



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 09:58 AM UTC

PDB ID : 7QJ6 / pdb_00007qj6
EMDB ID : EMD-14011
Title : Structure of recombinant human gamma-Tubulin Ring Complex 10-spoked assembly intermediate (spokes 3-12, substoichiometric spokes 13-14)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 7.80 Å(reported)
Based on initial models : 6V6S, 6L81, 6X0U, 7AS4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

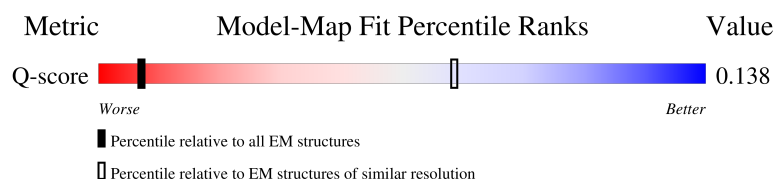
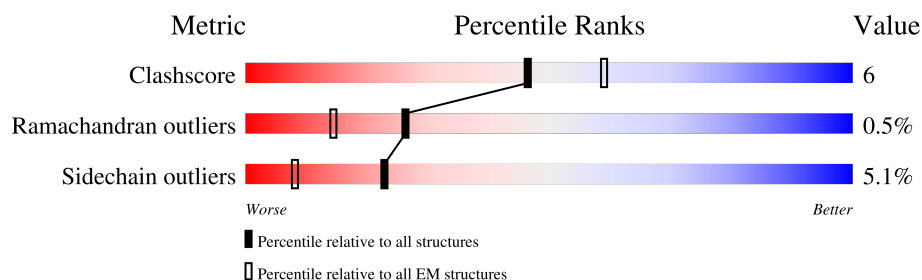
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.80 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	370 (7.30 - 8.30)

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.

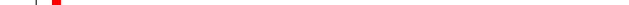
Mol	Chain	Length	Quality of chain
1	e	375	71% 75% 21% .
2	b	82	63% 16% 21%
2	d	82	38% 54% 18% 28%
2	i	82	18% 65% 12% . 21%

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Mol	Chain	Length	Quality of chain
2	k	82	
2	m	82	
3	D	907	
3	F	907	
3	H	907	
3	a	907	
3	h	907	
3	j	907	
4	C	902	
4	E	902	
4	G	902	
5	I	667	
5	K	667	
6	J	1024	
6	l	1024	
7	L	1819	
7	c	1819	
8	Q	451	
8	R	451	
8	S	451	
8	T	451	
8	U	451	
8	V	451	
8	W	451	
8	X	451	

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

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 91575 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 actin, cytoplasmic 1.

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

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

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

- 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	h	107	Total	C	N	O	S	0	0
			843	533	156	152	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		

- 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 Tubulin gamma-1 chain.

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

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

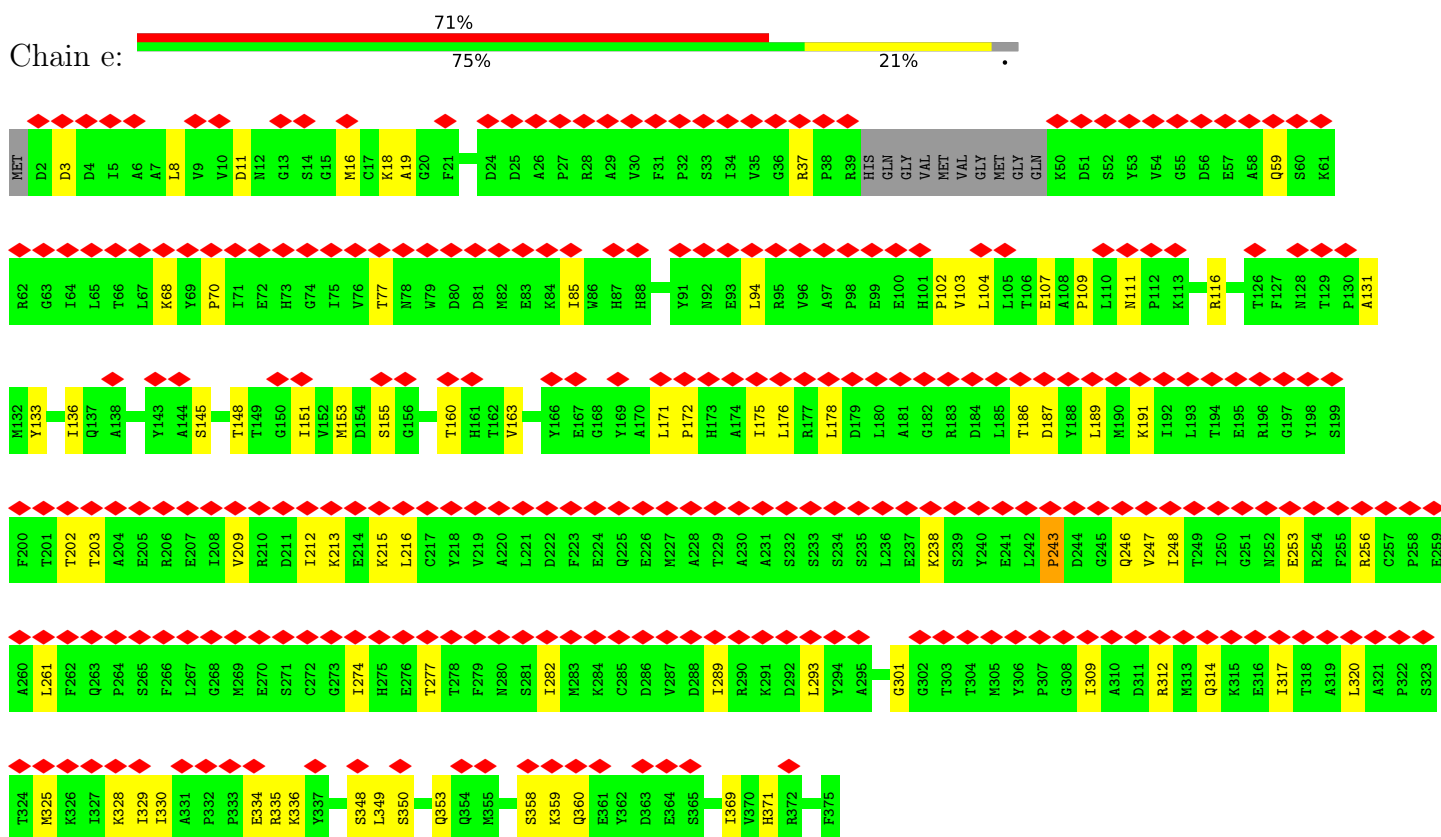
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	1	6	Total	O	0
			6	6	

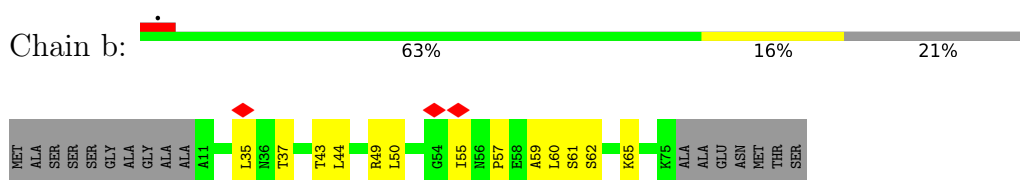
3 Residue-property plots

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: actin, cytoplasmic 1



- Molecule 2: Mitotic-spindle organizing protein 1



- Molecule 2: Mitotic-spindle organizing protein 1



[illegible]

- Molecule 3: Gamma-tubulin complex component 3

Chain D: 57% 7% 36%

ARG	VAL	Q739	L577	M411	GLY	THR	LEU	ALA	GLU	MET
VAL	LEU	Q740	L580	Q415	THR	MET	PRO	LEU	ILE	ALA
SER	GLY	H746	L581	Q416	GLU	GLU	GLN	ARG	THR	ALA
THR	THR	I747	L582	H417	THR	THR	ASN	ASP	ARG	GLN
ARG	ARG	A749	K582	I418	THR	THR	ALA	HIS	ARG	LYS
GLY	GLY		P583	L419	THR	THR	ALA	SER	GLU	SER
ARG	ARG	R761	E584	S420	THR	THR	PRO	ALA	ALA	PRO
SER	SER		L585	L421	THR	THR	VAL	THR	ASP	ASN
SER	SER	L763	V586	L434	THR	THR	GLY	TYR	LEU	VAL
HIS	HIS	L775	A589	I434	THR	THR	GLY	TYR	ALA	LEU
THR	THR		T590	Y464	THR	THR	CYS	ALA	PHE	GLN
		I782	T591	Y464	THR	THR	LEU	ARG	SER	ASN
		I783	L592	M470	THR	THR	GLN	PRO	GLU	LEU
			Y593	N491	THR	THR	GLN	GLN	LEU	CYS
		Q786	Q594	Y495	THR	THR	LEU	THR	HIS	CYS
		E799	H595	Q495	THR	THR	GLY	PRO	LEU	ILE
		R803	N596	P502	THR	THR	SER	LEU	LEU	LEU
			L597	P502	THR	THR	ARG	SER	HIS	GLY
		R811	A604	THR	THR	THR	LEU	TYR	SER	ARG
GLN	ARG		V605	THR	THR	THR	ALA	GLN	GLN	SER
GLU	GLU		N609	THR	THR	THR	TRP	ASP	GLY	GLU
ILE	ILE		P615	THR	THR	THR	LEU	ARG	VAL	ALA
GLY	GLY		R619	THR	THR	THR	LEU	SER	LEU	ASP
GLN	GLN		Y635	THR	THR	THR	ALA	ALA	LYS	VAL
TRP	TRP			GLU	THR	THR	ASN	GLN	ASN	ALA
VAL	VAL			GLU	THR	THR	ALA	GLN	ASN	ALA
THR	THR	A823	L640	PRO	THR	THR	ALA	GLN	ASN	GLN
		E829	D641	GLN	THR	THR	THR	VAL	LEU	VAL
		R837	Y642	ASP	THR	THR	THR	GLY	LEU	VAL
			P647	ALA	THR	THR	ASN	SER	SER	GLY
		R848	I648	ALA	THR	THR	LYS	SER	LEU	ASN
		T851	Y660	ASP	THR	THR	GLY	GLY	GLU	ASN
		Q855		LEU	THR	THR	VAL	ILE	ASP	PHE
			L676	PHE	THR	THR	PRO	SER	ASP	THR
		Q855	L677	THR	THR	THR	ALA	ILE	ARG	ALA
				LEU	THR	THR	VAL	GLY	ARG	THR
		F861	M685	ASN	THR	THR	LEU	GLN	GLN	VAL
				VAL	THR	THR	ARG	CYS	PRO	GLU
		T867		ALA	THR	THR	ASN	ALA	ARG	ARG
		S869	A688	ALA	THR	THR	MET	LEU	LYS	ASP
		L876	K689	PHE	THR	THR	THR	LEU	VAL	GLU
			R692	THR	THR	THR	ARG	GLY	SER	PHE
				GLU	THR	THR	SER	PRO	SER	THR
		R897	Q703	D535	THR	THR	ARG	ALA	TYR	VAL
				Y548	THR	THR	ARG	PRO	ALA	ALA
		E890	L706	K552	THR	THR	GLY	ALA	THR	GLU
PRO	ARG		L707	Y553	THR	THR	ASP	PRO	LEU	LYS
			E710	L566	THR	THR	THR	GLN	PHE	ILE
					THR	THR	GLY	LEU	ALA	LYS



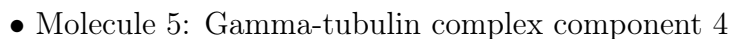
LEU	VAL	ARG	ASP	GLN	LYS	ASP	VAL	ARG	MET	PRO	THR	THR	ALA	ALA	GLN	SER	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN
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● Molecule 4: Gamma-tubulin complex component 2

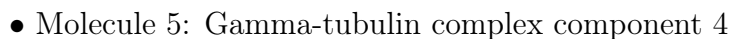


MET	SER	GLU	PHE	ARG	HIS	HIS	ASP	ASP	VAL	ASN	GLU	LEU	LEU	SER	LEU	LEU	VAL	HIS	GLY	GLY	ASP	GLY	ALA	ALA	GLU	GLY	VAL	THR	LYS	ASN	ARG	THR	THR	THR	VAL	SER	ALA	HIS	SER	ALA	LYS	VAL	LYS	ILE	GLU	GLU	PHE	ARG	PRO	
GLU	ASP	PHE	LEU	LYS	TYR	ASP	GLU	LEU	SER	ASN	ASN	THR	ARG	ASN	LEU	ASP	PRO	LEU	VAL	TYR	LEU	SER	SER	LEU	LEU	GLN	THR	ASP	LYS	GLY	THR	LEU	GLN	ASN	ALA	LYS	GLU	ARG	ALA	GLU	LEU	ALA	ALA	ALA	VAL	GLY	SER	THR	THR	ILE
ASN	VAL	PRO	ALA	ALA	ALA	SER	LYS	ILE	MET	GLN	GLU	LEU	GLU	GLU	GLU	LEU	GLN	LEU	GLY	VAL	SER	VAL	ALA	ALA	THR	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		
L150	L156	K159	N169	S170	G171	F177	L187	F191	ILE	GLY	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	ALA	GLY	ILE	

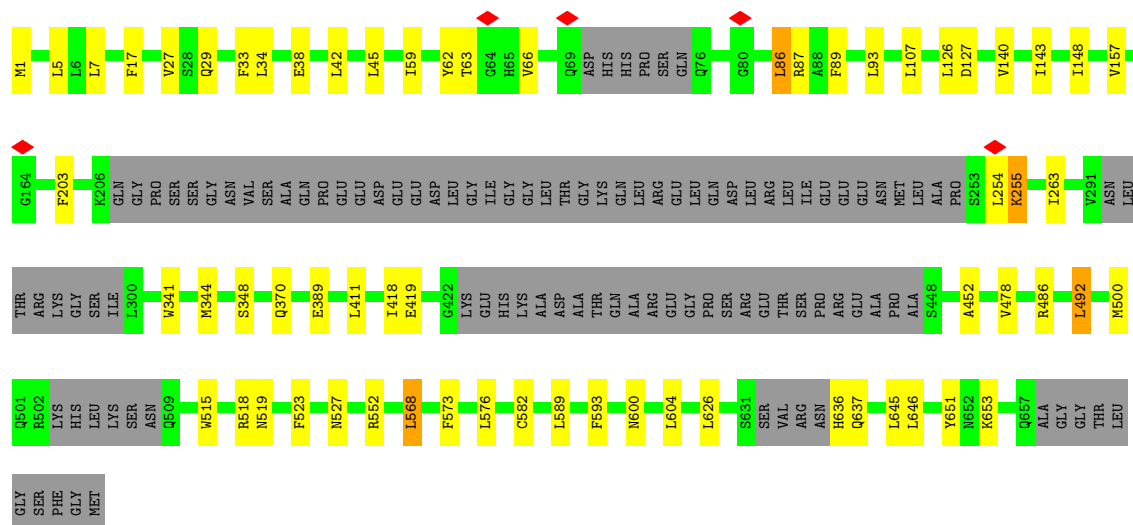
App Type	Percentage
Shopping app	61%
Social media app	10%
Productivity app	29%



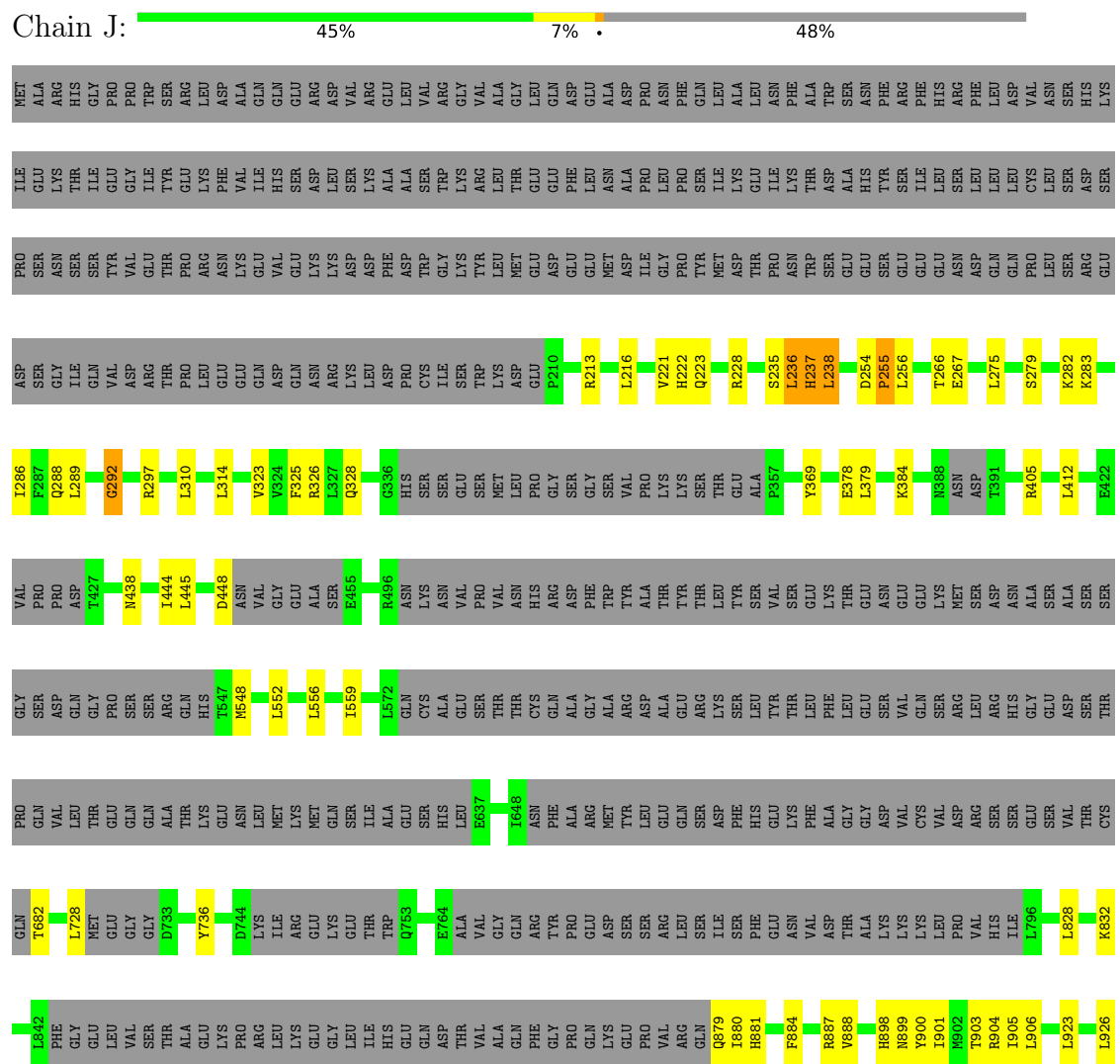
Response	Percentage
Doing a good job	68%
Not doing a good job	9%
Don't know	22%

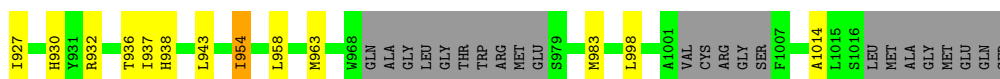


Frequency	Percentage
Often	75%
Sometimes	9%
Rarely	16%
Never	0%



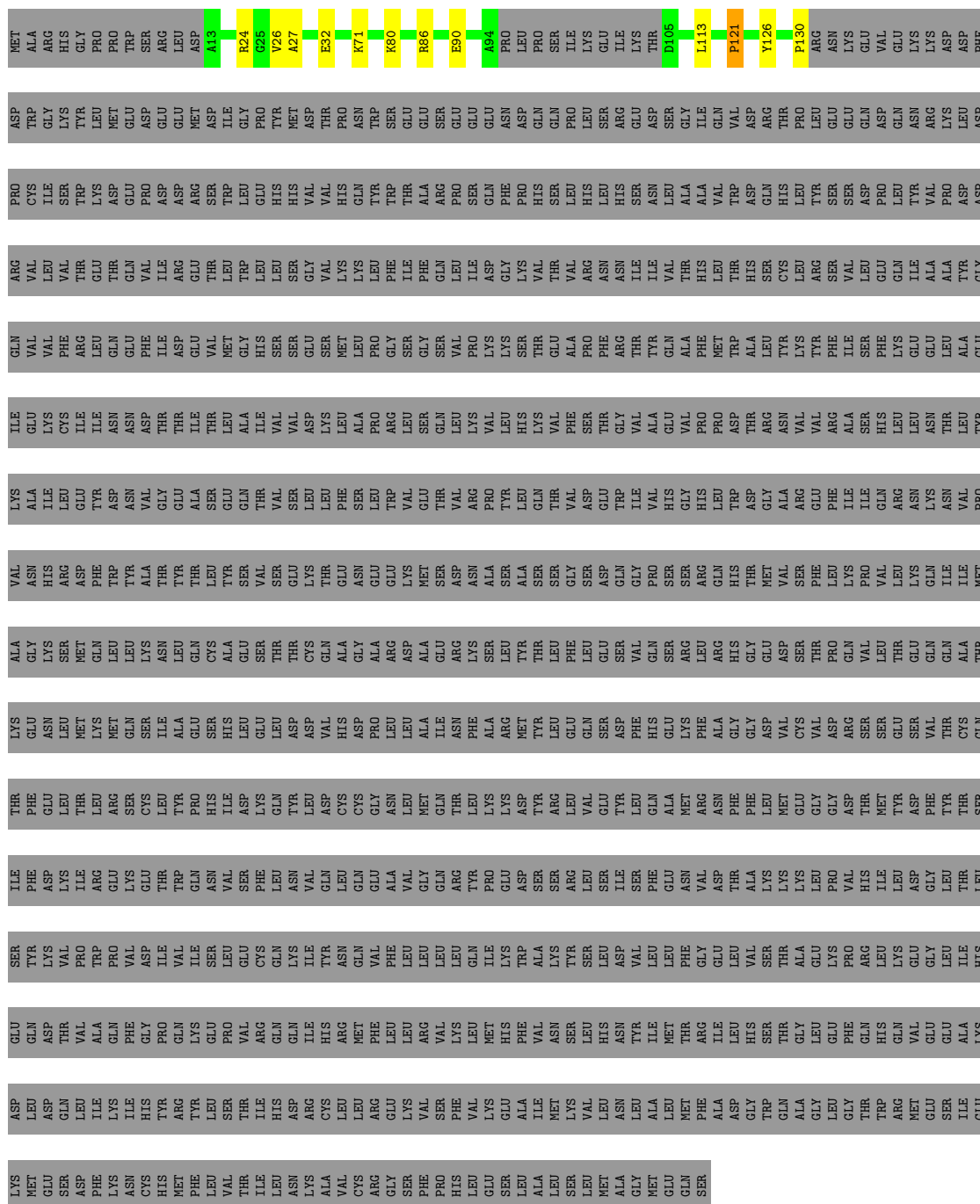
• Molecule 6: Gamma-tubulin complex component 5





