



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 02:35 AM UTC

PDB ID : 7QJ3 / pdb_00007qj3
EMDB ID : EMD-14008
Title : Structure of recombinant human gamma-Tubulin Ring Complex 8-spoked assembly intermediate (spokes 7-14)
Authors : Zupa, E.; Pfeffer, S.
Deposited on : 2021-12-16
Resolution : 7.60 Å (reported)
Based on initial models : 6X0U, 6L81, 7AS4, 6V6S

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

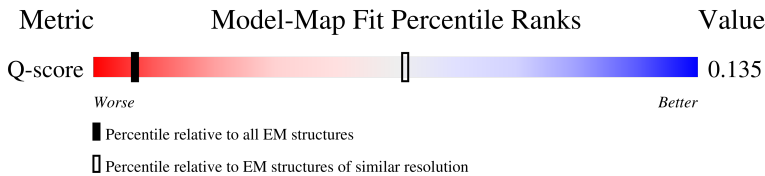
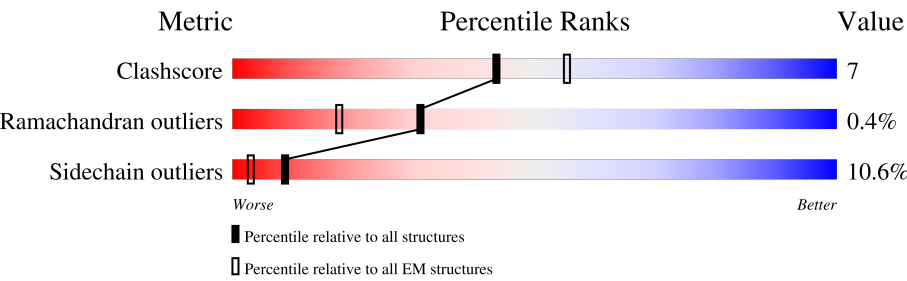
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 7.60 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.



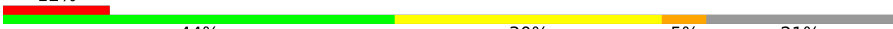
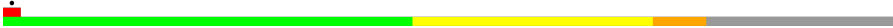
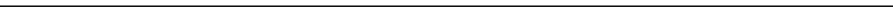
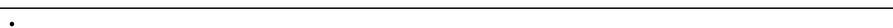
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	389 (7.10 - 8.10)

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

Mol	Chain	Length	Quality of chain
1	1	451	 15% 65% 25% 7%
1	2	451	 17% 65% 24% 7%
1	U	451	 67% 22% 7%
1	V	451	 66% 23% 7%

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Mol	Chain	Length	Quality of chain
1	W	451	
1	X	451	
1	Y	451	
1	Z	451	
2	b	82	
2	m	82	
2	o	82	
3	H	907	
3	N	907	
3	a	907	
3	n	907	
4	J	1024	
4	l	1024	
5	G	902	
5	M	902	
6	I	667	
6	K	667	
7	L	1819	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 69053 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	o	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
2	m	65	Total	C	N	O	S	0	0
			484	299	85	96	4		
2	b	65	Total	C	N	O	S	0	0
			484	299	85	96	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	n	99	Total	C	N	O	S	0	0
			803	509	148	144	2		
3	a	116	Total	C	N	O	S	0	0
			933	591	171	169	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		
3	N	594	Total	C	N	O	S	0	0
			4907	3130	864	888	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	108	Total	C	N	O	S	0	0
			875	556	151	167	1		
4	J	534	Total	C	N	O	S	0	0
			4429	2893	737	776	23		

- Molecule 5 is a protein called Gamma-tubulin complex component 2.

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

- Molecule 6 is a protein called Gamma-tubulin complex component 4.

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

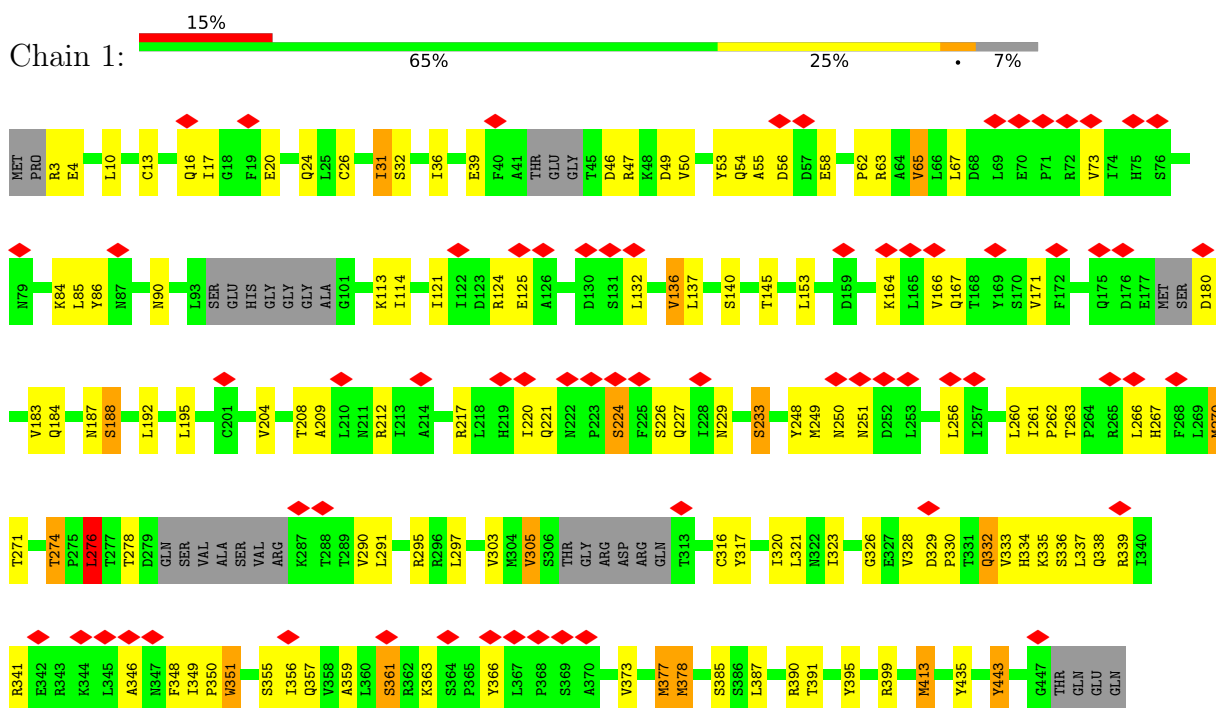
- Molecule 7 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	566	Total	C	N	O	S	0	0
			4587	3000	773	789	25		

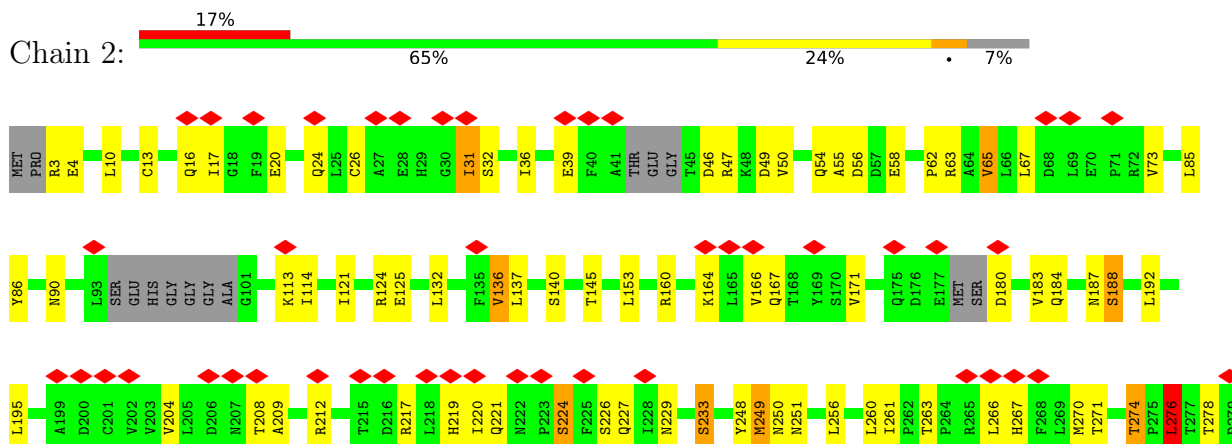
3 Residue-property plots

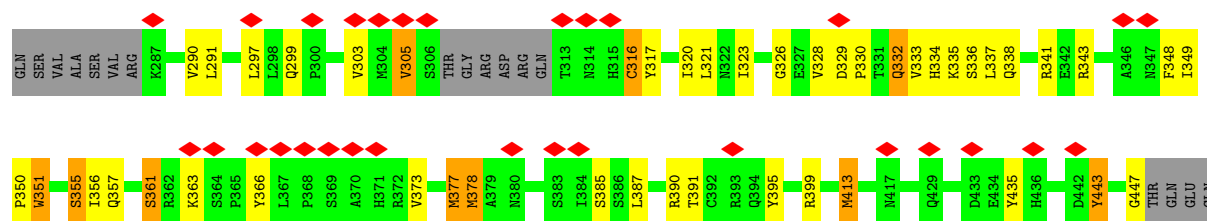
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Tubulin gamma-1 chain



