Q:172:PHE:N	2:Q:205:LEU:O	2.49	0.42
2:R:110:GLN:HA	2:R:113:LYS:HE3	2.01	0.42
2:V:69:LEU:HD12	2:V:69:LEU:HA	1.88	0.42
2:X:350:PRO:HG2	2:X:441:PRO:HG3	2.00	0.42
4:b:63:VAL:HG22	5:a:38:VAL:HG21	2.02	0.42
6:C:178:PRO:HB3	6:C:180:TRP:CE2	2.54	0.42
5:F:673:MET:HE3	5:F:779:PHE:HB3	2.01	0.42
6:G:180:TRP:HA	6:G:183:GLU:HB2	2.01	0.42
8:L:1804:PHE:HD1	2:Z:355:SER:HB3	1.82	0.42
6:M:660:ILE:HA	6:M:663:LYS:HA	2.01	0.42
6:M:711:LYS:HA	6:M:714:LYS:HG2	2.01	0.42
5:N:449:ALA:HB2	5:N:467:ARG:HD2	2.00	0.42
5:N:730:SER:HA	5:N:733:GLU:HG3	2.01	0.42
2:S:350:PRO:HG2	2:S:441:PRO:HG3	2.00	0.42
8:c:76:ASP:HA	8:c:79:VAL:HG22	2.01	0.42
3:e:31:PHE:HD2	3:e:54:VAL:HG23	1.83	0.42
3:e:211:ASP:O	3:e:215:LYS:HD3	2.19	0.42
5:D:587:ARG:HH22	5:D:591:THR:HB	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:i:18:LEU:HA	4:i:21:VAL:HG12	2.00	0.42
2:S:110:GLN:HA	2:S:113:LYS:HE3	2.01	0.42
2:S:343:ARG:HG3	2:S:345:LEU:HB2	1.99	0.42
2:S:352:GLY:HA2	2:S:353:PRO:HD3	1.88	0.42
2:V:237:SER:O	2:V:241:THR:OG1	2.25	0.42
2:V:350:PRO:HG2	2:V:441:PRO:HG3	2.00	0.42
2:W:110:GLN:HA	2:W:113:LYS:HE3	2.01	0.42
4:b:65:LYS:O	4:b:69:LYS:NZ	2.51	0.42
6:E:442:PHE:HE1	6:E:484:TYR:HE1	1.66	0.42
5:F:468:LYS:HA	5:F:471:ILE:HG13	2.01	0.42
6:G:818:PHE:O	6:G:822:ILE:HG12	2.20	0.42
7:I:118:SER:OG	7:I:119:ILE:N	2.53	0.42
5:N:463:LYS:HE2	5:N:495:GLN:HE22	1.83	0.42
4:i:74:LEU:HB3	5:h:23:ARG:HE	1.84	0.42
2:R:350:PRO:HG2	2:R:441:PRO:HG3	2.00	0.42
2:X:141:ILE:H	2:X:171:VAL:HG22	1.85	0.42
2:Z:20:GLU:OE1	2:Z:230:GLN:NE2	2.52	0.42
4:d:24:THR:HA	4:d:27:VAL:HG12	2.00	0.42
2:1:141:ILE:H	2:1:171:VAL:HG22	1.84	0.42
2:2:9:GLN:HE21	2:2:64:ALA:HB1	1.85	0.42
2:2:110:GLN:HA	2:2:113:LYS:HE3	2.01	0.42
4:b:57:PRO:HA	4:b:60:LEU:HD12	2.01	0.42
5:D:797:LEU:HA	5:D:800:LEU:HG	2.01	0.42
6:M:395:ILE:HD11	6:M:450:ILE:HG23	2.02	0.42
2:U:350:PRO:HG2	2:U:441:PRO:HG3	2.00	0.42
4:b:62:SER:O	4:b:66:GLU:HG2	2.19	0.42
5:F:319:LEU:O	5:F:323:SER:OG	2.37	0.42
1:J:237:HIS:O	1:J:239:HIS:N	2.53	0.42
2:Q:20:GLU:OE1	2:Q:230:GLN:NE2	2.52	0.42
2:U:141:ILE:H	2:U:171:VAL:HG22	1.85	0.42
2:Y:9:GLN:HE21	2:Y:64:ALA:HB1	1.85	0.42
2:Y:323:ILE:HD12	2:Y:323:ILE:HA	1.81	0.42
3:e:86:TRP:CH2	3:e:105:LEU:HB2	2.54	0.42
4:b:49:ARG:HH22	8:L:283:TRP:N	2.16	0.42
5:F:334:GLU:O	5:F:338:LEU:HD13	2.19	0.42
5:H:763:LEU:HD12	5:H:775:LEU:HD22	2.02	0.42
5:H:869:SER:HB3	5:H:873:LEU:HD13	2.01	0.42
7:I:172:LEU:HD23	7:I:175:ILE:HD12	2.01	0.42
6:M:739:LEU:HD13	6:M:739:LEU:HA	1.83	0.42
2:Q:237:SER:O	2:Q:241:THR:OG1	2.25	0.42
2:V:141:ILE:H	2:V:171:VAL:HG22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:141:ILE:H	2:W:171:VAL:HG22	1.85	0.42
2:Y:141:ILE:H	2:Y:171:VAL:HG22	1.85	0.42
2:Y:183:VAL:HG13	2:Y:187:ASN:HD21	1.83	0.42
2:Z:9:GLN:HE21	2:Z:64:ALA:HB1	1.85	0.42
2:Z:37:VAL:HG12	2:Z:59:HIS:CD2	2.54	0.42
5:j:35:ALA:HA	5:j:38:VAL:HG22	2.02	0.42
7:I:59:ILE:HD11	7:I:93:LEU:HG	2.00	0.42
2:R:9:GLN:HE21	2:R:64:ALA:HB1	1.85	0.42
2:T:20:GLU:OE1	2:T:230:GLN:NE2	2.52	0.42
2:T:37:VAL:HG12	2:T:59:HIS:CD2	2.54	0.42
2:U:397:LYS:HE2	2:U:401:ARG:HH11	1.85	0.42
2:Y:110:GLN:HA	2:Y:113:LYS:HE3	2.01	0.42
2:Y:397:LYS:HE2	2:Y:401:ARG:HH11	1.85	0.42
5:D:653:THR:HG22	5:D:655:GLU:H	1.85	0.42
6:E:577:LEU:HD13	6:E:611:SER:HB2	2.01	0.42
5:H:485:LEU:HD12	5:H:485:LEU:HA	1.93	0.42
7:K:305:ASP:N	7:K:305:ASP:OD2	2.53	0.42
5:N:871:GLU:HG2	5:N:874:ARG:NH2	2.34	0.42
2:Q:396:ASP:OD2	2:Q:425:ARG:NH2	2.47	0.42
2:Z:141:ILE:H	2:Z:171:VAL:HG22	1.85	0.42
1:l:108:TYR:HA	1:l:111:LEU:HD12	2.02	0.42
2:S:37:VAL:HG12	2:S:59:HIS:CD2	2.54	0.42
2:W:397:LYS:HE2	2:W:401:ARG:HH11	1.85	0.42
2:Z:397:LYS:HE2	2:Z:401:ARG:HH11	1.85	0.42
1:l:109:SER:HA	4:m:57:PRO:HG3	2.02	0.41
2:1:298:LEU:HD21	2:1:346:ALA:HB2	2.02	0.41
3:e:109:PRO:HD3	3:e:137:GLN:HB3	2.01	0.41
5:F:644:VAL:HG11	5:F:652:PHE:HB2	2.02	0.41
6:G:304:LEU:HB3	5:H:369:VAL:HG22	2.01	0.41
7:K:264:LEU:HD12	7:K:265:PRO:HD2	2.01	0.41
2:R:141:ILE:H	2:R:171:VAL:HG22	1.84	0.41
2:W:9:GLN:HE21	2:W:64:ALA:HB1	1.85	0.41
2:X:20:GLU:OE1	2:X:230:GLN:NE2	2.52	0.41
2:X:323:ILE:HD12	2:X:323:ILE:HA	1.81	0.41
2:2:141:ILE:H	2:2:171:VAL:HG22	1.85	0.41
3:e:20:GLY:HA2	3:e:28:ARG:HB3	2.01	0.41
6:C:520:PHE:HB2	6:C:638:TYR:CZ	2.55	0.41
6:E:427:TYR:HE1	6:E:628:LEU:HD13	1.85	0.41
7:I:586:ILE:HD13	7:I:622:GLN:HE21	1.85	0.41
1:J:886:LEU:HA	1:J:886:LEU:HD13	1.68	0.41
2:Q:66:LEU:HD21	2:Q:74:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:298:LEU:HD21	2:R:346:ALA:HB2	2.03	0.41
2:S:141:ILE:H	2:S:171:VAL:HG22	1.85	0.41
2:T:66:LEU:HD21	2:T:74:ILE:HG12	2.03	0.41
2:W:66:LEU:HD21	2:W:74:ILE:HG12	2.03	0.41
2:X:110:GLN:HA	2:X:113:LYS:HE3	2.01	0.41
2:Y:20:GLU:OE1	2:Y:230:GLN:NE2	2.52	0.41
2:Z:66:LEU:HD21	2:Z:74:ILE:HG12	2.03	0.41
2:1:66:LEU:HD21	2:1:74:ILE:HG12	2.02	0.41
3:e:189:LEU:HD11	3:e:213:LYS:HD2	2.01	0.41
2:Q:37:VAL:HG12	2:Q:59:HIS:CD2	2.54	0.41
2:Q:352:GLY:HA2	2:Q:353:PRO:HD3	1.88	0.41
2:R:37:VAL:HG12	2:R:59:HIS:CD2	2.54	0.41
2:U:298:LEU:HD21	2:U:346:ALA:HB2	2.02	0.41
2:V:20:GLU:OE1	2:V:230:GLN:NE2	2.52	0.41
2:V:110:GLN:HA	2:V:113:LYS:HE3	2.01	0.41
2:W:298:LEU:HD21	2:W:346:ALA:HB2	2.03	0.41
2:2:66:LEU:HD21	2:2:74:ILE:HG12	2.03	0.41
6:E:466:ASP:OD1	6:E:466:ASP:N	2.49	0.41
6:G:578:MET:HB3	6:G:578:MET:HE2	1.65	0.41
6:G:685:ARG:HD3	2:U:353:PRO:HG2	2.02	0.41
7:I:404:LEU:HD23	7:I:404:LEU:HA	1.76	0.41
6:M:439:ILE:HG22	6:M:441:SER:H	1.84	0.41
2:R:396:ASP:OD2	2:R:425:ARG:NH2	2.47	0.41
2:R:397:LYS:HE2	2:R:401:ARG:HH11	1.85	0.41
2:S:9:GLN:HE21	2:S:64:ALA:HB1	1.85	0.41
2:U:13:CYS:HB2	2:U:140:SER:HB3	2.03	0.41
2:X:66:LEU:HD21	2:X:74:ILE:HG12	2.03	0.41
6:C:277:ILE:HG12	6:C:293:ALA:HB1	2.01	0.41
5:H:336:TYR:HB2	7:I:124:TYR:CD1	2.55	0.41
1:J:275:LEU:O	1:J:279:SER:OG	2.35	0.41
2:Q:397:LYS:HE2	2:Q:401:ARG:HH11	1.85	0.41
2:R:66:LEU:HD21	2:R:74:ILE:HG12	2.02	0.41
2:V:383:SER:O	2:V:386:SER:OG	2.29	0.41
2:W:53:TYR:N	2:W:61:ILE:O	2.54	0.41
2:X:13:CYS:HB2	2:X:140:SER:HB3	2.03	0.41
2:Y:296:ARG:HB2	2:Y:296:ARG:HE	1.72	0.41
3:e:70:PRO:HG3	3:e:85:ILE:HG21	2.03	0.41
5:D:609:ASN:HD22	5:D:609:ASN:HA	1.63	0.41
1:J:762:LEU:HD22	1:J:801:LEU:HD11	2.03	0.41
2:Q:53:TYR:N	2:Q:61:ILE:O	2.54	0.41
2:Q:298:LEU:HD21	2:Q:346:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:53:TYR:N	2:R:61:ILE:O	2.54	0.41
2:R:297:LEU:HD12	2:R:297:LEU:HA	1.91	0.41
2:V:397:LYS:HE2	2:V:401:ARG:HH11	1.85	0.41
2:W:425:ARG:HA	2:W:428:VAL:HG12	2.03	0.41
2:Y:298:LEU:HD21	2:Y:346:ALA:HB2	2.02	0.41
1:l:71:LYS:HE3	5:H:630:PRO:HA	2.02	0.41
2:1:20:GLU:OE1	2:1:230:GLN:NE2	2.52	0.41
2:2:296:ARG:HB2	2:2:296:ARG:HE	1.72	0.41
3:e:226:GLU:HA	3:e:229:THR:HG22	2.03	0.41
6:E:700:GLU:OE1	2:S:334:HIS:HB3	2.20	0.41
1:J:493:ILE:HG13	1:J:494:ILE:HG12	2.03	0.41
7:K:648:ARG:HG3	7:K:649:LEU:HD23	2.02	0.41
2:S:53:TYR:N	2:S:61:ILE:O	2.54	0.41
2:S:425:ARG:HA	2:S:428:VAL:HG12	2.03	0.41