• Molecule 6: Gamma-tubulin complex component 5

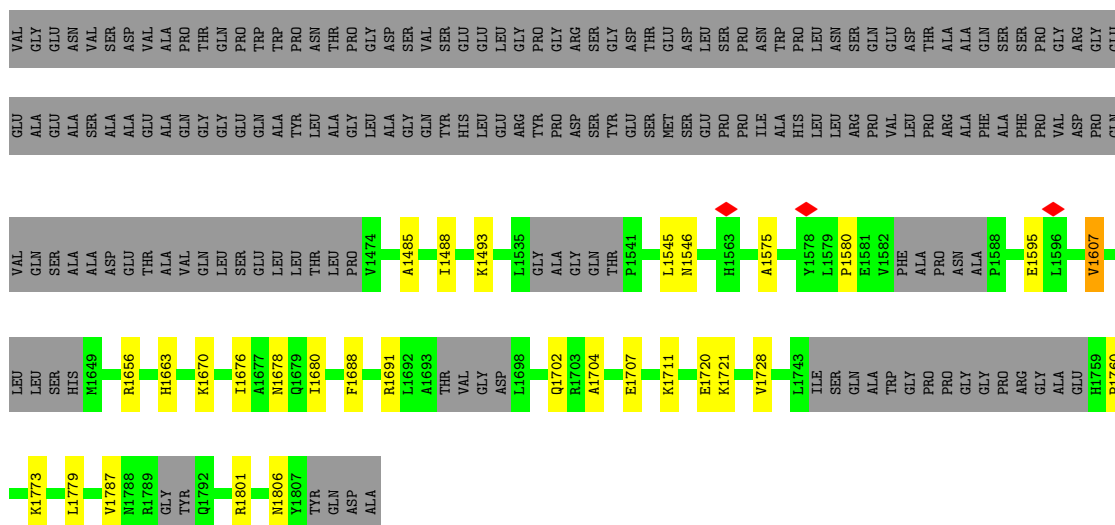
Chain 1: 9% . 89%



• Molecule 7: Gamma-tubulin complex component 6

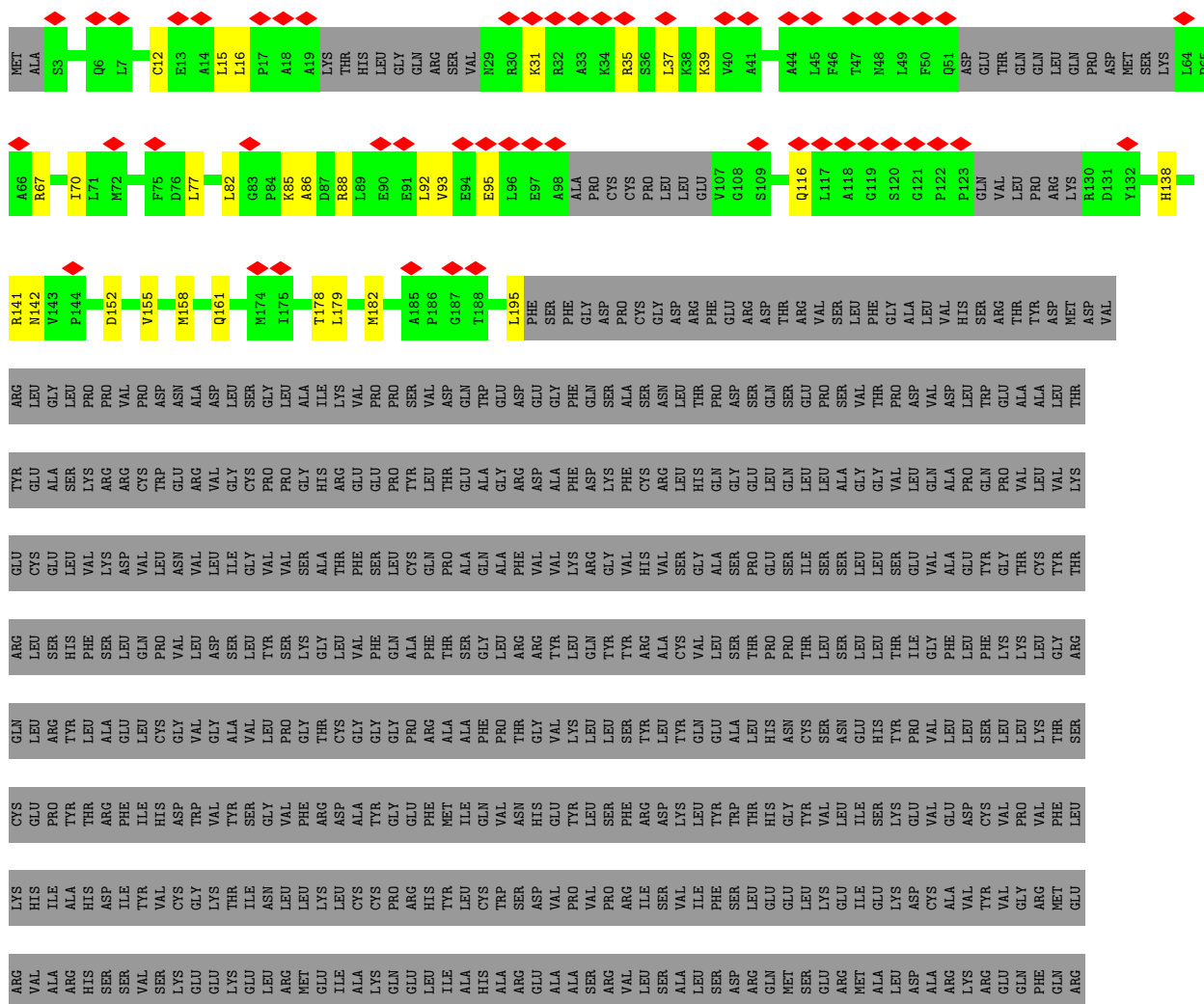
Chain L: 28% . 69%

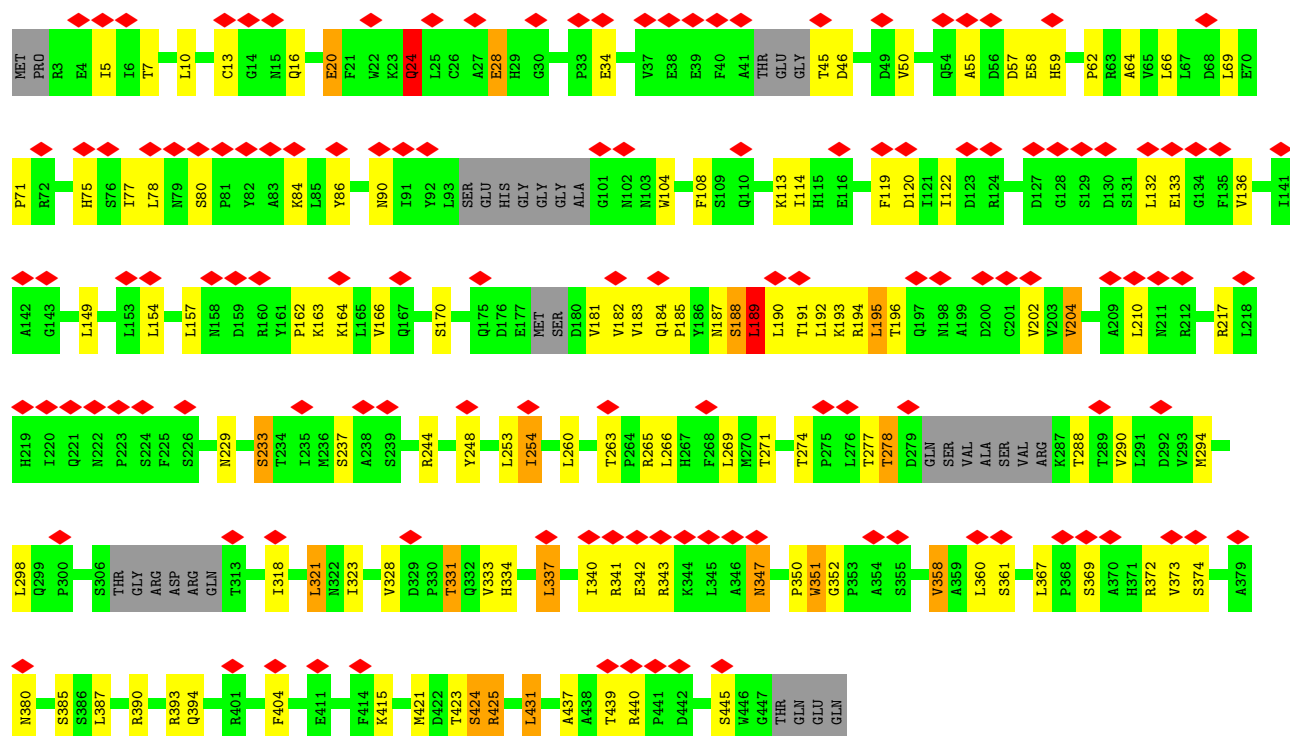




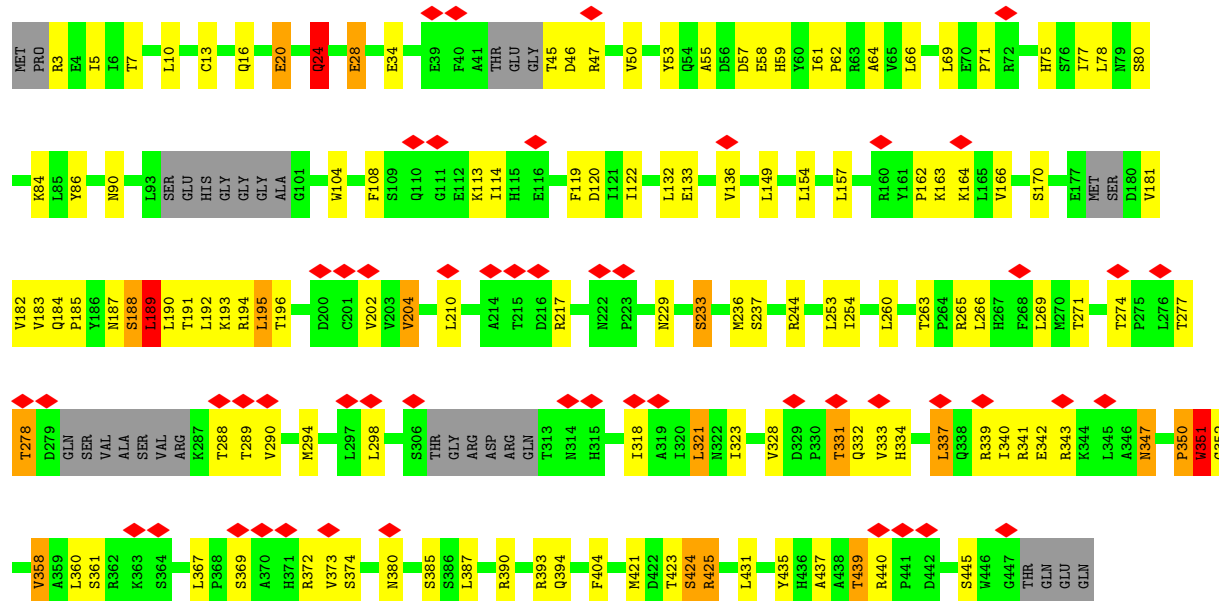
• Molecule 7: Gamma-tubulin complex component 6

Chain c: 7% . 91%



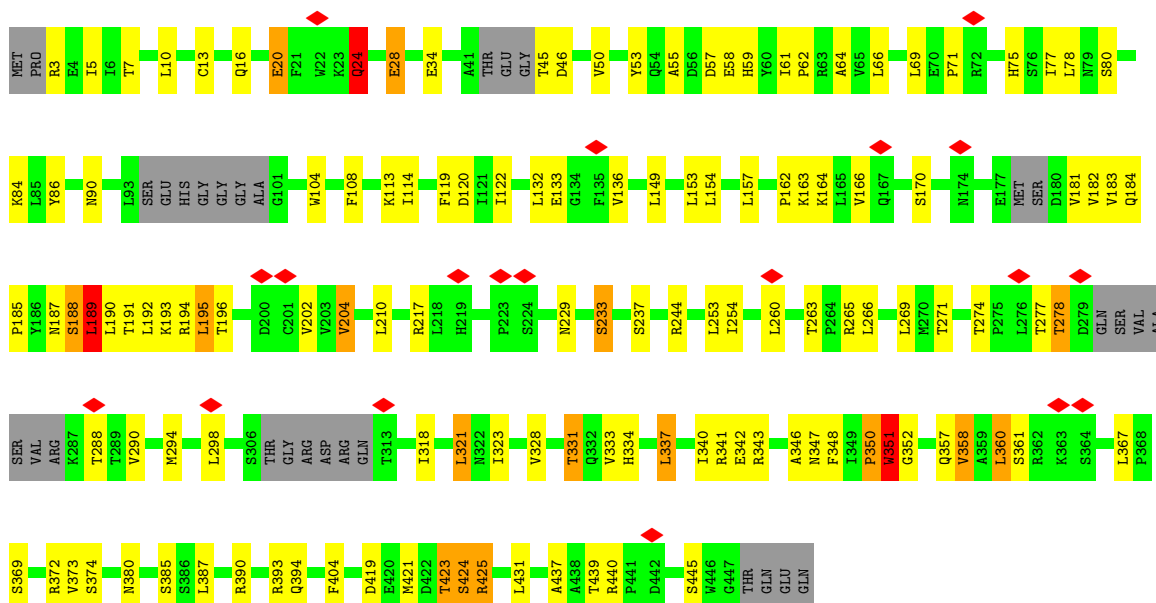


• Molecule 8: Tubulin gamma-1 chain



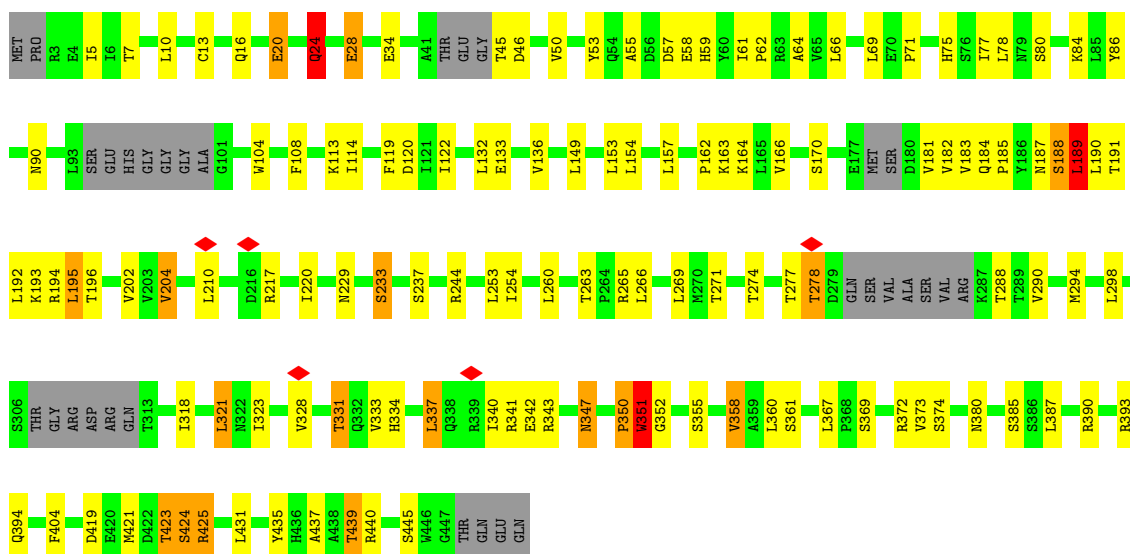
• Molecule 8: Tubulin gamma-1 chain





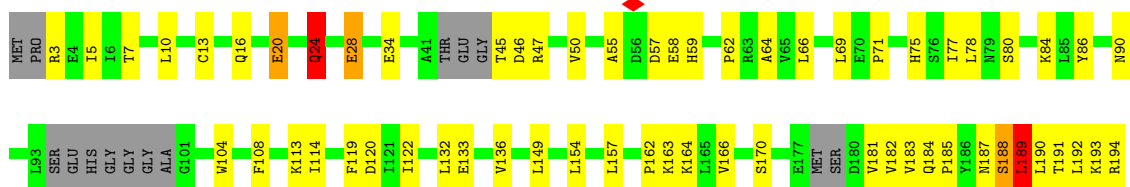
• Molecule 8: Tubulin gamma-1 chain

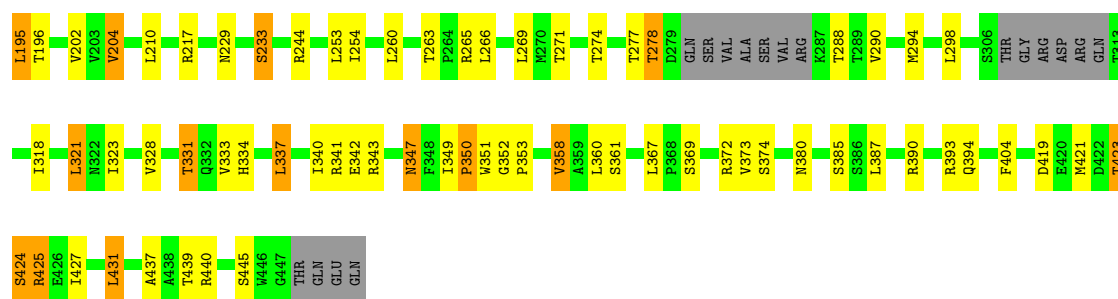
Chain T: 64% 25% 7%



• Molecule 8: Tubulin gamma-1 chain

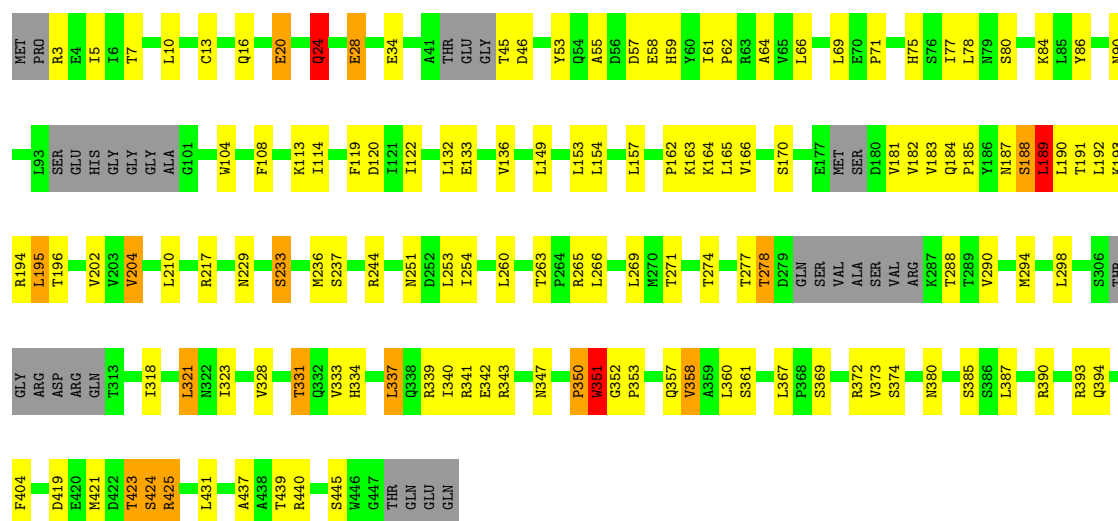
Chain U: 65% 24% 7%





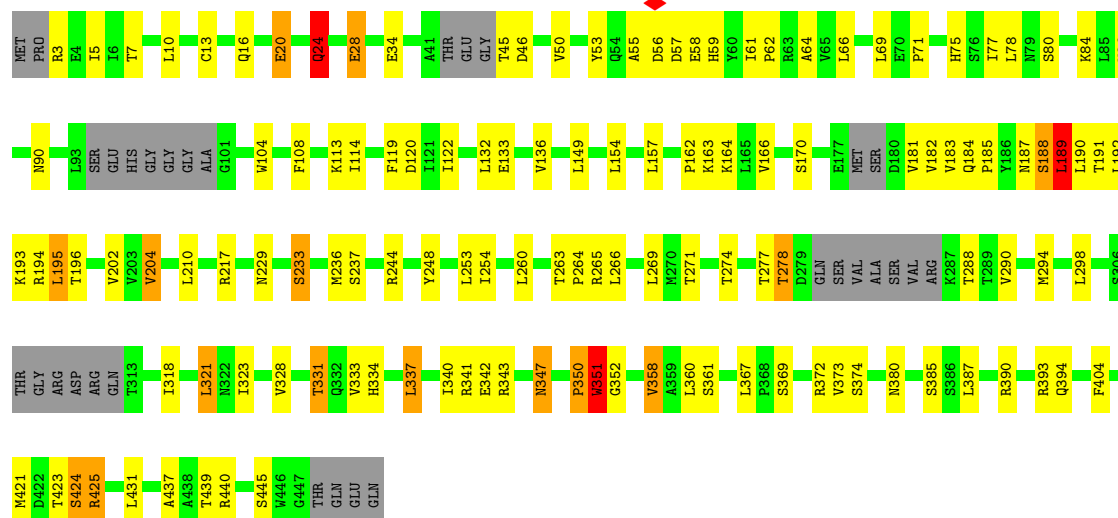
• Molecule 8: Tubulin gamma-1 chain

Chain V: 63% 26% 7%



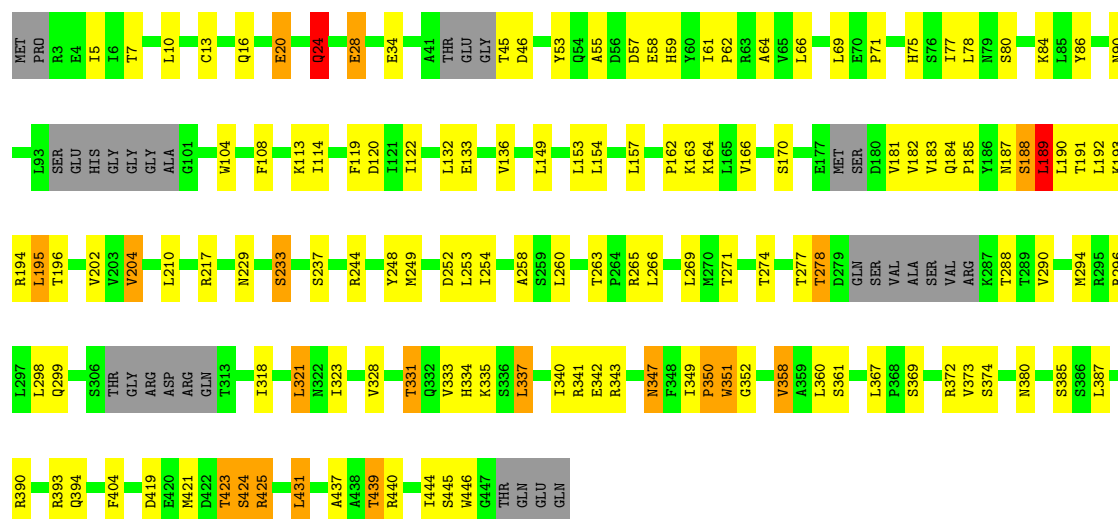
• Molecule 8: Tubulin gamma-1 chain

Chain W: 64% 25% 7%



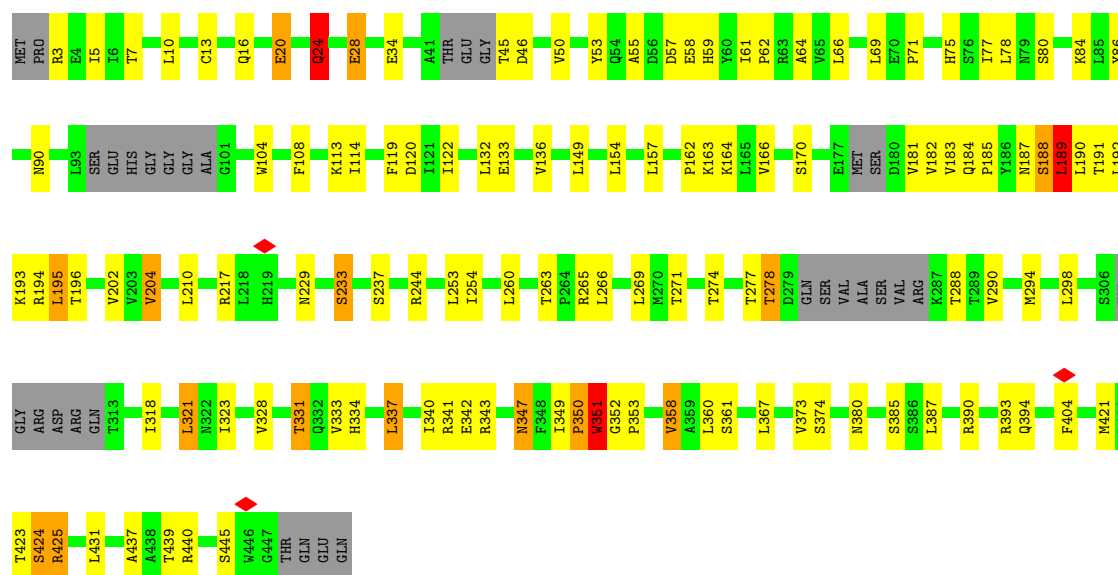
• Molecule 8: Tubulin gamma-1 chain

Chain X:  63% 26% 7%



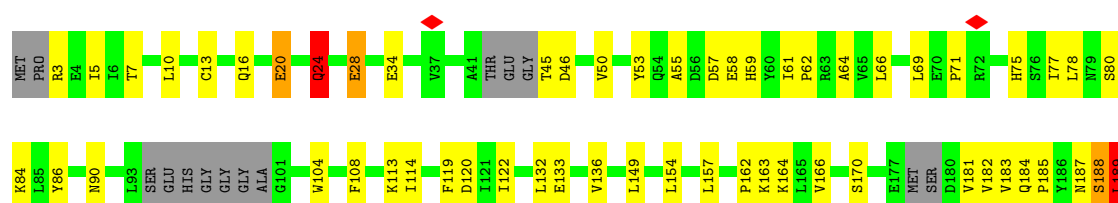
• Molecule 8: Tubulin gamma-1 chain

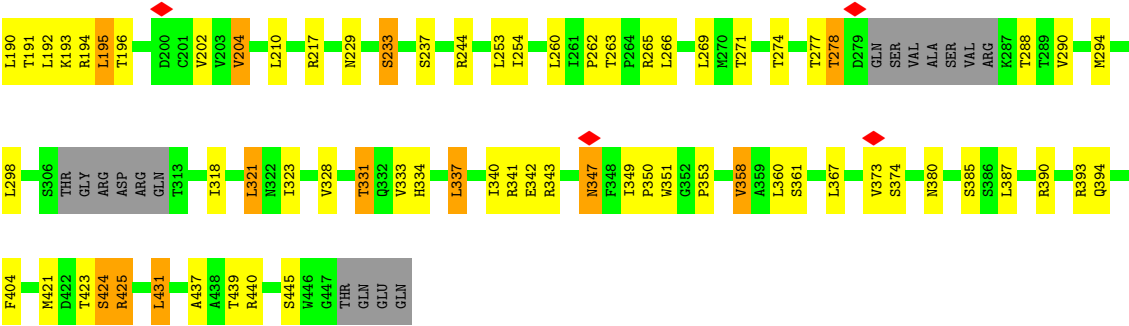
Chain Y:  65% 24% 7%



• Molecule 8: Tubulin gamma-1 chain

Chain Z:  65% 24% 7%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28611	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	0.247	Depositor
Minimum map value	-0.091	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0308	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	e	0.56	1/2908 (0.0%)	0.77	2/3938 (0.1%)
2	b	0.33	0/484	0.73	0/653
2	d	0.35	0/454	0.66	0/611
2	i	0.45	0/484	1.00	5/653 (0.8%)
2	k	0.28	0/484	0.62	0/653
2	m	0.31	0/484	0.70	0/653
3	D	0.33	0/4897	0.72	5/6610 (0.1%)
3	F	0.32	0/5044	0.71	4/6809 (0.1%)
3	H	0.34	0/5009	0.73	1/6761 (0.0%)
3	a	0.33	0/948	0.70	1/1277 (0.1%)
3	h	0.35	0/855	0.83	1/1152 (0.1%)
3	j	0.30	0/855	0.82	4/1152 (0.3%)
4	C	0.37	0/5151	0.82	11/6955 (0.2%)
4	E	0.38	1/5311 (0.0%)	0.75	8/7169 (0.1%)
4	G	0.35	0/5315	0.74	4/7175 (0.1%)
5	I	0.36	0/4322	0.75	1/5853 (0.0%)
5	K	0.35	1/4683 (0.0%)	0.75	5/6338 (0.1%)
6	J	0.39	0/4525	0.78	5/6119 (0.1%)
6	l	0.33	0/863	0.81	2/1166 (0.2%)
7	L	0.31	0/4697	0.72	5/6348 (0.1%)
7	c	0.32	0/1235	0.76	3/1664 (0.2%)
8	Q	0.28	0/3441	0.66	3/4661 (0.1%)
8	R	0.28	0/3441	0.66	3/4661 (0.1%)
8	S	0.28	0/3441	0.66	3/4661 (0.1%)
8	T	0.28	0/3441	0.66	3/4661 (0.1%)
8	U	0.29	0/3441	0.66	3/4661 (0.1%)
8	V	0.28	0/3441	0.66	3/4661 (0.1%)
8	W	0.28	0/3441	0.66	3/4661 (0.1%)
8	X	0.28	0/3441	0.66	3/4661 (0.1%)
8	Y	0.28	0/3441	0.66	3/4661 (0.1%)
8	Z	0.29	0/3441	0.68	6/4661 (0.1%)
All	All	0.34	3/93418 (0.0%)	0.72	100/126319 (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	H	0	1
4	E	0	2
4	G	0	2
5	I	0	4
5	K	0	1
6	J	0	1
7	L	0	2
8	Q	0	1
8	R	0	1
8	S	0	1
8	T	0	1
8	V	0	1
8	W	0	1
8	X	0	1
8	Y	0	1
All	All	0	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	243	PRO	N-CD	22.85	1.79	1.47
5	K	411	LEU	C-N	5.95	1.38	1.33
4	E	865	TYR	CD2-CE2	-5.67	1.21	1.38