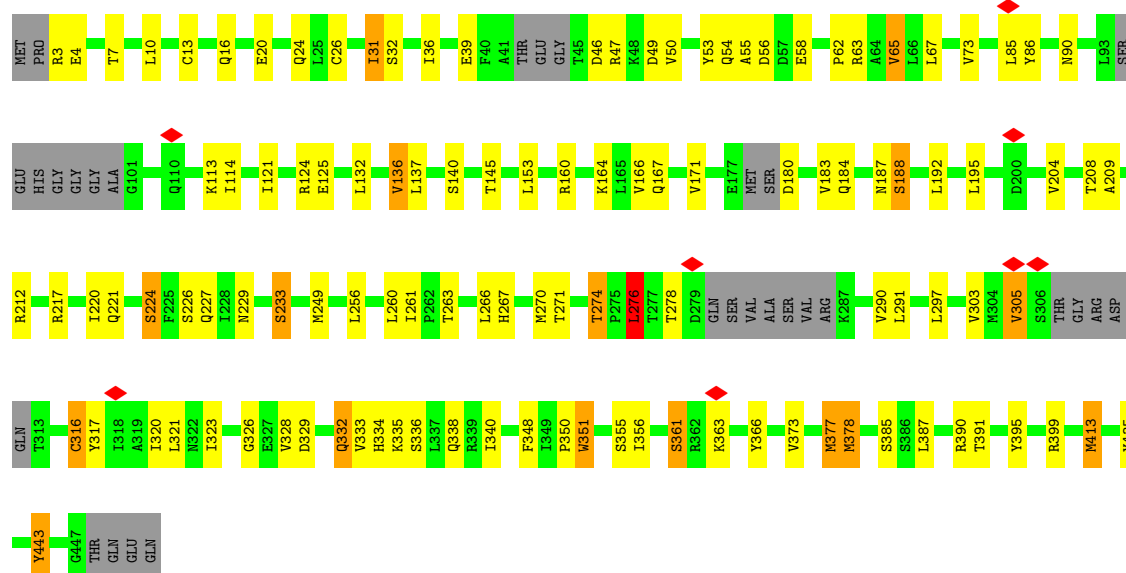
- Molecule 1: Tubulin gamma-1 chain





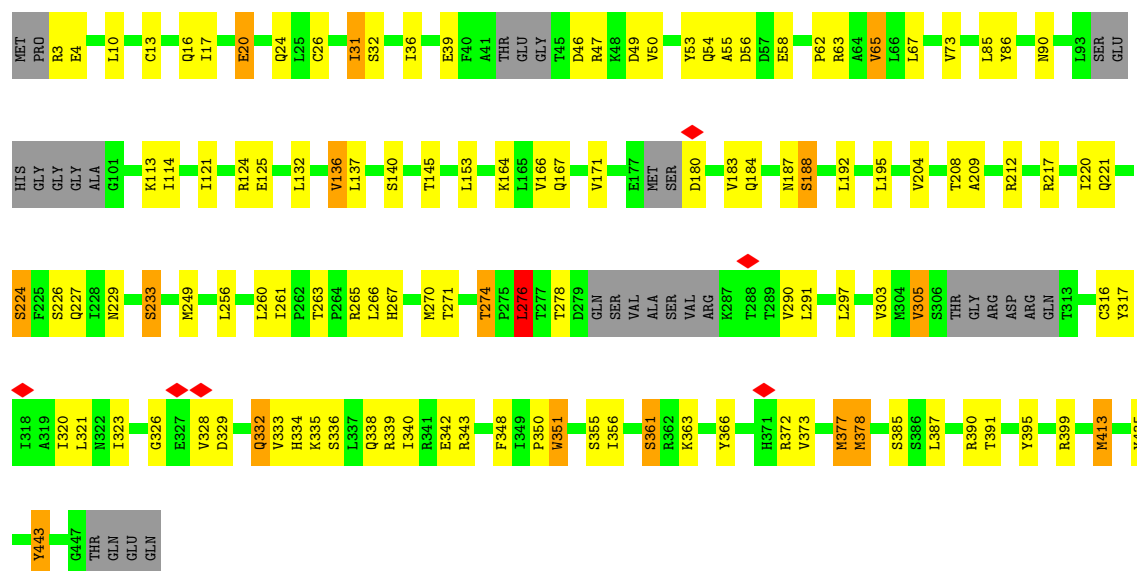
• Molecule 1: Tubulin gamma-1 chain

Chain U: 67% 22% 7%

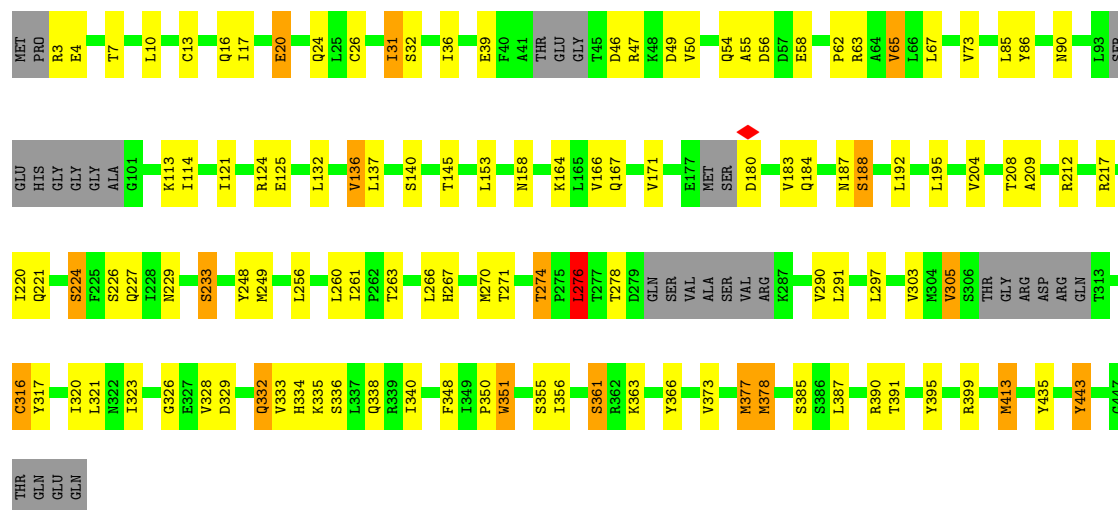


• Molecule 1: Tubulin gamma-1 chain

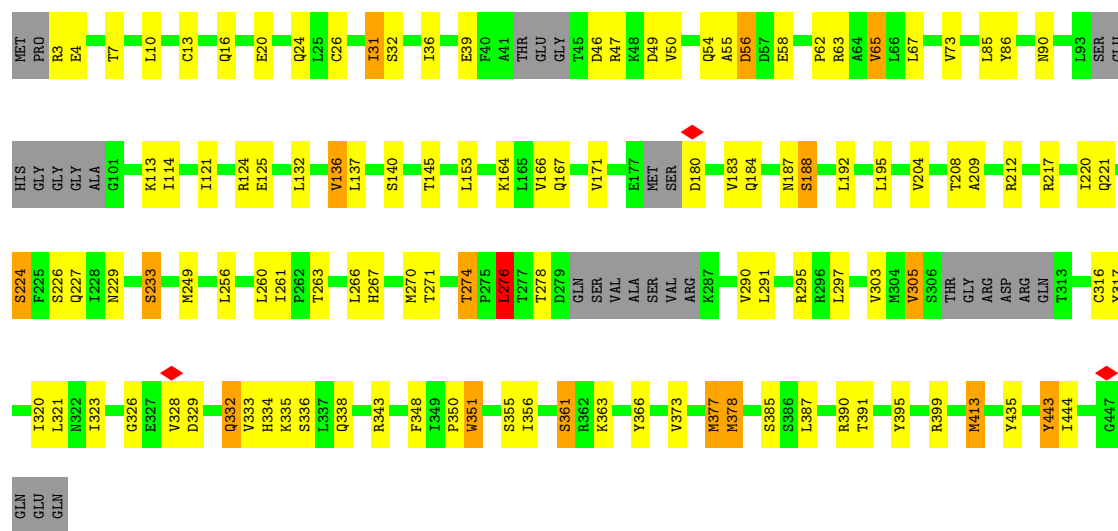
Chain V: 66% 23% 7%



