



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 11:32 AM UTC

PDB ID : 7QJC / pdb_00007qjc
EMDB ID : EMD-14017
Title : Structure of recombinant human gamma-Tubulin Ring Complex (spokes 1-14, homogeneous dataset)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 16.10 Å (reported)
Based on initial models : 6L81, 7AS4, 6V6S, 6X0U

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:

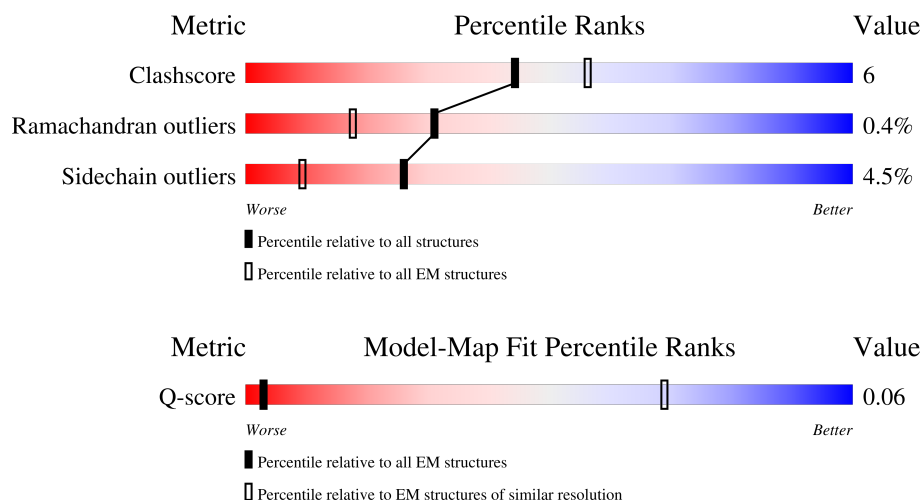
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 16.10 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.



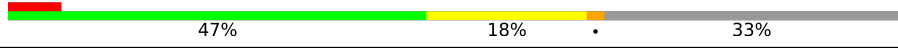
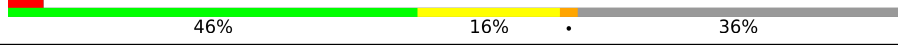
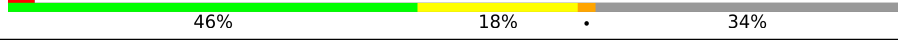
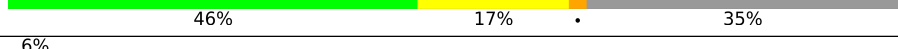
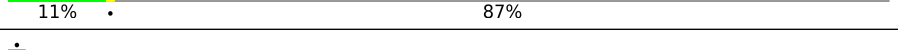
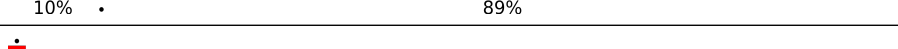
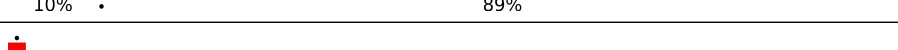
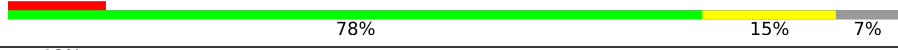
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	32 (15.90 - 16.50)

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	48% 94%
2	A	902	49% 17% 32%
2	C	902	6% 49% 18% 31%
2	E	902	52% 17% 29%

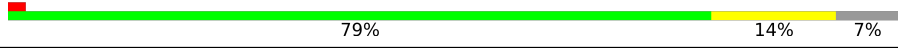
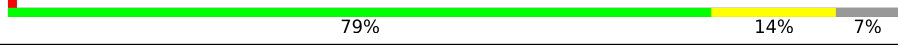
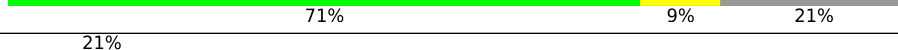
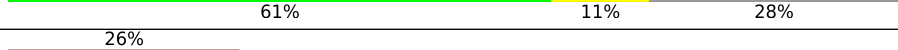
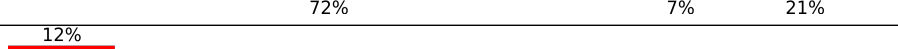
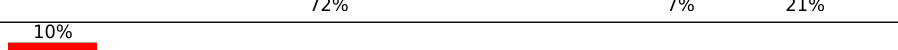
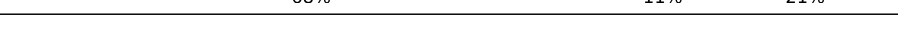
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Mol	Chain	Length	Quality of chain
2	G	902	
2	M	902	
3	B	907	
3	D	907	
3	F	907	
3	H	907	
3	N	907	
3	a	907	
3	f	907	
3	h	907	
3	j	907	
4	I	667	
4	K	667	
5	J	1024	
5	l	1024	
6	L	1819	
6	c	1819	
7	1	451	
7	2	451	
7	O	451	
7	P	451	
7	Q	451	
7	R	451	
7	S	451	
7	T	451	

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Mol	Chain	Length	Quality of chain
7	U	451	
7	V	451	
7	W	451	
7	X	451	
7	Y	451	
7	Z	451	
8	b	82	
8	d	82	
8	g	82	
8	i	82	
8	k	82	
8	m	82	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 125323 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
			1818	1083	364	370	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	613	Total	C	N	O	S	0	0
			4978	3212	831	903	32		
2	C	620	Total	C	N	O	S	0	0
			5044	3257	845	910	32		
2	E	638	Total	C	N	O	S	0	0
			5202	3354	873	942	33		
2	G	640	Total	C	N	O	S	0	0
			5217	3359	878	947	33		
2	M	636	Total	C	N	O	S	0	0
			5186	3342	871	940	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	610	Total	C	N	O	S	0	0
			5021	3198	888	910	25		
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
			4933	3146	871	891	25		
3	H	594	Total	C	N	O	S	0	0
			4899	3125	864	885	25		
3	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		
3	f	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
3	h	99	Total	C	N	O	S	0	0
			803	509	148	144	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	j	107	Total	C	N	O	S	0	0
			864	545	161	156	2		
3	N	594	Total	C	N	O	S	0	0
			4899	3125	864	885	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	521	Total	C	N	O	S	0	0
			4222	2734	720	750	18		
4	K	562	Total	C	N	O	S	0	0
			4579	2964	781	816	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	534	Total	C	N	O	S	0	0
			4406	2879	733	771	23		
5	l	108	Total	C	N	O	S	0	0
			876	556	151	168	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	566	Total	C	N	O	S	0	0
			4556	2977	767	788	24		
6	c	158	Total	C	N	O	S	0	0
			1220	771	209	232	8		

- Molecule 7 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		
7	P	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		
7	Q	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		
7	R	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		
7	S	420	Total	C	N	O	S	0	0
			3371	2133	586	637	15		

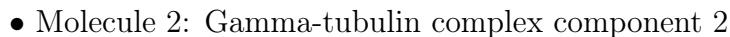
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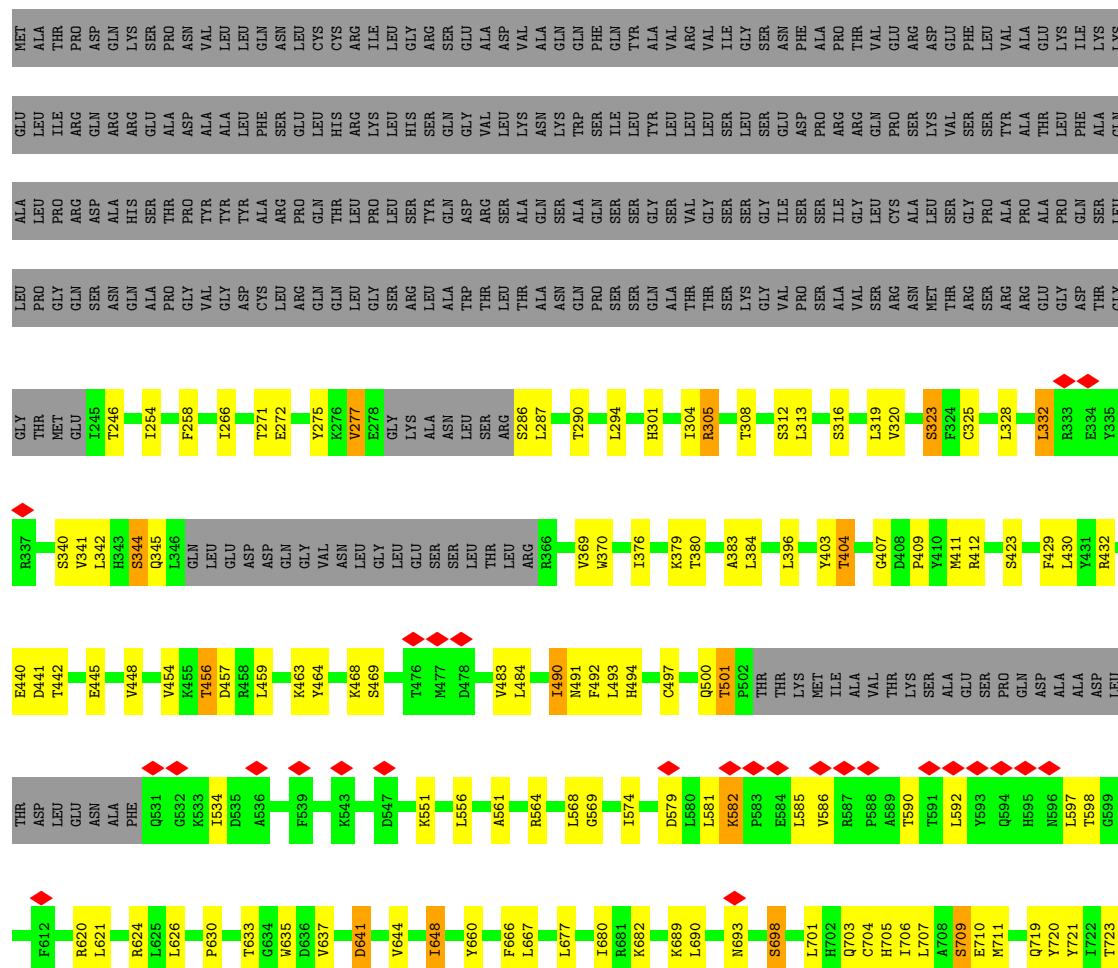
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Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	U	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	V	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	W	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	X	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	Y	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	Z	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	1	420	Total 3371	C 2133	N 586	O 637	S 15	0	0
7	2	420	Total 3371	C 2133	N 586	O 637	S 15	0	0

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

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



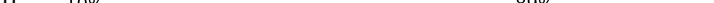




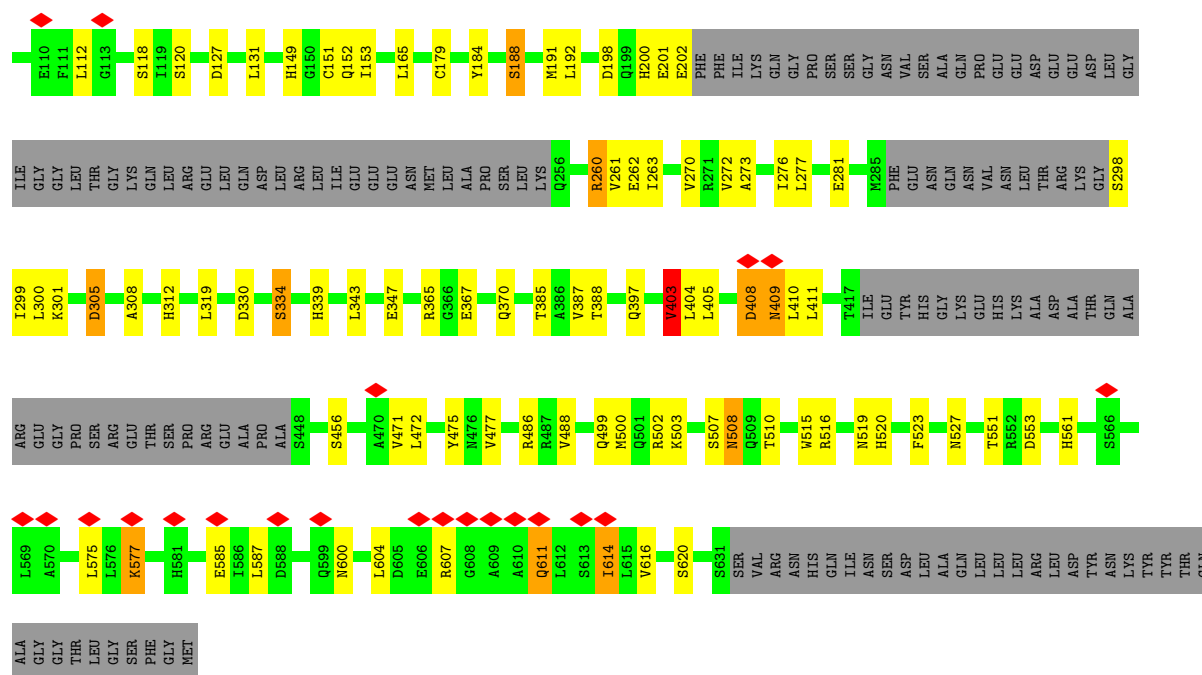


ARG	ARG	LYS	ILE	ILE	THR	ILE	ARG	GLU	SER
ARG	SER	MET	ILE	GLU	THR	THR	VAL	THR	LYS
SER	SER	CYS	GLU	PHE	GLU	PHE	PHE	ALA	TYR
HIS	THR	GLN	GLN	VAL	VAL	VAL	PHE	ARG	LEU
THR	LEU	ASN	ALA	ASN	LEU	LEU	LEU	ALA	ASP
	ARG	ALA	GLU	GLU	GLU	GLU	TRP	THR	VAL
	ARG	GLN	CYS	CYS	GLU	GLN	TRP	ASN	LEU
	ILE	ASP	GLN	ASP	GLN	ALA	ALA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

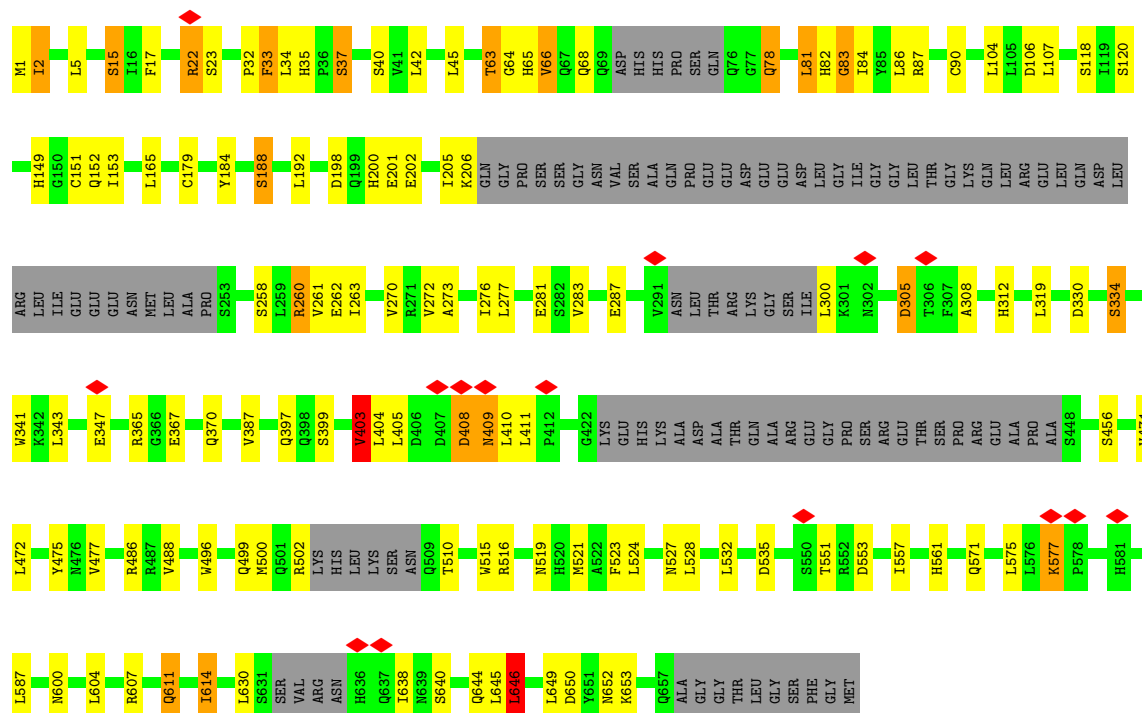
- Molecule 3: Gamma-tubulin complex component 3

Chain h:  10% 89%

LEU	ARG	GLU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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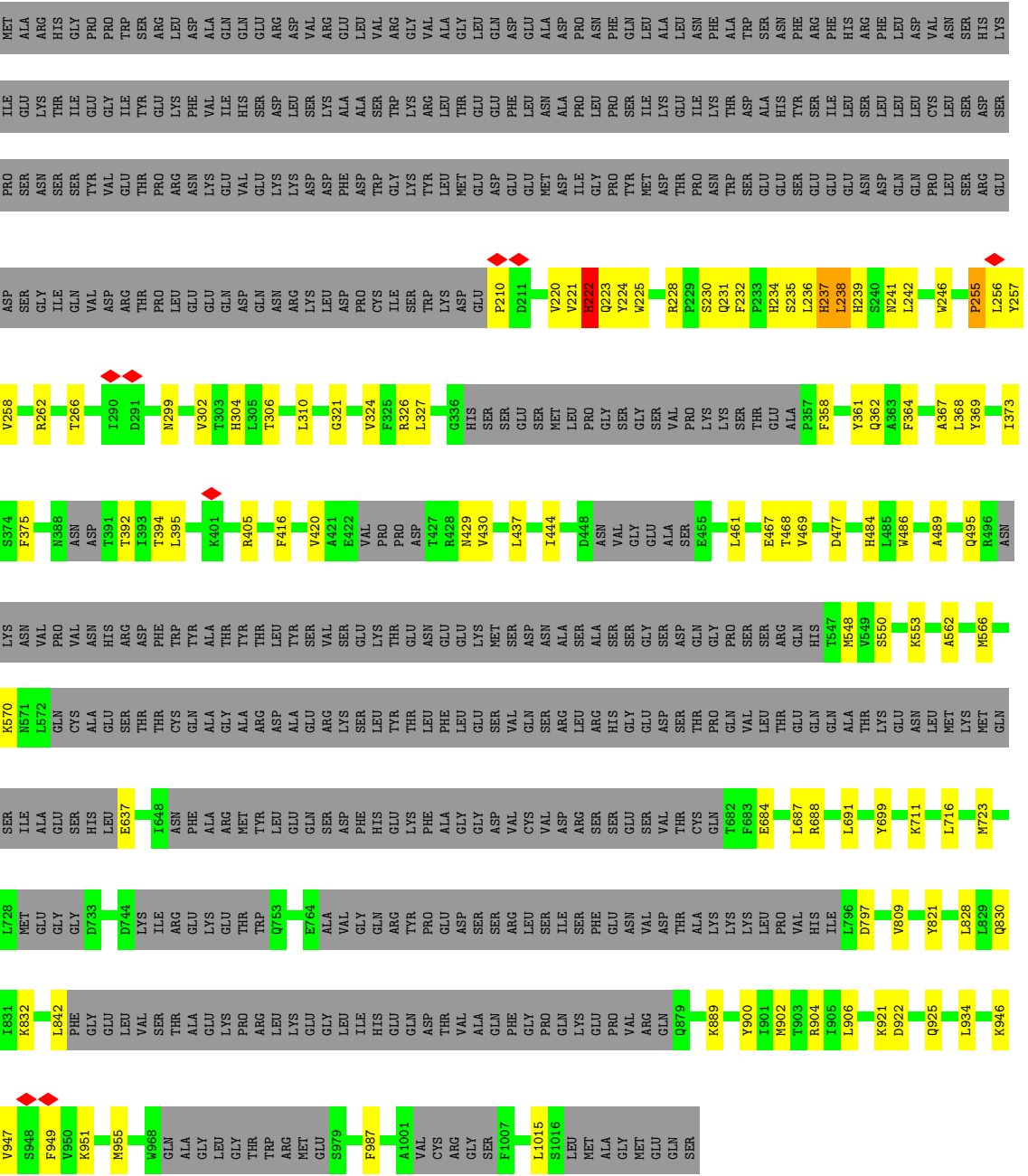


• Molecule 4: Gamma-tubulin complex component 4

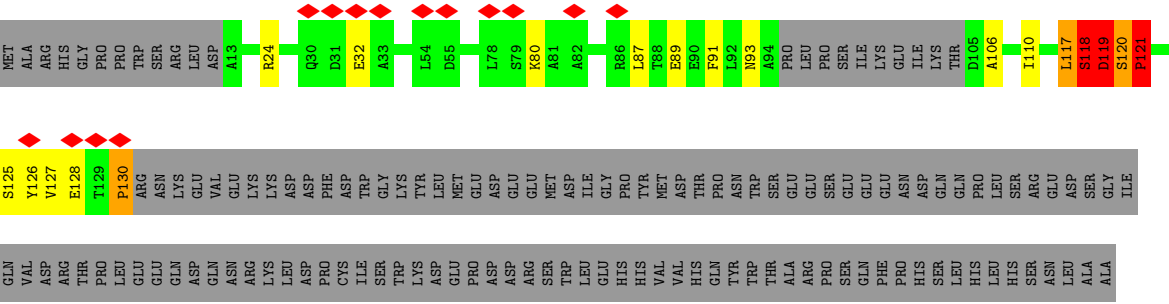


• Molecule 5: Gamma-tubulin complex component 5



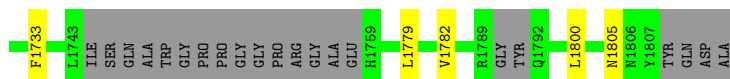


● Molecule 5: Gamma-tubulin complex component 5



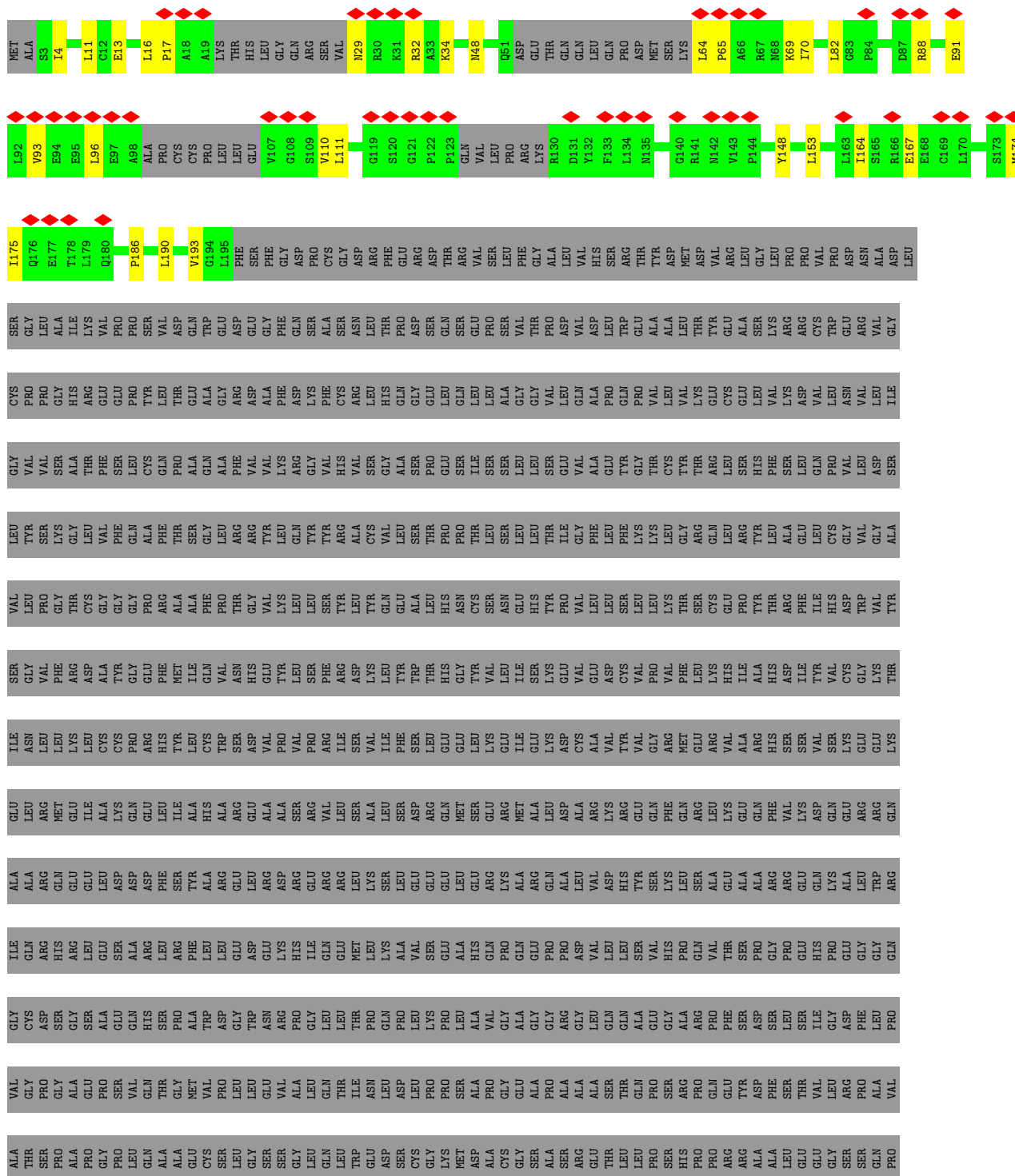


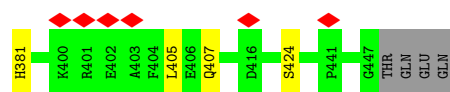




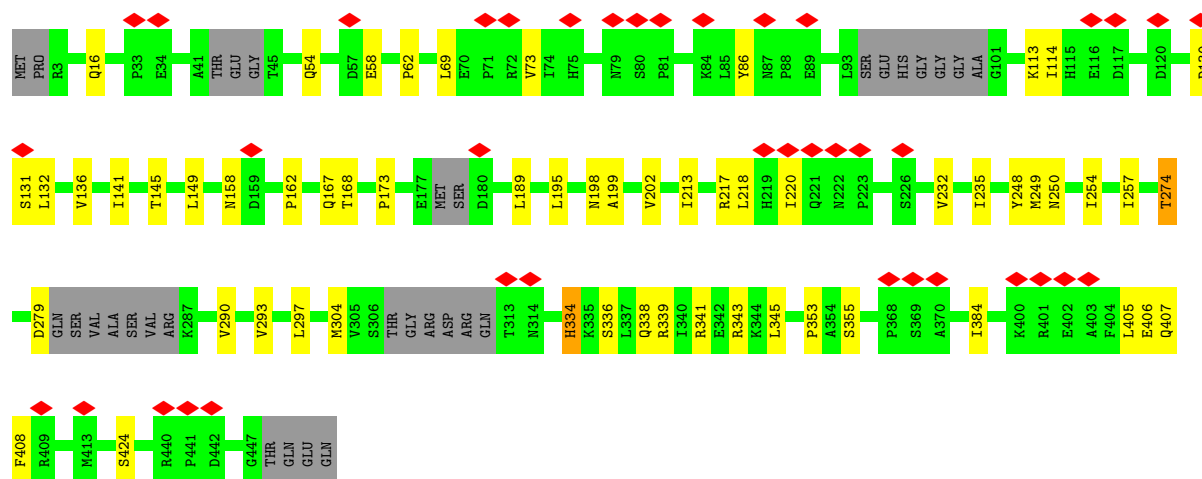
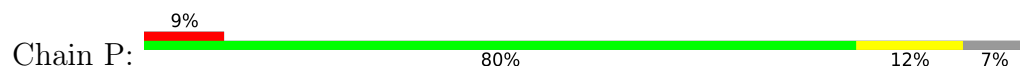
• Molecule 6: Gamma-tubulin complex component 6

Chain c: 91%

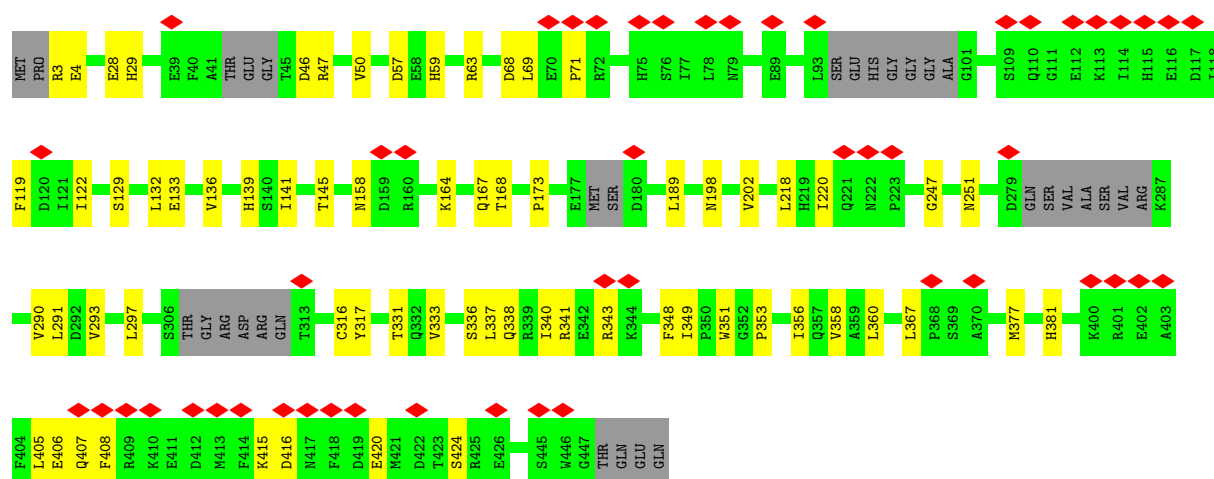
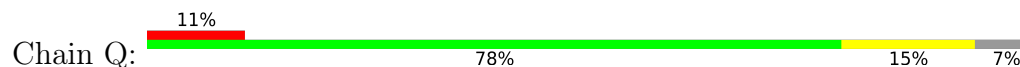




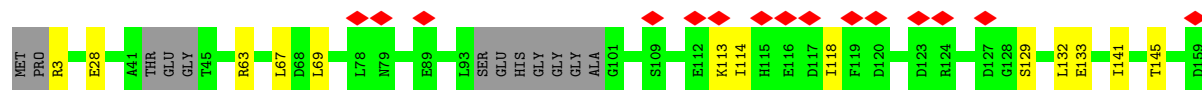
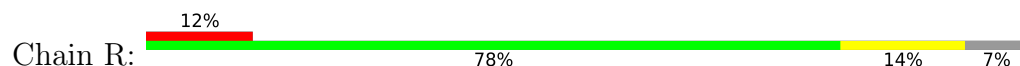
• Molecule 7: Tubulin gamma-1 chain