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	j	108	PRO	N-CA-CB	11.26	115.08	103.25
3	h	108	PRO	N-CA-CB	8.93	112.63	103.25
3	D	418	ILE	N-CA-C	-8.82	104.71	112.12
4	E	580	HIS	CA-C-N	8.73	138.22	121.54
4	E	580	HIS	C-N-CA	8.73	138.22	121.54
4	C	288	VAL	N-CA-C	-8.54	104.95	112.12
3	j	107	GLN	CA-C-N	8.12	129.99	119.84
3	j	107	GLN	C-N-CA	8.12	129.99	119.84
7	L	1787	VAL	N-CA-C	-8.01	105.39	112.12
3	D	434	ILE	N-CA-C	-8.00	105.69	113.53
8	X	24	GLN	CB-CG-CD	7.64	125.59	112.60
8	Y	24	GLN	CB-CG-CD	7.64	125.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	W	24	GLN	CB-CG-CD	7.63	125.57	112.60
8	U	24	GLN	CB-CG-CD	7.62	125.56	112.60
8	Q	24	GLN	CB-CG-CD	7.62	125.55	112.60
8	Z	24	GLN	CB-CG-CD	7.61	125.53	112.60
8	R	24	GLN	CB-CG-CD	7.61	125.53	112.60
8	V	24	GLN	CB-CG-CD	7.61	125.53	112.60
8	T	24	GLN	CB-CG-CD	7.60	125.53	112.60
8	S	24	GLN	CB-CG-CD	7.60	125.52	112.60
6	l	121	PRO	N-CA-CB	7.26	110.88	103.25
4	E	865	TYR	OH-CZ-CE2	-7.04	98.77	119.90
6	l	130	PRO	N-CA-CB	7.03	110.73	103.00
4	G	815	VAL	N-CA-C	-6.73	106.23	112.43
3	j	41	SER	N-CA-C	-6.53	107.18	114.62
1	e	243	PRO	CA-N-CD	-6.45	102.97	112.00
3	H	726	VAL	N-CA-C	-6.37	106.59	112.96
3	F	269	ASN	CA-C-N	6.34	133.17	123.47
3	F	269	ASN	C-N-CA	6.34	133.17	123.47
3	D	581	LEU	CA-CB-CG	6.28	138.27	116.30
5	I	530	TYR	CA-CB-CG	6.27	125.19	113.90
4	C	483	ALA	N-CA-C	-6.15	105.30	114.64
4	E	287	GLN	N-CA-C	-6.12	107.04	114.75
7	c	195	LEU	CA-CB-CG	6.10	137.65	116.30
6	J	237	HIS	CA-C-N	6.06	133.11	121.54
6	J	237	HIS	C-N-CA	6.06	133.11	121.54
2	i	36	ASN	N-CA-C	6.02	123.62	110.80
4	C	205	ILE	N-CA-C	-6.00	108.01	113.71
8	Z	351	TRP	CA-C-N	-5.96	112.51	121.87
8	Z	351	TRP	C-N-CA	-5.96	112.51	121.87
5	K	255	LYS	N-CA-CB	5.95	120.55	110.49
2	i	35	LEU	CA-C-N	5.90	132.82	121.54
2	i	35	LEU	C-N-CA	5.90	132.82	121.54
4	E	424	ASN	N-CA-C	-5.89	105.69	114.64
7	L	316	GLY	CA-C-N	5.83	132.68	121.54
7	L	316	GLY	C-N-CA	5.83	132.68	121.54
4	C	564	ALA	N-CA-C	-5.82	104.00	113.19
8	T	24	GLN	CA-CB-CG	5.82	125.73	114.10
8	Q	24	GLN	CA-CB-CG	5.82	125.73	114.10
8	Z	24	GLN	CA-CB-CG	5.81	125.72	114.10
8	S	24	GLN	CA-CB-CG	5.81	125.72	114.10
8	U	24	GLN	CA-CB-CG	5.81	125.72	114.10
8	V	24	GLN	CA-CB-CG	5.81	125.71	114.10
8	W	24	GLN	CA-CB-CG	5.80	125.70	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	24	GLN	CA-CB-CG	5.80	125.69	114.10
8	X	24	GLN	CA-CB-CG	5.79	125.69	114.10
8	Y	24	GLN	CA-CB-CG	5.79	125.67	114.10
4	E	840	LEU	CB-CG-CD2	-5.77	93.40	110.70
2	i	36	ASN	CA-C-N	5.74	132.50	121.54
2	i	36	ASN	C-N-CA	5.74	132.50	121.54
8	Q	189	LEU	CA-CB-CG	5.72	136.33	116.30
8	V	189	LEU	CA-CB-CG	5.72	136.33	116.30
8	Z	349	ILE	O-C-N	-5.72	117.72	121.72
8	R	189	LEU	CA-CB-CG	5.72	136.32	116.30
8	S	189	LEU	CA-CB-CG	5.72	136.32	116.30
8	U	189	LEU	CA-CB-CG	5.72	136.32	116.30
8	W	189	LEU	CA-CB-CG	5.72	136.32	116.30
8	X	189	LEU	CA-CB-CG	5.71	136.30	116.30
8	T	189	LEU	CA-CB-CG	5.71	136.29	116.30
8	Y	189	LEU	CA-CB-CG	5.71	136.29	116.30
8	Z	189	LEU	CA-CB-CG	5.71	136.28	116.30
4	C	464	GLY	CA-C-N	5.70	132.42	121.54
4	C	464	GLY	C-N-CA	5.70	132.42	121.54
4	C	766	THR	CA-C-N	5.67	130.46	122.46
4	C	766	THR	C-N-CA	5.67	130.46	122.46
1	e	243	PRO	N-CA-CB	5.63	108.69	103.46
4	E	865	TYR	CE1-CZ-OH	5.62	136.77	119.90
3	F	272	GLU	CA-C-N	5.59	132.22	121.54
3	F	272	GLU	C-N-CA	5.59	132.22	121.54
6	J	292	GLY	N-CA-C	-5.58	106.86	116.01
5	K	263	ILE	CA-C-N	5.51	128.70	120.83
5	K	263	ILE	C-N-CA	5.51	128.70	120.83
3	a	46	THR	N-CA-C	-5.50	106.28	114.64
5	K	203	PHE	CA-C-N	5.48	132.00	121.54
5	K	203	PHE	C-N-CA	5.48	132.00	121.54
4	E	581	ASP	O-C-N	-5.47	115.31	122.59
7	c	82	LEU	CA-CB-CG	5.43	135.32	116.30
4	G	264	LEU	N-CA-C	5.41	121.77	109.81
7	L	306	HIS	CA-C-N	5.34	131.74	121.54
7	L	306	HIS	C-N-CA	5.34	131.74	121.54
3	D	495	GLN	CA-C-N	-5.31	117.20	122.77
3	D	495	GLN	C-N-CA	-5.31	117.20	122.77
4	C	467	VAL	N-CA-C	-5.26	108.72	113.71
6	J	235	SER	N-CA-C	-5.19	105.62	112.94
7	c	31	LYS	N-CA-C	-5.13	106.85	114.64
4	C	743	GLU	CA-C-N	5.10	131.28	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	743	GLU	C-N-CA	5.10	131.28	121.54
4	G	240	GLY	CA-C-N	5.10	131.28	121.54
4	G	240	GLY	C-N-CA	5.10	131.28	121.54
6	J	238	LEU	N-CA-C	5.03	121.51	110.80

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	581	ASP	Mainchain
4	E	865	TYR	Peptide
4	G	240	GLY	Peptide
4	G	580	HIS	Peptide
3	H	364	LEU	Peptide
5	I	407	ASP	Peptide
5	I	408	ASP	Mainchain
5	I	499	GLN	Peptide
5	I	507	SER	Peptide
6	J	255	PRO	Peptide
5	K	254	LEU	Peptide
7	L	306	HIS	Peptide
7	L	346	LEU	Peptide
8	Q	351	TRP	Peptide
8	R	351	TRP	Peptide
8	S	351	TRP	Peptide
8	T	351	TRP	Peptide
8	V	351	TRP	Peptide
8	W	351	TRP	Peptide
8	X	351	TRP	Peptide
8	Y	351	TRP	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	e	2847	0	2810	68	0
2	b	484	0	512	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	454	0	482	12	0
2	i	484	0	512	8	0
2	k	484	0	512	4	0
2	m	484	0	512	4	0
3	D	4796	0	4775	37	0
3	F	4941	0	4935	49	0
3	H	4907	0	4896	36	0
3	a	933	0	953	9	0
3	h	843	0	846	14	0
3	j	843	0	846	7	0
4	C	5044	0	5081	55	0
4	E	5202	0	5241	37	0
4	G	5206	0	5230	54	0
5	I	4225	0	4259	36	0
5	K	4579	0	4586	37	0
6	J	4429	0	4482	46	0
6	l	847	0	789	7	0
7	L	4587	0	4636	33	0
7	c	1220	0	1231	27	0
8	Q	3373	0	3325	58	0
8	R	3373	0	3325	69	0
8	S	3373	0	3325	63	0
8	T	3373	0	3325	59	0
8	U	3373	0	3325	63	0
8	V	3373	0	3325	65	0
8	W	3373	0	3325	61	0
8	X	3373	0	3325	69	0
8	Y	3373	0	3325	60	0
8	Z	3373	0	3325	58	0
9	l	6	0	0	1	0
All	All	91575	0	91376	1122	0