2:U:84:LYS:HB2	2:U:84:LYS:HE3	1.90	0.41
2:X:53:TYR:N	2:X:61:ILE:O	2.54	0.41
2:1:425:ARG:HA	2:1:428:VAL:HG12	2.03	0.41
3:e:280:ASN:HD22	3:e:283:MET:HE2	1.85	0.41
6:C:840:LEU:HB2	6:C:856:ILE:HD11	2.02	0.41
6:E:547:THR:HA	6:E:548:PRO:HD3	1.93	0.41
5:F:679:ASP:HA	5:F:682:LYS:HB3	2.03	0.41
5:F:836:PHE:O	5:F:840:ILE:HG12	2.20	0.41
6:M:238:LEU:HA	6:M:238:LEU:HD12	1.68	0.41
2:Q:141:ILE:H	2:Q:171:VAL:HG22	1.85	0.41
5:h:56:GLU:O	5:h:60:LYS:HG2	2.20	0.41
1:l:15:GLN:HB2	4:m:53:GLN:HE22	1.86	0.41
2:1:53:TYR:N	2:1:61:ILE:O	2.54	0.41
2:1:396:ASP:OD2	2:1:425:ARG:NH2	2.47	0.41
2:2:397:LYS:HE2	2:2:401:ARG:HH11	1.85	0.41
2:2:425:ARG:HA	2:2:428:VAL:HG12	2.03	0.41
3:e:34:ILE:HG13	3:e:67:LEU:HA	2.03	0.41
6:C:864:PHE:CZ	2:Q:348:PHE:HD1	2.39	0.41
5:D:327:ALA:HB1	5:D:418:ILE:HA	2.03	0.41
5:F:619:ARG:HH12	5:F:620:ARG:NH1	2.18	0.41
1:J:884:PHE:O	1:J:888:VAL:HG23	2.21	0.41
7:K:190:TRP:CH2	7:K:280:GLY:HA3	2.56	0.41
6:M:356:LEU:HG	6:M:440:PRO:HB3	2.03	0.41
5:N:644:VAL:HG11	5:N:649:ALA:HB2	2.02	0.41
2:Q:187:ASN:O	2:Q:191:THR:OG1	2.33	0.41
2:T:53:TYR:N	2:T:61:ILE:O	2.54	0.41
2:V:425:ARG:HA	2:V:428:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:37:VAL:HG12	2:W:59:HIS:CD2	2.54	0.41
2:X:9:GLN:HE21	2:X:64:ALA:HB1	1.85	0.41
2:X:37:VAL:HG12	2:X:59:HIS:CD2	2.54	0.41
2:X:397:LYS:HE2	2:X:401:ARG:HH11	1.85	0.41
2:Y:396:ASP:OD2	2:Y:425:ARG:NH2	2.47	0.41
2:Y:425:ARG:HA	2:Y:428:VAL:HG12	2.03	0.41
2:Z:53:TYR:N	2:Z:61:ILE:O	2.54	0.41
2:Z:298:LEU:HD21	2:Z:346:ALA:HB2	2.02	0.41
2:1:9:GLN:HE21	2:1:64:ALA:HB1	1.85	0.41
2:1:37:VAL:HG12	2:1:59:HIS:CD2	2.54	0.41
2:2:298:LEU:HD21	2:2:346:ALA:HB2	2.03	0.41
3:e:132:MET:HE3	3:e:132:MET:HB2	1.83	0.41
3:e:295:ALA:O	3:e:328:LYS:HD2	2.21	0.41
6:E:384:SER:OG	6:E:477:TYR:HB3	2.21	0.41
6:G:652:GLU:HG2	6:G:694:GLN:HE22	1.86	0.41
1:J:719:TYR:HD1	1:J:809:VAL:HG21	1.85	0.41
7:K:181:GLY:HA2	7:K:315:LYS:HG3	2.02	0.41
2:T:425:ARG:HA	2:T:428:VAL:HG12	2.03	0.41
2:U:9:GLN:HE21	2:U:64:ALA:HB1	1.85	0.41
2:U:53:TYR:N	2:U:61:ILE:O	2.54	0.41
2:V:352:GLY:HA2	2:V:353:PRO:HD3	1.88	0.41
2:Y:13:CYS:HB2	2:Y:140:SER:HB3	2.03	0.41
6:C:767:GLN:HE21	6:C:814:LEU:HG	1.85	0.40
6:E:180:TRP:O	6:E:184:ARG:NH1	2.54	0.40
5:H:655:GLU:O	5:H:658:SER:OG	2.29	0.40
7:I:331:ARG:O	7:I:334:SER:OG	2.39	0.40
7:I:518:ARG:HD3	7:I:616:VAL:HG12	2.01	0.40
2:S:397:LYS:HE2	2:S:401:ARG:HH11	1.85	0.40
2:U:37:VAL:HG12	2:U:59:HIS:CD2	2.54	0.40
2:V:37:VAL:HG12	2:V:59:HIS:CD2	2.54	0.40
2:Z:84:LYS:HB2	2:Z:84:LYS:HE3	1.90	0.40
2:1:395:TYR:HE2	2:1:425:ARG:HG3	1.87	0.40
2:2:20:GLU:OE1	2:2:230:GLN:NE2	2.52	0.40
3:e:90:PHE:HZ	3:e:101:HIS:HB2	1.87	0.40
6:E:838:ALA:HB3	6:E:871:ARG:HH21	1.86	0.40
5:F:270:ASN:HD22	5:F:299:TRP:CD1	2.38	0.40
6:G:557:LEU:HD21	2:V:343:ARG:HD3	2.03	0.40
5:N:706:ILE:O	5:N:710:GLU:HG3	2.21	0.40
2:T:298:LEU:HD21	2:T:346:ALA:HB2	2.03	0.40
2:W:13:CYS:HB2	2:W:140:SER:HB3	2.03	0.40
2:1:397:LYS:HE2	2:1:401:ARG:HH11	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:53:TYR:N	2:2:61:ILE:O	2.54	0.40
3:e:240:TYR:CZ	3:e:242:LEU:HB2	2.57	0.40
1:J:216:LEU:HD22	1:J:222:HIS:NE2	2.36	0.40
8:L:1623:LEU:HD12	8:L:1623:LEU:HA	1.94	0.40
5:N:588:PRO:HA	5:N:634:GLY:H	1.86	0.40
2:Q:9:GLN:HE21	2:Q:64:ALA:HB1	1.85	0.40
2:S:298:LEU:HD21	2:S:346:ALA:HB2	2.03	0.40
2:T:9:GLN:HE21	2:T:64:ALA:HB1	1.85	0.40
2:T:252:ASP:OD1	2:T:252:ASP:N	2.55	0.40
2:U:66:LEU:HD21	2:U:74:ILE:HG12	2.02	0.40
2:V:9:GLN:HE21	2:V:64:ALA:HB1	1.85	0.40
2:V:337:LEU:HD12	2:V:337:LEU:HA	1.94	0.40
2:Y:53:TYR:N	2:Y:61:ILE:O	2.54	0.40
2:Z:252:ASP:OD1	2:Z:252:ASP:N	2.55	0.40
2:1:296:ARG:HG3	2:1:302:ASN:ND2	2.37	0.40
5:D:689:LYS:HA	5:D:692:ARG:HE	1.86	0.40
5:F:293:ARG:HD3	5:F:368:LEU:HD22	2.03	0.40
7:K:411:LEU:HD13	7:K:414:LEU:HD12	2.03	0.40
8:L:346:LEU:HD13	8:L:347:VAL:HA	2.02	0.40
5:N:553:TYR:O	5:N:558:HIS:HE1	2.04	0.40
2:Q:13:CYS:HB2	2:Q:140:SER:HB3	2.03	0.40
2:Q:323:ILE:HD12	2:Q:323:ILE:HA	1.81	0.40
2:R:252:ASP:OD1	2:R:252:ASP:N	2.55	0.40
2:V:53:TYR:N	2:V:61:ILE:O	2.54	0.40
2:V:66:LEU:HD21	2:V:74:ILE:HG12	2.03	0.40
2:Y:296:ARG:HG3	2:Y:302:ASN:ND2	2.37	0.40
2:Z:296:ARG:HG3	2:Z:302:ASN:ND2	2.37	0.40
2:Z:425:ARG:HA	2:Z:428:VAL:HG12	2.03	0.40
2:1:13:CYS:HB2	2:1:140:SER:HB3	2.02	0.40
2:1:252:ASP:OD1	2:1:252:ASP:N	2.55	0.40
2:2:395:TYR:HE2	2:2:425:ARG:HG3	1.87	0.40
6:C:217:VAL:HG12	6:C:321:LEU:HD21	2.03	0.40
5:D:391:ARG:HH21	5:D:399:ALA:HB2	1.85	0.40
5:F:572:ASP:O	5:F:575:ARG:HG3	2.22	0.40
5:H:799:GLU:HG2	5:H:802:ARG:HH11	1.85	0.40
1:J:998:LEU:HD11	1:J:1010:LEU:HB3	2.03	0.40
7:K:255:LYS:HD2	7:K:255:LYS:HA	1.87	0.40
2:S:84:LYS:HE3	2:S:84:LYS:HB2	1.90	0.40
2:T:397:LYS:HE2	2:T:401:ARG:HH11	1.85	0.40
2:W:323:ILE:HD12	2:W:323:ILE:HA	1.81	0.40
2:Z:13:CYS:HB2	2:Z:140:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:352:GLY:HA2	2:Z:353:PRO:HD3	1.88	0.40
8:c:90:GLU:HA	8:c:93:VAL:HG22	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	J	506/1024 (49%)	467 (92%)	35 (7%)	4 (1%)	16	54
1	l	104/1024 (10%)	94 (90%)	9 (9%)	1 (1%)	12	49
2	1	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	2	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	Q	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	R	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	S	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	T	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	U	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	V	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	W	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	X	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	Y	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
2	Z	408/451 (90%)	385 (94%)	21 (5%)	2 (0%)	24	63
3	e	360/375 (96%)	339 (94%)	21 (6%)	0	100	100
4	b	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
4	d	57/82 (70%)	57 (100%)	0	0	100	100
4	i	63/82 (77%)	62 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	k	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
4	m	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
5	D	571/907 (63%)	547 (96%)	24 (4%)	0	100	100
5	F	591/907 (65%)	556 (94%)	32 (5%)	3 (0%)	24	63
5	H	584/907 (64%)	565 (97%)	19 (3%)	0	100	100
5	N	584/907 (64%)	565 (97%)	19 (3%)	0	100	100
5	a	112/907 (12%)	108 (96%)	3 (3%)	1 (1%)	14	51
5	h	97/907 (11%)	95 (98%)	2 (2%)	0	100	100
5	j	105/907 (12%)	97 (92%)	7 (7%)	1 (1%)	12	49
6	C	606/902 (67%)	577 (95%)	26 (4%)	3 (0%)	24	63
6	E	626/902 (69%)	577 (92%)	47 (8%)	2 (0%)	36	72
6	G	624/902 (69%)	589 (94%)	32 (5%)	3 (0%)	24	63
6	M	624/902 (69%)	591 (95%)	28 (4%)	5 (1%)	16	54
7	I	511/667 (77%)	473 (93%)	32 (6%)	6 (1%)	10	44
7	K	548/667 (82%)	526 (96%)	21 (4%)	1 (0%)	43	78
8	L	540/1819 (30%)	493 (91%)	44 (8%)	3 (1%)	21	59
8	c	148/1819 (8%)	139 (94%)	9 (6%)	0	100	100
All	All	13046/23174 (56%)	12322 (94%)	667 (5%)	57 (0%)	31	67

