



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:54 AM UTC

PDB ID : 7QJB / pdb_00007qjb
EMDB ID : EMD-14016
Title : Structure of recombinant human gamma-Tubulin Ring Complex 12-spoked assembly intermediate (spokes 3-14, homogeneous dataset)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 9.20 Å (reported)
Based on initial models : 6X0U, 6V6S, 7AS4, 6L81

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

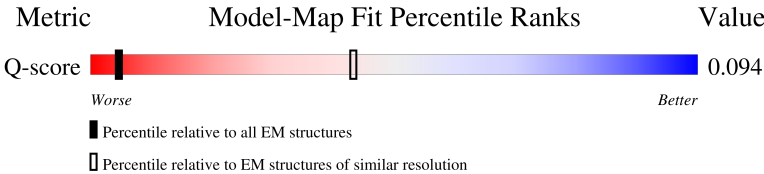
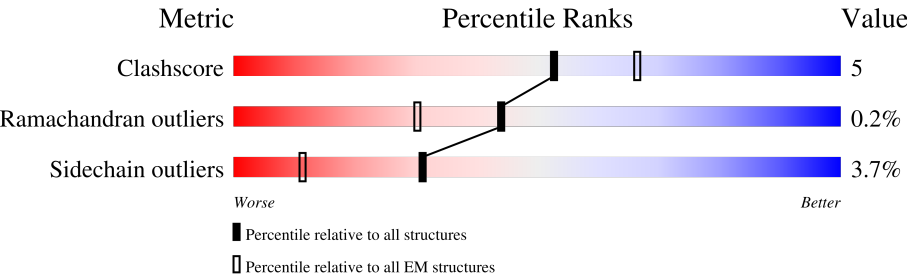
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 9.20 Å.

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



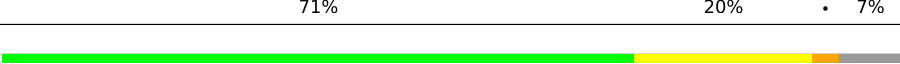
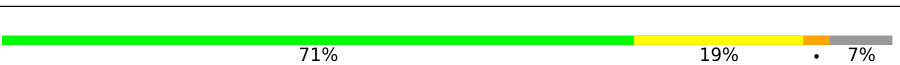
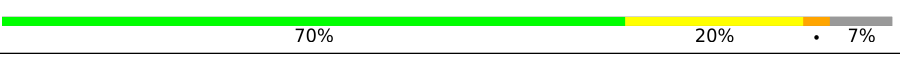
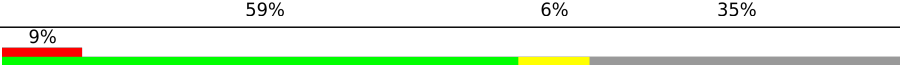
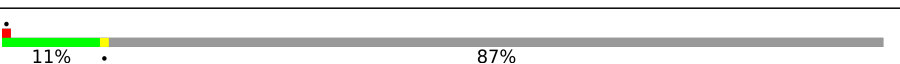
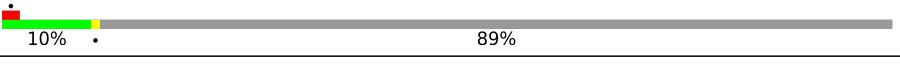
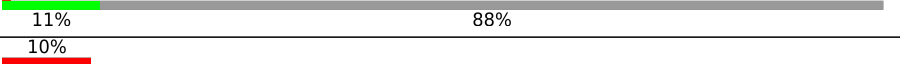
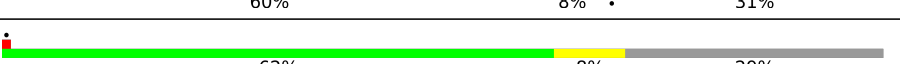
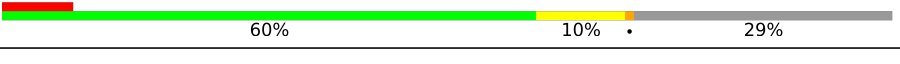
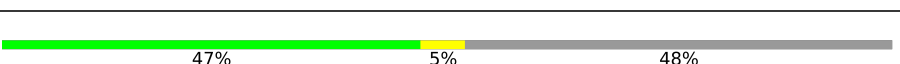
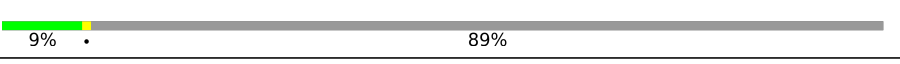
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	239 (8.70 - 9.70)

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	1	451	7% 69% 21% • 7%
1	2	451	10% 70% 20% • 7%
1	Q	451	36% 71% 19% • 7%
1	R	451	25% 72% 19% • 7%

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Mol	Chain	Length	Quality of chain
1	S	451	
1	T	451	
1	U	451	
1	V	451	
1	W	451	
1	X	451	
1	Y	451	
1	Z	451	
2	e	375	
3	D	907	
3	F	907	
3	H	907	
3	N	907	
3	a	907	
3	h	907	
3	j	907	
4	C	902	
4	E	902	
4	G	902	
4	M	902	
5	I	667	
5	K	667	
6	J	1024	
6	l	1024	
7	L	1819	

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Mol	Chain	Length	Quality of chain
7	c	1819	8% 91%
8	b	82	6% 61% 17% 21%
8	d	82	45% 61% 10% 28%
8	i	82	20% 68% 11% 21%
8	k	82	74% 5% 21%
8	m	82	68% 11% 21%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 108374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

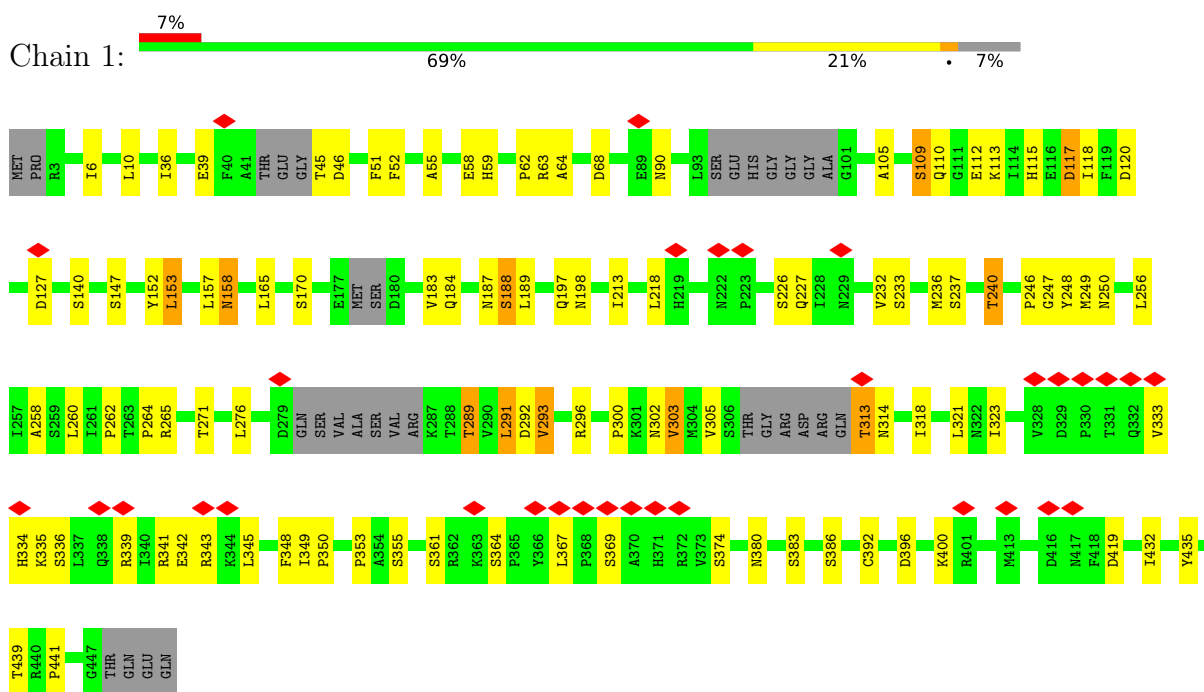
- Molecule 9 is water.

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

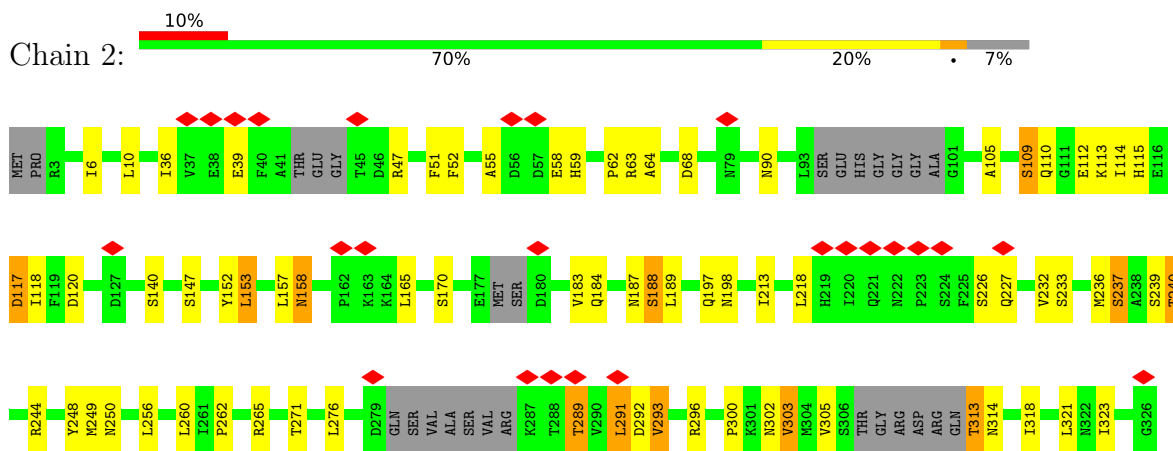
3 Residue-property plots

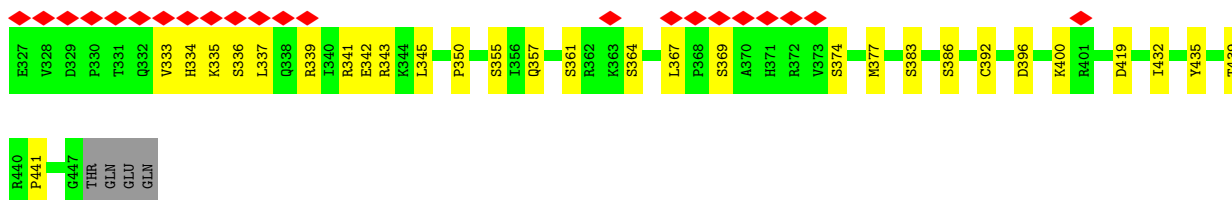
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Tubulin gamma-1 chain