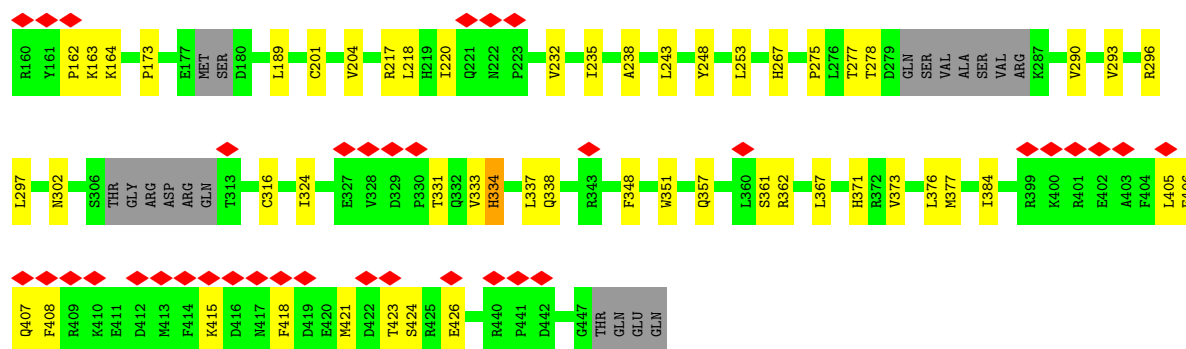


• Molecule 7: Tubulin gamma-1 chain

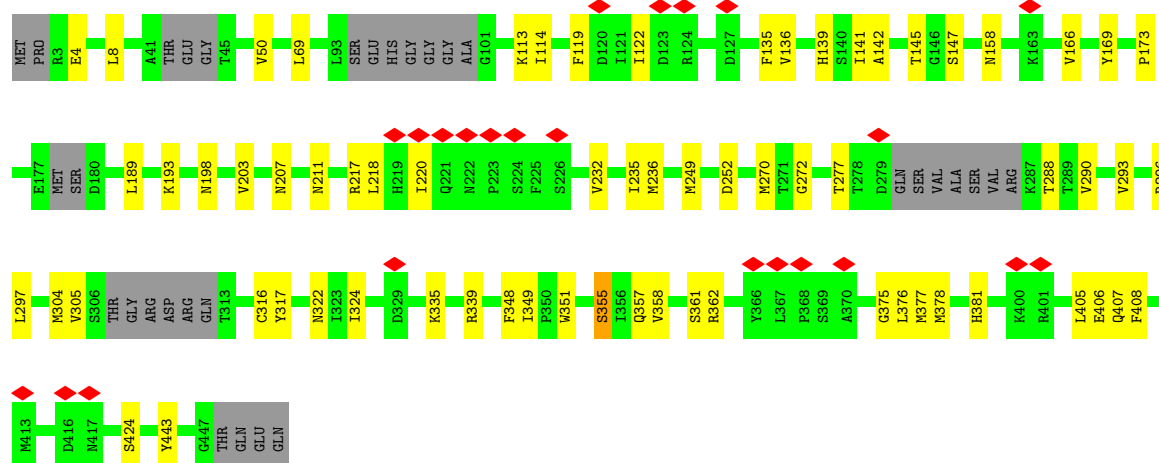
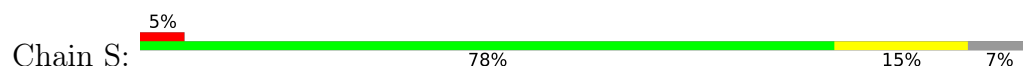


• Molecule 7: Tubulin gamma-1 chain

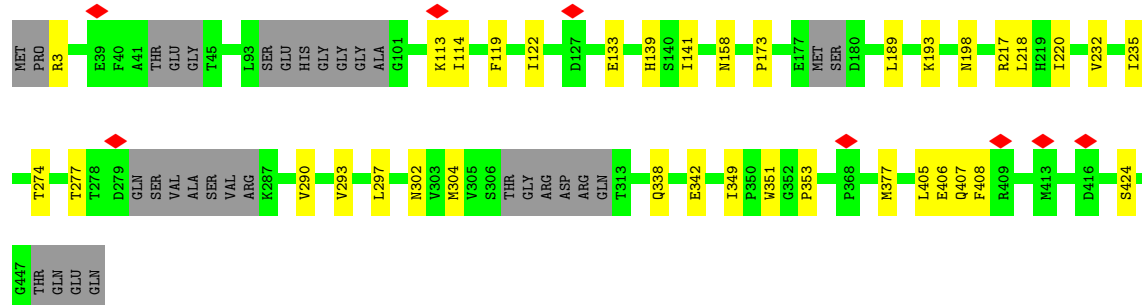
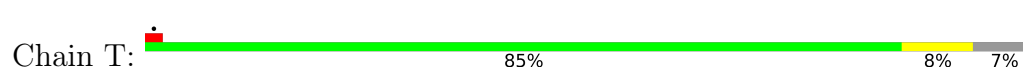




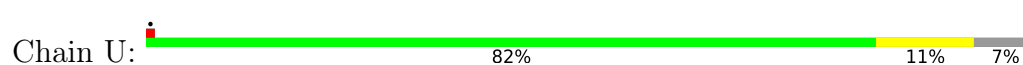
• Molecule 7: Tubulin gamma-1 chain

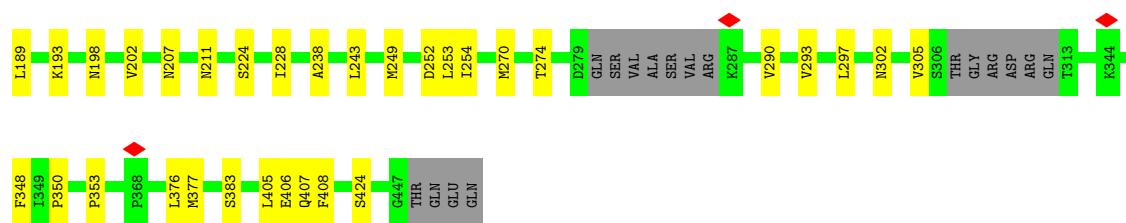


• Molecule 7: Tubulin gamma-1 chain



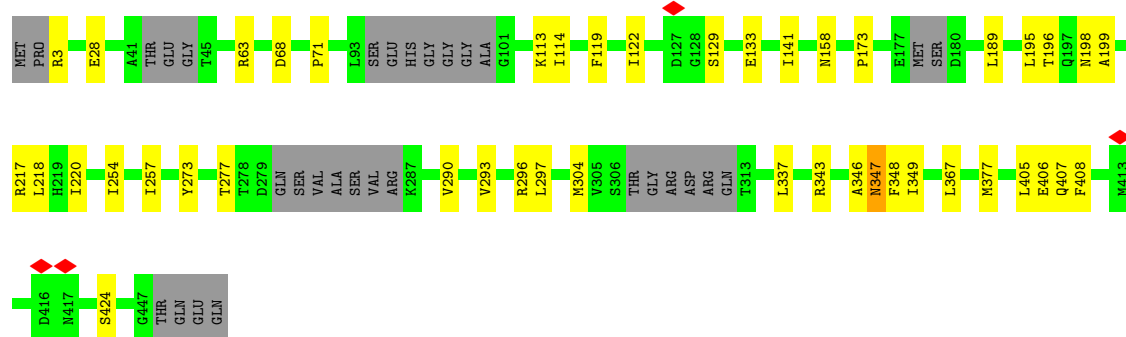
• Molecule 7: Tubulin gamma-1 chain





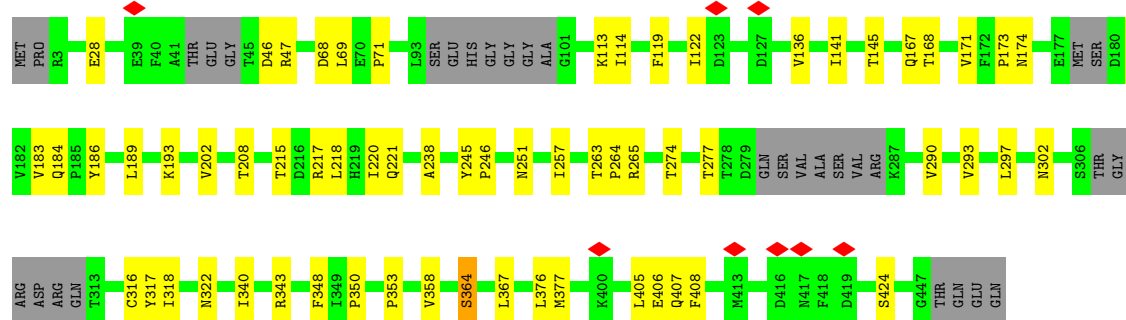
• Molecule 7: Tubulin gamma-1 chain

Chain V: 83% 10% 7%



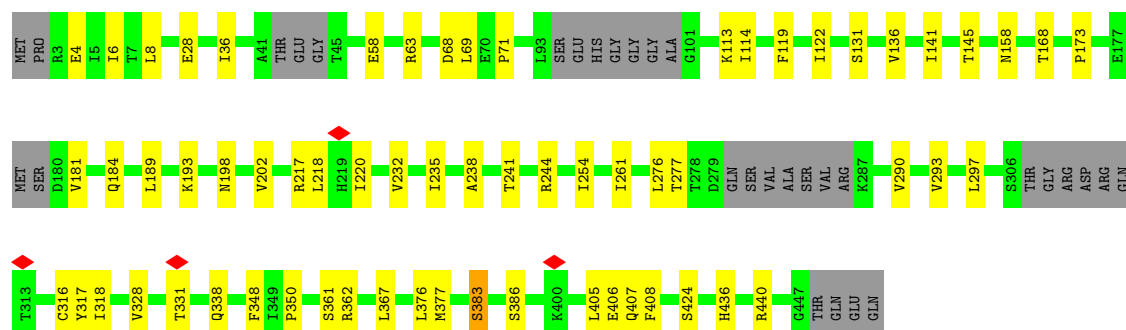
• Molecule 7: Tubulin gamma-1 chain

Chain W: 79% 14% 7%

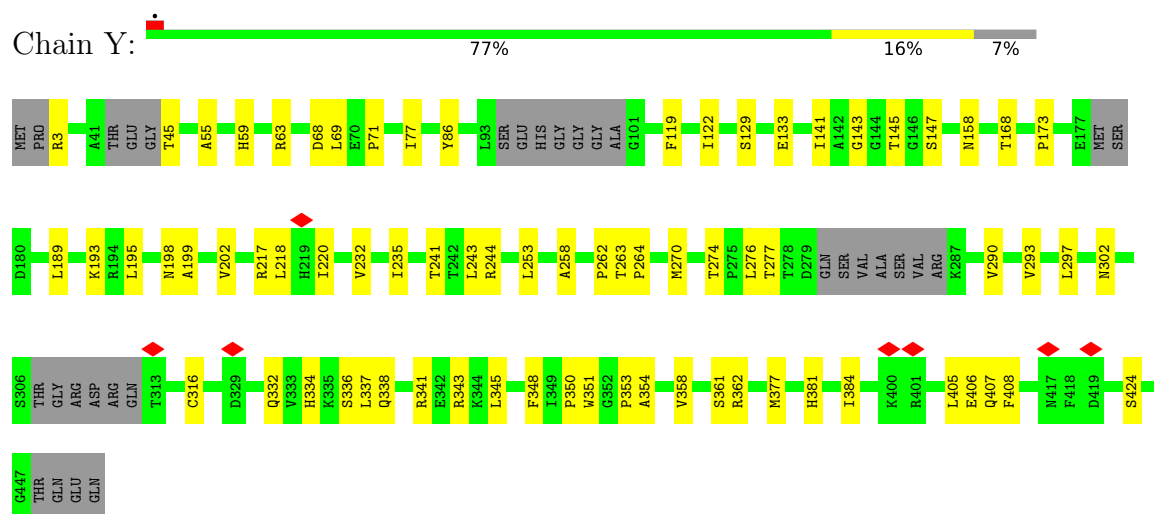


• Molecule 7: Tubulin gamma-1 chain

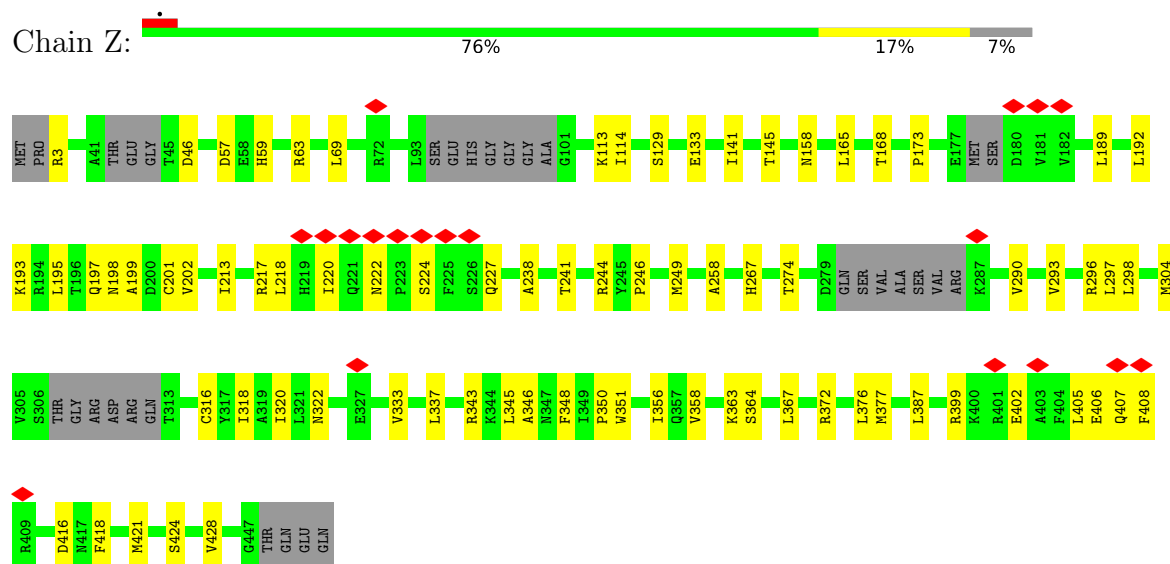
Chain X: 79% 14% 7%



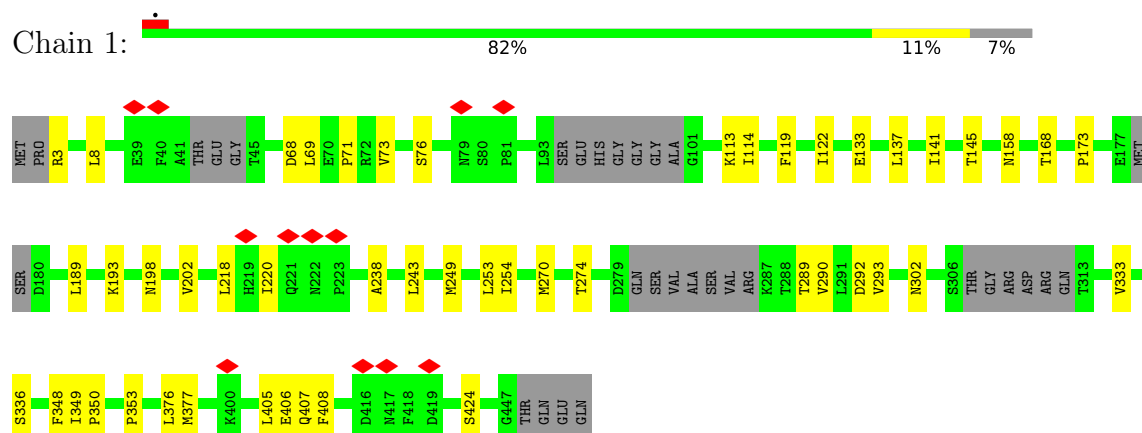
- Molecule 7: Tubulin gamma-1 chain



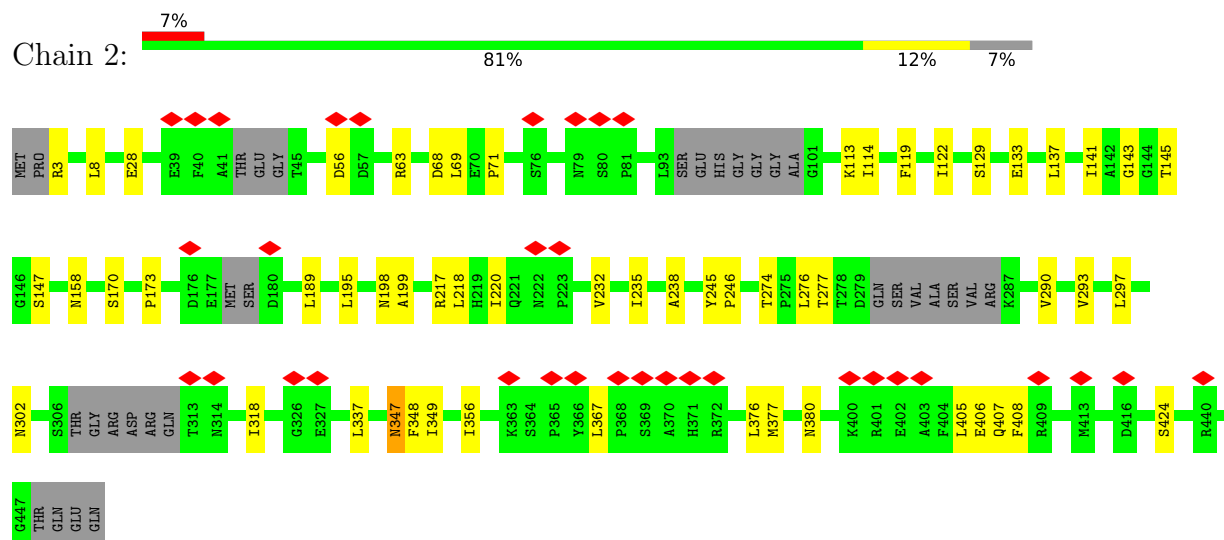
- Molecule 7: Tubulin gamma-1 chain



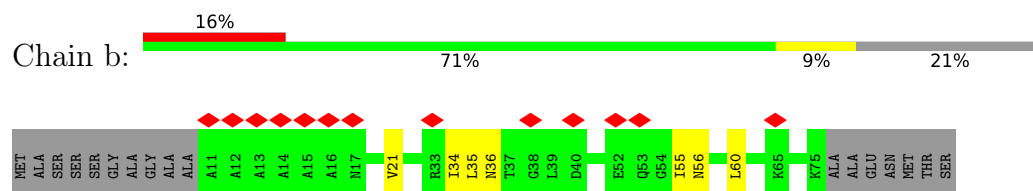
- Molecule 7: Tubulin gamma-1 chain



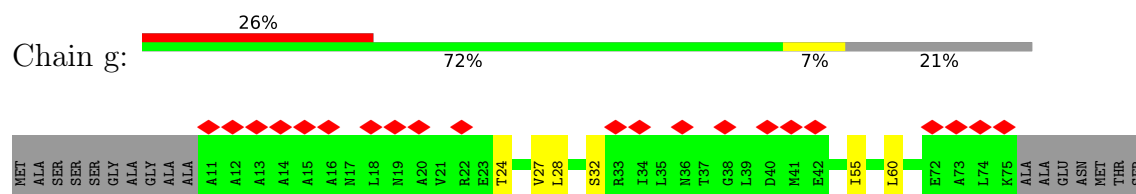
- Molecule 7: Tubulin gamma-1 chain



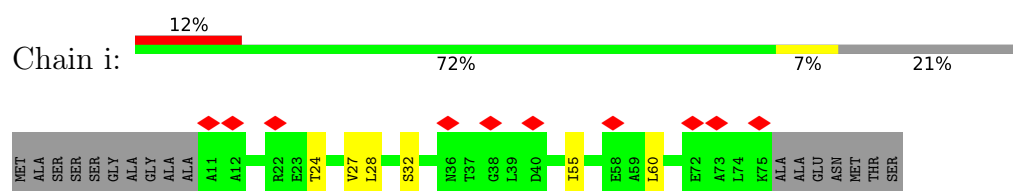
- Molecule 8: Mitotic-spindle organizing protein 1



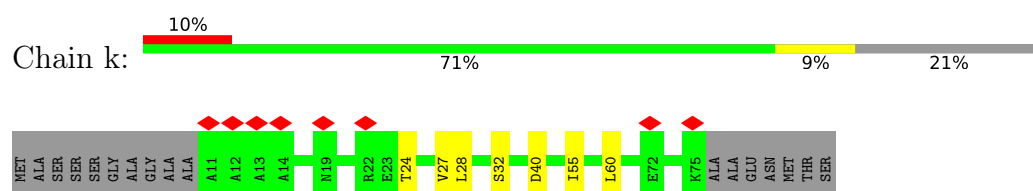
- Molecule 8: Mitotic-spindle organizing protein 1



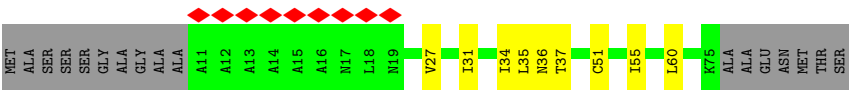
- Molecule 8: Mitotic-spindle organizing protein 1



- Molecule 8: Mitotic-spindle organizing protein 1



- Molecule 8: Mitotic-spindle organizing protein 1



● Molecule 8: Mitotic-spindle organizing protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2645	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	0.091	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0319	Depositor
Map size (Å)	532.0, 532.0, 532.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	e	0.45	1/1818 (0.1%)	0.43	1/2525 (0.0%)
2	A	0.29	0/5085	0.69	6/6866 (0.1%)
2	C	0.29	0/5151	0.68	4/6955 (0.1%)
2	E	0.29	0/5311	0.69	4/7169 (0.1%)
2	G	0.30	0/5326	0.69	5/7188 (0.1%)
2	M	0.29	0/5295	0.68	3/7147 (0.0%)
3	B	0.30	1/5125 (0.0%)	0.69	6/6919 (0.1%)
3	D	0.28	1/4897 (0.0%)	0.65	3/6610 (0.0%)
3	F	0.29	1/5036 (0.0%)	0.66	4/6798 (0.1%)
3	H	0.30	2/5001 (0.0%)	0.68	4/6750 (0.1%)
3	N	0.31	2/5001 (0.0%)	0.68	8/6750 (0.1%)
3	a	0.23	0/948	0.56	0/1277
3	f	0.23	0/815	0.57	0/1096
3	h	0.22	0/815	0.55	0/1096
3	j	0.42	0/877	0.82	3/1179 (0.3%)
4	I	0.32	0/4319	0.74	8/5849 (0.1%)
4	K	0.34	0/4683	0.76	8/6338 (0.1%)
5	J	0.35	0/4501	0.73	11/6089 (0.2%)
5	l	0.31	0/895	0.85	6/1210 (0.5%)
6	L	0.37	0/4666	0.72	9/6310 (0.1%)
6	c	0.33	0/1235	0.71	1/1664 (0.1%)
7	1	0.31	0/3439	0.69	2/4658 (0.0%)
7	2	0.31	0/3439	0.68	4/4658 (0.1%)
7	O	0.34	0/3439	0.72	2/4658 (0.0%)
7	P	0.36	0/3439	0.75	3/4658 (0.1%)
7	Q	0.35	0/3439	0.73	3/4658 (0.1%)
7	R	0.34	0/3439	0.72	2/4658 (0.0%)
7	S	0.34	0/3439	0.74	3/4658 (0.1%)
7	T	0.31	0/3439	0.67	2/4658 (0.0%)
7	U	0.32	0/3439	0.68	2/4658 (0.0%)
7	V	0.31	0/3439	0.68	5/4658 (0.1%)
7	W	0.30	0/3439	0.66	2/4658 (0.0%)
7	X	0.30	0/3439	0.66	2/4658 (0.0%)
7	Y	0.32	0/3439	0.71	2/4658 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	Z	0.32	0/3439	0.65	2/4658 (0.0%)
8	b	0.31	0/484	0.64	0/653
8	d	0.28	0/454	0.57	0/611
8	g	0.25	0/484	0.58	0/653
8	i	0.25	0/484	0.54	0/653
8	k	0.25	0/484	0.57	0/653
8	m	0.33	0/484	0.76	0/653
All	All	0.32	8/127820 (0.0%)	0.69	130/172873 (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
2	A	0	9
2	C	0	7
2	E	0	7
2	G	0	10
2	M	0	8
3	B	0	3
3	D	0	3
3	F	0	5
3	H	0	7
3	N	0	6
3	j	0	1
4	I	0	7
4	K	0	7
5	J	0	1
5	l	0	3
6	L	0	1
7	2	0	1
7	P	0	2
7	V	0	2
All	All	0	90

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	243	PRO	N-CD	17.82	1.72	1.47
3	N	503	THR	N-CA	5.68	1.53	1.46
3	B	840	ILE	CA-CB	5.38	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	840	ILE	CA-CB	5.37	1.57	1.53
3	H	840	ILE	CA-CB	5.37	1.57	1.53
3	N	840	ILE	CA-CB	5.37	1.57	1.53
3	F	840	ILE	CA-CB	5.21	1.57	1.53
3	H	503	THR	N-CA	5.14	1.52	1.46

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	577	LYS	CB-CG-CD	8.81	131.56	111.30
4	I	577	LYS	CB-CG-CD	8.78	131.48	111.30
5	l	121	PRO	CA-N-CD	-8.69	99.83	112.00
5	l	130	PRO	CA-N-CD	-8.69	99.83	112.00
3	H	871	GLU	CA-CB-CG	8.64	131.38	114.10
3	N	871	GLU	CA-CB-CG	8.64	131.38	114.10
3	D	871	GLU	CA-CB-CG	8.64	131.38	114.10
3	F	871	GLU	CA-CB-CG	8.63	131.36	114.10
3	B	871	GLU	CA-CB-CG	8.61	131.32	114.10
4	K	63	THR	N-CA-C	-8.48	102.94	113.20
6	L	306	HIS	CA-C-N	8.30	137.40	121.54
6	L	306	HIS	C-N-CA	8.30	137.40	121.54
2	E	151	GLN	CA-CB-CG	8.26	130.62	114.10
2	G	151	GLN	CA-CB-CG	8.26	130.61	114.10
2	M	151	GLN	CA-CB-CG	8.25	130.60	114.10
2	C	151	GLN	CA-CB-CG	8.25	130.59	114.10
2	A	151	GLN	CA-CB-CG	8.24	130.58	114.10
2	A	426	LYS	CA-C-N	8.22	137.24	121.54
2	A	426	LYS	C-N-CA	8.22	137.24	121.54
5	l	117	LEU	CA-C-N	-7.55	111.60	121.79
5	l	117	LEU	C-N-CA	-7.55	111.60	121.79
3	B	891	PRO	CA-N-CD	-7.37	101.68	112.00
7	V	347	ASN	CA-C-N	7.09	135.09	121.54
7	V	347	ASN	C-N-CA	7.09	135.09	121.54
5	J	256	LEU	CA-C-N	7.02	134.95	121.54
5	J	256	LEU	C-N-CA	7.02	134.95	121.54
5	J	235	SER	CA-C-N	7.01	134.92	121.54
5	J	235	SER	C-N-CA	7.01	134.92	121.54
7	W	405	LEU	CA-C-N	6.88	134.68	121.54
7	W	405	LEU	C-N-CA	6.88	134.68	121.54
7	T	405	LEU	CA-C-N	6.86	134.65	121.54
7	T	405	LEU	C-N-CA	6.86	134.65	121.54
7	X	405	LEU	CA-C-N	6.84	134.60	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	405	LEU	C-N-CA	6.84	134.60	121.54
7	1	405	LEU	CA-C-N	6.79	134.51	121.54
7	1	405	LEU	C-N-CA	6.79	134.51	121.54
7	P	405	LEU	CA-C-N	6.78	134.49	121.54
7	P	405	LEU	C-N-CA	6.78	134.49	121.54
7	U	405	LEU	CA-C-N	6.78	134.49	121.54
7	U	405	LEU	C-N-CA	6.78	134.49	121.54
7	R	405	LEU	CA-C-N	6.77	134.47	121.54
7	R	405	LEU	C-N-CA	6.77	134.47	121.54
7	V	405	LEU	CA-C-N	6.76	134.46	121.54
7	V	405	LEU	C-N-CA	6.76	134.46	121.54
7	S	405	LEU	CA-C-N	6.74	134.41	121.54
7	S	405	LEU	C-N-CA	6.74	134.41	121.54
7	O	405	LEU	CA-C-N	6.70	134.34	121.54
7	O	405	LEU	C-N-CA	6.70	134.34	121.54
7	2	347	ASN	CA-C-N	6.65	134.25	121.54
7	2	347	ASN	C-N-CA	6.65	134.25	121.54
6	L	306	HIS	N-CA-C	6.64	118.24	110.41
7	Z	405	LEU	CA-C-N	6.64	134.22	121.54
7	Z	405	LEU	C-N-CA	6.64	134.22	121.54
7	Q	405	LEU	CA-C-N	6.62	134.18	121.54
7	Q	405	LEU	C-N-CA	6.62	134.18	121.54
7	2	405	LEU	CA-C-N	6.60	134.15	121.54
7	2	405	LEU	C-N-CA	6.60	134.15	121.54
7	Y	405	LEU	CA-C-N	6.59	134.14	121.54
7	Y	405	LEU	C-N-CA	6.59	134.14	121.54
2	E	425	ASP	O-C-N	-6.57	113.85	122.59
4	I	577	LYS	CG-CD-CE	6.54	126.35	111.30
4	K	577	LYS	CG-CD-CE	6.52	126.29	111.30
3	B	365	ARG	CA-C-N	6.40	133.76	121.54
3	B	365	ARG	C-N-CA	6.40	133.76	121.54
3	N	346	LEU	CA-C-N	6.14	132.75	121.70
3	N	346	LEU	C-N-CA	6.14	132.75	121.70
4	I	83	GLY	N-CA-C	6.04	119.10	110.46
4	K	83	GLY	N-CA-C	6.04	119.10	110.46
7	P	339	ARG	CB-CG-CD	6.01	125.12	111.30
3	j	63	ILE	CA-C-N	-5.97	113.10	122.65
3	j	63	ILE	C-N-CA	-5.97	113.10	122.65
3	H	879	ARG	NE-CZ-NH2	5.86	124.47	119.20
3	N	879	ARG	NE-CZ-NH2	5.85	124.47	119.20
3	D	879	ARG	NE-CZ-NH2	5.84	124.46	119.20
3	F	879	ARG	NE-CZ-NH2	5.84	124.46	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	879	ARG	NE-CZ-NH2	5.82	124.44	119.20
7	Q	360	LEU	CA-CB-CG	5.78	136.54	116.30
4	K	403	VAL	CA-C-N	5.64	132.31	121.54
4	K	403	VAL	C-N-CA	5.64	132.31	121.54
4	I	403	VAL	CA-C-N	5.62	132.28	121.54
4	I	403	VAL	C-N-CA	5.62	132.28	121.54
6	L	346	LEU	CA-CB-CG	5.60	135.91	116.30
6	L	316	GLY	CA-C-N	5.60	132.24	121.54
6	L	316	GLY	C-N-CA	5.60	132.24	121.54
3	N	285	ARG	CA-C-N	5.58	128.53	120.38
3	N	285	ARG	C-N-CA	5.58	128.53	120.38
5	l	118	SER	CA-C-N	5.58	132.19	121.54
5	l	118	SER	C-N-CA	5.58	132.19	121.54
3	N	502	PRO	CA-C-O	5.51	130.63	120.60
2	C	674	GLN	CA-CB-CG	5.50	125.09	114.10
3	H	502	PRO	CA-C-O	5.49	130.59	120.60
4	I	81	LEU	CA-C-N	5.47	131.99	121.54
4	I	81	LEU	C-N-CA	5.47	131.99	121.54
4	K	81	LEU	CA-C-N	5.46	131.98	121.54
4	K	81	LEU	C-N-CA	5.46	131.98	121.54
6	c	82	LEU	CA-CB-CG	5.42	135.29	116.30
3	D	879	ARG	NE-CZ-NH1	-5.40	116.10	121.50
5	J	255	PRO	CA-C-N	5.39	131.40	121.70
5	J	255	PRO	C-N-CA	5.39	131.40	121.70
3	F	879	ARG	NE-CZ-NH1	-5.38	116.12	121.50
3	H	879	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	e	243	PRO	CA-N-CD	-5.35	104.51	112.00
3	N	879	ARG	NE-CZ-NH1	-5.35	116.15	121.50
6	L	308	GLU	CA-C-O	-5.33	115.97	122.64
6	L	287	LEU	CA-CB-CG	5.33	134.95	116.30
3	B	879	ARG	NE-CZ-NH1	-5.28	116.22	121.50
4	I	81	LEU	N-CA-C	-5.28	106.97	113.41
2	A	664	THR	N-CA-C	5.24	117.89	110.50
7	V	349	ILE	N-CA-C	5.20	114.68	108.96
7	S	355	SER	N-CA-C	5.20	121.88	110.80
5	J	237	HIS	CA-C-N	5.11	131.30	121.54
5	J	237	HIS	C-N-CA	5.11	131.30	121.54
3	j	108	PRO	N-CA-C	-5.10	104.91	112.26
3	F	501	THR	O-C-N	-5.10	116.78	121.42
5	J	420	VAL	N-CA-C	-5.09	108.54	113.53
6	L	306	HIS	CA-C-O	-5.08	116.45	121.02
5	J	224	TYR	CA-CB-CG	5.07	123.02	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	479	LEU	CA-C-N	5.07	131.22	121.54
2	E	479	LEU	C-N-CA	5.07	131.22	121.54
2	M	479	LEU	CA-C-N	5.06	131.21	121.54
2	M	479	LEU	C-N-CA	5.06	131.21	121.54
2	G	238	LEU	CA-C-N	5.05	131.19	121.54
2	G	238	LEU	C-N-CA	5.05	131.19	121.54
2	C	479	LEU	CA-C-N	5.05	131.19	121.54
2	C	479	LEU	C-N-CA	5.05	131.19	121.54
2	A	479	LEU	CA-C-N	5.04	131.17	121.54
2	A	479	LEU	C-N-CA	5.04	131.17	121.54
2	G	479	LEU	CA-C-N	5.04	131.16	121.54
2	G	479	LEU	C-N-CA	5.04	131.16	121.54
5	J	220	VAL	CG1-CB-CG2	-5.02	99.77	110.80