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	l	121	PRO
6	C	239	ALA
6	C	465	HIS
6	E	425	ASP
6	G	241	ARG
6	G	581	ASP
7	I	408	ASP
7	I	509	GLN
7	I	601	LEU
1	J	237	HIS
1	J	238	LEU
6	M	241	ARG
6	M	243	SER
5	j	108	PRO

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Mol	Chain	Res	Type
2	1	347	ASN
2	1	348	PHE
2	2	347	ASN
2	2	348	PHE
6	E	426	LYS
5	F	270	ASN
7	I	510	THR
8	L	307	ARG
6	M	676	PHE
2	Q	347	ASN
2	Q	348	PHE
2	R	347	ASN
2	R	348	PHE
2	S	347	ASN
2	S	348	PHE
2	T	347	ASN
2	T	348	PHE
2	U	347	ASN
2	U	348	PHE
2	V	347	ASN
2	V	348	PHE
2	W	347	ASN
2	W	348	PHE
2	X	347	ASN
2	X	348	PHE
2	Y	347	ASN
2	Y	348	PHE
2	Z	347	ASN
2	Z	348	PHE
6	G	582	LEU
7	I	259	LEU
1	J	255	PRO
8	L	345	VAL
5	a	44	ALA
6	M	238	LEU
6	M	242	GLN
6	C	240	GLY
7	I	508	ASN
7	K	409	ASN
8	L	343	GLN
5	F	501	THR
1	J	713	ASP

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Mol	Chain	Res	Type
5	F	502	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	498/933 (53%)	495 (99%)	3 (1%)	78	83
1	l	84/933 (9%)	84 (100%)	0	100	100
2	1	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	2	376/400 (94%)	346 (92%)	30 (8%)	11	31
2	Q	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	R	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	S	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	T	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	U	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	V	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	W	376/400 (94%)	346 (92%)	30 (8%)	11	31
2	X	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	Y	376/400 (94%)	345 (92%)	31 (8%)	10	31
2	Z	376/400 (94%)	346 (92%)	30 (8%)	11	31
3	e	310/318 (98%)	306 (99%)	4 (1%)	61	74
4	b	53/62 (86%)	53 (100%)	0	100	100
4	d	53/62 (86%)	52 (98%)	1 (2%)	50	67
4	i	53/62 (86%)	53 (100%)	0	100	100
4	k	53/62 (86%)	51 (96%)	2 (4%)	29	50
4	m	53/62 (86%)	53 (100%)	0	100	100
5	D	525/798 (66%)	523 (100%)	2 (0%)	84	84
5	F	542/798 (68%)	539 (99%)	3 (1%)	78	83
5	H	539/798 (68%)	536 (99%)	3 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	N	539/798 (68%)	539 (100%)	0	100	100
5	a	101/798 (13%)	101 (100%)	0	100	100
5	h	88/798 (11%)	88 (100%)	0	100	100
5	j	88/798 (11%)	88 (100%)	0	100	100
6	C	556/791 (70%)	552 (99%)	4 (1%)	76	81
6	E	574/791 (73%)	567 (99%)	7 (1%)	63	75
6	G	572/791 (72%)	568 (99%)	4 (1%)	76	81
6	M	572/791 (72%)	569 (100%)	3 (0%)	81	83
7	I	472/594 (80%)	471 (100%)	1 (0%)	87	87
7	K	509/594 (86%)	503 (99%)	6 (1%)	63	75
8	L	501/1546 (32%)	498 (99%)	3 (1%)	78	83
8	c	135/1546 (9%)	135 (100%)	0	100	100
All	All	11982/20324 (59%)	11567 (96%)	415 (4%)	32	53