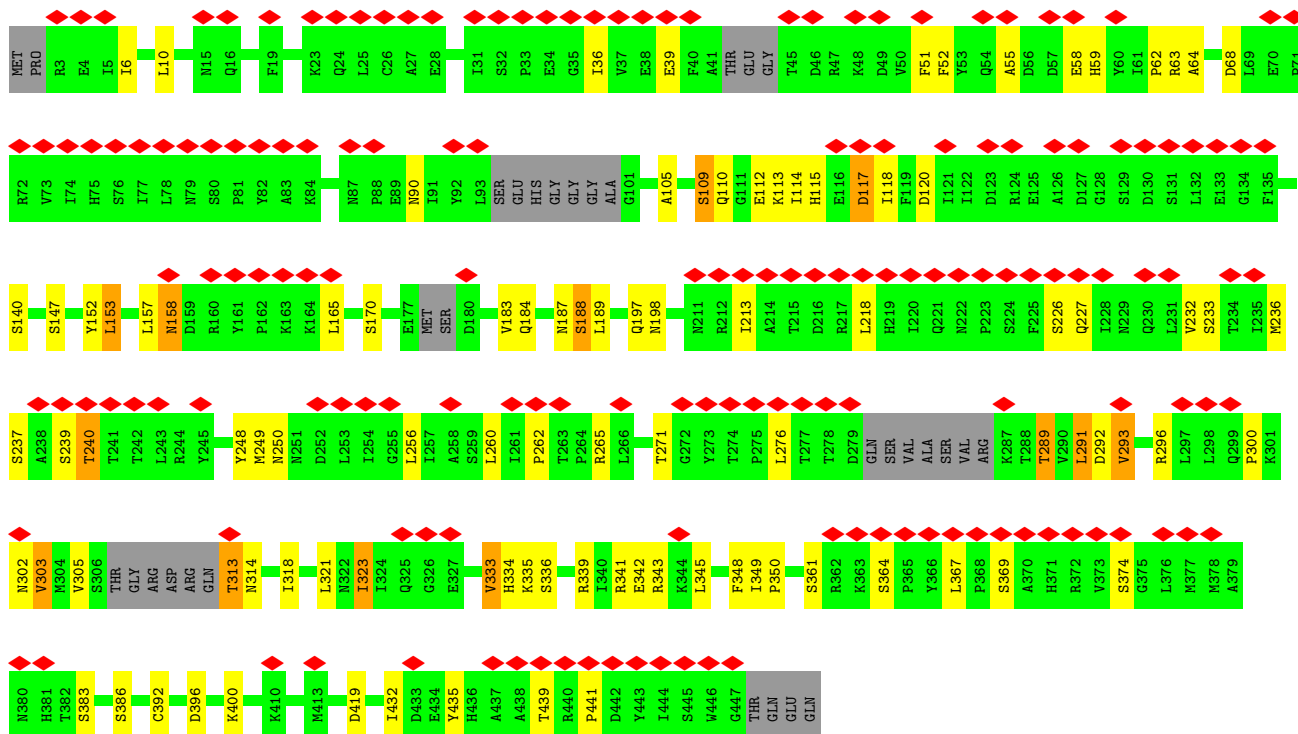


- Molecule 1: Tubulin gamma-1 chain

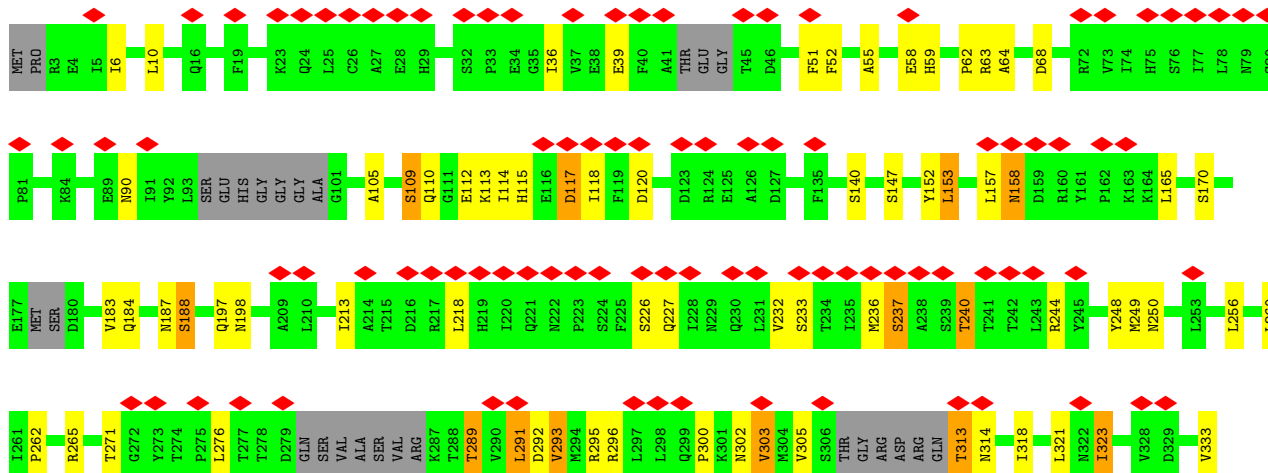


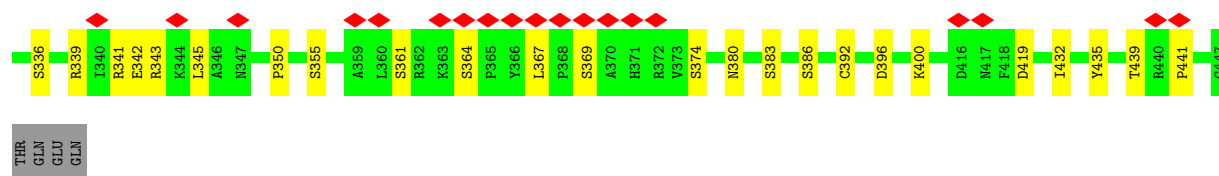


• Molecule 1: Tubulin gamma-1 chain

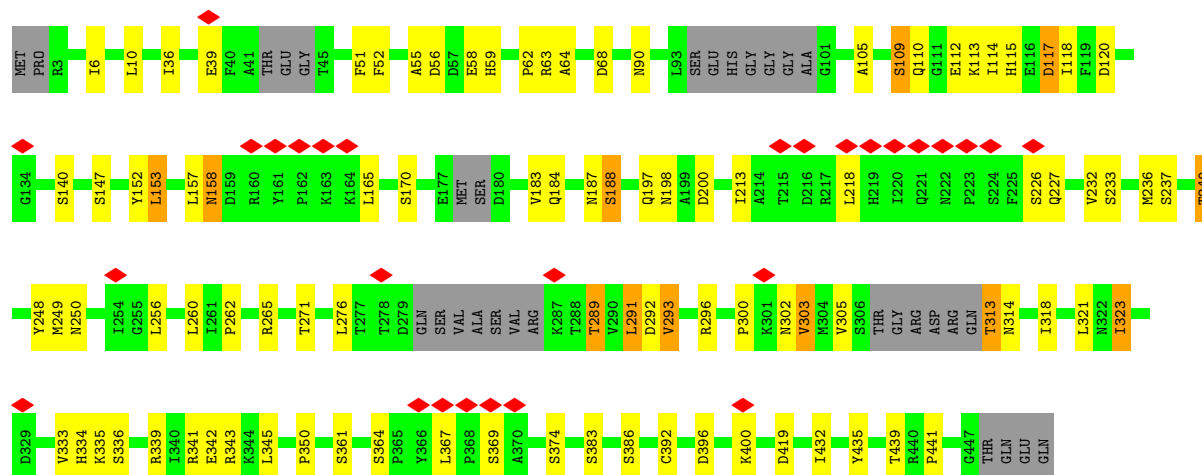


• Molecule 1: Tubulin gamma-1 chain

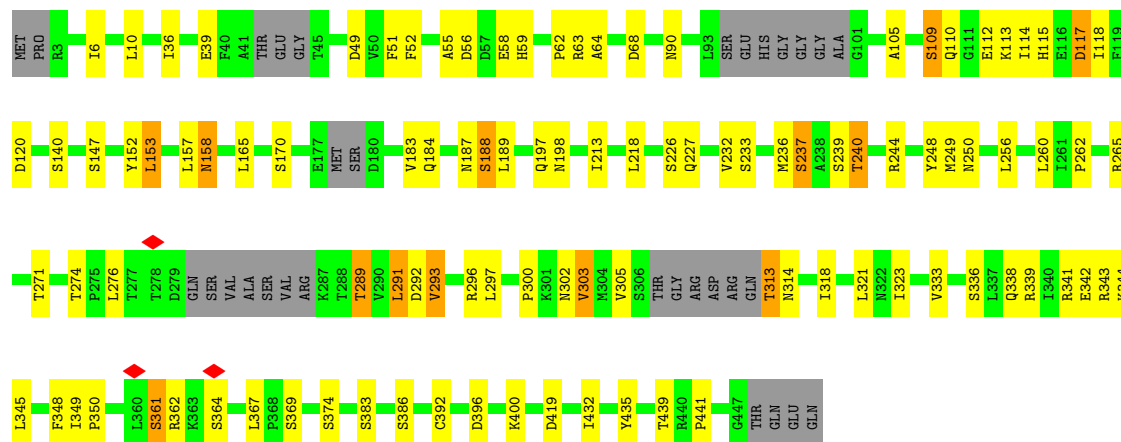




• Molecule 1: Tubulin gamma-1 chain

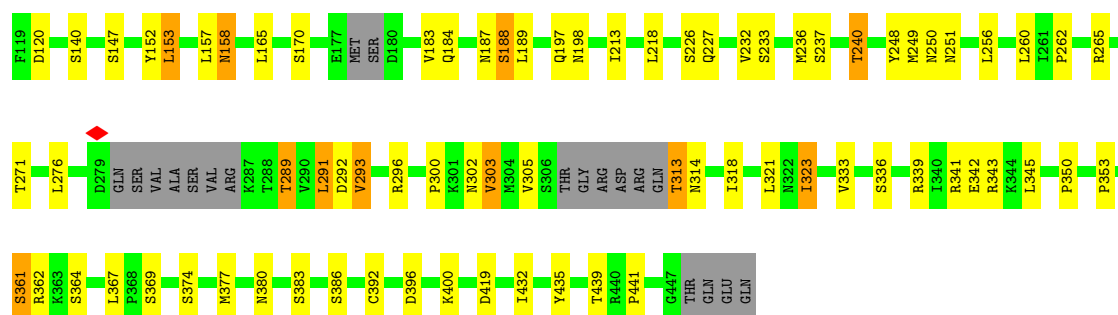


• Molecule 1: Tubulin gamma-1 chain



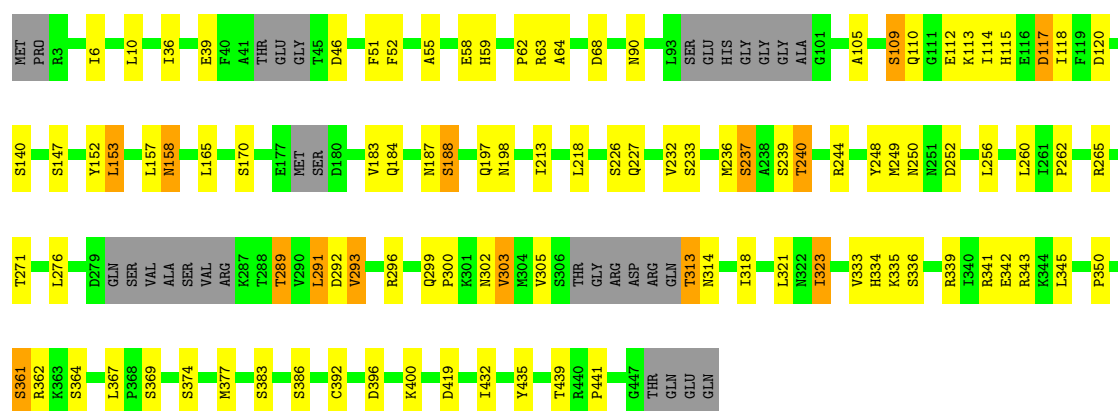
• Molecule 1: Tubulin gamma-1 chain





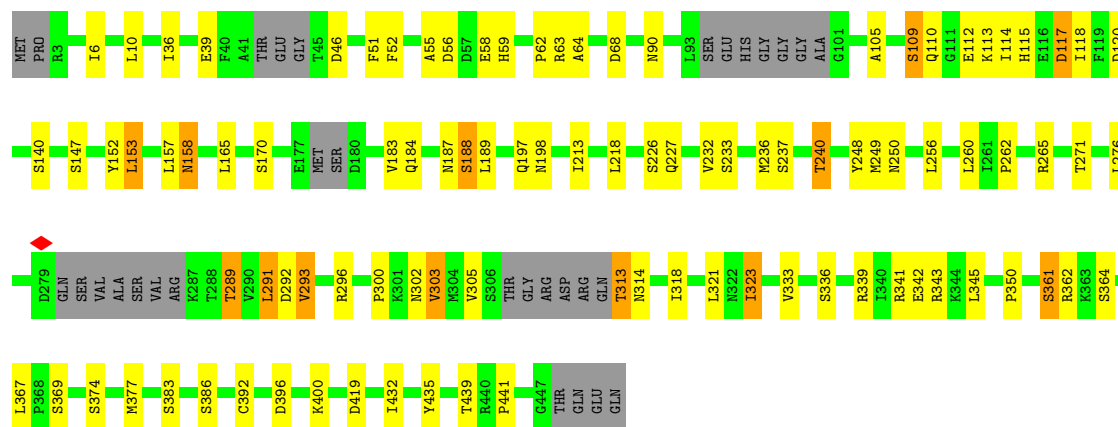
- Molecule 1: Tubulin gamma-1 chain

Chain V: 71% 20% 7%



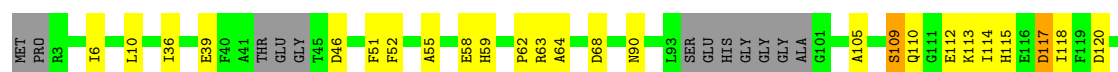
- Molecule 1: Tubulin gamma-1 chain

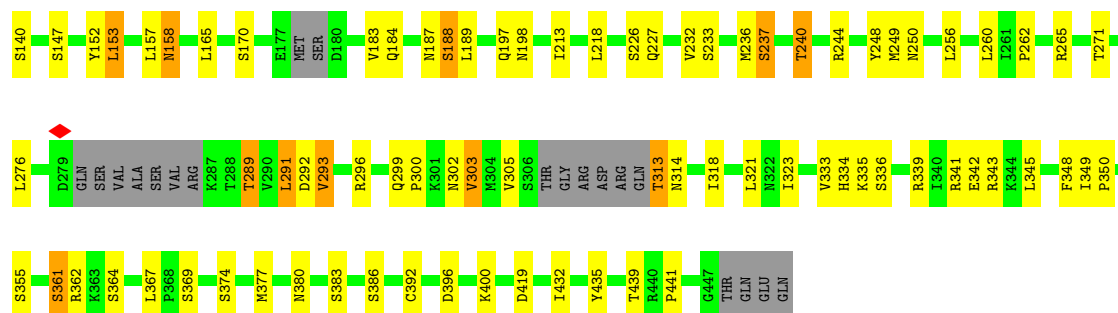
Chain W: 71% 19% 7%



- Molecule 1: Tubulin gamma-1 chain

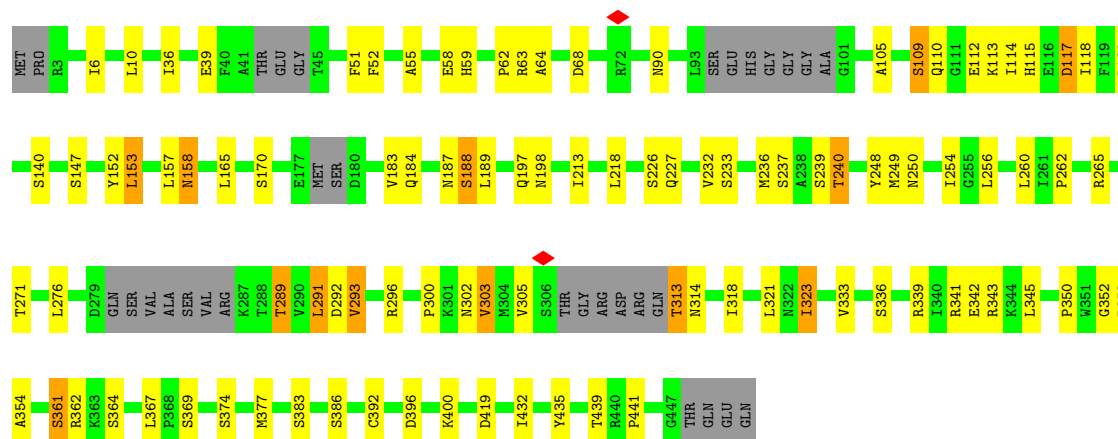
Chain X: 70% 20% 7%





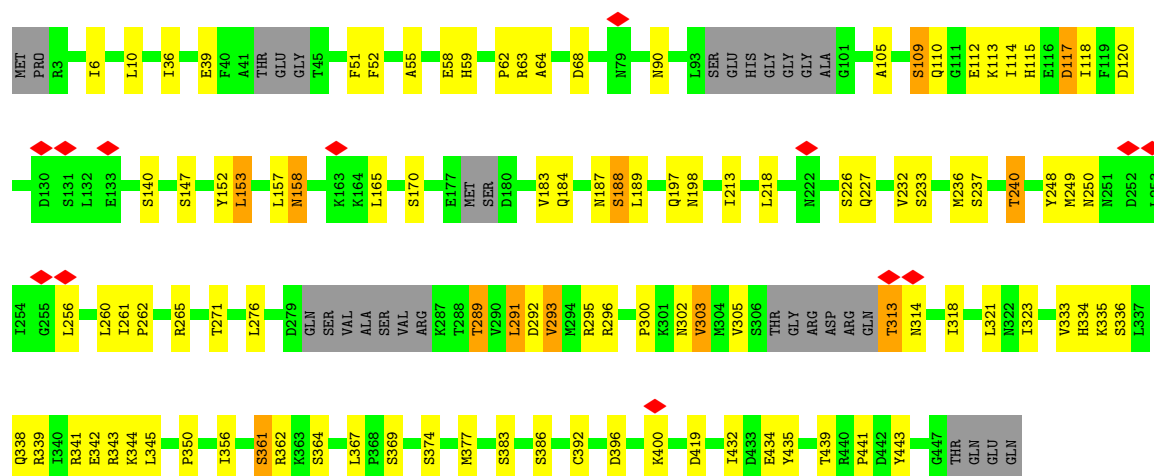
• Molecule 1: Tubulin gamma-1 chain

Chain Y: 71% 20% 7%



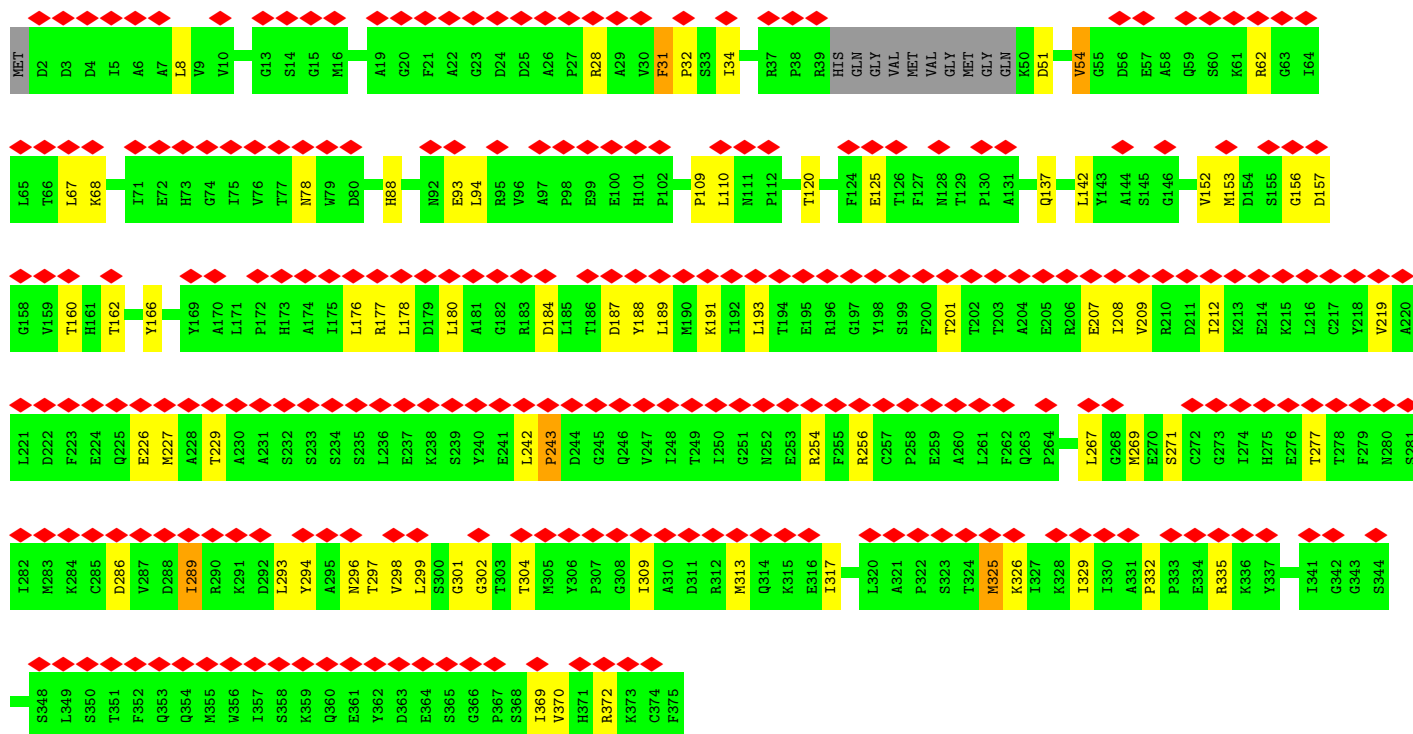
• Molecule 1: Tubulin gamma-1 chain

Chain Z: 70% 21% 7%

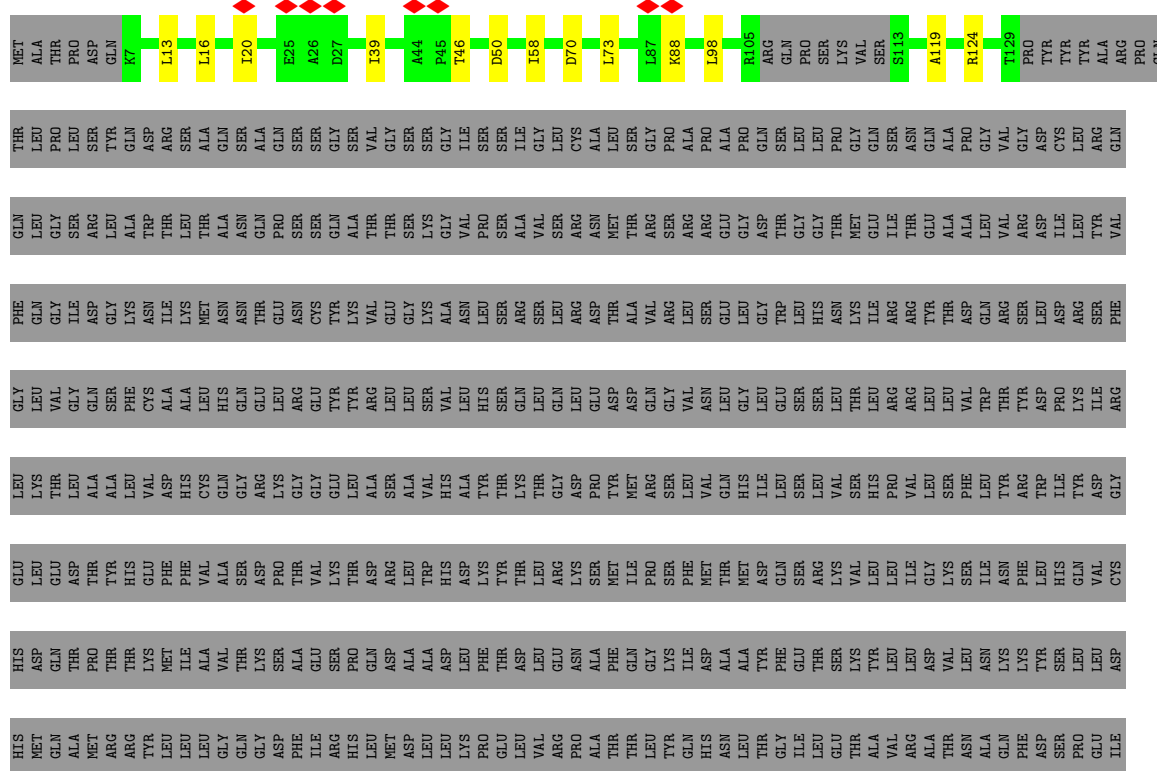


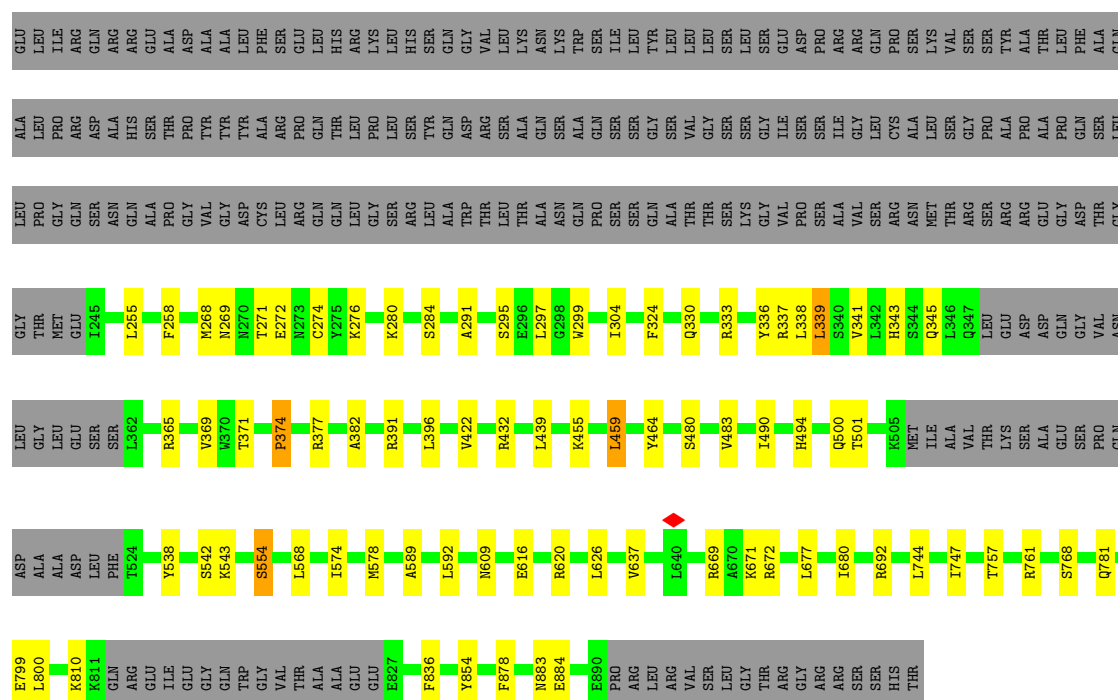
• Molecule 2: actin, cytoplasmic 1

Chain e: 69% 77% 19%



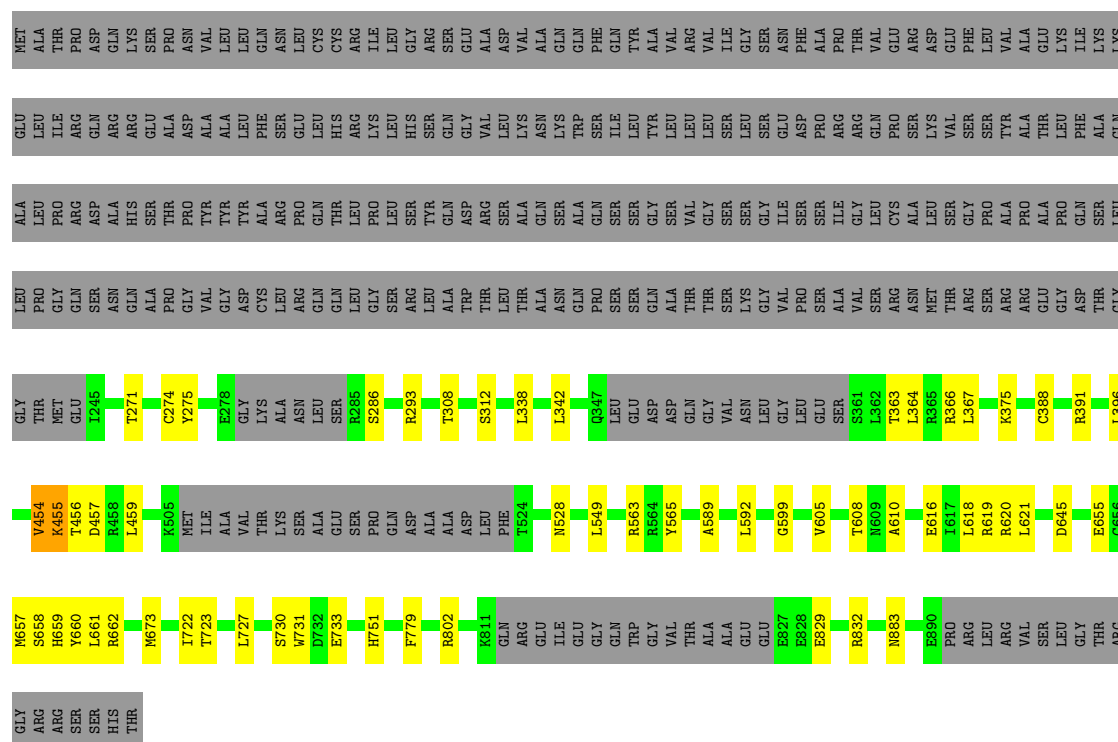
• Molecule 3: Gamma-tubulin complex component 3





• Molecule 3: Gamma-tubulin complex component 3

Chain H: 59% 6% 35%

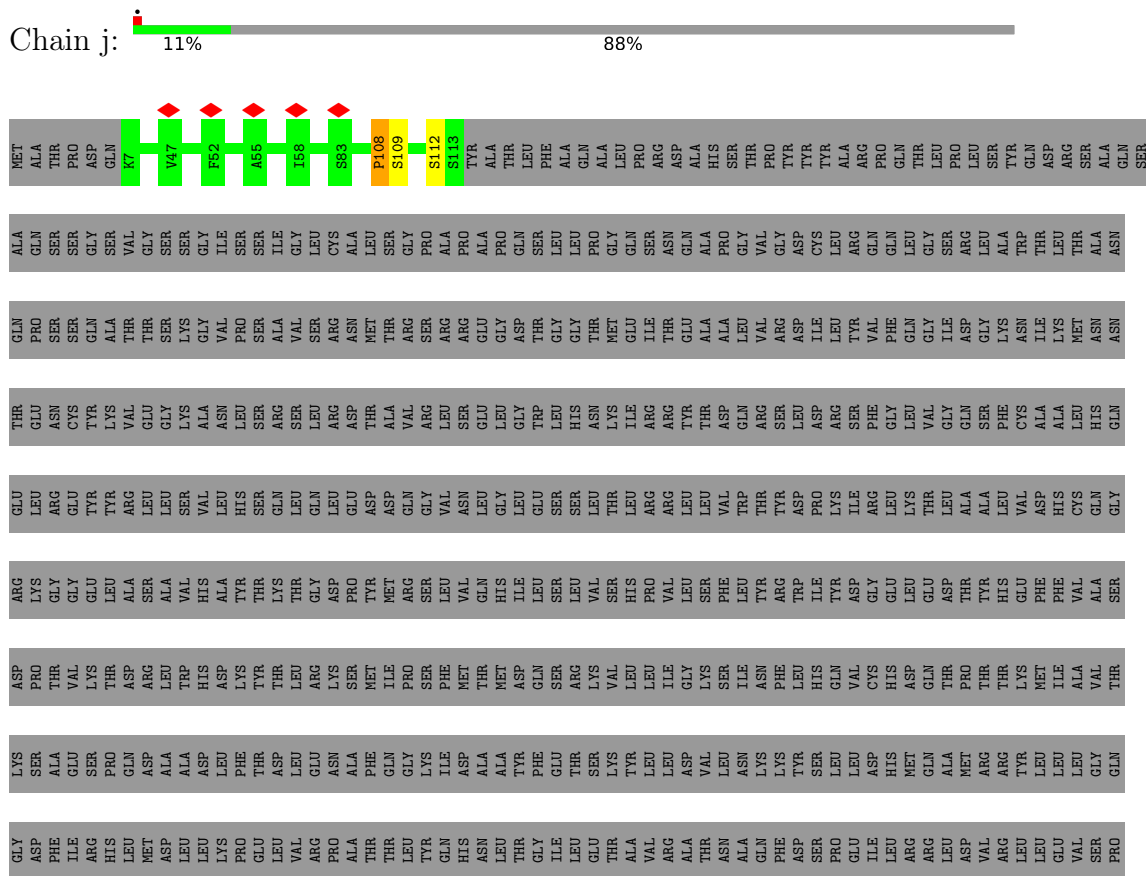


• Molecule 3: Gamma-tubulin complex component 3

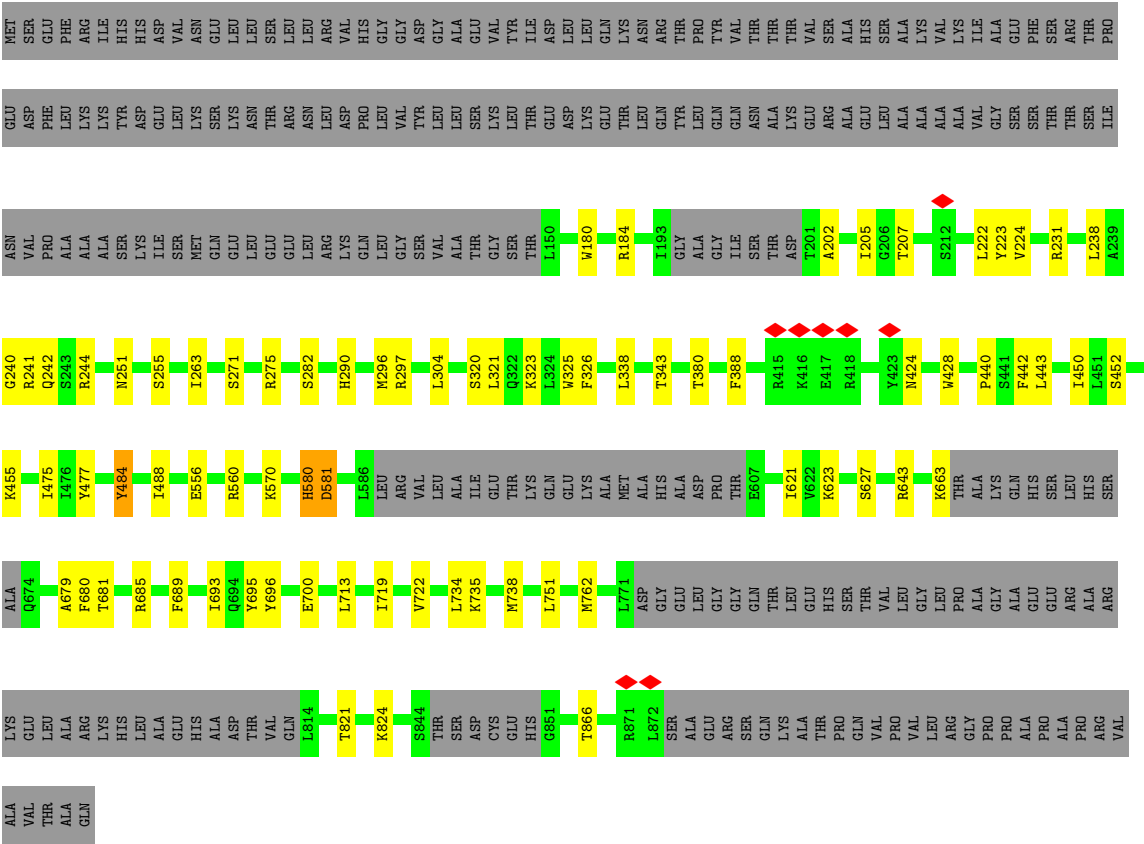
Chain N: 9% 58% 8% 35%

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

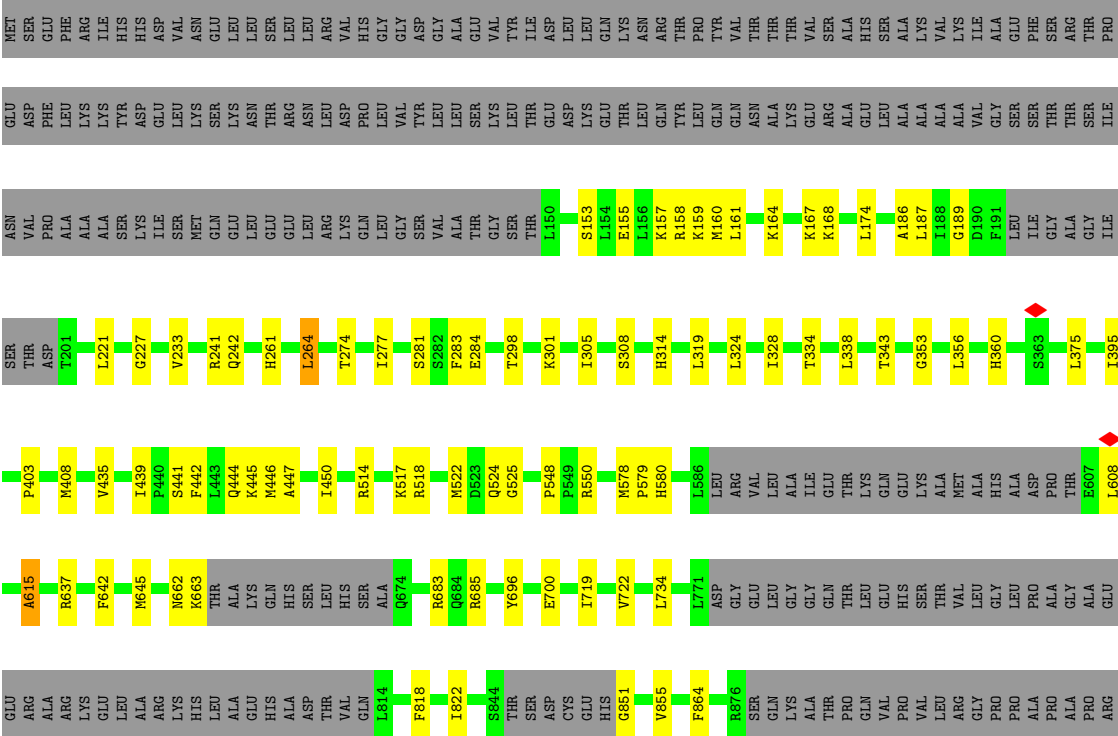
- Molecule 3: Gamma-tubulin complex component 3







● Molecule 4: Gamma-tubulin complex component 2



- Molecule 7: Gamma-tubulin complex component 6

[illegible]



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

• Molecule 8: Mitotic-spindle organizing protein 1



MET ALA SER SER SER GLY ALA GLY ALA ALA A11 A12 A13 A14 A15 A16 A20 V21 R22 D40 M41 E42 I46 C47 V48 C51 K65 E66 L67 R68 K69 A70 T71 E72 A73 L74 K75 ALA ALA GLU ASN MET THR SER

• Molecule 8: Mitotic-spindle organizing protein 1



MET ALA SER SER SER GLY ALA GLY ALA ALA A11 V21 T24 V27 I34 K75 ALA ALA GLU ASN MET THR SER

• Molecule 8: Mitotic-spindle organizing protein 1



MET ALA SER SER SER GLY ALA GLY ALA ALA A11 A12 M25 L39 D40 M41 L44 P57 S61 I64 K65 E66 L67 K75 ALA ALA GLU ASN MET THR SER

• Molecule 8: Mitotic-spindle organizing protein 1



MET ALA SER SER SER GLY ALA GLY ALA ALA A11 E23 T24 L28 L35 L39 E42 S45 I46 C47 V48 R49 D26 L50 C51 E52 Q53 Q54 I55 S61 S62 V63 I64 L67 R68 K75 ALA ALA GLU ASN MET THR SER