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	2	347	ASN	Peptide
2	A	238	LEU	Peptide
2	A	239	ALA	Peptide
2	A	426	LYS	Peptide
2	A	467	VAL	Peptide
2	A	580	HIS	Peptide
2	A	663	LYS	Peptide
2	A	664	THR	Peptide
2	A	852	MET	Peptide
2	A	861	PHE	Peptide
3	B	272	GLU	Peptide
3	B	630	PRO	Peptide
3	B	641	ASP	Peptide
2	C	238	LEU	Peptide
2	C	239	ALA	Peptide
2	C	467	VAL	Peptide
2	C	580	HIS	Peptide
2	C	674	GLN	Peptide
2	C	861	PHE	Peptide
2	C	868	ARG	Peptide
3	D	272	GLU	Peptide
3	D	630	PRO	Peptide
3	D	641	ASP	Peptide
2	E	238	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	E	239	ALA	Peptide
2	E	424	ASN	Peptide
2	E	425	ASP	Mainchain
2	E	467	VAL	Peptide
2	E	580	HIS	Peptide
2	E	861	PHE	Peptide
3	F	272	GLU	Peptide
3	F	285	ARG	Peptide
3	F	364	LEU	Peptide
3	F	630	PRO	Peptide
3	F	641	ASP	Peptide
2	G	202	ALA	Peptide
2	G	238	LEU	Peptide
2	G	239	ALA	Peptide
2	G	414	LEU	Peptide
2	G	425	ASP	Peptide
2	G	426	LYS	Peptide
2	G	467	VAL	Peptide
2	G	580	HIS	Peptide
2	G	585	GLN	Peptide
2	G	674	GLN	Peptide
3	H	272	GLU	Peptide
3	H	285	ARG	Peptide
3	H	502	PRO	Mainchain,Peptide
3	H	503	THR	Peptide
3	H	630	PRO	Peptide
3	H	641	ASP	Peptide
4	I	15	SER	Peptide
4	I	298	SER	Peptide
4	I	403	VAL	Peptide
4	I	408	ASP	Peptide
4	I	507	SER	Peptide
4	I	81	LEU	Peptide
4	I	83	GLY	Peptide
5	J	210	PRO	Peptide
4	K	15	SER	Peptide
4	K	403	VAL	Peptide
4	K	408	ASP	Peptide
4	K	64	GLY	Peptide
4	K	646	LEU	Peptide
4	K	81	LEU	Peptide
4	K	83	GLY	Peptide