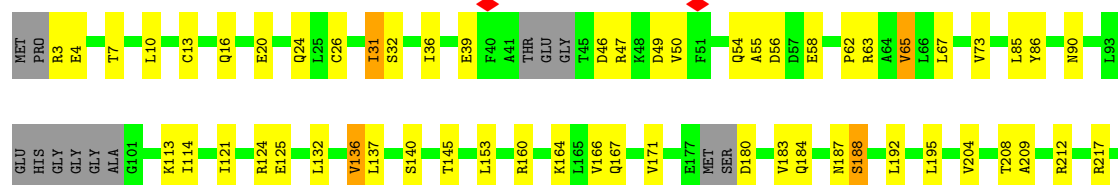
• Molecule 1: Tubulin gamma-1 chain

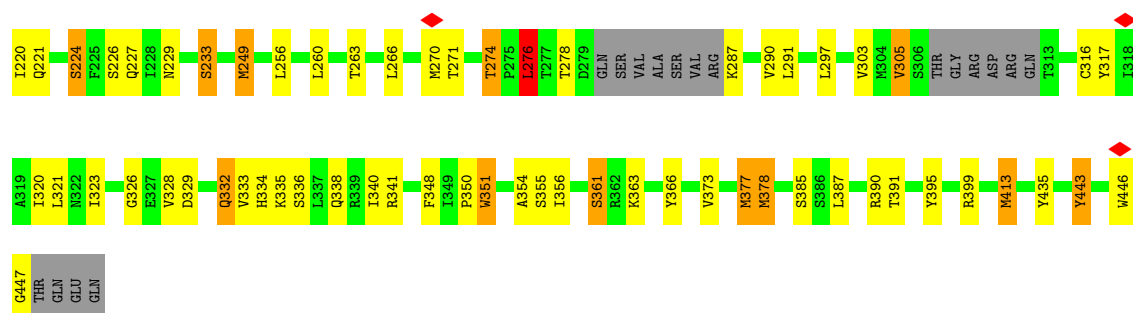
Chain W:  67% 22% 7%

• Molecule 1: Tubulin gamma-1 chain

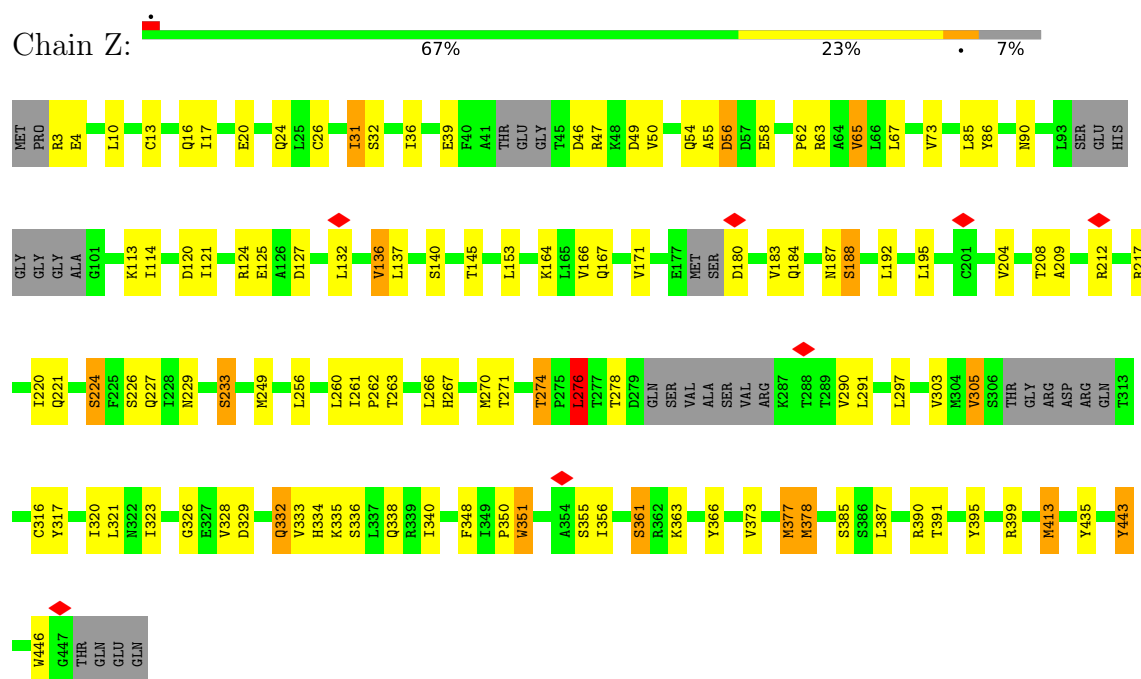
Chain X:  67% 22% 7%

• Molecule 1: Tubulin gamma-1 chain

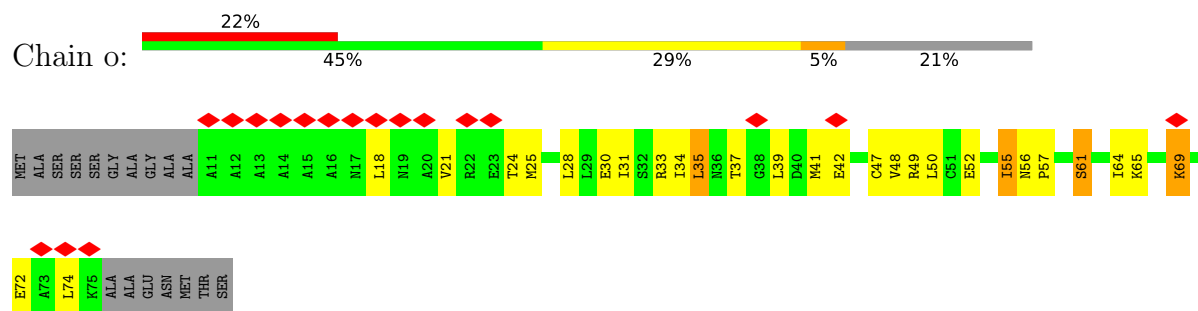
Chain Y:  67% 23% 7%