All (415) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	10	LEU
2	1	25	LEU
2	1	50	VAL
2	1	57	ASP
2	1	78	LEU
2	1	109	SER
2	1	131	SER
2	1	136	VAL
2	1	151	SER
2	1	168	THR
2	1	188	SER
2	1	201	CYS
2	1	204	VAL
2	1	222	ASN
2	1	237	SER
2	1	263	THR
2	1	267	HIS
2	1	274	THR
2	1	278	THR
2	1	296	ARG
2	1	298	LEU

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Mol	Chain	Res	Type
2	1	316	CYS
2	1	323	ILE
2	1	328	VAL
2	1	331	THR
2	1	333	VAL
2	1	349	ILE
2	1	367	LEU
2	1	374	SER
2	1	385	SER
2	1	424	SER
2	2	10	LEU
2	2	25	LEU
2	2	50	VAL
2	2	57	ASP
2	2	78	LEU
2	2	109	SER
2	2	131	SER
2	2	151	SER
2	2	168	THR
2	2	188	SER
2	2	201	CYS
2	2	204	VAL
2	2	222	ASN
2	2	237	SER
2	2	263	THR
2	2	267	HIS
2	2	274	THR
2	2	278	THR
2	2	296	ARG
2	2	298	LEU
2	2	316	CYS
2	2	323	ILE
2	2	328	VAL
2	2	331	THR
2	2	333	VAL
2	2	349	ILE
2	2	367	LEU
2	2	374	SER
2	2	385	SER
2	2	424	SER
3	e	105	LEU
3	e	129	THR

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Mol	Chain	Res	Type
3	e	200	PHE
3	e	282	ILE
6	C	287	GLN
6	C	288	VAL
6	C	399	ILE
6	C	547	THR
5	D	277	VAL
5	D	369	VAL
6	E	255	SER
6	E	328	ILE
6	E	467	VAL
6	E	468	THR
6	E	562	SER
6	E	628	LEU
6	E	674	GLN
5	F	304	ILE
5	F	404	THR
5	F	648	ILE
6	G	328	ILE
6	G	467	VAL
6	G	628	LEU
6	G	855	VAL
5	H	623	VAL
5	H	628	VAL
5	H	629	SER
7	I	475	TYR
1	J	220	VAL
1	J	222	HIS
1	J	306	THR
7	K	27	VAL
7	K	205	ILE
7	K	255	LYS
7	K	537	LEU
7	K	647	LEU
7	K	651	TYR
8	L	288	THR
8	L	346	LEU
8	L	357	LEU
6	M	243	SER
6	M	328	ILE
6	M	563	THR
4	k	48	VAL

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Mol	Chain	Res	Type
4	k	56	ASN
2	Q	10	LEU
2	Q	25	LEU
2	Q	50	VAL
2	Q	57	ASP
2	Q	78	LEU
2	Q	109	SER
2	Q	131	SER
2	Q	136	VAL
2	Q	151	SER
2	Q	168	THR
2	Q	188	SER
2	Q	201	CYS
2	Q	204	VAL
2	Q	222	ASN
2	Q	237	SER
2	Q	263	THR
2	Q	267	HIS
2	Q	274	THR
2	Q	278	THR
2	Q	296	ARG
2	Q	298	LEU
2	Q	316	CYS
2	Q	323	ILE
2	Q	328	VAL
2	Q	331	THR
2	Q	333	VAL
2	Q	349	ILE
2	Q	367	LEU
2	Q	374	SER
2	Q	385	SER
2	Q	424	SER
2	R	10	LEU
2	R	25	LEU
2	R	50	VAL
2	R	57	ASP
2	R	78	LEU
2	R	109	SER
2	R	131	SER
2	R	136	VAL
2	R	151	SER
2	R	168	THR

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Mol	Chain	Res	Type
2	R	188	SER
2	R	201	CYS
2	R	204	VAL
2	R	222	ASN
2	R	237	SER
2	R	263	THR
2	R	267	HIS
2	R	274	THR
2	R	278	THR
2	R	296	ARG
2	R	298	LEU
2	R	316	CYS
2	R	323	ILE
2	R	328	VAL
2	R	331	THR
2	R	333	VAL
2	R	349	ILE
2	R	367	LEU
2	R	374	SER
2	R	385	SER
2	R	424	SER
2	S	10	LEU
2	S	25	LEU
2	S	50	VAL
2	S	57	ASP
2	S	78	LEU
2	S	109	SER
2	S	131	SER
2	S	136	VAL
2	S	151	SER
2	S	168	THR
2	S	188	SER
2	S	201	CYS
2	S	204	VAL
2	S	222	ASN
2	S	237	SER
2	S	263	THR
2	S	267	HIS
2	S	274	THR
2	S	278	THR
2	S	296	ARG
2	S	298	LEU

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Mol	Chain	Res	Type
2	S	316	CYS
2	S	323	ILE
2	S	328	VAL
2	S	331	THR
2	S	333	VAL
2	S	349	ILE
2	S	367	LEU
2	S	374	SER
2	S	385	SER
2	S	424	SER
2	T	10	LEU
2	T	25	LEU
2	T	50	VAL
2	T	57	ASP
2	T	78	LEU
2	T	109	SER
2	T	131	SER
2	T	136	VAL
2	T	151	SER
2	T	168	THR
2	T	188	SER
2	T	201	CYS
2	T	204	VAL
2	T	222	ASN
2	T	237	SER
2	T	263	THR
2	T	267	HIS
2	T	274	THR
2	T	278	THR
2	T	296	ARG
2	T	298	LEU
2	T	316	CYS
2	T	323	ILE
2	T	328	VAL
2	T	331	THR
2	T	333	VAL
2	T	349	ILE
2	T	367	LEU
2	T	374	SER
2	T	385	SER
2	T	424	SER
2	U	10	LEU

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Mol	Chain	Res	Type
2	U	25	LEU
2	U	50	VAL
2	U	57	ASP
2	U	78	LEU
2	U	109	SER
2	U	131	SER
2	U	136	VAL
2	U	151	SER
2	U	168	THR
2	U	188	SER
2	U	201	CYS
2	U	204	VAL
2	U	222	ASN
2	U	237	SER
2	U	263	THR
2	U	267	HIS
2	U	274	THR
2	U	278	THR
2	U	296	ARG
2	U	298	LEU
2	U	316	CYS
2	U	323	ILE
2	U	328	VAL
2	U	331	THR
2	U	333	VAL
2	U	349	ILE
2	U	367	LEU
2	U	374	SER
2	U	385	SER
2	U	424	SER
2	V	10	LEU
2	V	25	LEU
2	V	50	VAL
2	V	57	ASP
2	V	78	LEU
2	V	109	SER
2	V	131	SER
2	V	136	VAL
2	V	151	SER
2	V	168	THR
2	V	188	SER
2	V	201	CYS

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Mol	Chain	Res	Type
2	V	204	VAL
2	V	222	ASN
2	V	237	SER
2	V	263	THR
2	V	267	HIS
2	V	274	THR
2	V	278	THR
2	V	296	ARG
2	V	298	LEU
2	V	316	CYS
2	V	323	ILE
2	V	328	VAL
2	V	331	THR
2	V	333	VAL
2	V	349	ILE
2	V	367	LEU
2	V	374	SER
2	V	385	SER
2	V	424	SER
2	W	10	LEU
2	W	25	LEU
2	W	50	VAL
2	W	57	ASP
2	W	78	LEU
2	W	109	SER
2	W	131	SER
2	W	151	SER
2	W	168	THR
2	W	188	SER
2	W	201	CYS
2	W	204	VAL
2	W	222	ASN
2	W	237	SER
2	W	263	THR
2	W	267	HIS
2	W	274	THR
2	W	278	THR
2	W	296	ARG
2	W	298	LEU
2	W	316	CYS
2	W	323	ILE
2	W	328	VAL

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Mol	Chain	Res	Type
2	W	331	THR
2	W	333	VAL
2	W	349	ILE
2	W	367	LEU
2	W	374	SER
2	W	385	SER
2	W	424	SER
2	X	10	LEU
2	X	25	LEU
2	X	50	VAL
2	X	57	ASP
2	X	78	LEU
2	X	109	SER
2	X	131	SER
2	X	136	VAL
2	X	151	SER
2	X	168	THR
2	X	188	SER
2	X	201	CYS
2	X	204	VAL
2	X	222	ASN
2	X	237	SER
2	X	263	THR
2	X	267	HIS
2	X	274	THR
2	X	278	THR
2	X	296	ARG
2	X	298	LEU
2	X	316	CYS
2	X	323	ILE
2	X	328	VAL
2	X	331	THR
2	X	333	VAL
2	X	349	ILE
2	X	367	LEU
2	X	374	SER
2	X	385	SER
2	X	424	SER
2	Y	10	LEU
2	Y	25	LEU
2	Y	50	VAL
2	Y	57	ASP