• Molecule 8: Mitotic-spindle organizing protein 1



MET ALA SER SER SER GLY ALA GLY ALA ALA ALA ALA ALA ALA N17 L18 N19 A20 V21 R22 E23 T24 M25 D26 V27 L28 I31 I34 L35 G38 L39 D40 M41 E42 T43 L44 S45 I46 C47 V48 R49 L50 C51 E52 Q53 Q54 I55 N56 P57 E58 A59 L60 V63 I64 K65 E66 L67 R68 T71 E72 A73 L74 K75 ALA ALA GLU ASN MET THR SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6456	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	0.170	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0318	Depositor
Map size ($\text{\AA}$)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.66, 2.66, 2.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.24	0/3441	0.60	0/4661
1	2	0.25	0/3441	0.60	0/4661
1	Q	0.24	0/3441	0.60	0/4661
1	R	0.24	0/3441	0.60	0/4661
1	S	0.24	0/3441	0.59	0/4661
1	T	0.25	0/3441	0.59	0/4661
1	U	0.24	0/3441	0.60	0/4661
1	V	0.24	0/3441	0.59	0/4661
1	W	0.24	0/3441	0.60	0/4661
1	X	0.24	0/3441	0.60	0/4661
1	Y	0.24	0/3441	0.59	0/4661
1	Z	0.24	0/3441	0.60	0/4661
2	e	0.55	1/2908 (0.0%)	0.84	4/3938 (0.1%)
3	D	0.35	1/4897 (0.0%)	0.73	5/6610 (0.1%)
3	F	0.38	1/5044 (0.0%)	0.78	6/6809 (0.1%)
3	H	0.32	0/5009	0.71	4/6761 (0.1%)
3	N	0.34	0/5009	0.76	6/6761 (0.1%)
3	a	0.31	0/948	0.76	1/1277 (0.1%)
3	h	0.30	0/815	0.65	0/1096
3	j	0.28	0/855	0.76	1/1152 (0.1%)
4	C	0.35	0/5151	0.77	7/6955 (0.1%)
4	E	0.41	2/5311 (0.0%)	0.75	7/7169 (0.1%)
4	G	0.34	1/5315 (0.0%)	0.71	4/7175 (0.1%)
4	M	0.38	0/5295	0.78	11/7147 (0.2%)
5	I	0.34	0/4322	0.77	7/5853 (0.1%)
5	K	0.42	2/4683 (0.0%)	0.76	10/6338 (0.2%)
6	J	0.36	0/4525	0.81	9/6119 (0.1%)
6	l	0.33	0/863	0.76	2/1166 (0.2%)
7	L	0.37	0/4697	0.79	8/6348 (0.1%)
7	c	0.40	0/1235	0.79	2/1664 (0.1%)
8	b	0.36	0/484	0.76	0/653
8	d	0.34	0/454	0.73	0/611
8	i	0.33	0/484	0.69	0/653
8	k	0.25	0/484	0.61	0/653

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
8	m	0.33	0/484	0.74	0/653
All	All	0.33	8/110564 (0.0%)	0.70	94/149493 (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
3	D	0	2
3	F	0	2
3	H	0	2
3	N	0	1
3	h	0	1
3	j	0	2
4	C	0	3
4	E	0	2
4	G	0	2
4	M	0	1
5	I	0	3
5	K	0	2
6	J	0	4
7	L	0	2
All	All	0	29

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	243	PRO	N-CD	20.77	1.76	1.47
4	E	184	ARG	CD-NE	7.35	1.56	1.46
4	E	184	ARG	NE-CZ	7.10	1.40	1.33
5	K	166	PRO	C-N	6.23	1.42	1.34
3	F	299	TRP	CZ3-CH2	5.61	1.54	1.40
5	K	651	TYR	CD2-CE2	-5.30	1.22	1.38
3	D	582	LYS	C-N	5.22	1.40	1.34
4	G	283	PHE	CA-C	-5.10	1.43	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	727	LEU	CB-CG-CD2	-9.48	82.25	110.70
4	M	464	GLY	CA-C-O	-8.43	116.74	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	456	THR	N-CA-C	-8.10	97.86	109.29
6	I	121	PRO	N-CA-CB	7.76	111.40	103.25
4	C	460	VAL	CG1-CB-CG2	-7.68	93.91	110.80
3	F	883	ASN	N-CA-C	-7.64	105.13	114.75
7	L	1800	LEU	CB-CG-CD1	-7.61	87.87	110.70
4	E	580	HIS	CA-C-N	7.54	135.95	121.54
4	E	580	HIS	C-N-CA	7.54	135.95	121.54
4	C	467	VAL	N-CA-C	-7.32	106.76	113.71
5	K	574	ILE	N-CA-C	-7.25	106.14	113.47
4	E	719	ILE	N-CA-C	-7.02	105.66	111.91
3	N	713	HIS	CA-CB-CG	-6.98	106.82	113.80
5	I	600	ASN	CA-C-N	6.95	134.82	121.54
5	I	600	ASN	C-N-CA	6.95	134.82	121.54
6	I	130	PRO	N-CA-CB	6.89	110.57	103.00
3	D	871	GLU	N-CA-C	-6.74	106.00	114.56
6	J	237	HIS	CA-C-N	6.70	134.34	121.54
6	J	237	HIS	C-N-CA	6.70	134.34	121.54
3	D	418	ILE	N-CA-C	-6.60	106.58	112.12
4	M	815	VAL	N-CA-C	-6.53	106.87	113.47
5	K	263	ILE	CA-C-N	6.53	129.98	120.51
5	K	263	ILE	C-N-CA	6.53	129.98	120.51
6	J	255	PRO	CA-C-N	6.52	133.43	121.70
6	J	255	PRO	C-N-CA	6.52	133.43	121.70
4	C	815	VAL	N-CA-C	-6.49	105.00	111.88
4	C	545	ASP	N-CA-C	-6.40	103.13	111.71
7	L	1689	ARG	N-CA-C	-6.32	106.53	114.56
6	J	905	ILE	CA-C-N	-6.30	111.72	122.56
6	J	905	ILE	C-N-CA	-6.30	111.72	122.56
5	K	409	ASN	CA-C-N	6.25	136.68	126.86
5	K	409	ASN	C-N-CA	6.25	136.68	126.86
7	L	1800	LEU	CB-CG-CD2	-6.16	92.23	110.70
3	j	108	PRO	N-CA-CB	6.12	109.67	103.25
3	N	433	TRP	N-CA-C	-5.96	106.99	114.56
7	c	82	LEU	CA-CB-CG	5.82	136.65	116.30
4	G	264	LEU	N-CA-C	5.79	122.60	109.81
5	K	203	PHE	CA-C-N	5.72	131.53	122.61
5	K	203	PHE	C-N-CA	5.72	131.53	122.61
4	M	264	LEU	N-CA-C	5.71	122.43	109.81
6	J	235	SER	CA-C-N	5.68	132.39	121.54
6	J	235	SER	C-N-CA	5.68	132.39	121.54
3	F	337	ARG	N-CA-C	-5.64	106.45	113.38
4	C	238	LEU	CA-C-N	5.62	132.27	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	238	LEU	C-N-CA	5.62	132.27	121.54
4	M	240	GLY	CA-C-N	5.61	132.25	121.54
4	M	240	GLY	C-N-CA	5.61	132.25	121.54
3	F	336	TYR	CB-CA-C	5.49	119.54	109.99
3	F	269	ASN	CA-C-N	5.44	132.31	123.93
3	F	269	ASN	C-N-CA	5.44	132.31	123.93
3	H	454	VAL	CA-C-N	5.43	131.91	121.54
3	H	454	VAL	C-N-CA	5.43	131.91	121.54
5	I	503	LYS	N-CA-C	-5.42	107.93	114.75
7	L	306	HIS	CA-C-N	5.38	131.81	121.54
7	L	306	HIS	C-N-CA	5.38	131.81	121.54
3	N	458	ARG	CA-C-N	5.38	127.80	120.54
3	N	458	ARG	C-N-CA	5.38	127.80	120.54
4	E	424	ASN	CA-C-N	5.37	131.80	121.54
4	E	424	ASN	C-N-CA	5.37	131.80	121.54
3	D	610	ALA	N-CA-C	-5.36	104.53	111.71
3	D	581	LEU	CA-CB-CG	5.36	135.06	116.30
4	M	543	VAL	CA-C-N	5.35	131.76	121.54
4	M	543	VAL	C-N-CA	5.35	131.76	121.54
5	K	68	GLN	CA-CB-CG	5.32	124.74	114.10
4	G	548	PRO	N-CA-C	5.31	117.18	110.70
3	H	883	ASN	N-CA-C	-5.31	106.69	114.39
4	E	184	ARG	NE-CZ-NH2	-5.29	114.44	119.20
7	L	567	LEU	CA-C-N	5.28	131.63	121.54
7	L	567	LEU	C-N-CA	5.28	131.63	121.54
3	F	336	TYR	N-CA-C	-5.26	105.72	113.61
5	I	628	LYS	N-CA-C	-5.26	106.64	114.64
5	I	515	TRP	CA-C-N	5.25	131.57	121.54
5	I	515	TRP	C-N-CA	5.25	131.57	121.54
4	E	866	THR	N-CA-C	-5.25	106.66	114.64
4	C	273	VAL	N-CA-C	-5.24	107.48	111.62
4	M	719	ILE	N-CA-C	-5.23	106.79	112.80
7	L	307	ARG	N-CA-C	-5.22	99.67	110.80
3	a	119	ALA	N-CA-C	5.21	118.03	110.42
2	e	166	TYR	CA-C-N	5.21	131.49	121.54
2	e	166	TYR	C-N-CA	5.21	131.49	121.54
7	c	148	TYR	CB-CA-C	5.18	118.26	109.50
2	e	51	ASP	N-CA-C	-5.16	106.79	114.64
2	e	243	PRO	CA-N-CD	-5.15	104.79	112.00
4	M	700	GLU	CA-C-N	-5.14	117.93	122.97
4	M	700	GLU	C-N-CA	-5.14	117.93	122.97
4	G	227	GLY	CA-C-N	5.14	131.22	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	227	GLY	C-N-CA	5.14	131.22	121.97
6	J	236	LEU	CA-CB-CG	5.14	134.28	116.30
5	K	67	GLN	CA-C-N	5.11	130.65	122.93
5	K	67	GLN	C-N-CA	5.11	130.65	122.93
3	D	866	THR	N-CA-C	-5.09	106.90	114.64
4	M	548	PRO	N-CA-C	5.09	116.91	110.70
5	I	408	ASP	N-CA-C	5.07	119.68	111.37
3	N	727	LEU	CA-CB-CG	5.03	133.90	116.30

There are no chirality outliers.