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

All (1122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:243:PRO:CD	1:e:243:PRO:N	1.79	1.39
1:e:3:ASP:OD1	7:c:35:ARG:NH2	1.69	1.23
1:e:160:THR:HG21	1:e:178:LEU:CD2	1.69	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:160:THR:HG21	1:e:178:LEU:HD23	1.37	1.05
1:e:3:ASP:OD1	7:c:35:ARG:CZ	2.04	1.05
1:e:160:THR:HG21	1:e:178:LEU:HD22	1.40	1.00
1:e:160:THR:HG22	1:e:178:LEU:O	1.65	0.95
1:e:3:ASP:CG	7:c:35:ARG:NH2	2.25	0.94
1:e:3:ASP:OD2	7:c:35:ARG:NE	2.04	0.89
1:e:160:THR:HG23	1:e:178:LEU:HB3	1.56	0.88
1:e:160:THR:CG2	1:e:178:LEU:CD2	2.53	0.87
1:e:160:THR:CG2	1:e:178:LEU:O	2.25	0.84
1:e:160:THR:CG2	1:e:178:LEU:HD23	2.07	0.84
1:e:3:ASP:CG	7:c:35:ARG:HH21	1.88	0.81
4:C:656:CYS:HB3	8:Q:254:ILE:HD11	1.63	0.80
7:L:1806:ASN:HD22	8:Z:353:PRO:HB3	1.47	0.80
4:E:414:LEU:HG	4:E:424:ASN:HB2	1.65	0.78
4:E:688:ASN:HD21	8:S:357:GLN:HE22	1.32	0.78
4:C:482:ARG:HH11	4:C:486:GLU:HG2	1.52	0.75
6:J:881:HIS:NE2	8:X:444:ILE:O	2.20	0.74
4:E:865:TYR:OH	8:S:350:PRO:O	2.03	0.74
1:e:3:ASP:CG	7:c:35:ARG:CZ	2.60	0.72
3:F:543:LYS:HD3	3:F:742:GLN:HG2	1.72	0.72
8:V:185:PRO:O	8:V:189:LEU:HB3	1.92	0.70
8:Z:185:PRO:O	8:Z:189:LEU:HB3	1.92	0.70
3:D:739:GLN:HE21	3:D:740:GLN:HE22	1.39	0.70
8:W:185:PRO:O	8:W:189:LEU:HB3	1.92	0.70
8:Q:185:PRO:O	8:Q:189:LEU:HB3	1.92	0.70
8:S:185:PRO:O	8:S:189:LEU:HB3	1.92	0.70
8:R:185:PRO:O	8:R:189:LEU:HB3	1.92	0.70
3:F:363:THR:OG1	3:F:366:ARG:NH2	2.25	0.69
3:H:829:GLU:HA	3:H:832:ARG:HD3	1.75	0.69
8:T:185:PRO:O	8:T:189:LEU:HB3	1.92	0.69
8:U:185:PRO:O	8:U:189:LEU:HB3	1.92	0.69
1:e:107:GLU:HB2	1:e:111:ASN:HD22	1.57	0.69
8:X:185:PRO:O	8:X:189:LEU:HB3	1.92	0.68
8:Y:185:PRO:O	8:Y:189:LEU:HB3	1.92	0.68
8:S:62:PRO:HD2	8:S:86:TYR:HB3	1.76	0.68
8:Y:62:PRO:HD2	8:Y:86:TYR:HB3	1.76	0.68
3:h:49:ARG:HE	3:h:91:TRP:HB3	1.58	0.68
8:X:62:PRO:HD2	8:X:86:TYR:HB3	1.76	0.68
4:E:613:LEU:HD11	4:E:647:TYR:HA	1.75	0.68
8:R:62:PRO:HD2	8:R:86:TYR:HB3	1.76	0.68
4:C:526:ASP:HB3	4:C:562:SER:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:62:PRO:HD2	8:T:86:TYR:HB3	1.76	0.67
8:W:56:ASP:O	8:X:296:ARG:NE	2.28	0.67
3:H:365:ARG:HB2	3:H:368:LEU:HB2	1.77	0.67
5:K:518:ARG:HH12	5:K:589:LEU:HD13	1.60	0.67
8:W:62:PRO:HD2	8:W:86:TYR:HB3	1.76	0.67
5:I:312:HIS:HA	5:I:315:LYS:HD2	1.76	0.66
8:Q:62:PRO:HD2	8:Q:86:TYR:HB3	1.76	0.66
8:Z:62:PRO:HD2	8:Z:86:TYR:HB3	1.76	0.66
5:I:85:TYR:OH	5:I:151:CYS:SG	2.54	0.66
8:U:62:PRO:HD2	8:U:86:TYR:HB3	1.76	0.66
8:V:62:PRO:HD2	8:V:86:TYR:HB3	1.76	0.66
6:J:279:SER:HB3	6:J:379:LEU:HD22	1.76	0.66
4:C:334:THR:OG1	4:C:371:GLN:NE2	2.30	0.65
5:I:515:TRP:HE1	5:I:519:ASN:H	1.44	0.65
6:J:222:HIS:HE1	5:K:33:PHE:HA	1.62	0.65
5:K:646:LEU:HB3	8:Y:341:ARG:HD2	1.79	0.65
6:J:898:HIS:NE2	8:X:249:MET:SD	2.69	0.64
8:S:217:ARG:HE	8:S:277:THR:HA	1.63	0.64
8:Q:217:ARG:HE	8:Q:277:THR:HA	1.63	0.63
8:V:217:ARG:HE	8:V:277:THR:HA	1.63	0.63
8:Z:217:ARG:HE	8:Z:277:THR:HA	1.63	0.63
8:U:217:ARG:HE	8:U:277:THR:HA	1.63	0.63
8:W:217:ARG:HE	8:W:277:THR:HA	1.63	0.63
2:i:73:ALA:H	3:h:23:ARG:HH21	1.46	0.63
4:C:645:MET:HE3	4:C:698:MET:HE3	1.80	0.63
4:G:863:GLY:HA2	8:U:353:PRO:HB3	1.79	0.63
8:V:24:GLN:HE21	8:V:24:GLN:HA	1.64	0.62
1:e:160:THR:CG2	1:e:178:LEU:HD22	2.23	0.62
4:C:696:TYR:O	4:C:700:GLU:HB2	1.99	0.62
8:T:217:ARG:HE	8:T:277:THR:HA	1.63	0.62
8:Z:24:GLN:HE21	8:Z:24:GLN:HA	1.64	0.62
8:U:24:GLN:HE21	8:U:24:GLN:HA	1.65	0.62
8:Y:217:ARG:HE	8:Y:277:THR:HA	1.63	0.62
1:e:186:THR:HA	1:e:189:LEU:HD12	1.81	0.62
4:C:534:LEU:HD13	4:C:557:LEU:HG	1.81	0.62
6:J:828:LEU:O	6:J:832:LYS:NZ	2.28	0.62
8:R:24:GLN:HE21	8:R:24:GLN:HA	1.64	0.62
8:X:217:ARG:HE	8:X:277:THR:HA	1.63	0.62
8:Y:24:GLN:HE21	8:Y:24:GLN:HA	1.64	0.62
8:Q:24:GLN:HA	8:Q:24:GLN:HE21	1.64	0.62
2:b:35:LEU:HD21	3:a:97:LEU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:193:LYS:HB2	8:V:424:SER:HB2	1.82	0.62
8:T:193:LYS:HB2	8:T:424:SER:HB2	1.82	0.62
8:T:24:GLN:HE21	8:T:24:GLN:HA	1.64	0.61
8:X:193:LYS:HB2	8:X:424:SER:HB2	1.82	0.61
7:c:70:ILE:HG21	7:c:93:VAL:HG21	1.81	0.61
8:R:193:LYS:HB2	8:R:424:SER:HB2	1.82	0.61
8:R:217:ARG:HE	8:R:277:THR:HA	1.63	0.61
1:e:246:GLN:HE22	1:e:248:ILE:HG23	1.65	0.61
8:Y:193:LYS:HB2	8:Y:424:SER:HB2	1.82	0.61
4:E:688:ASN:HD21	8:S:357:GLN:NE2	1.98	0.61
8:W:193:LYS:HB2	8:W:424:SER:HB2	1.82	0.61
8:Q:193:LYS:HB2	8:Q:424:SER:HB2	1.82	0.61
8:Z:193:LYS:HB2	8:Z:424:SER:HB2	1.82	0.61
3:h:58:ILE:HG12	3:h:98:LEU:HD21	1.83	0.61
1:e:16:MET:HE2	1:e:336:LYS:HE3	1.82	0.61
8:S:24:GLN:HE21	8:S:24:GLN:HA	1.64	0.61
8:U:193:LYS:HB2	8:U:424:SER:HB2	1.82	0.61
8:X:24:GLN:HA	8:X:24:GLN:HE21	1.65	0.61
3:F:553:TYR:HB3	3:F:648:ILE:HD11	1.82	0.60
8:S:193:LYS:HB2	8:S:424:SER:HB2	1.82	0.60
2:d:26:ASP:HA	2:d:29:LEU:HD12	1.83	0.60
4:G:578:MET:H	4:G:615:ALA:HB1	1.66	0.60
8:W:24:GLN:HE21	8:W:24:GLN:HA	1.64	0.60
5:I:184:TYR:HB3	5:I:315:LYS:HZ2	1.67	0.60
5:I:363:LEU:HD13	5:I:486:ARG:HH21	1.66	0.60
5:I:131:LEU:HB3	5:I:165:LEU:HD21	1.84	0.60
6:J:900:TYR:O	6:J:904:ARG:HB3	2.01	0.60
3:F:589:ALA:HA	3:F:592:LEU:HD13	1.82	0.59
4:E:294:ALA:HB1	7:c:138:HIS:HB3	1.83	0.59
4:E:862:ASN:ND2	8:S:346:ALA:O	2.34	0.59
1:e:176:LEU:HD22	1:e:277:THR:HG23	1.85	0.59
3:H:720:TYR:HE2	8:V:357:GLN:HB3	1.67	0.59
1:e:3:ASP:CG	7:c:35:ARG:NE	2.61	0.59
1:e:216:LEU:HD22	1:e:238:LYS:HE2	1.85	0.59
4:C:276:PHE:HB3	4:C:296:MET:HE1	1.85	0.59
4:G:511:ALA:HA	4:G:514:ARG:HE	1.68	0.59
5:I:154:LEU:O	5:I:158:TYR:HB2	2.03	0.59
7:L:1607:VAL:HG12	7:L:1702:GLN:HG2	1.83	0.59
3:H:431:TYR:HA	3:H:434:ILE:HG22	1.84	0.58
5:I:486:ARG:HH22	8:W:248:TYR:HE1	1.48	0.58
4:G:563:THR:HG21	8:U:47:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:582:CYS:HB2	5:K:626:LEU:HD13	1.86	0.58
6:J:266:THR:OG1	6:J:267:GLU:N	2.36	0.58
8:V:183:VAL:HG13	8:V:187:ASN:HD21	1.69	0.58
8:Y:64:ALA:O	8:Y:90:ASN:ND2	2.37	0.58
8:X:64:ALA:O	8:X:90:ASN:ND2	2.37	0.58
4:G:242:GLN:HE21	4:G:343:THR:HG23	1.68	0.58
6:J:963:MET:HE2	6:J:983:MET:HE2	1.84	0.58
5:K:62:TYR:HB3	5:K:86:LEU:HD21	1.86	0.58
8:R:183:VAL:HG13	8:R:187:ASN:HD21	1.69	0.58
8:S:183:VAL:HG13	8:S:187:ASN:HD21	1.69	0.58
8:X:183:VAL:HG13	8:X:187:ASN:HD21	1.69	0.58
6:J:438:ASN:ND2	6:J:548:MET:O	2.37	0.58
5:K:7:LEU:HD23	7:L:392:SER:HB3	1.84	0.58
8:T:183:VAL:HG13	8:T:187:ASN:HD21	1.69	0.58
8:Z:64:ALA:O	8:Z:90:ASN:ND2	2.37	0.58
5:K:653:LYS:HG2	8:Y:353:PRO:HB3	1.85	0.58
4:G:356:LEU:HG	4:G:440:PRO:HB3	1.87	0.57
8:R:64:ALA:O	8:R:90:ASN:ND2	2.37	0.57
8:Z:183:VAL:HG13	8:Z:187:ASN:HD21	1.69	0.57
8:S:64:ALA:O	8:S:90:ASN:ND2	2.37	0.57
8:T:217:ARG:HH21	8:T:278:THR:H	1.53	0.57
8:U:64:ALA:O	8:U:90:ASN:ND2	2.37	0.57
8:U:217:ARG:HH21	8:U:278:THR:H	1.53	0.57
4:E:356:LEU:HD23	4:E:359:LEU:HD21	1.85	0.57
8:Q:64:ALA:O	8:Q:90:ASN:ND2	2.37	0.57
8:V:64:ALA:O	8:V:90:ASN:ND2	2.37	0.57
7:L:294:ARG:HH11	7:L:305:GLY:HA2	1.67	0.57
8:Q:217:ARG:HH21	8:Q:278:THR:H	1.52	0.57
8:Y:217:ARG:HH21	8:Y:278:THR:H	1.53	0.57
1:e:282:ILE:HG21	1:e:320:LEU:HD21	1.84	0.57
8:U:183:VAL:HG13	8:U:187:ASN:HD21	1.69	0.57
8:W:217:ARG:HH21	8:W:278:THR:H	1.53	0.57
6:J:899:ASN:O	6:J:903:THR:OG1	2.23	0.57
4:E:559:LEU:HD21	4:E:570:LYS:HG3	1.86	0.57
5:K:17:PHE:HE1	5:K:42:LEU:HD21	1.69	0.57
4:G:709:LEU:HD13	4:G:729:PHE:HB2	1.87	0.57
8:T:64:ALA:O	8:T:90:ASN:ND2	2.37	0.57
8:V:217:ARG:HH21	8:V:278:THR:H	1.53	0.57
8:W:183:VAL:HG13	8:W:187:ASN:HD21	1.69	0.57
7:c:85:LYS:HG3	7:c:88:ARG:HH12	1.70	0.57
3:F:266:ILE:HD11	3:F:275:TYR:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:183:VAL:HG13	8:Y:187:ASN:HD21	1.69	0.57
8:Y:318:ILE:HB	8:Y:380:ASN:HB3	1.87	0.57
3:F:797:LEU:HA	3:F:800:LEU:HD12	1.85	0.57
8:Q:183:VAL:HG13	8:Q:187:ASN:HD21	1.69	0.57
8:S:318:ILE:HB	8:S:380:ASN:HB3	1.87	0.57
8:T:318:ILE:HB	8:T:380:ASN:HB3	1.87	0.57
8:W:64:ALA:O	8:W:90:ASN:ND2	2.37	0.57
8:Z:318:ILE:HB	8:Z:380:ASN:HB3	1.87	0.57
3:F:627:GLU:HG3	3:j:60:LYS:HD2	1.86	0.56
3:D:710:GLU:OE1	3:D:855:GLN:NE2	2.38	0.56
8:X:13:CYS:HA	8:X:16:GLN:HE21	1.71	0.56
7:c:77:LEU:HD22	7:c:86:ALA:HB2	1.88	0.56
4:E:359:LEU:HD13	4:E:380:THR:HG22	1.88	0.56
5:K:519:ASN:HD22	5:K:593:PHE:HE2	1.52	0.56
8:Q:13:CYS:HA	8:Q:16:GLN:HE21	1.71	0.56
8:R:318:ILE:HB	8:R:380:ASN:HB3	1.87	0.56
8:W:13:CYS:HA	8:W:16:GLN:HE21	1.71	0.56
8:X:217:ARG:HH21	8:X:278:THR:H	1.53	0.56
8:X:318:ILE:HB	8:X:380:ASN:HB3	1.87	0.56
3:D:320:VAL:HG21	3:D:393:GLY:H	1.70	0.56
8:Q:318:ILE:HB	8:Q:380:ASN:HB3	1.87	0.56
8:S:13:CYS:HA	8:S:16:GLN:HE21	1.71	0.56
3:F:879:ARG:NH1	8:T:355:SER:OG	2.39	0.56
5:K:523:PHE:O	5:K:527:ASN:ND2	2.38	0.56
8:R:13:CYS:HA	8:R:16:GLN:HE21	1.71	0.56
8:Z:217:ARG:HH21	8:Z:278:THR:H	1.52	0.56
4:C:335:MET:HG3	4:C:338:LEU:HD12	1.87	0.56
8:V:13:CYS:HA	8:V:16:GLN:HE21	1.71	0.56
3:F:798:GLU:HA	3:F:801:GLN:HE21	1.70	0.55
8:V:318:ILE:HB	8:V:380:ASN:HB3	1.87	0.55
3:D:566:LEU:HD21	3:D:660:TYR:HB3	1.88	0.55
6:J:288:GLN:HE21	6:J:297:ARG:HG3	1.71	0.55
8:W:182:VAL:HB	8:W:404:PHE:HB3	1.89	0.55
1:e:16:MET:SD	1:e:16:MET:N	2.79	0.55
4:C:273:VAL:HG13	4:C:296:MET:HE3	1.87	0.55
3:H:655:GLU:O	3:H:658:SER:OG	2.23	0.55
6:J:879:GLN:HG2	6:J:880:ILE:HG13	1.87	0.55
5:K:34:LEU:HD12	5:K:38:GLU:HG3	1.88	0.55
8:R:217:ARG:HH21	8:R:278:THR:H	1.53	0.55
8:U:13:CYS:HA	8:U:16:GLN:HE21	1.71	0.55
8:Z:13:CYS:HA	8:Z:16:GLN:HE21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:821:THR:HA	4:C:824:LYS:HG2	1.88	0.55
5:K:651:TYR:CE2	8:Y:349:ILE:HG22	2.41	0.55
8:X:182:VAL:HB	8:X:404:PHE:HB3	1.89	0.55
4:C:413:GLU:OE1	4:C:431:ARG:NH2	2.35	0.55
8:T:13:CYS:HA	8:T:16:GLN:HE21	1.71	0.55
8:W:318:ILE:HB	8:W:380:ASN:HB3	1.87	0.55
8:Y:13:CYS:HA	8:Y:16:GLN:HE21	1.71	0.55
1:e:68:LYS:HD2	1:e:77:THR:HG21	1.89	0.55
3:D:323:SER:HB3	3:D:421:LEU:HG	1.87	0.55
3:D:707:LEU:HG	3:D:711:MET:HE1	1.89	0.55
8:V:182:VAL:HB	8:V:404:PHE:HB3	1.89	0.55
8:U:318:ILE:HB	8:U:380:ASN:HB3	1.87	0.55
4:E:353:GLY:HA2	4:E:356:LEU:HD12	1.87	0.55
4:E:555:LEU:HD13	4:E:575:ILE:HD11	1.87	0.55
3:F:654:ARG:HH22	3:F:658:SER:HB3	1.70	0.55
3:H:455:LYS:HB3	3:H:459:LEU:HG	1.88	0.55
7:L:1801:ARG:HH11	8:Z:337:LEU:HD21	1.72	0.55
8:S:217:ARG:HH21	8:S:278:THR:H	1.52	0.55
8:T:182:VAL:HB	8:T:404:PHE:HB3	1.89	0.55
8:S:182:VAL:HB	8:S:404:PHE:HB3	1.89	0.55
8:Y:182:VAL:HB	8:Y:404:PHE:HB3	1.89	0.55
4:C:560:ARG:NH1	8:R:289:THR:OG1	2.40	0.54
8:U:182:VAL:HB	8:U:404:PHE:HB3	1.89	0.54
8:W:341:ARG:NH1	8:W:342:GLU:OE1	2.40	0.54
7:L:461:PHE:HA	7:L:464:LYS:HD2	1.88	0.54
7:L:1485:ALA:HA	7:L:1488:ILE:HD12	1.89	0.54
8:X:184:GLN:O	8:X:188:SER:OG	2.25	0.54
8:X:341:ARG:NH1	8:X:342:GLU:OE1	2.41	0.54
8:Y:341:ARG:NH1	8:Y:342:GLU:OE1	2.40	0.54
2:d:61:SER:OG	7:c:116:GLN:OE1	2.26	0.54
4:C:556:GLU:HB3	8:R:339:ARG:HH11	1.73	0.54
8:W:56:ASP:HB3	8:X:299:GLN:OE1	2.06	0.54
8:Y:184:GLN:O	8:Y:188:SER:OG	2.25	0.54
8:S:71:PRO:O	8:S:75:HIS:NE2	2.41	0.54
8:V:71:PRO:O	8:V:75:HIS:NE2	2.41	0.54
3:h:49:ARG:NH2	3:h:92:SER:OG	2.40	0.54
4:C:484:TYR:C	4:C:486:GLU:H	2.15	0.54
6:J:901:ILE:HA	6:J:905:ILE:HD12	1.88	0.54
8:Q:71:PRO:O	8:Q:75:HIS:NE2	2.41	0.54
8:R:182:VAL:HB	8:R:404:PHE:HB3	1.89	0.54
8:R:341:ARG:NH1	8:R:342:GLU:OE1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:71:PRO:O	8:X:75:HIS:NE2	2.41	0.54
7:c:16:LEU:HD21	7:c:37:LEU:HD12	1.89	0.54
4:C:359:LEU:HD21	4:C:379:LEU:HB3	1.88	0.54
3:F:594:GLN:NE2	3:F:623:VAL:O	2.36	0.54
8:R:229:ASN:O	8:R:233:SER:OG	2.25	0.54
5:K:27:VAL:HG13	5:K:29:GLN:HB3	1.90	0.54
1:e:348:SER:HB2	7:c:39:LYS:HE2	1.90	0.54
8:Q:182:VAL:HB	8:Q:404:PHE:HB3	1.89	0.54
8:U:437:ALA:HA	8:U:440:ARG:HG2	1.90	0.54
8:X:45:THR:OG1	8:X:46:ASP:N	2.41	0.54
8:Y:437:ALA:HA	8:Y:440:ARG:HG2	1.90	0.54
3:F:337:ARG:O	3:F:340:SER:OG	2.23	0.53
5:I:98:GLN:HA	5:I:101:ARG:HD2	1.90	0.53
2:k:57:PRO:HA	2:k:60:LEU:HB2	1.91	0.53
8:Q:341:ARG:NH1	8:Q:342:GLU:OE1	2.40	0.53
8:U:45:THR:OG1	8:U:46:ASP:N	2.41	0.53
8:V:341:ARG:NH1	8:V:342:GLU:OE1	2.40	0.53
8:Z:182:VAL:HB	8:Z:404:PHE:HB3	1.89	0.53
7:c:152:ASP:HA	7:c:155:VAL:HG22	1.90	0.53
3:D:548:VAL:HG22	3:D:552:LYS:HE2	1.90	0.53
3:D:586:VAL:HG12	3:D:635:TRP:HE1	1.72	0.53
5:K:515:TRP:O	5:K:519:ASN:HB2	2.08	0.53
8:T:341:ARG:NH1	8:T:342:GLU:OE1	2.40	0.53
8:T:437:ALA:HA	8:T:440:ARG:HG2	1.90	0.53
8:U:341:ARG:NH1	8:U:342:GLU:OE1	2.40	0.53
8:W:437:ALA:HA	8:W:440:ARG:HG2	1.90	0.53
7:L:1676:ILE:HG23	7:L:1680:ILE:HD12	1.89	0.53
8:Z:184:GLN:O	8:Z:188:SER:OG	2.25	0.53
8:Q:45:THR:OG1	8:Q:46:ASP:N	2.41	0.53
8:Y:71:PRO:O	8:Y:75:HIS:NE2	2.41	0.53
8:Z:71:PRO:O	8:Z:75:HIS:NE2	2.41	0.53
8:Z:341:ARG:NH1	8:Z:342:GLU:OE1	2.40	0.53
3:h:59:LYS:HD2	3:h:71:ALA:HB1	1.89	0.53
4:G:158:ARG:HA	4:G:161:LEU:HD12	1.90	0.53
6:J:881:HIS:ND1	8:X:446:TRP:HB3	2.24	0.53
8:Q:229:ASN:O	8:Q:233:SER:OG	2.25	0.53
8:W:71:PRO:O	8:W:75:HIS:NE2	2.41	0.53
4:C:473:LYS:HE2	4:C:474:GLU:HG3	1.91	0.53
8:S:341:ARG:NH1	8:S:342:GLU:OE1	2.40	0.53
8:T:71:PRO:O	8:T:75:HIS:NE2	2.41	0.53
2:b:59:ALA:O	2:b:62:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:71:PRO:O	8:R:75:HIS:NE2	2.41	0.53
8:U:71:PRO:O	8:U:75:HIS:NE2	2.41	0.53
4:E:297:ARG:NH1	3:F:408:ASP:OD2	2.39	0.53
8:S:437:ALA:HA	8:S:440:ARG:HG2	1.90	0.53
8:W:45:THR:OG1	8:W:46:ASP:N	2.41	0.53
4:C:835:ASP:OD1	4:C:871:ARG:NH2	2.42	0.53
4:E:454:GLY:HA2	4:E:457:LEU:HD12	1.91	0.53
3:F:736:ASN:HA	3:F:739:GLN:HE21	1.73	0.53
6:J:887:ARG:NH1	8:X:258:ALA:O	2.42	0.53
8:Q:184:GLN:O	8:Q:188:SER:OG	2.25	0.53
8:Q:437:ALA:HA	8:Q:440:ARG:HG2	1.90	0.53
8:V:437:ALA:HA	8:V:440:ARG:HG2	1.90	0.53
8:X:437:ALA:HA	8:X:440:ARG:HG2	1.90	0.53
3:H:712:VAL:O	3:H:716:HIS:ND1	2.33	0.53
7:L:1720:GLU:HG3	7:L:1721:LYS:HD2	1.89	0.53
8:Q:337:LEU:HD11	8:Q:358:VAL:HG11	1.92	0.53
8:X:162:PRO:HG2	8:X:163:LYS:HZ2	1.74	0.53
3:j:54:VAL:HA	3:j:57:LYS:HD3	1.89	0.53
4:C:638:TYR:HA	4:C:641:LEU:HD12	1.92	0.52
8:T:337:LEU:HD11	8:T:358:VAL:HG11	1.91	0.52
8:U:337:LEU:HD11	8:U:358:VAL:HG11	1.92	0.52
8:V:184:GLN:O	8:V:188:SER:OG	2.25	0.52
8:Y:77:ILE:O	8:Y:80:SER:OG	2.27	0.52
1:e:160:THR:HG23	1:e:178:LEU:CB	2.36	0.52
1:e:212:ILE:HG13	1:e:213:LYS:HE3	1.91	0.52
3:H:589:ALA:HB2	3:H:634:GLY:HA2	1.91	0.52
5:I:305:ASP:N	5:I:305:ASP:OD1	2.41	0.52
8:T:184:GLN:O	8:T:188:SER:OG	2.25	0.52
8:V:77:ILE:O	8:V:80:SER:OG	2.28	0.52
1:e:151:ILE:HG23	1:e:293:LEU:HB3	1.92	0.52
7:L:1688:PHE:HB2	7:L:1691:ARG:HH21	1.75	0.52
8:U:229:ASN:O	8:U:233:SER:OG	2.25	0.52
8:V:337:LEU:HD11	8:V:358:VAL:HG11	1.92	0.52
8:Q:77:ILE:O	8:Q:80:SER:OG	2.27	0.52
8:V:45:THR:OG1	8:V:46:ASP:N	2.41	0.52
8:Y:45:THR:OG1	8:Y:46:ASP:N	2.41	0.52
8:Z:437:ALA:HA	8:Z:440:ARG:HG2	1.90	0.52
4:E:417:GLU:HG2	4:E:418:ARG:HG3	1.92	0.52
4:C:557:LEU:HA	8:R:339:ARG:HD3	1.92	0.52
4:C:694:GLN:HB3	8:Q:248:TYR:CE2	2.44	0.52
4:E:427:TYR:HE2	4:E:455:LYS:HG3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:77:ILE:O	8:X:80:SER:OG	2.27	0.52
5:I:526:ASP:O	5:I:530:TYR:HB2	2.10	0.52
1:e:145:SER:HB2	1:e:330:ILE:HD13	1.91	0.52
3:H:677:LEU:HB2	3:H:782:ILE:HD11	1.92	0.52
8:R:45:THR:OG1	8:R:46:ASP:N	2.41	0.52
8:R:337:LEU:HD11	8:R:358:VAL:HG11	1.92	0.52
8:S:337:LEU:HD11	8:S:358:VAL:HG11	1.91	0.52
8:S:184:GLN:O	8:S:188:SER:OG	2.25	0.52
8:Z:77:ILE:O	8:Z:80:SER:OG	2.27	0.52
3:D:783:ILE:HD12	3:D:786:GLN:HG3	1.91	0.52
4:E:518:ARG:HG3	4:E:524:GLN:HG2	1.92	0.52
5:K:34:LEU:HD21	7:L:312:LEU:HD22	1.92	0.52
8:X:337:LEU:HD11	8:X:358:VAL:HG11	1.92	0.52
1:e:104:LEU:HG	1:e:133:TYR:HB3	1.92	0.51
1:e:314:GLN:HE22	1:e:329:ILE:HG12	1.76	0.51
3:H:608:THR:HG23	3:H:610:ALA:H	1.75	0.51
8:R:184:GLN:O	8:R:188:SER:OG	2.25	0.51
8:V:343:ARG:O	8:V:343:ARG:NH2	2.42	0.51
8:Z:45:THR:OG1	8:Z:46:ASP:N	2.41	0.51
8:Z:229:ASN:O	8:Z:233:SER:OG	2.25	0.51
3:H:590:THR:OG1	3:H:632:ASP:OD1	2.23	0.51
8:U:77:ILE:O	8:U:80:SER:OG	2.27	0.51
8:V:28:GLU:HA	8:V:367:LEU:HD13	1.93	0.51
8:V:229:ASN:O	8:V:233:SER:OG	2.25	0.51
8:W:184:GLN:O	8:W:188:SER:OG	2.25	0.51
4:C:203:LEU:HD11	4:C:231:ARG:HD2	1.92	0.51
5:K:344:MET:O	5:K:348:SER:OG	2.27	0.51
8:S:343:ARG:O	8:S:343:ARG:NH2	2.42	0.51
4:G:478:THR:HG21	4:G:483:ALA:H	1.75	0.51
8:Q:28:GLU:HA	8:Q:367:LEU:HD13	1.93	0.51
8:R:437:ALA:HA	8:R:440:ARG:HG2	1.90	0.51
4:G:415:ARG:NH2	4:G:427:TYR:OH	2.36	0.51
8:T:28:GLU:HA	8:T:367:LEU:HD13	1.93	0.51
8:T:77:ILE:O	8:T:80:SER:OG	2.27	0.51
8:W:337:LEU:HD11	8:W:358:VAL:HG11	1.91	0.51
2:d:56:ASN:ND2	2:d:58:GLU:OE2	2.43	0.51
4:C:177:PHE:HE2	4:C:282:SER:HA	1.76	0.51
8:W:77:ILE:O	8:W:80:SER:OG	2.27	0.51
8:Z:337:LEU:HD11	8:Z:358:VAL:HG11	1.92	0.51
5:K:89:PHE:HE1	5:K:157:VAL:HG11	1.75	0.51
8:S:77:ILE:O	8:S:80:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:162:PRO:HG2	8:T:163:LYS:HZ2	1.76	0.51
8:R:77:ILE:O	8:R:80:SER:OG	2.27	0.51
8:S:28:GLU:HA	8:S:367:LEU:HD13	1.93	0.51
8:W:28:GLU:HA	8:W:367:LEU:HD13	1.93	0.51
8:Y:337:LEU:HD11	8:Y:358:VAL:HG11	1.92	0.51
1:e:160:THR:CG2	1:e:178:LEU:HB3	2.36	0.51
1:e:309:ILE:HG13	1:e:312:ARG:HH11	1.76	0.51
5:K:45:LEU:HD22	5:K:126:LEU:HD12	1.93	0.51
2:m:67:LEU:HB3	6:l:27:ALA:HB2	1.92	0.51
5:I:128:GLN:HA	5:I:131:LEU:HD12	1.91	0.50
6:J:221:VAL:HG12	6:J:223:GLN:HG2	1.94	0.50
8:X:28:GLU:HA	8:X:367:LEU:HD13	1.93	0.50
7:L:1678:ASN:OD1	7:L:1801:ARG:NH1	2.45	0.50
4:E:517:LYS:HG3	4:E:521:LEU:HD12	1.93	0.50
4:G:408:MET:HG3	4:G:409:VAL:HG23	1.93	0.50