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Mol	Chain	Res	Type
2	Y	78	LEU
2	Y	109	SER
2	Y	131	SER
2	Y	136	VAL
2	Y	151	SER
2	Y	168	THR
2	Y	188	SER
2	Y	201	CYS
2	Y	204	VAL
2	Y	222	ASN
2	Y	237	SER
2	Y	263	THR
2	Y	267	HIS
2	Y	274	THR
2	Y	278	THR
2	Y	296	ARG
2	Y	298	LEU
2	Y	316	CYS
2	Y	323	ILE
2	Y	328	VAL
2	Y	331	THR
2	Y	333	VAL
2	Y	349	ILE
2	Y	367	LEU
2	Y	374	SER
2	Y	385	SER
2	Y	424	SER
2	Z	10	LEU
2	Z	25	LEU
2	Z	50	VAL
2	Z	57	ASP
2	Z	78	LEU
2	Z	109	SER
2	Z	131	SER
2	Z	151	SER
2	Z	168	THR
2	Z	188	SER
2	Z	201	CYS
2	Z	204	VAL
2	Z	222	ASN
2	Z	237	SER
2	Z	263	THR

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Mol	Chain	Res	Type
2	Z	267	HIS
2	Z	274	THR
2	Z	278	THR
2	Z	296	ARG
2	Z	298	LEU
2	Z	316	CYS
2	Z	323	ILE
2	Z	328	VAL
2	Z	331	THR
2	Z	333	VAL
2	Z	349	ILE
2	Z	367	LEU
2	Z	374	SER
2	Z	385	SER
2	Z	424	SER
4	d	46	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (305) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	107	HIS
2	1	29	HIS
2	1	59	HIS
2	1	102	ASN
2	1	110	GLN
2	1	167	GLN
2	1	229	ASN
2	1	314	ASN
2	1	325	GLN
2	1	338	GLN
2	1	357	GLN
2	1	430	GLN
2	2	29	HIS
2	2	59	HIS
2	2	102	ASN
2	2	110	GLN
2	2	167	GLN
2	2	207	ASN
2	2	229	ASN
2	2	314	ASN
2	2	325	GLN
2	2	430	GLN

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Mol	Chain	Res	Type
3	e	12	ASN
3	e	111	ASN
3	e	115	ASN
3	e	280	ASN
3	e	296	ASN
5	a	30	GLN
5	a	120	GLN
6	C	172	GLN
6	C	329	GLN
6	C	444	GLN
6	C	487	GLN
6	C	524	GLN
6	C	580	HIS
6	C	585	GLN
6	C	644	HIS
6	C	692	ASN
6	C	823	ASN
5	D	259	GLN
5	D	310	GLN
5	D	343	HIS
5	D	389	GLN
5	D	401	HIS
5	D	444	HIS
5	D	479	GLN
5	D	491	ASN
5	D	494	HIS
5	D	531	GLN
5	D	560	GLN
5	D	576	HIS
5	D	594	GLN
5	D	609	ASN
5	D	665	ASN
5	D	684	HIS
5	D	705	HIS
5	D	774	GLN
5	D	846	GLN
5	D	883	ASN
6	E	151	GLN
6	E	169	ASN
6	E	213	GLN
6	E	236	GLN
6	E	242	GLN

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Mol	Chain	Res	Type
6	E	289	ASN
6	E	316	GLN
6	E	322	GLN
6	E	329	GLN
6	E	371	GLN
6	E	438	GLN
6	E	565	ASN
6	E	585	GLN
6	E	726	HIS
6	E	741	ASN
6	E	823	ASN
5	F	302	ASN
5	F	322	GLN
5	F	330	GLN
5	F	347	GLN
5	F	416	GLN
5	F	461	HIS
5	F	558	HIS
5	F	560	GLN
5	F	576	HIS
5	F	594	GLN
5	F	643	HIS
5	F	713	HIS
5	F	739	GLN
5	F	742	GLN
5	F	781	GLN
5	F	786	GLN
5	F	855	GLN
5	F	860	GLN
6	G	166	ASN
6	G	172	GLN
6	G	309	GLN
6	G	329	GLN
6	G	436	GLN
6	G	644	HIS
6	G	688	ASN
6	G	694	GLN
6	G	741	ASN
6	G	862	ASN
5	H	269	ASN
5	H	310	GLN
5	H	389	GLN

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Mol	Chain	Res	Type
5	H	687	ASN
5	H	740	GLN
5	H	786	GLN
5	H	883	ASN
7	I	3	HIS
7	I	29	GLN
7	I	98	GLN
7	I	102	GLN
7	I	116	HIS
7	I	123	ASN
7	I	142	GLN
7	I	186	GLN
7	I	316	GLN
7	I	327	GLN
7	I	377	GLN
7	I	398	GLN
7	I	501	GLN
7	I	504	HIS
7	I	520	HIS
7	I	540	GLN
7	I	547	GLN
7	I	549	ASN
7	I	563	HIS
7	I	567	ASN
7	I	591	HIS
7	I	599	GLN
7	I	622	GLN
1	J	269	GLN
1	J	328	GLN
1	J	362	GLN
1	J	456	GLN
1	J	474	GLN
1	J	482	HIS
1	J	567	GLN
1	J	698	GLN
1	J	823	GLN
1	J	895	ASN
1	J	914	GLN
1	J	938	HIS
1	J	1009	HIS
7	K	26	GLN
7	K	65	HIS

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Mol	Chain	Res	Type
7	K	68	GLN
7	K	98	GLN
7	K	130	GLN
7	K	152	GLN
7	K	290	ASN
7	K	316	GLN
7	K	378	HIS
7	K	397	GLN
7	K	401	HIS
7	K	409	ASN
7	K	493	GLN
7	K	540	GLN
7	K	600	ASN
8	L	327	HIS
8	L	340	GLN
8	L	412	HIS
8	L	512	ASN
8	L	603	ASN
8	L	1657	GLN
8	L	1659	GLN
8	L	1673	GLN
8	L	1678	ASN
8	L	1679	GLN
8	L	1761	ASN
8	L	1767	GLN
8	L	1770	ASN
6	M	151	GLN
6	M	213	GLN
6	M	242	GLN
6	M	412	HIS
6	M	465	HIS
6	M	493	ASN
6	M	691	GLN
5	N	259	GLN
5	N	345	GLN
5	N	389	GLN
5	N	401	HIS
5	N	479	GLN
5	N	491	ASN
5	N	495	GLN
5	N	531	GLN
5	N	594	GLN

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Mol	Chain	Res	Type
5	N	702	HIS
5	N	717	GLN
5	N	855	GLN
4	k	53	GLN
2	Q	29	HIS
2	Q	59	HIS
2	Q	102	ASN
2	Q	110	GLN
2	Q	167	GLN
2	Q	229	ASN
2	Q	314	ASN
2	Q	325	GLN
2	Q	357	GLN
2	Q	430	GLN
2	R	29	HIS
2	R	59	HIS
2	R	102	ASN
2	R	110	GLN
2	R	167	GLN
2	R	187	ASN
2	R	229	ASN
2	R	302	ASN
2	R	314	ASN
2	R	325	GLN
2	R	338	GLN
2	R	430	GLN
2	R	436	HIS
2	S	29	HIS
2	S	59	HIS
2	S	102	ASN
2	S	110	GLN
2	S	167	GLN
2	S	229	ASN
2	S	314	ASN
2	S	325	GLN
2	S	338	GLN
2	S	430	GLN
2	T	29	HIS
2	T	59	HIS
2	T	102	ASN
2	T	110	GLN
2	T	167	GLN

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Mol	Chain	Res	Type
2	T	219	HIS
2	T	229	ASN
2	T	314	ASN
2	T	325	GLN
2	T	334	HIS
2	T	338	GLN
2	T	430	GLN
2	U	29	HIS
2	U	59	HIS
2	U	110	GLN
2	U	167	GLN
2	U	229	ASN
2	U	314	ASN
2	U	325	GLN
2	U	334	HIS
2	U	430	GLN
2	V	29	HIS
2	V	59	HIS
2	V	102	ASN
2	V	110	GLN
2	V	167	GLN
2	V	229	ASN
2	V	302	ASN
2	V	314	ASN
2	V	325	GLN
2	V	338	GLN
2	V	430	GLN
2	V	436	HIS
2	W	29	HIS
2	W	59	HIS
2	W	102	ASN
2	W	110	GLN
2	W	167	GLN
2	W	187	ASN
2	W	229	ASN
2	W	314	ASN
2	W	325	GLN
2	W	430	GLN
2	X	29	HIS
2	X	59	HIS
2	X	102	ASN
2	X	110	GLN

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Mol	Chain	Res	Type
2	X	229	ASN
2	X	251	ASN
2	X	314	ASN
2	X	325	GLN
2	X	334	HIS
2	X	338	GLN
2	X	430	GLN
2	Y	29	HIS
2	Y	59	HIS
2	Y	102	ASN
2	Y	110	GLN
2	Y	229	ASN
2	Y	314	ASN
2	Y	325	GLN
2	Y	334	HIS
2	Y	338	GLN
2	Y	430	GLN
2	Z	29	HIS
2	Z	59	HIS
2	Z	167	GLN
2	Z	229	ASN
2	Z	314	ASN
2	Z	325	GLN
2	Z	334	HIS
2	Z	338	GLN
2	Z	430	GLN
4	m	53	GLN
4	d	53	GLN
8	c	6	GLN
8	c	176	GLN
8	c	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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.