All (29) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3373	0	3325	55	0
1	2	3373	0	3325	59	0
1	Q	3373	0	3325	50	0
1	R	3373	0	3325	48	0
1	S	3373	0	3325	48	0
1	T	3373	0	3325	53	0
1	U	3373	0	3325	55	0
1	V	3373	0	3325	51	0
1	W	3373	0	3325	52	0
1	X	3373	0	3325	55	0
1	Y	3373	0	3325	53	0
1	Z	3373	0	3325	55	0
2	e	2847	0	2810	64	0
3	D	4796	0	4775	37	0
3	F	4941	0	4935	52	0
3	H	4907	0	4896	29	0
3	N	4907	0	4896	47	0
3	a	933	0	953	11	0
3	h	803	0	831	5	0
3	j	843	0	846	0	0
4	C	5044	0	5081	45	0
4	E	5202	0	5241	48	0
4	G	5206	0	5230	48	0
4	M	5186	0	5219	58	0
5	I	4225	0	4259	30	0
5	K	4579	0	4586	31	0
6	J	4429	0	4482	24	0
6	l	847	0	789	6	0
7	L	4587	0	4636	34	0
7	c	1220	0	1231	16	0
8	b	484	0	512	13	0
8	d	454	0	482	6	0
8	i	484	0	512	7	0
8	k	484	0	512	2	0
8	m	484	0	512	6	0
9	l	6	0	0	0	0
All	All	108374	0	108126	1150	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 (1150) 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)
2:e:243:PRO:CD	2:e:243:PRO:N	1.76	1.37
2:e:242:LEU:HD12	2:e:243:PRO:CD	1.68	1.24
2:e:242:LEU:CD1	2:e:243:PRO:HD2	1.75	1.15
2:e:160:THR:HG22	2:e:178:LEU:O	1.50	1.10
2:e:160:THR:HG23	2:e:178:LEU:CB	1.92	0.99
2:e:160:THR:HG23	2:e:178:LEU:HB2	1.44	0.97
2:e:160:THR:CG2	2:e:178:LEU:CB	2.51	0.89
2:e:160:THR:CG2	2:e:178:LEU:HB3	2.03	0.88
2:e:160:THR:HG21	2:e:178:LEU:HB3	1.59	0.83
2:e:160:THR:CG2	2:e:178:LEU:O	2.25	0.82
2:e:242:LEU:HD12	2:e:243:PRO:HD2	0.85	0.77
4:M:638:TYR:HH	4:M:726:HIS:HE2	1.29	0.76
1:T:56:ASP:OD1	1:U:296:ARG:NE	2.19	0.75
1:W:56:ASP:OD2	1:X:299:GLN:NE2	2.22	0.72
2:e:178:LEU:HD22	2:e:271:SER:OG	1.89	0.72
3:a:16:LEU:HD11	8:b:50:LEU:HD11	1.71	0.70
4:G:696:TYR:HH	4:G:851:GLY:N	1.87	0.70
5:K:401:HIS:HE1	1:Z:295:ARG:HH12	1.40	0.69
1:1:55:ALA:HB3	1:1:59:HIS:HB2	1.76	0.68
2:e:156:GLY:HA2	2:e:302:GLY:H	1.57	0.68
2:e:212:ILE:HG23	2:e:254:ARG:HH22	1.57	0.68
5:K:345:VAL:HA	5:K:350:LEU:HD13	1.75	0.68
1:U:55:ALA:HB3	1:U:59:HIS:HB2	1.76	0.68
1:S:55:ALA:HB3	1:S:59:HIS:HB2	1.76	0.68
1:2:342:GLU:HG3	4:M:549:PRO:HB2	1.73	0.68
1:X:55:ALA:HB3	1:X:59:HIS:HB2	1.76	0.68
1:Z:55:ALA:HB3	1:Z:59:HIS:HB2	1.76	0.68
1:R:55:ALA:HB3	1:R:59:HIS:HB2	1.76	0.68
1:Y:55:ALA:HB3	1:Y:59:HIS:HB2	1.76	0.68
1:2:55:ALA:HB3	1:2:59:HIS:HB2	1.76	0.67
2:e:62:ARG:HH12	2:e:207:GLU:HG3	1.59	0.67
4:E:244:ARG:HE	4:E:275:ARG:HE	1.42	0.67
1:W:55:ALA:HB3	1:W:59:HIS:HB2	1.76	0.67
4:E:696:TYR:O	4:E:700:GLU:HB2	1.95	0.67
1:Q:55:ALA:HB3	1:Q:59:HIS:HB2	1.76	0.67
1:V:55:ALA:HB3	1:V:59:HIS:HB2	1.76	0.67
8:d:43:THR:HA	8:d:46:ILE:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:56:ASP:OD1	1:T:296:ARG:HD3	1.94	0.67
1:T:55:ALA:HB3	1:T:59:HIS:HB2	1.76	0.66
2:e:176:LEU:HD23	2:e:277:THR:HG23	1.77	0.66
3:D:806:PHE:HA	3:D:809:LYS:HE3	1.76	0.66
2:e:369:ILE:HD12	2:e:372:ARG:HD2	1.77	0.65
1:1:36:ILE:HD13	1:1:59:HIS:HE1	1.62	0.65
1:V:36:ILE:HD13	1:V:59:HIS:HE1	1.62	0.65
1:S:36:ILE:HD13	1:S:59:HIS:HE1	1.62	0.65
1:2:36:ILE:HD13	1:2:59:HIS:HE1	1.62	0.65
2:e:160:THR:CG2	2:e:178:LEU:C	2.71	0.64
3:N:573:PHE:HB2	3:N:610:ALA:HB2	1.79	0.64
2:e:160:THR:HG22	2:e:178:LEU:C	2.21	0.64
4:G:864:PHE:HB3	1:U:353:PRO:HB3	1.77	0.64
1:Z:36:ILE:HD13	1:Z:59:HIS:HE1	1.62	0.64
4:C:460:VAL:HG23	4:C:465:HIS:CE1	2.33	0.64
1:U:36:ILE:HD13	1:U:59:HIS:HE1	1.62	0.64
1:W:36:ILE:HD13	1:W:59:HIS:HE1	1.62	0.64
1:Y:36:ILE:HD13	1:Y:59:HIS:HE1	1.62	0.64
1:Q:36:ILE:HD13	1:Q:59:HIS:HE1	1.62	0.64
1:T:36:ILE:HD13	1:T:59:HIS:HE1	1.62	0.64
2:e:326:LYS:HE3	8:d:54:GLY:HA3	1.80	0.63
6:J:391:THR:HA	7:L:293:LYS:HG3	1.79	0.63
1:R:36:ILE:HD13	1:R:59:HIS:HE1	1.62	0.63
3:a:13:LEU:HA	3:a:16:LEU:HD12	1.81	0.63
5:I:398:GLN:NE2	1:X:342:GLU:OE2	2.32	0.63
7:L:1722:ALA:HB2	7:L:1792:GLN:HE22	1.62	0.63
1:X:36:ILE:HD13	1:X:59:HIS:HE1	1.62	0.63
3:F:432:ARG:HH12	3:F:439:LEU:HD12	1.64	0.63
1:U:53:TYR:OH	1:V:299:GLN:NE2	2.24	0.62
2:e:34:ILE:HD11	2:e:67:LEU:HA	1.81	0.62
4:M:524:GLN:HE21	4:M:564:ALA:HA	1.63	0.62
2:e:153:MET:HE3	2:e:313:MET:HE3	1.82	0.62
4:M:459:VAL:HG11	4:M:628:LEU:HD11	1.81	0.62
5:K:1:MET:HA	5:K:5:LEU:HD23	1.81	0.62
3:a:20:ILE:HD13	8:b:67:LEU:HB2	1.81	0.62
8:d:71:THR:HG21	7:c:15:LEU:HD22	1.81	0.62
2:e:227:MET:HE2	2:e:256:ARG:HE	1.64	0.62
3:D:245:ILE:HG12	3:D:288:ARG:HH12	1.65	0.62
1:U:300:PRO:HA	1:U:303:VAL:HB	1.82	0.62
1:X:300:PRO:HA	1:X:303:VAL:HB	1.82	0.61
1:Z:300:PRO:HA	1:Z:303:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:293:VAL:HA	1:T:296:ARG:HD2	1.83	0.61
1:W:300:PRO:HA	1:W:303:VAL:HB	1.82	0.61
1:1:300:PRO:HA	1:1:303:VAL:HB	1.82	0.61
3:F:391:ARG:HB2	3:F:396:LEU:HD12	1.82	0.61
1:Y:300:PRO:HA	1:Y:303:VAL:HB	1.82	0.61
1:Q:300:PRO:HA	1:Q:303:VAL:HB	1.82	0.61
1:X:293:VAL:HA	1:X:296:ARG:HD2	1.83	0.61
1:2:293:VAL:HA	1:2:296:ARG:HD2	1.83	0.61
4:G:338:LEU:HD21	4:G:375:LEU:HD11	1.82	0.61
1:S:293:VAL:HA	1:S:296:ARG:HD2	1.83	0.61
5:I:618:GLY:HA2	5:I:621:ARG:HE	1.66	0.61
1:R:300:PRO:HA	1:R:303:VAL:HB	1.82	0.60
1:1:264:PRO:HB3	4:M:663:LYS:HG3	1.83	0.60
1:W:158:ASN:ND2	1:W:198:ASN:O	2.35	0.60
1:1:293:VAL:HA	1:1:296:ARG:HD2	1.83	0.60
5:K:339:HIS:HA	5:K:342:LYS:HD2	1.83	0.60
1:S:300:PRO:HA	1:S:303:VAL:HB	1.82	0.60
1:U:158:ASN:ND2	1:U:198:ASN:O	2.35	0.60
1:V:158:ASN:ND2	1:V:198:ASN:O	2.35	0.60
1:Y:293:VAL:HA	1:Y:296:ARG:HD2	1.83	0.60
1:2:300:PRO:HA	1:2:303:VAL:HB	1.82	0.60
5:I:313:ARG:HA	5:I:316:GLN:HE21	1.66	0.60
1:U:293:VAL:HA	1:U:296:ARG:HD2	1.83	0.60
1:X:158:ASN:ND2	1:X:198:ASN:O	2.35	0.60
4:G:167:LYS:HE3	4:G:168:LYS:HG3	1.82	0.60
6:J:707:MET:HE2	6:J:921:LYS:HA	1.84	0.60
1:S:158:ASN:ND2	1:S:198:ASN:O	2.35	0.60
1:V:300:PRO:HA	1:V:303:VAL:HB	1.82	0.60
1:W:293:VAL:HA	1:W:296:ARG:HD2	1.83	0.60
1:Z:158:ASN:ND2	1:Z:198:ASN:O	2.35	0.60
3:F:626:LEU:HB2	3:F:637:VAL:HG23	1.84	0.60
3:H:620:ARG:HH12	3:H:645:ASP:H	1.50	0.60
1:T:158:ASN:ND2	1:T:198:ASN:O	2.35	0.60
1:Z:293:VAL:HA	1:Z:296:ARG:HD2	1.83	0.60
1:V:183:VAL:HG13	1:V:187:ASN:HD21	1.67	0.60
1:Y:183:VAL:HG13	1:Y:187:ASN:HD21	1.67	0.60
1:V:293:VAL:HA	1:V:296:ARG:HD2	1.83	0.60
3:D:266:ILE:HG12	3:D:277:VAL:HG22	1.83	0.59
1:R:183:VAL:HG13	1:R:187:ASN:HD21	1.67	0.59
1:T:300:PRO:HA	1:T:303:VAL:HB	1.82	0.59
1:U:183:VAL:HG13	1:U:187:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:158:ASN:ND2	1:2:198:ASN:O	2.35	0.59
1:2:183:VAL:HG13	1:2:187:ASN:HD21	1.67	0.59
1:S:183:VAL:HG13	1:S:187:ASN:HD21	1.67	0.59
1:1:183:VAL:HG13	1:1:187:ASN:HD21	1.67	0.59
4:E:442:PHE:HE2	4:E:484:TYR:HE2	1.51	0.59
7:L:512:ASN:HD21	7:L:515:ASN:HD22	1.49	0.59
1:Q:293:VAL:HA	1:Q:296:ARG:HD2	1.83	0.59
1:R:293:VAL:HA	1:R:296:ARG:HD2	1.83	0.59
1:Z:183:VAL:HG13	1:Z:187:ASN:HD21	1.67	0.59
1:T:183:VAL:HG13	1:T:187:ASN:HD21	1.67	0.59
1:Y:158:ASN:ND2	1:Y:198:ASN:O	2.35	0.59
7:L:1633:LEU:HD22	7:L:1662:LYS:HZ3	1.66	0.59
1:R:158:ASN:ND2	1:R:198:ASN:O	2.35	0.59
4:C:464:GLY:O	4:C:465:HIS:ND1	2.30	0.59
1:I:247:GLY:O	4:M:525:GLY:N	2.35	0.59
1:U:213:ILE:HG21	1:U:276:LEU:HD22	1.85	0.59
1:W:213:ILE:HG21	1:W:276:LEU:HD22	1.85	0.59
1:X:183:VAL:HG13	1:X:187:ASN:HD21	1.67	0.59
1:X:213:ILE:HG21	1:X:276:LEU:HD22	1.85	0.59
1:2:213:ILE:HG21	1:2:276:LEU:HD22	1.85	0.59
1:2:357:GLN:OE1	3:N:716:HIS:ND1	2.36	0.59
2:e:153:MET:HG2	2:e:162:THR:HG23	1.84	0.59
1:S:213:ILE:HG21	1:S:276:LEU:HD22	1.85	0.59
4:C:695:TYR:HB2	4:C:858:ARG:HH22	1.68	0.58
6:J:221:VAL:O	6:J:228:ARG:NH2	2.36	0.58
1:Q:158:ASN:ND2	1:Q:198:ASN:O	2.35	0.58
1:R:213:ILE:HG21	1:R:276:LEU:HD22	1.85	0.58
1:1:158:ASN:ND2	1:1:198:ASN:O	2.35	0.58
1:1:213:ILE:HG21	1:1:276:LEU:HD22	1.85	0.58
1:Q:183:VAL:HG13	1:Q:187:ASN:HD21	1.67	0.58
1:V:350:PRO:HG2	1:V:441:PRO:HG3	1.85	0.58
3:H:363:THR:HB	3:H:366:ARG:H	1.69	0.58
8:i:48:VAL:HG13	3:h:87:LEU:HD13	1.85	0.58
1:S:350:PRO:HG2	1:S:441:PRO:HG3	1.85	0.58
7:L:1663:HIS:ND1	1:Z:261:ILE:O	2.37	0.58
1:2:350:PRO:HG2	1:2:441:PRO:HG3	1.85	0.58
3:a:46:THR:HG23	3:a:124:ARG:HH11	1.67	0.58
1:Y:350:PRO:HG2	1:Y:441:PRO:HG3	1.85	0.58
4:M:287:GLN:HB2	4:M:406:GLU:HG2	1.86	0.57
1:T:350:PRO:HG2	1:T:441:PRO:HG3	1.85	0.57
3:N:266:ILE:HG12	3:N:277:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:350:PRO:HG2	1:W:441:PRO:HG3	1.85	0.57
3:H:608:THR:HG23	3:H:610:ALA:H	1.69	0.57
1:T:184:GLN:O	1:T:188:SER:OG	2.23	0.57
1:T:213:ILE:HG21	1:T:276:LEU:HD22	1.85	0.57
1:V:184:GLN:O	1:V:188:SER:OG	2.23	0.57
1:W:184:GLN:O	1:W:188:SER:OG	2.23	0.57
1:X:184:GLN:O	1:X:188:SER:OG	2.23	0.57
1:X:350:PRO:HG2	1:X:441:PRO:HG3	1.85	0.57
1:Y:213:ILE:HG21	1:Y:276:LEU:HD22	1.85	0.57
1:Q:213:ILE:HG21	1:Q:276:LEU:HD22	1.85	0.57
1:S:260:LEU:HD21	1:S:321:LEU:HB3	1.87	0.57
1:W:183:VAL:HG13	1:W:187:ASN:HD21	1.67	0.57
4:M:560:ARG:HH21	4:M:570:LYS:HD2	1.70	0.57
1:Q:350:PRO:HG2	1:Q:441:PRO:HG3	1.85	0.57
1:Y:184:GLN:O	1:Y:188:SER:OG	2.23	0.57
1:Z:213:ILE:HG21	1:Z:276:LEU:HD22	1.85	0.57
1:2:184:GLN:O	1:2:188:SER:OG	2.23	0.57
5:I:18:THR:OG1	5:I:26:GLN:OE1	2.21	0.57
4:M:536:GLU:HA	4:M:539:LEU:HB2	1.87	0.57
4:E:282:SER:O	4:E:290:HIS:NE2	2.38	0.57
1:T:260:LEU:HD21	1:T:321:LEU:HB3	1.87	0.57
1:U:350:PRO:HG2	1:U:441:PRO:HG3	1.85	0.57
1:V:52:PHE:HA	1:V:62:PRO:HA	1.87	0.57
1:1:350:PRO:HG2	1:1:441:PRO:HG3	1.85	0.57
1:U:260:LEU:HD21	1:U:321:LEU:HB3	1.87	0.57
1:V:213:ILE:HG21	1:V:276:LEU:HD22	1.85	0.57
1:2:355:SER:HB2	3:N:713:HIS:CE1	2.40	0.57
7:L:1656:ARG:NH1	1:Z:434:GLU:OE1	2.38	0.57
1:R:350:PRO:HG2	1:R:441:PRO:HG3	1.85	0.57
1:Z:350:PRO:HG2	1:Z:441:PRO:HG3	1.85	0.57
4:E:231:ARG:NH1	3:F:284:SER:OG	2.38	0.56
6:I:118:SER:OG	6:I:119:ASP:N	2.37	0.56
1:2:260:LEU:HD21	1:2:321:LEU:HB3	1.87	0.56
1:U:184:GLN:O	1:U:188:SER:OG	2.23	0.56
1:Z:184:GLN:O	1:Z:188:SER:OG	2.23	0.56
1:1:45:THR:OG1	4:M:563:THR:OG1	2.23	0.56
4:E:240:GLY:O	4:E:241:ARG:NE	2.37	0.56
4:M:865:TYR:H	4:M:868:ARG:HD2	1.69	0.56
1:Q:64:ALA:O	1:Q:90:ASN:ND2	2.37	0.56
1:T:52:PHE:HA	1:T:62:PRO:HA	1.87	0.56
1:W:64:ALA:O	1:W:90:ASN:ND2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:260:LEU:HD21	1:W:321:LEU:HB3	1.87	0.56
1:1:184:GLN:O	1:1:188:SER:OG	2.23	0.56
1:1:260:LEU:HD21	1:1:321:LEU:HB3	1.87	0.56
4:C:440:PRO:HG2	4:C:443:LEU:HB2	1.87	0.56
4:M:446:MET:HE3	4:M:484:TYR:HE2	1.70	0.56
1:R:260:LEU:HD21	1:R:321:LEU:HB3	1.87	0.56
1:W:341:ARG:NH1	1:W:342:GLU:OE1	2.38	0.56
1:X:226:SER:OG	1:X:227:GLN:NE2	2.39	0.56
1:R:226:SER:OG	1:R:227:GLN:NE2	2.39	0.56
1:T:226:SER:OG	1:T:227:GLN:NE2	2.39	0.56
1:Z:226:SER:OG	1:Z:227:GLN:NE2	2.39	0.56
1:2:52:PHE:HA	1:2:62:PRO:HA	1.87	0.56
1:R:184:GLN:O	1:R:188:SER:OG	2.23	0.56
1:U:226:SER:OG	1:U:227:GLN:NE2	2.39	0.56
1:X:52:PHE:HA	1:X:62:PRO:HA	1.87	0.56
2:e:219:VAL:HG11	2:e:309:ILE:HG22	1.88	0.56
3:H:455:LYS:HE2	3:H:459:LEU:HA	1.88	0.56
4:M:638:TYR:OH	4:M:726:HIS:NE2	2.29	0.56
1:R:341:ARG:NH1	1:R:342:GLU:OE1	2.38	0.56
1:S:184:GLN:O	1:S:188:SER:OG	2.23	0.56
1:S:226:SER:OG	1:S:227:GLN:NE2	2.39	0.56
1:2:226:SER:OG	1:2:227:GLN:NE2	2.39	0.56
1:S:52:PHE:HA	1:S:62:PRO:HA	1.87	0.56
1:Y:226:SER:OG	1:Y:227:GLN:NE2	2.39	0.56
1:2:250:ASN:HB3	1:2:256:LEU:HB2	1.88	0.56
1:U:52:PHE:HA	1:U:62:PRO:HA	1.87	0.56
1:X:260:LEU:HD21	1:X:321:LEU:HB3	1.87	0.56
3:a:58:ILE:HD11	3:a:98:LEU:HB2	1.88	0.56
5:K:653:LYS:HG2	1:Y:350:PRO:HA	1.87	0.56
1:W:56:ASP:HB3	1:X:296:ARG:CG	2.36	0.56
1:Z:52:PHE:HA	1:Z:62:PRO:HA	1.87	0.56
1:2:355:SER:HB2	3:N:713:HIS:NE2	2.20	0.55
1:Q:184:GLN:O	1:Q:188:SER:OG	2.23	0.55
1:W:250:ASN:HB3	1:W:256:LEU:HB2	1.89	0.55
1:Y:250:ASN:HB3	1:Y:256:LEU:HB2	1.88	0.55
1:Y:260:LEU:HD21	1:Y:321:LEU:HB3	1.87	0.55
1:1:64:ALA:O	1:1:90:ASN:ND2	2.37	0.55
1:1:226:SER:OG	1:1:227:GLN:NE2	2.39	0.55
1:Q:52:PHE:HA	1:Q:62:PRO:HA	1.87	0.55
1:Q:250:ASN:HB3	1:Q:256:LEU:HB2	1.88	0.55
1:Y:52:PHE:HA	1:Y:62:PRO:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:161:LEU:HG	4:G:174:LEU:HD22	1.88	0.55
4:M:555:LEU:HD13	4:M:575:ILE:HD11	1.87	0.55
1:T:64:ALA:O	1:T:90:ASN:ND2	2.37	0.55
1:V:260:LEU:HD21	1:V:321:LEU:HB3	1.87	0.55
1:Q:260:LEU:HD21	1:Q:321:LEU:HB3	1.87	0.55
1:V:117:ASP:OD1	1:V:117:ASP:N	2.39	0.55
1:W:226:SER:OG	1:W:227:GLN:NE2	2.39	0.55
2:e:153:MET:HE1	2:e:317:ILE:HD11	1.89	0.55
1:V:250:ASN:HB3	1:V:256:LEU:HB2	1.89	0.55
5:I:448:SER:OG	5:I:449:GLY:N	2.39	0.55
4:M:577:LEU:HD13	4:M:611:SER:HB3	1.88	0.55
1:T:117:ASP:OD1	1:T:117:ASP:N	2.39	0.55
1:V:64:ALA:O	1:V:90:ASN:ND2	2.37	0.55
1:V:226:SER:OG	1:V:227:GLN:NE2	2.39	0.55
1:W:52:PHE:HA	1:W:62:PRO:HA	1.87	0.55
1:X:250:ASN:HB3	1:X:256:LEU:HB2	1.89	0.55
1:1:250:ASN:HB3	1:1:256:LEU:HB2	1.88	0.55
6:J:566:MET:HA	6:J:569:LEU:HD12	1.87	0.55
1:T:250:ASN:HB3	1:T:256:LEU:HB2	1.89	0.55
1:U:117:ASP:N	1:U:117:ASP:OD1	2.39	0.55
1:X:117:ASP:OD1	1:X:117:ASP:N	2.39	0.55
1:Z:117:ASP:OD1	1:Z:117:ASP:N	2.39	0.55
1:Z:260:LEU:HD21	1:Z:321:LEU:HB3	1.87	0.55
1:1:52:PHE:HA	1:1:62:PRO:HA	1.87	0.55
2:e:332:PRO:HA	7:c:5:THR:HG21	1.88	0.55
8:m:25:MET:HG3	8:m:41:MET:HE1	1.89	0.55
3:N:453:THR:OG1	3:N:455:LYS:NZ	2.40	0.55
8:i:66:GLU:HA	8:i:69:LYS:HG2	1.88	0.55
1:X:341:ARG:NH1	1:X:342:GLU:OE1	2.38	0.55
1:Z:341:ARG:NH1	1:Z:342:GLU:OE1	2.38	0.55
1:Q:226:SER:OG	1:Q:227:GLN:NE2	2.39	0.55
3:F:554:SER:O	3:F:554:SER:OG	2.24	0.54
3:F:799:GLU:HG2	3:F:836:PHE:CZ	2.43	0.54
3:H:589:ALA:HA	3:H:592:LEU:HG	1.90	0.54
1:Q:117:ASP:OD1	1:Q:117:ASP:N	2.39	0.54
1:Y:341:ARG:NH1	1:Y:342:GLU:OE1	2.38	0.54
4:C:160:MET:HE1	4:C:351:LEU:HD22	1.88	0.54
4:M:855:VAL:HA	4:M:858:ARG:HG2	1.88	0.54
1:R:52:PHE:HA	1:R:62:PRO:HA	1.87	0.54
1:S:250:ASN:HB3	1:S:256:LEU:HB2	1.88	0.54
1:Y:117:ASP:OD1	1:Y:117:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:662:ARG:HB3	3:N:764:LEU:HD21	1.89	0.54
3:N:801:GLN:OE1	3:N:802:ARG:NH2	2.40	0.54
3:F:799:GLU:HG2	3:F:836:PHE:HZ	1.72	0.54
4:M:445:LYS:HE3	4:M:446:MET:HE1	1.90	0.54
1:Z:250:ASN:HB3	1:Z:256:LEU:HB2	1.88	0.54
4:C:839:ARG:HG3	4:C:871:ARG:HH22	1.73	0.54
4:M:703:GLU:HG3	4:M:707:HIS:CE1	2.43	0.54
1:2:341:ARG:NH1	1:2:342:GLU:OE1	2.38	0.54
3:H:723:THR:HA	3:H:727:LEU:HG	1.89	0.54
1:U:250:ASN:HB3	1:U:256:LEU:HB2	1.88	0.54
5:K:107:LEU:HD11	5:K:126:LEU:HD21	1.90	0.54
3:N:581:LEU:HD11	3:N:597:LEU:HD12	1.90	0.53
8:d:60:LEU:HA	8:d:63:VAL:HG22	1.90	0.53
4:E:297:ARG:HE	7:c:138:HIS:HB3	1.74	0.53
4:C:658:VAL:HG23	4:C:765:PHE:HD1	1.73	0.53
1:S:64:ALA:O	1:S:90:ASN:ND2	2.37	0.53
8:d:28:LEU:HD23	8:d:31:ILE:HD11	1.90	0.53
4:G:353:GLY:HA2	4:G:356:LEU:HD12	1.91	0.53
4:G:578:MET:H	4:G:615:ALA:HB1	1.72	0.53
1:2:248:TYR:CE1	3:N:727:LEU:HD21	2.43	0.53
2:e:294:TYR:HD2	2:e:325:MET:HG2	1.73	0.53
8:i:42:GLU:HG3	3:h:19:ARG:HD3	1.90	0.53
1:Q:110:GLN:HA	1:Q:113:LYS:HE3	1.91	0.53
1:S:341:ARG:NH1	1:S:342:GLU:OE1	2.38	0.53
1:2:64:ALA:O	1:2:90:ASN:ND2	2.37	0.53
4:E:663:LYS:NZ	1:S:200:ASP:OD1	2.39	0.53
4:G:160:MET:HG3	4:G:284:GLU:HB2	1.89	0.53
5:I:492:LEU:HD11	5:I:590:CYS:HB3	1.89	0.53
1:R:250:ASN:HB3	1:R:256:LEU:HB2	1.88	0.53
1:1:110:GLN:HA	1:1:113:LYS:HE3	1.91	0.53
2:e:188:TYR:HA	2:e:191:LYS:HD2	1.90	0.53
4:G:153:SER:OG	4:G:157:LYS:NZ	2.40	0.53
4:M:233:VAL:HG12	4:M:248:VAL:HA	1.91	0.53
1:S:117:ASP:OD1	1:S:117:ASP:N	2.39	0.53
1:Y:105:ALA:O	1:Y:109:SER:OG	2.27	0.53
4:E:734:LEU:HB3	4:E:735:LYS:HZ2	1.73	0.53
7:L:1656:ARG:NH2	1:Z:443:TYR:OH	2.42	0.53
7:L:1663:HIS:CG	1:Z:262:PRO:HA	2.43	0.53
1:R:117:ASP:N	1:R:117:ASP:OD1	2.39	0.53
1:U:105:ALA:O	1:U:109:SER:OG	2.27	0.53
1:Z:110:GLN:HA	1:Z:113:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:ASP:OD1	1:1:117:ASP:N	2.40	0.53
1:2:110:GLN:HA	1:2:113:LYS:HE3	1.91	0.53
1:S:110:GLN:HA	1:S:113:LYS:HE3	1.91	0.53
1:X:64:ALA:O	1:X:90:ASN:ND2	2.37	0.53
1:R:110:GLN:HA	1:R:113:LYS:HE3	1.91	0.52
1:U:341:ARG:NH1	1:U:342:GLU:OE1	2.38	0.52
1:W:105:ALA:O	1:W:109:SER:OG	2.27	0.52
1:1:341:ARG:NH1	1:1:342:GLU:OE1	2.38	0.52
1:2:105:ALA:O	1:2:109:SER:OG	2.27	0.52
4:C:442:PHE:HB2	4:C:484:TYR:OH	2.09	0.52
1:T:105:ALA:O	1:T:109:SER:OG	2.27	0.52
1:W:117:ASP:N	1:W:117:ASP:OD1	2.40	0.52
4:C:492:PHE:O	4:C:496:SER:OG	2.27	0.52
3:D:304:ILE:HG12	3:D:332:LEU:HD13	1.91	0.52
1:V:110:GLN:HA	1:V:113:LYS:HE3	1.91	0.52
1:1:105:ALA:O	1:1:109:SER:OG	2.27	0.52
5:I:548:ILE:HD12	5:I:557:ILE:HG23	1.92	0.52
1:Q:341:ARG:NH1	1:Q:342:GLU:OE1	2.38	0.52
1:V:105:ALA:O	1:V:109:SER:OG	2.27	0.52
1:Z:64:ALA:O	1:Z:90:ASN:ND2	2.37	0.52
1:1:45:THR:HG1	4:M:563:THR:HG1	1.58	0.52
3:D:643:HIS:NE2	3:D:645:ASP:OD1	2.41	0.52
1:X:110:GLN:HA	1:X:113:LYS:HE3	1.91	0.52
1:2:117:ASP:N	1:2:117:ASP:OD1	2.39	0.52
1:2:337:LEU:HD23	3:N:875:PHE:CZ	2.45	0.52
1:T:341:ARG:NH1	1:T:342:GLU:OE1	2.38	0.52
1:Y:64:ALA:O	1:Y:90:ASN:ND2	2.37	0.52
1:Q:313:THR:OG1	1:Q:314:ASN:N	2.43	0.52
1:Z:105:ALA:O	1:Z:109:SER:OG	2.27	0.52
3:a:70:ASP:HA	3:a:73:LEU:HG	1.91	0.52
7:L:597:VAL:HA	7:L:600:LYS:HE2	1.92	0.52
7:L:1643:THR:HG21	7:L:1743:LEU:HD21	1.91	0.52
1:S:105:ALA:O	1:S:109:SER:OG	2.27	0.52
1:U:313:THR:OG1	1:U:314:ASN:N	2.43	0.52
2:e:209:VAL:HA	2:e:212:ILE:HG22	1.92	0.52
3:H:829:GLU:HA	3:H:832:ARG:HB2	1.92	0.52
7:L:498:GLY:HA3	7:L:551:GLU:HB2	1.91	0.52
1:Q:105:ALA:O	1:Q:109:SER:OG	2.27	0.52
1:R:105:ALA:O	1:R:109:SER:OG	2.27	0.52
1:Y:313:THR:OG1	1:Y:314:ASN:N	2.43	0.52
2:e:309:ILE:HD11	2:e:335:ARG:HH12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:356:VAL:HG13	7:L:400:VAL:HG11	1.91	0.52
1:V:341:ARG:NH1	1:V:342:GLU:OE1	2.38	0.52
1:Y:110:GLN:HA	1:Y:113:LYS:HE3	1.91	0.52
4:C:161:LEU:HG	4:C:284:GLU:HG3	1.91	0.51
4:M:164:LYS:HD2	4:M:405:SER:H	1.75	0.51
1:V:383:SER:O	1:V:386:SER:OG	2.28	0.51
7:c:70:ILE:HD11	7:c:111:LEU:HB3	1.92	0.51
1:Q:383:SER:O	1:Q:386:SER:OG	2.28	0.51
1:Z:313:THR:OG1	1:Z:314:ASN:N	2.43	0.51
1:2:313:THR:OG1	1:2:314:ASN:N	2.43	0.51
2:e:297:THR:HG21	2:e:317:ILE:HD13	1.93	0.51
3:F:455:LYS:HA	3:F:459:LEU:HB2	1.92	0.51
1:Q:336:SER:OG	1:Q:339:ARG:NH1	2.44	0.51
1:W:336:SER:OG	1:W:339:ARG:NH1	2.44	0.51
1:X:105:ALA:O	1:X:109:SER:OG	2.27	0.51
1:1:313:THR:OG1	1:1:314:ASN:N	2.43	0.51
3:a:88:LYS:HZ2	8:b:52:GLU:HA	1.75	0.51
7:L:602:ILE:HD13	7:L:605:LEU:HD12	1.93	0.51
1:T:110:GLN:HA	1:T:113:LYS:HE3	1.91	0.51
1:U:110:GLN:HA	1:U:113:LYS:HE3	1.91	0.51
1:V:313:THR:OG1	1:V:314:ASN:N	2.43	0.51
1:X:313:THR:OG1	1:X:314:ASN:N	2.43	0.51
3:D:869:SER:HB3	3:D:873:LEU:HD23	1.93	0.51
6:J:210:PRO:N	6:J:214:SER:HG	2.09	0.51
4:C:522:MET:HB3	1:Q:248:TYR:CE1	2.46	0.51
1:S:383:SER:O	1:S:386:SER:OG	2.28	0.51
1:X:336:SER:OG	1:X:339:ARG:NH1	2.44	0.51
2:e:304:THR:HG23	2:e:335:ARG:HD3	1.92	0.51
3:D:549:LEU:HB3	3:D:555:LEU:HG	1.93	0.51
5:I:184:TYR:HD2	5:I:315:LYS:HB3	1.76	0.51
1:V:197:GLN:HA	1:V:265:ARG:HH22	1.76	0.51
1:V:336:SER:OG	1:V:339:ARG:NH1	2.44	0.51
1:W:197:GLN:HA	1:W:265:ARG:HH22	1.76	0.51
1:Z:336:SER:OG	1:Z:339:ARG:NH1	2.44	0.51
1:Z:383:SER:O	1:Z:386:SER:OG	2.28	0.51
2:e:68:LYS:HZ1	2:e:78:ASN:H	1.59	0.51
4:E:380:THR:HB	4:E:477:TYR:HE2	1.76	0.51
4:G:685:ARG:HG2	1:U:353:PRO:HG2	1.93	0.51
1:S:197:GLN:HA	1:S:265:ARG:HH22	1.76	0.51
1:W:110:GLN:HA	1:W:113:LYS:HE3	1.91	0.51
1:W:383:SER:O	1:W:386:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:197:GLN:HA	1:X:265:ARG:HH22	1.76	0.51
1:Y:197:GLN:HA	1:Y:265:ARG:HH22	1.76	0.51
1:2:47:ARG:HH11	3:N:575:ARG:HH21	1.59	0.51
4:C:350:CYS:HG	4:C:355:THR:HG1	1.58	0.51
6:J:478:GLU:O	6:J:482:HIS:HB2	2.10	0.51
1:R:313:THR:OG1	1:R:314:ASN:N	2.43	0.51
1:2:336:SER:OG	1:2:339:ARG:NH1	2.44	0.51
4:E:581:ASP:HA	4:E:643:ARG:HH12	1.77	0.51
4:M:530:HIS:CD2	4:M:562:SER:HB3	2.45	0.51
3:N:621:LEU:HD11	3:N:640:LEU:HD13	1.92	0.51
8:k:21:VAL:HA	8:k:24:THR:HG22	1.93	0.51
8:m:39:LEU:HD13	8:m:44:LEU:HB2	1.93	0.51
2:e:157:ASP:OD2	2:e:157:ASP:N	2.43	0.50
4:E:428:TRP:CD1	4:E:455:LYS:HZ1	2.29	0.50
1:S:336:SER:OG	1:S:339:ARG:NH1	2.44	0.50
1:T:336:SER:OG	1:T:339:ARG:NH1	2.44	0.50
1:Z:197:GLN:HA	1:Z:265:ARG:HH22	1.76	0.50
8:b:61:SER:HA	8:b:64:ILE:HG22	1.93	0.50
2:e:153:MET:HE3	2:e:313:MET:CE	2.41	0.50
3:D:838:GLU:OE1	3:D:842:LYS:NZ	2.40	0.50
3:F:757:THR:O	3:F:761:ARG:NE	2.40	0.50
1:1:336:SER:OG	1:1:339:ARG:NH1	2.44	0.50
3:D:331:GLU:HG3	3:D:418:ILE:HD11	1.93	0.50
3:D:759:ILE:HG23	3:D:764:LEU:HD23	1.94	0.50
4:G:662:ASN:HD21	4:G:683:ARG:HH12	1.57	0.50
3:N:655:GLU:O	3:N:658:SER:OG	2.28	0.50
3:N:660:TYR:HA	3:N:663:VAL:HG12	1.93	0.50
1:R:336:SER:OG	1:R:339:ARG:NH1	2.44	0.50
1:2:197:GLN:HA	1:2:265:ARG:HH22	1.76	0.50
5:K:4:GLU:HG2	7:L:320:PHE:CE1	2.47	0.50
5:K:499:GLN:O	5:K:516:ARG:NH1	2.44	0.50
1:R:383:SER:O	1:R:386:SER:OG	2.28	0.50
1:U:336:SER:OG	1:U:339:ARG:NH1	2.44	0.50
1:Y:383:SER:O	1:Y:386:SER:OG	2.28	0.50
4:E:623:LYS:O	4:E:627:SER:N	2.45	0.50
4:G:522:MET:HB2	1:U:248:TYR:CE1	2.46	0.50
1:T:383:SER:O	1:T:386:SER:OG	2.28	0.50
1:1:197:GLN:HA	1:1:265:ARG:HH22	1.76	0.50
1:2:383:SER:O	1:2:386:SER:OG	2.28	0.50
3:F:878:PHE:HD2	1:T:338:GLN:HE22	1.59	0.50
4:M:157:LYS:HA	4:M:284:GLU:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:6:ILE:HG12	1:S:63:ARG:HB3	1.94	0.50
1:T:197:GLN:HA	1:T:265:ARG:HH22	1.76	0.50
1:1:383:SER:O	1:1:386:SER:OG	2.28	0.50
4:C:644:HIS:CE1	4:C:738:MET:HB2	2.47	0.50
1:W:313:THR:OG1	1:W:314:ASN:N	2.43	0.50
1:X:383:SER:O	1:X:386:SER:OG	2.28	0.50
1:Y:336:SER:OG	1:Y:339:ARG:NH1	2.44	0.50
3:N:737:LYS:HA	3:N:740:GLN:HE21	1.77	0.50
1:R:6:ILE:HG12	1:R:63:ARG:HB3	1.94	0.50
1:U:64:ALA:O	1:U:90:ASN:ND2	2.37	0.50
1:W:6:ILE:HG12	1:W:63:ARG:HB3	1.94	0.50
1:X:6:ILE:HG12	1:X:63:ARG:HB3	1.94	0.50
1:Q:6:ILE:HG12	1:Q:63:ARG:HB3	1.94	0.50
1:R:64:ALA:O	1:R:90:ASN:ND2	2.37	0.50
1:U:197:GLN:HA	1:U:265:ARG:HH22	1.76	0.50
1:Q:197:GLN:HA	1:Q:265:ARG:HH22	1.76	0.49
1:S:313:THR:OG1	1:S:314:ASN:N	2.43	0.49
1:V:6:ILE:HG12	1:V:63:ARG:HB3	1.94	0.49
2:e:142:LEU:HD11	2:e:296:ASN:HD21	1.77	0.49
4:M:538:GLU:HG2	4:M:550:ARG:CZ	2.42	0.49
1:X:112:GLU:O	1:X:115:HIS:ND1	2.45	0.49
4:G:514:ARG:HA	4:G:517:LYS:HG2	1.92	0.49
7:L:601:THR:HG23	7:L:1698:LEU:HD13	1.94	0.49
1:R:112:GLU:O	1:R:115:HIS:ND1	2.45	0.49
1:T:6:ILE:HG12	1:T:63:ARG:HB3	1.94	0.49
1:2:6:ILE:HG12	1:2:63:ARG:HB3	1.94	0.49
1:R:197:GLN:HA	1:R:265:ARG:HH22	1.76	0.49
3:F:274:CYS:SG	3:F:276:LYS:NZ	2.85	0.49
3:D:855:GLN:HB3	3:D:890:GLU:HG3	1.95	0.49
4:E:388:PHE:HD2	4:E:475:ILE:HD12	1.77	0.49
5:I:118:SER:OG	5:I:119:ILE:N	2.45	0.49
3:N:572:ASP:HA	3:N:575:ARG:NH1	2.28	0.49
1:W:56:ASP:HB3	1:X:296:ARG:HG3	1.93	0.49
4:E:320:SER:OG	4:E:321:LEU:N	2.46	0.49
7:L:1669:VAL:HA	7:L:1672:ILE:HG22	1.95	0.49
1:Y:112:GLU:O	1:Y:115:HIS:ND1	2.45	0.49
1:U:383:SER:O	1:U:386:SER:OG	2.28	0.49
6:J:313:VAL:O	6:J:316:GLN:HG2	2.13	0.49
5:K:470:ALA:O	5:K:473:GLU:HG2	2.12	0.49
1:V:112:GLU:O	1:V:115:HIS:ND1	2.45	0.49
1:1:6:ILE:HG12	1:1:63:ARG:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:112:GLU:O	1:1:115:HIS:ND1	2.46	0.48
4:C:221:LEU:HD11	4:C:260:VAL:HG22	1.95	0.48
3:D:581:LEU:HD12	3:D:584:GLU:HB3	1.93	0.48
4:M:860:ASP:HB3	4:M:866:THR:HB	1.95	0.48
3:N:270:ASN:HD21	3:N:273:ASN:HB2	1.78	0.48
1:U:6:ILE:HG12	1:U:63:ARG:HB3	1.94	0.48
1:Y:158:ASN:OD1	1:Y:158:ASN:N	2.46	0.48
4:E:222:LEU:HB3	3:F:365:ARG:HH22	1.78	0.48
4:E:475:ILE:HD13	4:E:484:TYR:HB3	1.94	0.48
8:k:24:THR:HA	8:k:27:VAL:HG22	1.95	0.48
2:e:301:GLY:O	2:e:304:THR:OG1	2.29	0.48
3:F:589:ALA:HA	3:F:592:LEU:HD13	1.93	0.48
4:G:155:GLU:HG3	4:G:158:ARG:HH21	1.78	0.48
4:G:525:GLY:HA3	1:U:251:ASN:HD22	1.77	0.48
3:H:388:CYS:HB3	3:H:396:LEU:HD11	1.95	0.48
6:J:902:MET:HA	6:J:906:LEU:HD23	1.94	0.48
1:T:313:THR:OG1	1:T:314:ASN:N	2.43	0.48
4:G:445:LYS:HE2	4:G:446:MET:HE1	1.94	0.48
1:W:112:GLU:O	1:W:115:HIS:ND1	2.45	0.48
3:N:456:THR:OG1	3:N:457:ASP:N	2.45	0.48
1:Q:158:ASN:N	1:Q:158:ASN:OD1	2.46	0.48
1:U:112:GLU:O	1:U:115:HIS:ND1	2.46	0.48
4:C:394:TRP:HB2	4:C:400:ILE:HD12	1.95	0.48
4:C:543:VAL:HA	4:C:546:ILE:HD12	1.93	0.48
3:F:669:ARG:HG2	3:F:672:ARG:HH22	1.78	0.48
4:G:298:THR:HA	4:G:301:LYS:HD3	1.94	0.48
1:Z:112:GLU:O	1:Z:115:HIS:ND1	2.46	0.48
7:c:131:ASP:OD1	7:c:131:ASP:N	2.47	0.48
4:E:205:ILE:HG23	4:E:207:THR:H	1.78	0.48
1:2:249:MET:HE1	3:N:671:LYS:HD3	1.95	0.48
4:C:738:MET:HA	4:C:741:ASN:HD21	1.78	0.48
1:Z:6:ILE:HG12	1:Z:63:ARG:HB3	1.94	0.48
3:D:721:TYR:OH	3:D:872:SER:OG	2.26	0.48
3:N:448:VAL:HG22	3:N:484:LEU:HD12	1.96	0.48
1:U:158:ASN:OD1	1:U:158:ASN:N	2.46	0.48
1:W:158:ASN:OD1	1:W:158:ASN:N	2.46	0.48
1:Y:6:ILE:HG12	1:Y:63:ARG:HB3	1.94	0.48
1:Z:158:ASN:OD1	1:Z:158:ASN:N	2.46	0.48
8:b:42:GLU:O	8:b:45:SER:OG	2.28	0.48
4:C:528:PHE:HB3	4:C:649:LYS:HE2	1.95	0.48
3:N:308:THR:O	3:N:312:SER:OG	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:158:ASN:N	1:1:158:ASN:OD1	2.46	0.47
4:E:304:LEU:HG	3:F:369:VAL:HG22	1.96	0.47
4:M:677:ALA:HA	4:M:680:PHE:CD2	2.50	0.47
1:S:158:ASN:N	1:S:158:ASN:OD1	2.46	0.47
3:h:15:ASN:O	3:h:19:ARG:HG2	2.14	0.47
1:V:158:ASN:N	1:V:158:ASN:OD1	2.46	0.47
3:N:578:MET:HE1	3:N:671:LYS:HG3	1.96	0.47
2:e:142:LEU:HD13	2:e:298:VAL:HG21	1.96	0.47
3:D:308:THR:HG21	3:D:332:LEU:HD22	1.97	0.47
4:E:242:GLN:HB2	4:E:343:THR:HB	1.96	0.47
3:H:605:VAL:HG11	3:H:618:LEU:HD11	1.96	0.47
1:X:158:ASN:N	1:X:158:ASN:OD1	2.46	0.47
1:2:158:ASN:OD1	1:2:158:ASN:N	2.46	0.47
1:T:112:GLU:O	1:T:115:HIS:ND1	2.45	0.47
1:2:291:LEU:HD21	4:M:560:ARG:HH12	1.79	0.47
4:C:868:ARG:HG3	4:C:869:LEU:HD23	1.96	0.47
4:G:395:ILE:HD11	4:G:450:ILE:HG23	1.96	0.47
3:H:391:ARG:HB2	3:H:396:LEU:HD13	1.96	0.47
5:K:497:ALA:HB2	1:Y:254:ILE:HD11	1.97	0.47
7:L:569:TRP:NE1	7:L:600:LYS:HD2	2.30	0.47
3:N:376:ILE:HA	3:N:379:LYS:HG2	1.97	0.47
3:N:691:LEU:HD11	3:N:797:LEU:HG	1.96	0.47
1:R:158:ASN:OD1	1:R:158:ASN:N	2.46	0.47
4:E:238:LEU:HD21	4:E:241:ARG:HB2	1.97	0.47
4:E:440:PRO:HD2	4:E:443:LEU:HD12	1.96	0.47
3:F:494:HIS:CD2	3:F:500:GLN:HA	2.49	0.47
3:N:535:ASP:N	3:N:535:ASP:OD1	2.45	0.47
1:Q:112:GLU:O	1:Q:115:HIS:ND1	2.45	0.47
1:Z:189:LEU:HD12	1:Z:189:LEU:HA	1.78	0.47
3:F:297:LEU:HD22	3:F:371:THR:HG22	1.96	0.47
7:L:1629:MET:HB2	7:L:1669:VAL:HG11	1.96	0.47
3:N:738:VAL:HG12	3:N:747:ILE:HG23	1.97	0.47
3:F:255:LEU:HD11	3:F:343:HIS:HB2	1.97	0.47
3:F:609:ASN:ND2	1:T:49:ASP:OD2	2.38	0.47
4:G:242:GLN:HG3	4:G:343:THR:HA	1.97	0.47
5:I:337:ALA:HB1	5:I:554:PHE:H	1.79	0.47
5:K:649:LEU:C	5:K:651:TYR:H	2.23	0.47
1:T:158:ASN:OD1	1:T:158:ASN:N	2.46	0.47
4:C:690:VAL:HG13	4:C:752:MET:HE1	1.98	0.46
3:F:345:GLN:HE22	7:c:150:CYS:HB2	1.80	0.46
5:K:511:ASP:HB3	5:K:603:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:333:ARG:HG2	4:E:326:PHE:HB2	1.97	0.46
4:G:314:HIS:HB2	4:G:319:LEU:HD23	1.97	0.46
3:H:616:GLU:OE1	3:H:619:ARG:NH1	2.44	0.46
5:K:380:LEU:HD22	5:K:453:LEU:HD11	1.97	0.46
7:L:1505:LEU:HD22	7:L:1604:LEU:HD22	1.96	0.46
4:M:312:GLN:HG3	3:N:364:LEU:HD12	1.97	0.46
1:U:289:THR:HG23	1:U:292:ASP:HB2	1.97	0.46
7:c:130:ARG:NH1	7:c:135:ASN:H	2.13	0.46
5:I:3:HIS:HB3	7:L:297:TRP:CH2	2.50	0.46
5:K:540:GLN:HE21	5:K:564:PHE:HA	1.80	0.46
3:N:737:LYS:HG3	3:N:750:ALA:HB1	1.98	0.46
1:T:289:THR:HG23	1:T:292:ASP:HB2	1.98	0.46
1:T:396:ASP:HB3	1:T:400:LYS:HE2	1.98	0.46
1:Z:289:THR:HG23	1:Z:292:ASP:HB2	1.98	0.46
6:J:262:ARG:HH11	6:J:301:ILE:HD12	1.79	0.46
1:S:112:GLU:O	1:S:115:HIS:ND1	2.46	0.46
1:2:47:ARG:NH1	3:N:575:ARG:HH21	2.12	0.46
1:2:112:GLU:O	1:2:115:HIS:ND1	2.45	0.46