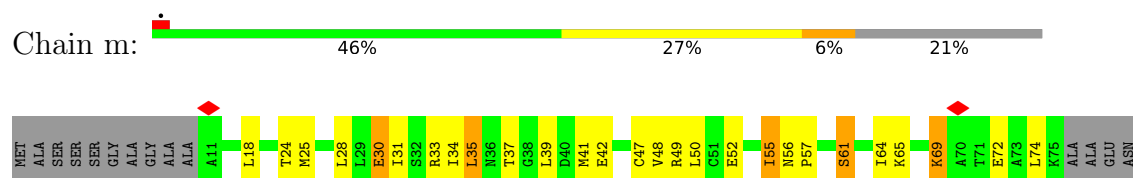
- Molecule 1: Tubulin gamma-1 chain

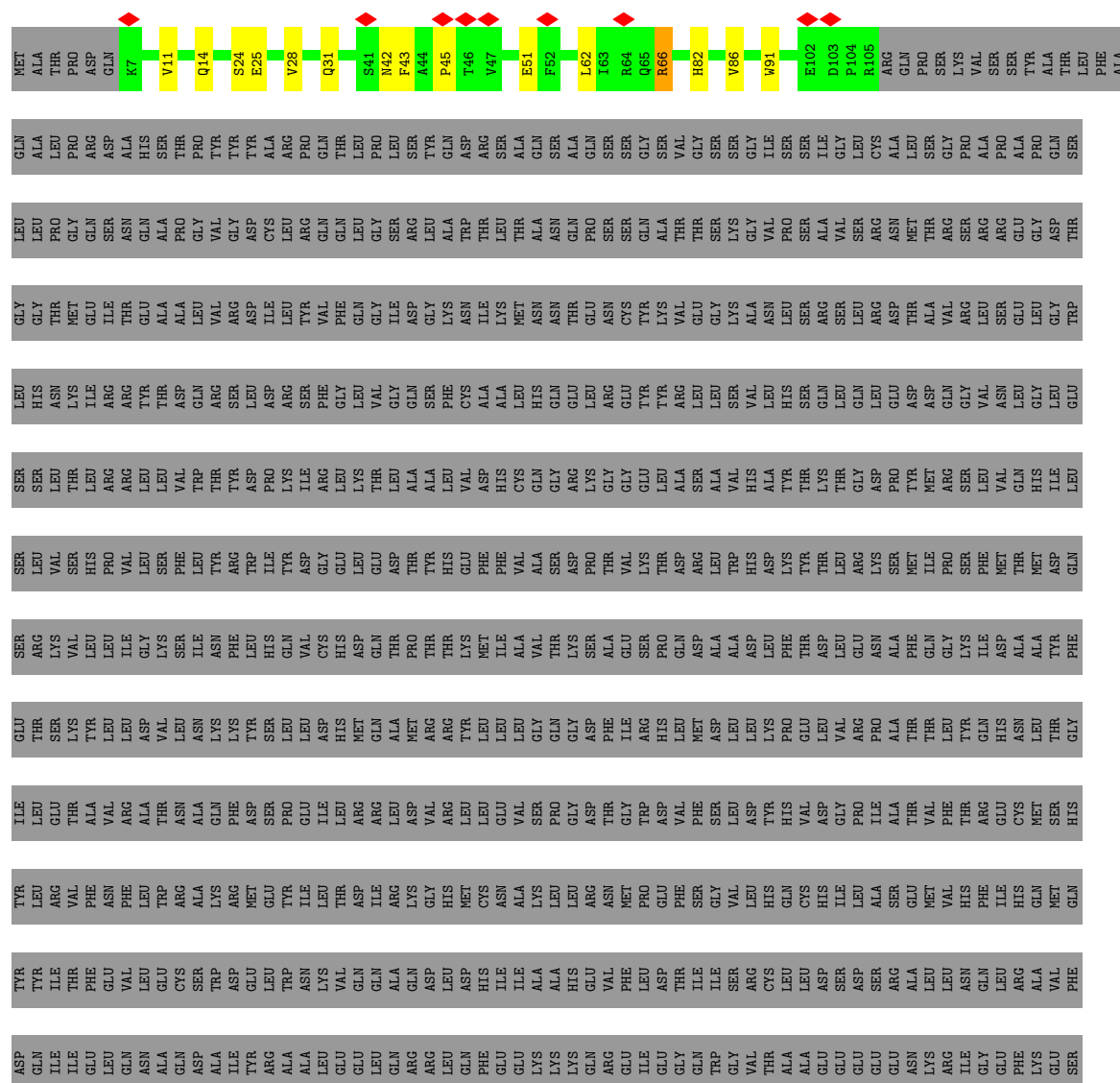


- Molecule 2: Mitotic-spindle organizing protein 1

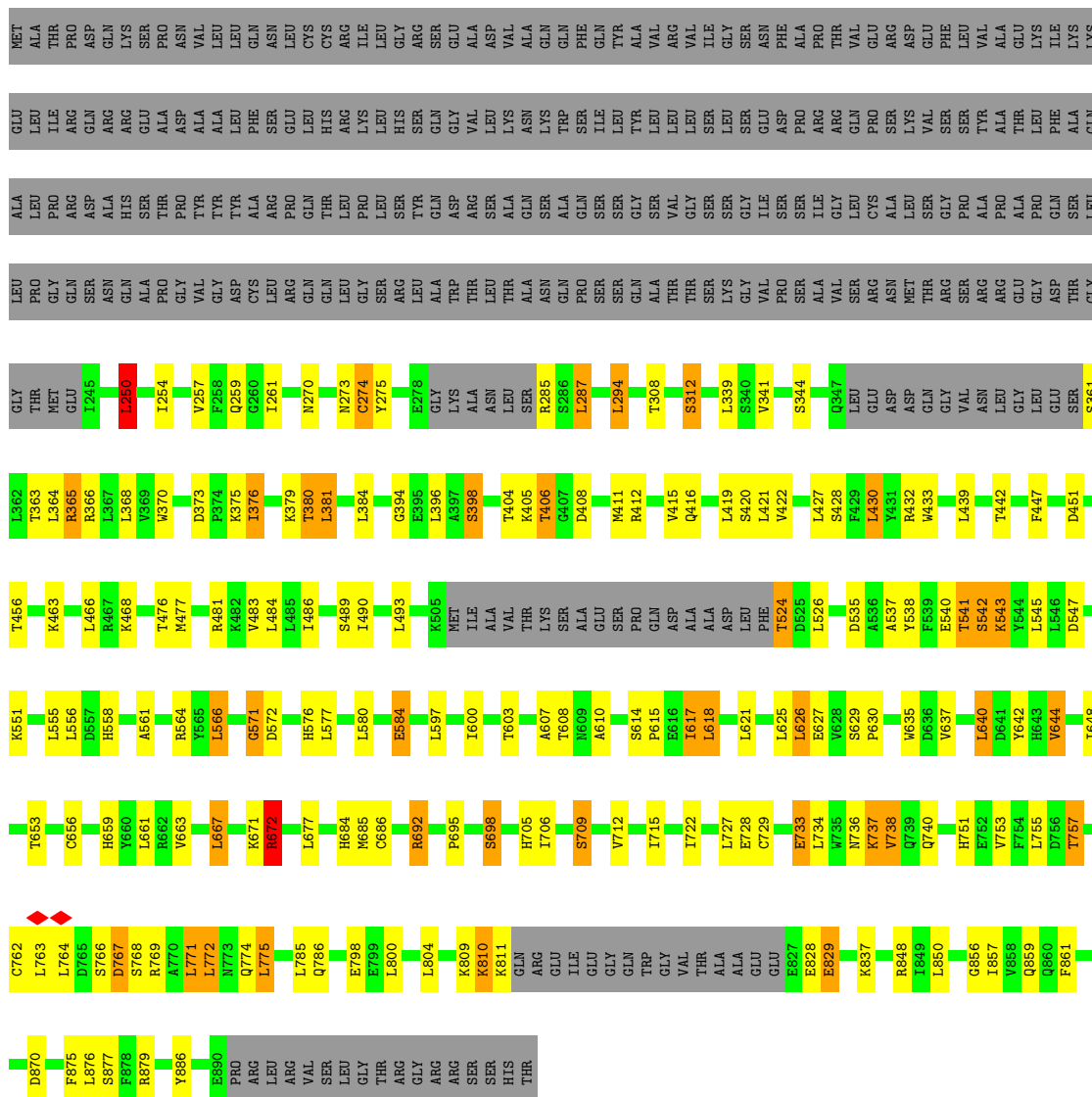


- Molecule 2: Mitotic-spindle organizing protein 1

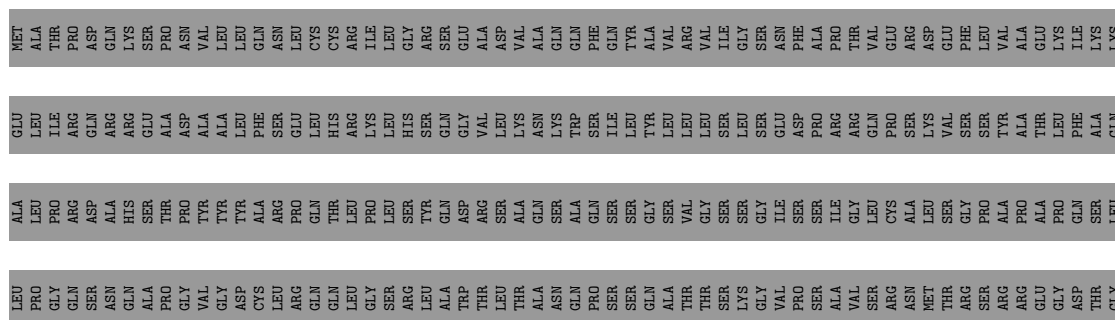


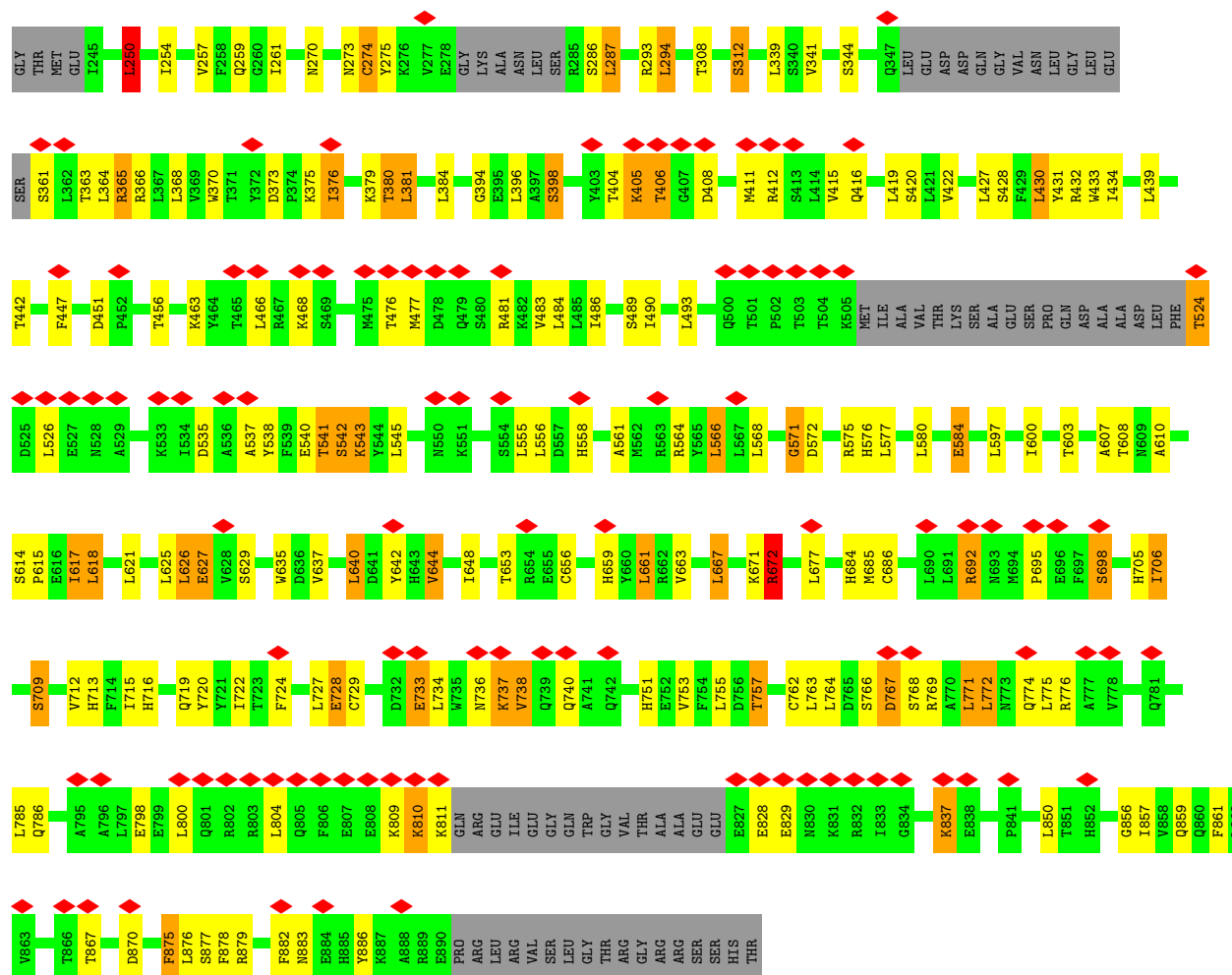