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Mol	Chain	Res	Type	Group
6	L	306	HIS	Peptide
2	M	238	LEU	Peptide
2	M	239	ALA	Peptide
2	M	414	LEU	Peptide
2	M	425	ASP	Peptide
2	M	426	LYS	Peptide
2	M	467	VAL	Peptide
2	M	580	HIS	Peptide
2	M	674	GLN	Peptide
3	N	272	GLU	Peptide
3	N	502	PRO	Mainchain,Peptide
3	N	503	THR	Peptide
3	N	630	PRO	Peptide
3	N	641	ASP	Peptide
7	P	334	HIS	Sidechain
7	P	355	SER	Peptide
7	V	346	ALA	Peptide
7	V	347	ASN	Peptide
3	j	112	SER	Peptide
5	l	117	LEU	Peptide
5	l	118	SER	Peptide
5	l	119	ASP	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	1818	0	860	7	0
2	A	4978	0	4996	83	0
2	C	5044	0	5081	99	0
2	E	5202	0	5241	82	0
2	G	5217	0	5248	91	0
2	M	5186	0	5219	86	0
3	B	5021	0	5002	90	0
3	D	4796	0	4775	98	0
3	F	4933	0	4919	104	0
3	H	4899	0	4880	84	0
3	N	4899	0	4880	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	a	933	0	953	10	0
3	f	803	0	831	8	0
3	h	803	0	831	5	0
3	j	864	0	894	34	0
4	I	4222	0	4250	59	0
4	K	4579	0	4586	60	0
5	J	4406	0	4452	58	0
5	l	876	0	842	39	0
6	L	4556	0	4559	43	0
6	c	1220	0	1231	27	0
7	1	3371	0	3320	27	0
7	2	3371	0	3320	28	0
7	O	3371	0	3320	42	0
7	P	3371	0	3320	34	0
7	Q	3371	0	3320	41	0
7	R	3371	0	3320	44	0
7	S	3371	0	3320	36	0
7	T	3371	0	3320	21	0
7	U	3371	0	3320	29	0
7	V	3371	0	3320	20	0
7	W	3371	0	3320	35	0
7	X	3371	0	3320	34	0
7	Y	3371	0	3320	44	0
7	Z	3371	0	3320	42	0
8	b	484	0	512	8	0
8	d	454	0	482	7	0
8	g	484	0	512	5	0
8	i	484	0	512	5	0
8	k	484	0	512	6	0
8	m	484	0	512	26	0
All	All	125323	0	124052	1591	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 (1591) 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)
8:m:36:ASN:HB2	5:l:121:PRO:CG	1.44	1.43
8:m:36:ASN:CB	5:l:121:PRO:CG	2.00	1.39
1:e:243:PRO:CD	1:e:243:PRO:N	1.72	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:776:ARG:NH2	3:j:106:ARG:HE	1.52	1.08
8:m:36:ASN:CB	5:l:121:PRO:HG3	1.76	1.06
8:m:35:LEU:O	5:l:121:PRO:HD3	1.59	1.01
8:m:36:ASN:CB	5:l:121:PRO:CD	2.41	0.98
3:F:780:ASP:CG	3:j:106:ARG:HH12	1.71	0.98
8:m:36:ASN:HB2	5:l:121:PRO:HG2	0.99	0.98
8:m:35:LEU:O	5:l:121:PRO:CD	2.13	0.95
2:G:876:ARG:CD	3:j:42:ASN:HD21	1.81	0.94
8:m:36:ASN:CB	5:l:121:PRO:HG2	1.83	0.94
8:m:36:ASN:HB3	5:l:121:PRO:CG	1.97	0.94
8:m:36:ASN:HB2	5:l:121:PRO:CD	1.98	0.91
8:m:36:ASN:HB3	5:l:121:PRO:HD3	1.51	0.90
3:F:776:ARG:NH2	3:j:106:ARG:NE	2.20	0.89
8:m:36:ASN:HB3	5:l:121:PRO:CD	2.02	0.89
8:m:36:ASN:CG	5:l:121:PRO:HG3	2.02	0.85
2:G:876:ARG:HD3	3:j:42:ASN:HD21	1.42	0.84
3:B:890:GLU:HA	3:B:893:LEU:HD12	1.61	0.80
8:m:36:ASN:HB3	5:l:121:PRO:HG3	1.59	0.80
5:l:127:VAL:HG12	5:l:127:VAL:O	1.80	0.80
2:G:876:ARG:HG2	3:j:42:ASN:ND2	1.98	0.79
3:N:345:GLN:HB2	3:N:362:LEU:HD22	1.65	0.77
3:F:776:ARG:HH22	3:j:106:ARG:HE	1.32	0.76
7:U:270:MET:HG2	7:U:305:VAL:HG21	1.69	0.75
3:j:105:ARG:HD2	3:j:106:ARG:HG3	1.68	0.74
3:D:879:ARG:HE	7:R:334:HIS:CE1	2.05	0.73
7:R:3:ARG:HB2	7:R:133:GLU:HB2	1.69	0.73
3:H:630:PRO:HG2	5:l:119:ASP:HB2	1.68	0.73
3:B:810:LYS:NZ	3:B:826:GLU:OE1	2.21	0.73
8:m:36:ASN:ND2	5:l:121:PRO:HG3	2.04	0.73
2:G:876:ARG:CG	3:j:42:ASN:HD21	2.03	0.72
5:J:222:HIS:CD2	5:J:225:TRP:HE1	2.05	0.72
7:S:141:ILE:HB	7:S:173:PRO:HD3	1.69	0.72
7:Q:3:ARG:HB2	7:Q:133:GLU:HB2	1.71	0.72
4:K:283:VAL:O	4:K:287:GLU:HB2	1.89	0.71
4:K:650:ASP:HA	7:Y:341:ARG:HG3	1.73	0.71
8:m:36:ASN:CB	5:l:121:PRO:HD3	2.15	0.71
2:A:649:LYS:HD3	7:O:249:MET:HE1	1.73	0.71
7:W:136:VAL:HG12	7:W:167:GLN:HB3	1.73	0.70
7:Z:290:VAL:HA	7:Z:293:VAL:HG22	1.73	0.70
7:Q:316:CYS:HB2	7:Q:348:PHE:HA	1.72	0.70
6:L:1571:ASN:HB3	6:L:1599:LYS:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:j:111:VAL:HG12	3:j:112:SER:N	2.07	0.70
3:F:665:ASN:HD21	3:j:66:ARG:HG2	1.57	0.69
5:l:121:PRO:HD2	5:l:121:PRO:O	1.93	0.69
7:2:3:ARG:HB2	7:2:133:GLU:HB2	1.76	0.68
7:O:3:ARG:HB2	7:O:133:GLU:HB2	1.77	0.67
6:L:507:GLN:O	6:L:511:HIS:HB2	1.95	0.67
5:l:126:TYR:O	5:l:128:GLU:HG3	1.94	0.67
7:1:3:ARG:HB2	7:1:133:GLU:HB2	1.77	0.67
3:F:629:SER:HB3	3:j:64:ARG:HH22	1.59	0.66
7:Q:132:LEU:HG	7:Q:164:LYS:HD3	1.77	0.66
3:F:780:ASP:CG	3:j:106:ARG:NH1	2.51	0.66
7:Z:3:ARG:HB2	7:Z:133:GLU:HB2	1.77	0.66
2:M:222:LEU:HB3	3:N:365:ARG:HH12	1.61	0.66
7:V:3:ARG:HB2	7:V:133:GLU:HB2	1.76	0.66
2:C:294:ALA:HB1	3:D:409:PRO:HD3	1.79	0.65
7:T:3:ARG:HB2	7:T:133:GLU:HB2	1.78	0.65
7:Y:316:CYS:HB2	7:Y:348:PHE:HA	1.77	0.65
4:K:305:ASP:N	4:K:305:ASP:OD1	2.30	0.65
7:O:320:ILE:HB	7:O:356:ILE:HG12	1.79	0.65
8:m:35:LEU:O	5:l:121:PRO:HD2	1.94	0.65
3:F:624:ARG:HB2	3:F:641:ASP:HB2	1.78	0.65
4:I:305:ASP:N	4:I:305:ASP:OD1	2.30	0.65
7:U:3:ARG:HB2	7:U:133:GLU:HB2	1.77	0.65
3:D:624:ARG:HB2	3:D:641:ASP:HB2	1.78	0.65
7:Z:316:CYS:HB2	7:Z:348:PHE:HA	1.78	0.65
3:B:624:ARG:HB2	3:B:641:ASP:HB2	1.78	0.65
3:D:689:LYS:NZ	7:R:162:PRO:O	2.30	0.64
3:N:624:ARG:HB2	3:N:641:ASP:HB2	1.78	0.64
2:C:858:ARG:HH12	7:Q:358:VAL:HG22	1.61	0.64
3:H:624:ARG:HB2	3:H:641:ASP:HB2	1.78	0.64
3:D:626:LEU:HD23	3:h:64:ARG:HD2	1.80	0.64
2:G:660:ILE:HG21	7:U:254:ILE:HD11	1.79	0.64
2:G:876:ARG:HG2	3:j:42:ASN:CG	2.23	0.63
3:H:345:GLN:HB2	3:H:362:LEU:HD22	1.79	0.63
6:L:444:ARG:HH22	2:M:322:GLN:HE22	1.46	0.63
2:C:526:ASP:HB2	7:Q:47:ARG:HD2	1.81	0.63
5:J:1015:LEU:HD13	7:X:338:GLN:HE22	1.63	0.63
7:O:270:MET:HG2	7:O:305:VAL:HG21	1.81	0.63
7:X:316:CYS:HB2	7:X:348:PHE:HA	1.81	0.63
2:M:233:VAL:HG12	2:M:248:VAL:HG12	1.81	0.62
2:E:233:VAL:HG12	2:E:248:VAL:HG12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:876:ARG:CG	3:j:42:ASN:ND2	2.61	0.62
8:m:34:ILE:HG22	5:l:125:SER:OG	1.99	0.62
2:G:233:VAL:HG12	2:G:248:VAL:HG12	1.81	0.62
7:1:254:ILE:HD11	2:M:660:ILE:HG21	1.81	0.62
2:A:664:THR:HG1	2:A:675:TRP:CD1	2.17	0.62
7:Z:224:SER:HA	7:Z:227:GLN:HE21	1.64	0.62
7:Z:158:ASN:HD21	7:Z:198:ASN:HD22	1.45	0.62
1:e:4:ASP:C	1:e:4:ASP:OD1	2.42	0.62
7:W:217:ARG:HH21	7:W:277:THR:HA	1.64	0.62
2:A:233:VAL:HG12	2:A:248:VAL:HG12	1.81	0.61
7:X:217:ARG:HH21	7:X:277:THR:HA	1.65	0.61
7:2:349:ILE:O	3:N:883:ASN:ND2	2.28	0.61
2:C:233:VAL:HG12	2:C:248:VAL:HG12	1.81	0.61
2:C:395:ILE:HD11	2:C:450:ILE:HG23	1.82	0.61
2:A:395:ILE:HD11	2:A:450:ILE:HG23	1.82	0.61
7:Y:217:ARG:HH21	7:Y:277:THR:HA	1.65	0.61
2:C:278:GLU:OE2	3:D:379:LYS:NZ	2.26	0.61
3:F:456:THR:OG1	3:F:457:ASP:N	2.32	0.61
3:H:456:THR:OG1	3:H:457:ASP:N	2.32	0.61
7:S:158:ASN:HD21	7:S:198:ASN:HD22	1.49	0.61
7:U:270:MET:HE1	7:U:383:SER:HB3	1.81	0.61
3:D:456:THR:OG1	3:D:457:ASP:N	2.32	0.61
3:F:736:ASN:OD1	3:F:736:ASN:N	2.34	0.61
2:M:395:ILE:HD11	2:M:450:ILE:HG23	1.82	0.61
3:B:736:ASN:N	3:B:736:ASN:OD1	2.34	0.61
2:G:395:ILE:HD11	2:G:450:ILE:HG23	1.82	0.61
4:I:523:PHE:O	4:I:527:ASN:ND2	2.34	0.61
8:b:55:ILE:HD13	8:b:60:LEU:HD12	1.83	0.61
2:M:390:VAL:HG22	2:M:401:HIS:HE1	1.66	0.61
2:C:390:VAL:HG22	2:C:401:HIS:HE1	1.66	0.60
3:D:682:LYS:HE2	7:R:163:LYS:HE3	1.83	0.60
4:I:367:GLU:HA	7:W:251:ASN:HD22	1.66	0.60
2:A:390:VAL:HG22	2:A:401:HIS:HE1	1.66	0.60
2:C:674:GLN:HA	2:C:675:TRP:CD1	2.36	0.60
7:Y:3:ARG:HB2	7:Y:133:GLU:HB2	1.84	0.60
2:M:509:LEU:HD21	2:M:629:ILE:HG21	1.84	0.60
2:E:395:ILE:HD11	2:E:450:ILE:HG23	1.82	0.60
7:X:28:GLU:HA	7:X:367:LEU:HD11	1.84	0.60
2:A:509:LEU:HD21	2:A:629:ILE:HG21	1.84	0.60
2:E:313:LEU:HD23	2:E:319:LEU:HD12	1.84	0.60
2:G:509:LEU:HD21	2:G:629:ILE:HG21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:736:ASN:OD1	3:D:736:ASN:N	2.34	0.60
7:X:36:ILE:HG23	7:X:58:GLU:HB3	1.84	0.60
3:D:345:GLN:HG2	6:c:175:ILE:HG13	1.84	0.60
2:G:313:LEU:HD23	2:G:319:LEU:HD12	1.84	0.60
8:b:55:ILE:HD11	3:a:39:ILE:HD12	1.83	0.60
3:B:456:THR:OG1	3:B:457:ASP:N	2.32	0.60
2:C:313:LEU:HD23	2:C:319:LEU:HD12	1.84	0.60
2:C:509:LEU:HD21	2:C:629:ILE:HG21	1.84	0.60
7:W:263:THR:HG22	7:W:265:ARG:H	1.66	0.60
2:G:238:LEU:HD21	2:G:245:THR:H	1.68	0.59
3:H:875:PHE:O	3:H:879:ARG:NH1	2.35	0.59
7:R:141:ILE:HB	7:R:173:PRO:HD3	1.84	0.59
2:M:238:LEU:HD21	2:M:245:THR:H	1.67	0.59
3:B:666:PHE:HB2	3:B:764:LEU:HD21	1.84	0.59
2:E:509:LEU:HD21	2:E:629:ILE:HG21	1.84	0.59
4:K:523:PHE:O	4:K:527:ASN:ND2	2.34	0.59
3:N:875:PHE:O	3:N:879:ARG:NH1	2.35	0.59
2:G:390:VAL:HG22	2:G:401:HIS:HE1	1.66	0.59
3:H:666:PHE:HB2	3:H:764:LEU:HD21	1.84	0.59
7:P:54:GLN:HE22	7:P:58:GLU:HA	1.66	0.59
7:Y:195:LEU:O	7:Y:199:ALA:HB3	2.02	0.59
2:E:238:LEU:HD21	2:E:245:THR:H	1.67	0.59
2:E:390:VAL:HG22	2:E:401:HIS:HE1	1.66	0.59
2:E:555:LEU:HD22	2:E:575:ILE:HG13	1.85	0.59
8:m:36:ASN:CG	5:l:121:PRO:CG	2.64	0.59
5:l:130:PRO:HD2	5:l:130:PRO:O	2.02	0.59
3:D:875:PHE:O	3:D:879:ARG:NH1	2.35	0.59
4:K:524:LEU:HD13	7:Y:354:ALA:HA	1.84	0.59
8:d:66:GLU:HA	8:d:69:LYS:HD2	1.84	0.59
2:M:313:LEU:HD23	2:M:319:LEU:HD12	1.84	0.59
2:A:238:LEU:HD21	2:A:245:THR:H	1.67	0.59
5:J:716:LEU:HG	5:J:809:VAL:HG13	1.84	0.59
7:1:158:ASN:HD21	7:1:198:ASN:HD22	1.50	0.59
2:E:427:TYR:HE1	2:E:455:LYS:HG3	1.68	0.59
3:F:875:PHE:O	3:F:879:ARG:NH1	2.35	0.59
3:B:266:ILE:HD11	3:B:275:TYR:HB3	1.85	0.59
2:E:489:GLU:O	2:E:493:ASN:ND2	2.36	0.59
7:O:217:ARG:HH21	7:O:277:THR:HA	1.67	0.59
3:B:879:ARG:HH21	3:B:879:ARG:HB3	1.68	0.59
3:H:380:THR:HG23	3:H:411:MET:HE3	1.85	0.59
7:S:270:MET:HG2	7:S:305:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:158:ASN:HD21	7:T:198:ASN:HD22	1.51	0.59
7:2:318:ILE:HB	7:2:380:ASN:HB3	1.85	0.59
2:M:427:TYR:HE1	2:M:455:LYS:HG3	1.68	0.59
3:B:380:THR:HG23	3:B:411:MET:HE3	1.85	0.59
3:D:666:PHE:HB2	3:D:764:LEU:HD21	1.84	0.59
3:D:879:ARG:HH21	3:D:879:ARG:HB3	1.68	0.58
3:N:266:ILE:HD11	3:N:275:TYR:HB3	1.85	0.58
7:Y:270:MET:HE3	7:Y:381:HIS:HB3	1.85	0.58
3:N:879:ARG:HH21	3:N:879:ARG:HB3	1.68	0.58
2:A:543:VAL:HG13	2:A:544:GLU:HG2	1.85	0.58
3:F:380:THR:HG23	3:F:411:MET:HE3	1.85	0.58
7:Q:141:ILE:HB	7:Q:173:PRO:HD3	1.85	0.58
7:Q:158:ASN:HD21	7:Q:198:ASN:HD22	1.51	0.58
2:M:555:LEU:HD22	2:M:575:ILE:HG13	1.84	0.58
2:A:663:LYS:HD3	2:A:664:THR:HA	1.85	0.58
2:G:427:TYR:HE1	2:G:455:LYS:HG3	1.68	0.58
7:Z:297:LEU:HD13	7:Z:377:MET:HB3	1.86	0.58
3:N:380:THR:HG23	3:N:411:MET:HE3	1.85	0.58
3:B:875:PHE:O	3:B:879:ARG:NH1	2.35	0.58
2:G:489:GLU:O	2:G:493:ASN:ND2	2.36	0.58
7:W:316:CYS:HB2	7:W:348:PHE:HA	1.86	0.58
6:c:164:ILE:HA	6:c:167:GLU:HG3	1.86	0.58
2:G:454:GLY:HA2	2:G:457:LEU:HD12	1.86	0.58
6:L:1805:ASN:ND2	7:Z:348:PHE:O	2.37	0.58
7:O:232:VAL:HA	7:O:235:ILE:HD12	1.85	0.58
2:A:454:GLY:HA2	2:A:457:LEU:HD12	1.86	0.58
2:C:427:TYR:HE1	2:C:455:LYS:HG3	1.68	0.58
3:F:776:ARG:HH21	3:j:106:ARG:HE	1.47	0.58
3:F:879:ARG:HH21	3:F:879:ARG:HB3	1.68	0.58
3:H:266:ILE:HD11	3:H:275:TYR:HB3	1.85	0.58
3:H:879:ARG:HB3	3:H:879:ARG:HH21	1.68	0.58
5:J:242:LEU:HB3	5:J:304:HIS:HA	1.85	0.58
7:R:316:CYS:HB2	7:R:348:PHE:HA	1.84	0.58
7:V:290:VAL:HA	7:V:293:VAL:HG22	1.84	0.58
7:X:6:ILE:HG12	7:X:63:ARG:HB3	1.85	0.58
7:1:68:ASP:HB2	7:1:71:PRO:HB3	1.84	0.58
2:A:313:LEU:HD23	2:A:319:LEU:HD12	1.84	0.58
2:C:238:LEU:HD21	2:C:245:THR:H	1.67	0.58
2:G:555:LEU:HD22	2:G:575:ILE:HG13	1.85	0.58
3:H:404:THR:O	3:H:404:THR:OG1	2.22	0.58
7:P:334:HIS:NE2	7:P:338:GLN:HG2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:158:ASN:HD21	7:X:198:ASN:HD22	1.51	0.58
2:M:454:GLY:HA2	2:M:457:LEU:HD12	1.86	0.58
3:N:666:PHE:HB2	3:N:764:LEU:HD21	1.84	0.58
2:A:555:LEU:HD22	2:A:575:ILE:HG13	1.84	0.58
3:D:266:ILE:HD11	3:D:275:TYR:HB3	1.85	0.58
3:H:736:ASN:OD1	3:H:736:ASN:N	2.34	0.58
5:J:477:ASP:OD2	5:J:637:GLU:N	2.37	0.58
7:O:270:MET:HE3	7:O:305:VAL:HB	1.86	0.58
8:g:60:LEU:HD22	3:f:96:LEU:HD11	1.85	0.58
3:N:456:THR:OG1	3:N:457:ASP:N	2.32	0.58
2:C:555:LEU:HD22	2:C:575:ILE:HG13	1.85	0.58
3:D:380:THR:HG23	3:D:411:MET:HE3	1.85	0.58
3:F:666:PHE:HB2	3:F:764:LEU:HD21	1.84	0.58
3:F:719:GLN:O	3:F:723:THR:OG1	2.22	0.58
7:U:68:ASP:HB2	7:U:71:PRO:HB3	1.86	0.58
7:U:158:ASN:HD21	7:U:198:ASN:HD22	1.51	0.58
2:M:231:ARG:HE	3:N:285:ARG:HE	1.51	0.58
3:B:719:GLN:O	3:B:723:THR:OG1	2.22	0.57
2:C:330:PRO:HG2	6:c:193:VAL:HA	1.86	0.57
3:D:266:ILE:HB	3:D:277:VAL:HG23	1.86	0.57
4:I:405:LEU:HD21	7:W:47:ARG:HA	1.86	0.57
4:K:532:LEU:HD22	4:K:644:GLN:HG2	1.85	0.57
8:i:60:LEU:HD22	3:h:96:LEU:HD11	1.85	0.57
2:M:645:MET:HE3	2:M:697:MET:HE3	1.86	0.57
3:N:266:ILE:HB	3:N:277:VAL:HG23	1.86	0.57
7:Q:47:ARG:NH1	7:Q:251:ASN:O	2.37	0.57
2:A:489:GLU:O	2:A:493:ASN:ND2	2.36	0.57
2:C:489:GLU:O	2:C:493:ASN:ND2	2.36	0.57
3:D:501:THR:O	3:D:501:THR:OG1	2.22	0.57
3:N:736:ASN:OD1	3:N:736:ASN:N	2.34	0.57
2:A:645:MET:HE3	2:A:697:MET:HE3	1.86	0.57
3:H:266:ILE:HB	3:H:277:VAL:HG23	1.86	0.57
8:b:60:LEU:HD22	3:a:96:LEU:HD11	1.85	0.57
8:k:60:LEU:HD22	3:j:96:LEU:HD11	1.85	0.57
2:M:489:GLU:O	2:M:493:ASN:ND2	2.36	0.57
3:N:719:GLN:O	3:N:723:THR:OG1	2.22	0.57
7:R:217:ARG:HH21	7:R:277:THR:HA	1.68	0.57
8:m:27:VAL:HG13	5:l:87:LEU:HD13	1.86	0.57
7:W:168:THR:HB	7:W:202:VAL:HG22	1.87	0.57
2:C:543:VAL:HG13	2:C:544:GLU:HG2	1.85	0.57
2:E:543:VAL:HG13	2:E:544:GLU:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:306:THR:O	5:J:306:THR:OG1	2.20	0.57
7:Q:290:VAL:HA	7:Q:293:VAL:HG22	1.86	0.57
2:C:454:GLY:HA2	2:C:457:LEU:HD12	1.86	0.57
2:G:543:VAL:HG13	2:G:544:GLU:HG2	1.85	0.57
5:J:904:ARG:HH22	7:X:331:THR:HG23	1.69	0.57
7:P:16:GLN:HE21	7:P:73:VAL:HG11	1.69	0.57
3:F:266:ILE:HD11	3:F:275:TYR:HB3	1.85	0.57
7:R:418:PHE:HB3	7:R:421:MET:HE2	1.87	0.57
7:S:290:VAL:HA	7:S:293:VAL:HG22	1.86	0.57
7:Y:68:ASP:HB2	7:Y:71:PRO:HB3	1.86	0.57
3:F:266:ILE:HB	3:F:277:VAL:HG23	1.86	0.57
5:J:688:ARG:HH11	5:J:691:LEU:HD22	1.69	0.57
7:R:28:GLU:HA	7:R:367:LEU:HD11	1.85	0.57
7:T:290:VAL:HA	7:T:293:VAL:HG22	1.85	0.57
7:2:217:ARG:HH21	7:2:277:THR:HA	1.70	0.57
2:M:543:VAL:HG13	2:M:544:GLU:HG2	1.85	0.57
1:e:153:MET:HE1	1:e:274:ILE:O	2.04	0.56
2:E:645:MET:HE3	2:E:697:MET:HE3	1.86	0.56
4:I:184:TYR:O	4:I:188:SER:OG	2.23	0.56
7:X:290:VAL:HA	7:X:293:VAL:HG22	1.85	0.56
3:B:266:ILE:HB	3:B:277:VAL:HG23	1.86	0.56
7:V:28:GLU:HA	7:V:367:LEU:HD11	1.86	0.56
8:d:31:ILE:HD12	6:c:111:LEU:HD13	1.86	0.56
2:E:454:GLY:HA2	2:E:457:LEU:HD12	1.86	0.56
7:Z:193:LYS:HE2	7:Z:197:GLN:HE22	1.70	0.56
5:J:392:THR:HB	6:L:295:ARG:HB3	1.86	0.56
5:J:900:TYR:O	5:J:904:ARG:HB3	2.05	0.56
2:E:311:GLU:OE2	3:F:365:ARG:NH1	2.39	0.56
2:E:421:GLU:O	2:E:426:LYS:NZ	2.32	0.56
7:S:135:PHE:HB2	7:S:166:VAL:HG22	1.88	0.56
5:l:89:GLU:O	5:l:93:ASN:ND2	2.38	0.56
3:F:581:LEU:HG	3:F:585:LEU:HG	1.88	0.56
7:Z:63:ARG:NE	7:Z:129:SER:OG	2.39	0.56
3:N:404:THR:O	3:N:404:THR:OG1	2.22	0.56
5:J:394:THR:OG1	5:J:395:LEU:N	2.38	0.56
7:P:158:ASN:HD21	7:P:198:ASN:HD22	1.52	0.56
2:A:427:TYR:HE1	2:A:455:LYS:HG3	1.68	0.56
2:C:685:ARG:HA	7:Q:353:PRO:HG3	1.86	0.56
3:D:660:TYR:OH	3:D:751:HIS:NE2	2.36	0.56
4:K:652:ASN:OD1	7:Y:341:ARG:NH2	2.39	0.56
5:J:375:PHE:HE1	5:J:405:ARG:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:287:LEU:HD12	8:b:21:VAL:HG13	1.87	0.56
7:O:158:ASN:HD21	7:O:198:ASN:HD22	1.53	0.56
7:Q:28:GLU:HA	7:Q:367:LEU:HD11	1.86	0.56
7:Q:218:LEU:HB2	7:Q:220:ILE:HG12	1.86	0.56
7:S:322:ASN:HD21	7:S:358:VAL:HG12	1.70	0.56
2:C:645:MET:HE3	2:C:697:MET:HE3	1.87	0.56
7:Y:158:ASN:HD21	7:Y:198:ASN:HD22	1.53	0.56
3:j:111:VAL:CG1	3:j:112:SER:N	2.68	0.56
3:D:404:THR:O	3:D:404:THR:OG1	2.22	0.55
3:D:879:ARG:HD3	7:R:337:LEU:HD23	1.87	0.55
7:Y:141:ILE:HB	7:Y:173:PRO:HD3	1.88	0.55
8:d:60:LEU:HA	8:d:63:VAL:HG22	1.88	0.55
4:K:37:SER:O	4:K:40:SER:OG	2.21	0.55
4:K:184:TYR:O	4:K:188:SER:OG	2.23	0.55
2:M:623:LYS:O	2:M:627:SER:OG	2.24	0.55
3:N:608:THR:OG1	3:N:609:ASN:N	2.40	0.55
2:G:307:VAL:HG12	3:H:365:ARG:HH11	1.71	0.55
5:J:255:PRO:HD2	5:J:257:TYR:H	1.72	0.55
7:R:218:LEU:HB2	7:R:220:ILE:HG12	1.87	0.55
3:F:286:SER:O	3:F:290:THR:OG1	2.25	0.55
2:G:645:MET:HE3	2:G:697:MET:HE3	1.86	0.55
5:J:223:GLN:HB2	5:J:230:SER:HB3	1.89	0.55
3:B:404:THR:O	3:B:404:THR:OG1	2.22	0.55
3:D:581:LEU:HG	3:D:585:LEU:HG	1.88	0.55
3:F:404:THR:O	3:F:404:THR:OG1	2.22	0.55
3:H:660:TYR:OH	3:H:751:HIS:NE2	2.36	0.55
7:T:218:LEU:HB2	7:T:220:ILE:HG12	1.88	0.55
2:C:306:LEU:HB2	6:c:190:LEU:HD22	1.88	0.55
2:E:623:LYS:O	2:E:627:SER:OG	2.24	0.55
7:O:218:LEU:HB2	7:O:220:ILE:HG12	1.89	0.55
3:B:320:VAL:HG13	3:B:396:LEU:HD23	1.89	0.55
3:H:501:THR:O	3:H:501:THR:OG1	2.22	0.55
3:H:592:LEU:HD21	3:H:597:LEU:HD21	1.89	0.55
4:K:571:GLN:HE22	4:K:638:ILE:HD13	1.72	0.55
4:K:646:LEU:HB3	7:Y:341:ARG:HD2	1.89	0.55
7:T:141:ILE:HB	7:T:173:PRO:HD3	1.88	0.55
3:B:286:SER:O	3:B:290:THR:OG1	2.25	0.55
7:S:316:CYS:HB2	7:S:349:ILE:H	1.72	0.55
2:A:623:LYS:O	2:A:627:SER:OG	2.24	0.55
2:C:623:LYS:O	2:C:627:SER:OG	2.24	0.55
3:H:608:THR:OG1	3:H:609:ASN:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:444:ILE:HG12	5:J:461:LEU:HB3	1.89	0.55
3:N:320:VAL:HG13	3:N:396:LEU:HD23	1.89	0.55
1:e:331:ALA:H	6:c:4:ILE:HD13	1.71	0.55
2:A:160:MET:HB2	2:A:284:GLU:HB3	1.90	0.55
2:A:819:GLU:O	2:A:823:ASN:ND2	2.41	0.55
3:H:286:SER:O	3:H:290:THR:OG1	2.25	0.55
5:J:238:LEU:HA	5:J:241:ASN:H	1.72	0.55
7:S:288:THR:HB	7:S:296:ARG:HH12	1.72	0.55
3:B:345:GLN:HB2	3:B:362:LEU:HD13	1.87	0.54
3:H:581:LEU:HG	3:H:585:LEU:HG	1.88	0.54
6:L:299:ARG:HB3	6:L:303:PRO:HB3	1.90	0.54
7:S:8:LEU:N	7:S:136:VAL:O	2.34	0.54
7:W:46:ASP:HA	7:W:246:PRO:HD3	1.87	0.54
3:N:779:PHE:HA	3:N:782:ILE:HD12	1.90	0.54
2:A:637:ARG:HB2	2:A:730:LEU:HD21	1.90	0.54
2:E:507:LYS:HE3	2:E:625:PRO:HG2	1.90	0.54
3:H:320:VAL:HG13	3:H:396:LEU:HD23	1.89	0.54
3:D:608:THR:OG1	3:D:609:ASN:N	2.40	0.54
3:D:719:GLN:O	3:D:723:THR:OG1	2.22	0.54
3:H:719:GLN:O	3:H:723:THR:OG1	2.22	0.54
3:H:779:PHE:HA	3:H:782:ILE:HD12	1.89	0.54
7:O:335:LYS:O	7:O:339:ARG:HB2	2.07	0.54
7:U:141:ILE:HB	7:U:173:PRO:HD3	1.88	0.54
7:2:218:LEU:HB2	7:2:220:ILE:HG12	1.89	0.54
2:M:819:GLU:O	2:M:823:ASN:ND2	2.41	0.54
2:A:434:ILE:HB	2:A:451:LEU:HD22	1.90	0.54
3:D:286:SER:O	3:D:290:THR:OG1	2.25	0.54
3:F:320:VAL:HG13	3:F:396:LEU:HD23	1.89	0.54
3:F:592:LEU:HD21	3:F:597:LEU:HD21	1.89	0.54
2:G:623:LYS:O	2:G:627:SER:OG	2.24	0.54
7:Z:141:ILE:HB	7:Z:173:PRO:HD3	1.89	0.54
2:M:434:ILE:HB	2:M:451:LEU:HD22	1.90	0.54
3:B:581:LEU:HG	3:B:585:LEU:HG	1.88	0.54
3:B:592:LEU:HD21	3:B:597:LEU:HD21	1.89	0.54
3:F:448:VAL:HG22	3:F:484:LEU:HD12	1.89	0.54
7:Y:168:THR:HB	7:Y:202:VAL:HG22	1.89	0.54
3:B:779:PHE:HA	3:B:782:ILE:HD12	1.89	0.54
2:C:819:GLU:O	2:C:823:ASN:ND2	2.41	0.54
2:G:819:GLU:O	2:G:823:ASN:ND2	2.41	0.54
7:P:290:VAL:HA	7:P:293:VAL:HG22	1.90	0.54
7:R:232:VAL:HA	7:R:235:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:218:LEU:HB2	7:Y:220:ILE:HG12	1.89	0.54
2:A:691:GLN:NE2	7:O:255:GLY:O	2.40	0.54
2:E:160:MET:HB2	2:E:284:GLU:HB3	1.90	0.54
2:E:833:LEU:HD11	2:E:859:LEU:HD21	1.90	0.54
3:H:448:VAL:HG22	3:H:484:LEU:HD12	1.89	0.54
7:R:243:LEU:HD21	7:R:253:LEU:HB3	1.90	0.54
7:W:141:ILE:HB	7:W:173:PRO:HD3	1.88	0.54
7:Y:243:LEU:HD21	7:Y:253:LEU:HB3	1.89	0.54
2:M:637:ARG:HB2	2:M:730:LEU:HD21	1.90	0.54
3:N:448:VAL:HG22	3:N:484:LEU:HD12	1.89	0.54
2:A:507:LYS:HE3	2:A:625:PRO:HG2	1.89	0.54
2:C:637:ARG:HB2	2:C:730:LEU:HD21	1.90	0.54
2:E:819:GLU:O	2:E:823:ASN:ND2	2.41	0.54
2:G:637:ARG:HB2	2:G:730:LEU:HD21	1.90	0.54
3:N:286:SER:O	3:N:290:THR:OG1	2.25	0.54
3:B:608:THR:OG1	3:B:609:ASN:N	2.40	0.54
7:P:136:VAL:HG22	7:P:167:GLN:HB3	1.90	0.54
7:V:217:ARG:HH21	7:V:277:THR:HA	1.73	0.54
7:Z:218:LEU:HB2	7:Z:220:ILE:HG12	1.89	0.54
7:1:243:LEU:HD21	7:1:253:LEU:HB3	1.89	0.54
3:D:320:VAL:HG13	3:D:396:LEU:HD23	1.89	0.54
7:U:297:LEU:HD21	7:U:377:MET:HB3	1.89	0.54
8:d:59:ALA:HB2	6:c:48:ASN:HD22	1.72	0.54
1:e:144:ALA:HB2	1:e:342:GLY:HA2	1.90	0.53
2:C:434:ILE:HB	2:C:451:LEU:HD22	1.90	0.53
2:G:160:MET:HB2	2:G:284:GLU:HB3	1.90	0.53
2:G:434:ILE:HB	2:G:451:LEU:HD22	1.90	0.53
7:O:34:GLU:HG3	7:O:84:LYS:HE3	1.90	0.53
3:N:592:LEU:HD21	3:N:597:LEU:HD21	1.89	0.53
3:D:779:PHE:HA	3:D:782:ILE:HD12	1.89	0.53
2:E:637:ARG:HB2	2:E:730:LEU:HD21	1.90	0.53
3:F:660:TYR:OH	3:F:751:HIS:NE2	2.36	0.53
4:K:630:LEU:HB3	4:K:645:LEU:HG	1.91	0.53
7:T:217:ARG:HH21	7:T:277:THR:HA	1.73	0.53
7:V:218:LEU:HB2	7:V:220:ILE:HG12	1.90	0.53
7:X:68:ASP:HB2	7:X:71:PRO:HB3	1.90	0.53
2:C:446:MET:HE3	2:C:485:VAL:HA	1.91	0.53
4:I:502:ARG:O	4:I:508:ASN:ND2	2.42	0.53
4:K:330:ASP:O	4:K:334:SER:OG	2.25	0.53
7:V:68:ASP:HB2	7:V:71:PRO:HB3	1.89	0.53
2:M:160:MET:HB2	2:M:284:GLU:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:581:LEU:HG	3:N:585:LEU:HG	1.88	0.53
2:A:446:MET:HE3	2:A:485:VAL:HA	1.91	0.53
2:E:446:MET:HE3	2:E:485:VAL:HA	1.91	0.53
2:G:833:LEU:HD11	2:G:859:LEU:HD21	1.90	0.53
3:B:448:VAL:HG22	3:B:484:LEU:HD12	1.89	0.53
2:C:290:HIS:HB3	3:D:407:GLY:HA3	1.90	0.53
3:D:448:VAL:HG22	3:D:484:LEU:HD12	1.89	0.53
3:D:592:LEU:HD21	3:D:597:LEU:HD21	1.89	0.53
5:J:947:VAL:HA	5:J:951:LYS:HB3	1.90	0.53
7:P:218:LEU:HB2	7:P:220:ILE:HG12	1.89	0.53
3:F:779:PHE:HA	3:F:782:ILE:HD12	1.89	0.53
7:Q:338:GLN:HE22	7:Q:341:ARG:HD2	1.74	0.53
7:X:436:HIS:O	7:X:440:ARG:NH2	2.42	0.53
3:N:342:LEU:HD11	3:N:370:TRP:HB3	1.91	0.53
3:N:454:VAL:HB	3:N:463:LYS:HD2	1.91	0.53
3:D:342:LEU:HD11	3:D:370:TRP:HB3	1.91	0.53
2:E:434:ILE:HB	2:E:451:LEU:HD22	1.90	0.53
3:H:454:VAL:HB	3:H:463:LYS:HD2	1.91	0.53
2:M:833:LEU:HD11	2:M:859:LEU:HD21	1.90	0.53
2:A:833:LEU:HD11	2:A:859:LEU:HD21	1.90	0.53
2:C:833:LEU:HD11	2:C:859:LEU:HD21	1.90	0.53
4:I:330:ASP:O	4:I:334:SER:OG	2.25	0.53
7:X:218:LEU:HB2	7:X:220:ILE:HG12	1.91	0.53
7:2:28:GLU:HA	7:2:367:LEU:HD11	1.90	0.53
7:2:297:LEU:HD21	7:2:377:MET:HB3	1.91	0.53
2:M:446:MET:HE3	2:M:485:VAL:HA	1.91	0.53
2:C:507:LYS:HE3	2:C:625:PRO:HG2	1.89	0.53
2:E:500:LEU:HA	2:E:719:ILE:HD11	1.91	0.53
4:I:16:ILE:HG12	5:J:246:TRP:HZ3	1.74	0.53
7:O:297:LEU:HD21	7:O:377:MET:HB3	1.90	0.53
7:W:218:LEU:HB2	7:W:220:ILE:HG12	1.90	0.53
7:Y:332:GLN:O	7:Y:336:SER:HB3	2.09	0.53
2:M:500:LEU:HA	2:M:719:ILE:HD11	1.91	0.53
3:B:342:LEU:HD11	3:B:370:TRP:HB3	1.91	0.52
2:C:160:MET:HB2	2:C:284:GLU:HB3	1.90	0.52
4:K:206:LYS:N	4:K:258:SER:O	2.34	0.52
7:P:130:ASP:OD1	7:P:130:ASP:N	2.38	0.52
7:W:322:ASN:HD21	7:W:358:VAL:HG12	1.74	0.52
2:G:446:MET:HE3	2:G:485:VAL:HA	1.91	0.52
4:K:403:VAL:O	4:K:405:LEU:N	2.43	0.52
7:U:243:LEU:HD21	7:U:253:LEU:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:g:55:ILE:HD13	8:g:60:LEU:HD12	1.92	0.52
2:A:500:LEU:HA	2:A:719:ILE:HD11	1.91	0.52
3:D:454:VAL:HB	3:D:463:LYS:HD2	1.91	0.52
4:K:283:VAL:O	4:K:287:GLU:CB	2.56	0.52
4:K:521:MET:HA	7:Y:353:PRO:HG3	1.91	0.52
7:Y:297:LEU:HD21	7:Y:377:MET:HB3	1.91	0.52
2:M:507:LYS:HE3	2:M:625:PRO:HG2	1.90	0.52
3:D:409:PRO:HA	3:D:412:ARG:HB3	1.92	0.52
2:E:277:ILE:HD13	2:E:297:ARG:HG2	1.91	0.52
7:V:141:ILE:HB	7:V:173:PRO:HD3	1.90	0.52
7:1:290:VAL:HA	7:1:293:VAL:HG22	1.91	0.52
2:A:277:ILE:HD13	2:A:297:ARG:HG2	1.91	0.52
3:B:340:SER:O	3:B:344:SER:OG	2.28	0.52
3:B:454:VAL:HB	3:B:463:LYS:HD2	1.91	0.52
3:H:409:PRO:HA	3:H:412:ARG:HB3	1.91	0.52
4:I:37:SER:O	4:I:40:SER:OG	2.21	0.52
4:I:149:HIS:HE1	4:I:201:GLU:HA	1.75	0.52
7:Z:298:LEU:HD22	7:Z:346:ALA:HB2	1.90	0.52
2:M:418:ARG:HB2	2:M:426:LYS:HD3	1.91	0.52
3:F:409:PRO:HA	3:F:412:ARG:HB3	1.92	0.52
2:G:500:LEU:HA	2:G:719:ILE:HD11	1.91	0.52
3:H:705:HIS:O	3:H:709:SER:OG	2.28	0.52
6:L:595:ILE:HD11	6:L:1484:LEU:HD21	1.92	0.52
7:P:141:ILE:HB	7:P:173:PRO:HD3	1.91	0.52
7:R:67:LEU:HD22	7:R:118:ILE:HD12	1.92	0.52
7:R:296:ARG:O	7:R:302:ASN:ND2	2.37	0.52
7:S:217:ARG:HH21	7:S:277:THR:HA	1.74	0.52
7:U:238:ALA:HB3	7:U:376:LEU:HD13	1.91	0.52
7:W:245:TYR:OH	7:W:364:SER:OG	2.25	0.52
3:N:705:HIS:O	3:N:709:SER:OG	2.28	0.52
2:C:865:TYR:HE2	7:Q:353:PRO:HB3	1.75	0.52
3:D:561:ALA:HA	3:D:564:ARG:HD3	1.92	0.52
3:H:329:HIS:CE1	4:I:131:LEU:HD21	2.45	0.52
5:l:91:PHE:HZ	5:l:110:ILE:HD12	1.75	0.52
3:B:585:LEU:O	3:B:633:THR:OG1	2.28	0.52
4:K:499:GLN:OE1	4:K:502:ARG:NH2	2.43	0.52
7:T:297:LEU:HD21	7:T:377:MET:HB3	1.92	0.52
7:Z:168:THR:HB	7:Z:202:VAL:HG22	1.91	0.52
7:1:238:ALA:HB3	7:1:376:LEU:HD13	1.92	0.52
2:C:441:SER:HA	2:C:444:GLN:HG3	1.91	0.52
3:F:342:LEU:HD11	3:F:370:TRP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:695:TYR:HE1	7:U:249:MET:HG2	1.74	0.52
4:I:403:VAL:O	4:I:405:LEU:N	2.43	0.52
7:R:189:LEU:O	7:R:424:SER:OG	2.28	0.52
3:N:501:THR:O	3:N:501:THR:OG1	2.22	0.52
2:A:441:SER:HA	2:A:444:GLN:HG3	1.91	0.52
3:D:340:SER:O	3:D:344:SER:OG	2.28	0.52
2:E:441:SER:HA	2:E:444:GLN:HG3	1.91	0.52
3:F:454:VAL:HB	3:F:463:LYS:HD2	1.91	0.52
2:G:441:SER:HA	2:G:444:GLN:HG3	1.91	0.52
2:G:507:LYS:HE3	2:G:625:PRO:HG2	1.90	0.52
6:L:1678:ASN:ND2	6:L:1679:GLN:OE1	2.42	0.52
7:Z:364:SER:HB2	7:Z:367:LEU:HD22	1.92	0.52
5:I:127:VAL:O	5:I:127:VAL:CG1	2.54	0.52
3:N:585:LEU:O	3:N:633:THR:OG1	2.28	0.52
2:C:500:LEU:HA	2:C:719:ILE:HD11	1.91	0.51
4:I:202:GLU:OE1	4:I:260:ARG:NH2	2.43	0.51
7:Q:4:GLU:HG3	7:Q:50:VAL:HA	1.92	0.51
7:X:168:THR:HB	7:X:202:VAL:HG22	1.92	0.51
3:N:340:SER:O	3:N:344:SER:OG	2.28	0.51
3:N:561:ALA:HA	3:N:564:ARG:HD3	1.92	0.51
3:H:342:LEU:HD11	3:H:370:TRP:HB3	1.91	0.51
3:H:561:ALA:HA	3:H:564:ARG:HD3	1.92	0.51
7:O:141:ILE:HB	7:O:173:PRO:HD3	1.92	0.51
2:M:277:ILE:HD13	2:M:297:ARG:HG2	1.91	0.51
2:C:297:ARG:HH21	3:D:376:ILE:HD11	1.74	0.51
3:D:494:HIS:O	3:D:500:GLN:NE2	2.44	0.51
3:D:585:LEU:O	3:D:633:THR:OG1	2.28	0.51
3:D:680:ILE:HD11	3:D:786:GLN:HA	1.92	0.51
3:D:802:ARG:O	3:D:806:PHE:N	2.42	0.51
3:H:376:ILE:HA	3:H:379:LYS:HE2	1.92	0.51
4:K:202:GLU:OE1	4:K:260:ARG:NH2	2.43	0.51
7:X:241:THR:OG1	7:X:244:ARG:NH2	2.42	0.51
3:N:409:PRO:HA	3:N:412:ARG:HB3	1.91	0.51
3:B:409:PRO:HA	3:B:412:ARG:HB3	1.91	0.51
3:F:585:LEU:O	3:F:633:THR:OG1	2.28	0.51
2:G:277:ILE:HD13	2:G:297:ARG:HG2	1.91	0.51
4:I:499:GLN:OE1	4:I:502:ARG:NH2	2.43	0.51
5:J:326:ARG:HE	5:J:416:PHE:HE2	1.57	0.51
7:P:334:HIS:CE1	7:P:338:GLN:HG2	2.45	0.51
7:X:141:ILE:HB	7:X:173:PRO:HD3	1.92	0.51
7:I:189:LEU:O	7:I:424:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:376:ILE:HA	3:N:379:LYS:HE2	1.92	0.51
2:A:282:SER:OG	2:A:284:GLU:OE1	2.25	0.51
3:B:705:HIS:O	3:B:709:SER:OG	2.28	0.51
3:D:705:HIS:O	3:D:709:SER:OG	2.28	0.51
4:K:149:HIS:HE1	4:K:201:GLU:HA	1.75	0.51
3:N:494:HIS:O	3:N:500:GLN:NE2	2.44	0.51
3:B:881:ASP:O	7:P:341:ARG:NH2	2.37	0.51
2:C:277:ILE:HD13	2:C:297:ARG:HG2	1.91	0.51
3:F:376:ILE:HA	3:F:379:LYS:HE2	1.92	0.51
3:F:608:THR:OG1	3:F:609:ASN:N	2.40	0.51
3:F:705:HIS:O	3:F:709:SER:OG	2.28	0.51
7:Q:415:LYS:HD3	7:Q:420:GLU:HB2	1.93	0.51
2:M:441:SER:HA	2:M:444:GLN:HG3	1.91	0.51
3:B:660:TYR:OH	3:B:751:HIS:NE2	2.36	0.51
3:F:340:SER:O	3:F:344:SER:OG	2.28	0.51
3:F:680:ILE:HD11	3:F:786:GLN:HA	1.92	0.51
3:H:340:SER:O	3:H:344:SER:OG	2.28	0.51
3:H:585:LEU:O	3:H:633:THR:OG1	2.28	0.51
5:J:367:ALA:HB2	5:J:467:GLU:HB2	1.92	0.51
7:2:68:ASP:HB2	7:2:71:PRO:HB3	1.92	0.51
2:A:395:ILE:HG22	2:A:491:ALA:HB3	1.93	0.51
3:B:308:THR:OG1	3:B:325:CYS:SG	2.68	0.51
3:D:723:THR:HG23	7:R:248:TYR:CD2	2.45	0.51
4:I:551:THR:HG23	4:I:553:ASP:H	1.76	0.51
7:Q:168:THR:HB	7:Q:202:VAL:HG22	1.93	0.51
3:N:660:TYR:OH	3:N:751:HIS:NE2	2.36	0.51
3:N:680:ILE:HD11	3:N:786:GLN:HA	1.92	0.51
3:B:376:ILE:HA	3:B:379:LYS:HE2	1.92	0.51
3:B:561:ALA:HA	3:B:564:ARG:HD3	1.92	0.51
2:C:282:SER:OG	2:C:284:GLU:OE1	2.25	0.51
2:C:283:PHE:HZ	3:D:403:TYR:HA	1.76	0.51
3:D:723:THR:HG23	7:R:248:TYR:HD2	1.76	0.51
3:F:494:HIS:O	3:F:500:GLN:NE2	2.44	0.51
2:G:395:ILE:HG22	2:G:491:ALA:HB3	1.93	0.51
7:U:168:THR:HB	7:U:202:VAL:HG22	1.93	0.51
3:B:677:LEU:HD21	3:B:711:MET:HB3	1.93	0.51
3:D:677:LEU:HD21	3:D:711:MET:HB3	1.93	0.51
3:F:308:THR:HB	3:F:328:LEU:HD23	1.93	0.51
5:J:562:ALA:HB2	5:J:699:TYR:HD1	1.75	0.51
5:J:922:ASP:HB3	5:J:925:GLN:HG2	1.93	0.51
4:K:82:HIS:O	4:K:200:HIS:NE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:R:290:VAL:HA	7:R:293:VAL:HG22	1.92	0.51
7:U:113:LYS:HG3	7:U:114:ILE:HG23	1.93	0.51
3:B:494:HIS:O	3:B:500:GLN:NE2	2.44	0.50
3:B:680:ILE:HD11	3:B:786:GLN:HA	1.92	0.50
3:D:301:HIS:NE2	3:D:336:TYR:OH	2.30	0.50
3:D:308:THR:OG1	3:D:325:CYS:SG	2.68	0.50
3:D:603:THR:HG23	7:S:339:ARG:HH22	1.76	0.50
4:I:365:ARG:HH22	4:I:367:GLU:HB2	1.76	0.50
7:P:168:THR:HB	7:P:202:VAL:HG22	1.93	0.50
7:T:113:LYS:HG3	7:T:114:ILE:HG23	1.92	0.50
7:V:158:ASN:HD21	7:V:198:ASN:HD22	1.58	0.50
7:Y:406:GLU:HB3	7:Y:408:PHE:HD2	1.76	0.50
3:F:665:ASN:ND2	3:j:66:ARG:HG2	2.25	0.50
3:H:308:THR:HB	3:H:328:LEU:HD23	1.93	0.50
4:K:104:LEU:HD12	4:K:107:LEU:HD12	1.93	0.50
4:K:551:THR:HG23	4:K:553:ASP:H	1.76	0.50
6:L:308:GLU:O	6:L:309:GLU:C	2.54	0.50
2:M:395:ILE:HG22	2:M:491:ALA:HB3	1.93	0.50
3:B:308:THR:HB	3:B:328:LEU:HD23	1.94	0.50
5:J:684:GLU:H	5:J:687:LEU:HB3	1.76	0.50
7:Z:320:ILE:HB	7:Z:356:ILE:HG12	1.93	0.50
5:J:562:ALA:HB2	5:J:699:TYR:CD1	2.47	0.50
5:J:842:LEU:HD11	7:X:254:ILE:HD11	1.93	0.50
7:O:318:ILE:HA	7:O:350:PRO:HG3	1.93	0.50
7:P:406:GLU:HB3	7:P:408:PHE:HD2	1.77	0.50
7:Q:291:LEU:HG	7:Q:336:SER:HA	1.92	0.50
7:X:8:LEU:N	7:X:136:VAL:O	2.37	0.50
7:1:218:LEU:HB2	7:1:220:ILE:HG12	1.93	0.50
3:N:361:SER:OG	3:N:362:LEU:N	2.43	0.50
2:A:233:VAL:HA	2:A:248:VAL:HA	1.94	0.50
3:F:301:HIS:NE2	3:F:336:TYR:OH	2.30	0.50
2:G:418:ARG:HG3	2:G:426:LYS:HB3	1.94	0.50
3:H:494:HIS:O	3:H:500:GLN:NE2	2.44	0.50
4:K:365:ARG:HH22	4:K:367:GLU:HB2	1.76	0.50
7:O:290:VAL:HA	7:O:293:VAL:HG22	1.92	0.50
7:R:415:LYS:HB2	7:R:418:PHE:HA	1.92	0.50
7:1:348:PHE:HB3	7:1:350:PRO:HD3	1.94	0.50
3:B:581:LEU:HD13	3:B:600:ILE:HG21	1.94	0.50
3:B:698:SER:HA	3:B:701:LEU:HB3	1.94	0.50
3:D:376:ILE:HA	3:D:379:LYS:HE2	1.92	0.50
3:F:802:ARG:O	3:F:806:PHE:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:394:THR:HB	6:L:297:TRP:HE1	1.77	0.50
5:J:902:MET:HA	5:J:906:LEU:HB2	1.94	0.50
4:K:488:VAL:HG21	4:K:587:LEU:HB3	1.94	0.50
7:V:297:LEU:HD21	7:V:377:MET:HB3	1.92	0.50
5:J:437:LEU:HD21	5:J:469:VAL:HG23	1.94	0.50
6:L:533:THR:O	6:L:537:HIS:HB2	2.12	0.50
6:L:1570:SER:OG	6:L:1571:ASN:N	2.45	0.50
7:Q:189:LEU:O	7:Q:424:SER:OG	2.29	0.50
3:N:308:THR:HB	3:N:328:LEU:HD23	1.94	0.50
3:N:581:LEU:HD13	3:N:600:ILE:HG21	1.94	0.50
2:C:395:ILE:HG22	2:C:491:ALA:HB3	1.93	0.50
2:E:675:TRP:HZ2	2:E:770:LYS:HE2	1.77	0.50
7:U:189:LEU:O	7:U:424:SER:OG	2.30	0.50
7:W:317:TYR:HB2	7:W:348:PHE:HB3	1.94	0.50
2:M:282:SER:OG	2:M:284:GLU:OE1	2.25	0.50
3:N:677:LEU:HD21	3:N:711:MET:HB3	1.93	0.50
3:F:334:GLU:OE2	6:c:148:TYR:N	2.45	0.50
4:I:22:ARG:HH21	4:I:23:SER:HB3	1.77	0.50
4:K:152:GLN:NE2	4:K:262:GLU:O	2.45	0.50
7:X:189:LEU:O	7:X:424:SER:OG	2.29	0.50
3:j:105:ARG:C	3:j:106:ARG:HG3	2.37	0.50
5:l:121:PRO:CD	5:l:121:PRO:O	2.59	0.50
3:B:723:THR:HA	7:P:248:TYR:HD1	1.76	0.49
2:C:233:VAL:HA	2:C:248:VAL:HA	1.94	0.49
2:C:864:PHE:HE1	7:Q:349:ILE:HD12	1.77	0.49
3:F:561:ALA:HA	3:F:564:ARG:HD3	1.92	0.49
3:F:698:SER:HA	3:F:701:LEU:HB3	1.94	0.49
7:Z:189:LEU:O	7:Z:424:SER:OG	2.30	0.49
8:b:36:ASN:HD21	3:a:67:ARG:HH12	1.60	0.49
3:B:720:TYR:OH	7:P:250:ASN:ND2	2.45	0.49
3:D:698:SER:HA	3:D:701:LEU:HB3	1.94	0.49
4:I:273:ALA:HA	4:I:276:ILE:HD12	1.94	0.49
5:J:232:PHE:HE2	6:L:298:GLU:HB3	1.77	0.49
7:S:324:ILE:HD12	7:S:375:GLY:HA3	1.94	0.49
7:1:141:ILE:HB	7:1:173:PRO:HD3	1.94	0.49
7:1:168:THR:HB	7:1:202:VAL:HG22	1.95	0.49
3:H:432:ARG:NH2	3:H:440:GLU:O	2.45	0.49
3:H:677:LEU:HD21	3:H:711:MET:HB3	1.93	0.49
3:H:680:ILE:HD11	3:H:786:GLN:HA	1.92	0.49
6:L:447:VAL:HG22	6:L:448:LEU:HG	1.95	0.49
7:T:235:ILE:HG12	7:T:304:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:290:VAL:HA	7:Y:293:VAL:HG22	1.94	0.49
8:m:51:CYS:SG	5:l:110:ILE:HG12	2.52	0.49
2:M:517:LYS:NZ	2:M:703:GLU:OE2	2.44	0.49
3:D:677:LEU:HD13	3:D:782:ILE:HG23	1.95	0.49
3:D:879:ARG:HH11	7:R:334:HIS:CE1	2.31	0.49
2:E:728:GLY:O	2:E:732:THR:OG1	2.29	0.49
3:F:581:LEU:HD13	3:F:600:ILE:HG21	1.94	0.49
3:F:677:LEU:HD21	3:F:711:MET:HB3	1.93	0.49
4:I:488:VAL:HG21	4:I:587:LEU:HB3	1.94	0.49
4:K:273:ALA:HA	4:K:276:ILE:HD12	1.94	0.49
4:K:611:GLN:HA	4:K:614:ILE:HB	1.94	0.49
4:K:308:ALA:O	4:K:312:HIS:N	2.41	0.49
3:j:65:GLN:HE22	3:j:104:PRO:HD2	1.77	0.49
2:A:692:ASN:HD21	7:O:355:SER:HB2	1.77	0.49
3:H:698:SER:HA	3:H:701:LEU:HB3	1.94	0.49
5:J:327:LEU:HD22	5:J:368:LEU:HD21	1.95	0.49
7:P:189:LEU:O	7:P:424:SER:OG	2.30	0.49
7:S:189:LEU:O	7:S:424:SER:OG	2.31	0.49
3:N:441:ASP:OD1	3:N:441:ASP:N	2.46	0.49
2:A:517:LYS:NZ	2:A:703:GLU:OE2	2.44	0.49
3:F:432:ARG:NH2	3:F:440:GLU:O	2.45	0.49
2:G:233:VAL:HA	2:G:248:VAL:HA	1.94	0.49
3:H:677:LEU:HD13	3:H:782:ILE:HG23	1.95	0.49
4:I:104:LEU:HD12	4:I:107:LEU:HD12	1.93	0.49
6:L:444:ARG:HH21	2:M:325:TRP:CD1	2.31	0.49
7:T:349:ILE:HD11	7:T:351:TRP:CE2	2.47	0.49
7:Z:363:LYS:HG2	7:Z:372:ARG:HD2	1.95	0.49
3:B:312:SER:OG	3:B:325:CYS:SG	2.67	0.49
3:D:432:ARG:NH2	3:D:440:GLU:O	2.45	0.49
2:G:629:ILE:HA	2:G:723:LEU:HD11	1.95	0.49
4:I:82:HIS:O	4:I:200:HIS:NE2	2.42	0.49
4:I:151:CYS:HB2	4:I:263:ILE:HG13	1.95	0.49
4:K:515:TRP:O	4:K:519:ASN:N	2.40	0.49
7:P:274:THR:HG22	7:P:297:LEU:HD13	1.94	0.49
7:U:290:VAL:HA	7:U:293:VAL:HG22	1.94	0.49
7:X:113:LYS:HG3	7:X:114:ILE:HG23	1.95	0.49
8:k:55:ILE:HD13	8:k:60:LEU:HD12	1.94	0.49
2:M:233:VAL:HA	2:M:248:VAL:HA	1.94	0.49
3:N:432:ARG:NH2	3:N:440:GLU:O	2.45	0.49
3:D:441:ASP:N	3:D:441:ASP:OD1	2.46	0.49
3:D:581:LEU:HD13	3:D:600:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:713:HIS:CE1	7:T:353:PRO:HB2	2.48	0.49
3:H:333:ARG:HD3	4:I:127:ASP:HB3	1.95	0.49
7:O:246:PRO:O	7:O:362:ARG:NH1	2.42	0.49
7:2:406:GLU:HB3	7:2:408:PHE:HD2	1.78	0.49
3:N:698:SER:HA	3:N:701:LEU:HB3	1.94	0.49
3:B:677:LEU:HD13	3:B:782:ILE:HG23	1.95	0.49
5:J:358:PHE:HD2	5:J:361:TYR:H	1.61	0.49
7:Y:232:VAL:HA	7:Y:235:ILE:HD12	1.94	0.49
7:Z:213:ILE:HD13	7:Z:304:MET:HE2	1.95	0.49
3:N:677:LEU:HD13	3:N:782:ILE:HG23	1.95	0.49
2:E:233:VAL:HA	2:E:248:VAL:HA	1.94	0.48
2:G:282:SER:OG	2:G:284:GLU:OE1	2.25	0.48
7:2:113:LYS:HG3	7:2:114:ILE:HG23	1.94	0.48
2:A:629:ILE:HA	2:A:723:LEU:HD11	1.95	0.48
3:B:432:ARG:NH2	3:B:440:GLU:O	2.45	0.48
3:B:885:HIS:CD2	7:P:353:PRO:HB3	2.48	0.48
2:E:395:ILE:HG22	2:E:491:ALA:HB3	1.93	0.48
7:O:274:THR:O	7:O:302:ASN:ND2	2.45	0.48
7:S:218:LEU:HB2	7:S:220:ILE:HG12	1.94	0.48
7:X:232:VAL:HA	7:X:235:ILE:HD12	1.94	0.48
3:B:774:GLN:HE22	3:B:860:GLN:HB3	1.79	0.48
3:D:345:GLN:HE21	6:c:175:ILE:HA	1.79	0.48
3:F:677:LEU:HD13	3:F:782:ILE:HG23	1.95	0.48
2:G:320:SER:H	2:G:323:LYS:HB2	1.78	0.48
3:H:774:GLN:HE22	3:H:860:GLN:HB3	1.78	0.48
4:I:515:TRP:O	4:I:519:ASN:N	2.40	0.48
5:J:266:THR:OG1	6:L:298:GLU:OE1	2.29	0.48
6:L:346:LEU:HA	6:L:347:VAL:HA	1.63	0.48
6:L:1630:MET:SD	6:L:1673:GLN:NE2	2.81	0.48
6:L:1800:LEU:HD21	7:Z:337:LEU:HB3	1.95	0.48
7:O:113:LYS:HG3	7:O:114:ILE:HG23	1.94	0.48
7:R:297:LEU:HD21	7:R:377:MET:HB3	1.94	0.48
7:V:113:LYS:HG3	7:V:114:ILE:HG23	1.94	0.48
4:K:151:CYS:HB2	4:K:263:ILE:HG13	1.95	0.48
7:S:406:GLU:HB3	7:S:408:PHE:HD2	1.79	0.48
2:M:629:ILE:HA	2:M:723:LEU:HD11	1.95	0.48
2:A:320:SER:H	2:A:323:LYS:HB2	1.78	0.48
3:B:441:ASP:OD1	3:B:441:ASP:N	2.46	0.48
2:E:629:ILE:HA	2:E:723:LEU:HD11	1.95	0.48
4:K:22:ARG:HH21	4:K:23:SER:HB3	1.77	0.48
7:U:274:THR:O	7:U:302:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:m:35:LEU:O	5:l:120:SER:N	2.46	0.48
7:1:113:LYS:HG3	7:1:114:ILE:HG23	1.95	0.48
7:2:158:ASN:HD21	7:2:198:ASN:HD22	1.61	0.48
2:C:629:ILE:HA	2:C:723:LEU:HD11	1.95	0.48
2:G:517:LYS:NZ	2:G:703:GLU:OE2	2.44	0.48
4:K:649:LEU:HD12	4:K:652:ASN:HA	1.94	0.48
7:S:113:LYS:HG3	7:S:114:ILE:HG23	1.95	0.48
3:a:48:GLU:HG2	3:a:124:ARG:HG3	1.96	0.48
3:N:774:GLN:HE22	3:N:860:GLN:HB3	1.79	0.48
3:B:459:LEU:HD21	3:B:492:PHE:HA	1.96	0.48
3:B:802:ARG:O	3:B:806:PHE:N	2.42	0.48
3:B:827:GLU:N	3:B:827:GLU:OE1	2.47	0.48
2:C:320:SER:H	2:C:323:LYS:HB2	1.78	0.48
3:D:626:LEU:HD22	3:D:637:VAL:HG12	1.96	0.48
4:I:611:GLN:HA	4:I:614:ILE:HB	1.94	0.48
7:W:406:GLU:HB3	7:W:408:PHE:HD2	1.79	0.48
7:Z:113:LYS:HG3	7:Z:114:ILE:HG23	1.96	0.48
8:d:48:VAL:HG12	6:c:110:VAL:HG11	1.96	0.48
3:N:827:GLU:N	3:N:827:GLU:OE1	2.47	0.48
3:D:308:THR:HB	3:D:328:LEU:HD23	1.93	0.48
3:D:459:LEU:HD21	3:D:492:PHE:HA	1.96	0.48
2:E:307:VAL:HG12	3:F:365:ARG:HH21	1.79	0.48
2:E:320:SER:H	2:E:323:LYS:HB2	1.78	0.48
3:H:581:LEU:HD13	3:H:600:ILE:HG21	1.94	0.48
7:Y:45:THR:OG1	7:Y:362:ARG:NH1	2.46	0.48
2:M:728:GLY:O	2:M:732:THR:OG1	2.29	0.48
2:A:728:GLY:O	2:A:732:THR:OG1	2.29	0.48
2:E:517:LYS:NZ	2:E:703:GLU:OE2	2.44	0.48
3:F:827:GLU:N	3:F:827:GLU:OE1	2.47	0.48
3:H:626:LEU:HD22	3:H:637:VAL:HG12	1.96	0.48
7:R:423:THR:HA	7:R:426:GLU:HG3	1.96	0.48
7:W:274:THR:O	7:W:302:ASN:ND2	2.47	0.48
3:B:626:LEU:HD22	3:B:637:VAL:HG12	1.96	0.47
2:E:446:MET:SD	2:E:446:MET:N	2.87	0.47
3:F:441:ASP:N	3:F:441:ASP:OD1	2.46	0.47
5:J:830:GLN:HE22	5:J:955:MET:HE1	1.78	0.47
4:K:653:LYS:HZ2	7:Y:353:PRO:HB3	1.79	0.47
6:L:294:ARG:HH12	6:L:306:HIS:CE1	2.32	0.47
7:O:189:LEU:O	7:O:424:SER:OG	2.30	0.47
7:Z:217:ARG:HG3	7:Z:218:LEU:HG	1.96	0.47
7:Z:399:ARG:NH1	7:Z:402:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:838:ALA:HB1	2:M:871:ARG:HD2	1.96	0.47
3:H:301:HIS:NE2	3:H:336:TYR:OH	2.30	0.47
4:I:112:LEU:HD21	6:L:295:ARG:HG2	1.96	0.47
5:J:364:PHE:HA	5:J:468:THR:HG22	1.96	0.47
7:Y:270:MET:HE2	7:Y:384:ILE:HB	1.95	0.47
7:Z:343:ARG:HB3	7:Z:345:LEU:HG	1.96	0.47
3:B:889:ARG:HD3	3:B:889:ARG:HA	1.66	0.47
2:C:446:MET:SD	2:C:446:MET:N	2.87	0.47
3:D:774:GLN:HE22	3:D:860:GLN:HB3	1.78	0.47
2:A:446:MET:SD	2:A:446:MET:N	2.87	0.47
2:C:517:LYS:NZ	2:C:703:GLU:OE2	2.44	0.47
2:C:728:GLY:O	2:C:732:THR:OG1	2.29	0.47
3:H:827:GLU:OE1	3:H:827:GLU:N	2.47	0.47
7:S:207:ASN:O	7:S:211:ASN:HB2	2.14	0.47
7:S:297:LEU:HD21	7:S:377:MET:HB2	1.95	0.47
7:X:406:GLU:HB3	7:X:408:PHE:HD2	1.79	0.47
2:M:320:SER:H	2:M:323:LYS:HB2	1.78	0.47