4:G:693:ILE:HG23	4:G:738:MET:HE1	1.93	0.50
8:U:28:GLU:HA	8:U:367:LEU:HD13	1.93	0.50
8:X:229:ASN:O	8:X:233:SER:OG	2.25	0.50
8:Z:28:GLU:HA	8:Z:367:LEU:HD13	1.93	0.50
4:E:738:MET:HG3	4:E:745:LEU:HD12	1.93	0.50
8:Q:119:PHE:HA	8:Q:122:ILE:HD12	1.94	0.50
5:I:499:GLN:HE22	8:W:265:ARG:HH12	1.59	0.50
8:R:119:PHE:HA	8:R:122:ILE:HD12	1.94	0.50
8:S:45:THR:OG1	8:S:46:ASP:N	2.41	0.50
8:V:119:PHE:HA	8:V:122:ILE:HD12	1.94	0.50
2:m:67:LEU:HB2	6:l:26:VAL:HG12	1.94	0.50
2:i:38:GLY:H	3:h:102:GLU:HA	1.77	0.50
8:U:119:PHE:HA	8:U:122:ILE:HD12	1.94	0.50
3:F:419:LEU:HA	3:F:422:VAL:HG22	1.93	0.50
4:G:156:LEU:HD12	4:G:160:MET:HE3	1.94	0.50
4:G:241:ARG:HG3	4:G:243:SER:H	1.76	0.50
3:H:304:ILE:HG22	3:H:328:LEU:HD21	1.93	0.50
3:H:327:ALA:HB1	3:H:418:ILE:HD12	1.94	0.50
5:I:586:ILE:HD13	5:I:622:GLN:HE21	1.77	0.50
8:R:28:GLU:HA	8:R:367:LEU:HD13	1.93	0.50
8:S:191:THR:O	8:S:195:LEU:HB2	2.12	0.50
8:V:393:ARG:HH12	8:V:394:GLN:HE21	1.60	0.50
7:c:179:LEU:HD13	7:c:182:MET:HE2	1.93	0.50
4:C:655:LEU:HD11	4:C:687:LEU:HD13	1.94	0.50
7:L:1545:LEU:HD11	7:L:1580:PRO:HD2	1.94	0.50
8:S:119:PHE:HA	8:S:122:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:191:THR:O	8:T:195:LEU:HB2	2.12	0.50
8:U:387:LEU:HD13	8:U:390:ARG:HD3	1.94	0.50
8:U:393:ARG:HH12	8:U:394:GLN:HE21	1.60	0.50
8:W:387:LEU:HD13	8:W:390:ARG:HD3	1.94	0.50
8:X:119:PHE:HA	8:X:122:ILE:HD12	1.94	0.50
8:Y:387:LEU:HD13	8:Y:390:ARG:HD3	1.94	0.50
6:J:213:ARG:HA	6:J:216:LEU:HD12	1.93	0.50
8:Q:191:THR:O	8:Q:195:LEU:HB2	2.12	0.50
8:R:191:THR:O	8:R:195:LEU:HB2	2.12	0.50
8:R:387:LEU:HD13	8:R:390:ARG:HD3	1.94	0.50
8:U:191:THR:O	8:U:195:LEU:HB2	2.12	0.50
8:Y:28:GLU:HA	8:Y:367:LEU:HD13	1.93	0.50
8:Z:119:PHE:HA	8:Z:122:ILE:HD12	1.94	0.50
2:d:67:LEU:HD22	7:c:15:LEU:HB2	1.94	0.50
4:G:277:ILE:HD11	4:G:296:MET:HB2	1.94	0.49
6:J:938:HIS:CE1	6:J:943:LEU:HB2	2.47	0.49
5:K:389:GLU:HB2	5:K:418:ILE:HG22	1.94	0.49
8:Q:113:LYS:HG3	8:Q:114:ILE:HG23	1.94	0.49
8:Q:290:VAL:HG11	8:Q:333:VAL:HG12	1.94	0.49
8:T:45:THR:OG1	8:T:46:ASP:N	2.41	0.49
8:Y:113:LYS:HG3	8:Y:114:ILE:HG23	1.94	0.49
1:e:8:LEU:HD11	1:e:94:LEU:HD22	1.93	0.49
2:b:49:ARG:HE	7:L:284:GLU:HB2	1.76	0.49
5:K:1:MET:HA	5:K:5:LEU:HD23	1.93	0.49
8:Z:290:VAL:HG11	8:Z:333:VAL:HG12	1.95	0.49
8:Z:387:LEU:HD13	8:Z:390:ARG:HD3	1.94	0.49
1:e:349:LEU:O	1:e:353:GLN:NE2	2.45	0.49
3:F:448:VAL:HG22	3:F:484:LEU:HD12	1.94	0.49
8:Q:387:LEU:HD13	8:Q:390:ARG:HD3	1.94	0.49
8:R:347:ASN:OD1	8:R:347:ASN:N	2.45	0.49
8:T:387:LEU:HD13	8:T:390:ARG:HD3	1.94	0.49
8:W:191:THR:O	8:W:195:LEU:HB2	2.12	0.49
3:j:14:GLN:HG3	3:j:32:PHE:HB2	1.94	0.49
4:E:422:ASP:OD2	4:E:422:ASP:N	2.42	0.49
4:G:201:THR:OG1	4:G:202:ALA:N	2.39	0.49
8:Q:393:ARG:HH12	8:Q:394:GLN:HE21	1.60	0.49
8:T:290:VAL:HG11	8:T:333:VAL:HG12	1.95	0.49
8:U:343:ARG:O	8:U:343:ARG:NH2	2.42	0.49
8:Z:191:THR:O	8:Z:195:LEU:HB2	2.12	0.49
8:X:191:THR:O	8:X:195:LEU:HB2	2.12	0.49
8:Y:290:VAL:HG11	8:Y:333:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:261:LEU:HG	1:e:274:ILE:HD12	1.94	0.49
3:F:848:ARG:HH21	3:F:852:HIS:HE1	1.59	0.49
4:G:452:SER:HA	4:G:455:LYS:HE2	1.95	0.49
8:Q:55:ALA:HB3	8:Q:59:HIS:HB2	1.95	0.49
8:R:113:LYS:HG3	8:R:114:ILE:HG23	1.95	0.49
8:S:290:VAL:HG11	8:S:333:VAL:HG12	1.95	0.49
8:S:387:LEU:HD13	8:S:390:ARG:HD3	1.94	0.49
8:X:55:ALA:HB3	8:X:59:HIS:HB2	1.95	0.49
8:R:290:VAL:HG11	8:R:333:VAL:HG12	1.95	0.49
8:U:113:LYS:HG3	8:U:114:ILE:HG23	1.95	0.49
6:l:71:LYS:NZ	9:l:1102:HOH:O	2.45	0.49
3:D:275:TYR:HB2	3:D:295:SER:HB2	1.95	0.49
8:V:55:ALA:HB3	8:V:59:HIS:HB2	1.95	0.49
8:Y:191:THR:O	8:Y:195:LEU:HB2	2.12	0.49
3:D:676:ILE:HD12	3:D:786:GLN:HE21	1.78	0.49
3:F:554:SER:O	3:F:554:SER:OG	2.31	0.49
6:J:289:LEU:HD23	6:J:292:GLY:HA2	1.95	0.49
8:T:119:PHE:HA	8:T:122:ILE:HD12	1.94	0.49
8:U:34:GLU:HG3	8:U:84:LYS:HE3	1.95	0.49
8:U:290:VAL:HG11	8:U:333:VAL:HG12	1.95	0.49
8:W:343:ARG:O	8:W:343:ARG:NH2	2.42	0.49
4:C:156:LEU:HD23	4:C:159:LYS:HZ2	1.78	0.49
4:C:687:LEU:O	4:C:691:GLN:HB2	2.13	0.49
8:Q:34:GLU:HG3	8:Q:84:LYS:HE3	1.95	0.49
8:Q:343:ARG:O	8:Q:343:ARG:NH2	2.42	0.49
8:S:162:PRO:HG2	8:S:163:LYS:HZ2	1.78	0.49
8:S:393:ARG:HH12	8:S:394:GLN:HE21	1.60	0.49
8:V:113:LYS:HG3	8:V:114:ILE:HG23	1.94	0.49
3:H:568:LEU:HD11	3:H:664:PHE:HA	1.95	0.48
8:S:34:GLU:HG3	8:S:84:LYS:HE3	1.95	0.48
8:W:290:VAL:HG11	8:W:333:VAL:HG12	1.95	0.48
8:Y:229:ASN:O	8:Y:233:SER:OG	2.25	0.48
8:Z:113:LYS:HG3	8:Z:114:ILE:HG23	1.94	0.48
1:e:116:ARG:HH21	1:e:371:HIS:HA	1.77	0.48
5:K:59:ILE:HD11	5:K:93:LEU:HD22	1.95	0.48
8:S:113:LYS:HG3	8:S:114:ILE:HG23	1.94	0.48
8:U:347:ASN:OD1	8:U:347:ASN:N	2.45	0.48
8:V:387:LEU:HD13	8:V:390:ARG:HD3	1.94	0.48
8:X:343:ARG:O	8:X:343:ARG:NH2	2.42	0.48
3:a:49:ARG:HH21	3:a:91:TRP:H	1.60	0.48
3:H:419:LEU:HA	3:H:422:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:T:55:ALA:HB3	8:T:59:HIS:HB2	1.95	0.48
8:T:393:ARG:HH12	8:T:394:GLN:HE21	1.60	0.48
8:U:55:ALA:HB3	8:U:59:HIS:HB2	1.95	0.48
8:V:34:GLU:HG3	8:V:84:LYS:HE3	1.95	0.48
8:V:191:THR:O	8:V:195:LEU:HB2	2.12	0.48
8:Y:55:ALA:HB3	8:Y:59:HIS:HB2	1.95	0.48
8:Y:119:PHE:HA	8:Y:122:ILE:HD12	1.94	0.48
1:e:70:PRO:HG3	1:e:85:ILE:HG21	1.95	0.48
8:T:34:GLU:HG3	8:T:84:LYS:HE3	1.95	0.48
8:X:34:GLU:HG3	8:X:84:LYS:HE3	1.95	0.48
8:X:393:ARG:HH12	8:X:394:GLN:HE21	1.60	0.48
8:Z:55:ALA:HB3	8:Z:59:HIS:HB2	1.95	0.48
3:F:281:ALA:HB3	3:F:287:LEU:HD11	1.95	0.48
8:S:55:ALA:HB3	8:S:59:HIS:HB2	1.95	0.48
8:U:184:GLN:O	8:U:188:SER:OG	2.25	0.48
8:W:113:LYS:HG3	8:W:114:ILE:HG23	1.95	0.48
8:Z:393:ARG:HH12	8:Z:394:GLN:HE21	1.60	0.48
8:T:343:ARG:O	8:T:343:ARG:NH2	2.42	0.48
8:W:119:PHE:HA	8:W:122:ILE:HD12	1.94	0.48
8:W:229:ASN:O	8:W:233:SER:OG	2.25	0.48
8:Y:34:GLU:HG3	8:Y:84:LYS:HE3	1.95	0.48
8:Y:393:ARG:HH12	8:Y:394:GLN:HE21	1.60	0.48
3:a:31:GLN:O	3:a:31:GLN:NE2	2.47	0.48
3:F:626:LEU:HB2	3:F:637:VAL:HG13	1.95	0.48
5:K:478:VAL:HG21	5:K:568:LEU:HD21	1.95	0.48
8:T:113:LYS:HG3	8:T:114:ILE:HG23	1.94	0.48
8:W:34:GLU:HG3	8:W:84:LYS:HE3	1.95	0.48
8:W:55:ALA:HB3	8:W:59:HIS:HB2	1.95	0.48
8:Z:34:GLU:HG3	8:Z:84:LYS:HE3	1.95	0.48
7:c:67:ARG:HA	7:c:70:ILE:HD12	1.95	0.48
7:c:179:LEU:HA	7:c:182:MET:HG2	1.96	0.48
8:X:113:LYS:HG3	8:X:114:ILE:HG23	1.94	0.48
1:e:163:VAL:HG13	1:e:175:ILE:HG12	1.96	0.48
6:J:275:LEU:HB3	6:J:379:LEU:HD21	1.96	0.48
2:i:39:LEU:HD22	2:i:64:ILE:HD12	1.95	0.48
8:X:387:LEU:HD13	8:X:390:ARG:HD3	1.94	0.48
4:G:460:VAL:HB	4:G:499:LEU:HD13	1.96	0.48
7:L:1493:LYS:HD2	7:L:1493:LYS:HA	1.66	0.48
8:V:290:VAL:HG11	8:V:333:VAL:HG12	1.94	0.48
8:X:290:VAL:HG11	8:X:333:VAL:HG12	1.94	0.48
3:D:609:ASN:HB2	8:R:47:ARG:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:522:MET:HE1	4:E:645:MET:HB2	1.96	0.47
3:F:683:GLY:O	3:F:687:ASN:HB2	2.13	0.47
5:I:621:ARG:O	5:I:624:SER:OG	2.32	0.47
8:Q:195:LEU:HD21	8:Q:202:VAL:HG11	1.97	0.47
8:Y:343:ARG:O	8:Y:343:ARG:NH2	2.42	0.47
8:Y:347:ASN:OD1	8:Y:347:ASN:N	2.45	0.47
4:C:522:MET:HE1	4:C:649:LYS:HD3	1.96	0.47
4:G:418:ARG:HE	4:G:424:ASN:HB2	1.78	0.47
8:W:393:ARG:HH12	8:W:394:GLN:HE21	1.60	0.47
4:E:864:PHE:CZ	8:S:348:PHE:HB2	2.49	0.47
3:F:799:GLU:HG2	3:F:832:ARG:HE	1.78	0.47
5:I:102:GLN:HE22	5:I:105:LEU:HD23	1.78	0.47
5:K:500:MET:HE3	5:K:500:MET:HB3	1.86	0.47
8:R:55:ALA:HB3	8:R:59:HIS:HB2	1.95	0.47
8:R:393:ARG:HH12	8:R:394:GLN:HE21	1.60	0.47
8:V:350:PRO:HB2	8:V:351:TRP:H	1.49	0.47
3:D:738:VAL:HG23	3:D:747:ILE:HG12	1.95	0.47
6:J:221:VAL:O	6:J:228:ARG:NH2	2.47	0.47
7:L:1663:HIS:CG	8:Z:262:PRO:HA	2.49	0.47
8:R:237:SER:O	8:R:244:ARG:NH2	2.41	0.47
8:Z:195:LEU:HD21	8:Z:202:VAL:HG11	1.97	0.47
3:h:28:VAL:HG11	3:h:31:GLN:HG2	1.96	0.47
6:l:24:ARG:NH1	6:l:32:GLU:OE2	2.45	0.47
3:D:685:MET:HE3	3:D:685:MET:HB3	1.84	0.47
4:G:709:LEU:HD12	4:G:709:LEU:HA	1.79	0.47
8:W:195:LEU:HD21	8:W:202:VAL:HG11	1.96	0.47
8:Z:343:ARG:O	8:Z:343:ARG:NH2	2.42	0.47
4:E:650:HIS:HA	4:E:653:ARG:HE	1.79	0.47
5:K:370:GLN:HG3	5:K:486:ARG:HH21	1.79	0.47
7:L:433:THR:HA	7:L:436:LEU:HD12	1.96	0.47
1:e:109:PRO:HA	1:e:136:ILE:HD11	1.97	0.47
1:e:358:SER:OG	1:e:359:LYS:N	2.48	0.47
4:C:641:LEU:HG	4:C:734:LEU:HD13	1.96	0.47
3:D:799:GLU:OE1	3:D:803:ARG:NH1	2.48	0.47
4:G:624:TRP:O	4:G:627:SER:OG	2.32	0.47
7:L:1691:ARG:HG2	7:L:1704:ALA:HB1	1.97	0.47
8:T:195:LEU:HD21	8:T:202:VAL:HG11	1.96	0.47
8:U:162:PRO:HG2	8:U:163:LYS:HZ2	1.79	0.47
8:V:195:LEU:HD21	8:V:202:VAL:HG11	1.96	0.47
8:W:347:ASN:OD1	8:W:347:ASN:N	2.45	0.47
8:X:347:ASN:OD1	8:X:347:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:237:SER:O	8:Y:244:ARG:NH2	2.41	0.47
3:h:99:SER:HB2	3:h:100:LEU:HD22	1.97	0.47
4:E:447:ALA:HA	4:E:450:ILE:HD12	1.96	0.47
4:G:221:LEU:HA	4:G:224:VAL:HG22	1.95	0.47
4:G:737:CYS:SG	4:G:738:MET:N	2.88	0.47
8:R:34:GLU:HG3	8:R:84:LYS:HE3	1.95	0.47
8:R:195:LEU:HD21	8:R:202:VAL:HG11	1.96	0.47
8:Z:347:ASN:OD1	8:Z:347:ASN:N	2.45	0.47
1:e:171:LEU:HD12	1:e:172:PRO:HD2	1.95	0.47
4:C:560:ARG:HH22	8:R:332:GLN:HB3	1.78	0.47
3:D:394:GLY:H	3:D:470:MET:HA	1.80	0.47
4:E:738:MET:SD	4:E:738:MET:N	2.87	0.47
3:F:713:HIS:O	3:F:717:GLN:HG2	2.15	0.47
8:U:195:LEU:HD21	8:U:202:VAL:HG11	1.96	0.47
2:d:29:LEU:HD23	2:d:44:LEU:HD13	1.97	0.47
1:e:153:MET:HE1	1:e:317:ILE:HD11	1.96	0.47
4:C:560:ARG:NE	8:R:339:ARG:HH22	2.13	0.47
3:H:588:PRO:HB3	3:H:632:ASP:HB3	1.97	0.47
6:J:923:LEU:HA	6:J:926:LEU:HD12	1.96	0.47
6:J:998:LEU:HD23	6:J:1014:ALA:HB2	1.97	0.47
8:R:162:PRO:HG2	8:R:163:LYS:HZ2	1.80	0.47
8:V:263:THR:HB	8:V:266:LEU:HD12	1.97	0.47
4:C:289:ASN:HA	4:C:292:LEU:HD12	1.96	0.46
4:G:562:SER:OG	4:G:563:THR:N	2.48	0.46
1:e:202:THR:OG1	1:e:203:THR:N	2.48	0.46
4:G:655:LEU:HD22	4:G:687:LEU:HD13	1.97	0.46
8:Q:263:THR:HB	8:Q:266:LEU:HD12	1.98	0.46
8:S:53:TYR:N	8:S:61:ILE:O	2.44	0.46
8:X:195:LEU:HD21	8:X:202:VAL:HG11	1.97	0.46
3:H:572:ASP:OD1	8:V:251:ASN:ND2	2.42	0.46
8:S:263:THR:HB	8:S:266:LEU:HD12	1.98	0.46
1:e:160:THR:HG23	1:e:178:LEU:O	2.10	0.46
1:e:359:LYS:NZ	1:e:360:GLN:OE1	2.46	0.46
8:V:90:ASN:OD1	8:V:90:ASN:N	2.49	0.46
8:W:263:THR:HB	8:W:266:LEU:HD12	1.98	0.46
8:X:53:TYR:N	8:X:61:ILE:O	2.44	0.46
1:e:3:ASP:OD2	7:c:35:ARG:CZ	2.58	0.46
1:e:215:LYS:HB3	1:e:215:LYS:HE2	1.67	0.46
4:C:517:LYS:HA	4:C:521:LEU:HD13	1.98	0.46
4:C:713:LEU:HG	4:C:722:VAL:HG13	1.96	0.46
5:K:107:LEU:HD11	5:K:126:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:464:TYR:OH	3:D:491:ASN:ND2	2.48	0.46
3:D:746:HIS:HA	3:D:749:ALA:HB3	1.96	0.46
5:I:34:LEU:HD22	5:I:38:GLU:HG2	1.97	0.46
2:i:47:CYS:HB3	2:i:60:LEU:HD21	1.97	0.46
8:R:90:ASN:OD1	8:R:90:ASN:N	2.49	0.46
3:h:61:GLU:OE2	3:h:64:ARG:NH2	2.49	0.46
8:R:343:ARG:O	8:R:343:ARG:NH2	2.42	0.46
2:b:43:THR:HG22	3:a:19:ARG:HB3	1.97	0.46
7:L:295:ARG:HD3	7:L:303:PRO:HD2	1.96	0.46
8:S:154:LEU:HD23	8:S:194:ARG:HB3	1.98	0.46
8:T:154:LEU:HD23	8:T:194:ARG:HB3	1.98	0.46
8:Z:53:TYR:N	8:Z:61:ILE:O	2.44	0.46
3:H:710:GLU:HG2	8:V:353:PRO:HD2	1.98	0.46
8:S:195:LEU:HD21	8:S:202:VAL:HG11	1.97	0.46
8:Z:154:LEU:HD23	8:Z:194:ARG:HB3	1.98	0.46
4:C:737:CYS:HB2	4:C:739:LEU:HD22	1.98	0.46
4:G:439:ILE:HG22	4:G:441:SER:H	1.81	0.46
5:K:63:THR:HG23	5:K:87:ARG:HG3	1.98	0.46
2:i:16:ALA:HA	3:h:84:GLN:NE2	2.31	0.46
8:S:229:ASN:O	8:S:233:SER:OG	2.25	0.46
8:X:263:THR:HB	8:X:266:LEU:HD12	1.98	0.46
6:J:378:GLU:HG2	6:J:405:ARG:HH11	1.81	0.45
5:K:651:TYR:CD2	8:Y:349:ILE:HG22	2.51	0.45
8:Q:162:PRO:HG2	8:Q:163:LYS:HZ2	1.81	0.45
8:X:154:LEU:HD23	8:X:194:ARG:HB3	1.98	0.45
8:Y:263:THR:HB	8:Y:266:LEU:HD12	1.98	0.45
6:l:80:LYS:HE3	6:l:126:TYR:HA	1.96	0.45
8:Q:323:ILE:HD11	8:Q:361:SER:HB3	1.98	0.45
8:R:154:LEU:HD23	8:R:194:ARG:HB3	1.98	0.45
8:R:263:THR:HB	8:R:266:LEU:HD12	1.98	0.45
8:V:162:PRO:HG2	8:V:163:LYS:HZ2	1.81	0.45
8:W:323:ILE:HD11	8:W:361:SER:HB3	1.98	0.45
8:Y:195:LEU:HD21	8:Y:202:VAL:HG11	1.97	0.45
1:e:253:GLU:OE1	1:e:256:ARG:NH1	2.50	0.45
4:G:320:SER:OG	4:G:323:LYS:NZ	2.37	0.45
4:G:864:PHE:CG	8:U:351:TRP:HA	2.51	0.45
3:H:718:MET:HE3	3:H:718:MET:HB3	1.84	0.45
8:T:263:THR:HB	8:T:266:LEU:HD12	1.98	0.45
8:U:187:ASN:O	8:U:191:THR:OG1	2.34	0.45
4:E:580:HIS:O	4:E:584:THR:OG1	2.21	0.45
3:H:364:LEU:H	3:H:367:LEU:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:310:LEU:HG	6:J:314:LEU:HD13	1.97	0.45
8:S:90:ASN:OD1	8:S:90:ASN:N	2.49	0.45
3:j:7:LYS:HD2	3:j:12:LEU:HD13	1.97	0.45
4:E:188:ILE:HG12	4:E:278:GLU:HG3	1.98	0.45
4:G:305:ILE:O	4:G:308:SER:OG	2.34	0.45
5:K:419:GLU:HG2	5:K:452:ALA:HB1	1.98	0.45
8:R:323:ILE:HD11	8:R:361:SER:HB3	1.98	0.45
8:T:323:ILE:HD11	8:T:361:SER:HB3	1.98	0.45
8:U:3:ARG:NH1	8:U:132:LEU:O	2.35	0.45
3:H:361:SER:OG	3:H:362:LEU:N	2.47	0.45
7:L:307:ARG:HD2	7:L:307:ARG:HA	1.64	0.45
8:V:154:LEU:HD23	8:V:194:ARG:HB3	1.98	0.45
4:G:186:ALA:HB1	3:H:293:ARG:HG2	1.99	0.45
8:U:263:THR:HB	8:U:266:LEU:HD12	1.98	0.45
8:Z:263:THR:HB	8:Z:266:LEU:HD12	1.98	0.45
1:e:189:LEU:HD13	1:e:213:LYS:HG3	1.98	0.45
3:a:34:TYR:HA	3:a:37:ARG:HD3	1.99	0.45
3:D:803:ARG:HH11	3:D:829:GLU:HB3	1.81	0.45
4:E:550:ARG:HE	4:E:554:LEU:HD11	1.82	0.45
4:E:699:PHE:CZ	8:S:360:LEU:HB3	2.52	0.45
6:J:444:ILE:HG13	6:J:445:LEU:HG	1.99	0.45
6:J:552:LEU:HG	6:J:556:LEU:HG	1.99	0.45
8:T:350:PRO:HB2	8:T:351:TRP:H	1.49	0.45
4:G:499:LEU:HD23	4:G:719:ILE:HD13	1.99	0.45
4:G:633:LYS:O	4:G:637:ARG:HG2	2.16	0.45
4:G:719:ILE:HA	4:G:722:VAL:HG22	1.97	0.45
6:J:286:ILE:HD12	6:J:297:ARG:HD2	1.99	0.45
4:C:461:ARG:HD3	4:C:467:VAL:HG21	2.00	0.45
4:C:550:ARG:O	4:C:553:ALA:HB3	2.17	0.45
3:D:370:TRP:CH2	7:c:178:THR:HG21	2.51	0.45
3:D:647:PRO:HG2	3:D:648:ILE:HD12	1.99	0.45
8:U:323:ILE:HD11	8:U:361:SER:HB3	1.98	0.45
8:X:237:SER:O	8:X:244:ARG:NH2	2.41	0.45
4:C:555:LEU:HD21	4:C:573:LEU:HD22	1.99	0.44
8:R:236:MET:HE2	8:R:236:MET:HB3	1.85	0.44
8:T:5:ILE:HG12	8:T:133:GLU:HB3	1.99	0.44
8:T:229:ASN:O	8:T:233:SER:OG	2.25	0.44
3:F:480:SER:HA	3:F:483:VAL:HG12	1.99	0.44
4:G:542:PRO:HA	4:G:610:LEU:HG	1.99	0.44
4:G:556:GLU:HB3	8:V:339:ARG:HE	1.82	0.44
5:I:59:ILE:HD11	5:I:93:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:573:PHE:HD1	5:K:576:LEU:HD13	1.82	0.44
7:L:1688:PHE:HD1	7:L:1691:ARG:HE	1.66	0.44
7:L:1728:VAL:HB	7:L:1779:LEU:HD12	1.98	0.44
8:Q:5:ILE:HG12	8:Q:133:GLU:HB3	1.99	0.44
8:T:347:ASN:OD1	8:T:347:ASN:N	2.45	0.44
8:V:3:ARG:NH1	8:V:132:LEU:O	2.35	0.44
8:X:323:ILE:HD11	8:X:361:SER:HB3	1.98	0.44
8:Z:5:ILE:HG12	8:Z:133:GLU:HB3	1.99	0.44
1:e:215:LYS:HE3	1:e:216:LEU:HD23	1.99	0.44
3:F:546:LEU:HD23	3:F:546:LEU:HA	1.83	0.44
8:R:5:ILE:HG12	8:R:133:GLU:HB3	1.99	0.44
8:X:5:ILE:HG12	8:X:133:GLU:HB3	1.99	0.44
4:C:429:ASP:OD1	4:C:429:ASP:N	2.50	0.44
7:L:1691:ARG:HH12	7:L:1711:LYS:HD2	1.82	0.44
8:Q:237:SER:O	8:Q:244:ARG:NH2	2.41	0.44
8:S:323:ILE:HD11	8:S:361:SER:HB3	1.98	0.44
8:W:154:LEU:HD23	8:W:194:ARG:HB3	1.98	0.44
8:X:132:LEU:HD23	8:X:164:LYS:HE3	2.00	0.44
8:X:189:LEU:HD12	8:X:190:LEU:HG	2.00	0.44
8:Y:132:LEU:HD23	8:Y:164:LYS:HE3	2.00	0.44
2:d:25:MET:HE2	2:d:48:VAL:HG11	2.00	0.44
6:J:445:LEU:HA	6:J:448:ASP:HB2	2.00	0.44
5:K:636:HIS:HB2	5:K:637:GLN:H	1.60	0.44
7:L:1656:ARG:H	7:L:1656:ARG:HG2	1.65	0.44
8:Q:154:LEU:HD23	8:Q:194:ARG:HB3	1.98	0.44
8:Q:189:LEU:HD12	8:Q:190:LEU:HG	2.00	0.44
8:U:196:THR:O	8:U:265:ARG:NH1	2.51	0.44
8:V:189:LEU:HD12	8:V:190:LEU:HG	2.00	0.44
8:V:323:ILE:HD11	8:V:361:SER:HB3	1.98	0.44
8:Z:162:PRO:HG2	8:Z:163:LYS:HZ2	1.81	0.44
8:Z:196:THR:O	8:Z:265:ARG:NH1	2.51	0.44
1:e:11:ASP:HB3	1:e:18:LYS:HB2	1.99	0.44
3:D:837:LYS:HA	3:D:837:LYS:HD3	1.91	0.44
4:G:503:LEU:HD11	4:G:625:PRO:HB2	1.98	0.44
6:J:323:VAL:HG13	6:J:326:ARG:HH22	1.82	0.44
5:K:515:TRP:HE1	5:K:604:LEU:HD11	1.82	0.44
8:R:196:THR:O	8:R:265:ARG:NH1	2.51	0.44
8:S:5:ILE:HG12	8:S:133:GLU:HB3	1.99	0.44
8:T:132:LEU:HD23	8:T:164:LYS:HE3	2.00	0.44
8:V:196:THR:O	8:V:265:ARG:NH1	2.51	0.44
8:V:237:SER:O	8:V:244:ARG:NH2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:236:MET:HE2	8:W:236:MET:HB3	1.85	0.44
8:X:90:ASN:OD1	8:X:90:ASN:N	2.49	0.44
8:Y:5:ILE:HG12	8:Y:133:GLU:HB3	1.99	0.44
7:L:1773:LYS:HA	7:L:1773:LYS:HD2	1.85	0.44
8:R:3:ARG:NH1	8:R:132:LEU:O	2.35	0.44
8:V:294:MET:HE2	8:V:340:ILE:HG13	2.00	0.44
8:Y:154:LEU:HD23	8:Y:194:ARG:HB3	1.98	0.44
8:Y:323:ILE:HD11	8:Y:361:SER:HB3	1.98	0.44
8:Z:237:SER:O	8:Z:244:ARG:NH2	2.41	0.44
4:C:296:MET:HB3	4:C:296:MET:HE2	1.71	0.44
4:C:522:MET:HG2	4:C:528:PHE:CZ	2.52	0.44
3:D:383:ALA:O	3:D:387:HIS:ND1	2.46	0.44
8:Q:132:LEU:HD23	8:Q:164:LYS:HE3	2.00	0.44
8:S:196:THR:O	8:S:265:ARG:NH1	2.51	0.44
8:U:154:LEU:HD23	8:U:194:ARG:HB3	1.98	0.44
8:V:132:LEU:HD23	8:V:164:LYS:HE3	2.00	0.44
8:W:196:THR:O	8:W:265:ARG:NH1	2.51	0.44
4:C:482:ARG:HA	4:C:485:VAL:HG23	2.00	0.44
4:C:691:GLN:HG2	4:C:695:TYR:CZ	2.53	0.44
4:E:187:LEU:HD23	3:F:375:LYS:HE2	2.00	0.44
6:J:556:LEU:HD23	6:J:559:ILE:HD12	2.00	0.44
2:m:41:MET:O	2:m:45:SER:OG	2.26	0.44
8:S:3:ARG:NH1	8:S:132:LEU:O	2.35	0.44
8:U:431:LEU:HD13	8:U:431:LEU:HA	1.87	0.44
8:X:196:THR:O	8:X:265:ARG:NH1	2.51	0.44
8:X:294:MET:HE2	8:X:340:ILE:HG13	2.00	0.44
8:Y:294:MET:HE2	8:Y:340:ILE:HG13	2.00	0.44
8:Z:323:ILE:HD11	8:Z:361:SER:HB3	1.98	0.44
2:d:60:LEU:HA	2:d:63:VAL:HG22	2.00	0.44
1:e:328:LYS:HZ2	2:d:52:GLU:HA	1.83	0.43
5:I:165:LEU:HD12	5:I:166:PRO:HD2	1.99	0.43
8:R:132:LEU:HD23	8:R:164:LYS:HE3	2.00	0.43