Response	Percentage
Yes, the U.S. is a democracy	45%
No, the U.S. is not a democracy	16%
Don't know	1%
Refused to answer	35%



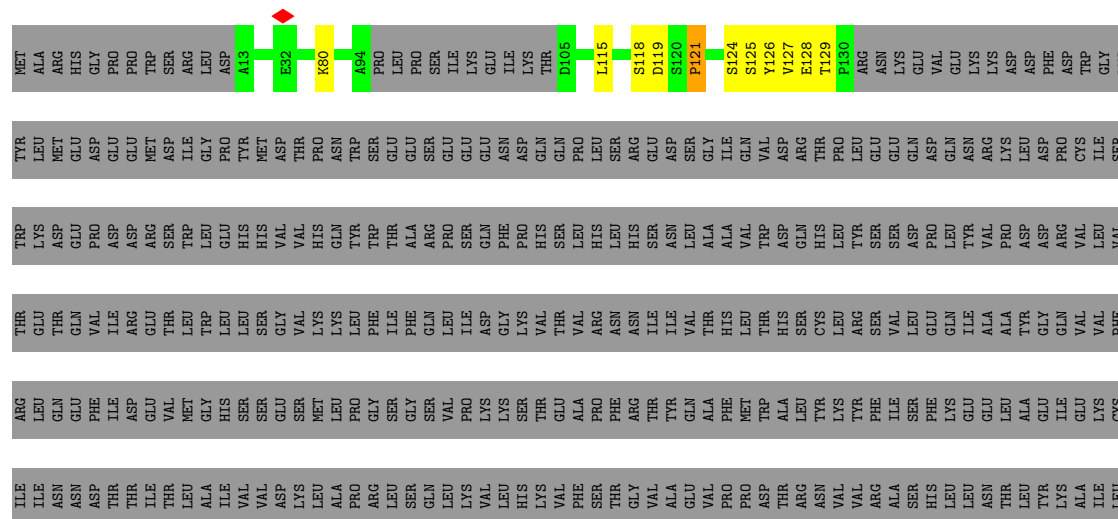
Chain N:

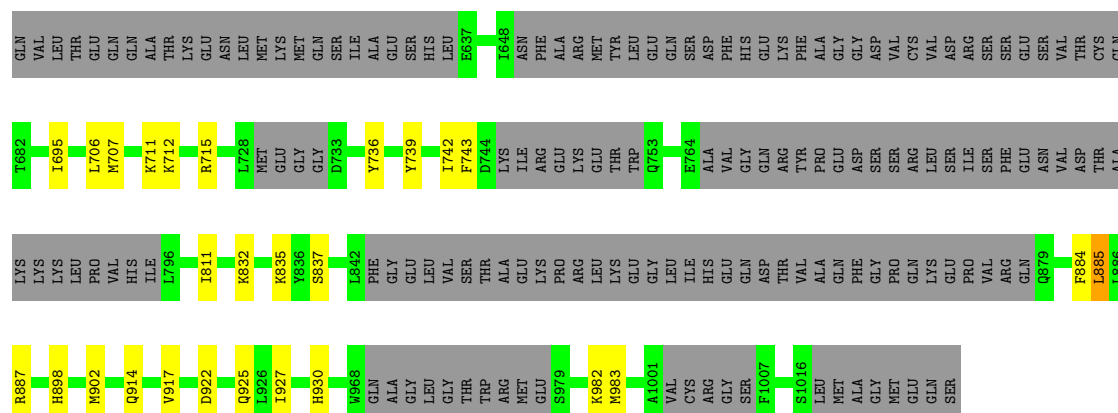




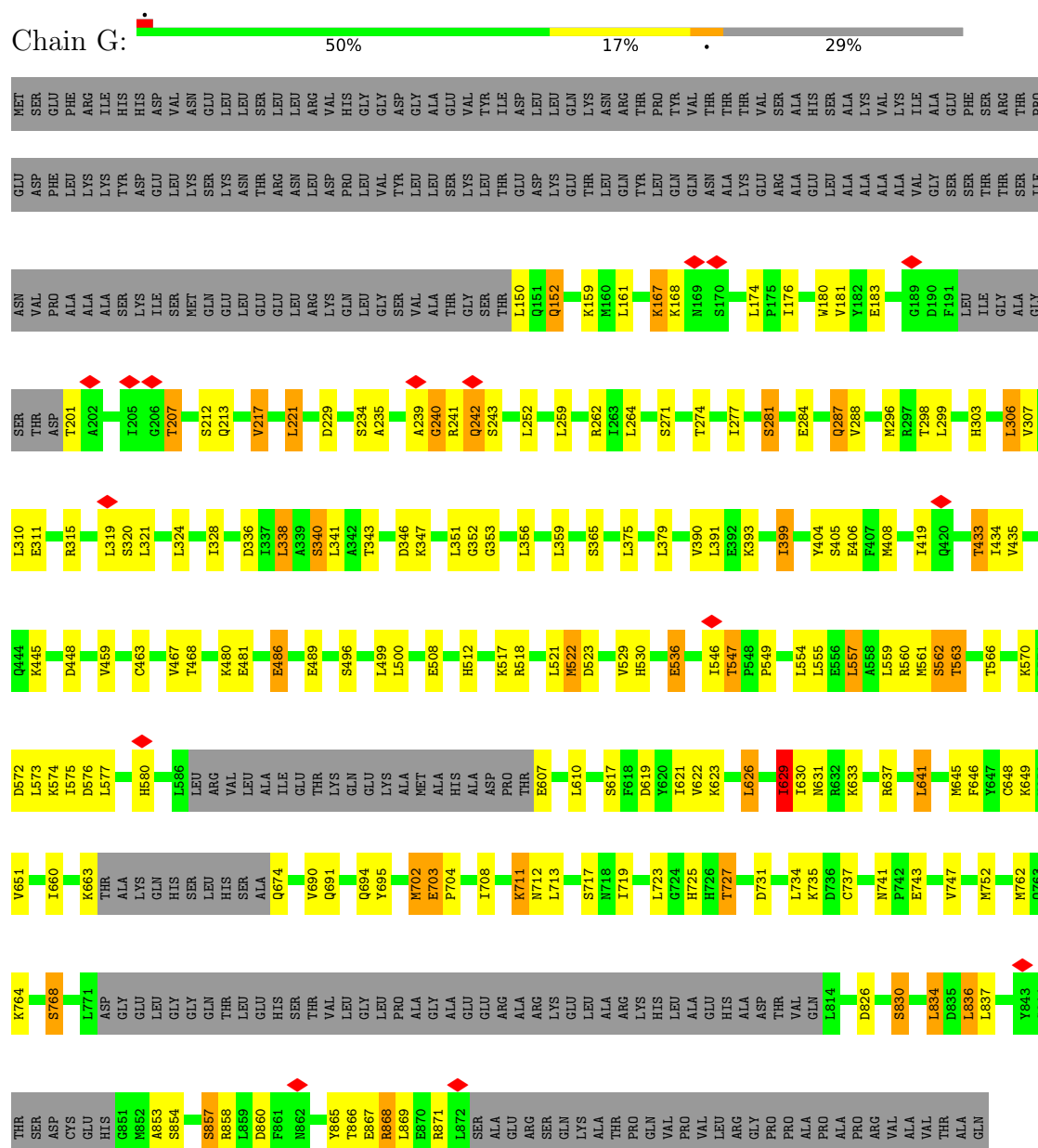
• Molecule 4: Gamma-tubulin complex component 5