2:A:679:ALA:HB1	2:A:762:MET:HE2	1.97	0.47
4:I:367:GLU:HG3	7:W:251:ASN:HB2	1.95	0.47
3:a:115:ALA:O	3:a:120:GLN:NE2	2.47	0.47
3:a:116:THR:HG23	3:a:117:LEU:HD12	1.97	0.47
3:N:626:LEU:HD22	3:N:637:VAL:HG12	1.96	0.47
1:e:73:HIS:HA	1:e:158:GLY:HA3	1.94	0.47
2:A:633:LYS:NZ	2:A:727:THR:OG1	2.48	0.47
4:K:600:ASN:HB2	4:K:604:LEU:HD11	1.97	0.47
7:V:189:LEU:O	7:V:424:SER:OG	2.32	0.47
7:W:113:LYS:HG3	7:W:114:ILE:HG23	1.95	0.47
2:A:509:LEU:HD13	2:A:626:LEU:HD22	1.97	0.47
2:E:633:LYS:NZ	2:E:727:THR:OG1	2.48	0.47
2:G:415:ARG:HG3	2:G:419:ILE:HD12	1.97	0.47
2:G:446:MET:SD	2:G:446:MET:N	2.87	0.47
2:G:536:GLU:HA	2:G:539:LEU:HB2	1.97	0.47
5:J:946:LYS:HA	5:J:949:PHE:HD2	1.79	0.47
7:P:213:ILE:HD13	7:P:304:MET:HG2	1.97	0.47
7:Q:69:LEU:HD23	7:Q:145:THR:HB	1.96	0.47
7:W:318:ILE:HA	7:W:350:PRO:HB3	1.97	0.47
7:X:69:LEU:HD23	7:X:145:THR:HB	1.97	0.47
7:Y:133:GLU:HG2	7:Y:253:LEU:HD21	1.97	0.47
7:Z:46:ASP:HA	7:Z:246:PRO:HD3	1.95	0.47
7:Z:351:TRP:H	7:Z:351:TRP:CD1	2.33	0.47
8:i:55:ILE:HD13	8:i:60:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:509:LEU:HD13	2:M:626:LEU:HD22	1.97	0.47
2:M:536:GLU:HA	2:M:539:LEU:HB2	1.97	0.47
3:H:441:ASP:N	3:H:441:ASP:OD1	2.46	0.47
3:N:308:THR:OG1	3:N:325:CYS:SG	2.68	0.47
3:N:312:SER:OG	3:N:325:CYS:SG	2.67	0.47
3:N:802:ARG:O	3:N:806:PHE:N	2.42	0.47
2:A:191:PHE:CD1	3:B:289:ASP:HB3	2.50	0.47
2:A:536:GLU:HA	2:A:539:LEU:HB2	1.97	0.47
3:B:661:LEU:HD21	3:f:64:ARG:HH12	1.78	0.47
2:C:311:GLU:OE1	2:C:315:ARG:NH1	2.48	0.47
2:C:705:THR:HG1	2:C:733:CYS:HG	1.58	0.47
3:F:308:THR:OG1	3:F:325:CYS:SG	2.68	0.47
3:F:774:GLN:HE22	3:F:860:GLN:HB3	1.78	0.47
4:I:409:ASN:O	4:I:411:LEU:N	2.47	0.47
7:W:189:LEU:O	7:W:424:SER:OG	2.29	0.47
2:M:446:MET:N	2:M:446:MET:SD	2.87	0.47
2:M:633:LYS:NZ	2:M:727:THR:OG1	2.48	0.47
2:A:213:GLN:HE22	2:A:253:ASP:H	1.63	0.47
3:F:660:TYR:HH	3:F:751:HIS:HE2	1.61	0.47
2:G:633:LYS:NZ	2:G:727:THR:OG1	2.48	0.47
2:G:728:GLY:O	2:G:732:THR:OG1	2.29	0.47
7:O:37:VAL:HG23	7:O:58:GLU:HB3	1.96	0.47
3:N:459:LEU:HD21	3:N:492:PHE:HA	1.96	0.47
4:K:1:MET:HE1	6:L:312:LEU:HG	1.97	0.46
4:K:397:GLN:HE22	4:K:411:LEU:HD13	1.80	0.46
7:O:168:THR:HB	7:O:202:VAL:HG22	1.96	0.46
7:P:69:LEU:HD11	7:P:149:LEU:HD13	1.97	0.46
2:M:302:GLU:H	2:M:302:GLU:HG3	1.56	0.46
2:M:311:GLU:OE1	2:M:315:ARG:NH1	2.48	0.46
2:M:428:TRP:CD1	2:M:455:LYS:HD3	2.51	0.46
2:A:311:GLU:OE1	2:A:315:ARG:NH1	2.48	0.46
2:C:428:TRP:CD1	2:C:455:LYS:HD3	2.51	0.46
2:E:694:GLN:HG2	7:S:249:MET:HE3	1.98	0.46
2:A:428:TRP:CD1	2:A:455:LYS:HD3	2.51	0.46
3:F:626:LEU:HD22	3:F:637:VAL:HG12	1.96	0.46
3:H:459:LEU:HD21	3:H:492:PHE:HA	1.96	0.46
4:I:600:ASN:HB2	4:I:604:LEU:HD11	1.97	0.46
6:L:361:ILE:HB	6:L:363:VAL:HG13	1.97	0.46
7:1:349:ILE:HA	2:M:864:PHE:HZ	1.80	0.46
2:C:327:TYR:CE2	6:c:186:PRO:HG2	2.51	0.46
3:D:464:TYR:OH	3:D:491:ASN:ND2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:152:GLN:NE2	4:I:262:GLU:O	2.45	0.46
6:L:1676:ILE:HG23	6:L:1680:ILE:HD12	1.98	0.46
6:c:16:LEU:HD12	6:c:17:PRO:HD2	1.97	0.46
2:M:241:ARG:HD2	2:M:241:ARG:HA	1.43	0.46
2:A:618:PHE:O	2:A:639:GLN:NE2	2.45	0.46
2:C:633:LYS:NZ	2:C:727:THR:OG1	2.48	0.46
3:D:889:ARG:HA	3:D:889:ARG:HD3	1.65	0.46
2:E:428:TRP:CD1	2:E:455:LYS:HD3	2.51	0.46
3:F:879:ARG:HH22	7:T:338:GLN:HE22	1.63	0.46
2:G:509:LEU:HD13	2:G:626:LEU:HD22	1.97	0.46
7:Z:406:GLU:HB3	7:Z:408:PHE:HD2	1.80	0.46
7:2:238:ALA:HB3	7:2:376:LEU:HD13	1.97	0.46
2:E:282:SER:OG	2:E:284:GLU:OE1	2.25	0.46
2:E:509:LEU:HD13	2:E:626:LEU:HD22	1.97	0.46
5:J:723:MET:HE3	5:J:723:MET:HB3	1.87	0.46
4:K:496:TRP:CE2	7:Y:258:ALA:HA	2.51	0.46
6:L:1699:GLU:HA	6:L:1702:GLN:HE21	1.81	0.46
7:Z:195:LEU:O	7:Z:199:ALA:HB3	2.14	0.46
6:c:29:ASN:HD21	6:c:32:ARG:HB2	1.81	0.46
2:M:618:PHE:O	2:M:639:GLN:NE2	2.45	0.46
2:C:325:TRP:O	2:C:329:GLN:NE2	2.46	0.46
2:C:674:GLN:HA	2:C:675:TRP:HD1	1.81	0.46
2:E:213:GLN:HE22	2:E:253:ASP:H	1.63	0.46
3:F:886:TYR:HA	3:F:890:GLU:HB3	1.98	0.46
2:G:241:ARG:HD2	2:G:241:ARG:HA	1.43	0.46
4:I:397:GLN:HE22	4:I:411:LEU:HD13	1.80	0.46
4:I:471:VAL:HG21	4:I:561:HIS:HE1	1.80	0.46
7:P:113:LYS:HG3	7:P:114:ILE:HG23	1.96	0.46
7:W:297:LEU:HD21	7:W:377:MET:HB3	1.98	0.46
8:g:24:THR:OG1	3:f:84:GLN:OE1	2.33	0.46
8:k:24:THR:OG1	3:j:84:GLN:OE1	2.33	0.46
3:j:60:LYS:HA	3:j:63:ILE:HG22	1.98	0.46
3:N:886:TYR:HA	3:N:890:GLU:HB3	1.98	0.46
2:A:664:THR:HG1	2:A:675:TRP:CG	2.33	0.46
2:C:221:LEU:HA	2:C:224:VAL:HG12	1.98	0.46
2:C:864:PHE:CE1	7:Q:349:ILE:HD12	2.50	0.46
3:F:459:LEU:HD21	3:F:492:PHE:HA	1.96	0.46
2:G:428:TRP:CD1	2:G:455:LYS:HD3	2.51	0.46
6:L:357:LEU:HD21	6:L:459:ILE:HD12	1.96	0.46
7:S:119:PHE:HA	7:S:122:ILE:HG12	1.98	0.46
7:T:189:LEU:O	7:T:424:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:252:ASP:N	7:U:252:ASP:OD1	2.48	0.46
8:k:40:ASP:OD1	8:k:40:ASP:N	2.49	0.46
3:j:105:ARG:O	3:j:106:ARG:HG3	2.16	0.46
2:A:221:LEU:HA	2:A:224:VAL:HG12	1.98	0.46
2:C:310:LEU:HD11	6:c:186:PRO:HB3	1.98	0.46
5:J:369:TYR:CE2	5:J:373:ILE:HD11	2.51	0.46
7:R:406:GLU:HB3	7:R:408:PHE:HD2	1.81	0.46
7:S:69:LEU:HD23	7:S:145:THR:HB	1.98	0.46
7:T:193:LYS:HG3	7:T:424:SER:HA	1.98	0.46
7:Y:63:ARG:NE	7:Y:129:SER:OG	2.49	0.46
3:j:106:ARG:O	3:j:107:GLN:C	2.59	0.46
2:M:682:LEU:HD11	2:M:686:MET:HE3	1.98	0.46
2:C:679:ALA:HB1	2:C:762:MET:HE2	1.97	0.46
3:D:886:TYR:HA	3:D:890:GLU:HB3	1.98	0.46
2:G:221:LEU:HA	2:G:224:VAL:HG12	1.98	0.46
2:G:311:GLU:OE1	2:G:315:ARG:NH1	2.48	0.46
2:G:679:ALA:HB1	2:G:762:MET:HE2	1.97	0.46
5:J:566:MET:HE3	5:J:570:LYS:HE2	1.98	0.46
4:K:471:VAL:HG21	4:K:561:HIS:HE1	1.80	0.46
7:O:317:TYR:HA	7:O:381:HIS:HA	1.98	0.46
7:R:63:ARG:NE	7:R:129:SER:OG	2.48	0.46
7:W:68:ASP:HB2	7:W:71:PRO:HB3	1.97	0.46
2:C:180:TRP:HZ2	3:D:383:ALA:HA	1.81	0.45
3:F:733:GLU:HG2	3:F:737:LYS:HE2	1.98	0.45
3:H:733:GLU:HG2	3:H:737:LYS:HE2	1.98	0.45
6:L:1635:ASP:O	6:L:1639:HIS:HB2	2.15	0.45
7:O:238:ALA:HB3	7:O:376:LEU:HD13	1.98	0.45
7:Q:29:HIS:ND1	7:Q:46:ASP:OD2	2.49	0.45
7:S:376:LEU:HD21	7:S:378:MET:HE2	1.99	0.45
7:U:56:ASP:OD1	7:V:296:ARG:NH1	2.50	0.45
8:i:24:THR:OG1	3:h:84:GLN:OE1	2.34	0.45
7:1:406:GLU:HB3	7:1:408:PHE:HD2	1.81	0.45
2:M:213:GLN:HE22	2:M:253:ASP:H	1.63	0.45
3:N:733:GLU:HG2	3:N:737:LYS:HE2	1.98	0.45
2:A:698:MET:HB2	7:O:248:TYR:HB3	1.97	0.45
3:B:490:ILE:HG22	3:B:503:THR:HG21	1.97	0.45
2:E:682:LEU:HD11	2:E:686:MET:HE3	1.98	0.45
3:F:883:ASN:ND2	7:T:349:ILE:O	2.25	0.45
7:O:252:ASP:OD1	7:O:252:ASP:N	2.48	0.45
7:X:4:GLU:OE2	7:X:131:SER:N	2.48	0.45
2:C:509:LEU:HD13	2:C:626:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:536:GLU:HA	2:E:539:LEU:HB2	1.97	0.45
2:G:618:PHE:O	2:G:639:GLN:NE2	2.45	0.45
4:I:472:LEU:HA	4:I:475:TYR:HB2	1.99	0.45
7:X:238:ALA:HB3	7:X:376:LEU:HD13	1.98	0.45
8:i:28:LEU:O	8:i:32:SER:OG	2.33	0.45
3:j:13:LEU:HD11	3:j:39:ILE:HG21	1.98	0.45
6:c:93:VAL:HA	6:c:96:LEU:HD12	1.98	0.45
2:M:221:LEU:HA	2:M:224:VAL:HG12	1.98	0.45
2:A:682:LEU:HD11	2:A:686:MET:HE3	1.98	0.45
3:B:661:LEU:HD21	3:f:64:ARG:HH22	1.81	0.45
2:E:221:LEU:HA	2:E:224:VAL:HG12	1.98	0.45
2:E:679:ALA:HB1	2:E:762:MET:HE2	1.97	0.45
3:H:889:ARG:HA	3:H:889:ARG:HD3	1.65	0.45
7:O:249:MET:HB3	7:O:250:ASN:H	1.65	0.45
7:T:119:PHE:HA	7:T:122:ILE:HG12	1.98	0.45
2:M:679:ALA:HB1	2:M:762:MET:HE2	1.97	0.45
2:E:311:GLU:OE1	2:E:315:ARG:NH1	2.48	0.45
3:F:483:VAL:HG12	3:F:534:ILE:HD12	1.99	0.45
2:G:682:LEU:HD11	2:G:686:MET:HE3	1.98	0.45
3:H:464:TYR:OH	3:H:491:ASN:ND2	2.45	0.45
7:R:132:LEU:HG	7:R:164:LYS:NZ	2.31	0.45
7:S:351:TRP:NE1	7:S:443:TYR:HB3	2.32	0.45
3:a:13:LEU:HD11	3:a:39:ILE:HG21	1.99	0.45
2:C:701:VAL:HG13	2:C:736:ASP:HB3	1.99	0.45
3:H:886:TYR:HA	3:H:890:GLU:HB3	1.98	0.45
4:I:308:ALA:O	4:I:312:HIS:N	2.41	0.45
5:J:225:TRP:HD1	4:K:35:HIS:CD2	2.34	0.45
4:K:34:LEU:HB3	6:L:312:LEU:HD22	1.98	0.45
4:K:409:ASN:O	4:K:411:LEU:N	2.47	0.45
7:O:69:LEU:HD23	7:O:145:THR:HB	1.98	0.45
7:Q:340:ILE:HD13	7:Q:343:ARG:HD2	1.99	0.45
1:e:20:GLY:HA3	1:e:28:ARG:H	1.81	0.45
3:F:620:ARG:HH21	3:F:644:VAL:HA	1.82	0.45
2:G:213:GLN:HE22	2:G:253:ASP:H	1.63	0.45
2:G:701:VAL:HG13	2:G:736:ASP:HB3	1.99	0.45
5:J:302:VAL:HG23	5:J:310:LEU:HD22	1.97	0.45
7:P:131:SER:OG	7:P:132:LEU:N	2.48	0.45
7:Q:297:LEU:HD21	7:Q:377:MET:HB3	1.97	0.45
7:V:195:LEU:O	7:V:199:ALA:HB3	2.17	0.45
7:X:318:ILE:HA	7:X:350:PRO:HB3	1.98	0.45
2:C:305:ILE:HA	3:D:369:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:682:LEU:HD11	2:C:686:MET:HE3	1.98	0.45
3:D:483:VAL:HG12	3:D:534:ILE:HD12	1.99	0.45
2:G:734:LEU:O	2:G:740:THR:OG1	2.35	0.45
7:S:335:LYS:O	7:S:339:ARG:HB2	2.17	0.45
7:T:139:HIS:CE1	7:T:141:ILE:HD13	2.52	0.45
7:Y:189:LEU:O	7:Y:424:SER:OG	2.31	0.45
8:b:35:LEU:HD21	3:a:58:ILE:HG23	1.99	0.45
8:k:28:LEU:O	8:k:32:SER:OG	2.33	0.45
2:C:290:HIS:HB3	3:D:407:GLY:H	1.81	0.45
2:C:659:TRP:HB2	2:C:683:ARG:HD2	1.99	0.45
7:2:143:GLY:H	7:2:147:SER:HB3	1.82	0.45
2:M:701:VAL:HG13	2:M:736:ASP:HB3	1.99	0.45
3:B:483:VAL:HG12	3:B:534:ILE:HD12	1.99	0.45
3:D:620:ARG:HH21	3:D:644:VAL:HA	1.82	0.45
2:E:701:VAL:HG13	2:E:736:ASP:HB3	1.99	0.45
3:F:707:LEU:HD13	3:F:851:THR:HG22	1.99	0.45
3:F:780:ASP:OD2	3:j:106:ARG:NH1	2.50	0.45
2:G:659:TRP:HB2	2:G:683:ARG:HD2	1.99	0.45
4:I:299:ILE:HG13	4:I:339:HIS:CD2	2.52	0.45
7:W:28:GLU:HA	7:W:367:LEU:HD11	1.98	0.45
7:W:340:ILE:HD13	7:W:343:ARG:HE	1.82	0.45
7:X:193:LYS:HG3	7:X:424:SER:HA	1.99	0.45
2:A:356:LEU:HB3	2:A:440:PRO:HB3	1.99	0.44
2:A:659:TRP:HB2	2:A:683:ARG:HD2	1.99	0.44
2:C:356:LEU:HB3	2:C:440:PRO:HB3	2.00	0.44
2:C:536:GLU:HA	2:C:539:LEU:HB2	1.97	0.44
2:E:734:LEU:O	2:E:740:THR:OG1	2.35	0.44
5:J:797:ASP:OD1	5:J:797:ASP:N	2.47	0.44
7:R:69:LEU:HD23	7:R:145:THR:HB	1.98	0.44
7:Y:274:THR:O	7:Y:302:ASN:ND2	2.51	0.44
7:1:289:THR:HG23	7:1:292:ASP:H	1.82	0.44
2:M:356:LEU:HB3	2:M:440:PRO:HB3	2.00	0.44
3:B:733:GLU:HG2	3:B:737:LYS:HE2	1.98	0.44
2:C:339:ALA:O	2:C:343:THR:OG1	2.36	0.44
2:C:350:CYS:HB3	2:C:355:THR:HB	1.99	0.44
3:D:707:LEU:HD13	3:D:851:THR:HG22	1.99	0.44
2:E:350:CYS:HB3	2:E:355:THR:HB	1.99	0.44
3:F:464:TYR:OH	3:F:491:ASN:ND2	2.45	0.44
3:F:776:ARG:HH21	3:j:106:ARG:NE	2.09	0.44
3:H:620:ARG:HH21	3:H:644:VAL:HA	1.82	0.44
3:H:721:TYR:OH	3:H:761:ARG:O	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:13:GLU:HB2	6:c:34:LYS:HE3	1.98	0.44
2:M:659:TRP:HB2	2:M:683:ARG:HD2	1.99	0.44
2:C:529:VAL:HG21	7:Q:251:ASN:HB2	1.99	0.44
2:E:485:VAL:HG23	2:E:486:GLU:HG3	2.00	0.44
2:G:705:THR:OG1	2:G:733:CYS:SG	2.68	0.44
3:H:707:LEU:HD13	3:H:851:THR:HG22	1.99	0.44
6:L:1679:GLN:HA	6:L:1683:VAL:HG22	1.98	0.44
7:R:351:TRP:CD1	7:R:351:TRP:H	2.35	0.44
7:S:4:GLU:HA	7:S:50:VAL:HA	1.98	0.44
6:c:88:ARG:NH1	6:c:91:GLU:OE1	2.50	0.44
3:N:620:ARG:HH21	3:N:644:VAL:HA	1.82	0.44
3:B:648:ILE:H	3:B:648:ILE:HG13	1.45	0.44
2:G:356:LEU:HB3	2:G:440:PRO:HB3	2.00	0.44
3:H:802:ARG:O	3:H:806:PHE:N	2.42	0.44
6:L:444:ARG:O	6:L:444:ARG:NH1	2.47	0.44
7:Q:406:GLU:HB3	7:Q:408:PHE:HD2	1.81	0.44
7:S:361:SER:OG	7:S:362:ARG:N	2.50	0.44
7:W:238:ALA:HB3	7:W:376:LEU:HD13	1.99	0.44
2:M:339:ALA:O	2:M:343:THR:OG1	2.36	0.44
2:A:485:VAL:HG23	2:A:486:GLU:HG3	2.00	0.44
3:B:429:PHE:HE2	3:B:445:GLU:HB2	1.83	0.44
3:B:674:GLU:CD	7:P:249:MET:HE1	2.43	0.44
3:D:703:GLN:HA	3:D:706:ILE:HG12	2.00	0.44
3:F:710:GLU:HG2	3:F:854:TYR:HE2	1.83	0.44
3:H:254:ILE:HD13	3:H:254:ILE:HA	1.88	0.44
3:h:13:LEU:HD11	3:h:39:ILE:HG21	1.99	0.44
7:2:232:VAL:HA	7:2:235:ILE:HD12	1.98	0.44
3:N:408:ASP:O	3:N:412:ARG:N	2.48	0.44
3:B:707:LEU:HD13	3:B:851:THR:HG22	1.99	0.44
3:B:710:GLU:HG2	3:B:854:TYR:HE2	1.83	0.44
4:I:2:ILE:H	4:I:2:ILE:HG12	1.58	0.44
7:Q:247:GLY:O	7:Q:251:ASN:ND2	2.38	0.44
7:R:361:SER:OG	7:R:362:ARG:N	2.51	0.44
3:B:703:GLN:HA	3:B:706:ILE:HG12	2.00	0.44
2:C:734:LEU:O	2:C:740:THR:OG1	2.35	0.44
3:D:733:GLU:HG2	3:D:737:LYS:HE2	1.98	0.44
7:R:275:PRO:HB2	7:R:278:THR:HB	2.00	0.44
7:W:181:VAL:HB	7:W:184:GLN:HB2	1.99	0.44
2:M:325:TRP:O	2:M:329:GLN:NE2	2.46	0.44
2:M:734:LEU:O	2:M:740:THR:OG1	2.35	0.44
3:N:647:PRO:O	3:N:650:THR:OG1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:890:GLU:O	3:B:891:PRO:C	2.61	0.44
2:C:241:ARG:HD2	2:C:241:ARG:HA	1.43	0.44
2:C:485:VAL:HG23	2:C:486:GLU:HG3	2.00	0.44
3:D:305:ARG:HG3	3:D:332:LEU:HD21	2.00	0.44
3:D:429:PHE:HE2	3:D:445:GLU:HB2	1.83	0.44
3:D:581:LEU:HD12	3:D:581:LEU:HA	1.87	0.44
3:D:710:GLU:HG2	3:D:854:TYR:HE2	1.83	0.44
2:E:325:TRP:O	2:E:329:GLN:NE2	2.46	0.44
2:E:659:TRP:HB2	2:E:683:ARG:HD2	1.99	0.44
3:F:578:MET:HE2	3:F:578:MET:HB3	1.91	0.44
2:G:543:VAL:HA	2:G:546:ILE:HG22	2.00	0.44
5:J:237:HIS:O	5:J:239:HIS:N	2.50	0.44
7:Q:68:ASP:HB2	7:Q:71:PRO:HB3	2.00	0.44
7:V:119:PHE:HA	7:V:122:ILE:HG12	1.99	0.44
7:W:193:LYS:HG3	7:W:424:SER:HA	2.00	0.44
7:X:119:PHE:HA	7:X:122:ILE:HG12	1.99	0.44
7:X:290:VAL:HG21	7:X:328:VAL:HG13	1.99	0.44
7:Y:193:LYS:HG3	7:Y:424:SER:HA	2.00	0.44
7:Y:334:HIS:O	7:Y:338:GLN:HG2	2.18	0.44
7:Y:348:PHE:HB2	7:Y:350:PRO:HD3	2.00	0.44
7:1:249:MET:HG2	2:M:695:TYR:HE1	1.83	0.44
7:2:56:ASP:OD2	7:2:56:ASP:N	2.51	0.44
2:A:350:CYS:HB3	2:A:355:THR:HB	1.99	0.44
2:A:543:VAL:HA	2:A:546:ILE:HG22	2.00	0.44
2:A:701:VAL:HG13	2:A:736:ASP:HB3	1.99	0.44
2:A:734:LEU:O	2:A:740:THR:OG1	2.35	0.44
3:B:305:ARG:HG3	3:B:332:LEU:HD21	2.00	0.44
3:D:743:ASP:OD1	3:D:743:ASP:N	2.51	0.44
2:G:350:CYS:HB3	2:G:355:THR:HB	1.99	0.44
3:H:743:ASP:N	3:H:743:ASP:OD1	2.51	0.44
7:Q:416:ASP:N	7:Q:416:ASP:OD2	2.46	0.44
7:V:254:ILE:HA	7:V:257:ILE:HB	1.99	0.44
7:W:290:VAL:HA	7:W:293:VAL:HG22	1.99	0.44
5:l:106:ALA:O	5:l:110:ILE:HG13	2.17	0.44
7:1:73:VAL:O	7:1:76:SER:OG	2.33	0.44
7:1:274:THR:O	7:1:302:ASN:ND2	2.51	0.44
2:M:543:VAL:HA	2:M:546:ILE:HG22	2.00	0.44
2:C:213:GLN:HE22	2:C:253:ASP:H	1.63	0.43
3:F:501:THR:O	3:F:501:THR:OG1	2.22	0.43
3:H:483:VAL:HG12	3:H:534:ILE:HD12	1.99	0.43
3:H:710:GLU:HG2	3:H:854:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:274:THR:O	7:T:302:ASN:ND2	2.51	0.43
3:j:53:LEU:HA	3:j:56:GLU:HG3	2.00	0.43
3:N:429:PHE:HE2	3:N:445:GLU:HB2	1.83	0.43
3:N:464:TYR:OH	3:N:491:ASN:ND2	2.45	0.43
3:N:490:ILE:H	3:N:490:ILE:HG12	1.64	0.43
3:N:578:MET:HE2	3:N:578:MET:HB3	1.91	0.43
2:E:513:LEU:HB3	2:E:706:TRP:HH2	1.84	0.43
3:F:254:ILE:HD13	3:F:254:ILE:HA	1.89	0.43
3:F:429:PHE:HE2	3:F:445:GLU:HB2	1.83	0.43
3:H:308:THR:OG1	3:H:325:CYS:SG	2.68	0.43
3:H:312:SER:OG	3:H:325:CYS:SG	2.67	0.43
5:J:262:ARG:HA	5:J:299:ASN:HB3	2.00	0.43
4:K:528:LEU:O	4:K:644:GLN:NE2	2.52	0.43
7:T:232:VAL:HA	7:T:235:ILE:HD12	1.99	0.43
3:N:483:VAL:HG12	3:N:534:ILE:HD12	1.99	0.43
3:N:743:ASP:OD1	3:N:743:ASP:N	2.51	0.43
3:B:620:ARG:HH21	3:B:644:VAL:HA	1.82	0.43
2:C:543:VAL:HA	2:C:546:ILE:HG22	2.00	0.43
2:E:339:ALA:O	2:E:343:THR:OG1	2.36	0.43
2:E:543:VAL:HA	2:E:546:ILE:HG22	2.00	0.43
2:G:352:GLY:HA3	2:G:406:GLU:HB2	2.01	0.43
4:K:472:LEU:HA	4:K:475:TYR:HB2	1.99	0.43
6:L:390:PRO:HB2	6:L:391:GLU:H	1.64	0.43
3:N:710:GLU:HG2	3:N:854:TYR:HE2	1.83	0.43
2:A:414:LEU:HD23	2:A:414:LEU:HA	1.90	0.43
3:D:341:VAL:HB	6:c:174:MET:HE3	2.00	0.43
2:E:309:GLN:NE2	6:c:164:ILE:HB	2.33	0.43
2:E:415:ARG:HD3	2:E:415:ARG:HA	1.86	0.43
4:I:5:LEU:HD21	4:I:45:LEU:HD13	2.01	0.43
4:I:520:HIS:HE1	7:W:353:PRO:HD2	1.84	0.43
7:U:63:ARG:NE	7:U:129:SER:OG	2.52	0.43
7:Y:276:LEU:HA	7:Y:276:LEU:HD23	1.83	0.43
8:m:37:THR:HA	5:l:118:SER:HB3	2.00	0.43
7:1:69:LEU:HD23	7:1:145:THR:HB	2.00	0.43
7:2:189:LEU:O	7:2:424:SER:OG	2.35	0.43
2:A:665:ALA:HB1	7:O:197:GLN:HG2	2.00	0.43
3:D:312:SER:OG	3:D:325:CYS:SG	2.67	0.43
3:D:319:LEU:O	3:D:323:SER:OG	2.36	0.43
3:F:408:ASP:O	3:F:412:ARG:N	2.48	0.43
3:F:626:LEU:HB3	3:j:64:ARG:HG3	2.00	0.43
3:F:742:GLN:H	3:F:742:GLN:HG3	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:188:SER:HA	4:K:192:LEU:HD23	2.00	0.43
6:L:1666:GLN:HE22	7:Z:258:ALA:HB3	1.83	0.43
7:P:69:LEU:HD22	7:P:145:THR:HB	1.99	0.43
7:Q:351:TRP:CD1	7:Q:351:TRP:H	2.36	0.43
7:W:69:LEU:HD23	7:W:145:THR:HB	2.01	0.43
2:M:350:CYS:HB3	2:M:355:THR:HB	1.99	0.43
2:M:513:LEU:HB3	2:M:706:TRP:HH2	1.83	0.43
3:B:568:LEU:HG	3:B:574:ILE:HG13	2.01	0.43
3:B:689:LYS:NZ	7:P:162:PRO:O	2.38	0.43
3:F:312:SER:OG	3:F:325:CYS:SG	2.67	0.43
2:G:391:LEU:HD21	2:G:488:ILE:HD11	2.01	0.43
3:H:305:ARG:HG3	3:H:332:LEU:HD21	2.00	0.43
7:U:69:LEU:HD23	7:U:145:THR:HB	2.01	0.43
5:I:130:PRO:O	5:I:130:PRO:CD	2.66	0.43
7:1:353:PRO:HD2	2:M:684:GLN:HE21	1.83	0.43
2:M:166:ASN:O	2:M:169:ASN:ND2	2.46	0.43
2:M:391:LEU:HD21	2:M:488:ILE:HD11	2.01	0.43
2:M:485:VAL:HG23	2:M:486:GLU:HG3	2.00	0.43
3:N:319:LEU:O	3:N:323:SER:OG	2.36	0.43
2:E:307:VAL:HG12	3:F:365:ARG:NH2	2.33	0.43
2:G:513:LEU:HB3	2:G:706:TRP:HH2	1.84	0.43
2:G:861:PHE:O	2:G:863:GLY:N	2.52	0.43
3:H:429:PHE:HE2	3:H:445:GLU:HB2	1.83	0.43
7:O:243:LEU:HD21	7:O:253:LEU:HB2	2.01	0.43
7:Y:77:ILE:O	7:Y:86:TYR:OH	2.35	0.43
2:A:513:LEU:HB3	2:A:706:TRP:HH2	1.84	0.43
2:A:861:PHE:O	2:A:863:GLY:N	2.52	0.43
2:E:234:SER:O	2:E:247:LEU:N	2.40	0.43
2:E:419:ILE:HD12	2:E:424:ASN:HB3	2.01	0.43
2:G:427:TYR:OH	2:G:458:ASN:HB3	2.19	0.43
7:R:113:LYS:HG3	7:R:114:ILE:HG23	2.01	0.43
7:Y:241:THR:OG1	7:Y:244:ARG:NH2	2.51	0.43
8:m:31:ILE:HA	8:m:34:ILE:HG12	2.01	0.43
7:1:290:VAL:HG13	7:1:336:SER:HB2	2.00	0.43
7:2:290:VAL:HA	7:2:293:VAL:HG22	2.00	0.43
2:M:769:MET:HG3	2:M:770:LYS:HD3	2.01	0.43
2:A:241:ARG:HA	2:A:241:ARG:HD2	1.43	0.43
3:B:578:MET:HE2	3:B:578:MET:HB3	1.91	0.43
3:B:647:PRO:O	3:B:650:THR:OG1	2.36	0.43
2:C:277:ILE:HA	2:C:293:ALA:HB1	2.01	0.43
2:C:391:LEU:HD21	2:C:488:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:352:GLY:HA3	2:E:406:GLU:HB2	2.01	0.43
2:E:861:PHE:O	2:E:863:GLY:N	2.52	0.43
3:F:568:LEU:HG	3:F:574:ILE:HG13	2.01	0.43
3:H:326:ALA:HB2	4:I:165:LEU:HD23	2.01	0.43
4:K:535:ASP:OD2	4:K:640:SER:OG	2.35	0.43
3:N:254:ILE:HD13	3:N:254:ILE:HA	1.89	0.43
3:N:703:GLN:HA	3:N:706:ILE:HG12	2.00	0.43
2:A:277:ILE:HA	2:A:293:ALA:HB1	2.01	0.43
3:B:319:LEU:O	3:B:323:SER:OG	2.36	0.43
3:F:703:GLN:HA	3:F:706:ILE:HG12	2.00	0.43
3:F:743:ASP:N	3:F:743:ASP:OD1	2.51	0.43
2:G:339:ALA:O	2:G:343:THR:OG1	2.36	0.43
3:H:319:LEU:O	3:H:323:SER:OG	2.36	0.43
4:K:2:ILE:H	4:K:2:ILE:HG12	1.58	0.43
7:V:273:TYR:HB2	7:V:304:MET:HE1	2.01	0.43
7:X:383:SER:O	7:X:386:SER:OG	2.36	0.43
3:N:707:LEU:HD13	3:N:851:THR:HG22	2.00	0.43
2:A:745:LEU:HD12	2:A:745:LEU:HA	1.88	0.42
3:D:725:GLU:OE1	7:R:334:HIS:CE1	2.72	0.42
3:D:781:GLN:HA	3:D:784:GLU:HB3	2.01	0.42
3:F:680:ILE:HD13	3:F:680:ILE:HA	1.94	0.42
3:H:311:ARG:HD3	3:H:311:ARG:HA	1.81	0.42
5:J:821:TYR:CZ	5:J:934:LEU:HD21	2.53	0.42
4:K:84:ILE:HD12	4:K:87:ARG:HD2	2.01	0.42
7:P:62:PRO:HD2	7:P:86:TYR:HA	2.00	0.42
7:P:290:VAL:HG23	7:P:336:SER:HB2	2.01	0.42
7:2:274:THR:O	7:2:302:ASN:ND2	2.52	0.42
3:B:311:ARG:HA	3:B:311:ARG:HD3	1.81	0.42
2:C:352:GLY:HA3	2:C:406:GLU:HB2	2.01	0.42
2:C:682:LEU:HD13	2:C:826:ASP:HA	2.02	0.42
2:E:391:LEU:HD21	2:E:488:ILE:HD11	2.01	0.42
2:G:325:TRP:O	2:G:329:GLN:NE2	2.46	0.42
5:J:484:HIS:CE1	5:J:486:TRP:HB2	2.54	0.42
7:O:348:PHE:HD2	7:O:350:PRO:HD2	1.84	0.42
8:m:55:ILE:HD13	8:m:60:LEU:HD12	2.00	0.42
2:M:352:GLY:HA3	2:M:406:GLU:HB2	2.01	0.42
2:M:422:ASP:CG	2:M:426:LYS:H	2.27	0.42
2:M:861:PHE:O	2:M:863:GLY:N	2.52	0.42
3:N:305:ARG:HG3	3:N:332:LEU:HD21	2.00	0.42
2:C:234:SER:O	2:C:247:LEU:N	2.40	0.42
2:C:645:MET:HE2	2:C:645:MET:HB3	1.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:568:LEU:HG	3:D:574:ILE:HG13	2.01	0.42
3:D:721:TYR:OH	3:D:761:ARG:O	2.30	0.42
2:E:166:ASN:O	2:E:169:ASN:ND2	2.45	0.42
2:E:277:ILE:HA	2:E:293:ALA:HB1	2.01	0.42
2:G:485:VAL:HG23	2:G:486:GLU:HG3	2.00	0.42
2:G:682:LEU:HD13	2:G:826:ASP:HA	2.02	0.42
5:J:889:LYS:HG2	5:J:987:PHE:HE2	1.84	0.42
5:J:921:LYS:H	5:J:925:GLN:HE21	1.66	0.42
6:L:1590:VAL:HG11	6:L:1733:PHE:HB3	2.01	0.42
7:R:290:VAL:HG21	7:R:333:VAL:HG23	2.02	0.42
7:W:119:PHE:HA	7:W:122:ILE:HG12	2.01	0.42
7:Y:361:SER:OG	7:Y:362:ARG:N	2.52	0.42
5:l:118:SER:OG	5:l:119:ASP:N	2.43	0.42
2:M:427:TYR:OH	2:M:458:ASN:HB3	2.19	0.42
2:M:682:LEU:HD13	2:M:826:ASP:HA	2.01	0.42
2:A:152:GLN:OE1	2:A:152:GLN:N	2.50	0.42
2:A:391:LEU:HD21	2:A:488:ILE:HD11	2.01	0.42
2:C:152:GLN:OE1	2:C:152:GLN:N	2.50	0.42
4:I:84:ILE:HD12	4:I:87:ARG:HD2	2.01	0.42
5:J:394:THR:HB	6:L:297:TRP:NE1	2.34	0.42
4:K:516:ARG:HD2	7:Y:264:PRO:HD3	2.00	0.42
7:O:235:ILE:O	7:O:239:SER:OG	2.31	0.42
7:Q:63:ARG:NE	7:Q:129:SER:OG	2.53	0.42
7:S:193:LYS:HG3	7:S:424:SER:HA	2.00	0.42
5:l:91:PHE:CZ	5:l:110:ILE:HD12	2.53	0.42
2:A:234:SER:O	2:A:247:LEU:N	2.40	0.42
2:A:339:ALA:O	2:A:343:THR:OG1	2.36	0.42
2:C:861:PHE:O	2:C:863:GLY:N	2.52	0.42
3:F:319:LEU:O	3:F:323:SER:OG	2.36	0.42
3:H:285:ARG:NH2	3:H:288:ARG:HB2	2.33	0.42
4:I:503:LYS:HA	4:I:503:LYS:HD2	1.76	0.42
6:L:393:ILE:O	6:L:397:LEU:HB2	2.19	0.42
7:Q:139:HIS:CE1	7:Q:141:ILE:HD13	2.54	0.42
7:R:201:CYS:HA	7:R:267:HIS:HB2	2.01	0.42
7:R:204:VAL:HG11	7:R:384:ILE:HD11	2.01	0.42
7:S:232:VAL:HA	7:S:235:ILE:HD12	2.00	0.42
7:Y:262:PRO:HB2	7:Y:351:TRP:CH2	2.54	0.42
8:m:51:CYS:HA	8:m:55:ILE:HG22	2.00	0.42
7:2:195:LEU:O	7:2:199:ALA:HB3	2.19	0.42
2:C:166:ASN:O	2:C:169:ASN:ND2	2.45	0.42
2:C:180:TRP:CZ2	3:D:383:ALA:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:356:LEU:HB3	2:E:440:PRO:HB3	1.99	0.42
3:H:781:GLN:HA	3:H:784:GLU:HB3	2.01	0.42
4:I:370:GLN:HB2	4:I:486:ARG:HH21	1.85	0.42
7:O:316:CYS:HB2	7:O:349:ILE:H	1.83	0.42
7:S:272:GLY:HA2	7:S:304:MET:HG3	2.02	0.42
7:X:317:TYR:HB2	7:X:348:PHE:HB3	2.02	0.42
7:Z:69:LEU:HD23	7:Z:145:THR:HB	2.01	0.42
8:b:56:ASN:ND2	3:a:44:ALA:O	2.53	0.42
2:M:234:SER:O	2:M:247:LEU:N	2.40	0.42
3:D:827:GLU:OE1	3:D:827:GLU:N	2.47	0.42
3:F:581:LEU:HD12	3:F:581:LEU:HA	1.88	0.42
3:H:261:ILE:HG21	4:I:37:SER:HA	2.02	0.42
4:I:385:THR:O	4:I:388:THR:OG1	2.30	0.42
6:L:299:ARG:HH21	6:L:306:HIS:HB3	1.83	0.42
7:P:195:LEU:O	7:P:199:ALA:HB3	2.19	0.42
7:U:119:PHE:HA	7:U:122:ILE:HG12	2.02	0.42
7:X:181:VAL:HB	7:X:184:GLN:HB2	2.02	0.42
7:Z:193:LYS:HG3	7:Z:424:SER:HA	2.01	0.42
7:Z:274:THR:HG23	7:Z:296:ARG:HB3	2.02	0.42
7:Z:418:PHE:HB3	7:Z:421:MET:HE2	2.02	0.42
3:N:568:LEU:HG	3:N:574:ILE:HG13	2.01	0.42
3:N:729:CYS:O	3:N:733:GLU:N	2.49	0.42
2:A:352:GLY:HA3	2:A:406:GLU:HB2	2.01	0.42
2:C:390:VAL:HG22	2:C:401:HIS:CE1	2.52	0.42
2:C:427:TYR:OH	2:C:458:ASN:HB3	2.19	0.42
2:C:513:LEU:HB3	2:C:706:TRP:HH2	1.84	0.42
2:E:390:VAL:HG22	2:E:401:HIS:CE1	2.52	0.42
3:F:627:GLU:HG3	3:j:64:ARG:HD2	2.02	0.42
2:G:871:ARG:HA	2:G:871:ARG:HD3	1.83	0.42
3:H:408:ASP:O	3:H:412:ARG:N	2.48	0.42
3:H:568:LEU:HG	3:H:574:ILE:HG13	2.01	0.42
4:K:370:GLN:HB2	4:K:486:ARG:HH21	1.84	0.42
7:U:406:GLU:HB3	7:U:408:PHE:HD2	1.84	0.42
3:B:408:ASP:O	3:B:412:ARG:N	2.48	0.42
2:E:201:THR:N	3:F:282:ASN:O	2.53	0.42
2:E:427:TYR:OH	2:E:458:ASN:HB3	2.19	0.42
2:E:519:TYR:CG	2:E:573:LEU:HD11	2.55	0.42
4:I:188:SER:HA	4:I:192:LEU:HD23	2.00	0.42
4:K:5:LEU:HD21	4:K:45:LEU:HD13	2.01	0.42
4:K:17:PHE:HE2	4:K:42:LEU:HD22	1.85	0.42
6:L:296:CYS:SG	6:L:297:TRP:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Q:57:ASP:HB3	7:Q:59:HIS:CD2	2.55	0.42
7:R:371:HIS:ND1	7:R:373:VAL:O	2.48	0.42
7:S:169:TYR:CD1	7:S:236:MET:HG2	2.55	0.42
7:T:406:GLU:HB3	7:T:408:PHE:HD2	1.85	0.42
7:X:276:LEU:HD23	7:X:276:LEU:HA	1.81	0.42
2:A:159:LYS:HA	2:A:159:LYS:HD3	1.92	0.42
2:A:519:TYR:CG	2:A:573:LEU:HD11	2.55	0.42
3:B:781:GLN:HA	3:B:784:GLU:HB3	2.01	0.42
2:G:277:ILE:HA	2:G:293:ALA:HB1	2.02	0.42
2:G:837:LEU:HD21	2:G:859:LEU:HD22	2.02	0.42
3:H:490:ILE:H	3:H:490:ILE:HG12	1.64	0.42
3:H:703:GLN:HA	3:H:706:ILE:HG12	2.00	0.42
4:I:17:PHE:HE2	4:I:42:LEU:HD22	1.85	0.42
4:I:22:ARG:HE	4:I:22:ARG:HB3	1.29	0.42
4:K:205:ILE:O	4:K:260:ARG:NH2	2.53	0.42
7:O:8:LEU:HD12	7:O:137:LEU:HD11	2.02	0.42
7:O:333:VAL:HG23	7:O:334:HIS:CE1	2.54	0.42
7:P:232:VAL:HA	7:P:235:ILE:HD12	2.02	0.42
7:S:322:ASN:ND2	7:S:357:GLN:O	2.52	0.42
7:Y:343:ARG:HB3	7:Y:345:LEU:HG	2.02	0.42
7:Z:57:ASP:HB3	7:Z:59:HIS:CD2	2.55	0.42
7:Z:192:LEU:HD22	7:Z:428:VAL:HG23	2.02	0.42
6:c:64:LEU:HD21	6:c:69:LYS:HE3	2.01	0.42
5:l:24:ARG:NH1	5:l:32:GLU:OE2	2.49	0.42
7:2:119:PHE:HA	7:2:122:ILE:HG12	2.01	0.42
7:2:141:ILE:HD11	7:2:170:SER:HB2	2.02	0.42
2:A:427:TYR:OH	2:A:458:ASN:HB3	2.19	0.41
2:E:662:ASN:ND2	2:E:762:MET:SD	2.93	0.41
3:F:334:GLU:HG2	6:c:148:TYR:CD2	2.54	0.41
2:G:234:SER:O	2:G:247:LEU:N	2.40	0.41
5:J:550:SER:HA	5:J:553:LYS:HB2	2.01	0.41
4:K:500:MET:HE1	4:K:516:ARG:HD3	2.02	0.41
3:N:781:GLN:HA	3:N:784:GLU:HB3	2.01	0.41
2:A:662:ASN:ND2	2:A:762:MET:SD	2.93	0.41
2:E:682:LEU:HD13	2:E:826:ASP:HA	2.01	0.41
3:F:305:ARG:HG3	3:F:332:LEU:HD21	2.00	0.41
3:F:647:PRO:O	3:F:650:THR:OG1	2.35	0.41
3:F:763:LEU:HB3	3:F:772:LEU:HB2	2.02	0.41
5:J:228:ARG:NH1	5:J:231:GLN:H	2.18	0.41
5:J:321:GLY:HA2	5:J:324:VAL:HG12	2.02	0.41
6:L:532:TYR:HA	6:L:535:PHE:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:343:ARG:HB3	7:P:345:LEU:HG	2.01	0.41
7:Q:136:VAL:HG22	7:Q:167:GLN:HB3	2.02	0.41
7:S:142:ALA:N	7:S:147:SER:OG	2.53	0.41
6:c:70:ILE:HD11	6:c:111:LEU:HD11	2.02	0.41
7:2:141:ILE:HB	7:2:173:PRO:HD3	2.01	0.41
2:A:682:LEU:HD13	2:A:826:ASP:HA	2.01	0.41
3:B:742:GLN:H	3:B:742:GLN:HG3	1.69	0.41
2:C:519:TYR:CG	2:C:573:LEU:HD11	2.55	0.41
2:C:837:LEU:HD22	2:C:856:ILE:HG23	2.02	0.41
3:D:734:LEU:HB2	3:D:754:PHE:HB2	2.03	0.41
4:I:299:ILE:HG22	4:I:301:LYS:HG2	2.02	0.41
5:J:362:GLN:HE22	4:K:165:LEU:N	2.18	0.41
5:J:429:ASN:ND2	5:J:489:ALA:O	2.53	0.41
7:S:139:HIS:HE1	7:S:141:ILE:HD13	1.85	0.41
7:S:252:ASP:OD1	7:S:252:ASP:N	2.52	0.41
7:S:317:TYR:HA	7:S:381:HIS:HA	2.01	0.41
7:U:207:ASN:O	7:U:211:ASN:HB2	2.20	0.41
7:U:224:SER:O	7:U:228:ILE:HB	2.20	0.41
7:X:361:SER:OG	7:X:362:ARG:N	2.52	0.41
7:Z:201:CYS:HA	7:Z:267:HIS:HB2	2.02	0.41
8:k:27:VAL:HG13	3:j:77:LEU:HD22	2.02	0.41
7:1:119:PHE:HA	7:1:122:ILE:HG12	2.02	0.41
3:N:493:LEU:HA	3:N:497:CYS:HB2	2.02	0.41
2:C:618:PHE:O	2:C:639:GLN:NE2	2.45	0.41
2:E:770:LYS:HB2	2:E:771:LEU:HD12	2.03	0.41
3:F:803:ARG:HH12	3:F:833:ILE:HD11	1.85	0.41
3:H:258:PHE:HZ	3:H:294:LEU:HD22	1.86	0.41
5:J:548:MET:HB3	5:J:548:MET:HE2	1.80	0.41
5:J:828:LEU:O	5:J:832:LYS:HG2	2.20	0.41
7:U:193:LYS:HG3	7:U:424:SER:HA	2.02	0.41
7:V:406:GLU:HB3	7:V:408:PHE:HD2	1.85	0.41
7:W:257:ILE:HD13	7:W:257:ILE:HA	1.94	0.41
7:Z:238:ALA:HB3	7:Z:376:LEU:HD13	2.02	0.41
7:2:337:LEU:HD11	7:2:356:ILE:HG23	2.01	0.41
3:N:258:PHE:HZ	3:N:294:LEU:HD22	1.86	0.41
3:N:311:ARG:HD3	3:N:311:ARG:HA	1.81	0.41
2:A:434:ILE:HD13	2:A:451:LEU:HB2	2.03	0.41
2:A:662:ASN:O	2:A:664:THR:N	2.53	0.41
3:B:661:LEU:HD21	3:f:64:ARG:NH1	2.35	0.41
3:B:710:GLU:CD	7:P:353:PRO:HG3	2.45	0.41
2:C:704:PRO:HB3	7:Q:331:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:258:PHE:HZ	3:D:294:LEU:HD22	1.86	0.41
3:D:648:ILE:H	3:D:648:ILE:HG13	1.45	0.41
3:D:680:ILE:HD13	3:D:680:ILE:HA	1.94	0.41
2:G:486:GLU:HG3	2:G:486:GLU:H	1.63	0.41
2:G:876:ARG:HD3	3:j:42:ASN:ND2	2.22	0.41
4:K:32:PRO:HD2	4:K:33:PHE:CE2	2.56	0.41
7:P:384:ILE:HD12	7:P:384:ILE:HA	1.95	0.41
7:V:63:ARG:NE	7:V:129:SER:OG	2.53	0.41
7:Y:69:LEU:HD23	7:Y:145:THR:HB	2.02	0.41
7:1:290:VAL:HG21	7:1:333:VAL:HG12	2.02	0.41
3:B:301:HIS:NE2	3:B:336:TYR:OH	2.30	0.41
2:C:408:MET:HE3	2:C:439:ILE:HG12	2.03	0.41
2:E:408:MET:HE3	2:E:439:ILE:HG12	2.03	0.41
3:F:627:GLU:O	3:j:64:ARG:NH2	2.38	0.41
3:F:729:CYS:O	3:F:733:GLU:N	2.49	0.41
3:F:781:GLN:HA	3:F:784:GLU:HB3	2.01	0.41
4:I:500:MET:HE1	4:I:516:ARG:HD3	2.02	0.41
5:J:711:LYS:HA	5:J:711:LYS:HD3	1.85	0.41
5:J:902:MET:HE3	5:J:902:MET:HB3	1.87	0.41
7:Z:318:ILE:HA	7:Z:350:PRO:HG3	2.03	0.41
3:f:13:LEU:HD11	3:f:39:ILE:HG21	2.01	0.41
7:2:276:LEU:HA	7:2:276:LEU:HD23	1.86	0.41
2:M:277:ILE:HA	2:M:293:ALA:HB1	2.02	0.41
3:B:729:CYS:O	3:B:733:GLU:N	2.49	0.41
3:B:803:ARG:HH12	3:B:833:ILE:HD11	1.85	0.41
2:C:770:LYS:HB3	2:C:770:LYS:HE2	1.47	0.41
3:D:569:GLY:HA2	7:R:248:TYR:CE1	2.56	0.41
3:D:879:ARG:HH12	7:R:338:GLN:HE22	1.68	0.41
2:E:302:GLU:H	2:E:302:GLU:HG3	1.56	0.41
4:I:86:LEU:HG	4:I:153:ILE:HD13	2.03	0.41
4:I:191:MET:HE2	4:I:191:MET:HB3	1.82	0.41
7:O:290:VAL:HG11	7:O:328:VAL:HG13	2.03	0.41
7:R:238:ALA:HB3	7:R:376:LEU:HD13	2.02	0.41
7:U:139:HIS:CE1	7:U:141:ILE:HD13	2.56	0.41
7:Z:274:THR:HG21	7:Z:293:VAL:HB	2.02	0.41
8:g:27:VAL:HG13	3:f:77:LEU:HD22	2.02	0.41
7:2:8:LEU:HD12	7:2:137:LEU:HD11	2.03	0.41
7:2:69:LEU:HD23	7:2:145:THR:HB	2.02	0.41
3:B:464:TYR:OH	3:B:491:ASN:ND2	2.45	0.41
2:C:210:LEU:HD13	2:C:210:LEU:HA	1.95	0.41
2:C:837:LEU:HD21	2:C:859:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:709:LEU:HB2	2:E:729:PHE:HB2	2.02	0.41
2:G:519:TYR:CG	2:G:573:LEU:HD11	2.55	0.41
2:G:837:LEU:HD22	2:G:856:ILE:HG23	2.02	0.41
4:I:503:LYS:HG2	7:W:264:PRO:HG3	2.02	0.41
7:Q:317:TYR:HA	7:Q:381:HIS:HA	2.03	0.41
7:Q:337:LEU:HG	7:Q:356:ILE:HD11	2.03	0.41
7:S:317:TYR:HD1	7:S:348:PHE:HB3	1.86	0.41
7:W:174:ASN:O	7:W:208:THR:OG1	2.35	0.41
8:i:27:VAL:HG13	3:h:77:LEU:HD22	2.02	0.41
3:f:51:GLU:CD	3:f:82:HIS:HE2	2.29	0.41
8:d:46:ILE:HG21	6:c:11:LEU:HB2	2.03	0.41
2:M:519:TYR:CG	2:M:573:LEU:HD11	2.55	0.41
2:M:709:LEU:HB2	2:M:729:PHE:HB2	2.02	0.41
3:N:721:TYR:OH	3:N:761:ARG:O	2.30	0.41
3:N:763:LEU:HB3	3:N:772:LEU:HB2	2.02	0.41
3:N:803:ARG:HH12	3:N:833:ILE:HD11	1.85	0.41
2:A:704:PRO:HA	7:O:330:PRO:HB2	2.02	0.41
2:A:709:LEU:HB2	2:A:729:PHE:HB2	2.02	0.41
2:A:837:LEU:HD22	2:A:856:ILE:HG23	2.02	0.41
2:A:840:LEU:HB3	2:A:856:ILE:HD11	2.03	0.41
3:B:274:CYS:SG	3:B:275:TYR:N	2.93	0.41
3:B:493:LEU:HA	3:B:497:CYS:HB2	2.02	0.41
3:B:543:LYS:HD2	3:B:543:LYS:HA	1.86	0.41
3:B:734:LEU:HB2	3:B:754:PHE:HB2	2.03	0.41
3:B:763:LEU:HB3	3:B:772:LEU:HB2	2.02	0.41
3:D:701:LEU:O	3:D:705:HIS:ND1	2.54	0.41
2:E:543:VAL:HG12	2:E:609:ALA:HA	2.03	0.41
2:E:618:PHE:O	2:E:639:GLN:NE2	2.45	0.41
3:F:283:LEU:HD13	3:F:286:SER:HB2	2.03	0.41
3:F:734:LEU:HB2	3:F:754:PHE:HB2	2.02	0.41
2:G:434:ILE:HD13	2:G:451:LEU:HB2	2.03	0.41
2:G:543:VAL:HG12	2:G:609:ALA:HA	2.03	0.41
2:G:865:TYR:HB3	2:G:868:ARG:CZ	2.51	0.41
3:H:729:CYS:O	3:H:733:GLU:N	2.49	0.41
3:H:763:LEU:HB3	3:H:772:LEU:HB2	2.02	0.41
3:H:848:ARG:O	3:H:851:THR:OG1	2.37	0.41
4:I:343:LEU:HD12	4:I:347:GLU:HG3	2.03	0.41
6:L:1623:LEU:HD12	6:L:1623:LEU:HA	1.88	0.41
7:O:63:ARG:NE	7:O:129:SER:OG	2.54	0.41
7:O:68:ASP:HB2	7:O:71:PRO:HB3	2.03	0.41
7:X:297:LEU:HD21	7:X:377:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:55:ALA:HB3	7:Y:59:HIS:HB2	2.03	0.41
7:Z:322:ASN:HD21	7:Z:358:VAL:HG12	1.86	0.41
8:g:28:LEU:O	8:g:32:SER:OG	2.34	0.41
8:d:71:THR:HG23	6:c:17:PRO:HD3	2.02	0.41
5:l:80:LYS:HE2	5:l:125:SER:OG	2.21	0.41
7:2:63:ARG:NE	7:2:129:SER:OG	2.54	0.41
2:C:486:GLU:HG3	2:C:486:GLU:H	1.63	0.41
3:D:493:LEU:HA	3:D:497:CYS:HB2	2.03	0.41
3:F:274:CYS:SG	3:F:275:TYR:N	2.93	0.41
2:G:234:SER:N	2:G:247:LEU:O	2.54	0.41
2:G:400:ILE:HD11	2:G:411:GLU:HB2	2.03	0.41
2:G:684:GLN:HE21	7:U:353:PRO:HD2	1.86	0.41
3:H:276:LYS:HA	3:H:276:LYS:HD3	1.87	0.41
4:I:409:ASN:C	4:I:411:LEU:H	2.29	0.41
4:K:343:LEU:HD12	4:K:347:GLU:HG3	2.03	0.41
7:1:193:LYS:HG3	7:1:424:SER:HA	2.03	0.41
2:M:234:SER:N	2:M:247:LEU:O	2.54	0.41
2:M:415:ARG:HG3	2:M:419:ILE:HD12	2.03	0.41
2:M:486:GLU:HG3	2:M:486:GLU:H	1.63	0.41
2:M:662:ASN:ND2	2:M:762:MET:SD	2.93	0.41
3:N:701:LEU:O	3:N:705:HIS:ND1	2.54	0.41
2:E:434:ILE:HD13	2:E:451:LEU:HB2	2.03	0.40
2:G:662:ASN:ND2	2:G:762:MET:SD	2.93	0.40
3:H:803:ARG:HH12	3:H:833:ILE:HD11	1.85	0.40
4:I:32:PRO:HD2	4:I:33:PHE:CE2	2.55	0.40
4:I:277:LEU:O	4:I:281:GLU:HG2	2.21	0.40
4:I:585:GLU:OE1	4:I:585:GLU:N	2.51	0.40
7:1:8:LEU:HD12	7:1:137:LEU:HD11	2.03	0.40
3:N:582:LYS:HD3	3:N:635:TRP:HZ2	1.86	0.40
2:A:234:SER:N	2:A:247:LEU:O	2.54	0.40
2:A:837:LEU:HD21	2:A:859:LEU:HD22	2.02	0.40
3:B:258:PHE:HZ	3:B:294:LEU:HD22	1.86	0.40
3:B:850:LEU:HD12	3:B:850:LEU:HA	1.94	0.40
2:C:187:LEU:HG	3:D:379:LYS:HD2	2.02	0.40
2:C:745:LEU:HD12	2:C:745:LEU:HA	1.88	0.40
2:C:861:PHE:HZ	7:Q:340:ILE:HG22	1.86	0.40
3:D:729:CYS:HB3	7:R:331:THR:HB	2.03	0.40
2:E:553:ALA:HB1	7:T:342:GLU:HG3	2.03	0.40
2:E:837:LEU:HD21	2:E:859:LEU:HD22	2.02	0.40
3:F:258:PHE:HZ	3:F:294:LEU:HD22	1.86	0.40
3:F:582:LYS:HD3	3:F:635:TRP:HZ2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:840:LEU:HB3	2:G:856:ILE:HD11	2.03	0.40
3:H:701:LEU:O	3:H:705:HIS:ND1	2.54	0.40
3:H:734:LEU:HB2	3:H:754:PHE:HB2	2.03	0.40
5:J:430:VAL:HG11	5:J:495:GLN:HE21	1.86	0.40
4:K:277:LEU:O	4:K:281:GLU:HG2	2.21	0.40
4:K:341:TRP:HE1	4:K:557:ILE:HD11	1.86	0.40
7:O:193:LYS:HG3	7:O:424:SER:HA	2.02	0.40
7:P:254:ILE:HA	7:P:257:ILE:HB	2.02	0.40
7:R:293:VAL:HG21	7:R:324:ILE:HD13	2.03	0.40
7:R:337:LEU:HD12	7:R:337:LEU:HA	1.90	0.40
7:V:337:LEU:HD12	7:V:337:LEU:HA	1.84	0.40
7:W:215:THR:HG22	7:W:221:GLN:HG2	2.03	0.40
6:c:190:LEU:HD23	6:c:193:VAL:HG23	2.02	0.40
7:1:270:MET:HE2	7:1:377:MET:HE2	2.02	0.40
7:2:245:TYR:HA	7:2:246:PRO:HD3	1.93	0.40
2:M:400:ILE:HD11	2:M:411:GLU:HB2	2.03	0.40
2:M:414:LEU:HD23	2:M:414:LEU:HA	1.90	0.40
2:M:543:VAL:HG12	2:M:609:ALA:HA	2.03	0.40
2:M:837:LEU:HD21	2:M:859:LEU:HD22	2.02	0.40
2:A:400:ILE:HD11	2:A:411:GLU:HB2	2.03	0.40
3:B:743:ASP:OD1	3:B:743:ASP:N	2.51	0.40
2:C:699:PHE:HB3	7:Q:333:VAL:HG11	2.03	0.40
3:D:582:LYS:HD3	3:D:635:TRP:HZ2	1.86	0.40
3:D:803:ARG:HH12	3:D:833:ILE:HD11	1.85	0.40
3:F:832:ARG:HA	3:F:835:GLU:HG3	2.04	0.40
2:G:152:GLN:OE1	2:G:152:GLN:N	2.49	0.40
4:I:27:VAL:HG12	4:I:43:ASN:HD21	1.86	0.40
6:L:1627:LYS:HZ1	7:Z:249:MET:HE1	1.87	0.40
6:L:1779:LEU:HA	6:L:1782:VAL:HG12	2.02	0.40
7:Q:119:PHE:HA	7:Q:122:ILE:HG12	2.04	0.40
7:U:130:ASP:OD1	7:V:343:ARG:NH1	2.47	0.40
7:U:348:PHE:HB3	7:U:350:PRO:HD3	2.03	0.40
7:Y:119:PHE:HA	7:Y:122:ILE:HG12	2.03	0.40
7:Z:416:ASP:N	7:Z:416:ASP:OD2	2.53	0.40
8:b:34:ILE:O	3:a:67:ARG:NH2	2.54	0.40
6:c:64:LEU:HD12	6:c:65:PRO:HD2	2.03	0.40
2:C:234:SER:N	2:C:247:LEU:O	2.54	0.40
3:D:490:ILE:H	3:D:490:ILE:HG12	1.64	0.40
3:D:720:TYR:HE2	7:R:357:GLN:HB3	1.85	0.40
3:F:276:LYS:HD3	3:F:276:LYS:HA	1.87	0.40
3:F:369:VAL:HG12	6:c:153:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:466:LEU:HD12	3:F:466:LEU:HA	1.93	0.40
3:F:701:LEU:O	3:F:705:HIS:ND1	2.54	0.40
3:F:889:ARG:HD3	3:F:889:ARG:HA	1.65	0.40
2:G:207:THR:OG1	2:G:251:ASN:O	2.40	0.40
3:H:482:LYS:HE3	3:H:482:LYS:HB2	1.90	0.40
3:H:582:LYS:HD3	3:H:635:TRP:HZ2	1.86	0.40
6:L:444:ARG:NH2	2:M:322:GLN:HE22	2.16	0.40
7:R:163:LYS:HA	7:R:163:LYS:HD2	1.88	0.40
7:W:183:VAL:HG22	7:W:186:TYR:HB2	2.03	0.40
7:Y:143:GLY:H	7:Y:147:SER:HB3	1.85	0.40
7:Z:241:THR:OG1	7:Z:244:ARG:NH2	2.55	0.40
5:I:120:SER:N	5:I:121:PRO:HD3	2.36	0.40
3:N:543:LYS:HD2	3:N:543:LYS:HA	1.86	0.40
3:N:889:ARG:HD3	3:N:889:ARG:HA	1.65	0.40
2:A:210:LEU:HD13	2:A:210:LEU:HA	1.95	0.40
3:B:832:ARG:HA	3:B:835:GLU:HG3	2.04	0.40
2:E:234:SER:N	2:E:247:LEU:O	2.54	0.40
2:E:546:ILE:HD11	2:E:551:LEU:HD21	2.03	0.40
2:G:299:LEU:HB2	2:G:338:LEU:HD11	2.04	0.40
2:G:311:GLU:HB2	3:H:365:ARG:HH12	1.87	0.40
2:G:390:VAL:HG22	2:G:401:HIS:CE1	2.52	0.40
2:G:745:LEU:HD12	2:G:745:LEU:HA	1.88	0.40
4:I:616:VAL:O	4:I:620:SER:OG	2.29	0.40
4:K:86:LEU:HG	4:K:153:ILE:HD13	2.03	0.40
7:O:260:LEU:HD21	7:O:321:LEU:HB3	2.04	0.40
7:P:217:ARG:HH22	7:P:279:ASP:HB2	1.87	0.40
7:Y:337:LEU:HD12	7:Y:358:VAL:HG13	2.03	0.40
2:M:434:ILE:HD13	2:M:451:LEU:HB2	2.03	0.40
2:M:837:LEU:HD22	2:M:856:ILE:HG23	2.02	0.40
3:N:734:LEU:HB2	3:N:754:PHE:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	360/375 (96%)	345 (96%)	15 (4%)	0	100	100
2	A	599/902 (66%)	567 (95%)	31 (5%)	1 (0%)	43	78
2	C	606/902 (67%)	573 (95%)	30 (5%)	3 (0%)	24	63
2	E	626/902 (69%)	587 (94%)	36 (6%)	3 (0%)	24	63
2	G	628/902 (70%)	594 (95%)	33 (5%)	1 (0%)	43	78
2	M	624/902 (69%)	592 (95%)	31 (5%)	1 (0%)	43	78
3	B	602/907 (66%)	568 (94%)	31 (5%)	3 (0%)	24	63
3	D	571/907 (63%)	546 (96%)	25 (4%)	0	100	100
3	F	591/907 (65%)	561 (95%)	29 (5%)	1 (0%)	43	78
3	H	584/907 (64%)	550 (94%)	32 (6%)	2 (0%)	36	72
3	N	584/907 (64%)	551 (94%)	31 (5%)	2 (0%)	36	72
3	a	112/907 (12%)	106 (95%)	6 (5%)	0	100	100
3	f	97/907 (11%)	92 (95%)	5 (5%)	0	100	100
3	h	97/907 (11%)	92 (95%)	5 (5%)	0	100	100
3	j	105/907 (12%)	94 (90%)	11 (10%)	0	100	100
4	I	511/667 (77%)	483 (94%)	23 (4%)	5 (1%)	12	49
4	K	548/667 (82%)	515 (94%)	27 (5%)	6 (1%)	11	46
5	J	506/1024 (49%)	476 (94%)	25 (5%)	5 (1%)	12	49
5	l	104/1024 (10%)	95 (91%)	6 (6%)	3 (3%)	3	23
6	L	540/1819 (30%)	506 (94%)	29 (5%)	5 (1%)	14	51
6	c	148/1819 (8%)	141 (95%)	7 (5%)	0	100	100
7	1	408/451 (90%)	389 (95%)	18 (4%)	1 (0%)	43	78
7	2	408/451 (90%)	388 (95%)	18 (4%)	2 (0%)	24	63
7	O	408/451 (90%)	392 (96%)	14 (3%)	2 (0%)	24	63
7	P	408/451 (90%)	396 (97%)	11 (3%)	1 (0%)	43	78
7	Q	408/451 (90%)	391 (96%)	16 (4%)	1 (0%)	43	78
7	R	408/451 (90%)	390 (96%)	17 (4%)	1 (0%)	43	78
7	S	408/451 (90%)	391 (96%)	15 (4%)	2 (0%)	24	63
7	T	408/451 (90%)	393 (96%)	14 (3%)	1 (0%)	43	78
7	U	408/451 (90%)	390 (96%)	17 (4%)	1 (0%)	43	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	V	408/451 (90%)	389 (95%)	17 (4%)	2 (0%)	24	63
7	W	408/451 (90%)	386 (95%)	21 (5%)	1 (0%)	43	78
7	X	408/451 (90%)	393 (96%)	14 (3%)	1 (0%)	43	78
7	Y	408/451 (90%)	391 (96%)	16 (4%)	1 (0%)	43	78
7	Z	408/451 (90%)	396 (97%)	11 (3%)	1 (0%)	43	78
8	b	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
8	d	57/82 (70%)	56 (98%)	1 (2%)	0	100	100
8	g	63/82 (77%)	63 (100%)	0	0	100	100
8	i	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
8	k	63/82 (77%)	62 (98%)	1 (2%)	0	100	100
8	m	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
All	All	15227/26874 (57%)	14475 (95%)	693 (5%)	59 (0%)	31	67