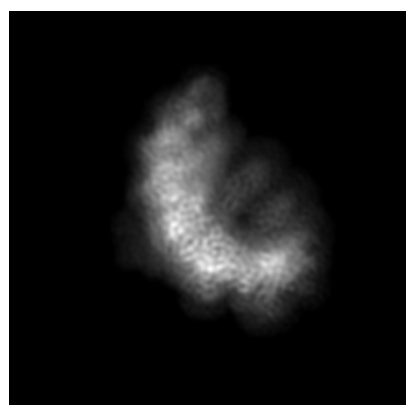
6 Map visualisation [i](#)

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

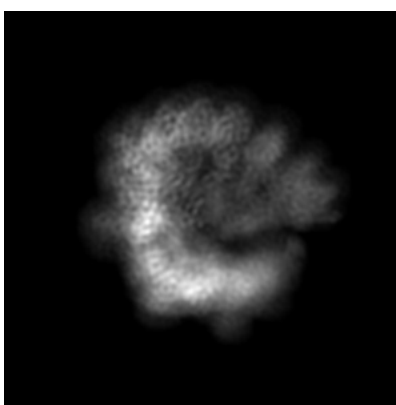
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

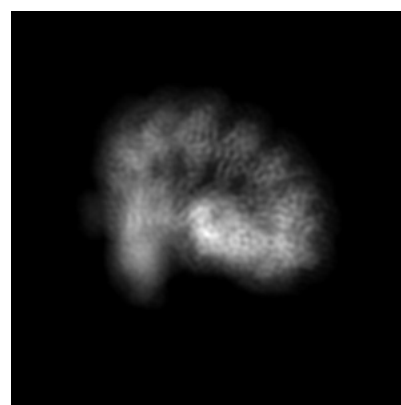
6.1.1 Primary map



X



Y

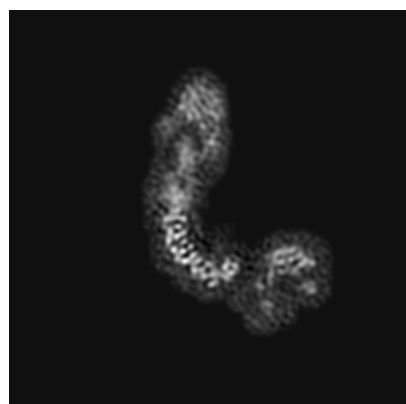


Z

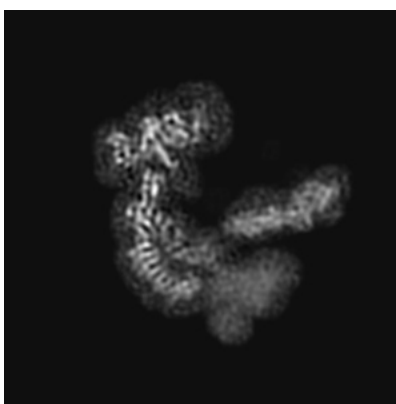
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

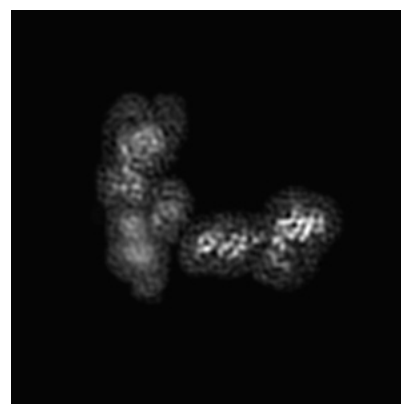
6.2.1 Primary map



X Index: 100



Y Index: 100

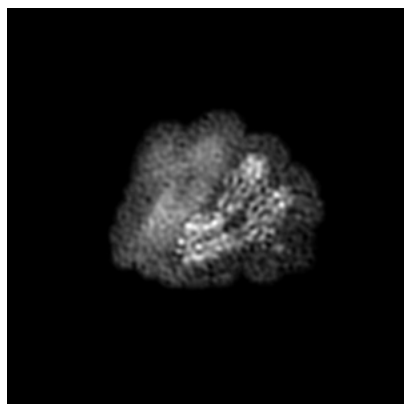


Z Index: 100

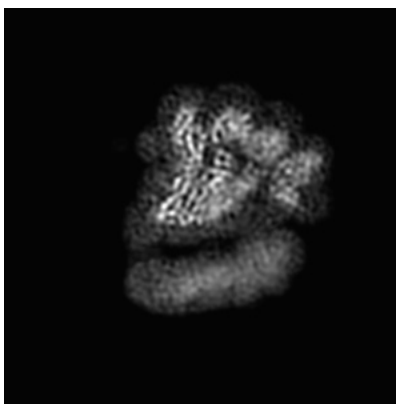
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

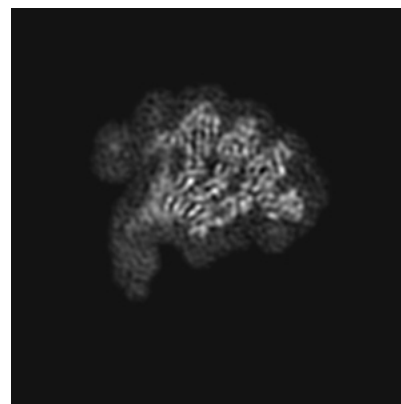
6.3.1 Primary map



X Index: 63



Y Index: 82

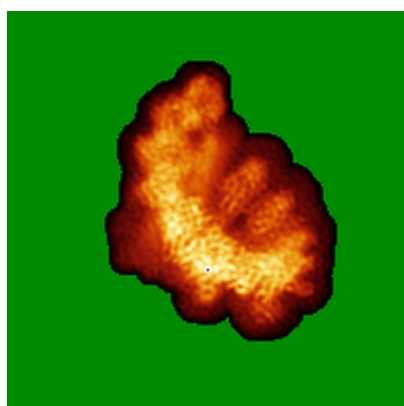


Z Index: 71

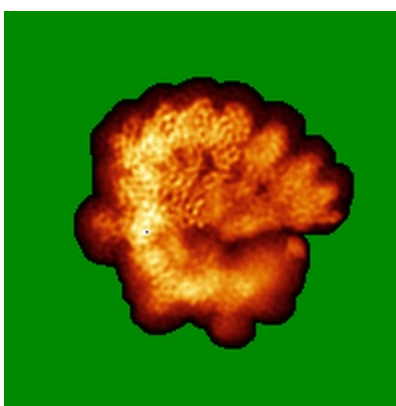
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

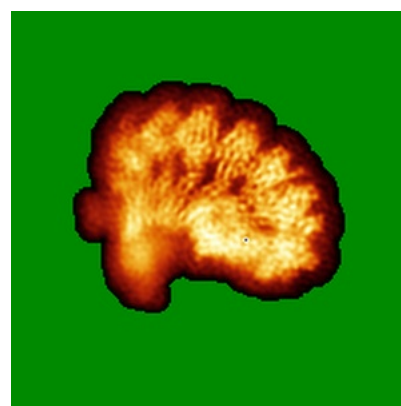
6.4.1 Primary map



X



Y



Z

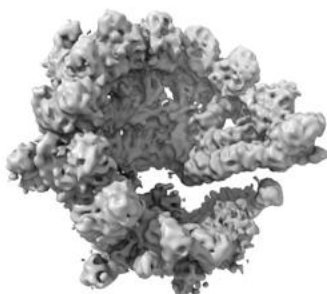
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