Chain 1:  9%  89%





Molecule 5: Gamma-tubulin complex component 2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17337	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	0.281	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0379	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	1	0.29	0/3441	0.73	7/4661 (0.2%)
1	2	0.29	0/3441	0.73	7/4661 (0.2%)
1	U	0.29	0/3441	0.73	7/4661 (0.2%)
1	V	0.29	0/3441	0.73	7/4661 (0.2%)
1	W	0.29	0/3441	0.73	7/4661 (0.2%)
1	X	0.29	0/3441	0.73	7/4661 (0.2%)
1	Y	0.29	0/3441	0.73	7/4661 (0.2%)
1	Z	0.29	0/3441	0.73	7/4661 (0.2%)
2	b	0.31	0/484	0.82	1/653 (0.2%)
2	m	0.31	0/484	0.82	1/653 (0.2%)
2	o	0.31	0/484	0.82	1/653 (0.2%)
3	H	0.35	0/5009	0.86	7/6761 (0.1%)
3	N	0.35	0/5009	0.86	7/6761 (0.1%)
3	a	0.31	0/948	0.72	0/1277
3	n	0.33	0/815	0.69	1/1096 (0.1%)
4	J	0.31	0/4525	0.77	6/6119 (0.1%)
4	l	0.28	0/894	0.74	1/1209 (0.1%)
5	G	0.35	0/5295	0.86	13/7147 (0.2%)
5	M	0.35	0/5295	0.86	13/7147 (0.2%)
6	I	0.31	0/4322	0.71	4/5853 (0.1%)
6	K	0.34	0/4683	0.74	5/6338 (0.1%)
7	L	0.31	0/4697	0.72	7/6348 (0.1%)
All	All	0.32	0/70472	0.77	123/95303 (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	b	0	1
2	m	0	1
2	o	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	2
3	N	0	2
4	J	0	3
5	G	0	3
5	M	0	3
6	I	0	1
7	L	0	1
All	All	0	18

There are no bond length outliers.