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	891	PRO
2	E	425	ASP
3	H	503	THR
4	I	404	LEU
5	J	236	LEU
5	J	238	LEU
4	K	65	HIS
4	K	404	LEU
6	L	307	ARG
6	L	310	PRO
7	O	407	GLN
7	U	407	GLN
7	V	348	PHE
7	V	407	GLN
5	l	119	ASP
5	l	121	PRO
7	2	348	PHE
3	N	502	PRO
3	N	503	THR
2	E	427	TYR
3	H	502	PRO
4	I	409	ASN

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Mol	Chain	Res	Type
5	J	222	HIS
5	J	234	HIS
4	K	66	VAL
4	K	409	ASN
7	Q	407	GLN
7	R	407	GLN
7	S	407	GLN
7	T	407	GLN
7	W	407	GLN
7	X	407	GLN
7	1	407	GLN
4	I	410	LEU
4	I	508	ASN
4	K	410	LEU
6	L	303	PRO
7	P	407	GLN
7	Y	407	GLN
7	Z	407	GLN
7	2	407	GLN
3	B	366	ARG
2	C	675	TRP
4	K	78	GLN
6	L	309	GLU
2	A	862	ASN
3	B	502	PRO
2	C	862	ASN
2	E	862	ASN
3	F	285	ARG
2	G	862	ASN
7	O	350	PRO
7	S	355	SER
5	1	120	SER
2	M	862	ASN
6	L	452	PRO
4	I	80	GLY
5	J	258	VAL
2	C	204	PRO