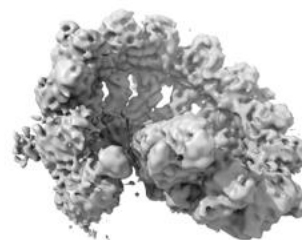
6.5.1 Primary map



X



Y



Z

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

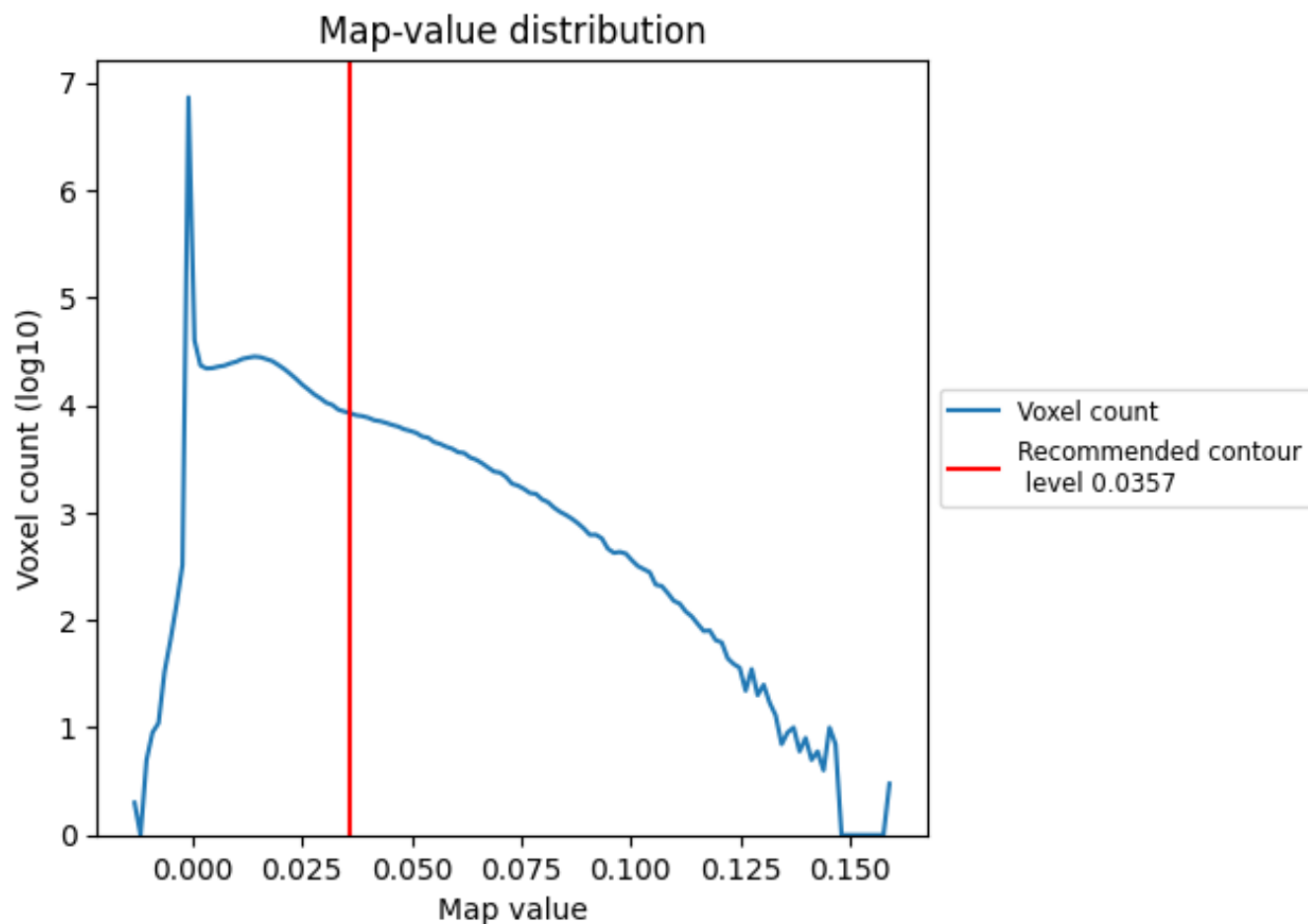
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

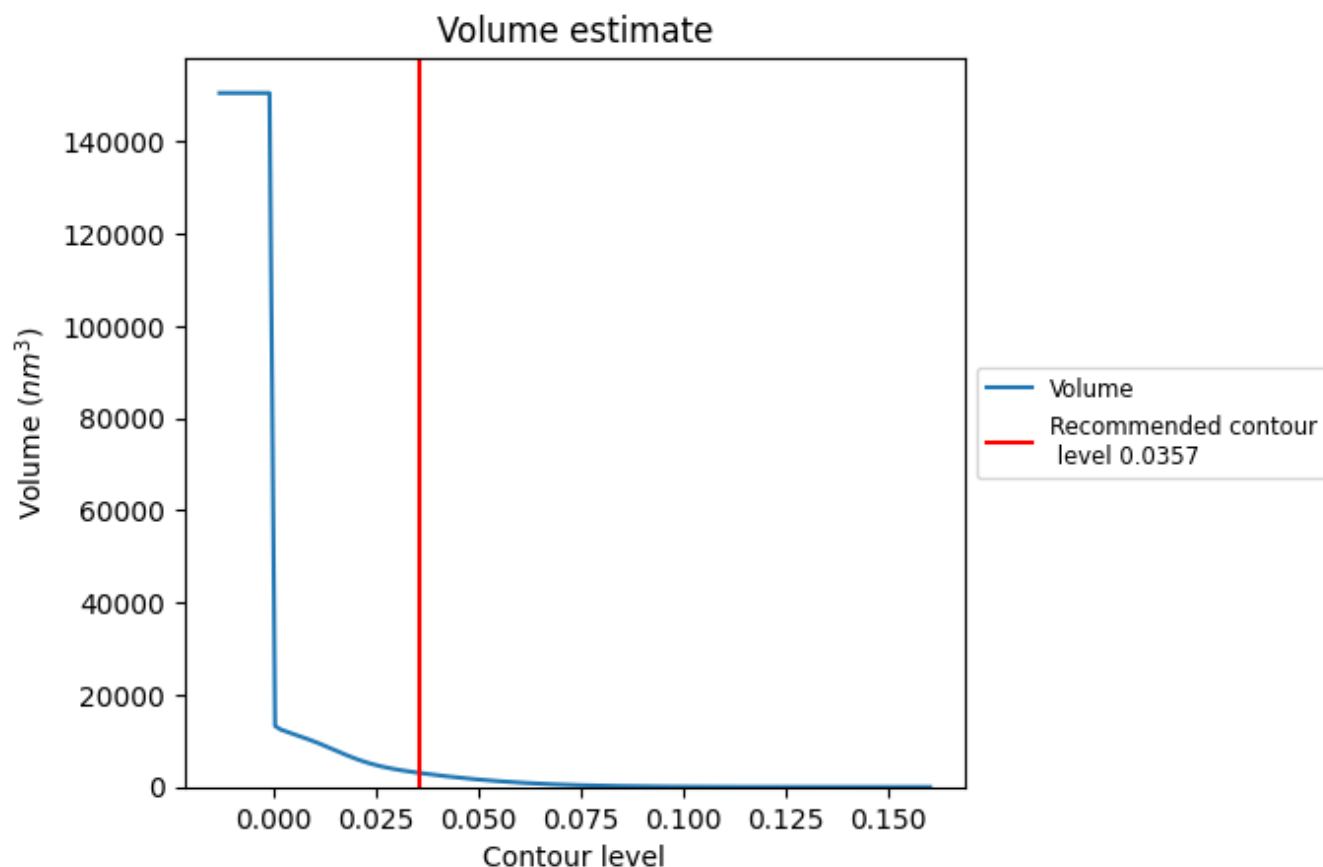
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

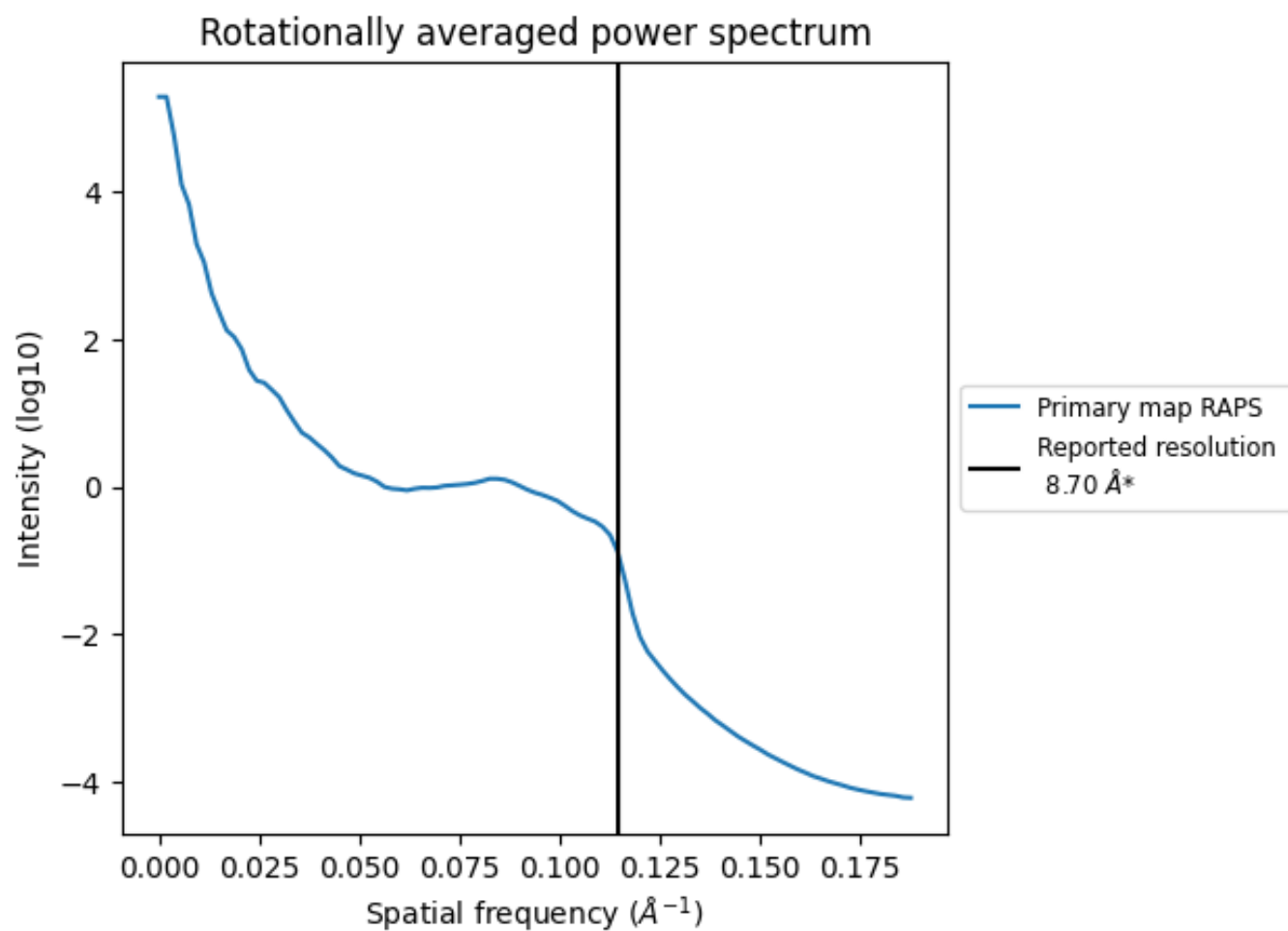
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3032 nm^3 ; this corresponds to an approximate mass of 2739 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.115 Å⁻¹