8:R:189:LEU:HD12	8:R:190:LEU:HG	2.00	0.43
8:T:189:LEU:HD12	8:T:190:LEU:HG	2.00	0.43
8:V:5:ILE:HG12	8:V:133:GLU:HB3	1.99	0.43
8:W:132:LEU:HD23	8:W:164:LYS:HE3	2.00	0.43
8:Z:294:MET:HE2	8:Z:340:ILE:HG13	2.00	0.43
2:b:62:SER:HA	2:b:65:LYS:HD2	1.99	0.43
3:F:620:ARG:HH11	3:F:644:VAL:HA	1.83	0.43
3:F:744:LEU:HA	3:F:747:ILE:HD12	2.00	0.43
3:H:562:MET:HG2	3:H:566:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:879:GLN:HE22	8:X:446:TRP:CD1	2.37	0.43
2:i:19:ASN:HB2	3:h:84:GLN:HB2	1.99	0.43
8:T:202:VAL:HG12	8:T:204:VAL:HG22	2.00	0.43
8:U:28:GLU:HG2	8:U:367:LEU:HD22	2.01	0.43
8:U:132:LEU:HD23	8:U:164:LYS:HE3	2.00	0.43
8:W:5:ILE:HG12	8:W:133:GLU:HB3	1.99	0.43
8:X:153:LEU:HD13	8:X:153:LEU:HA	1.92	0.43
8:Y:28:GLU:HG2	8:Y:367:LEU:HD22	2.01	0.43
3:D:615:PRO:O	3:D:619:ARG:HB2	2.18	0.43
8:Q:196:THR:O	8:Q:265:ARG:NH1	2.51	0.43
8:Y:162:PRO:HG2	8:Y:163:LYS:HZ2	1.84	0.43
2:d:67:LEU:HD11	7:c:12:CYS:HA	2.01	0.43
4:C:298:THR:HA	4:C:301:LYS:HD2	2.00	0.43
4:G:530:HIS:CE1	8:U:47:ARG:HH12	2.36	0.43
3:H:486:ILE:HD11	3:H:538:TYR:HB2	1.99	0.43
7:L:531:PRO:HA	7:L:534:ARG:HE	1.83	0.43
2:i:74:LEU:H	3:h:23:ARG:HH21	1.66	0.43
8:Q:187:ASN:O	8:Q:191:THR:OG1	2.34	0.43
8:Q:294:MET:HE2	8:Q:340:ILE:HG13	2.00	0.43
8:Q:369:SER:O	8:Q:372:ARG:NE	2.49	0.43
8:T:196:THR:O	8:T:265:ARG:NH1	2.51	0.43
8:U:20:GLU:O	8:U:24:GLN:HB2	2.19	0.43
8:U:189:LEU:HD12	8:U:190:LEU:HG	2.00	0.43
8:W:294:MET:HE2	8:W:340:ILE:HG13	2.00	0.43
8:X:202:VAL:HG12	8:X:204:VAL:HG22	2.00	0.43
8:Y:196:THR:O	8:Y:265:ARG:NH1	2.51	0.43
8:Y:202:VAL:HG12	8:Y:204:VAL:HG22	2.00	0.43
7:c:141:ARG:HG3	7:c:142:ASN:H	1.83	0.43
4:E:439:ILE:HG22	4:E:441:SER:H	1.83	0.43
3:F:336:TYR:HA	3:F:339:LEU:HD12	2.00	0.43
8:T:294:MET:HE2	8:T:340:ILE:HG13	2.00	0.43
8:U:5:ILE:HG12	8:U:133:GLU:HB3	1.99	0.43
8:V:236:MET:HE2	8:V:236:MET:HB3	1.85	0.43
3:D:848:ARG:HD2	3:D:848:ARG:HA	1.82	0.43
4:G:823:ASN:HD21	4:G:827:LYS:HE3	1.84	0.43
3:H:546:LEU:O	3:H:550:ASN:ND2	2.52	0.43
5:I:345:VAL:HG22	5:I:350:LEU:HD12	2.00	0.43
5:I:408:ASP:HB2	5:I:409:ASN:H	1.62	0.43
8:S:132:LEU:HD23	8:S:164:LYS:HE3	2.00	0.43
8:S:237:SER:O	8:S:244:ARG:NH2	2.41	0.43
8:W:53:TYR:N	8:W:61:ILE:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:56:ASP:HA	8:X:296:ARG:NH1	2.34	0.43
8:W:162:PRO:HG2	8:W:163:LYS:HZ2	1.83	0.43
8:Z:3:ARG:NH1	8:Z:132:LEU:O	2.35	0.43
1:e:160:THR:HG23	1:e:160:THR:O	2.18	0.43
4:G:427:TYR:HD1	4:G:431:ARG:HD3	1.83	0.43
3:H:472:PRO:HD2	3:H:475:MET:HE3	2.00	0.43
3:H:878:PHE:HB2	3:H:879:ARG:NH2	2.34	0.43
6:J:221:VAL:HG22	7:L:309:GLU:HB3	2.00	0.43
6:J:728:LEU:HA	8:X:248:TYR:CZ	2.54	0.43
2:m:61:SER:HB3	6:l:113:LEU:HD12	1.98	0.43
8:R:20:GLU:O	8:R:24:GLN:HB2	2.19	0.43
8:R:294:MET:HE2	8:R:340:ILE:HG13	2.00	0.43
8:S:20:GLU:O	8:S:24:GLN:HB2	2.19	0.43
8:S:294:MET:HE2	8:S:340:ILE:HG13	2.00	0.43
8:S:369:SER:O	8:S:372:ARG:NE	2.49	0.43
8:U:294:MET:HE2	8:U:340:ILE:HG13	2.00	0.43
8:Z:28:GLU:HG2	8:Z:367:LEU:HD22	2.00	0.43
1:e:107:GLU:HG3	1:e:136:ILE:HD12	1.99	0.43
1:e:189:LEU:HD22	1:e:213:LYS:NZ	2.33	0.43
4:C:862:ASN:HB3	8:Q:341:ARG:HG3	2.00	0.43
3:F:364:LEU:HD13	3:F:370:TRP:HE1	1.84	0.43
4:G:229:ASP:O	3:H:286:SER:OG	2.33	0.43
8:W:189:LEU:HD12	8:W:190:LEU:HG	2.00	0.43
8:X:28:GLU:HG2	8:X:367:LEU:HD22	2.00	0.43
8:Z:202:VAL:HG12	8:Z:204:VAL:HG22	2.00	0.43
8:Z:431:LEU:HD13	8:Z:431:LEU:HA	1.87	0.43
4:C:346:ASP:OD2	4:C:347:LYS:N	2.52	0.43
4:G:613:LEU:HA	4:G:613:LEU:HD23	1.70	0.43
5:I:351:LEU:HA	5:I:354:LEU:HD12	1.99	0.43
5:K:492:LEU:HD22	5:K:523:PHE:HB2	2.00	0.43
8:Q:28:GLU:HG2	8:Q:367:LEU:HD22	2.01	0.43
8:Q:57:ASP:HB3	8:Q:59:HIS:CD2	2.54	0.43
8:S:28:GLU:HG2	8:S:367:LEU:HD22	2.01	0.43
8:T:90:ASN:OD1	8:T:90:ASN:N	2.49	0.43
8:V:28:GLU:HG2	8:V:367:LEU:HD22	2.01	0.43
8:W:28:GLU:HG2	8:W:367:LEU:HD22	2.00	0.43
8:Y:20:GLU:O	8:Y:24:GLN:HB2	2.19	0.43
8:Y:90:ASN:OD1	8:Y:90:ASN:N	2.49	0.43
8:Z:132:LEU:HD23	8:Z:164:LYS:HE3	2.00	0.43
2:b:57:PRO:O	2:b:61:SER:OG	2.29	0.43
4:G:610:LEU:HD23	4:G:613:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:564:PHE:O	5:I:568:LEU:HG	2.19	0.43
5:I:578:PRO:HA	5:I:581:HIS:CD2	2.54	0.43
6:J:736:TYR:OH	8:X:252:ASP:OD2	2.20	0.43
8:R:28:GLU:HG2	8:R:367:LEU:HD22	2.01	0.43
8:S:57:ASP:HB3	8:S:59:HIS:CD2	2.54	0.43
8:T:20:GLU:O	8:T:24:GLN:HB2	2.19	0.43
8:T:28:GLU:HG2	8:T:367:LEU:HD22	2.01	0.43
8:T:57:ASP:HB3	8:T:59:HIS:CD2	2.54	0.43
8:T:369:SER:O	8:T:372:ARG:NE	2.49	0.43
8:X:20:GLU:O	8:X:24:GLN:HB2	2.19	0.43
3:h:8:SER:HA	3:h:9:PRO:HD3	1.91	0.43
1:e:19:ALA:HB1	1:e:94:LEU:HD11	2.01	0.42
4:C:635:LEU:HA	4:C:638:TYR:HD2	1.84	0.42
4:C:814:LEU:HB3	4:C:815:VAL:H	1.63	0.42
3:F:754:PHE:O	3:F:758:ILE:HG12	2.19	0.42
4:G:556:GLU:HB3	8:V:339:ARG:NE	2.34	0.42
4:G:694:GLN:O	4:G:698:MET:HG2	2.19	0.42
5:I:511:ASP:HA	5:I:514:LYS:HD3	2.01	0.42
7:L:1575:ALA:HB3	7:L:1595:GLU:HB2	2.00	0.42
8:Q:20:GLU:O	8:Q:24:GLN:HB2	2.19	0.42
8:R:202:VAL:HG12	8:R:204:VAL:HG22	2.00	0.42
8:S:189:LEU:HD12	8:S:190:LEU:HG	2.00	0.42
8:X:57:ASP:HB3	8:X:59:HIS:CD2	2.54	0.42
8:Y:57:ASP:HB3	8:Y:59:HIS:CD2	2.54	0.42
8:Z:57:ASP:HB3	8:Z:59:HIS:CD2	2.54	0.42
3:D:707:LEU:HD13	3:D:851:THR:HG22	2.00	0.42
4:G:518:ARG:HA	4:G:523:ASP:HB3	2.00	0.42
2:k:42:GLU:O	2:k:45:SER:OG	2.31	0.42
2:k:62:SER:HA	2:k:65:LYS:HG3	2.01	0.42
8:V:369:SER:O	8:V:372:ARG:NE	2.49	0.42
8:W:237:SER:O	8:W:244:ARG:NH2	2.41	0.42
6:l:86:ARG:HD2	6:l:90:GLU:OE2	2.19	0.42
4:C:556:GLU:HB3	8:R:339:ARG:HE	1.83	0.42
3:D:692:ARG:NH1	8:R:265:ARG:HG2	2.35	0.42
4:E:533:ASP:N	4:E:533:ASP:OD1	2.50	0.42
3:H:253:ASP:HB3	3:H:263:GLY:HA3	2.00	0.42
8:W:20:GLU:O	8:W:24:GLN:HB2	2.19	0.42
2:b:37:THR:HG23	3:a:100:LEU:HB3	2.00	0.42
3:a:19:ARG:HD2	3:a:19:ARG:HA	1.86	0.42
4:C:326:PHE:O	4:C:329:GLN:HG2	2.20	0.42
4:E:174:LEU:HD21	4:E:283:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:190:TRP:CE2	5:I:280:GLY:HA3	2.55	0.42
5:K:143:ILE:HA	5:K:148:ILE:HD12	2.01	0.42
2:k:51:CYS:SG	3:j:92:SER:HB2	2.59	0.42
8:R:57:ASP:HB3	8:R:59:HIS:CD2	2.54	0.42
8:S:202:VAL:HG12	8:S:204:VAL:HG22	2.00	0.42
8:V:20:GLU:O	8:V:24:GLN:HB2	2.19	0.42
8:W:202:VAL:HG12	8:W:204:VAL:HG22	2.00	0.42
1:e:289:ILE:HD12	1:e:289:ILE:HA	1.83	0.42
6:J:828:LEU:HD13	6:J:832:LYS:HE2	2.01	0.42
8:T:153:LEU:HD13	8:T:153:LEU:HA	1.92	0.42
8:T:237:SER:O	8:T:244:ARG:NH2	2.41	0.42
8:V:202:VAL:HG12	8:V:204:VAL:HG22	2.00	0.42
8:Z:189:LEU:HD12	8:Z:190:LEU:HG	2.00	0.42
4:G:497:LYS:HD3	4:G:497:LYS:HA	1.86	0.42
6:J:954:ILE:O	6:J:958:LEU:HG	2.18	0.42
8:S:260:LEU:HD21	8:S:321:LEU:HB2	2.02	0.42
8:T:104:TRP:O	8:T:108:PHE:HB2	2.20	0.42
8:U:202:VAL:HG12	8:U:204:VAL:HG22	2.00	0.42
8:Y:189:LEU:HD12	8:Y:190:LEU:HG	2.00	0.42
3:F:543:LYS:HA	3:F:543:LYS:HD2	1.79	0.42
4:G:521:LEU:HD21	4:G:702:MET:HB3	2.01	0.42
3:H:685:MET:SD	8:V:165:LEU:HD21	2.59	0.42
8:Q:260:LEU:HD21	8:Q:321:LEU:HB2	2.02	0.42
8:V:421:MET:O	8:V:425:ARG:HB2	2.20	0.42
8:W:421:MET:O	8:W:425:ARG:HB2	2.20	0.42
8:Y:104:TRP:O	8:Y:108:PHE:HB2	2.20	0.42
2:b:55:ILE:HG12	2:b:60:LEU:HG	2.01	0.42
4:E:389:GLU:OE2	3:F:412:ARG:NH1	2.51	0.42
3:F:255:LEU:HD21	3:F:343:HIS:HB2	2.02	0.42
3:F:874:ARG:HG2	3:F:878:PHE:CE2	2.55	0.42
3:H:447:PHE:HA	3:H:467:ARG:HB3	2.01	0.42
3:H:455:LYS:HZ3	3:H:463:LYS:HA	1.84	0.42
8:S:421:MET:O	8:S:425:ARG:HB2	2.20	0.42
8:T:331:THR:O	8:T:334:HIS:NE2	2.53	0.42
8:U:104:TRP:O	8:U:108:PHE:HB2	2.20	0.42
8:V:260:LEU:HD21	8:V:321:LEU:HB2	2.02	0.42
8:Z:20:GLU:O	8:Z:24:GLN:HB2	2.19	0.42
1:e:155:SER:H	1:e:301:GLY:HA3	1.83	0.42
1:e:350:SER:HA	1:e:353:GLN:HG2	2.02	0.42
3:D:677:LEU:HB2	3:D:782:ILE:HD11	2.01	0.42
3:F:397:ALA:O	3:F:473:SER:OG	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:283:LYS:HD2	6:J:283:LYS:HA	1.70	0.42
8:Q:347:ASN:OD1	8:Q:347:ASN:N	2.45	0.42
8:Q:431:LEU:HD13	8:Q:431:LEU:HA	1.87	0.42
8:R:369:SER:O	8:R:372:ARG:NE	2.49	0.42
8:S:331:THR:O	8:S:334:HIS:NE2	2.53	0.42
8:V:104:TRP:O	8:V:108:PHE:HB2	2.20	0.42
8:X:421:MET:O	8:X:425:ARG:HB2	2.20	0.42
1:e:325:MET:H	1:e:325:MET:HG2	1.70	0.42
3:F:338:LEU:O	3:F:342:LEU:HG	2.20	0.42
5:I:37:SER:O	5:I:40:SER:OG	2.38	0.42
8:R:331:THR:O	8:R:334:HIS:NE2	2.53	0.42
8:V:57:ASP:HB3	8:V:59:HIS:CD2	2.54	0.42
4:C:718:ASN:OD1	4:C:719:ILE:N	2.48	0.41
3:F:613:ASP:HB3	3:F:617:ILE:HD11	2.02	0.41
3:H:333:ARG:HH11	5:I:127:ASP:HB3	1.85	0.41
7:L:448:LEU:HD23	7:L:448:LEU:HA	1.87	0.41
7:L:1691:ARG:HH11	7:L:1707:GLU:HG3	1.85	0.41
8:R:421:MET:O	8:R:425:ARG:HB2	2.20	0.41
8:S:350:PRO:HB2	8:S:351:TRP:H	1.49	0.41
8:T:53:TYR:N	8:T:61:ILE:O	2.44	0.41
8:U:421:MET:O	8:U:425:ARG:HB2	2.20	0.41
8:W:3:ARG:NH1	8:W:132:LEU:O	2.35	0.41
8:Z:104:TRP:O	8:Z:108:PHE:HB2	2.20	0.41
1:e:187:ASP:O	1:e:191:LYS:HG2	2.20	0.41
3:F:308:THR:O	3:F:312:SER:OG	2.30	0.41
8:Q:202:VAL:HG12	8:Q:204:VAL:HG22	2.00	0.41
8:V:53:TYR:N	8:V:61:ILE:O	2.44	0.41
8:W:331:THR:O	8:W:334:HIS:NE2	2.53	0.41
8:X:349:ILE:HA	8:X:350:PRO:HD2	1.93	0.41
1:e:209:VAL:HA	1:e:212:ILE:HG12	2.02	0.41
4:C:236:GLN:HG3	4:C:245:THR:HG23	2.01	0.41
8:Q:104:TRP:O	8:Q:108:PHE:HB2	2.20	0.41
8:R:350:PRO:HB2	8:R:351:TRP:H	1.49	0.41
8:U:57:ASP:HB3	8:U:59:HIS:CD2	2.54	0.41
8:V:331:THR:O	8:V:334:HIS:NE2	2.53	0.41
8:Y:260:LEU:HD21	8:Y:321:LEU:HB2	2.02	0.41
3:F:636:ASP:HB3	3:j:64:ARG:HH11	1.86	0.41
5:I:184:TYR:O	5:I:188:SER:OG	2.24	0.41
8:U:331:THR:O	8:U:334:HIS:NE2	2.53	0.41
8:U:369:SER:O	8:U:372:ARG:NE	2.49	0.41
8:W:57:ASP:HB3	8:W:59:HIS:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:260:LEU:HD21	8:X:321:LEU:HB2	2.02	0.41
8:Y:331:THR:O	8:Y:334:HIS:NE2	2.53	0.41
3:j:54:VAL:H	3:j:54:VAL:HG22	1.62	0.41
1:e:334:GLU:OE2	1:e:335:ARG:N	2.52	0.41
6:J:325:PHE:O	6:J:328:GLN:HG2	2.20	0.41
6:J:884:PHE:O	6:J:888:VAL:HG23	2.21	0.41
6:J:927:ILE:HA	6:J:930:HIS:CE1	2.56	0.41
6:J:932:ARG:HH21	6:J:936:THR:HB	1.85	0.41
8:R:53:TYR:N	8:R:61:ILE:O	2.44	0.41
8:U:90:ASN:OD1	8:U:90:ASN:N	2.49	0.41
8:X:331:THR:O	8:X:334:HIS:NE2	2.53	0.41
8:X:369:SER:O	8:X:372:ARG:NE	2.49	0.41
8:X:439:THR:H	8:X:439:THR:HG1	1.55	0.41
8:Y:349:ILE:HA	8:Y:350:PRO:HD2	1.93	0.41
2:b:50:LEU:HD13	2:b:60:LEU:HD21	2.02	0.41
4:C:682:LEU:O	4:C:686:MET:HG2	2.21	0.41
3:D:416:GLN:HA	3:D:419:LEU:HG	2.02	0.41
3:F:876:LEU:HG	3:F:880:LEU:HD11	2.03	0.41
5:I:339:HIS:HA	5:I:342:LYS:HE2	2.01	0.41
8:Q:421:MET:O	8:Q:425:ARG:HB2	2.20	0.41
8:S:104:TRP:O	8:S:108:PHE:HB2	2.20	0.41
8:Y:50:VAL:HG21	8:Y:244:ARG:HG2	2.03	0.41
8:Z:421:MET:O	8:Z:425:ARG:HB2	2.20	0.41
4:C:219:GLU:OE2	4:C:314:HIS:ND1	2.53	0.41
3:D:703:GLN:HA	3:D:706:ILE:HG12	2.03	0.41
3:D:876:LEU:HD12	3:D:876:LEU:HA	1.89	0.41
3:F:719:GLN:O	3:F:723:THR:OG1	2.34	0.41
7:L:459:ILE:HG13	7:L:460:GLY:N	2.36	0.41
8:Q:337:LEU:HD12	8:Q:337:LEU:HA	1.92	0.41
8:R:187:ASN:O	8:R:191:THR:OG1	2.34	0.41
8:R:337:LEU:HD12	8:R:337:LEU:HA	1.92	0.41
2:d:71:THR:HG23	7:c:16:LEU:HD13	2.03	0.41
7:c:88:ARG:O	7:c:92:LEU:HG	2.21	0.41
3:a:58:ILE:HG12	3:a:98:LEU:HD13	2.03	0.41
4:E:607:GLU:HG3	4:E:608:LEU:HD23	2.02	0.41
3:H:274:CYS:SG	3:H:275:TYR:N	2.91	0.41
8:Q:50:VAL:HG21	8:Q:244:ARG:HG2	2.03	0.41
8:Q:415:LYS:HD2	8:Q:415:LYS:HA	1.92	0.41
8:R:425:ARG:HA	8:R:425:ARG:HD2	1.91	0.41
8:T:260:LEU:HD21	8:T:321:LEU:HB2	2.02	0.41
8:W:104:TRP:O	8:W:108:PHE:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:260:LEU:HD21	8:Z:321:LEU:HB2	2.02	0.41
1:e:102:PRO:HB3	1:e:131:ALA:HB3	2.02	0.41
3:D:548:VAL:O	3:D:552:LYS:HG2	2.21	0.41
3:F:466:LEU:HD11	3:F:471:ILE:HD11	2.03	0.41
3:F:546:LEU:O	3:F:550:ASN:HB2	2.20	0.41
4:G:427:TYR:CD1	4:G:431:ARG:HD3	2.55	0.41
4:G:444:GLN:H	4:G:444:GLN:HG3	1.70	0.41
4:G:644:HIS:HE1	4:G:697:MET:HE1	1.85	0.41
6:J:906:LEU:HD22	6:J:937:ILE:HD11	2.03	0.41
5:K:645:LEU:HB2	5:K:646:LEU:HD22	2.02	0.41
2:i:20:ALA:HB2	3:h:84:GLN:HB3	2.03	0.41
8:Q:331:THR:O	8:Q:334:HIS:NE2	2.53	0.41
8:R:260:LEU:HD21	8:R:321:LEU:HB2	2.02	0.41
8:S:419:ASP:O	8:S:423:THR:OG1	2.39	0.41
8:T:50:VAL:HG21	8:T:244:ARG:HG2	2.03	0.41
8:T:419:ASP:O	8:T:423:THR:OG1	2.39	0.41
8:T:421:MET:O	8:T:425:ARG:HB2	2.20	0.41
8:U:50:VAL:HG21	8:U:244:ARG:HG2	2.03	0.41
8:U:349:ILE:HA	8:U:350:PRO:HD2	1.93	0.41
8:W:260:LEU:HD21	8:W:321:LEU:HB2	2.02	0.41
8:W:350:PRO:HB2	8:W:351:TRP:H	1.49	0.41
8:Z:331:THR:O	8:Z:334:HIS:NE2	2.53	0.41
3:D:577:LEU:O	3:D:581:LEU:HB3	2.21	0.41
4:E:338:LEU:HD21	4:E:375:LEU:HD11	2.03	0.41
3:H:677:LEU:HD11	3:H:712:VAL:HA	2.03	0.41
5:K:600:ASN:HD22	5:K:604:LEU:HD23	1.85	0.41
7:L:1546:ASN:OD1	7:L:1546:ASN:N	2.54	0.41
7:L:1670:LYS:HA	7:L:1670:LYS:HD2	1.89	0.41
8:R:50:VAL:HG21	8:R:244:ARG:HG2	2.03	0.41
8:R:104:TRP:O	8:R:108:PHE:HB2	2.20	0.41
8:V:153:LEU:HD13	8:V:153:LEU:HA	1.92	0.41
8:X:189:LEU:HD13	8:X:424:SER:OG	2.21	0.41
8:Y:3:ARG:NH1	8:Y:132:LEU:O	2.35	0.41
8:Z:294:MET:HE3	8:Z:294:MET:HB3	2.00	0.41
3:D:411:MET:HE3	3:D:415:VAL:HG13	2.02	0.40
4:E:425:ASP:HB2	4:E:631:ASN:HB2	2.03	0.40
3:F:627:GLU:HG3	3:F:627:GLU:H	1.71	0.40
3:F:879:ARG:HH21	3:F:879:ARG:HD2	1.76	0.40
8:U:189:LEU:HD13	8:U:424:SER:OG	2.22	0.40
8:U:294:MET:HE3	8:U:294:MET:HB3	2.00	0.40
8:U:419:ASP:O	8:U:423:THR:OG1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:104:TRP:O	8:X:108:PHE:HB2	2.20	0.40
8:X:431:LEU:HD13	8:X:431:LEU:HA	1.87	0.40
8:Y:421:MET:O	8:Y:425:ARG:HB2	2.20	0.40
2:d:58:GLU:HG3	7:c:116:GLN:NE2	2.36	0.40
7:c:158:MET:HA	7:c:161:GLN:HB2	2.03	0.40
1:e:8:LEU:HB3	1:e:103:VAL:HA	2.03	0.40
4:G:277:ILE:HD11	4:G:296:MET:HE2	2.02	0.40
4:G:306:LEU:O	4:G:310:LEU:HG	2.21	0.40
5:I:165:LEU:HG	5:I:167:PRO:HD2	2.03	0.40
5:I:594:CYS:SG	5:I:595:SER:N	2.94	0.40
8:S:153:LEU:HD13	8:S:153:LEU:HA	1.92	0.40
8:V:84:LYS:HE3	8:V:84:LYS:HB2	1.94	0.40
8:V:189:LEU:HD13	8:V:424:SER:OG	2.22	0.40
8:V:343:ARG:HA	8:V:343:ARG:HD2	1.90	0.40
8:X:419:ASP:O	8:X:423:THR:OG1	2.39	0.40
8:Z:90:ASN:OD1	8:Z:90:ASN:N	2.49	0.40
4:C:252:LEU:HD22	4:C:257:ARG:HG3	2.04	0.40
3:D:688:ALA:HB3	3:D:689:LYS:NZ	2.35	0.40
3:F:526:LEU:HB3	3:F:529:ALA:HB3	2.03	0.40
4:G:164:LYS:HD2	4:G:404:TYR:HB3	2.02	0.40
3:H:827:GLU:OE2	3:H:831:LYS:NZ	2.44	0.40
5:I:346:GLU:OE2	5:I:346:GLU:N	2.53	0.40
5:I:478:VAL:O	5:I:482:LEU:HG	2.21	0.40
6:J:369:TYR:OH	5:K:127:ASP:O	2.38	0.40
8:R:189:LEU:HD13	8:R:424:SER:OG	2.21	0.40
8:S:189:LEU:HD13	8:S:424:SER:OG	2.22	0.40
8:T:435:TYR:O	8:T:439:THR:OG1	2.40	0.40
8:X:335:LYS:H	8:X:335:LYS:HG2	1.73	0.40
8:Y:53:TYR:N	8:Y:61:ILE:O	2.44	0.40
8:Y:189:LEU:HD13	8:Y:424:SER:OG	2.22	0.40
3:D:552:LYS:HG3	3:D:553:TYR:CD1	2.56	0.40
3:F:729:CYS:SG	3:F:730:SER:N	2.95	0.40
5:K:341:TRP:CE2	5:K:552:ARG:HA	2.55	0.40
8:T:220:ILE:H	8:T:220:ILE:HG13	1.77	0.40
8:U:260:LEU:HD21	8:U:321:LEU:HB2	2.02	0.40
8:Z:50:VAL:HG21	8:Z:244:ARG:HG2	2.03	0.40
2:b:43:THR:HG22	3:a:19:ARG:HE	1.86	0.40
4:C:839:ARG:HA	4:C:842:ILE:HG12	2.04	0.40
3:D:535:ASP:OD1	3:D:535:ASP:N	2.55	0.40
3:F:887:LYS:HA	3:F:887:LYS:HD2	1.83	0.40
4:G:658:VAL:O	4:G:661:SER:OG	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:179:CYS:O	5:I:183:MET:HG2	2.21	0.40
5:I:499:GLN:HB2	8:W:264:PRO:HB3	2.04	0.40
6:J:282:LYS:HE3	6:J:328:GLN:HE21	1.85	0.40
6:J:384:LYS:HB3	6:J:384:LYS:HE3	1.79	0.40
8:R:435:TYR:O	8:R:439:THR:OG1	2.40	0.40
8:S:50:VAL:HG21	8:S:244:ARG:HG2	2.03	0.40
8:U:427:ILE:HD13	8:U:427:ILE:HA	1.96	0.40
8:V:419:ASP:O	8:V:423:THR:OG1	2.39	0.40
8:W:50:VAL:HG21	8:W:244:ARG:HG2	2.03	0.40
8:W:369:SER:O	8:W:372:ARG:NE	2.49	0.40
8:Y:350:PRO:HB2	8:Y:351:TRP:H	1.49	0.40
2:d:20:ALA:O	2:d:23:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	e	360/375 (96%)	336 (93%)	23 (6%)	1 (0%)	36	72
2	b	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
2	d	57/82 (70%)	55 (96%)	2 (4%)	0	100	100
2	i	63/82 (77%)	57 (90%)	5 (8%)	1 (2%)	7	38
2	k	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
2	m	63/82 (77%)	60 (95%)	3 (5%)	0	100	100
3	D	571/907 (63%)	552 (97%)	19 (3%)	0	100	100
3	F	591/907 (65%)	563 (95%)	28 (5%)	0	100	100
3	H	584/907 (64%)	565 (97%)	19 (3%)	0	100	100
3	a	112/907 (12%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	h	105/907 (12%)	94 (90%)	8 (8%)	3 (3%)	3	23
3	j	105/907 (12%)	100 (95%)	4 (4%)	1 (1%)	12	49
4	C	606/902 (67%)	567 (94%)	38 (6%)	1 (0%)	43	78
4	E	626/902 (69%)	587 (94%)	38 (6%)	1 (0%)	43	78
4	G	628/902 (70%)	590 (94%)	34 (5%)	4 (1%)	21	59
5	I	511/667 (77%)	490 (96%)	15 (3%)	6 (1%)	10	44
5	K	548/667 (82%)	533 (97%)	14 (3%)	1 (0%)	43	78
6	J	506/1024 (49%)	466 (92%)	35 (7%)	5 (1%)	12	49
6	l	104/1024 (10%)	96 (92%)	7 (7%)	1 (1%)	12	49
7	L	540/1819 (30%)	498 (92%)	39 (7%)	3 (1%)	21	59
7	c	148/1819 (8%)	142 (96%)	6 (4%)	0	100	100
8	Q	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	18	56
8	R	408/451 (90%)	381 (93%)	24 (6%)	3 (1%)	18	56
8	S	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	18	56
8	T	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	18	56
8	U	408/451 (90%)	382 (94%)	24 (6%)	2 (0%)	24	63
8	V	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	18	56
8	W	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	18	56
8	X	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	18	56
8	Y	408/451 (90%)	382 (94%)	23 (6%)	3 (1%)	18	56
8	Z	408/451 (90%)	383 (94%)	24 (6%)	1 (0%)	43	78
All	All	11034/20463 (54%)	10397 (94%)	582 (5%)	55 (0%)	26	63