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	l	121	PRO	CA-N-CD	-8.48	100.13	112.00
1	X	377	MET	CB-CG-SD	8.32	137.66	112.70
1	1	377	MET	CB-CG-SD	8.31	137.65	112.70
1	2	377	MET	CB-CG-SD	8.31	137.64	112.70
1	Z	377	MET	CB-CG-SD	8.31	137.64	112.70
1	V	377	MET	CB-CG-SD	8.31	137.63	112.70
1	U	377	MET	CB-CG-SD	8.31	137.62	112.70
1	W	377	MET	CB-CG-SD	8.30	137.62	112.70
1	Y	377	MET	CB-CG-SD	8.30	137.61	112.70
6	K	409	ASN	CA-C-N	8.08	136.97	121.54
6	K	409	ASN	C-N-CA	8.08	136.97	121.54
5	M	536	GLU	CA-CB-CG	7.98	130.06	114.10
5	G	536	GLU	CA-CB-CG	7.96	130.03	114.10
5	G	287	GLN	CA-CB-CG	7.25	128.60	114.10
5	M	287	GLN	CA-CB-CG	7.24	128.59	114.10
3	H	672	ARG	CG-CD-NE	6.87	127.12	112.00
3	N	672	ARG	CG-CD-NE	6.85	127.06	112.00
1	W	377	MET	CA-CB-CG	6.79	127.67	114.10
1	U	377	MET	CA-CB-CG	6.78	127.66	114.10
1	2	377	MET	CA-CB-CG	6.77	127.65	114.10
1	Z	377	MET	CA-CB-CG	6.77	127.65	114.10
1	V	377	MET	CA-CB-CG	6.76	127.63	114.10
1	1	377	MET	CA-CB-CG	6.76	127.63	114.10
1	X	377	MET	CA-CB-CG	6.76	127.62	114.10
1	Y	377	MET	CA-CB-CG	6.76	127.62	114.10
6	I	404	LEU	CA-C-N	6.72	134.37	121.54
6	I	404	LEU	C-N-CA	6.72	134.37	121.54
7	L	1480	ILE	N-CA-C	-6.70	106.26	112.96
5	M	152	GLN	CA-CB-CG	6.58	127.25	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	152	GLN	CA-CB-CG	6.56	127.22	114.10
1	V	378	MET	CB-CG-SD	6.48	132.15	112.70
5	M	629	ILE	N-CA-C	-6.48	105.51	111.67
1	Y	378	MET	CB-CG-SD	6.48	132.15	112.70
1	Z	378	MET	CB-CG-SD	6.48	132.15	112.70
1	U	378	MET	CB-CG-SD	6.48	132.14	112.70
1	2	378	MET	CB-CG-SD	6.48	132.14	112.70
1	W	378	MET	CB-CG-SD	6.48	132.14	112.70
1	X	378	MET	CB-CG-SD	6.47	132.12	112.70
1	1	378	MET	CB-CG-SD	6.47	132.10	112.70
5	G	629	ILE	N-CA-C	-6.44	105.55	111.67
5	M	641	LEU	CA-CB-CG	6.35	138.53	116.30
5	G	641	LEU	CA-CB-CG	6.35	138.52	116.30
4	J	237	HIS	CA-C-N	6.30	133.58	121.54
4	J	237	HIS	C-N-CA	6.30	133.58	121.54
3	H	667	LEU	CA-CB-CG	6.13	137.77	116.30
3	N	667	LEU	CA-CB-CG	6.13	137.77	116.30
3	N	886	TYR	CA-CB-CG	6.11	124.89	113.90
3	H	886	TYR	CA-CB-CG	6.10	124.87	113.90
3	N	584	GLU	CA-CB-CG	6.01	126.12	114.10
3	H	584	GLU	CA-CB-CG	5.98	126.06	114.10
4	J	305	LEU	CA-C-N	5.93	131.86	122.61
4	J	305	LEU	C-N-CA	5.93	131.86	122.61
1	2	276	LEU	CB-CA-C	-5.88	100.92	110.79
1	X	276	LEU	CB-CA-C	-5.88	100.92	110.79
1	Z	276	LEU	CB-CA-C	-5.87	100.92	110.79
1	1	276	LEU	CB-CA-C	-5.86	100.94	110.79
1	Y	276	LEU	CB-CA-C	-5.86	100.94	110.79
1	U	276	LEU	CB-CA-C	-5.85	100.96	110.79
1	W	276	LEU	CB-CA-C	-5.85	100.96	110.79
1	V	276	LEU	CB-CA-C	-5.85	100.97	110.79
5	G	834	LEU	CA-CB-CG	5.82	136.66	116.30
5	M	834	LEU	CA-CB-CG	5.80	136.61	116.30
7	L	1590	VAL	N-CA-C	-5.80	107.61	113.47
3	n	66	ARG	CB-CG-CD	5.71	124.42	111.30
7	L	307	ARG	CA-C-N	5.68	132.40	121.54
7	L	307	ARG	C-N-CA	5.68	132.40	121.54
3	H	677	LEU	CB-CG-CD2	-5.61	93.88	110.70
6	I	378	HIS	N-CA-C	-5.60	106.13	114.64
3	N	677	LEU	CB-CG-CD2	-5.59	93.91	110.70
1	V	413	MET	CA-CB-CG	5.58	125.26	114.10
1	2	413	MET	CA-CB-CG	5.57	125.23	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	413	MET	CA-CB-CG	5.56	125.23	114.10
1	W	413	MET	CA-CB-CG	5.56	125.23	114.10
1	1	413	MET	CA-CB-CG	5.56	125.23	114.10
1	X	413	MET	CA-CB-CG	5.56	125.23	114.10
1	Y	413	MET	CA-CB-CG	5.56	125.23	114.10
1	Z	413	MET	CA-CB-CG	5.56	125.22	114.10
4	J	255	PRO	CA-C-N	5.56	131.71	121.70
4	J	255	PRO	C-N-CA	5.56	131.71	121.70
5	M	836	LEU	CA-CB-CG	5.47	135.43	116.30
5	G	836	LEU	CA-CB-CG	5.45	135.38	116.30
6	I	465	ILE	N-CA-C	-5.43	107.83	113.10
5	M	240	GLY	N-CA-C	-5.38	104.34	112.41
5	G	240	GLY	N-CA-C	-5.35	104.38	112.41
5	G	287	GLN	CB-CG-CD	5.35	121.70	112.60
5	M	287	GLN	CB-CG-CD	5.34	121.67	112.60
2	o	35	LEU	CB-CG-CD2	-5.30	94.81	110.70
2	m	35	LEU	CB-CG-CD2	-5.29	94.82	110.70
2	b	35	LEU	CB-CG-CD2	-5.29	94.82	110.70
6	K	68	GLN	CA-C-N	5.29	131.23	121.70
6	K	68	GLN	C-N-CA	5.29	131.23	121.70
7	L	345	VAL	CA-C-N	5.28	131.62	121.54
7	L	345	VAL	C-N-CA	5.28	131.62	121.54
6	K	651	TYR	CA-CB-CG	-5.27	104.42	113.90
3	N	250	LEU	CA-CB-CG	5.24	134.65	116.30
3	H	250	LEU	CA-CB-CG	5.23	134.62	116.30
5	G	264	LEU	N-CA-C	5.20	120.67	113.45
5	M	264	LEU	N-CA-C	5.20	120.67	113.45
1	U	443	TYR	N-CA-C	-5.16	105.29	112.30
1	W	443	TYR	N-CA-C	-5.16	105.29	112.30
1	Z	443	TYR	N-CA-C	-5.14	105.30	112.30
3	N	786	GLN	CA-CB-CG	5.14	124.38	114.10
1	X	443	TYR	N-CA-C	-5.14	105.31	112.30
3	H	786	GLN	CA-CB-CG	5.13	124.37	114.10
1	V	443	TYR	N-CA-C	-5.13	105.32	112.30
1	2	443	TYR	N-CA-C	-5.12	105.34	112.30
7	L	1688	PHE	N-CA-C	-5.11	108.79	114.62
1	Y	443	TYR	N-CA-C	-5.11	105.34	112.30
1	1	443	TYR	N-CA-C	-5.11	105.35	112.30
5	M	240	GLY	CA-C-N	5.10	131.28	121.54
5	M	240	GLY	C-N-CA	5.10	131.28	121.54
5	G	240	GLY	CA-C-N	5.05	131.19	121.54
5	G	240	GLY	C-N-CA	5.05	131.19	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	335	LYS	CA-CB-CG	5.05	124.20	114.10
1	Y	335	LYS	CA-CB-CG	5.05	124.20	114.10
1	W	335	LYS	CA-CB-CG	5.04	124.18	114.10
1	U	335	LYS	CA-CB-CG	5.04	124.18	114.10
1	X	335	LYS	CA-CB-CG	5.03	124.17	114.10
1	V	335	LYS	CA-CB-CG	5.03	124.15	114.10
1	2	335	LYS	CA-CB-CG	5.02	124.15	114.10
5	M	152	GLN	CB-CG-CD	5.02	121.13	112.60
1	Z	335	LYS	CA-CB-CG	5.02	124.14	114.10
5	G	152	GLN	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	G	239	ALA	Peptide
5	G	240	GLY	Peptide
5	G	580	HIS	Peptide
3	H	571	GLY	Peptide
3	H	627	GLU	Peptide
6	I	407	ASP	Peptide
4	J	235	SER	Peptide
4	J	256	LEU	Peptide
4	J	302	VAL	Peptide
7	L	345	VAL	Peptide
5	M	239	ALA	Peptide
5	M	240	GLY	Peptide
5	M	580	HIS	Peptide
3	N	571	GLY	Peptide
3	N	627	GLU	Peptide
2	b	69	LYS	Peptide
2	m	69	LYS	Peptide
2	o	69	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3373	0	3325	64	0
1	2	3373	0	3325	64	0
1	U	3373	0	3325	46	0
1	V	3373	0	3325	52	0
1	W	3373	0	3325	51	0
1	X	3373	0	3325	49	0
1	Y	3373	0	3325	50	0
1	Z	3373	0	3325	53	0
2	b	484	0	512	14	0
2	m	484	0	512	29	0
2	o	484	0	512	11	0
3	H	4907	0	4896	67	0
3	N	4907	0	4896	88	0
3	a	933	0	953	19	0
3	n	803	0	831	12	0
4	J	4429	0	4482	36	0
4	l	875	0	842	43	0
5	G	5186	0	5219	70	0
5	M	5186	0	5219	84	0
6	I	4225	0	4259	33	0
6	K	4579	0	4586	40	0
7	L	4587	0	4636	33	0
All	All	69053	0	68955	902	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 7.