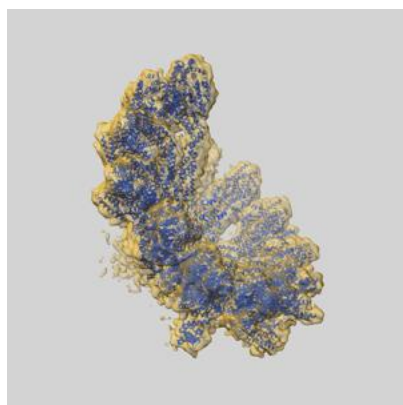
8 Fourier-Shell correlation ⓘ

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

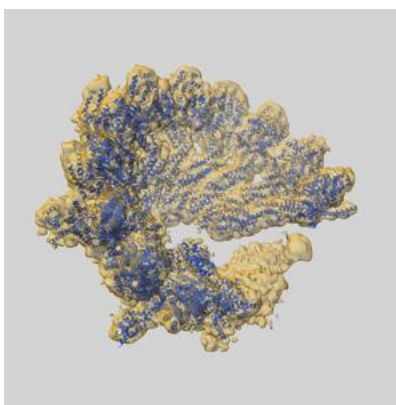
9 Map-model fit [i](#)

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

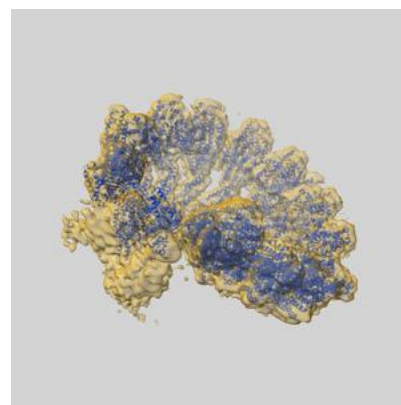
9.1 Map-model overlay [i](#)



X



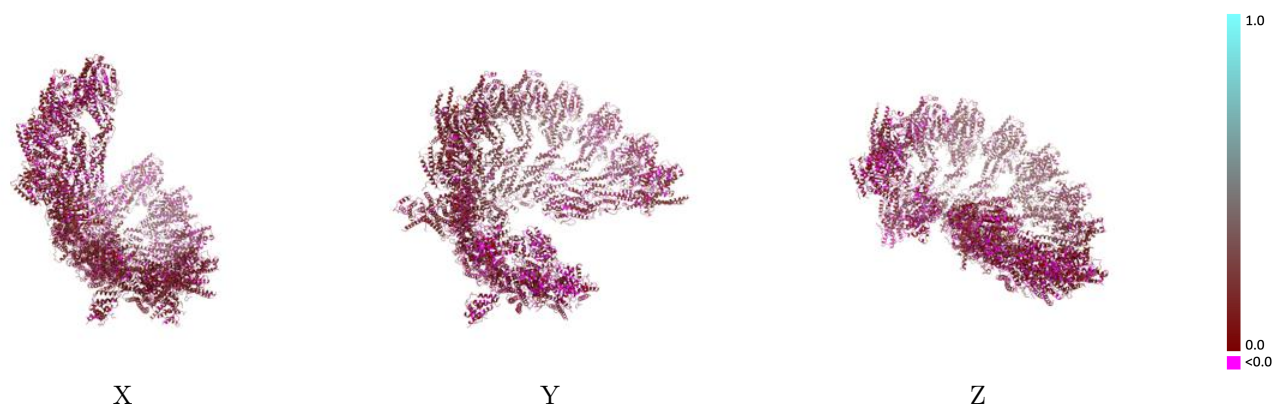
Y



Z

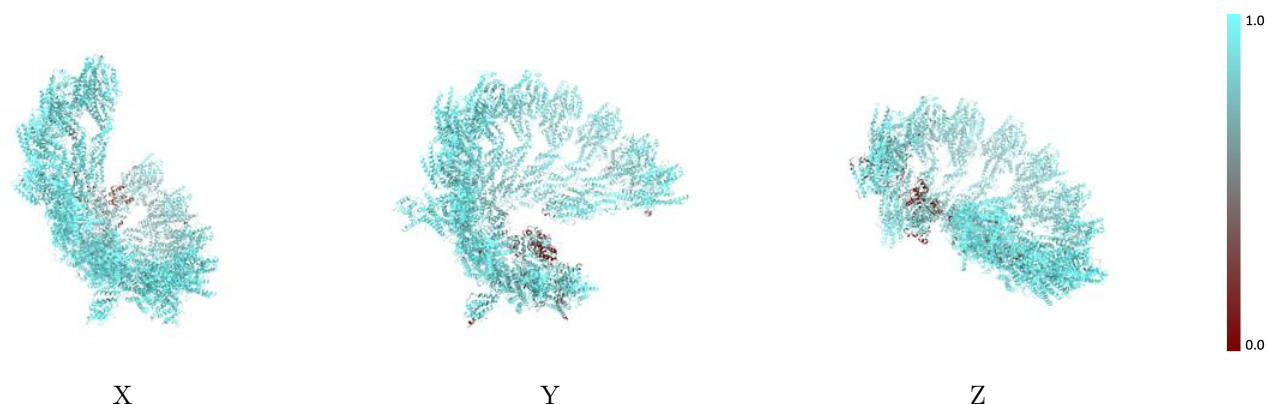
The images above show the 3D surface view of the map at the recommended contour level 0.0357 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



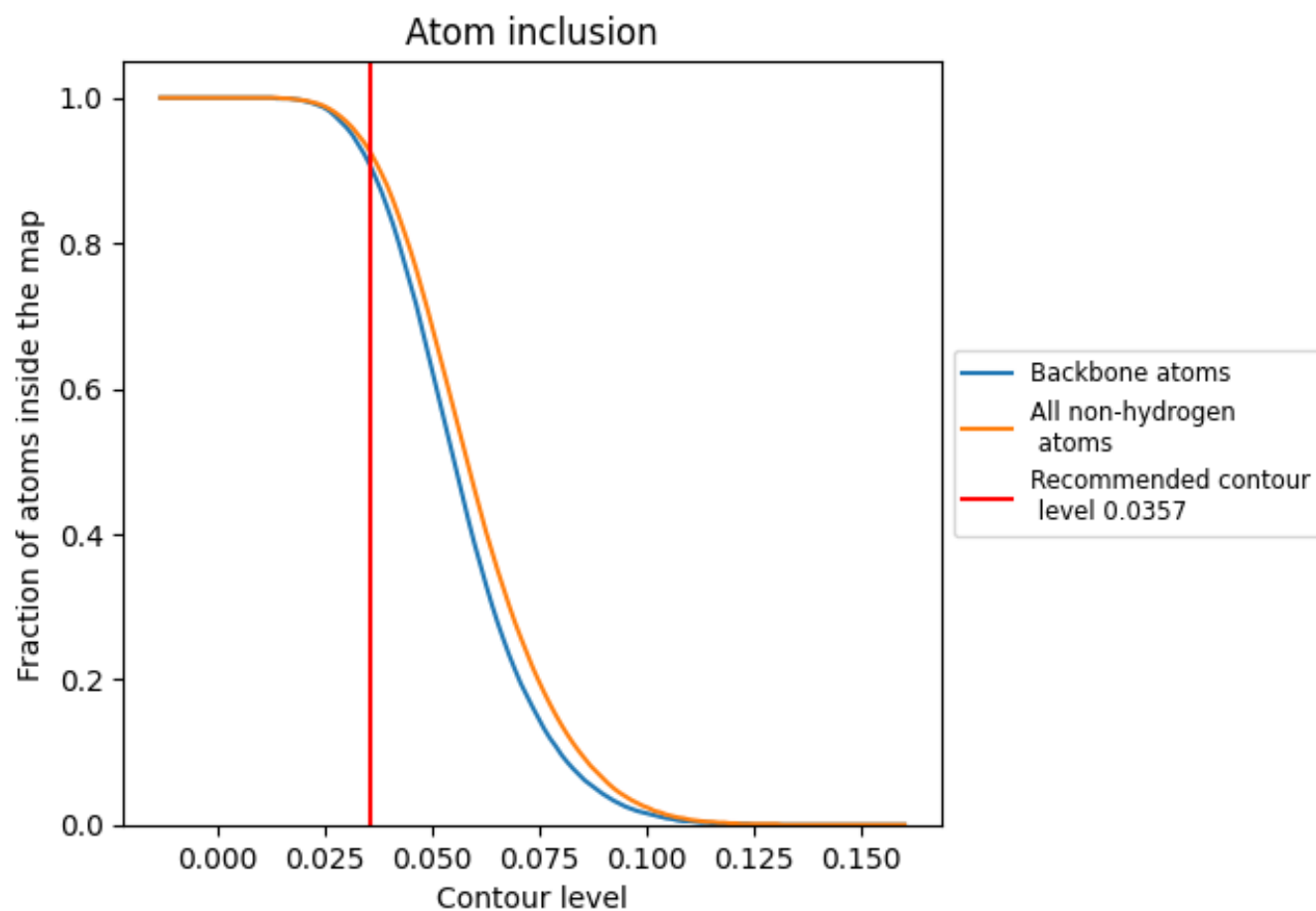
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0357).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0357) and Q-score for the entire model and for each chain.

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