4:G:164:LYS:HB2	4:G:174:LEU:HD21	1.97	0.46
6:J:892:HIS:HE1	1:X:355:SER:HB2	1.81	0.46
1:Q:289:THR:HG23	1:Q:292:ASP:HB2	1.97	0.46
1:Q:396:ASP:HB3	1:Q:400:LYS:HE2	1.98	0.46
1:S:289:THR:HG23	1:S:292:ASP:HB2	1.98	0.46
1:V:289:THR:HG23	1:V:292:ASP:HB2	1.98	0.46
1:W:289:THR:HG23	1:W:292:ASP:HB2	1.98	0.46
1:2:337:LEU:HD23	3:N:875:PHE:HZ	1.79	0.46
2:e:120:THR:HG21	2:e:370:VAL:HG11	1.97	0.46
4:C:180:TRP:HA	4:C:183:GLU:HG3	1.98	0.46
4:E:680:PHE:HB3	1:S:262:PRO:O	2.15	0.46
3:F:768:SER:O	3:F:768:SER:OG	2.31	0.46
5:I:164:GLY:H	5:I:169:ARG:HD2	1.79	0.46
1:R:248:TYR:HD2	1:R:249:MET:HG2	1.81	0.46
1:S:396:ASP:HB3	1:S:400:LYS:HE2	1.98	0.46
2:e:160:THR:CG2	2:e:178:LEU:HB2	2.26	0.46
3:a:20:ILE:HD11	8:b:68:ARG:HG3	1.97	0.46
4:C:160:MET:O	4:C:164:LYS:HG2	2.15	0.46
3:D:832:ARG:HA	3:D:835:GLU:HG3	1.98	0.46
5:K:483:LEU:HD12	5:K:483:LEU:HA	1.81	0.46
4:M:558:ALA:O	4:M:562:SER:OG	2.26	0.46
1:2:248:TYR:HD2	1:2:249:MET:HG2	1.81	0.46
1:2:396:ASP:HB3	1:2:400:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:193:LEU:HD23	2:e:193:LEU:HA	1.82	0.46
3:D:684:HIS:CE1	3:D:705:HIS:HA	2.51	0.46
4:E:244:ARG:HD2	4:E:271:SER:HB3	1.97	0.46
4:E:713:LEU:HD22	4:E:722:VAL:HG13	1.97	0.46
1:W:377:MET:HE3	1:W:377:MET:HB2	1.89	0.46
3:F:377:ARG:HH12	7:c:146:SER:H	1.64	0.46
7:L:1780:PHE:HB2	7:L:1803:ASN:HD22	1.81	0.46
7:c:130:ARG:HD3	7:c:156:PHE:CZ	2.51	0.46
2:e:54:VAL:HG22	2:e:88:HIS:CD2	2.51	0.46
5:I:488:VAL:HG21	5:I:587:LEU:HD22	1.97	0.46
4:M:467:VAL:HG21	4:M:498:VAL:HG11	1.98	0.46
1:Q:248:TYR:HD2	1:Q:249:MET:HG2	1.81	0.46
1:T:248:TYR:HD2	1:T:249:MET:HG2	1.81	0.46
8:m:64:ILE:HG23	6:l:26:VAL:HG11	1.98	0.46
3:F:268:MET:HE2	3:F:272:GLU:HB2	1.97	0.45
3:F:439:LEU:HD22	3:F:464:TYR:HE1	1.82	0.45
4:G:168:LYS:HE3	4:G:403:PRO:HA	1.97	0.45
5:I:37:SER:O	5:I:40:SER:OG	2.33	0.45
5:K:15:SER:OG	7:L:391:GLU:OE2	2.32	0.45
5:K:301:LYS:NZ	5:K:336:VAL:HA	2.32	0.45
3:N:490:ILE:HD13	3:N:541:THR:HG22	1.97	0.45
4:E:442:PHE:CE2	4:E:484:TYR:HE2	2.33	0.45
3:H:659:HIS:HA	3:H:662:ARG:HD3	1.97	0.45
3:H:673:MET:HE3	3:H:779:PHE:HB3	1.97	0.45
3:H:802:ARG:HE	3:H:832:ARG:HE	1.64	0.45
4:G:719:ILE:HA	4:G:722:VAL:HG22	1.99	0.45
6:J:812:VAL:HG23	6:J:813:ILE:HG12	1.98	0.45
5:K:649:LEU:CB	1:Y:341:ARG:HH21	2.29	0.45
1:X:396:ASP:HB3	1:X:400:LYS:HE2	1.98	0.45
1:Y:289:THR:HG23	1:Y:292:ASP:HB2	1.98	0.45
8:m:57:PRO:HG3	6:l:109:SER:HA	1.99	0.45
1:1:248:TYR:HD2	1:1:249:MET:HG2	1.81	0.45
7:L:1629:MET:HB3	7:L:1629:MET:HE3	1.65	0.45
1:R:396:ASP:HB3	1:R:400:LYS:HE2	1.98	0.45
1:Z:248:TYR:HD2	1:Z:249:MET:HG2	1.81	0.45
1:Z:303:VAL:HG12	1:Z:305:VAL:H	1.81	0.45
1:Z:377:MET:HE3	1:Z:377:MET:HB2	1.90	0.45
2:e:267:LEU:HD22	2:e:269:MET:HB2	1.97	0.45
4:C:770:LYS:HG3	4:C:771:LEU:HG	1.99	0.45
3:D:454:VAL:HG13	3:D:463:LYS:HG3	1.99	0.45
1:S:248:TYR:HD2	1:S:249:MET:HG2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:303:VAL:HG12	1:V:305:VAL:H	1.81	0.45
1:X:248:TYR:HD2	1:X:249:MET:HG2	1.81	0.45
1:X:303:VAL:HG12	1:X:305:VAL:H	1.81	0.45
1:1:396:ASP:HB3	1:1:400:LYS:HE2	1.98	0.45
4:E:263:ILE:HD11	4:E:325:TRP:HB2	1.98	0.45
3:F:339:LEU:H	3:F:339:LEU:HG	1.48	0.45
7:L:1641:LYS:HA	7:L:1641:LYS:HD3	1.76	0.45
1:U:248:TYR:HD2	1:U:249:MET:HG2	1.81	0.45
1:Y:303:VAL:HG12	1:Y:305:VAL:H	1.82	0.45
1:Z:396:ASP:HB3	1:Z:400:LYS:HE2	1.98	0.45
1:1:262:PRO:HG3	1:1:318:ILE:HG21	1.99	0.45
3:D:261:ILE:HD13	4:E:255:SER:HA	1.98	0.45
4:G:444:GLN:HA	4:G:447:ALA:HB2	1.99	0.45
6:J:266:THR:HA	6:J:302:VAL:HG13	1.97	0.45
1:R:289:THR:HG23	1:R:292:ASP:HB2	1.98	0.45
1:U:377:MET:HE3	1:U:377:MET:HB2	1.89	0.45
1:V:232:VAL:HG12	1:V:236:MET:HE2	1.99	0.45
1:W:56:ASP:HB3	1:X:296:ARG:HG2	1.99	0.45
1:Y:396:ASP:HB3	1:Y:400:LYS:HE2	1.98	0.45
3:a:50:ASP:OD1	3:a:50:ASP:N	2.49	0.45
4:C:557:LEU:HD13	1:R:295:ARG:HH12	1.82	0.45
4:C:632:ARG:HE	4:C:636:THR:HG23	1.82	0.45
3:F:578:MET:HE1	3:F:671:LYS:HB3	1.99	0.45
4:M:749:SER:O	4:M:753:SER:OG	2.30	0.45
8:i:21:VAL:HG12	8:i:22:ARG:HH21	1.81	0.45
1:Q:262:PRO:HG3	1:Q:318:ILE:HG21	1.99	0.45
1:W:262:PRO:HG3	1:W:318:ILE:HG21	1.99	0.45
6:l:24:ARG:NH1	6:l:32:GLU:OE2	2.48	0.45
1:1:276:LEU:HD23	1:1:276:LEU:HA	1.83	0.45
1:1:289:THR:HG23	1:1:292:ASP:HB2	1.98	0.45
1:2:291:LEU:HD13	1:2:339:ARG:HB3	1.99	0.45
3:D:377:ARG:O	3:D:380:THR:OG1	2.32	0.45
4:G:277:ILE:O	4:G:281:SER:OG	2.29	0.45
4:G:663:LYS:NZ	1:U:265:ARG:HH12	2.14	0.45
5:K:84:ILE:HA	5:K:87:ARG:HE	1.81	0.45
7:L:1792:GLN:HE21	7:L:1794:HIS:CE1	2.34	0.45
3:N:653:THR:HG23	3:N:655:GLU:H	1.82	0.45
3:N:703:GLN:HE21	3:N:847:LEU:HD23	1.81	0.45
1:R:276:LEU:HD23	1:R:276:LEU:HA	1.83	0.45
1:T:262:PRO:HG3	1:T:318:ILE:HG21	1.99	0.45
1:U:396:ASP:HB3	1:U:400:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:396:ASP:HB3	1:W:400:LYS:HE2	1.98	0.45
4:E:323:LYS:HA	4:E:326:PHE:CE1	2.51	0.45
3:H:274:CYS:SG	3:H:275:TYR:N	2.89	0.45
5:I:548:ILE:HD12	5:I:557:ILE:HD12	1.98	0.45
3:N:375:LYS:HG3	3:N:379:LYS:HE3	1.99	0.45
8:i:51:CYS:SG	3:h:92:SER:OG	2.72	0.45
1:U:189:LEU:HD12	1:U:189:LEU:HA	1.78	0.45
1:U:262:PRO:HG3	1:U:318:ILE:HG21	1.99	0.45
1:V:396:ASP:HB3	1:V:400:LYS:HE2	1.98	0.45
1:W:248:TYR:HD2	1:W:249:MET:HG2	1.81	0.45
1:Y:276:LEU:HD23	1:Y:276:LEU:HA	1.83	0.45
3:D:639:SER:HA	3:D:664:PHE:CE1	2.52	0.44
3:F:692:ARG:NH1	1:T:197:GLN:HB3	2.32	0.44
7:L:1783:VAL:HG21	7:L:1798:PHE:HD2	1.82	0.44
1:T:303:VAL:HG12	1:T:305:VAL:H	1.81	0.44
1:U:291:LEU:HD13	1:U:339:ARG:HB3	1.99	0.44
1:V:291:LEU:HD13	1:V:339:ARG:HB3	1.99	0.44
1:V:377:MET:HE3	1:V:377:MET:HB2	1.89	0.44
8:b:45:SER:HA	8:b:48:VAL:HG22	1.98	0.44
1:2:289:THR:HG23	1:2:292:ASP:HB2	1.97	0.44
1:2:303:VAL:HG12	1:2:305:VAL:H	1.81	0.44
1:2:342:GLU:HB3	4:M:550:ARG:HA	1.98	0.44
4:C:522:MET:HB3	1:Q:248:TYR:HE1	1.81	0.44
5:I:5:LEU:HD11	5:I:119:ILE:HD12	1.97	0.44
8:i:40:ASP:OD2	8:i:40:ASP:N	2.50	0.44
1:Q:291:LEU:HD13	1:Q:339:ARG:HB3	1.99	0.44
1:R:303:VAL:HG12	1:R:305:VAL:H	1.81	0.44
1:X:189:LEU:HD12	1:X:189:LEU:HA	1.78	0.44
1:X:289:THR:HG23	1:X:292:ASP:HB2	1.98	0.44
1:1:343:ARG:HG3	1:1:345:LEU:HB2	2.00	0.44
4:E:556:GLU:O	4:E:560:ARG:HG2	2.18	0.44
4:E:679:ALA:HB1	4:E:762:MET:HG3	1.99	0.44
6:J:922:ASP:HB3	6:J:925:GLN:HG2	1.98	0.44
1:S:232:VAL:HG12	1:S:236:MET:HE2	1.99	0.44
1:U:232:VAL:HG12	1:U:236:MET:HE2	1.99	0.44
1:X:262:PRO:HG3	1:X:318:ILE:HG21	1.99	0.44
1:X:377:MET:HE3	1:X:377:MET:HB2	1.89	0.44
1:Y:291:LEU:HD13	1:Y:339:ARG:HB3	1.99	0.44
4:E:296:MET:HG2	4:E:338:LEU:HD22	1.98	0.44
4:E:452:SER:HA	4:E:455:LYS:HB3	1.99	0.44
3:F:884:GLU:OE1	1:T:344:LYS:NZ	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:303:VAL:HG12	1:1:305:VAL:H	1.81	0.44
1:2:39:GLU:N	1:2:39:GLU:OE1	2.51	0.44
2:e:32:PRO:HB2	2:e:34:ILE:HG22	1.98	0.44
3:H:308:THR:O	3:H:312:SER:OG	2.32	0.44
4:M:695:TYR:HA	4:M:698:MET:HE2	1.99	0.44
1:U:39:GLU:OE1	1:U:39:GLU:N	2.51	0.44
1:V:39:GLU:N	1:V:39:GLU:OE1	2.51	0.44
1:V:262:PRO:HG3	1:V:318:ILE:HG21	1.99	0.44
1:Y:189:LEU:HA	1:Y:189:LEU:HD12	1.78	0.44
1:Y:248:TYR:HD2	1:Y:249:MET:HG2	1.81	0.44
1:Z:291:LEU:HD13	1:Z:339:ARG:HB3	1.99	0.44
1:1:109:SER:H	1:1:109:SER:HG	1.52	0.44
1:1:291:LEU:HD13	1:1:339:ARG:HB3	1.99	0.44
1:2:262:PRO:HG3	1:2:318:ILE:HG21	1.99	0.44
4:G:439:ILE:HG22	4:G:441:SER:H	1.83	0.44
3:H:730:SER:O	3:H:733:GLU:HG2	2.18	0.44
1:Q:39:GLU:N	1:Q:39:GLU:OE1	2.51	0.44
1:T:232:VAL:HG12	1:T:236:MET:HE2	1.99	0.44
1:U:276:LEU:HD23	1:U:276:LEU:HA	1.83	0.44
1:W:291:LEU:HD13	1:W:339:ARG:HB3	1.99	0.44
1:W:303:VAL:HG12	1:W:305:VAL:H	1.82	0.44
1:X:232:VAL:HG12	1:X:236:MET:HE2	1.99	0.44
1:X:291:LEU:HD13	1:X:339:ARG:HB3	1.99	0.44
1:Z:262:PRO:HG3	1:Z:318:ILE:HG21	1.99	0.44
1:Z:343:ARG:HG3	1:Z:345:LEU:HB2	2.00	0.44
7:c:173:SER:HA	7:c:176:GLN:HG3	1.99	0.44
1:1:232:VAL:HG12	1:1:236:MET:HE2	1.99	0.44
1:1:353:PRO:HB3	4:M:864:PHE:O	2.18	0.44
1:2:232:VAL:HG12	1:2:236:MET:HE2	1.99	0.44
2:e:226:GLU:HA	2:e:229:THR:HG22	1.99	0.44
2:e:293:LEU:HD12	2:e:293:LEU:HA	1.90	0.44
2:e:297:THR:HB	2:e:329:ILE:HG12	1.99	0.44
4:E:380:THR:HB	4:E:477:TYR:CE2	2.53	0.44
3:F:258:PHE:HB3	3:F:339:LEU:HD22	2.00	0.44
6:J:215:TRP:HE1	7:L:319:ALA:HB2	1.81	0.44
5:K:278:PHE:O	5:K:282:SER:OG	2.32	0.44
7:L:359:VAL:HG12	7:L:404:GLY:HA3	2.00	0.44
4:M:439:ILE:HG22	4:M:441:SER:H	1.82	0.44
1:S:39:GLU:OE1	1:S:39:GLU:N	2.51	0.44
1:S:323:ILE:HD13	1:S:323:ILE:HA	1.91	0.44
1:V:248:TYR:HD2	1:V:249:MET:HG2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:232:VAL:HG12	1:W:236:MET:HE2	1.99	0.44
3:D:677:LEU:HD21	3:D:712:VAL:HA	1.99	0.44
4:E:821:THR:HA	4:E:824:LYS:HG2	1.99	0.44
4:G:186:ALA:HB1	3:H:293:ARG:HG2	1.99	0.44
5:K:358:LYS:HA	5:K:362:LEU:HD12	1.99	0.44
4:M:358:LEU:HG	4:M:362:ARG:HE	1.82	0.44
1:Q:303:VAL:HG12	1:Q:305:VAL:H	1.81	0.44
1:U:51:PHE:HZ	1:U:240:THR:HG21	1.83	0.44
1:X:39:GLU:N	1:X:39:GLU:OE1	2.51	0.44
3:D:255:LEU:HD13	3:D:346:LEU:HD22	2.00	0.44
3:F:494:HIS:HD2	3:F:500:GLN:HA	1.82	0.44
3:F:543:LYS:HD2	3:F:543:LYS:HA	1.78	0.44
1:Q:51:PHE:HZ	1:Q:240:THR:HG21	1.83	0.44
1:Q:323:ILE:HD13	1:Q:323:ILE:HA	1.91	0.44
1:Y:39:GLU:N	1:Y:39:GLU:OE1	2.51	0.44
1:Y:343:ARG:HG3	1:Y:345:LEU:HB2	2.00	0.44
1:Y:377:MET:HE3	1:Y:377:MET:HB2	1.89	0.44
1:2:68:ASP:OD1	1:2:68:ASP:N	2.51	0.43
2:e:109:PRO:HD3	2:e:137:GLN:HB3	2.00	0.43
4:C:443:LEU:HD22	4:C:450:ILE:HD11	2.00	0.43
3:F:330:GLN:HA	3:F:333:ARG:HE	1.82	0.43
5:I:48:LEU:HD11	5:I:129:PHE:HB2	2.00	0.43
5:I:481:TYR:O	5:I:484:SER:OG	2.33	0.43
5:K:344:MET:HG2	5:K:350:LEU:HD11	2.00	0.43
3:N:247:GLU:OE2	3:N:366:ARG:NH1	2.51	0.43
1:T:39:GLU:N	1:T:39:GLU:OE1	2.51	0.43
1:T:68:ASP:OD1	1:T:68:ASP:N	2.51	0.43
1:T:291:LEU:HD13	1:T:339:ARG:HB3	1.99	0.43
8:m:67:LEU:HD22	6:l:27:ALA:HB2	1.99	0.43
3:D:717:GLN:HB3	3:D:879:ARG:HB3	2.00	0.43
5:K:540:GLN:OE1	5:K:543:GLN:NE2	2.50	0.43
4:M:395:ILE:HD11	4:M:450:ILE:HG23	2.00	0.43
1:Q:232:VAL:HG12	1:Q:236:MET:HE2	1.99	0.43
1:S:51:PHE:HZ	1:S:240:THR:HG21	1.83	0.43
1:S:262:PRO:HG3	1:S:318:ILE:HG21	1.99	0.43
1:S:291:LEU:HD13	1:S:339:ARG:HB3	1.99	0.43
1:U:303:VAL:HG12	1:U:305:VAL:H	1.81	0.43
1:W:51:PHE:HZ	1:W:240:THR:HG21	1.83	0.43
1:X:343:ARG:HG3	1:X:345:LEU:HB2	2.00	0.43
1:Y:262:PRO:HG3	1:Y:318:ILE:HG21	1.99	0.43
1:Z:39:GLU:OE1	1:Z:39:GLU:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:246:PRO:HB2	4:M:524:GLN:HG3	2.01	0.43
1:2:51:PHE:HZ	1:2:240:THR:HG21	1.83	0.43
3:F:374:PRO:HD3	7:c:148:TYR:OH	2.19	0.43
3:F:490:ILE:HG12	3:F:494:HIS:CE1	2.54	0.43
3:F:677:LEU:HA	3:F:680:ILE:HD12	2.00	0.43
1:R:262:PRO:HG3	1:R:318:ILE:HG21	1.99	0.43
1:S:303:VAL:HG12	1:S:305:VAL:H	1.82	0.43
1:X:51:PHE:HZ	1:X:240:THR:HG21	1.83	0.43
4:C:699:PHE:HB3	1:Q:333:VAL:HG21	1.99	0.43
3:D:861:PHE:HA	3:D:864:LEU:HD12	1.99	0.43
4:G:189:GLY:H	4:G:274:THR:HG21	1.82	0.43
3:H:655:GLU:O	3:H:658:SER:OG	2.32	0.43
3:N:581:LEU:HG	3:N:585:LEU:HG	1.99	0.43
1:X:118:ILE:HD12	1:X:153:LEU:HD11	2.01	0.43
2:e:68:LYS:HZ1	2:e:78:ASN:N	2.17	0.43
3:D:709:SER:HA	3:D:712:VAL:HG12	2.00	0.43
3:H:563:ARG:HD3	3:H:731:TRP:CD2	2.54	0.43
5:I:6:LEU:HD23	5:I:9:LEU:HD21	2.00	0.43
4:M:415:ARG:HD2	4:M:419:ILE:HD13	2.01	0.43
1:R:291:LEU:HD13	1:R:339:ARG:HB3	1.99	0.43
1:R:343:ARG:HG3	1:R:345:LEU:HB2	2.00	0.43
1:Y:232:VAL:HG12	1:Y:236:MET:HE2	1.99	0.43
1:1:39:GLU:N	1:1:39:GLU:OE1	2.51	0.43
5:K:203:PHE:H	5:K:260:ARG:HH12	1.66	0.43
5:K:651:TYR:CE2	1:Y:354:ALA:HB3	2.54	0.43
7:L:1594:LEU:HG	7:L:1620:PHE:HE2	1.83	0.43
1:S:118:ILE:HD12	1:S:153:LEU:HD11	2.01	0.43
1:T:118:ILE:HD12	1:T:153:LEU:HD11	2.01	0.43
1:U:118:ILE:HD12	1:U:153:LEU:HD11	2.01	0.43
1:U:343:ARG:HG3	1:U:345:LEU:HB2	2.00	0.43
1:V:118:ILE:HD12	1:V:153:LEU:HD11	2.01	0.43
1:Z:232:VAL:HG12	1:Z:236:MET:HE2	1.99	0.43
6:l:108:TYR:HA	6:l:111:LEU:HD12	2.01	0.43
3:D:333:ARG:HB3	3:D:337:ARG:HH22	1.84	0.43
3:D:543:LYS:NZ	3:D:742:GLN:OE1	2.48	0.43
3:F:538:TYR:O	3:F:542:SER:OG	2.32	0.43
4:M:637:ARG:HB2	4:M:730:LEU:HD21	2.01	0.43
1:Q:68:ASP:N	1:Q:68:ASP:OD1	2.51	0.43
1:S:343:ARG:HG3	1:S:345:LEU:HB2	2.00	0.43
1:W:39:GLU:N	1:W:39:GLU:OE1	2.51	0.43
1:W:118:ILE:HD12	1:W:153:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:189:LEU:HD12	1:1:189:LEU:HA	1.78	0.43
2:e:152:VAL:HG12	2:e:298:VAL:HB	2.00	0.43
4:C:460:VAL:H	4:C:460:VAL:HG12	1.55	0.43
3:F:341:VAL:HG11	7:c:149:ASP:HA	2.00	0.43
5:I:518:ARG:HE	5:I:616:VAL:HG12	1.83	0.43
6:J:222:HIS:O	6:J:228:ARG:NE	2.52	0.43
1:R:68:ASP:OD1	1:R:68:ASP:N	2.51	0.43
1:R:232:VAL:HG12	1:R:236:MET:HE2	1.99	0.43
1:S:112:GLU:HA	1:S:152:TYR:CZ	2.54	0.43
1:V:51:PHE:HZ	1:V:240:THR:HG21	1.83	0.43
1:V:323:ILE:HD13	1:V:323:ILE:HA	1.91	0.43
1:W:68:ASP:OD1	1:W:68:ASP:N	2.51	0.43
8:b:63:VAL:O	8:b:67:LEU:HG	2.18	0.43
1:2:112:GLU:HA	1:2:152:TYR:CZ	2.54	0.43
4:C:306:LEU:O	4:C:310:LEU:HG	2.18	0.43
3:H:722:ILE:HG22	3:H:727:LEU:HD23	2.00	0.43
7:L:1796:GLU:OE2	1:Z:338:GLN:NE2	2.52	0.43
1:Q:118:ILE:HD12	1:Q:153:LEU:HD11	2.01	0.43
1:T:51:PHE:HZ	1:T:240:THR:HG21	1.83	0.43
1:T:343:ARG:HG3	1:T:345:LEU:HB2	2.00	0.43
1:V:343:ARG:HG3	1:V:345:LEU:HB2	2.00	0.43
8:d:63:VAL:O	8:d:67:LEU:HG	2.19	0.43
7:c:130:ARG:HB2	7:c:134:LEU:HD23	2.01	0.43
1:2:343:ARG:HG3	1:2:345:LEU:HB2	2.00	0.43
2:e:110:LEU:HD23	2:e:177:ARG:HH21	1.84	0.43
1:R:39:GLU:N	1:R:39:GLU:OE1	2.51	0.43
1:W:343:ARG:HG3	1:W:345:LEU:HB2	2.00	0.43
1:Y:323:ILE:HD13	1:Y:323:ILE:HA	1.91	0.43
1:Z:118:ILE:HD12	1:Z:153:LEU:HD11	2.01	0.43
8:b:48:VAL:O	8:b:52:GLU:HG2	2.18	0.43
4:C:663:LYS:HB3	4:C:663:LYS:HE3	1.80	0.42
4:C:837:LEU:HB3	4:C:856:ILE:HG12	2.01	0.42
3:D:721:TYR:OH	3:D:872:SER:O	2.36	0.42
3:F:490:ILE:HG12	3:F:494:HIS:HE1	1.84	0.42
6:J:402:LEU:HD13	6:J:405:ARG:HG3	2.01	0.42
5:K:159:LYS:HA	5:K:159:LYS:HD3	1.80	0.42
1:T:348:PHE:HB3	1:T:349:ILE:H	1.71	0.42
1:U:68:ASP:OD1	1:U:68:ASP:N	2.51	0.42
1:U:323:ILE:HD13	1:U:323:ILE:HA	1.91	0.42
1:X:68:ASP:N	1:X:68:ASP:OD1	2.51	0.42
1:Z:51:PHE:HZ	1:Z:240:THR:HG21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:68:ASP:N	1:1:68:ASP:OD1	2.51	0.42
4:G:319:LEU:HD11	4:G:324:LEU:HB2	1.99	0.42
5:I:491:GLU:HA	5:I:494:HIS:CE1	2.54	0.42
4:M:443:LEU:HD22	4:M:450:ILE:HD11	2.00	0.42
3:N:635:TRP:CG	3:N:672:ARG:HG3	2.54	0.42
8:i:46:ILE:HG21	3:h:16:LEU:HB2	2.00	0.42
1:1:432:ILE:HD13	1:1:435:TYR:HD2	1.84	0.42
5:I:489:GLN:HB3	5:I:530:TYR:OH	2.19	0.42
4:M:261:HIS:HA	4:M:264:LEU:HD12	2.02	0.42
4:M:693:ILE:HD13	4:M:859:LEU:HD11	2.00	0.42
1:R:112:GLU:HA	1:R:152:TYR:CZ	2.54	0.42
1:R:118:ILE:HD12	1:R:153:LEU:HD11	2.01	0.42
1:W:112:GLU:HA	1:W:152:TYR:CZ	2.54	0.42
1:2:276:LEU:HD11	1:2:302:ASN:HA	2.02	0.42
2:e:286:ASP:HB2	2:e:289:ILE:HG22	2.00	0.42
4:C:302:GLU:HA	4:C:305:ILE:HD12	2.02	0.42
3:D:494:HIS:CD2	3:D:500:GLN:HA	2.54	0.42
5:I:601:LEU:HD23	5:I:601:LEU:HA	1.77	0.42
5:I:628:LYS:HD2	5:I:628:LYS:HA	1.87	0.42
5:K:651:TYR:HE2	1:Y:354:ALA:HB3	1.83	0.42
4:M:479:LEU:HG	4:M:480:LYS:HG2	2.00	0.42
4:M:623:LYS:H	4:M:626:LEU:HB2	1.85	0.42
1:Q:112:GLU:HA	1:Q:152:TYR:CZ	2.54	0.42
1:T:189:LEU:HD12	1:T:189:LEU:HA	1.78	0.42
1:1:51:PHE:HZ	1:1:240:THR:HG21	1.83	0.42
4:C:205:ILE:HD12	4:C:208:LEU:HD12	2.01	0.42
4:C:651:VAL:HG23	4:C:690:VAL:HG11	2.01	0.42
3:D:833:ILE:O	3:D:837:LYS:HG2	2.20	0.42
4:E:681:THR:O	4:E:685:ARG:HG3	2.20	0.42
4:G:579:PRO:HA	4:G:608:LEU:HG	2.01	0.42
1:T:112:GLU:HA	1:T:152:TYR:CZ	2.54	0.42
1:V:432:ILE:HD13	1:V:435:TYR:HD2	1.85	0.42
1:W:432:ILE:HD13	1:W:435:TYR:HD2	1.85	0.42
1:Y:68:ASP:OD1	1:Y:68:ASP:N	2.51	0.42
1:Z:68:ASP:OD1	1:Z:68:ASP:N	2.51	0.42
3:F:568:LEU:HD23	3:F:574:ILE:HG21	2.02	0.42
4:G:637:ARG:HD3	4:G:734:LEU:HD22	2.02	0.42
5:I:141:GLU:HA	5:I:144:LYS:HG3	2.02	0.42
1:R:51:PHE:HZ	1:R:240:THR:HG21	1.83	0.42
1:S:68:ASP:OD1	1:S:68:ASP:N	2.51	0.42
1:T:432:ILE:HD13	1:T:435:TYR:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:276:LEU:HD11	1:W:302:ASN:HA	2.02	0.42
4:C:220:ASP:HB2	4:C:233:VAL:HG12	2.02	0.42
4:G:408:MET:O	4:G:435:VAL:N	2.51	0.42
6:J:331:ILE:HD11	6:J:368:LEU:HD12	2.02	0.42
1:R:113:LYS:HG3	1:R:114:ILE:HG23	2.02	0.42
1:V:112:GLU:HA	1:V:152:TYR:CZ	2.54	0.42
1:X:112:GLU:HA	1:X:152:TYR:CZ	2.54	0.42
1:Y:51:PHE:HZ	1:Y:240:THR:HG21	1.83	0.42
1:Z:112:GLU:HA	1:Z:152:TYR:CZ	2.54	0.42
1:2:432:ILE:HD13	1:2:435:TYR:HD2	1.85	0.42
2:e:208:ILE:HD11	2:e:242:LEU:HD23	2.02	0.42
4:E:693:ILE:HG23	4:E:738:MET:HE3	2.00	0.42
4:G:167:LYS:HE2	4:G:167:LYS:HB3	1.90	0.42
5:I:54:ARG:HG3	5:I:137:MET:HE1	2.01	0.42
6:J:325:PHE:O	6:J:328:GLN:HG3	2.19	0.42
4:M:698:MET:HE2	4:M:698:MET:HB2	1.87	0.42
1:Q:343:ARG:HG3	1:Q:345:LEU:HB2	2.00	0.42
1:Q:348:PHE:HB3	1:Q:349:ILE:H	1.70	0.42
1:Q:432:ILE:HD13	1:Q:435:TYR:HD2	1.85	0.42
1:T:113:LYS:HG3	1:T:114:ILE:HG23	2.02	0.42
1:U:113:LYS:HG3	1:U:114:ILE:HG23	2.02	0.42
1:U:276:LEU:HD11	1:U:302:ASN:HA	2.02	0.42
1:U:432:ILE:HD13	1:U:435:TYR:HD2	1.85	0.42
1:2:189:LEU:HD12	1:2:189:LEU:HA	1.78	0.42
4:C:547:THR:HG21	4:C:550:ARG:CZ	2.49	0.42
3:F:480:SER:HA	3:F:483:VAL:HG22	2.02	0.42
4:G:305:ILE:O	4:G:308:SER:OG	2.38	0.42
3:N:568:LEU:HD13	3:N:667:LEU:HB3	2.01	0.42
1:Q:113:LYS:HG3	1:Q:114:ILE:HG23	2.02	0.42
1:R:276:LEU:HD11	1:R:302:ASN:HA	2.02	0.42
1:R:432:ILE:HD13	1:R:435:TYR:HD2	1.85	0.42
1:U:112:GLU:HA	1:U:152:TYR:CZ	2.54	0.42
1:1:46:ASP:OD1	1:1:46:ASP:N	2.53	0.42
1:1:118:ILE:HD12	1:1:153:LEU:HD11	2.01	0.42
3:a:39:ILE:HD11	8:b:55:ILE:HD11	2.02	0.42
3:F:744:LEU:HA	3:F:747:ILE:HD12	2.01	0.42
3:H:657:MET:O	3:H:661:LEU:HG	2.19	0.42
1:Q:276:LEU:HD23	1:Q:276:LEU:HA	1.83	0.42
1:Q:276:LEU:HD11	1:Q:302:ASN:HA	2.02	0.42
1:X:276:LEU:HD11	1:X:302:ASN:HA	2.02	0.42
2:e:34:ILE:HD12	2:e:34:ILE:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:550:ARG:CZ	1:V:342:GLU:HB3	2.50	0.41
4:G:696:TYR:O	4:G:700:GLU:HB2	2.20	0.41
3:H:549:LEU:HD23	3:H:549:LEU:HA	1.92	0.41
3:H:565:TYR:HB3	3:H:621:LEU:HD12	2.02	0.41
4:M:315:ARG:NH2	3:N:363:THR:OG1	2.52	0.41
1:Q:189:LEU:HD12	1:Q:189:LEU:HA	1.78	0.41
1:S:432:ILE:HD13	1:S:435:TYR:HD2	1.85	0.41
1:X:46:ASP:OD1	1:X:46:ASP:N	2.53	0.41
4:C:364:PHE:HA	4:C:367:THR:HG23	2.02	0.41
3:D:332:LEU:HG	3:D:336:TYR:HE2	1.84	0.41
4:E:689:PHE:HE2	4:E:751:LEU:HD13	1.85	0.41
3:F:781:GLN:HE22	3:F:854:TYR:HA	1.85	0.41
6:J:297:ARG:HG2	6:J:299:ASN:H	1.85	0.41
4:M:696:TYR:HB2	4:M:858:ARG:HD3	2.02	0.41
3:N:665:ASN:HD21	3:N:669:ARG:HE	1.68	0.41
3:N:681:ARG:HD3	3:N:685:MET:HE3	2.02	0.41
1:X:113:LYS:HG3	1:X:114:ILE:HG23	2.02	0.41
1:Z:432:ILE:HD13	1:Z:435:TYR:HD2	1.85	0.41
1:I:355:SER:HA	4:M:861:PHE:HB3	2.03	0.41
2:e:299:LEU:HD22	2:e:335:ARG:CZ	2.50	0.41
4:C:583:ILE:HA	4:C:586:LEU:HD22	2.03	0.41
4:G:663:LYS:HE3	4:G:663:LYS:HB2	1.95	0.41
3:H:338:LEU:O	3:H:342:LEU:HG	2.20	0.41
5:I:34:LEU:HD13	5:I:38:GLU:HG2	2.02	0.41
6:J:413:HIS:O	6:J:417:SER:OG	2.34	0.41
1:S:113:LYS:HG3	1:S:114:ILE:HG23	2.02	0.41
1:S:276:LEU:HD11	1:S:302:ASN:HA	2.02	0.41
1:T:361:SER:OG	1:T:362:ARG:N	2.54	0.41
1:X:361:SER:OG	1:X:362:ARG:N	2.54	0.41
1:Y:118:ILE:HD12	1:Y:153:LEU:HD11	2.01	0.41
1:Z:113:LYS:HG3	1:Z:114:ILE:HG23	2.02	0.41
4:C:176:ILE:HA	4:C:284:GLU:OE2	2.20	0.41
3:F:324:PHE:CD2	3:F:422:VAL:HG21	2.55	0.41
4:M:751:LEU:HD13	4:M:836:LEU:HD13	2.02	0.41
4:M:865:TYR:H	4:M:868:ARG:HH11	1.67	0.41
1:X:432:ILE:HD13	1:X:435:TYR:HD2	1.84	0.41
1:Y:112:GLU:HA	1:Y:152:TYR:CZ	2.54	0.41
1:Y:276:LEU:HD11	1:Y:302:ASN:HA	2.02	0.41
1:I:112:GLU:HA	1:I:152:TYR:CZ	2.54	0.41
3:D:671:LYS:HE2	1:R:248:TYR:OH	2.21	0.41
3:D:799:GLU:HG2	3:D:832:ARG:HE	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:360:HIS:CE1	4:G:442:PHE:HB3	2.55	0.41
4:G:408:MET:HE2	4:G:439:ILE:HG12	2.02	0.41
4:G:522:MET:HE3	4:G:645:MET:HE3	2.02	0.41
6:J:359:ARG:HD2	5:K:163:GLY:HA2	2.02	0.41
6:J:951:LYS:HE2	6:J:955:MET:HG2	2.01	0.41
7:L:346:LEU:HA	7:L:347:VAL:HA	1.68	0.41
7:c:148:TYR:HD1	7:c:148:TYR:HA	1.68	0.41
2:e:31:PHE:CE2	2:e:93:GLU:HB2	2.55	0.41
2:e:184:ASP:HA	2:e:187:ASP:HB2	2.02	0.41
2:e:309:ILE:HD13	2:e:309:ILE:HG21	1.90	0.41
4:C:310:LEU:HD22	4:C:327:TYR:CD2	2.56	0.41
4:E:205:ILE:HA	4:E:251:ASN:HD21	1.85	0.41
3:F:291:ALA:O	3:F:295:SER:OG	2.32	0.41
1:U:361:SER:OG	1:U:362:ARG:N	2.54	0.41
1:V:252:ASP:OD1	1:V:252:ASP:N	2.54	0.41
1:W:113:LYS:HG3	1:W:114:ILE:HG23	2.02	0.41
1:W:189:LEU:HD12	1:W:189:LEU:HA	1.78	0.41
1:W:361:SER:OG	1:W:362:ARG:N	2.54	0.41
8:m:61:SER:HB3	8:m:65:LYS:HZ3	1.85	0.41
1:1:348:PHE:HB3	1:1:349:ILE:H	1.71	0.41
1:2:118:ILE:HD12	1:2:153:LEU:HD11	2.01	0.41
2:e:31:PHE:HD1	2:e:31:PHE:HA	1.74	0.41
5:K:500:MET:HE2	5:K:500:MET:HB2	1.93	0.41
1:Y:113:LYS:HG3	1:Y:114:ILE:HG23	2.02	0.41
1:Y:432:ILE:HD13	1:Y:435:TYR:HD2	1.85	0.41
4:E:700:GLU:OE2	1:S:334:HIS:HB3	2.21	0.41
3:H:364:LEU:HB2	3:H:367:LEU:HD23	2.02	0.41
1:V:68:ASP:N	1:V:68:ASP:OD1	2.51	0.41
1:V:276:LEU:HD11	1:V:302:ASN:HA	2.02	0.41
1:W:46:ASP:OD1	1:W:46:ASP:N	2.53	0.41
1:Y:361:SER:OG	1:Y:362:ARG:N	2.54	0.41
2:e:189:LEU:HD23	2:e:189:LEU:HA	1.93	0.41
3:D:605:VAL:HG11	3:D:618:LEU:HD13	2.02	0.41
3:D:882:PHE:HB3	1:R:355:SER:OG	2.20	0.41
4:E:180:TRP:CH2	3:F:382:ALA:HB1	2.55	0.41
4:E:180:TRP:HH2	3:F:382:ALA:HB1	1.85	0.41
4:E:223:TYR:HA	3:F:365:ARG:NH1	2.35	0.41
4:E:450:ILE:HG12	4:E:488:ILE:HD13	2.02	0.41
4:G:155:GLU:O	4:G:159:LYS:HG2	2.20	0.41
4:G:187:LEU:HD12	3:H:375:LYS:HE3	2.03	0.41
4:G:261:HIS:HA	4:G:264:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:334:THR:O	4:G:338:LEU:HG	2.21	0.41
4:G:642:PHE:HA	4:G:645:MET:HE2	2.02	0.41
5:I:544:LEU:O	5:I:548:ILE:HG12	2.21	0.41
7:L:1804:PHE:CE2	1:Z:341:ARG:HB2	2.56	0.41
4:M:306:LEU:O	4:M:310:LEU:HG	2.20	0.41
4:M:532:MET:SD	4:M:649:LYS:HG3	2.61	0.41
4:M:539:LEU:HD23	4:M:539:LEU:HA	1.85	0.41
1:V:113:LYS:HG3	1:V:114:ILE:HG23	2.02	0.41
1:V:334:HIS:HE1	1:V:335:LYS:HE2	1.86	0.41
1:Y:352:GLY:HA2	1:Y:353:PRO:HD3	1.90	0.41
1:Z:276:LEU:HD11	1:Z:302:ASN:HA	2.02	0.41
8:b:35:LEU:HD23	8:b:35:LEU:HA	1.83	0.41
7:c:77:LEU:HD21	7:c:85:LYS:HB3	2.01	0.41
1:1:258:ALA:HB1	4:M:687:LEU:HD13	2.02	0.41
1:1:318:ILE:HB	1:1:380:ASN:HB3	2.03	0.41
2:e:28:ARG:CZ	2:e:94:LEU:HD22	2.50	0.41
3:H:599:GLY:HA3	1:W:342:GLU:HG3	2.03	0.41
6:J:490:ARG:HA	6:J:490:ARG:HD2	1.88	0.41
7:L:1805:ASN:HD22	1:Z:344:LYS:HD3	1.85	0.41
3:N:247:GLU:HB3	3:N:366:ARG:HH11	1.86	0.41
1:Q:236:MET:O	1:Q:239:SER:OG	2.39	0.41
1:T:236:MET:O	1:T:239:SER:OG	2.39	0.41
1:T:237:SER:O	1:T:244:ARG:NH2	2.54	0.41
1:Y:236:MET:O	1:Y:239:SER:OG	2.39	0.41
1:Z:276:LEU:HD23	1:Z:276:LEU:HA	1.83	0.41
1:1:334:HIS:HE1	1:1:335:LYS:HE2	1.86	0.40
1:2:113:LYS:HG3	1:2:114:ILE:HG23	2.02	0.40
1:2:237:SER:O	1:2:244:ARG:NH2	2.55	0.40
1:2:276:LEU:HA	1:2:276:LEU:HD23	1.83	0.40
4:C:517:LYS:HE3	4:C:706:TRP:CD1	2.56	0.40
4:C:814:LEU:HB3	4:C:815:VAL:H	1.63	0.40
4:C:855:VAL:HA	4:C:858:ARG:HG2	2.03	0.40
4:E:560:ARG:HH22	4:E:570:LYS:HD2	1.85	0.40
3:N:696:GLU:HG3	3:N:840:ILE:HG13	2.02	0.40
1:T:276:LEU:HD11	1:T:302:ASN:HA	2.02	0.40
1:V:361:SER:OG	1:V:362:ARG:N	2.54	0.40
1:W:276:LEU:HD23	1:W:276:LEU:HA	1.83	0.40
1:Z:361:SER:OG	1:Z:362:ARG:N	2.54	0.40
1:1:276:LEU:HD11	1:1:302:ASN:HA	2.02	0.40
1:2:334:HIS:HE1	1:2:335:LYS:HE2	1.86	0.40
2:e:8:LEU:HD11	2:e:28:ARG:HH22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:333:ARG:HB3	3:D:337:ARG:NH2	2.37	0.40
3:F:324:PHE:HD2	3:F:422:VAL:HG21	1.86	0.40
4:G:518:ARG:NH1	4:G:524:GLN:OE1	2.53	0.40
3:H:660:TYR:OH	3:H:751:HIS:NE2	2.28	0.40
5:I:115:PRO:HG2	5:I:116:HIS:ND1	2.36	0.40
5:I:560:ALA:HA	5:I:563:HIS:CD2	2.56	0.40
6:J:422:GLU:HG3	6:J:432:ARG:HH21	1.85	0.40
5:K:109:GLN:HA	5:K:112:LEU:HD12	2.02	0.40
4:M:203:LEU:H	4:M:232:TYR:HE1	1.70	0.40
1:R:318:ILE:HB	1:R:380:ASN:HB3	2.03	0.40
1:V:236:MET:O	1:V:239:SER:OG	2.39	0.40
1:W:323:ILE:HD13	1:W:323:ILE:HA	1.91	0.40
1:X:237:SER:O	1:X:244:ARG:NH2	2.55	0.40
1:2:377:MET:HE3	1:2:377:MET:HB2	1.89	0.40
4:E:695:TYR:HE1	1:S:249:MET:HG3	1.86	0.40
3:F:280:LYS:HD2	3:F:280:LYS:HA	1.94	0.40
3:F:836:PHE:HD1	3:F:836:PHE:HA	1.70	0.40
3:N:297:LEU:HA	3:N:300:LEU:HD12	2.04	0.40
3:N:793:TYR:HB3	3:N:797:LEU:HD12	2.03	0.40
1:V:46:ASP:OD1	1:V:46:ASP:N	2.53	0.40
1:V:237:SER:O	1:V:244:ARG:NH2	2.55	0.40
1:X:318:ILE:HB	1:X:380:ASN:HB3	2.03	0.40
1:X:334:HIS:HE1	1:X:335:LYS:HE2	1.86	0.40
1:X:348:PHE:HB3	1:X:349:ILE:H	1.71	0.40
7:c:38:LYS:HA	7:c:38:LYS:HD3	1.76	0.40
3:a:16:LEU:HG	8:b:46:ILE:HG21	2.04	0.40
4:C:350:CYS:SG	4:C:355:THR:OG1	2.69	0.40
4:E:202:ALA:HB2	4:E:231:ARG:HH21	1.86	0.40
3:F:616:GLU:O	3:F:620:ARG:HG2	2.21	0.40
4:G:818:PHE:O	4:G:822:ILE:HG12	2.22	0.40
7:L:1804:PHE:HB3	1:Z:356:ILE:H	1.86	0.40
4:M:252:LEU:HB3	4:M:257:ARG:HD2	2.02	0.40
1:Q:334:HIS:HE1	1:Q:335:LYS:HE2	1.86	0.40
1:R:323:ILE:HD13	1:R:323:ILE:HA	1.91	0.40
1:T:274:THR:HB	1:T:297:LEU:HD13	2.04	0.40
1:U:46:ASP:OD1	1:U:46:ASP:N	2.53	0.40
1:U:318:ILE:HB	1:U:380:ASN:HB3	2.03	0.40
1:Z:334:HIS:HE1	1:Z:335:LYS:HE2	1.86	0.40
8:b:24:THR:O	8:b:28:LEU:HG	2.21	0.40
1:2:236:MET:O	1:2:239:SER:OG	2.40	0.40
2:e:254:ARG:HA	2:e:254:ARG:HD3	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:810:LYS:HA	3:F:810:LYS:HD2	1.89	0.40
5:K:377:GLN:O	5:K:381:LYS:HB2	2.22	0.40
4:M:238:LEU:HG	4:M:240:GLY:H	1.86	0.40
3:N:681:ARG:O	3:N:685:MET:HG2	2.21	0.40
1:R:237:SER:O	1:R:244:ARG:NH2	2.55	0.40
1:S:334:HIS:HE1	1:S:335:LYS:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	2	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	Q	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	R	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	S	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	T	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	U	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	V	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	W	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	X	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	Y	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
1	Z	408/451 (90%)	386 (95%)	22 (5%)	0	100	100
2	e	360/375 (96%)	345 (96%)	15 (4%)	0	100	100
3	D	571/907 (63%)	546 (96%)	25 (4%)	0	100	100
3	F	591/907 (65%)	556 (94%)	35 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	584/907 (64%)	557 (95%)	25 (4%)	2 (0%)	36	72
3	N	584/907 (64%)	568 (97%)	16 (3%)	0	100	100
3	a	112/907 (12%)	108 (96%)	4 (4%)	0	100	100
3	h	97/907 (11%)	93 (96%)	4 (4%)	0	100	100
3	j	105/907 (12%)	94 (90%)	10 (10%)	1 (1%)	12	49
4	C	606/902 (67%)	571 (94%)	32 (5%)	3 (0%)	24	63
4	E	626/902 (69%)	577 (92%)	48 (8%)	1 (0%)	43	78
4	G	628/902 (70%)	585 (93%)	43 (7%)	0	100	100
4	M	624/902 (69%)	591 (95%)	31 (5%)	2 (0%)	36	72
5	I	511/667 (77%)	482 (94%)	27 (5%)	2 (0%)	30	67
5	K	548/667 (82%)	525 (96%)	20 (4%)	3 (0%)	24	63
6	J	506/1024 (49%)	472 (93%)	31 (6%)	3 (1%)	21	59
6	l	104/1024 (10%)	96 (92%)	7 (7%)	1 (1%)	12	49
7	L	540/1819 (30%)	501 (93%)	36 (7%)	3 (1%)	21	59
7	c	148/1819 (8%)	139 (94%)	9 (6%)	0	100	100
8	b	63/82 (77%)	63 (100%)	0	0	100	100
8	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
8	i	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
8	k	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
8	m	63/82 (77%)	63 (100%)	0	0	100	100
All	All	13050/23174 (56%)	12341 (95%)	688 (5%)	21 (0%)	44	78