5.3.2 Protein sidechains [i](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	8/318 (2%)	8 (100%)	0	100	100
2	A	549/791 (69%)	496 (90%)	53 (10%)	8	24
2	C	556/791 (70%)	504 (91%)	52 (9%)	8	26
2	E	574/791 (73%)	523 (91%)	51 (9%)	9	28
2	G	575/791 (73%)	521 (91%)	54 (9%)	8	26
2	M	572/791 (72%)	520 (91%)	52 (9%)	9	27
3	B	548/798 (69%)	493 (90%)	55 (10%)	7	24
3	D	525/798 (66%)	474 (90%)	51 (10%)	8	24
3	F	539/798 (68%)	487 (90%)	52 (10%)	8	25
3	H	536/798 (67%)	485 (90%)	51 (10%)	8	25
3	N	536/798 (67%)	485 (90%)	51 (10%)	8	25
3	a	101/798 (13%)	101 (100%)	0	100	100
3	f	88/798 (11%)	88 (100%)	0	100	100
3	h	88/798 (11%)	88 (100%)	0	100	100
3	j	96/798 (12%)	95 (99%)	1 (1%)	68	78
4	I	471/594 (79%)	441 (94%)	30 (6%)	16	37
4	K	509/594 (86%)	473 (93%)	36 (7%)	13	35
5	J	493/933 (53%)	491 (100%)	2 (0%)	84	84
5	l	96/933 (10%)	96 (100%)	0	100	100
6	L	492/1546 (32%)	486 (99%)	6 (1%)	63	75
6	c	135/1546 (9%)	135 (100%)	0	100	100
7	1	375/400 (94%)	375 (100%)	0	100	100
7	2	375/400 (94%)	375 (100%)	0	100	100
7	O	375/400 (94%)	375 (100%)	0	100	100
7	P	375/400 (94%)	374 (100%)	1 (0%)	86	86
7	Q	375/400 (94%)	375 (100%)	0	100	100
7	R	375/400 (94%)	374 (100%)	1 (0%)	86	86
7	S	375/400 (94%)	374 (100%)	1 (0%)	86	86
7	T	375/400 (94%)	375 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	375/400 (94%)	375 (100%)	0	100	100
7	V	375/400 (94%)	374 (100%)	1 (0%)	86	86
7	W	375/400 (94%)	373 (100%)	2 (0%)	81	83
7	X	375/400 (94%)	373 (100%)	2 (0%)	81	83
7	Y	375/400 (94%)	374 (100%)	1 (0%)	86	86
7	Z	375/400 (94%)	371 (99%)	4 (1%)	65	76
8	b	53/62 (86%)	53 (100%)	0	100	100
8	d	53/62 (86%)	53 (100%)	0	100	100
8	g	53/62 (86%)	53 (100%)	0	100	100
8	i	53/62 (86%)	53 (100%)	0	100	100
8	k	53/62 (86%)	53 (100%)	0	100	100
8	m	53/62 (86%)	53 (100%)	0	100	100
All	All	13655/23573 (58%)	13045 (96%)	610 (4%)	26	46

All (610) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	150	LEU
2	A	151	GLN
2	A	153	SER
2	A	165	GLN
2	A	170	SER
2	A	210	LEU
2	A	212	SER
2	A	221	LEU
2	A	229	ASP
2	A	241	ARG
2	A	243	SER
2	A	255	SER
2	A	258	GLU
2	A	271	SER
2	A	302	GLU
2	A	308	SER
2	A	320	SER
2	A	334	THR
2	A	343	THR
2	A	357	SER
2	A	401	HIS

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Mol	Chain	Res	Type
2	A	402	ASP
2	A	435	VAL
2	A	436	GLN
2	A	452	SER
2	A	459	VAL
2	A	475	ILE
2	A	481	GLU
2	A	485	VAL
2	A	486	GLU
2	A	501	ASP
2	A	505	GLU
2	A	515	SER
2	A	526	ASP
2	A	545	ASP
2	A	547	THR
2	A	571	ASP
2	A	622	VAL
2	A	627	SER
2	A	660	ILE
2	A	664	THR
2	A	712	ASN
2	A	714	LYS
2	A	717	SER
2	A	723	LEU
2	A	727	THR
2	A	732	THR
2	A	740	THR
2	A	755	CYS
2	A	764	LYS
2	A	840	LEU
2	A	859	LEU
2	A	866	THR
3	B	246	THR
3	B	254	ILE
3	B	271	THR
3	B	277	VAL
3	B	285	ARG
3	B	287	LEU
3	B	304	ILE
3	B	305	ARG
3	B	313	LEU
3	B	316	SER

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Mol	Chain	Res	Type
3	B	323	SER
3	B	332	LEU
3	B	344	SER
3	B	384	LEU
3	B	404	THR
3	B	423	SER
3	B	430	LEU
3	B	442	THR
3	B	456	THR
3	B	468	LYS
3	B	469	SER
3	B	490	ILE
3	B	503	THR
3	B	551	LYS
3	B	556	LEU
3	B	579	ASP
3	B	582	LYS
3	B	586	VAL
3	B	590	THR
3	B	598	THR
3	B	621	LEU
3	B	648	ILE
3	B	667	LEU
3	B	690	LEU
3	B	693	ASN
3	B	698	SER
3	B	704	CYS
3	B	709	SER
3	B	725	GLU
3	B	736	ASN
3	B	742	GLN
3	B	762	CYS
3	B	810	LYS
3	B	827	GLU
3	B	837	LYS
3	B	838	GLU
3	B	845	SER
3	B	866	THR
3	B	868	SER
3	B	871	GLU
3	B	877	SER
3	B	879	ARG

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Mol	Chain	Res	Type
3	B	890	GLU
3	B	891	PRO
3	B	892	ARG
2	C	150	LEU
2	C	151	GLN
2	C	153	SER
2	C	165	GLN
2	C	170	SER
2	C	210	LEU
2	C	212	SER
2	C	221	LEU
2	C	229	ASP
2	C	241	ARG
2	C	243	SER
2	C	255	SER
2	C	258	GLU
2	C	271	SER
2	C	302	GLU
2	C	308	SER
2	C	320	SER
2	C	334	THR
2	C	343	THR
2	C	357	SER
2	C	401	HIS
2	C	402	ASP
2	C	435	VAL
2	C	436	GLN
2	C	452	SER
2	C	459	VAL
2	C	475	ILE
2	C	481	GLU
2	C	485	VAL
2	C	486	GLU
2	C	501	ASP
2	C	505	GLU
2	C	515	SER
2	C	526	ASP
2	C	545	ASP
2	C	547	THR
2	C	571	ASP
2	C	622	VAL
2	C	627	SER

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Mol	Chain	Res	Type
2	C	660	ILE
2	C	712	ASN
2	C	714	LYS
2	C	717	SER
2	C	723	LEU
2	C	727	THR
2	C	732	THR
2	C	740	THR
2	C	755	CYS
2	C	764	LYS
2	C	840	LEU
2	C	859	LEU
2	C	866	THR
3	D	246	THR
3	D	254	ILE
3	D	271	THR
3	D	277	VAL
3	D	287	LEU
3	D	304	ILE
3	D	305	ARG
3	D	313	LEU
3	D	316	SER
3	D	323	SER
3	D	332	LEU
3	D	344	SER
3	D	384	LEU
3	D	404	THR
3	D	423	SER
3	D	430	LEU
3	D	442	THR
3	D	456	THR
3	D	468	LYS
3	D	469	SER
3	D	490	ILE
3	D	501	THR
3	D	551	LYS
3	D	556	LEU
3	D	579	ASP
3	D	582	LYS
3	D	586	VAL
3	D	590	THR
3	D	598	THR

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Mol	Chain	Res	Type
3	D	621	LEU
3	D	648	ILE
3	D	667	LEU
3	D	690	LEU
3	D	693	ASN
3	D	698	SER
3	D	704	CYS
3	D	709	SER
3	D	725	GLU
3	D	736	ASN
3	D	742	GLN
3	D	762	CYS
3	D	810	LYS
3	D	827	GLU
3	D	837	LYS
3	D	838	GLU
3	D	845	SER
3	D	866	THR
3	D	868	SER
3	D	871	GLU
3	D	877	SER
3	D	879	ARG
2	E	150	LEU
2	E	151	GLN
2	E	153	SER
2	E	165	GLN
2	E	170	SER
2	E	210	LEU
2	E	212	SER
2	E	221	LEU
2	E	229	ASP
2	E	241	ARG
2	E	243	SER
2	E	255	SER
2	E	258	GLU
2	E	271	SER
2	E	302	GLU
2	E	308	SER
2	E	320	SER
2	E	334	THR
2	E	343	THR
2	E	357	SER

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Mol	Chain	Res	Type
2	E	401	HIS
2	E	402	ASP
2	E	435	VAL
2	E	436	GLN
2	E	452	SER
2	E	459	VAL
2	E	475	ILE
2	E	481	GLU
2	E	485	VAL
2	E	486	GLU
2	E	501	ASP
2	E	505	GLU
2	E	515	SER
2	E	526	ASP
2	E	545	ASP
2	E	547	THR
2	E	571	ASP
2	E	622	VAL
2	E	627	SER
2	E	660	ILE
2	E	714	LYS
2	E	717	SER
2	E	723	LEU
2	E	727	THR
2	E	732	THR
2	E	740	THR
2	E	755	CYS
2	E	764	LYS
2	E	840	LEU
2	E	859	LEU
2	E	866	THR
3	F	246	THR
3	F	254	ILE
3	F	271	THR
3	F	277	VAL
3	F	287	LEU
3	F	304	ILE
3	F	305	ARG
3	F	313	LEU
3	F	316	SER
3	F	323	SER
3	F	332	LEU

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Mol	Chain	Res	Type
3	F	344	SER
3	F	384	LEU
3	F	404	THR
3	F	423	SER
3	F	430	LEU
3	F	442	THR
3	F	456	THR
3	F	468	LYS
3	F	469	SER
3	F	490	ILE
3	F	501	THR
3	F	503	THR
3	F	551	LYS
3	F	556	LEU
3	F	579	ASP
3	F	582	LYS
3	F	586	VAL
3	F	590	THR
3	F	598	THR
3	F	621	LEU
3	F	648	ILE
3	F	667	LEU
3	F	690	LEU
3	F	693	ASN
3	F	698	SER
3	F	704	CYS
3	F	709	SER
3	F	725	GLU
3	F	736	ASN
3	F	742	GLN
3	F	762	CYS
3	F	810	LYS
3	F	827	GLU
3	F	837	LYS
3	F	838	GLU
3	F	845	SER
3	F	866	THR
3	F	868	SER
3	F	871	GLU
3	F	877	SER
3	F	879	ARG
2	G	150	LEU

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Mol	Chain	Res	Type
2	G	151	GLN
2	G	153	SER
2	G	165	GLN
2	G	170	SER
2	G	203	LEU
2	G	210	LEU
2	G	212	SER
2	G	221	LEU
2	G	229	ASP
2	G	241	ARG
2	G	243	SER
2	G	255	SER
2	G	258	GLU
2	G	271	SER
2	G	302	GLU
2	G	308	SER
2	G	320	SER
2	G	334	THR
2	G	343	THR
2	G	357	SER
2	G	401	HIS
2	G	402	ASP
2	G	435	VAL
2	G	436	GLN
2	G	452	SER
2	G	459	VAL
2	G	475	ILE
2	G	481	GLU
2	G	485	VAL
2	G	486	GLU
2	G	501	ASP
2	G	505	GLU
2	G	515	SER
2	G	526	ASP
2	G	545	ASP
2	G	547	THR
2	G	571	ASP
2	G	622	VAL
2	G	627	SER
2	G	660	ILE
2	G	712	ASN
2	G	714	LYS

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Mol	Chain	Res	Type
2	G	717	SER
2	G	723	LEU
2	G	727	THR
2	G	732	THR
2	G	740	THR
2	G	755	CYS
2	G	764	LYS
2	G	840	LEU
2	G	859	LEU
2	G	866	THR
2	G	868	ARG
3	H	246	THR
3	H	254	ILE
3	H	271	THR
3	H	277	VAL
3	H	287	LEU
3	H	304	ILE
3	H	305	ARG
3	H	313	LEU
3	H	316	SER
3	H	323	SER
3	H	332	LEU
3	H	344	SER
3	H	384	LEU
3	H	404	THR
3	H	423	SER
3	H	430	LEU
3	H	442	THR
3	H	456	THR
3	H	468	LYS
3	H	469	SER
3	H	490	ILE
3	H	501	THR
3	H	551	LYS
3	H	556	LEU
3	H	579	ASP
3	H	582	LYS
3	H	586	VAL
3	H	590	THR
3	H	598	THR
3	H	621	LEU
3	H	648	ILE

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Mol	Chain	Res	Type
3	H	667	LEU
3	H	690	LEU
3	H	693	ASN
3	H	698	SER
3	H	704	CYS
3	H	709	SER
3	H	725	GLU
3	H	736	ASN
3	H	742	GLN
3	H	762	CYS
3	H	810	LYS
3	H	827	GLU
3	H	837	LYS
3	H	838	GLU
3	H	845	SER
3	H	866	THR
3	H	868	SER
3	H	871	GLU
3	H	877	SER
3	H	879	ARG
4	I	2	ILE
4	I	15	SER
4	I	22	ARG
4	I	33	PHE
4	I	37	SER
4	I	90	CYS
4	I	106	ASP
4	I	118	SER
4	I	120	SER
4	I	179	CYS
4	I	188	SER
4	I	198	ASP
4	I	260	ARG
4	I	261	VAL
4	I	270	VAL
4	I	272	VAL
4	I	300	LEU
4	I	305	ASP
4	I	319	LEU
4	I	334	SER
4	I	387	VAL
4	I	408	ASP

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Mol	Chain	Res	Type
4	I	456	SER
4	I	477	VAL
4	I	510	THR
4	I	575	LEU
4	I	577	LYS
4	I	607	ARG
4	I	611	GLN
4	I	614	ILE
5	J	221	VAL
5	J	222	HIS
4	K	2	ILE
4	K	15	SER
4	K	22	ARG
4	K	33	PHE
4	K	37	SER
4	K	63	THR
4	K	66	VAL
4	K	68	GLN
4	K	78	GLN
4	K	90	CYS
4	K	106	ASP
4	K	118	SER
4	K	120	SER
4	K	179	CYS
4	K	188	SER
4	K	198	ASP
4	K	260	ARG
4	K	261	VAL
4	K	270	VAL
4	K	272	VAL
4	K	300	LEU
4	K	305	ASP
4	K	319	LEU
4	K	334	SER
4	K	387	VAL
4	K	399	SER
4	K	408	ASP
4	K	456	SER
4	K	477	VAL
4	K	510	THR
4	K	575	LEU
4	K	577	LYS

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Mol	Chain	Res	Type
4	K	607	ARG
4	K	611	GLN
4	K	614	ILE
4	K	646	LEU
6	L	309	GLU
6	L	310	PRO
6	L	347	VAL
6	L	363	VAL
6	L	586	VAL
6	L	1612	CYS
7	P	274	THR
7	R	334	HIS
7	S	203	VAL
7	V	196	THR
7	W	171	VAL
7	W	364	SER
7	X	261	ILE
7	X	383	SER
7	Y	263	THR
7	Z	165	LEU
7	Z	222	ASN
7	Z	333	VAL
7	Z	387	LEU
3	j	107	GLN
2	M	150	LEU
2	M	151	GLN
2	M	153	SER
2	M	165	GLN
2	M	170	SER
2	M	210	LEU
2	M	212	SER
2	M	221	LEU
2	M	229	ASP
2	M	241	ARG
2	M	243	SER
2	M	255	SER
2	M	258	GLU
2	M	271	SER
2	M	302	GLU
2	M	308	SER
2	M	320	SER
2	M	334	THR

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Mol	Chain	Res	Type
2	M	343	THR
2	M	357	SER
2	M	401	HIS
2	M	402	ASP
2	M	435	VAL
2	M	436	GLN
2	M	452	SER
2	M	459	VAL
2	M	475	ILE
2	M	481	GLU
2	M	485	VAL
2	M	486	GLU
2	M	501	ASP
2	M	505	GLU
2	M	515	SER
2	M	526	ASP
2	M	545	ASP
2	M	547	THR
2	M	571	ASP
2	M	622	VAL
2	M	627	SER
2	M	660	ILE
2	M	712	ASN
2	M	714	LYS
2	M	717	SER
2	M	723	LEU
2	M	727	THR
2	M	732	THR
2	M	740	THR
2	M	755	CYS
2	M	764	LYS
2	M	840	LEU
2	M	859	LEU
2	M	866	THR
3	N	246	THR
3	N	254	ILE
3	N	271	THR
3	N	277	VAL
3	N	287	LEU
3	N	304	ILE
3	N	305	ARG
3	N	313	LEU

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Mol	Chain	Res	Type
3	N	316	SER
3	N	323	SER
3	N	332	LEU
3	N	344	SER
3	N	384	LEU
3	N	404	THR
3	N	423	SER
3	N	430	LEU
3	N	442	THR
3	N	456	THR
3	N	468	LYS
3	N	469	SER
3	N	490	ILE
3	N	501	THR
3	N	551	LYS
3	N	556	LEU
3	N	579	ASP
3	N	582	LYS
3	N	586	VAL
3	N	590	THR
3	N	598	THR
3	N	621	LEU
3	N	648	ILE
3	N	667	LEU
3	N	690	LEU
3	N	693	ASN
3	N	698	SER
3	N	704	CYS
3	N	709	SER
3	N	725	GLU
3	N	736	ASN
3	N	742	GLN
3	N	762	CYS
3	N	810	LYS
3	N	827	GLU
3	N	837	LYS
3	N	838	GLU
3	N	845	SER
3	N	866	THR
3	N	868	SER
3	N	871	GLU
3	N	877	SER

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Mol	Chain	Res	Type
3	N	879	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (329) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	213	GLN
2	A	322	GLN
2	A	373	GLN
2	A	692	ASN
2	A	707	HIS
2	A	718	ASN
2	A	823	ASN
3	B	270	ASN
3	B	302	ASN
3	B	389	GLN
3	B	417	HIS
3	B	444	HIS
3	B	491	ASN
3	B	494	HIS
3	B	576	HIS
3	B	713	HIS
3	B	719	GLN
3	B	773	ASN
3	B	787	ASN
3	B	860	GLN
3	B	885	HIS
2	C	213	GLN
2	C	322	GLN
2	C	373	GLN
2	C	688	ASN
2	C	707	HIS
2	C	718	ASN
2	C	862	ASN
3	D	259	GLN
3	D	270	ASN
3	D	302	ASN
3	D	389	GLN
3	D	401	HIS
3	D	417	HIS
3	D	444	HIS
3	D	479	GLN
3	D	491	ASN