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	581	ASP
5	I	408	ASP
6	J	238	LEU
5	K	255	LYS
2	i	36	ASN
8	Q	350	PRO
8	Q	351	TRP
8	R	350	PRO
8	R	351	TRP

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Mol	Chain	Res	Type
8	S	350	PRO
8	S	351	TRP
8	T	350	PRO
8	T	351	TRP
8	U	350	PRO
8	V	350	PRO
8	V	351	TRP
8	W	350	PRO
8	W	351	TRP
8	X	350	PRO
8	X	351	TRP
8	Y	350	PRO
8	Y	351	TRP
3	h	107	GLN
3	h	108	PRO
3	j	108	PRO
5	I	508	ASN
7	L	307	ARG
8	Q	352	GLY
8	R	352	GLY
8	S	352	GLY
8	T	352	GLY
8	U	352	GLY
8	V	352	GLY
8	W	352	GLY
8	X	352	GLY
8	Y	352	GLY
5	I	405	LEU
6	J	236	LEU
6	J	237	HIS
6	J	255	PRO
4	G	241	ARG
4	G	370	SER
6	l	121	PRO
1	e	37	ARG
4	G	741	ASN
5	I	404	LEU
5	I	409	ASN
5	I	603	PRO
4	C	466	ASP
8	Z	350	PRO
3	h	104	PRO

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Mol	Chain	Res	Type
4	G	742	PRO
6	J	254	ASP
7	L	452	PRO
7	L	1760	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	310/318 (98%)	306 (99%)	4 (1%)	61	74
2	b	53/62 (86%)	52 (98%)	1 (2%)	50	67
2	d	53/62 (86%)	53 (100%)	0	100	100
2	i	53/62 (86%)	52 (98%)	1 (2%)	50	67
2	k	53/62 (86%)	51 (96%)	2 (4%)	29	50
2	m	53/62 (86%)	53 (100%)	0	100	100
3	D	525/798 (66%)	523 (100%)	2 (0%)	84	84
3	F	542/798 (68%)	540 (100%)	2 (0%)	84	84
3	H	539/798 (68%)	535 (99%)	4 (1%)	76	81
3	a	101/798 (13%)	101 (100%)	0	100	100
3	h	88/798 (11%)	86 (98%)	2 (2%)	44	64
3	j	88/798 (11%)	88 (100%)	0	100	100
4	C	556/791 (70%)	550 (99%)	6 (1%)	65	76
4	E	574/791 (73%)	569 (99%)	5 (1%)	70	79
4	G	572/791 (72%)	568 (99%)	4 (1%)	76	81
5	I	472/594 (80%)	469 (99%)	3 (1%)	78	83
5	K	509/594 (86%)	504 (99%)	5 (1%)	68	78
6	J	498/933 (53%)	493 (99%)	5 (1%)	68	78
6	l	84/933 (9%)	84 (100%)	0	100	100
7	L	501/1546 (32%)	498 (99%)	3 (1%)	78	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	c	135/1546 (9%)	134 (99%)	1 (1%)	76	81
8	Q	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	R	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	S	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	T	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	U	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	V	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	W	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	X	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	Y	376/400 (94%)	329 (88%)	47 (12%)	4	16
8	Z	376/400 (94%)	329 (88%)	47 (12%)	4	16
All	All	10119/17935 (56%)	9599 (95%)	520 (5%)	23	42

All (520) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	59	GLN
1	e	148	THR
1	e	247	VAL
1	e	369	ILE
2	b	44	LEU
4	C	282	SER
4	C	308	SER
4	C	328	ILE
4	C	481	GLU
4	C	485	VAL
4	C	532	MET
3	D	385	VAL
3	D	775	LEU
4	E	424	ASN
4	E	547	THR
4	E	635	LEU
4	E	734	LEU
4	E	855	VAL
3	F	426	VAL
3	F	503	THR
4	G	233	VAL
4	G	478	THR

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Mol	Chain	Res	Type
4	G	551	LEU
4	G	584	THR
3	H	308	THR
3	H	368	LEU
3	H	651	VAL
3	H	778	VAL
5	I	18	THR
5	I	530	TYR
5	I	603	PRO
6	J	236	LEU
6	J	256	LEU
6	J	412	LEU
6	J	682	THR
6	J	954	ILE
5	K	66	VAL
5	K	86	LEU
5	K	140	VAL
5	K	492	LEU
5	K	568	LEU
7	L	450	THR
7	L	570	THR
7	L	1607	VAL
2	k	24	THR
2	k	43	THR
2	i	35	LEU
8	Q	7	THR
8	Q	10	LEU
8	Q	20	GLU
8	Q	24	GLN
8	Q	28	GLU
8	Q	58	GLU
8	Q	66	LEU
8	Q	69	LEU
8	Q	78	LEU
8	Q	120	ASP
8	Q	136	VAL
8	Q	149	LEU
8	Q	157	LEU
8	Q	166	VAL
8	Q	170	SER
8	Q	181	VAL
8	Q	188	SER

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Mol	Chain	Res	Type
8	Q	189	LEU
8	Q	192	LEU
8	Q	195	LEU
8	Q	204	VAL
8	Q	210	LEU
8	Q	233	SER
8	Q	253	LEU
8	Q	254	ILE
8	Q	269	LEU
8	Q	271	THR
8	Q	274	THR
8	Q	278	THR
8	Q	288	THR
8	Q	298	LEU
8	Q	321	LEU
8	Q	328	VAL
8	Q	331	THR
8	Q	337	LEU
8	Q	347	ASN
8	Q	358	VAL
8	Q	360	LEU
8	Q	373	VAL
8	Q	374	SER
8	Q	385	SER
8	Q	423	THR
8	Q	424	SER
8	Q	425	ARG
8	Q	431	LEU
8	Q	439	THR
8	Q	445	SER
8	R	7	THR
8	R	10	LEU
8	R	20	GLU
8	R	24	GLN
8	R	28	GLU
8	R	58	GLU
8	R	66	LEU
8	R	69	LEU
8	R	78	LEU
8	R	120	ASP
8	R	136	VAL
8	R	149	LEU

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Mol	Chain	Res	Type
8	R	157	LEU
8	R	166	VAL
8	R	170	SER
8	R	181	VAL
8	R	188	SER
8	R	189	LEU
8	R	192	LEU
8	R	195	LEU
8	R	204	VAL
8	R	210	LEU
8	R	233	SER
8	R	253	LEU
8	R	254	ILE
8	R	269	LEU
8	R	271	THR
8	R	274	THR
8	R	278	THR
8	R	288	THR
8	R	298	LEU
8	R	321	LEU
8	R	328	VAL
8	R	331	THR
8	R	337	LEU
8	R	347	ASN
8	R	358	VAL
8	R	360	LEU
8	R	373	VAL
8	R	374	SER
8	R	385	SER
8	R	423	THR
8	R	424	SER
8	R	425	ARG
8	R	431	LEU
8	R	439	THR
8	R	445	SER
8	S	7	THR
8	S	10	LEU
8	S	20	GLU
8	S	24	GLN
8	S	28	GLU
8	S	58	GLU
8	S	66	LEU

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Mol	Chain	Res	Type
8	S	69	LEU
8	S	78	LEU
8	S	120	ASP
8	S	136	VAL
8	S	149	LEU
8	S	157	LEU
8	S	166	VAL
8	S	170	SER
8	S	181	VAL
8	S	188	SER
8	S	189	LEU
8	S	192	LEU
8	S	195	LEU
8	S	204	VAL
8	S	210	LEU
8	S	233	SER
8	S	253	LEU
8	S	254	ILE
8	S	269	LEU
8	S	271	THR
8	S	274	THR
8	S	278	THR
8	S	288	THR
8	S	298	LEU
8	S	321	LEU
8	S	328	VAL
8	S	331	THR
8	S	337	LEU
8	S	347	ASN
8	S	358	VAL
8	S	360	LEU
8	S	373	VAL
8	S	374	SER
8	S	385	SER
8	S	423	THR
8	S	424	SER
8	S	425	ARG
8	S	431	LEU
8	S	439	THR
8	S	445	SER
8	T	7	THR
8	T	10	LEU

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Mol	Chain	Res	Type
8	T	20	GLU
8	T	24	GLN
8	T	28	GLU
8	T	58	GLU
8	T	66	LEU
8	T	69	LEU
8	T	78	LEU
8	T	120	ASP
8	T	136	VAL
8	T	149	LEU
8	T	157	LEU
8	T	166	VAL
8	T	170	SER
8	T	181	VAL
8	T	188	SER
8	T	189	LEU
8	T	192	LEU
8	T	195	LEU
8	T	204	VAL
8	T	210	LEU
8	T	233	SER
8	T	253	LEU
8	T	254	ILE
8	T	269	LEU
8	T	271	THR
8	T	274	THR
8	T	278	THR
8	T	288	THR
8	T	298	LEU
8	T	321	LEU
8	T	328	VAL
8	T	331	THR
8	T	337	LEU
8	T	347	ASN
8	T	358	VAL
8	T	360	LEU
8	T	373	VAL
8	T	374	SER
8	T	385	SER
8	T	423	THR
8	T	424	SER
8	T	425	ARG

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Mol	Chain	Res	Type
8	T	431	LEU
8	T	439	THR
8	T	445	SER
8	U	7	THR
8	U	10	LEU
8	U	20	GLU
8	U	24	GLN
8	U	28	GLU
8	U	58	GLU
8	U	66	LEU
8	U	69	LEU
8	U	78	LEU
8	U	120	ASP
8	U	136	VAL
8	U	149	LEU
8	U	157	LEU
8	U	166	VAL
8	U	170	SER
8	U	181	VAL
8	U	188	SER
8	U	189	LEU
8	U	192	LEU
8	U	195	LEU
8	U	204	VAL
8	U	210	LEU
8	U	233	SER
8	U	253	LEU
8	U	254	ILE
8	U	269	LEU
8	U	271	THR
8	U	274	THR
8	U	278	THR
8	U	288	THR
8	U	298	LEU
8	U	321	LEU
8	U	328	VAL
8	U	331	THR
8	U	337	LEU
8	U	347	ASN
8	U	358	VAL
8	U	360	LEU
8	U	373	VAL

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Mol	Chain	Res	Type
8	U	374	SER
8	U	385	SER
8	U	423	THR
8	U	424	SER
8	U	425	ARG
8	U	431	LEU
8	U	439	THR
8	U	445	SER
8	V	7	THR
8	V	10	LEU
8	V	20	GLU
8	V	24	GLN
8	V	28	GLU
8	V	58	GLU
8	V	66	LEU
8	V	69	LEU
8	V	78	LEU
8	V	120	ASP
8	V	136	VAL
8	V	149	LEU
8	V	157	LEU
8	V	166	VAL
8	V	170	SER
8	V	181	VAL
8	V	188	SER
8	V	189	LEU
8	V	192	LEU
8	V	195	LEU
8	V	204	VAL
8	V	210	LEU
8	V	233	SER
8	V	253	LEU
8	V	254	ILE
8	V	269	LEU
8	V	271	THR
8	V	274	THR
8	V	278	THR
8	V	288	THR
8	V	298	LEU
8	V	321	LEU
8	V	328	VAL
8	V	331	THR

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Mol	Chain	Res	Type
8	V	337	LEU
8	V	347	ASN
8	V	358	VAL
8	V	360	LEU
8	V	373	VAL
8	V	374	SER
8	V	385	SER
8	V	423	THR
8	V	424	SER
8	V	425	ARG
8	V	431	LEU
8	V	439	THR
8	V	445	SER
8	W	7	THR
8	W	10	LEU
8	W	20	GLU
8	W	24	GLN
8	W	28	GLU
8	W	58	GLU
8	W	66	LEU
8	W	69	LEU
8	W	78	LEU
8	W	120	ASP
8	W	136	VAL
8	W	149	LEU
8	W	157	LEU
8	W	166	VAL
8	W	170	SER
8	W	181	VAL
8	W	188	SER
8	W	189	LEU
8	W	192	LEU
8	W	195	LEU
8	W	204	VAL
8	W	210	LEU
8	W	233	SER
8	W	253	LEU
8	W	254	ILE
8	W	269	LEU
8	W	271	THR
8	W	274	THR
8	W	278	THR

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Mol	Chain	Res	Type
8	W	288	THR
8	W	298	LEU
8	W	321	LEU
8	W	328	VAL
8	W	331	THR
8	W	337	LEU
8	W	347	ASN
8	W	358	VAL
8	W	360	LEU
8	W	373	VAL
8	W	374	SER
8	W	385	SER
8	W	423	THR
8	W	424	SER
8	W	425	ARG
8	W	431	LEU
8	W	439	THR
8	W	445	SER
8	X	7	THR
8	X	10	LEU
8	X	20	GLU
8	X	24	GLN
8	X	28	GLU
8	X	58	GLU
8	X	66	LEU
8	X	69	LEU
8	X	78	LEU
8	X	120	ASP
8	X	136	VAL
8	X	149	LEU
8	X	157	LEU
8	X	166	VAL
8	X	170	SER
8	X	181	VAL
8	X	188	SER
8	X	189	LEU
8	X	192	LEU
8	X	195	LEU
8	X	204	VAL
8	X	210	LEU
8	X	233	SER
8	X	253	LEU

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Mol	Chain	Res	Type
8	X	254	ILE
8	X	269	LEU
8	X	271	THR
8	X	274	THR
8	X	278	THR
8	X	288	THR
8	X	298	LEU
8	X	321	LEU
8	X	328	VAL
8	X	331	THR
8	X	337	LEU
8	X	347	ASN
8	X	358	VAL
8	X	360	LEU
8	X	373	VAL
8	X	374	SER
8	X	385	SER
8	X	423	THR
8	X	424	SER
8	X	425	ARG
8	X	431	LEU
8	X	439	THR
8	X	445	SER
8	Y	7	THR
8	Y	10	LEU
8	Y	20	GLU
8	Y	24	GLN
8	Y	28	GLU
8	Y	58	GLU
8	Y	66	LEU
8	Y	69	LEU
8	Y	78	LEU
8	Y	120	ASP
8	Y	136	VAL
8	Y	149	LEU
8	Y	157	LEU
8	Y	166	VAL
8	Y	170	SER
8	Y	181	VAL
8	Y	188	SER
8	Y	189	LEU
8	Y	192	LEU

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Mol	Chain	Res	Type
8	Y	195	LEU
8	Y	204	VAL
8	Y	210	LEU
8	Y	233	SER
8	Y	253	LEU
8	Y	254	ILE
8	Y	269	LEU
8	Y	271	THR
8	Y	274	THR
8	Y	278	THR
8	Y	288	THR
8	Y	298	LEU
8	Y	321	LEU
8	Y	328	VAL
8	Y	331	THR
8	Y	337	LEU
8	Y	347	ASN
8	Y	358	VAL
8	Y	360	LEU
8	Y	373	VAL
8	Y	374	SER
8	Y	385	SER
8	Y	423	THR
8	Y	424	SER
8	Y	425	ARG
8	Y	431	LEU
8	Y	439	THR
8	Y	445	SER
8	Z	7	THR
8	Z	10	LEU
8	Z	20	GLU
8	Z	24	GLN
8	Z	28	GLU
8	Z	58	GLU
8	Z	66	LEU
8	Z	69	LEU
8	Z	78	LEU
8	Z	120	ASP
8	Z	136	VAL
8	Z	149	LEU
8	Z	157	LEU
8	Z	166	VAL

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Mol	Chain	Res	Type
8	Z	170	SER
8	Z	181	VAL
8	Z	188	SER
8	Z	189	LEU
8	Z	192	LEU
8	Z	195	LEU
8	Z	204	VAL
8	Z	210	LEU
8	Z	233	SER
8	Z	253	LEU
8	Z	254	ILE
8	Z	269	LEU
8	Z	271	THR
8	Z	274	THR
8	Z	278	THR
8	Z	288	THR
8	Z	298	LEU
8	Z	321	LEU
8	Z	328	VAL
8	Z	331	THR
8	Z	337	LEU
8	Z	347	ASN
8	Z	358	VAL
8	Z	360	LEU
8	Z	373	VAL
8	Z	374	SER
8	Z	385	SER
8	Z	423	THR
8	Z	424	SER
8	Z	425	ARG
8	Z	431	LEU
8	Z	439	THR
8	Z	445	SER
7	c	95	GLU
3	h	28	VAL
3	h	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (280) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	12	ASN
1	e	73	HIS

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Mol	Chain	Res	Type
1	e	88	HIS
1	e	92	ASN
1	e	111	ASN
1	e	246	GLN
1	e	275	HIS
1	e	296	ASN
1	e	314	GLN
2	b	19	ASN
2	b	56	ASN
3	a	14	GLN
3	a	84	GLN
4	C	165	GLN
4	C	236	GLN
4	C	287	GLN
4	C	309	GLN
4	C	316	GLN
4	C	371	GLN
4	C	401	HIS
4	C	436	GLN
4	C	437	GLN
4	C	684	GLN
4	C	688	ASN
4	C	691	GLN
4	C	694	GLN
4	C	862	ASN
3	D	345	GLN
3	D	491	ASN
3	D	495	GLN
3	D	596	ASN
3	D	665	ASN
3	D	687	ASN
3	D	693	ASN
3	D	705	HIS
3	D	713	HIS
3	D	739	GLN
3	D	742	GLN
3	D	773	ASN
3	D	786	GLN
3	D	885	HIS
4	E	166	ASN
4	E	213	GLN
4	E	236	GLN

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Mol	Chain	Res	Type
4	E	242	GLN
4	E	303	HIS
4	E	329	GLN
4	E	401	HIS
4	E	420	GLN
4	E	438	GLN
4	E	585	GLN
4	E	662	ASN
4	E	688	ASN
4	E	691	GLN
3	F	301	HIS
3	F	302	ASN
3	F	322	GLN
3	F	343	HIS
3	F	345	GLN
3	F	500	GLN
3	F	531	GLN
3	F	558	HIS
3	F	596	ASN
3	F	659	HIS
3	F	703	GLN
3	F	717	GLN
3	F	719	GLN
3	F	739	GLN
3	F	742	GLN
3	F	773	ASN
3	F	786	GLN
3	F	801	GLN
3	F	852	HIS
3	F	855	GLN
3	F	859	GLN
3	F	860	GLN
4	G	151	GLN
4	G	152	GLN
4	G	236	GLN
4	G	289	ASN
4	G	303	HIS
4	G	371	GLN
4	G	438	GLN
4	G	530	HIS
4	G	644	HIS
4	G	692	ASN

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Mol	Chain	Res	Type
4	G	823	ASN
4	G	862	ASN
3	H	259	GLN
3	H	273	ASN
3	H	310	GLN
3	H	558	HIS
3	H	570	GLN
3	H	693	ASN
3	H	717	GLN
3	H	751	HIS
3	H	786	GLN
3	H	787	ASN
3	H	830	ASN
3	H	883	ASN
5	I	102	GLN
5	I	152	GLN
5	I	339	HIS
5	I	377	GLN
5	I	398	GLN
5	I	489	GLN
5	I	494	HIS
5	I	546	HIS
5	I	571	GLN
5	I	581	HIS
5	I	622	GLN
6	J	222	HIS
6	J	248	GLN
6	J	269	GLN
6	J	288	GLN
6	J	298	ASN
6	J	299	ASN
6	J	362	GLN
6	J	456	GLN
6	J	474	GLN
6	J	484	HIS
6	J	705	ASN
6	J	725	ASN
6	J	818	GLN
6	J	822	ASN
6	J	830	GLN
6	J	938	HIS
6	J	959	ASN

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Mol	Chain	Res	Type
5	K	3	HIS
5	K	29	GLN
5	K	43	ASN
5	K	67	GLN
5	K	68	GLN
5	K	69	GLN
5	K	78	GLN
5	K	98	GLN
5	K	109	GLN
5	K	123	ASN
5	K	128	GLN
5	K	130	GLN
5	K	146	GLN
5	K	180	HIS
5	K	193	HIS
5	K	199	GLN
5	K	303	GLN
5	K	316	GLN
5	K	327	GLN
5	K	377	GLN
5	K	493	GLN
5	K	519	ASN
5	K	533	GLN
5	K	547	GLN
5	K	591	HIS
5	K	600	ASN
7	L	327	HIS
7	L	416	GLN
7	L	571	HIS
7	L	1508	HIS
7	L	1663	HIS
7	L	1666	GLN
7	L	1673	GLN
7	L	1730	HIS
7	L	1742	GLN
7	L	1770	ASN
7	L	1788	ASN
2	k	53	GLN
2	i	19	ASN
8	Q	15	ASN
8	Q	16	GLN
8	Q	24	GLN

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Mol	Chain	Res	Type
8	Q	54	GLN
8	Q	187	ASN
8	Q	207	ASN
8	Q	219	HIS
8	Q	229	ASN
8	Q	251	ASN
8	Q	314	ASN
8	Q	332	GLN
8	R	15	ASN
8	R	16	GLN
8	R	24	GLN
8	R	54	GLN
8	R	187	ASN
8	R	207	ASN
8	R	229	ASN
8	R	251	ASN
8	R	314	ASN
8	R	332	GLN
8	S	15	ASN
8	S	16	GLN
8	S	24	GLN
8	S	54	GLN
8	S	187	ASN
8	S	207	ASN
8	S	219	HIS
8	S	229	ASN
8	S	251	ASN
8	S	314	ASN
8	S	332	GLN
8	S	357	GLN
8	T	15	ASN
8	T	16	GLN
8	T	24	GLN
8	T	54	GLN
8	T	187	ASN
8	T	207	ASN
8	T	229	ASN
8	T	251	ASN
8	T	314	ASN
8	T	332	GLN
8	U	15	ASN
8	U	16	GLN

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Mol	Chain	Res	Type
8	U	24	GLN
8	U	54	GLN
8	U	187	ASN
8	U	207	ASN
8	U	219	HIS
8	U	229	ASN
8	U	251	ASN
8	U	314	ASN
8	U	332	GLN
8	V	15	ASN
8	V	16	GLN
8	V	24	GLN
8	V	54	GLN
8	V	187	ASN
8	V	207	ASN
8	V	219	HIS
8	V	229	ASN
8	V	314	ASN
8	V	332	GLN
8	W	15	ASN
8	W	16	GLN
8	W	24	GLN
8	W	54	GLN
8	W	187	ASN
8	W	207	ASN
8	W	229	ASN
8	W	251	ASN
8	W	314	ASN
8	W	332	GLN
8	X	15	ASN
8	X	16	GLN
8	X	24	GLN
8	X	54	GLN
8	X	187	ASN
8	X	207	ASN
8	X	229	ASN
8	X	314	ASN
8	X	332	GLN
8	Y	15	ASN
8	Y	16	GLN
8	Y	24	GLN
8	Y	54	GLN

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Mol	Chain	Res	Type
8	Y	187	ASN
8	Y	207	ASN
8	Y	229	ASN
8	Y	251	ASN
8	Y	314	ASN
8	Y	332	GLN
8	Z	15	ASN
8	Z	16	GLN
8	Z	24	GLN
8	Z	54	GLN
8	Z	187	ASN
8	Z	207	ASN
8	Z	229	ASN
8	Z	251	ASN
8	Z	314	ASN
8	Z	332	GLN
8	Z	357	GLN
2	d	56	ASN
3	h	14	GLN
3	h	42	ASN
3	j	14	GLN
3	j	15	ASN
3	j	42	ASN
6	l	38	GLN
6	l	42	ASN
6	l	107	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

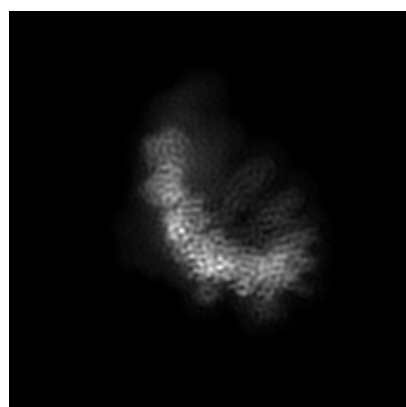
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14011. These allow visual inspection of the internal detail of the map and identification of artifacts.