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	239	ALA
4	C	465	HIS
4	E	581	ASP
3	H	455	LYS
5	I	601	LEU
6	J	236	LEU
6	J	238	LEU
5	K	254	LEU
7	L	307	ARG
4	M	241	ARG

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	376/400 (94%)	342 (91%)	34 (9%)	9	27
1	2	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	Q	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	R	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	S	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	T	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	U	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	V	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	W	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	X	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	Y	376/400 (94%)	343 (91%)	33 (9%)	9	28
1	Z	376/400 (94%)	343 (91%)	33 (9%)	9	28
2	e	310/318 (98%)	303 (98%)	7 (2%)	44	64
3	D	525/798 (66%)	524 (100%)	1 (0%)	87	87
3	F	542/798 (68%)	535 (99%)	7 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	539/798 (68%)	537 (100%)	2 (0%)	84	84
3	N	539/798 (68%)	538 (100%)	1 (0%)	87	87
3	a	101/798 (13%)	101 (100%)	0	100	100
3	h	88/798 (11%)	88 (100%)	0	100	100
3	j	88/798 (11%)	88 (100%)	0	100	100
4	C	556/791 (70%)	551 (99%)	5 (1%)	70	79
4	E	574/791 (73%)	572 (100%)	2 (0%)	86	86
4	G	572/791 (72%)	567 (99%)	5 (1%)	70	79
4	M	572/791 (72%)	567 (99%)	5 (1%)	70	79
5	I	472/594 (80%)	472 (100%)	0	100	100
5	K	509/594 (86%)	507 (100%)	2 (0%)	84	84
6	J	498/933 (53%)	497 (100%)	1 (0%)	87	87
6	l	84/933 (9%)	84 (100%)	0	100	100
7	L	501/1546 (32%)	501 (100%)	0	100	100
7	c	135/1546 (9%)	133 (98%)	2 (2%)	57	72
8	b	53/62 (86%)	52 (98%)	1 (2%)	50	67
8	d	53/62 (86%)	52 (98%)	1 (2%)	50	67
8	i	53/62 (86%)	53 (100%)	0	100	100
8	k	53/62 (86%)	52 (98%)	1 (2%)	50	67
8	m	53/62 (86%)	53 (100%)	0	100	100
All	All	11982/20324 (59%)	11542 (96%)	440 (4%)	31	51