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Mol	Chain	Res	Type
3	D	494	HIS
3	D	773	ASN
3	D	787	ASN
3	D	860	GLN
3	D	885	HIS
2	E	213	GLN
2	E	236	GLN
2	E	373	GLN
2	E	412	HIS
2	E	430	GLN
2	E	530	HIS
2	E	718	ASN
2	E	823	ASN
3	F	270	ASN
3	F	302	ASN
3	F	387	HIS
3	F	389	GLN
3	F	401	HIS
3	F	417	HIS
3	F	444	HIS
3	F	479	GLN
3	F	491	ASN
3	F	494	HIS
3	F	576	HIS
3	F	773	ASN
3	F	787	ASN
3	F	860	GLN
3	F	885	HIS
2	G	213	GLN
2	G	322	GLN
2	G	373	GLN
2	G	420	GLN
2	G	430	GLN
2	G	530	HIS
2	G	684	GLN
2	G	718	ASN
3	H	270	ASN
3	H	302	ASN
3	H	389	GLN
3	H	401	HIS
3	H	417	HIS
3	H	444	HIS

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Mol	Chain	Res	Type
3	H	479	GLN
3	H	494	HIS
3	H	773	ASN
3	H	787	ASN
3	H	860	GLN
3	H	885	HIS
4	I	29	GLN
4	I	43	ASN
4	I	116	HIS
4	I	121	HIS
4	I	149	HIS
4	I	180	HIS
4	I	316	GLN
4	I	397	GLN
4	I	398	GLN
4	I	401	HIS
4	I	493	GLN
4	I	520	HIS
4	I	529	GLN
4	I	533	GLN
4	I	540	GLN
4	I	547	GLN
4	I	561	HIS
4	I	563	HIS
4	I	567	ASN
4	I	571	GLN
4	I	600	ASN
4	I	622	GLN
5	J	222	HIS
5	J	223	GLN
5	J	239	HIS
5	J	241	ASN
5	J	328	GLN
5	J	413	HIS
5	J	474	GLN
5	J	705	ASN
5	J	822	ASN
5	J	830	GLN
5	J	925	GLN
5	J	938	HIS
4	K	29	GLN
4	K	35	HIS

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Mol	Chain	Res	Type
4	K	43	ASN
4	K	65	HIS
4	K	67	GLN
4	K	68	GLN
4	K	121	HIS
4	K	149	HIS
4	K	180	HIS
4	K	289	GLN
4	K	316	GLN
4	K	397	GLN
4	K	401	HIS
4	K	493	GLN
4	K	529	GLN
4	K	533	GLN
4	K	540	GLN
4	K	547	GLN
4	K	561	HIS
4	K	563	HIS
4	K	567	ASN
4	K	571	GLN
4	K	600	ASN
4	K	622	GLN
4	K	644	GLN
6	L	328	GLN
6	L	441	GLN
6	L	593	HIS
6	L	1492	ASN
6	L	1525	GLN
6	L	1559	GLN
6	L	1568	HIS
6	L	1666	GLN
6	L	1678	ASN
6	L	1679	GLN
6	L	1702	GLN
6	L	1705	HIS
6	L	1777	HIS
7	O	9	GLN
7	O	139	HIS
7	O	167	GLN
7	O	198	ASN
7	O	302	ASN
7	O	334	HIS

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Mol	Chain	Res	Type
7	O	338	GLN
7	O	357	GLN
7	P	9	GLN
7	P	16	GLN
7	P	24	GLN
7	P	54	GLN
7	P	75	HIS
7	P	110	GLN
7	P	139	HIS
7	P	167	GLN
7	P	198	ASN
7	P	250	ASN
7	P	302	ASN
7	P	371	HIS
7	P	380	ASN
7	P	407	GLN
7	Q	9	GLN
7	Q	54	GLN
7	Q	103	ASN
7	Q	139	HIS
7	Q	167	GLN
7	Q	174	ASN
7	Q	198	ASN
7	Q	322	ASN
7	Q	338	GLN
7	Q	357	GLN
7	Q	380	ASN
7	R	9	GLN
7	R	54	GLN
7	R	139	HIS
7	R	174	ASN
7	R	322	ASN
7	R	338	GLN
7	R	380	ASN
7	S	9	GLN
7	S	54	GLN
7	S	198	ASN
7	S	207	ASN
7	S	314	ASN
7	S	322	ASN
7	T	9	GLN
7	T	54	GLN

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Mol	Chain	Res	Type
7	T	139	HIS
7	T	174	ASN
7	T	198	ASN
7	T	302	ASN
7	T	338	GLN
7	T	357	GLN
7	T	380	ASN
7	U	54	GLN
7	U	139	HIS
7	U	174	ASN
7	U	198	ASN
7	U	302	ASN
7	U	338	GLN
7	U	380	ASN
7	V	9	GLN
7	V	24	GLN
7	V	54	GLN
7	V	139	HIS
7	V	167	GLN
7	V	174	ASN
7	V	197	GLN
7	V	198	ASN
7	V	302	ASN
7	V	322	ASN
7	W	9	GLN
7	W	24	GLN
7	W	54	GLN
7	W	139	HIS
7	W	167	GLN
7	W	267	HIS
7	W	302	ASN
7	W	314	ASN
7	W	322	ASN
7	W	338	GLN
7	X	9	GLN
7	X	139	HIS
7	X	167	GLN
7	X	174	ASN
7	X	198	ASN
7	X	302	ASN
7	X	314	ASN
7	X	338	GLN

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Mol	Chain	Res	Type
7	Y	9	GLN
7	Y	54	GLN
7	Y	139	HIS
7	Y	167	GLN
7	Y	174	ASN
7	Y	198	ASN
7	Y	221	GLN
7	Y	302	ASN
7	Y	357	GLN
7	Y	407	GLN
7	Z	9	GLN
7	Z	198	ASN
7	Z	227	GLN
7	Z	302	ASN
7	Z	338	GLN
7	Z	380	ASN
8	b	36	ASN
8	i	56	ASN
8	k	19	ASN
8	m	17	ASN
8	m	19	ASN
8	m	36	ASN
3	a	31	GLN
3	a	65	GLN
3	a	84	GLN
3	f	30	GLN
3	f	31	GLN
3	f	42	ASN
3	h	30	GLN
3	h	31	GLN
3	h	42	ASN
3	h	65	GLN
3	j	14	GLN
3	j	30	GLN
3	j	31	GLN
3	j	42	ASN
3	j	65	GLN
8	d	17	ASN
8	d	19	ASN
8	d	53	GLN
6	c	48	ASN
6	c	138	HIS

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Mol	Chain	Res	Type
6	c	176	GLN
5	1	93	ASN
7	1	54	GLN
7	1	139	HIS
7	1	167	GLN
7	1	174	ASN
7	1	198	ASN
7	1	222	ASN
7	1	338	GLN
7	1	347	ASN
7	2	9	GLN
7	2	54	GLN
7	2	79	ASN
7	2	174	ASN
7	2	197	GLN
7	2	198	ASN
7	2	302	ASN
7	2	407	GLN
2	M	213	GLN
2	M	322	GLN
2	M	373	GLN
2	M	684	GLN
2	M	688	ASN
2	M	718	ASN
3	N	270	ASN
3	N	302	ASN
3	N	347	GLN
3	N	389	GLN
3	N	401	HIS
3	N	417	HIS
3	N	444	HIS
3	N	479	GLN
3	N	491	ASN
3	N	494	HIS
3	N	570	GLN
3	N	576	HIS
3	N	773	ASN
3	N	787	ASN
3	N	860	GLN
3	N	885	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

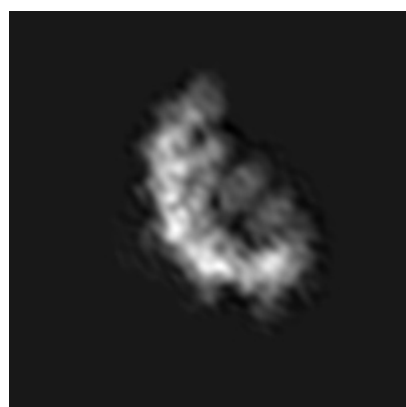
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14017. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

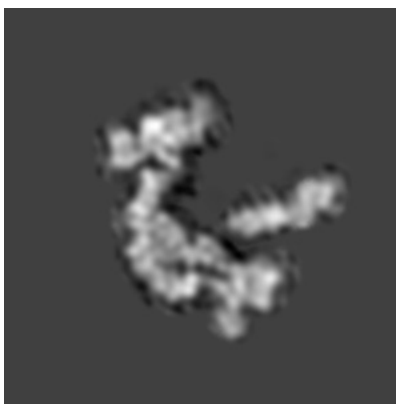
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100



Z Index: 100

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 63



Y Index: 81

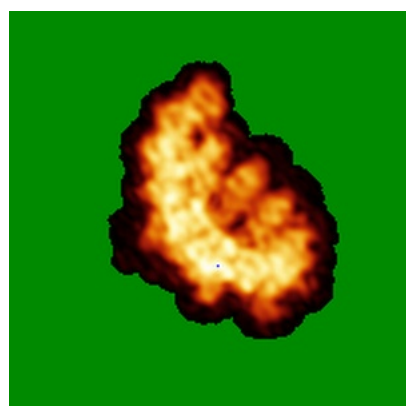


Z Index: 71

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

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

6.4.1 Primary map



X



Y

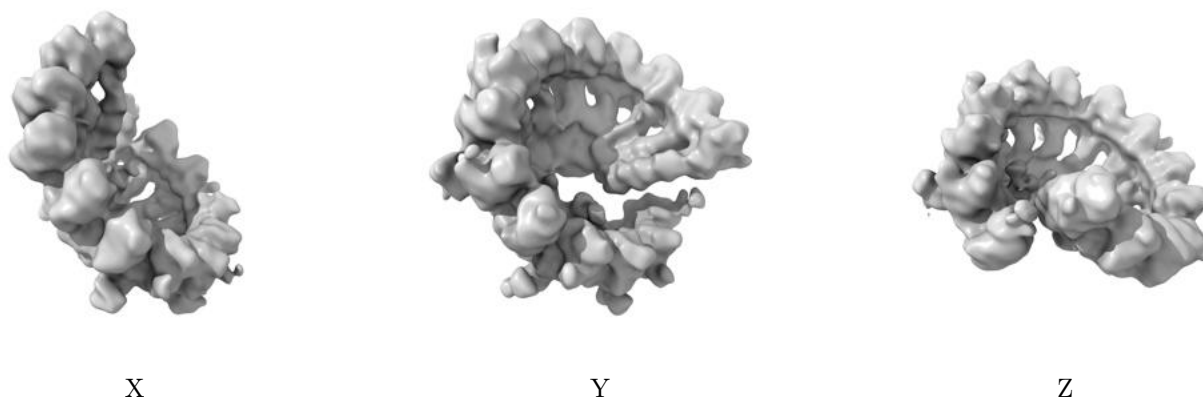


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0319. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

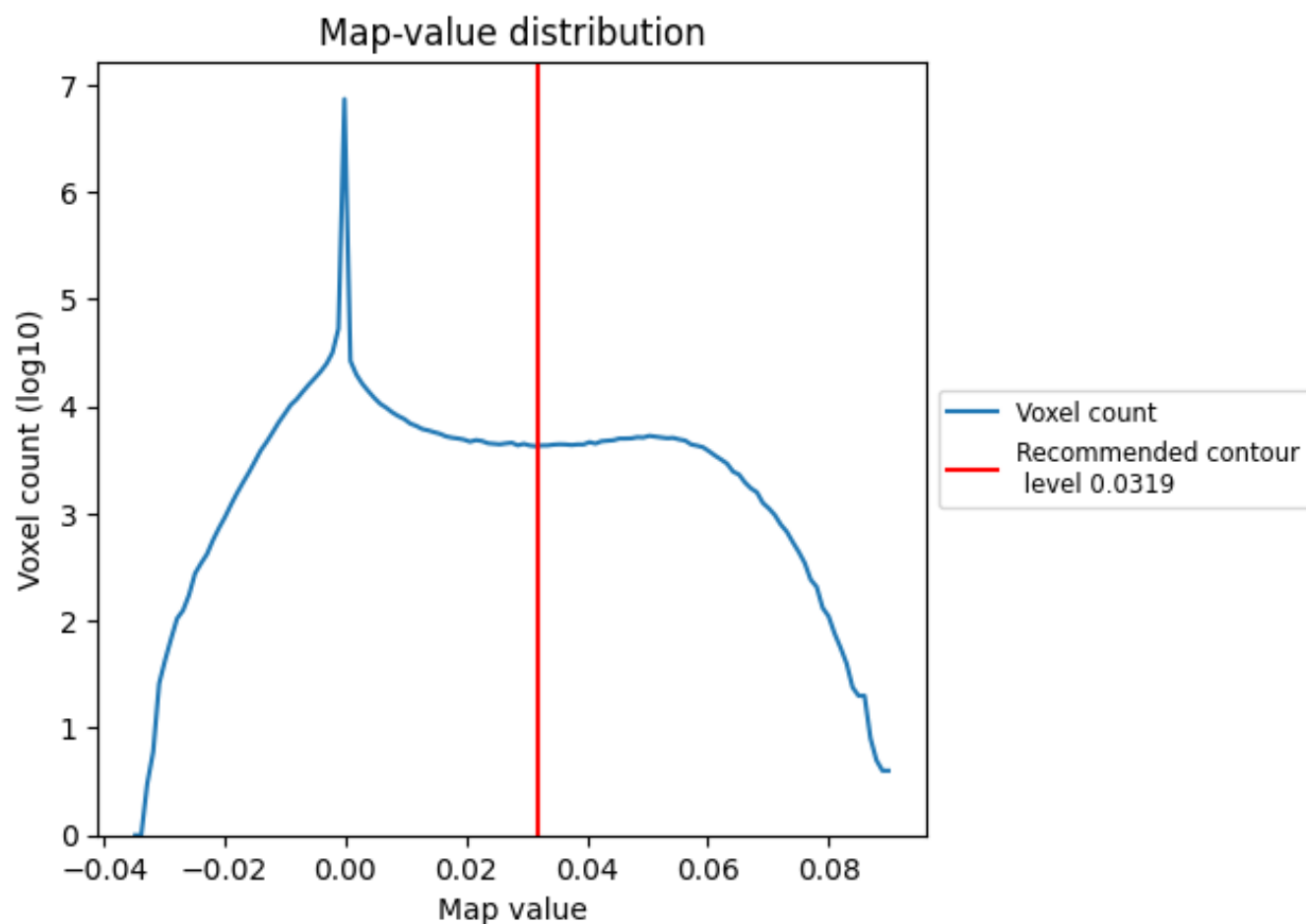
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

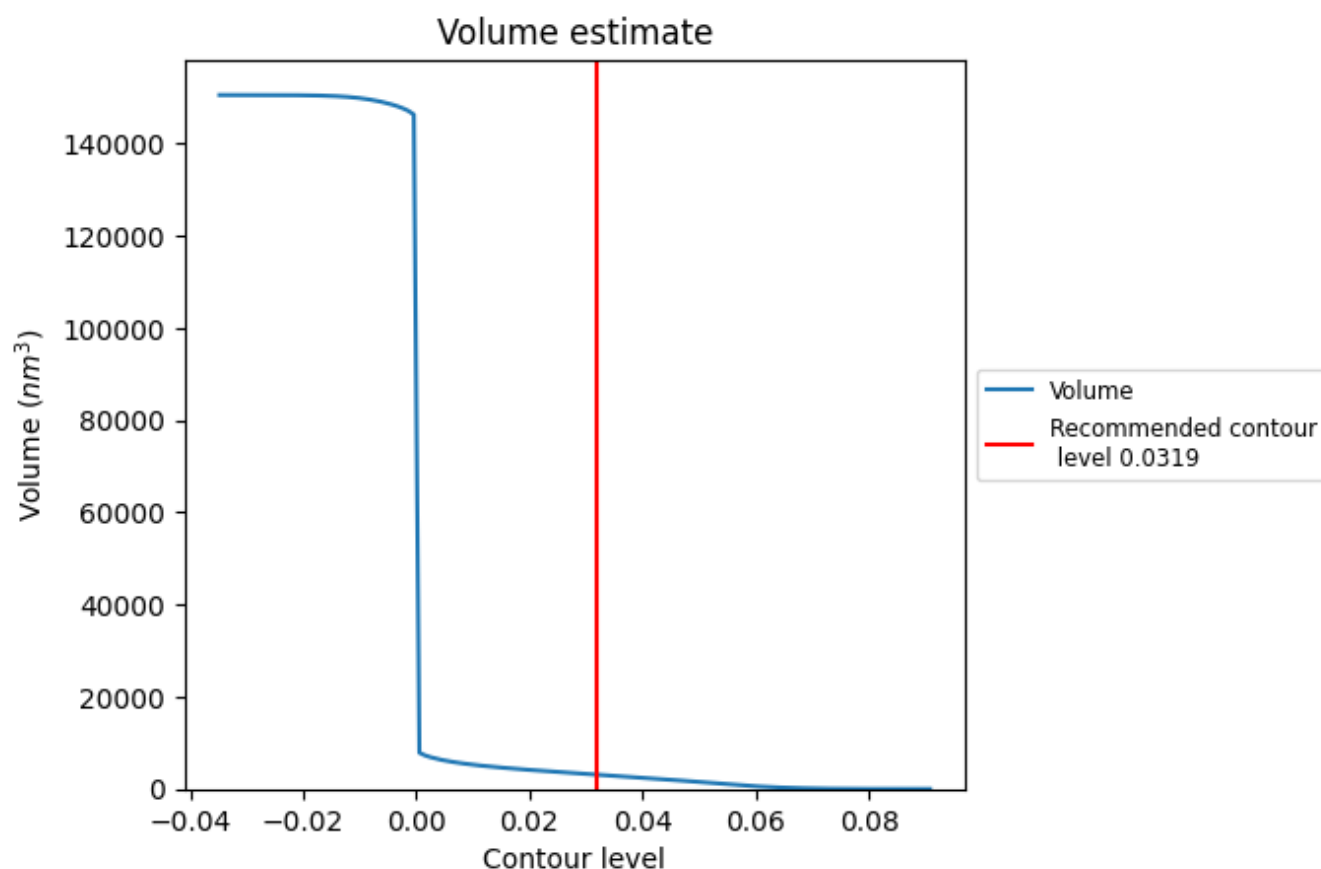
This section contains the results of statistical analysis of the map.

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.

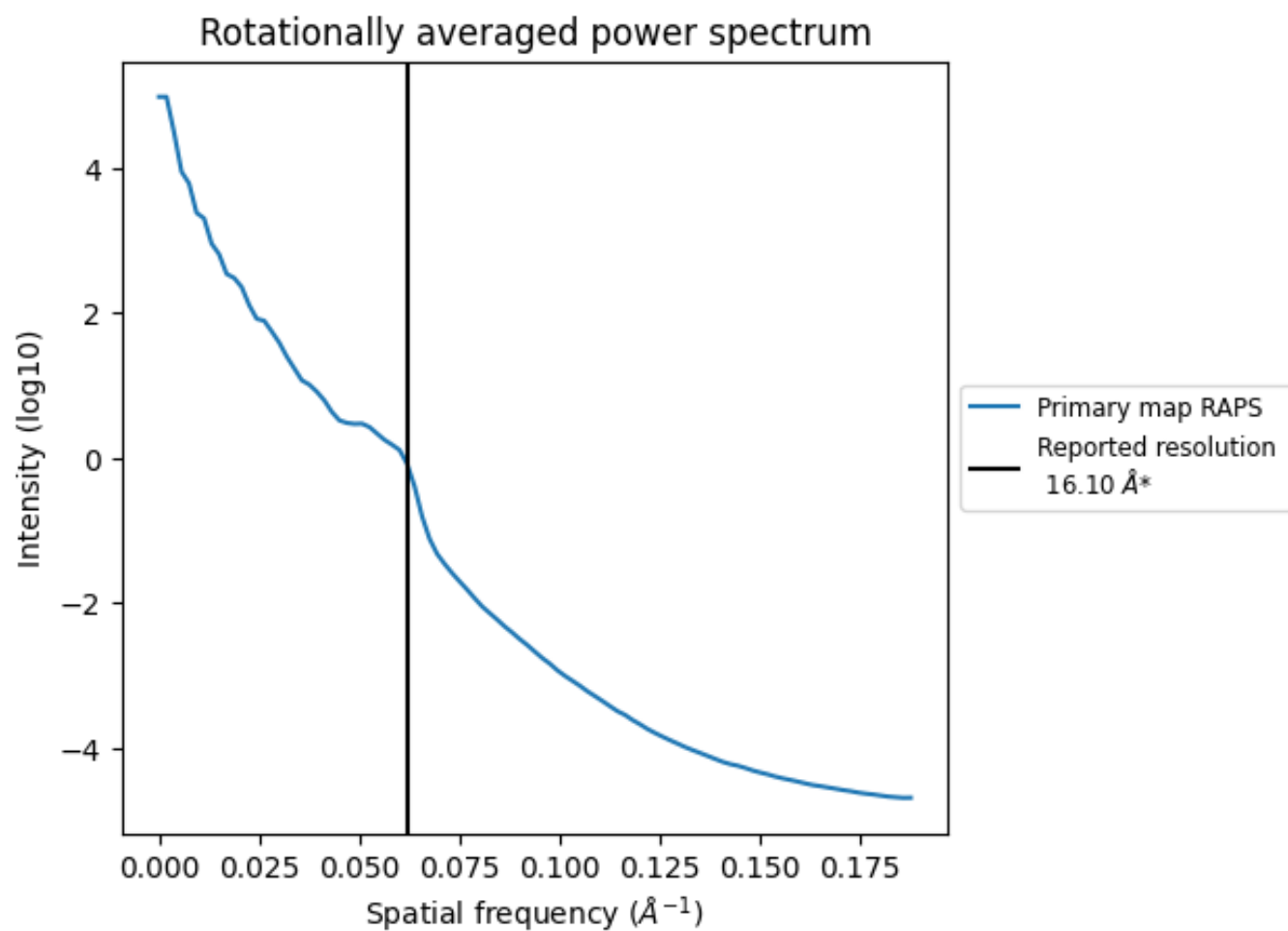
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3109 nm³; this corresponds to an approximate mass of 2809 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.062 Å⁻¹

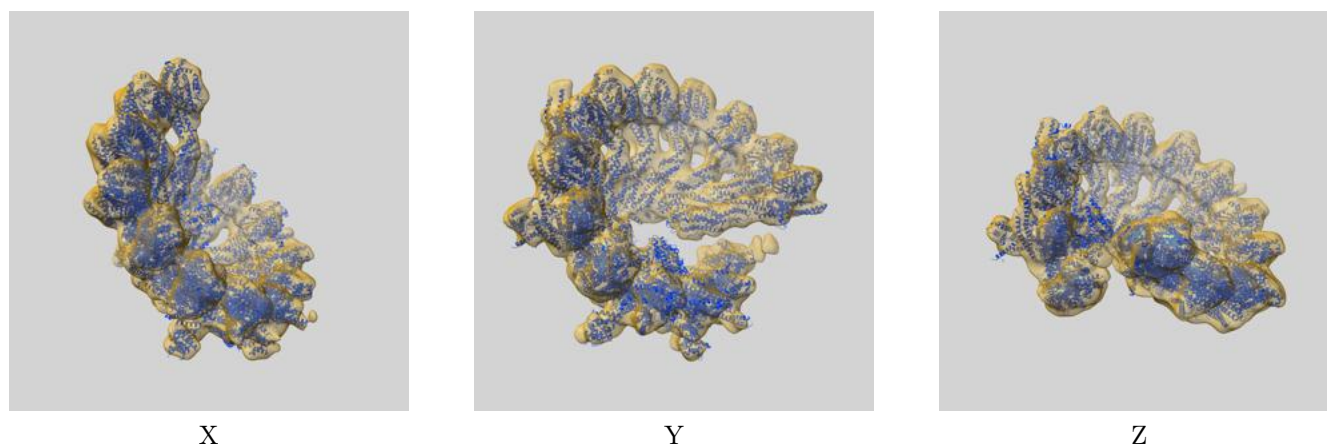
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

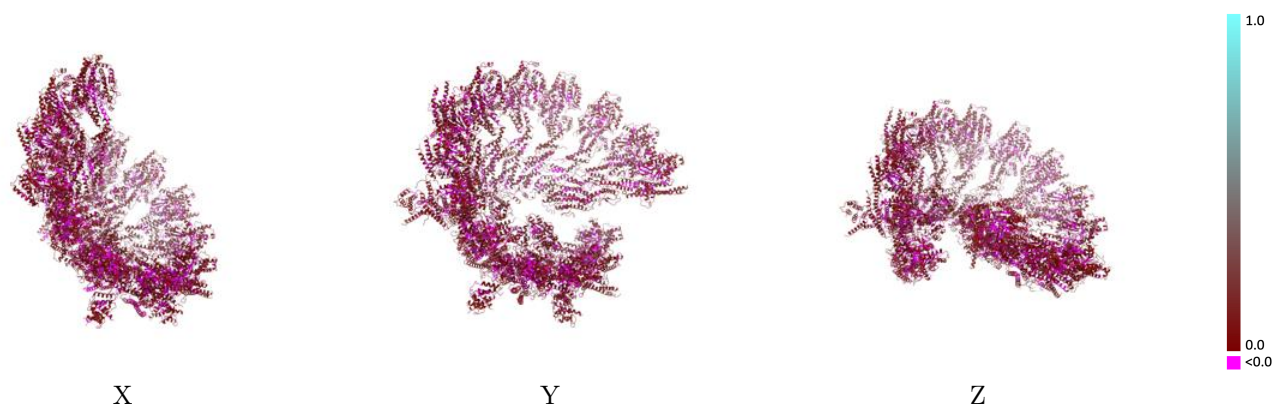
This section contains information regarding the fit between EMDB map EMD-14017 and PDB model 7QJC. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



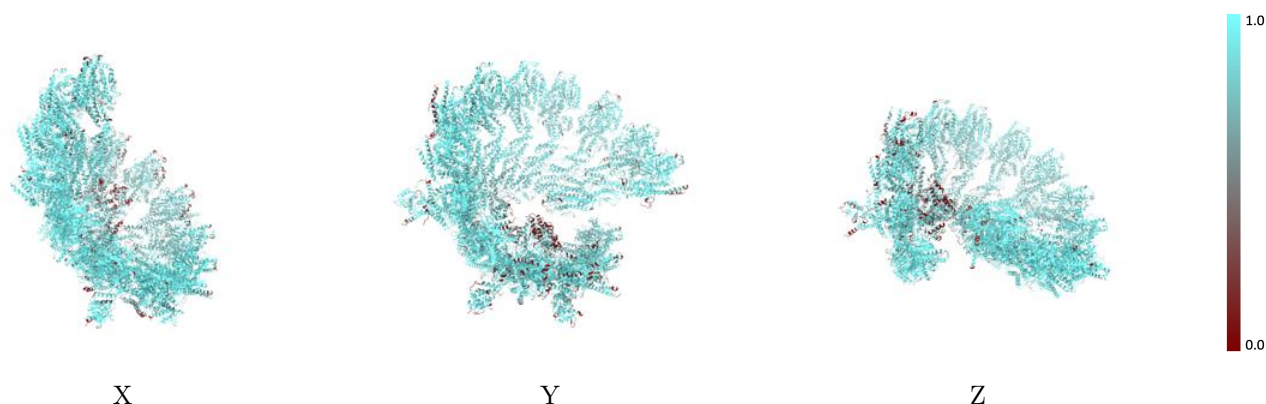
The images above show the 3D surface view of the map at the recommended contour level 0.0319 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



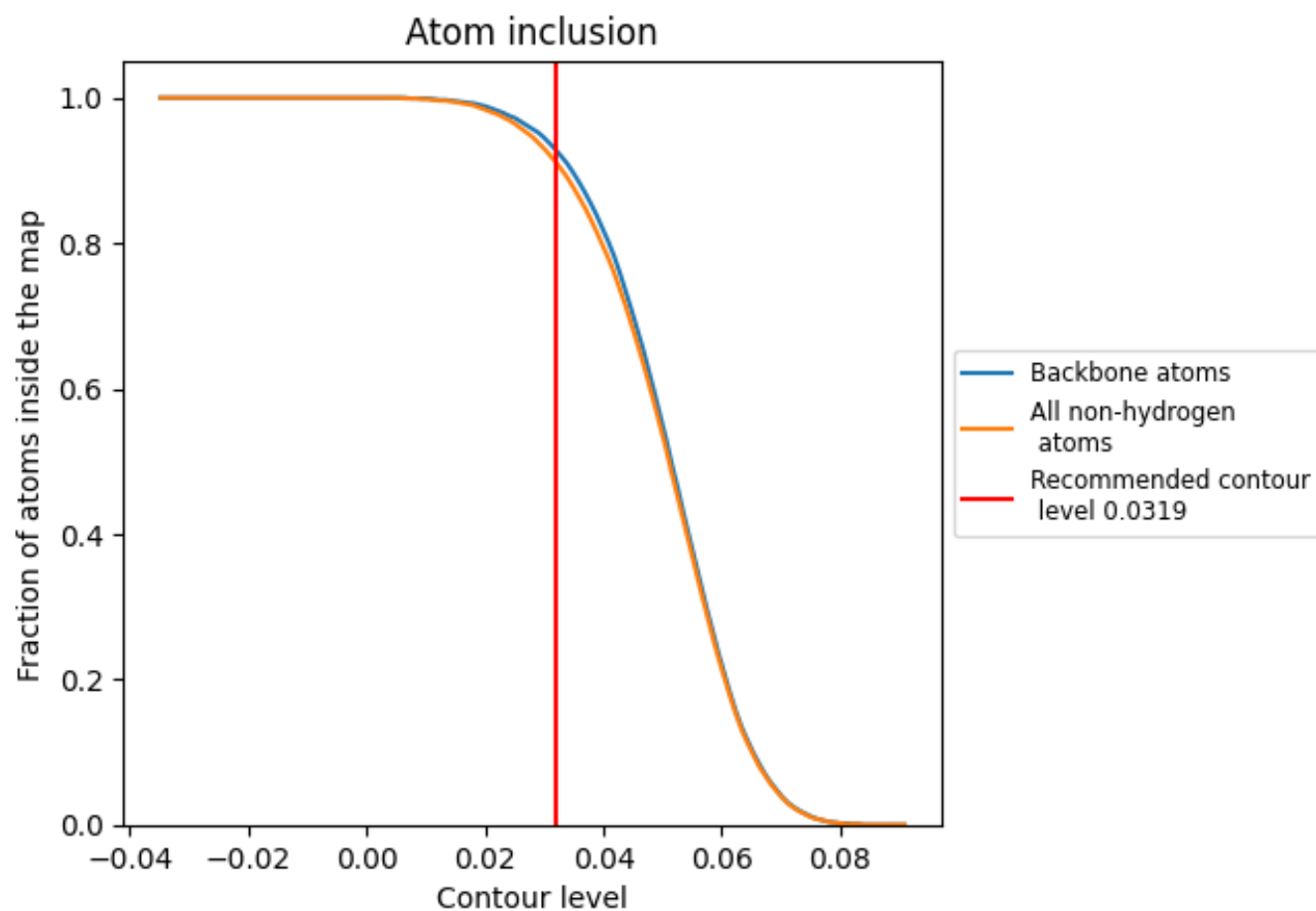
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0319).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.0319) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9120	 0.0600
1	 0.9560	 0.0550
2	 0.9120	 0.0460
A	 0.9530	 0.0720
B	 0.9060	 0.0580
C	 0.8960	 0.0590
D	 0.9160	 0.0600
E	 0.9370	 0.0600
F	 0.9370	 0.0650
G	 0.9230	 0.0630
H	 0.9160	 0.0650
I	 0.9330	 0.0620
J	 0.9640	 0.0680
K	 0.9490	 0.0730
L	 0.9440	 0.0630
M	 0.9160	 0.0630
N	 0.8850	 0.0630
O	 0.9230	 0.0440
P	 0.8770	 0.0430
Q	 0.8460	 0.0540
R	 0.8550	 0.0500
S	 0.9260	 0.0570
T	 0.9640	 0.0520
U	 0.9760	 0.0510
V	 0.9770	 0.0550
W	 0.9650	 0.0510
X	 0.9780	 0.0590
Y	 0.9660	 0.0550
Z	 0.9400	 0.0550
a	 0.8090	 0.0610
b	 0.7480	 0.0860
c	 0.6540	 0.0660
d	 0.6260	 0.0820
e	 0.4940	 0.0720
f	 0.8260	 0.0770



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Chain	Atom inclusion	Q-score
g	 0.6680	 0.0710
h	 0.7740	 0.0630
i	 0.7750	 0.0790
j	 0.8360	 0.0650
k	 0.8760	 0.0850
l	 0.8380	 0.0790
m	 0.8510	 0.0660