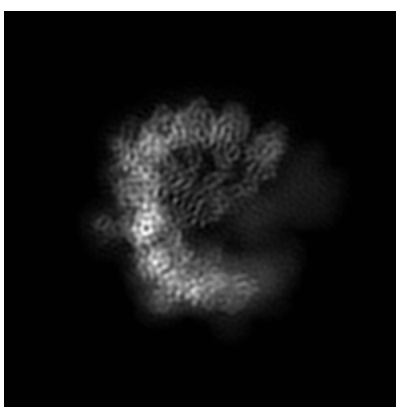
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

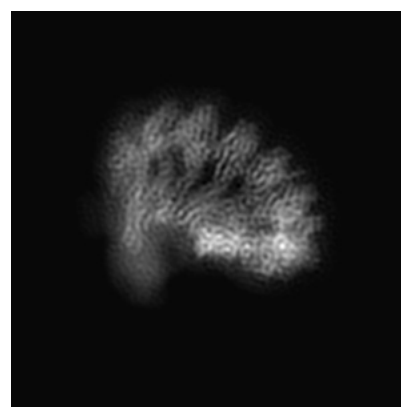
6.1.1 Primary map



X



Y



Z

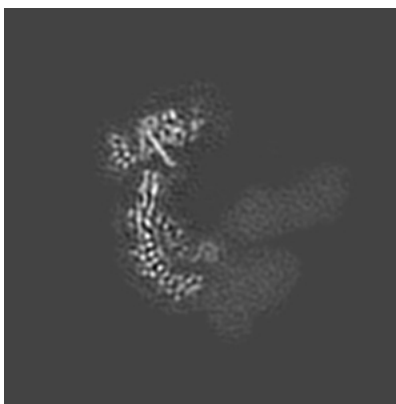
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

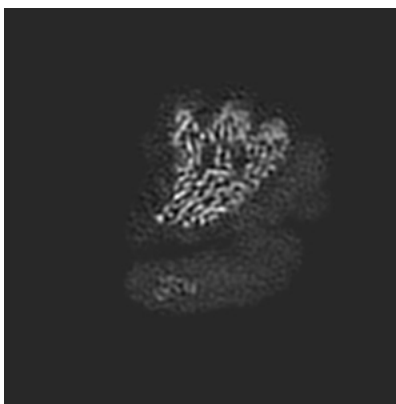
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

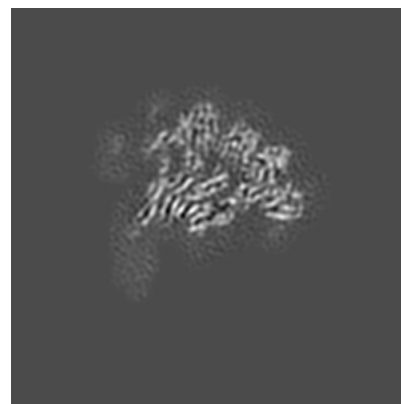
6.3.1 Primary map



X Index: 135



Y Index: 81

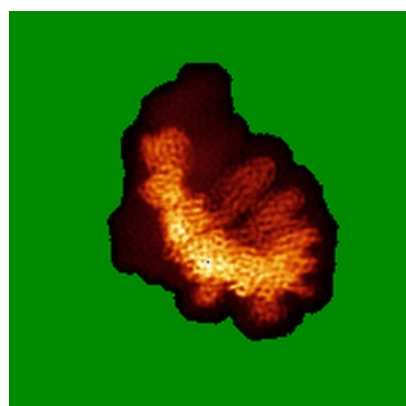


Z Index: 72

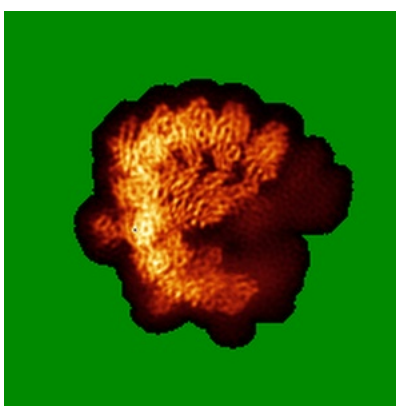
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.0308. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

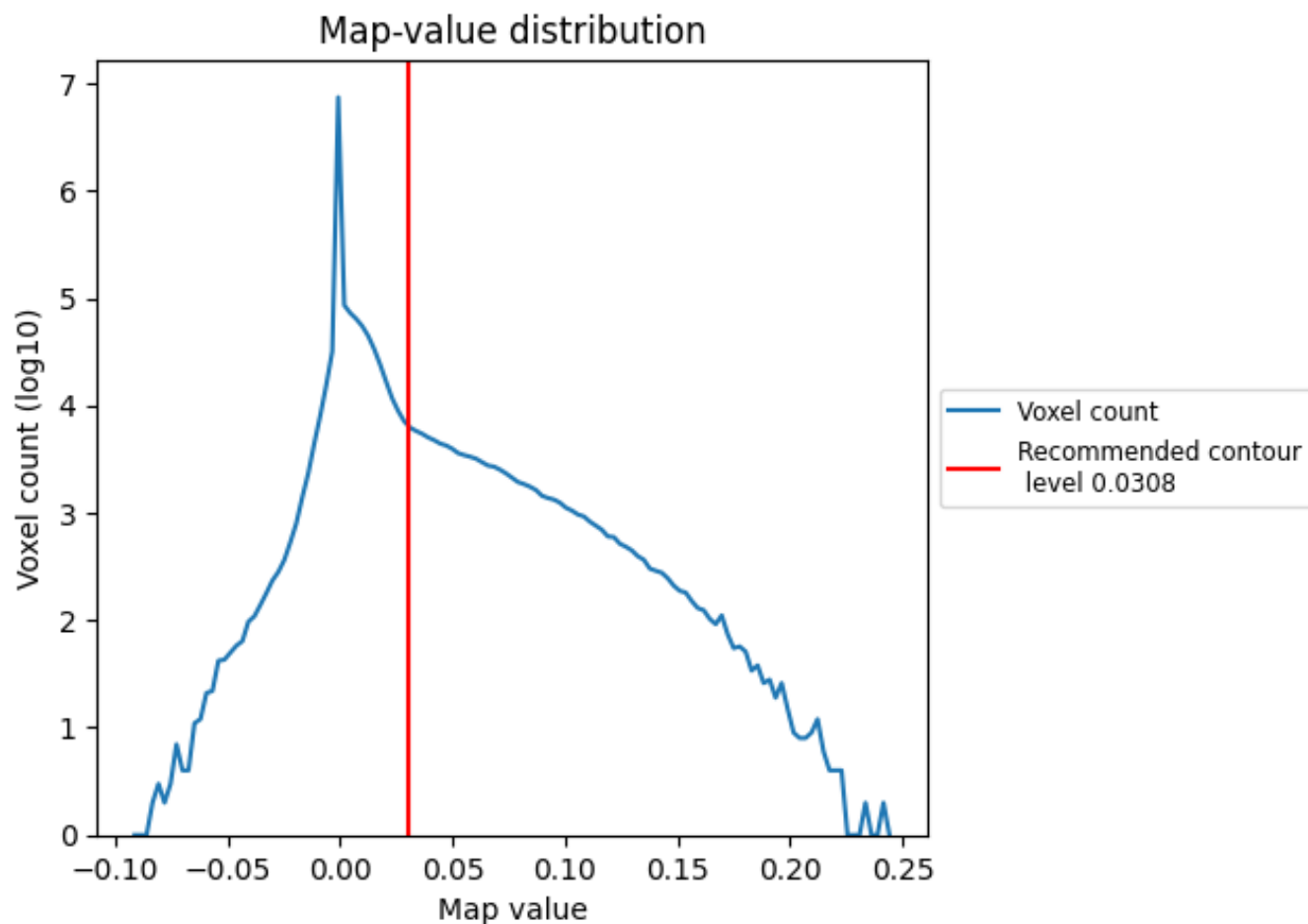
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

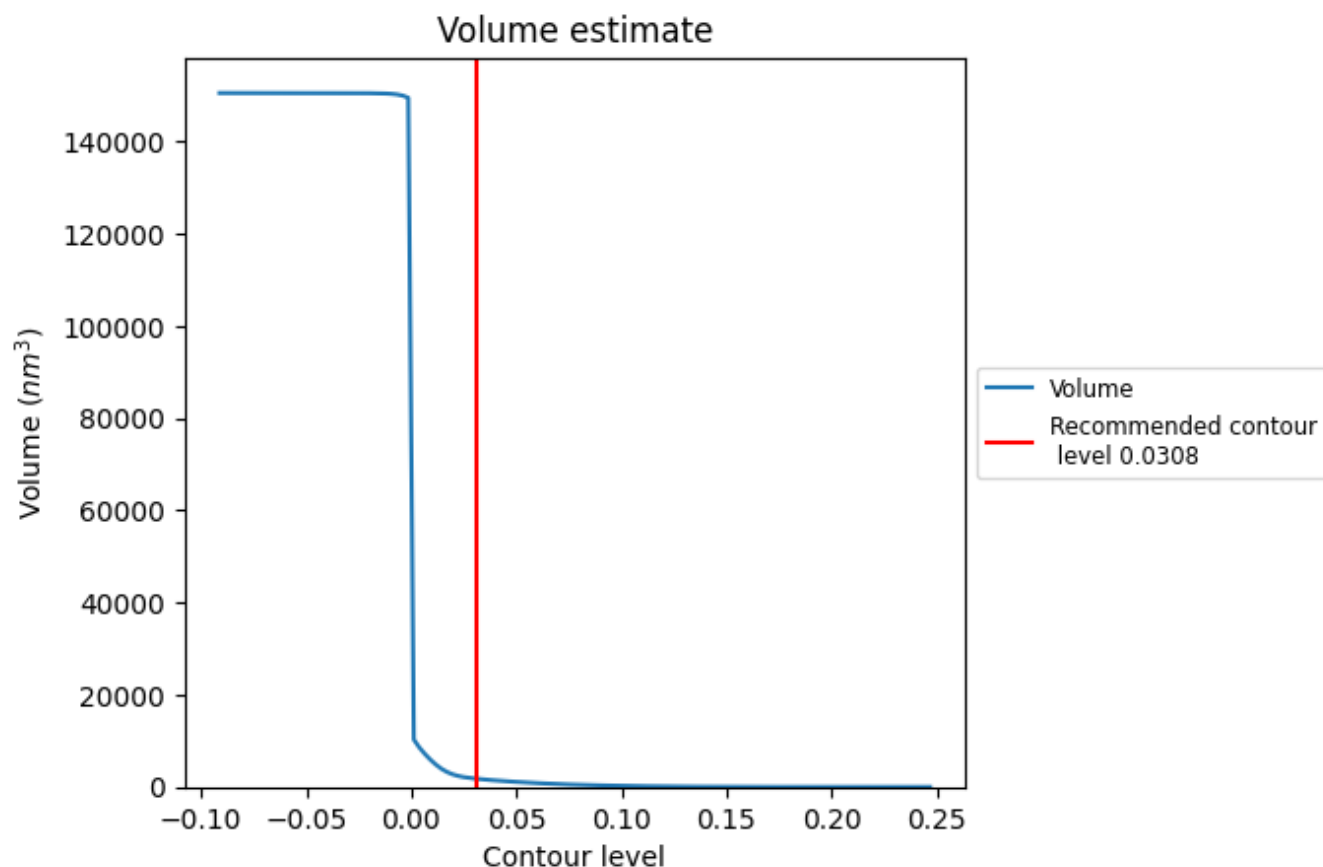
This section contains the results of statistical analysis of the map.

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.

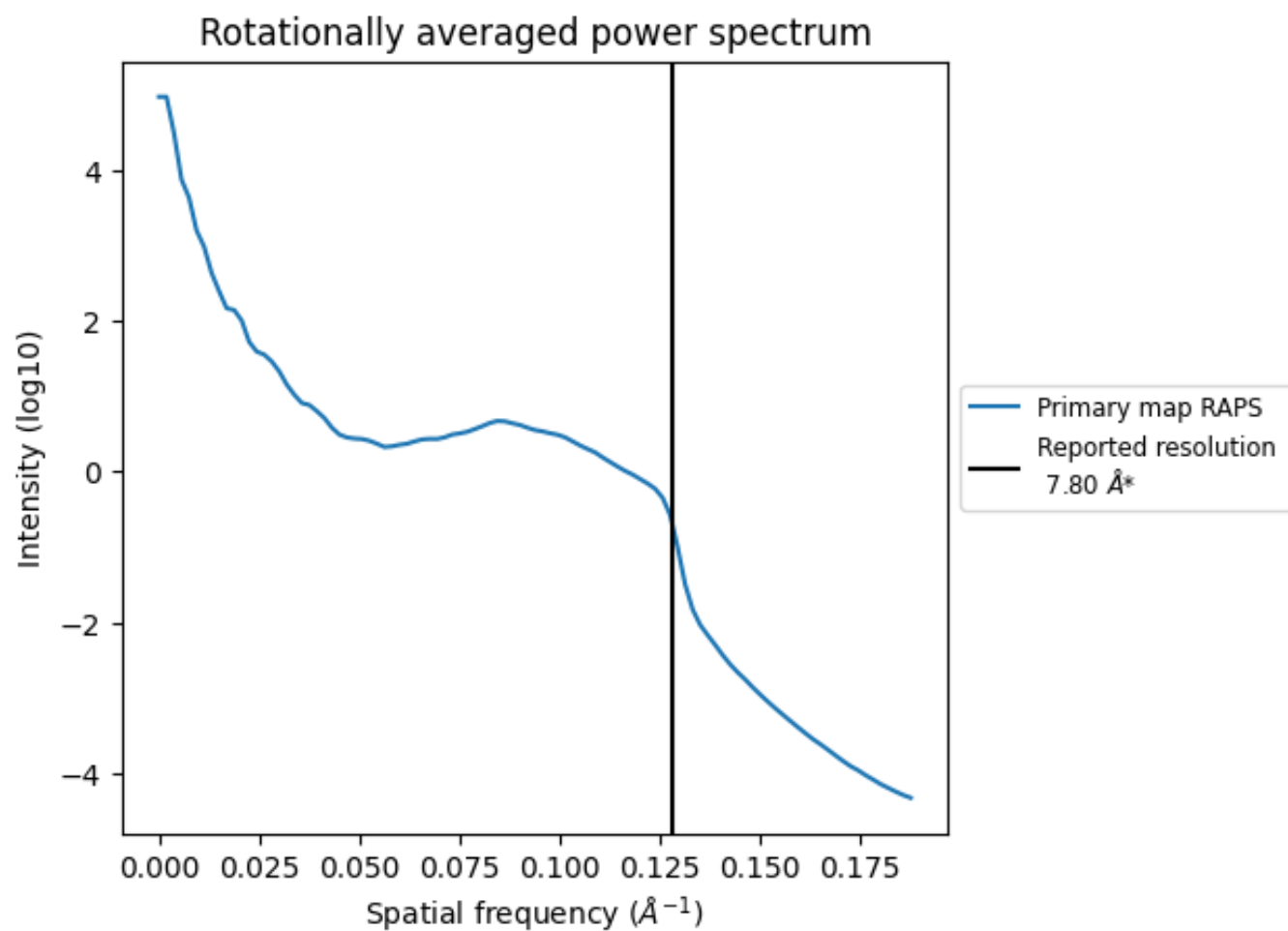
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1794 nm^3 ; this corresponds to an approximate mass of 1620 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 0.128 Å⁻¹

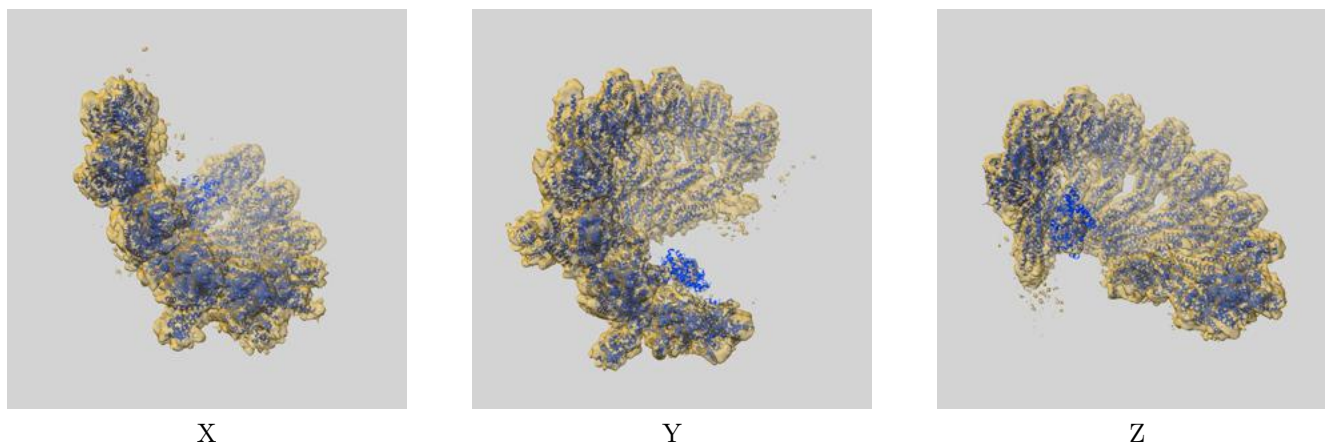
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

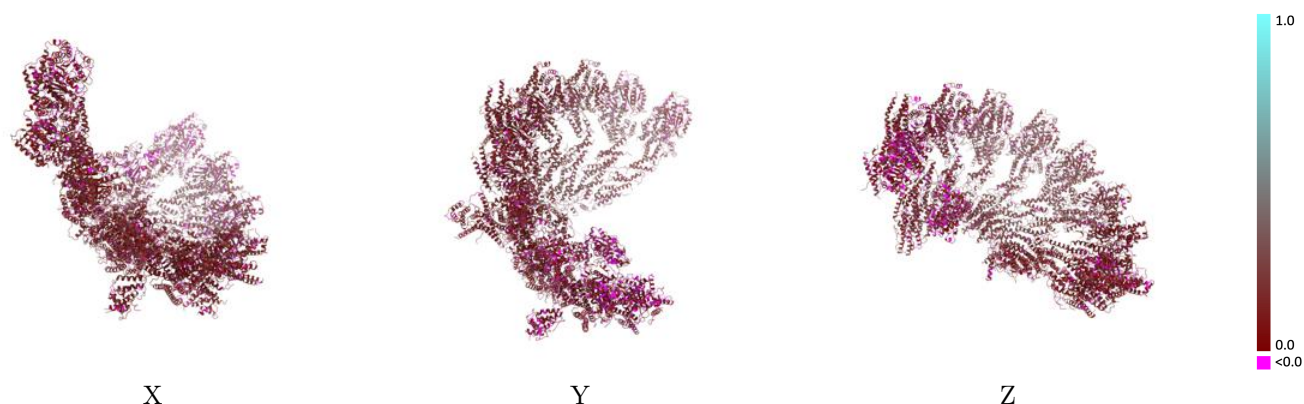
This section contains information regarding the fit between EMDB map EMD-14011 and PDB model 7QJ6. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



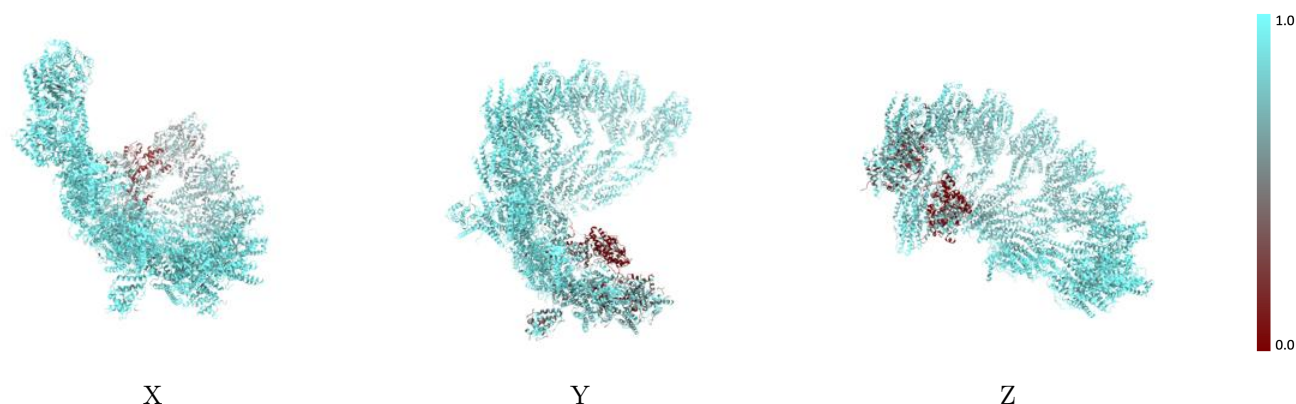
The images above show the 3D surface view of the map at the recommended contour level 0.0308 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



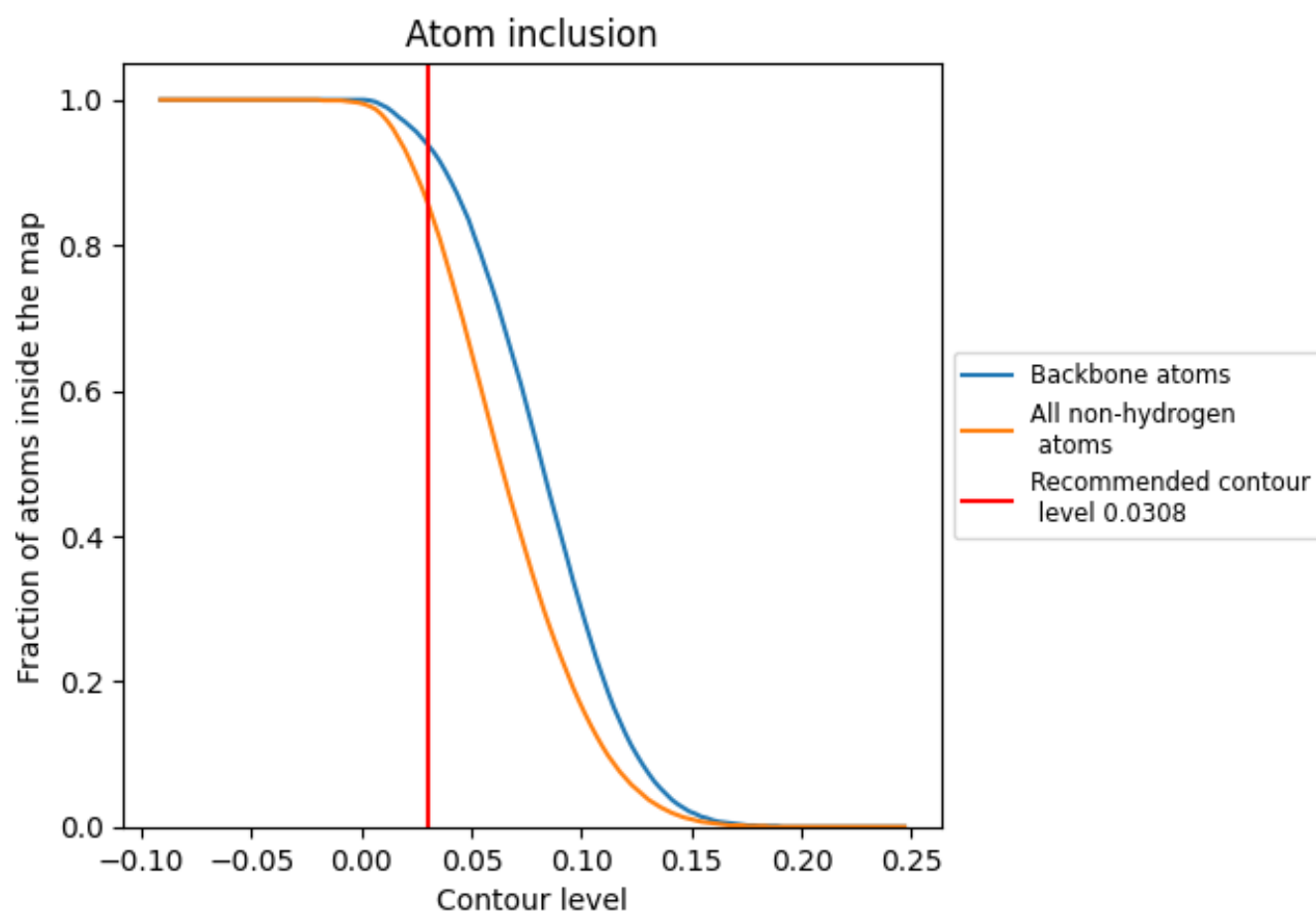
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0308).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.1380
C	 0.8000	 0.1270
D	 0.8250	 0.1380
E	 0.9110	 0.1430
F	 0.9210	 0.1500
G	 0.9150	 0.1580
H	 0.9160	 0.1510
I	 0.9220	 0.1610
J	 0.9130	 0.1610
K	 0.9190	 0.1570
L	 0.9180	 0.1520
Q	 0.5820	 0.0660
R	 0.7550	 0.0990
S	 0.8680	 0.1160
T	 0.9170	 0.1330
U	 0.9320	 0.1460
V	 0.9350	 0.1620
W	 0.9370	 0.1540
X	 0.9280	 0.1470
Y	 0.9390	 0.1370
Z	 0.8930	 0.1270
a	 0.7650	 0.1430
b	 0.7860	 0.1780
c	 0.5530	 0.1260
d	 0.4080	 0.1350
e	 0.2260	 0.0740
h	 0.6710	 0.1000
i	 0.7040	 0.0960
j	 0.8780	 0.1300
k	 0.9080	 0.1500
l	 0.9100	 0.1610
m	 0.9160	 0.1580