All (440) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	LEU
1	1	58	GLU
1	1	109	SER
1	1	117	ASP
1	1	120	ASP
1	1	127	ASP
1	1	140	SER
1	1	147	SER
1	1	153	LEU
1	1	157	LEU

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Mol	Chain	Res	Type
1	1	158	ASN
1	1	165	LEU
1	1	170	SER
1	1	188	SER
1	1	218	LEU
1	1	233	SER
1	1	237	SER
1	1	240	THR
1	1	271	THR
1	1	289	THR
1	1	291	LEU
1	1	293	VAL
1	1	303	VAL
1	1	313	THR
1	1	323	ILE
1	1	333	VAL
1	1	361	SER
1	1	364	SER
1	1	367	LEU
1	1	369	SER
1	1	374	SER
1	1	392	CYS
1	1	419	ASP
1	1	439	THR
1	2	10	LEU
1	2	58	GLU
1	2	109	SER
1	2	117	ASP
1	2	120	ASP
1	2	140	SER
1	2	147	SER
1	2	153	LEU
1	2	157	LEU
1	2	158	ASN
1	2	165	LEU
1	2	170	SER
1	2	188	SER
1	2	218	LEU
1	2	233	SER
1	2	237	SER
1	2	240	THR
1	2	271	THR

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Mol	Chain	Res	Type
1	2	289	THR
1	2	291	LEU
1	2	293	VAL
1	2	303	VAL
1	2	313	THR
1	2	323	ILE
1	2	333	VAL
1	2	361	SER
1	2	364	SER
1	2	367	LEU
1	2	369	SER
1	2	374	SER
1	2	392	CYS
1	2	419	ASP
1	2	439	THR
2	e	31	PHE
2	e	54	VAL
2	e	125	GLU
2	e	180	LEU
2	e	201	THR
2	e	289	ILE
2	e	325	MET
4	C	224	VAL
4	C	367	THR
4	C	510	VAL
4	C	547	THR
4	C	766	THR
3	D	706	ILE
4	E	224	VAL
4	E	621	ILE
3	F	271	THR
3	F	304	ILE
3	F	338	LEU
3	F	339	LEU
3	F	459	LEU
3	F	554	SER
3	F	800	LEU
4	G	221	LEU
4	G	233	VAL
4	G	241	ARG
4	G	328	ILE
4	G	855	VAL

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Mol	Chain	Res	Type
3	H	271	THR
3	H	286	SER
6	J	221	VAL
5	K	28	SER
5	K	253	SER
4	M	318	LEU
4	M	328	ILE
4	M	459	VAL
4	M	465	HIS
4	M	815	VAL
3	N	591	THR
8	k	34	ILE
1	Q	10	LEU
1	Q	58	GLU
1	Q	109	SER
1	Q	117	ASP
1	Q	120	ASP
1	Q	140	SER
1	Q	147	SER
1	Q	153	LEU
1	Q	157	LEU
1	Q	158	ASN
1	Q	165	LEU
1	Q	170	SER
1	Q	188	SER
1	Q	218	LEU
1	Q	233	SER
1	Q	237	SER
1	Q	240	THR
1	Q	271	THR
1	Q	289	THR
1	Q	291	LEU
1	Q	293	VAL
1	Q	303	VAL
1	Q	313	THR
1	Q	323	ILE
1	Q	333	VAL
1	Q	361	SER
1	Q	364	SER
1	Q	367	LEU
1	Q	369	SER
1	Q	374	SER

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Mol	Chain	Res	Type
1	Q	392	CYS
1	Q	419	ASP
1	Q	439	THR
1	R	10	LEU
1	R	58	GLU
1	R	109	SER
1	R	117	ASP
1	R	120	ASP
1	R	140	SER
1	R	147	SER
1	R	153	LEU
1	R	157	LEU
1	R	158	ASN
1	R	165	LEU
1	R	170	SER
1	R	188	SER
1	R	218	LEU
1	R	233	SER
1	R	237	SER
1	R	240	THR
1	R	271	THR
1	R	289	THR
1	R	291	LEU
1	R	293	VAL
1	R	303	VAL
1	R	313	THR
1	R	323	ILE
1	R	333	VAL
1	R	361	SER
1	R	364	SER
1	R	367	LEU
1	R	369	SER
1	R	374	SER
1	R	392	CYS
1	R	419	ASP
1	R	439	THR
1	S	10	LEU
1	S	58	GLU
1	S	109	SER
1	S	117	ASP
1	S	120	ASP
1	S	140	SER

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Mol	Chain	Res	Type
1	S	147	SER
1	S	153	LEU
1	S	157	LEU
1	S	158	ASN
1	S	165	LEU
1	S	170	SER
1	S	188	SER
1	S	218	LEU
1	S	233	SER
1	S	237	SER
1	S	240	THR
1	S	271	THR
1	S	289	THR
1	S	291	LEU
1	S	293	VAL
1	S	303	VAL
1	S	313	THR
1	S	323	ILE
1	S	333	VAL
1	S	361	SER
1	S	364	SER
1	S	367	LEU
1	S	369	SER
1	S	374	SER
1	S	392	CYS
1	S	419	ASP
1	S	439	THR
1	T	10	LEU
1	T	58	GLU
1	T	109	SER
1	T	117	ASP
1	T	120	ASP
1	T	140	SER
1	T	147	SER
1	T	153	LEU
1	T	157	LEU
1	T	158	ASN
1	T	165	LEU
1	T	170	SER
1	T	188	SER
1	T	218	LEU
1	T	233	SER

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Mol	Chain	Res	Type
1	T	237	SER
1	T	240	THR
1	T	271	THR
1	T	289	THR
1	T	291	LEU
1	T	293	VAL
1	T	303	VAL
1	T	313	THR
1	T	323	ILE
1	T	333	VAL
1	T	361	SER
1	T	364	SER
1	T	367	LEU
1	T	369	SER
1	T	374	SER
1	T	392	CYS
1	T	419	ASP
1	T	439	THR
1	U	10	LEU
1	U	58	GLU
1	U	109	SER
1	U	117	ASP
1	U	120	ASP
1	U	140	SER
1	U	147	SER
1	U	153	LEU
1	U	157	LEU
1	U	158	ASN
1	U	165	LEU
1	U	170	SER
1	U	188	SER
1	U	218	LEU
1	U	233	SER
1	U	237	SER
1	U	240	THR
1	U	271	THR
1	U	289	THR
1	U	291	LEU
1	U	293	VAL
1	U	303	VAL
1	U	313	THR
1	U	323	ILE

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Mol	Chain	Res	Type
1	U	333	VAL
1	U	361	SER
1	U	364	SER
1	U	367	LEU
1	U	369	SER
1	U	374	SER
1	U	392	CYS
1	U	419	ASP
1	U	439	THR
1	V	10	LEU
1	V	58	GLU
1	V	109	SER
1	V	117	ASP
1	V	120	ASP
1	V	140	SER
1	V	147	SER
1	V	153	LEU
1	V	157	LEU
1	V	158	ASN
1	V	165	LEU
1	V	170	SER
1	V	188	SER
1	V	218	LEU
1	V	233	SER
1	V	237	SER
1	V	240	THR
1	V	271	THR
1	V	289	THR
1	V	291	LEU
1	V	293	VAL
1	V	303	VAL
1	V	313	THR
1	V	323	ILE
1	V	333	VAL
1	V	361	SER
1	V	364	SER
1	V	367	LEU
1	V	369	SER
1	V	374	SER
1	V	392	CYS
1	V	419	ASP
1	V	439	THR

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Mol	Chain	Res	Type
1	W	10	LEU
1	W	58	GLU
1	W	109	SER
1	W	117	ASP
1	W	120	ASP
1	W	140	SER
1	W	147	SER
1	W	153	LEU
1	W	157	LEU
1	W	158	ASN
1	W	165	LEU
1	W	170	SER
1	W	188	SER
1	W	218	LEU
1	W	233	SER
1	W	237	SER
1	W	240	THR
1	W	271	THR
1	W	289	THR
1	W	291	LEU
1	W	293	VAL
1	W	303	VAL
1	W	313	THR
1	W	323	ILE
1	W	333	VAL
1	W	361	SER
1	W	364	SER
1	W	367	LEU
1	W	369	SER
1	W	374	SER
1	W	392	CYS
1	W	419	ASP
1	W	439	THR
1	X	10	LEU
1	X	58	GLU
1	X	109	SER
1	X	117	ASP
1	X	120	ASP
1	X	140	SER
1	X	147	SER
1	X	153	LEU
1	X	157	LEU

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Mol	Chain	Res	Type
1	X	158	ASN
1	X	165	LEU
1	X	170	SER
1	X	188	SER
1	X	218	LEU
1	X	233	SER
1	X	237	SER
1	X	240	THR
1	X	271	THR
1	X	289	THR
1	X	291	LEU
1	X	293	VAL
1	X	303	VAL
1	X	313	THR
1	X	323	ILE
1	X	333	VAL
1	X	361	SER
1	X	364	SER
1	X	367	LEU
1	X	369	SER
1	X	374	SER
1	X	392	CYS
1	X	419	ASP
1	X	439	THR
1	Y	10	LEU
1	Y	58	GLU
1	Y	109	SER
1	Y	117	ASP
1	Y	120	ASP
1	Y	140	SER
1	Y	147	SER
1	Y	153	LEU
1	Y	157	LEU
1	Y	158	ASN
1	Y	165	LEU
1	Y	170	SER
1	Y	188	SER
1	Y	218	LEU
1	Y	233	SER
1	Y	237	SER
1	Y	240	THR
1	Y	271	THR

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Mol	Chain	Res	Type
1	Y	289	THR
1	Y	291	LEU
1	Y	293	VAL
1	Y	303	VAL
1	Y	313	THR
1	Y	323	ILE
1	Y	333	VAL
1	Y	361	SER
1	Y	364	SER
1	Y	367	LEU
1	Y	369	SER
1	Y	374	SER
1	Y	392	CYS
1	Y	419	ASP
1	Y	439	THR
1	Z	10	LEU
1	Z	58	GLU
1	Z	109	SER
1	Z	117	ASP
1	Z	120	ASP
1	Z	140	SER
1	Z	147	SER
1	Z	153	LEU
1	Z	157	LEU
1	Z	158	ASN
1	Z	165	LEU
1	Z	170	SER
1	Z	188	SER
1	Z	218	LEU
1	Z	233	SER
1	Z	237	SER
1	Z	240	THR
1	Z	271	THR
1	Z	289	THR
1	Z	291	LEU
1	Z	293	VAL
1	Z	303	VAL
1	Z	313	THR
1	Z	323	ILE
1	Z	333	VAL
1	Z	361	SER
1	Z	364	SER

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Mol	Chain	Res	Type
1	Z	367	LEU
1	Z	369	SER
1	Z	374	SER
1	Z	392	CYS
1	Z	419	ASP
1	Z	439	THR
8	b	64	ILE
8	d	46	ILE
7	c	47	THR
7	c	149	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (281) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	175	GLN
1	1	187	ASN
1	1	221	GLN
1	1	227	GLN
1	1	229	ASN
1	1	267	HIS
1	1	314	ASN
1	1	315	HIS
1	1	338	GLN
1	1	407	GLN
1	1	430	GLN
1	2	175	GLN
1	2	187	ASN
1	2	221	GLN
1	2	227	GLN
1	2	229	ASN
1	2	250	ASN
1	2	267	HIS
1	2	315	HIS
1	2	430	GLN
2	e	88	HIS
2	e	111	ASN
2	e	161	HIS
2	e	225	GLN
2	e	263	GLN
2	e	296	ASN
2	e	353	GLN
4	C	172	GLN

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Mol	Chain	Res	Type
4	C	173	HIS
4	C	242	GLN
4	C	261	HIS
4	C	329	GLN
4	C	401	HIS
4	C	412	HIS
4	C	639	GLN
4	C	650	HIS
4	C	654	GLN
4	C	718	ASN
4	C	741	ASN
4	C	763	GLN
3	D	491	ASN
3	D	500	GLN
3	D	531	GLN
3	D	596	ASN
3	D	684	HIS
3	D	705	HIS
3	D	740	GLN
3	D	773	ASN
3	D	774	GLN
3	D	781	GLN
3	D	852	HIS
3	D	885	HIS
4	E	172	GLN
4	E	251	ASN
4	E	631	ASN
4	E	644	HIS
4	E	684	GLN
4	E	691	GLN
4	E	692	ASN
3	F	302	ASN
3	F	322	GLN
3	F	345	GLN
3	F	528	ASN
3	F	705	HIS
3	F	713	HIS
3	F	773	ASN
3	F	774	GLN
3	F	801	GLN
3	F	805	GLN
3	F	855	GLN

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Mol	Chain	Res	Type
4	G	165	GLN
4	G	166	ASN
4	G	236	GLN
4	G	287	GLN
4	G	322	GLN
4	G	424	ASN
4	G	430	GLN
4	G	465	HIS
4	G	530	HIS
4	G	639	GLN
4	G	644	HIS
4	G	662	ASN
4	G	694	GLN
4	G	741	ASN
3	H	322	GLN
3	H	329	HIS
3	H	347	GLN
3	H	389	GLN
3	H	401	HIS
3	H	444	HIS
3	H	479	GLN
3	H	684	HIS
3	H	693	ASN
3	H	703	GLN
3	H	705	HIS
3	H	716	HIS
3	H	717	GLN
3	H	860	GLN
5	I	142	GLN
5	I	160	HIS
5	I	186	GLN
5	I	200	HIS
5	I	316	GLN
5	I	327	GLN
5	I	409	ASN
5	I	519	ASN
5	I	533	GLN
5	I	581	HIS
5	I	622	GLN
6	J	322	GLN
6	J	362	GLN
6	J	484	HIS

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Mol	Chain	Res	Type
6	J	698	GLN
6	J	708	GLN
6	J	725	ASN
6	J	818	GLN
6	J	823	GLN
6	J	830	GLN
6	J	892	HIS
5	K	35	HIS
5	K	61	GLN
5	K	67	GLN
5	K	82	HIS
5	K	102	GLN
5	K	256	GLN
5	K	289	GLN
5	K	303	GLN
5	K	353	GLN
5	K	393	ASN
5	K	401	HIS
5	K	409	ASN
5	K	501	GLN
5	K	540	GLN
5	K	543	GLN
5	K	547	GLN
5	K	561	HIS
5	K	571	GLN
5	K	622	GLN
7	L	340	GLN
7	L	343	GLN
7	L	515	ASN
7	L	517	HIS
7	L	1492	ASN
7	L	1766	GLN
7	L	1770	ASN
7	L	1792	GLN
7	L	1803	ASN
7	L	1805	ASN
7	L	1806	ASN
4	M	287	GLN
4	M	322	GLN
4	M	512	HIS
4	M	530	HIS
4	M	565	ASN

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Mol	Chain	Res	Type
4	M	654	GLN
4	M	823	ASN
3	N	310	GLN
3	N	343	HIS
3	N	345	GLN
3	N	389	GLN
3	N	401	HIS
3	N	491	ASN
3	N	500	GLN
3	N	560	GLN
3	N	576	HIS
3	N	665	ASN
3	N	684	HIS
3	N	687	ASN
3	N	693	ASN
3	N	703	GLN
3	N	717	GLN
3	N	740	GLN
3	N	781	GLN
3	N	830	ASN
3	N	855	GLN
8	i	53	GLN
1	Q	175	GLN
1	Q	187	ASN
1	Q	221	GLN
1	Q	227	GLN
1	Q	229	ASN
1	Q	267	HIS
1	Q	315	HIS
1	Q	430	GLN
1	R	175	GLN
1	R	187	ASN
1	R	221	GLN
1	R	227	GLN
1	R	229	ASN
1	R	267	HIS
1	R	315	HIS
1	R	430	GLN
1	S	175	GLN
1	S	187	ASN
1	S	221	GLN
1	S	227	GLN

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Mol	Chain	Res	Type
1	S	229	ASN
1	S	267	HIS
1	S	314	ASN
1	S	315	HIS
1	S	338	GLN
1	S	357	GLN
1	S	430	GLN
1	T	175	GLN
1	T	187	ASN
1	T	221	GLN
1	T	227	GLN
1	T	229	ASN
1	T	267	HIS
1	T	315	HIS
1	T	338	GLN
1	T	430	GLN
1	U	175	GLN
1	U	187	ASN
1	U	221	GLN
1	U	227	GLN
1	U	229	ASN
1	U	251	ASN
1	U	267	HIS
1	U	315	HIS
1	U	338	GLN
1	U	407	GLN
1	U	430	GLN
1	V	175	GLN
1	V	187	ASN
1	V	221	GLN
1	V	227	GLN
1	V	229	ASN
1	V	267	HIS
1	V	314	ASN
1	V	315	HIS
1	V	430	GLN
1	W	24	GLN
1	W	175	GLN
1	W	187	ASN
1	W	221	GLN
1	W	227	GLN
1	W	229	ASN

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Mol	Chain	Res	Type
1	W	267	HIS
1	W	315	HIS
1	W	338	GLN
1	W	430	GLN
1	X	175	GLN
1	X	187	ASN
1	X	221	GLN
1	X	227	GLN
1	X	229	ASN
1	X	267	HIS
1	X	299	GLN
1	X	315	HIS
1	X	338	GLN
1	X	430	GLN
1	Y	54	GLN
1	Y	175	GLN
1	Y	187	ASN
1	Y	221	GLN
1	Y	227	GLN
1	Y	229	ASN
1	Y	267	HIS
1	Y	314	ASN
1	Y	315	HIS
1	Y	430	GLN
1	Z	175	GLN
1	Z	187	ASN
1	Z	221	GLN
1	Z	227	GLN
1	Z	229	ASN
1	Z	267	HIS
1	Z	314	ASN
1	Z	315	HIS
1	Z	338	GLN
1	Z	407	GLN
1	Z	430	GLN
8	d	17	ASN
7	c	43	ASN
7	c	51	GLN
7	c	135	ASN
7	c	138	HIS
3	j	42	ASN
6	l	15	GLN

Continued on next page...

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Mol	Chain	Res	Type
6	1	107	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

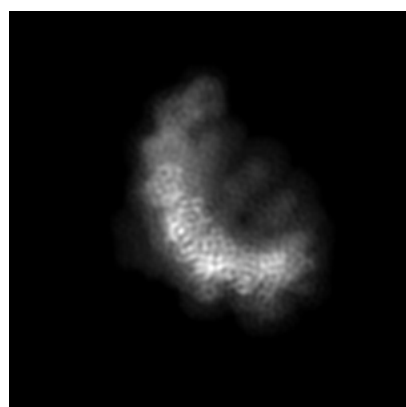
6 Map visualisation [i](#)

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

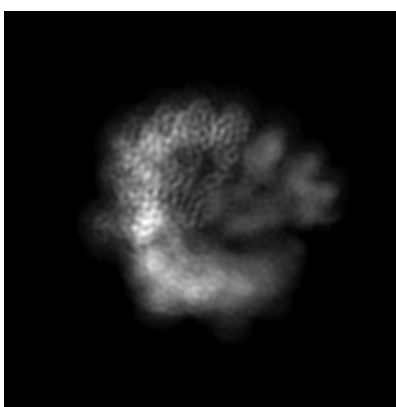
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

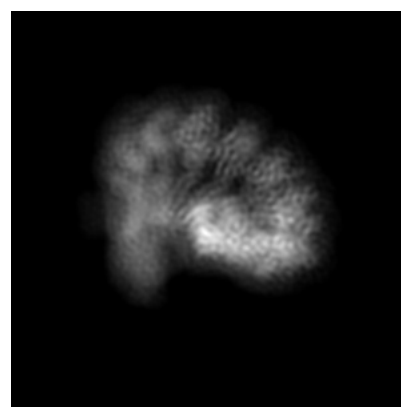
6.1.1 Primary map



X



Y

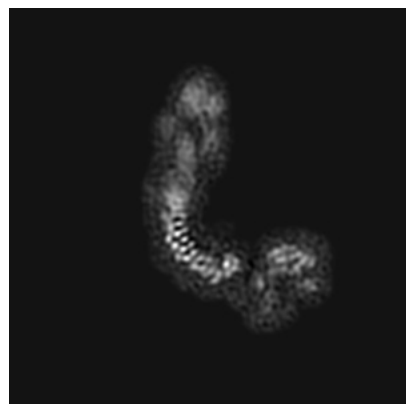


Z

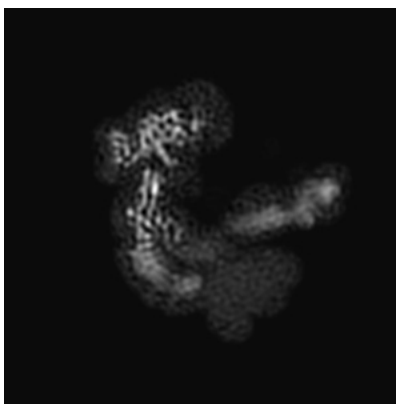
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

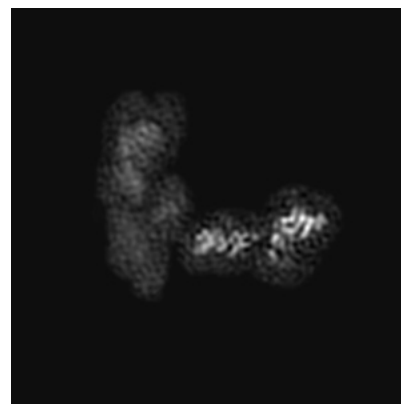
6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

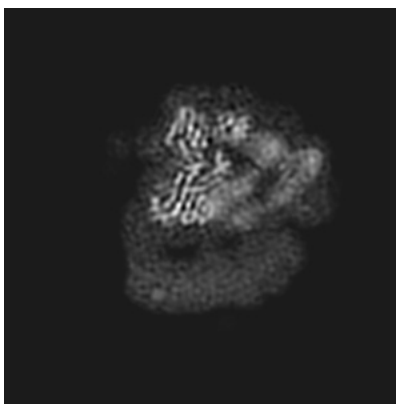
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

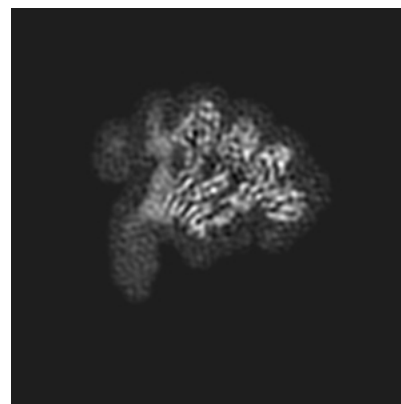
6.3.1 Primary map



X Index: 134



Y Index: 84

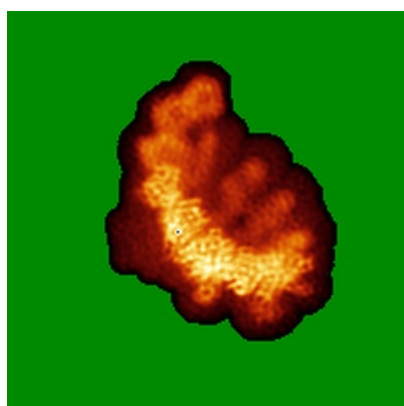


Z Index: 72

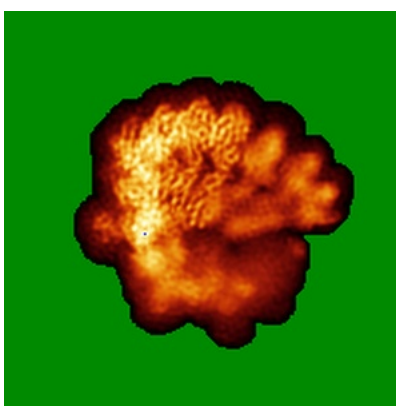
The images above show the largest variance slices of the map in three orthogonal directions.

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

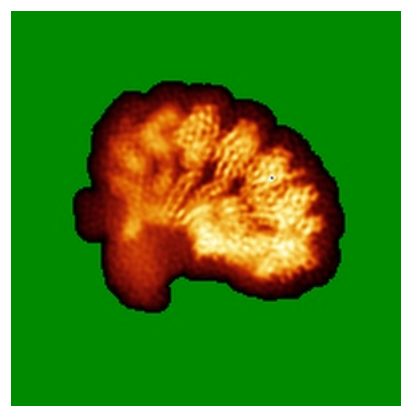
6.4.1 Primary map



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



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

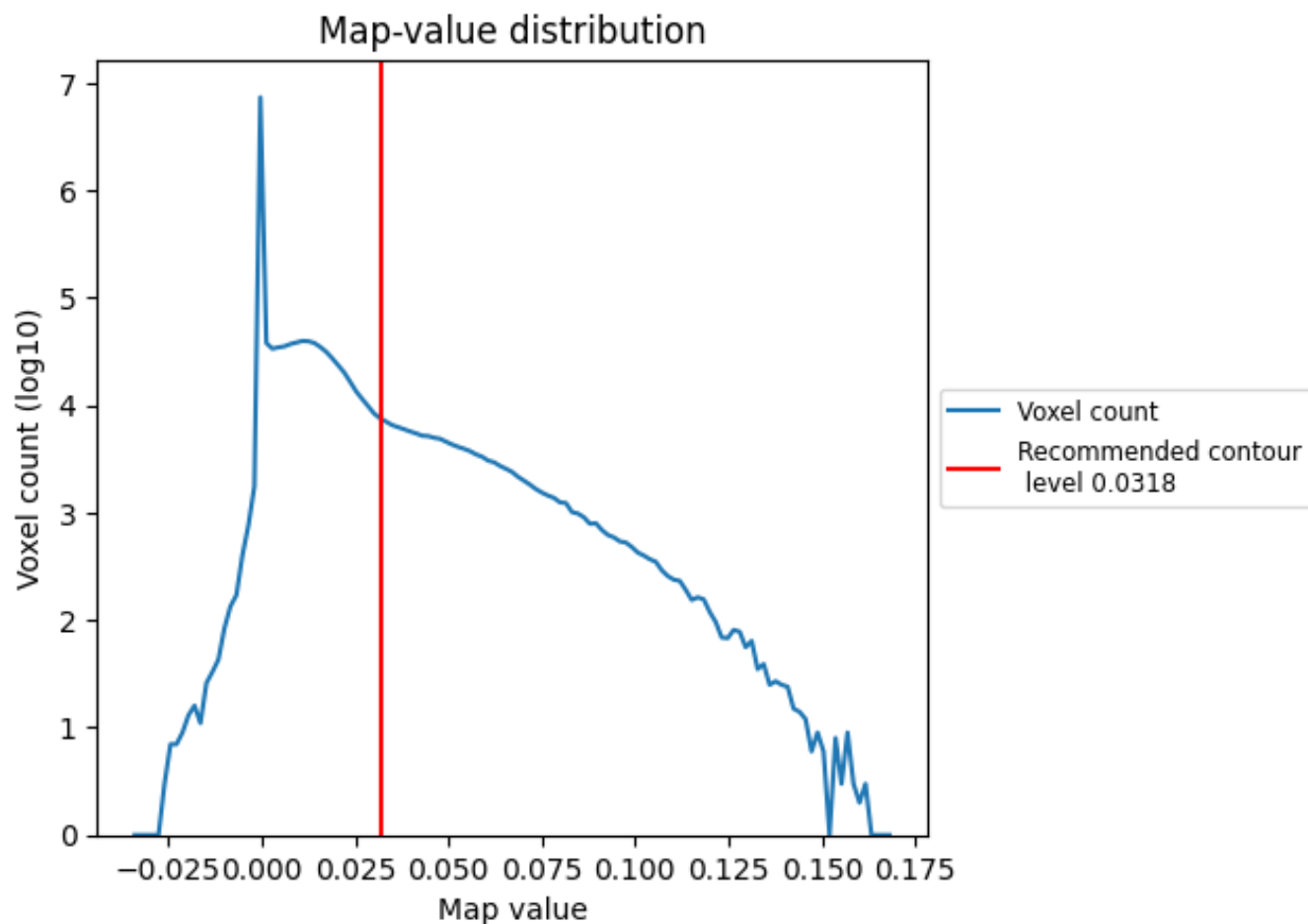
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

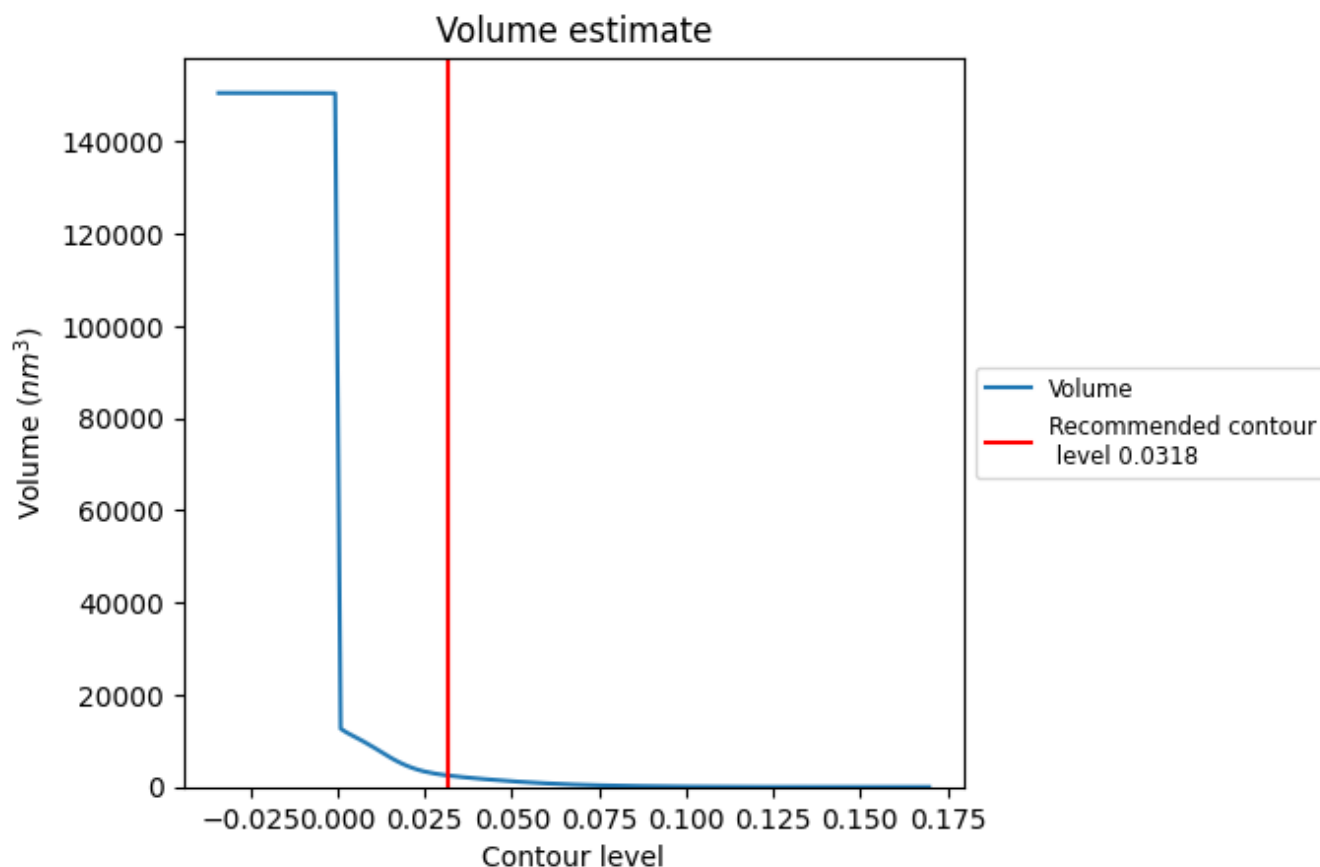
This section contains the results of statistical analysis of the map.

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.

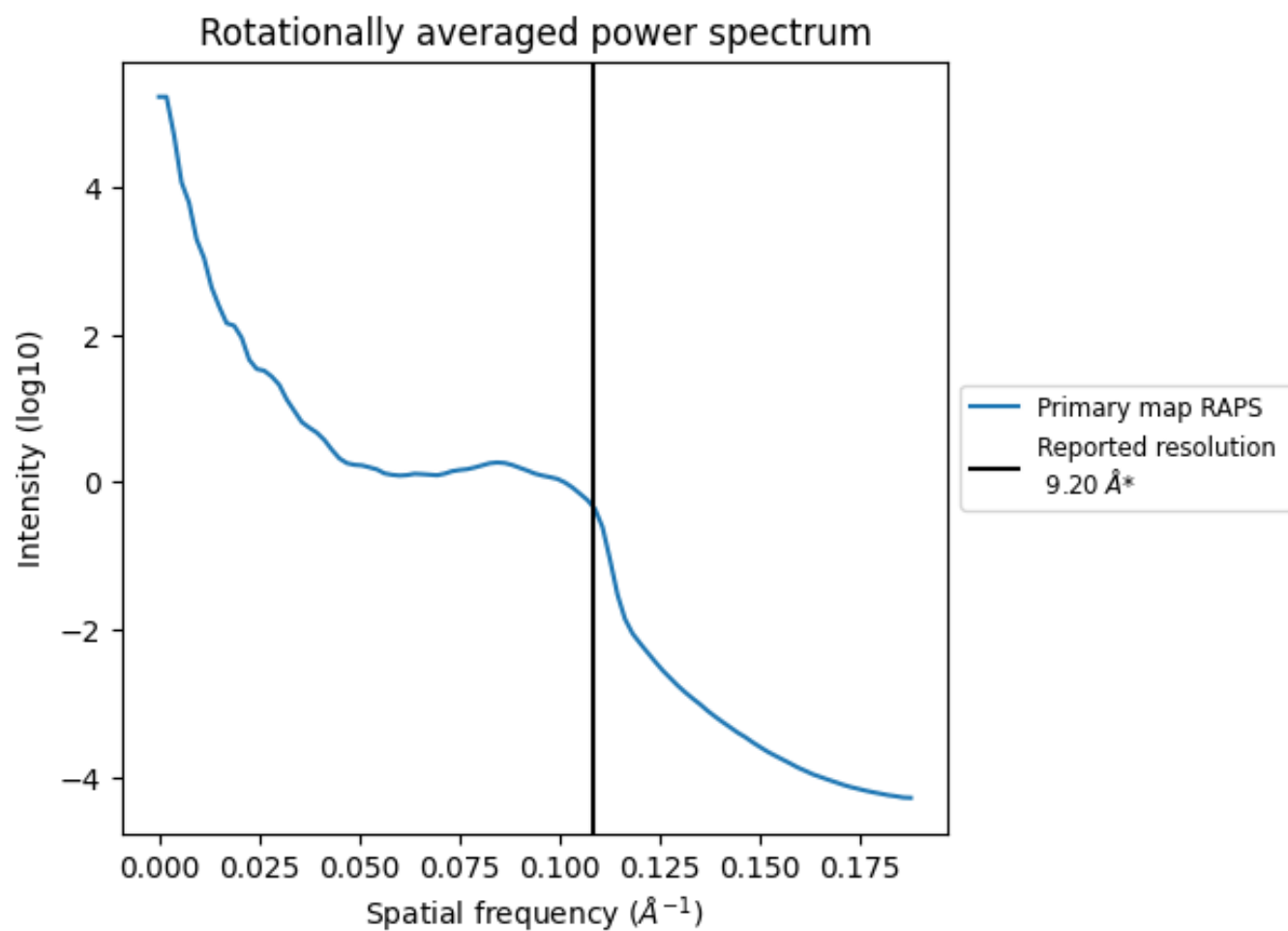
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2484 nm^3 ; this corresponds to an approximate mass of 2244 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.109 Å⁻¹

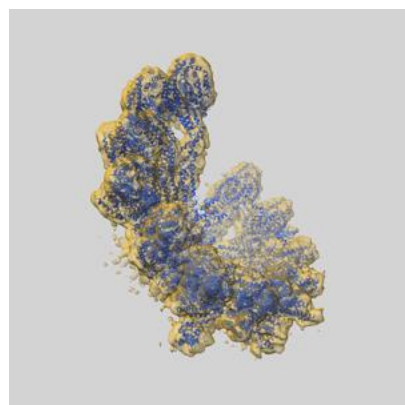
8 Fourier-Shell correlation

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

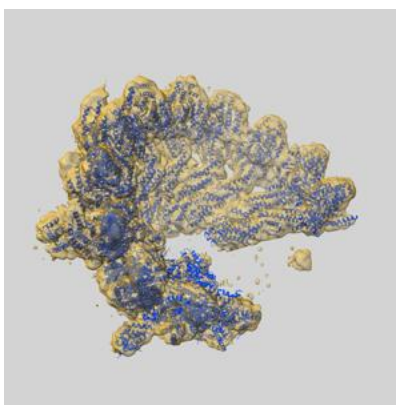
9 Map-model fit [i](#)

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

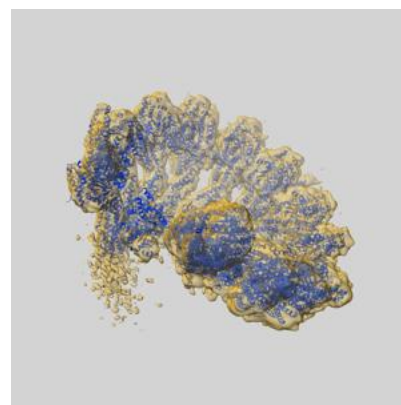
9.1 Map-model overlay [i](#)



X



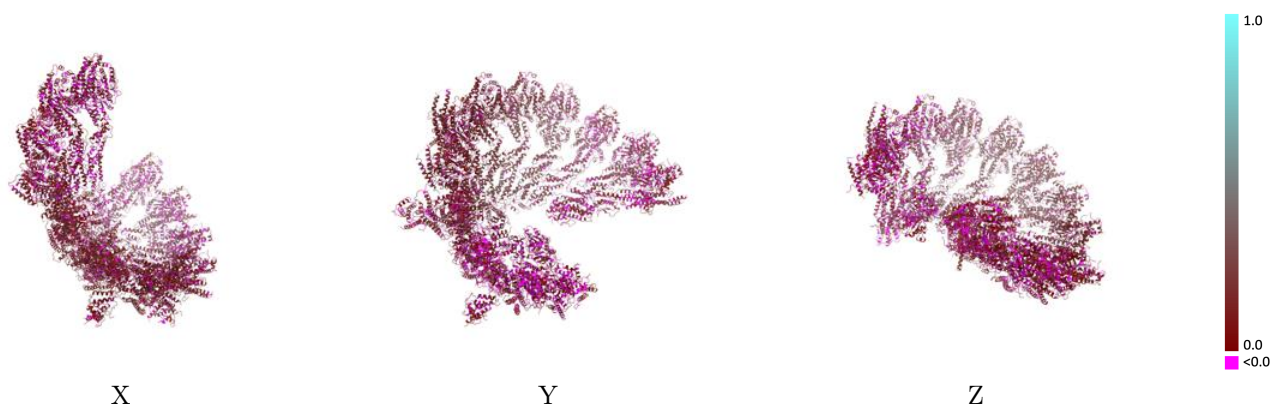
Y



Z

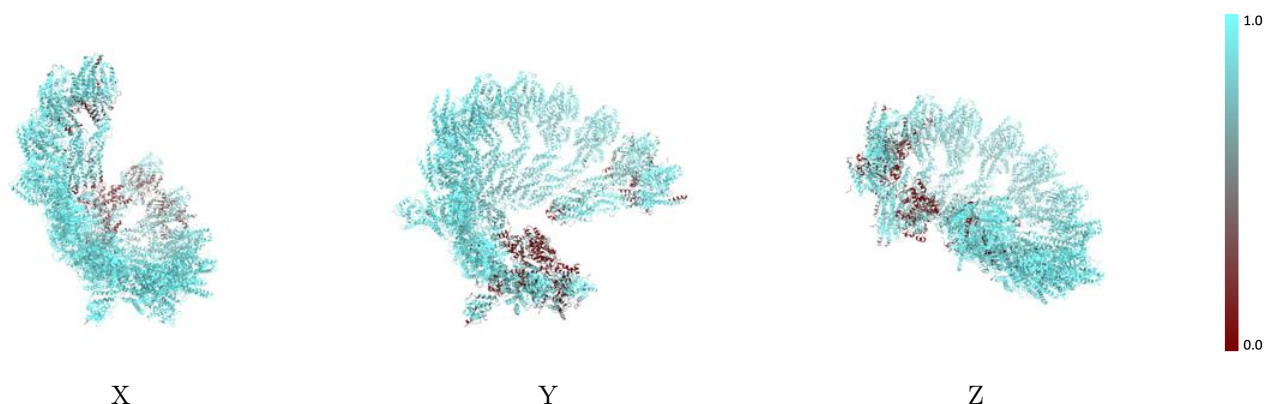
The images above show the 3D surface view of the map at the recommended contour level 0.0318 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



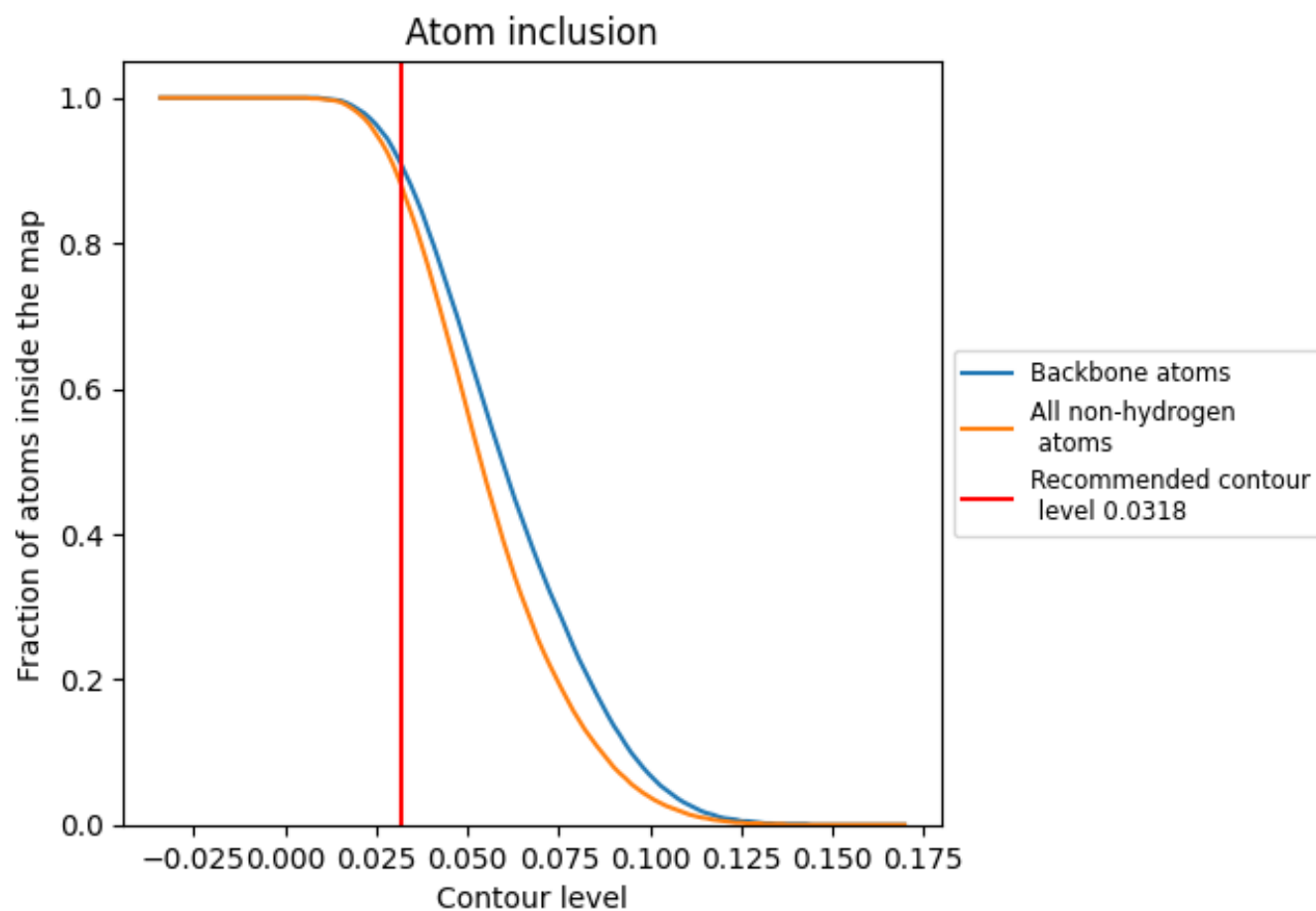
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0318).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 88% 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 (0.0318) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.0940
1	 0.8850	 0.0630
2	 0.8610	 0.0530
C	 0.8160	 0.0630
D	 0.8430	 0.0730
E	 0.9700	 0.0760
F	 0.9610	 0.1220
G	 0.9630	 0.1340
H	 0.9690	 0.1370
I	 0.9610	 0.1390
J	 0.9630	 0.1440
K	 0.9630	 0.1360
L	 0.9830	 0.0860
M	 0.8480	 0.0670
N	 0.8220	 0.0630
Q	 0.5840	 0.0400
R	 0.6810	 0.0380
S	 0.9050	 0.0460
T	 0.9680	 0.1100
U	 0.9700	 0.1220
V	 0.9760	 0.1260
W	 0.9680	 0.1180
X	 0.9690	 0.1300
Y	 0.9600	 0.1060
Z	 0.9450	 0.0400
a	 0.8020	 0.1210
b	 0.7960	 0.1370
c	 0.4660	 0.0670
d	 0.3210	 0.0920
e	 0.2530	 0.0500
h	 0.7670	 0.0760
i	 0.7290	 0.1030
j	 0.9150	 0.0860
k	 0.9430	 0.1250
l	 0.9630	 0.1320
m	 0.9480	 0.1580