All (902) 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)
4:l:80:LYS:HG3	4:l:126:TYR:CE2	1.38	1.53
2:m:30:GLU:HG2	4:l:128:GLU:CD	1.49	1.37
2:m:34:ILE:HG21	4:l:126:TYR:CE1	1.64	1.32
2:m:30:GLU:CG	4:l:128:GLU:OE2	1.74	1.31
4:l:80:LYS:CG	4:l:126:TYR:CE2	2.35	1.10
2:m:30:GLU:CG	4:l:128:GLU:CD	2.23	1.03
2:m:34:ILE:CG2	4:l:126:TYR:CE1	2.44	1.00
2:m:30:GLU:HG2	4:l:128:GLU:OE2	1.39	0.99
4:l:80:LYS:CG	4:l:126:TYR:HE2	1.73	0.99
2:m:30:GLU:CD	4:l:128:GLU:OE2	2.10	0.94
2:m:30:GLU:CB	4:l:128:GLU:OE2	2.21	0.88
2:m:30:GLU:HG2	4:l:128:GLU:OE1	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:34:ILE:HG21	4:l:126:TYR:CZ	2.10	0.86
4:l:127:VAL:HG12	4:l:127:VAL:O	1.74	0.86
2:m:34:ILE:CG2	4:l:126:TYR:CZ	2.59	0.85
2:m:30:GLU:CD	4:l:128:GLU:CD	2.45	0.85
2:m:34:ILE:HA	4:l:125:SER:OG	1.77	0.84
4:l:124:SER:O	4:l:126:TYR:CD2	2.30	0.84
4:l:119:ASP:HB2	3:H:630:PRO:HD3	1.63	0.81
1:2:357:GLN:HG2	3:N:716:HIS:HB3	1.65	0.77
4:l:80:LYS:NZ	4:l:121:PRO:CD	2.50	0.75
5:G:521:LEU:HD22	5:G:702:MET:HG2	1.69	0.75
5:M:521:LEU:HD22	5:M:702:MET:HG2	1.69	0.73
3:N:774:GLN:NE2	3:N:857:ILE:O	2.22	0.73
3:H:774:GLN:NE2	3:H:857:ILE:O	2.22	0.73
1:1:250:ASN:ND2	5:M:695:TYR:OH	2.20	0.72
2:m:30:GLU:HB2	4:l:128:GLU:OE2	1.88	0.72
4:l:80:LYS:NZ	4:l:121:PRO:HD2	2.04	0.72
4:l:118:SER:O	4:l:119:ASP:OD1	2.08	0.72
4:l:80:LYS:HZ1	4:l:121:PRO:HD3	1.55	0.71
4:l:80:LYS:HG3	4:l:126:TYR:CZ	2.19	0.71
3:H:608:THR:HG23	3:H:610:ALA:H	1.55	0.71
4:l:124:SER:O	4:l:126:TYR:CE2	2.44	0.70
1:1:251:ASN:HB2	5:M:529:VAL:HG11	1.74	0.70
3:N:274:CYS:SG	3:N:275:TYR:N	2.65	0.69
3:N:608:THR:HG23	3:N:610:ALA:H	1.55	0.69
2:b:27:VAL:HG13	3:a:77:LEU:HB3	1.74	0.69
3:H:274:CYS:SG	3:H:275:TYR:N	2.65	0.69
3:N:250:LEU:HD21	3:N:287:LEU:HD12	1.75	0.68
3:H:250:LEU:HD21	3:H:287:LEU:HD12	1.75	0.68
4:l:80:LYS:HZ1	4:l:121:PRO:CD	2.07	0.68
7:L:468:ARG:NH1	7:L:516:GLU:OE1	2.27	0.68
5:M:517:LYS:HA	5:M:521:LEU:HB2	1.74	0.68
5:G:517:LYS:HA	5:G:521:LEU:HB2	1.74	0.68
1:2:250:ASN:ND2	3:N:720:TYR:OH	2.27	0.67
1:1:341:ARG:HD2	5:M:857:SER:HB3	1.75	0.66
5:G:607:GLU:N	5:G:610:LEU:O	2.28	0.66
5:M:607:GLU:N	5:M:610:LEU:O	2.28	0.66
5:G:307:VAL:HA	5:G:310:LEU:HD12	1.78	0.66
5:M:307:VAL:HA	5:M:310:LEU:HD12	1.78	0.66
4:l:80:LYS:HG3	4:l:126:TYR:HE2	0.87	0.65
5:M:869:LEU:HD23	5:M:871:ARG:HE	1.62	0.65
6:K:639:ASN:O	6:K:643:ALA:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:876:LEU:HA	3:H:879:ARG:HG3	1.79	0.65
4:J:480:ILE:HG13	4:J:695:ILE:HD11	1.78	0.65
5:M:629:ILE:HG22	5:M:630:ILE:HG12	1.79	0.65
3:N:644:VAL:HG22	3:N:648:ILE:HG13	1.79	0.65
3:N:876:LEU:HA	3:N:879:ARG:HG3	1.79	0.65
6:I:586:ILE:HD13	6:I:622:GLN:HE21	1.62	0.65
3:N:709:SER:HA	3:N:712:VAL:HG22	1.79	0.65
3:a:65:GLN:HE21	3:a:67:ARG:HD2	1.59	0.64
5:G:629:ILE:HG22	5:G:630:ILE:HG12	1.79	0.64
2:m:30:GLU:OE2	4:l:128:GLU:OE2	2.16	0.64
3:H:644:VAL:HG22	3:H:648:ILE:HG13	1.79	0.63
4:l:127:VAL:O	4:l:127:VAL:CG1	2.46	0.63
2:b:22:ARG:HB2	7:L:287:LEU:HD22	1.81	0.63
5:G:869:LEU:HD23	5:G:871:ARG:HE	1.62	0.63
3:H:709:SER:HA	3:H:712:VAL:HG22	1.79	0.63
1:1:262:PRO:HB3	5:M:684:GLN:HG2	1.81	0.63
5:G:695:TYR:HB2	5:G:858:ARG:HH22	1.64	0.63
6:I:337:ALA:HB1	6:I:554:PHE:H	1.64	0.63
6:I:92:GLY:HA3	6:I:175:ILE:HG12	1.82	0.62
1:V:316:CYS:HB3	1:V:348:PHE:HA	1.81	0.62
1:X:316:CYS:HB3	1:X:348:PHE:HA	1.81	0.62
5:M:695:TYR:HB2	5:M:858:ARG:HH22	1.64	0.62
6:K:513:ILE:HD13	1:Y:446:TRP:HA	1.81	0.62
1:W:316:CYS:HB3	1:W:348:PHE:HA	1.81	0.62
3:H:558:HIS:ND1	3:H:642:TYR:OH	2.33	0.61
7:L:347:VAL:HG12	7:L:348:LYS:HG2	1.81	0.61
5:M:559:LEU:HD23	5:M:560:ARG:HD3	1.83	0.61
1:1:53:TYR:OH	1:2:299:GLN:NE2	2.32	0.61
1:1:316:CYS:HB3	1:1:348:PHE:HA	1.81	0.61
1:Y:316:CYS:HB3	1:Y:348:PHE:HA	1.81	0.61
5:G:559:LEU:HD23	5:G:560:ARG:HD3	1.83	0.61
1:2:316:CYS:HB3	1:2:348:PHE:HA	1.81	0.61
5:G:229:ASP:OD1	5:G:235:ALA:N	2.33	0.61
1:U:316:CYS:HB3	1:U:348:PHE:HA	1.81	0.61
1:Z:316:CYS:HB3	1:Z:348:PHE:HA	1.81	0.61
4:J:412:LEU:HA	4:J:415:VAL:HG22	1.83	0.61
3:N:558:HIS:ND1	3:N:642:TYR:OH	2.33	0.61
3:N:364:LEU:HD13	3:N:370:TRP:HE1	1.65	0.61
4:J:884:PHE:O	4:J:887:ARG:HB3	2.01	0.61
4:l:80:LYS:HZ2	4:l:121:PRO:HD2	1.66	0.60
5:M:229:ASP:OD1	5:M:235:ALA:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:364:LEU:HD13	3:H:370:TRP:HE1	1.65	0.60
3:H:538:TYR:O	3:H:542:SER:OG	2.20	0.60
1:V:274:THR:HG23	1:V:297:LEU:HD13	1.84	0.60
1:2:274:THR:HG23	1:2:297:LEU:HD13	1.84	0.59
6:K:199:GLN:O	6:K:200:HIS:ND1	2.35	0.59
3:N:538:TYR:O	3:N:542:SER:OG	2.20	0.59
1:W:274:THR:HG23	1:W:297:LEU:HD13	1.84	0.59
6:I:414:LEU:HD23	6:I:455:LEU:HD13	1.85	0.59
2:m:30:GLU:CD	4:l:128:GLU:HG3	2.27	0.59
6:K:651:TYR:OH	1:Y:354:ALA:O	2.16	0.59
3:N:659:HIS:HB2	3:N:755:LEU:HD21	1.85	0.59
1:U:274:THR:HG23	1:U:297:LEU:HD13	1.84	0.59
1:1:274:THR:HG23	1:1:297:LEU:HD13	1.84	0.59
5:G:555:LEU:HD22	5:G:575:ILE:HG13	1.85	0.59
4:J:394:THR:H	4:J:397:ILE:HD12	1.68	0.59
4:J:712:LYS:HA	4:J:715:ARG:HG2	1.85	0.58
5:M:555:LEU:HD22	5:M:575:ILE:HG13	1.85	0.58
2:b:49:ARG:HH21	7:L:283:TRP:H	1.52	0.58
3:H:270:ASN:HB3	3:H:273:ASN:HB2	1.86	0.58
4:J:225:TRP:CD1	4:J:226:THR:HG1	2.20	0.58
1:Y:274:THR:HG23	1:Y:297:LEU:HD13	1.84	0.58
2:m:30:GLU:CD	4:l:128:GLU:CG	2.77	0.58
5:G:311:GLU:HB2	3:H:365:ARG:NH2	2.18	0.58
7:L:433:THR:HA	7:L:436:LEU:HD12	1.86	0.58
5:G:559:LEU:HD11	5:G:570:LYS:HB2	1.85	0.58
1:Z:274:THR:HG23	1:Z:297:LEU:HD13	1.84	0.58
1:2:355:SER:OG	3:N:713:HIS:NE2	2.35	0.58
1:X:274:THR:HG23	1:X:297:LEU:HD13	1.84	0.58
4:l:80:LYS:HZ2	4:l:121:PRO:CD	2.17	0.58
5:M:559:LEU:HD11	5:M:570:LYS:HB2	1.85	0.58
2:b:36:ASN:ND2	3:a:102:GLU:OE1	2.36	0.58
5:G:623:LYS:HB2	5:G:626:LEU:HD12	1.87	0.57
3:N:270:ASN:HB3	3:N:273:ASN:HB2	1.86	0.57
5:G:691:GLN:HG3	5:G:694:GLN:HE21	1.69	0.57
3:H:659:HIS:HB2	3:H:755:LEU:HD21	1.85	0.57
6:I:345:VAL:HG23	6:I:346:GLU:HG3	1.85	0.57
1:2:355:SER:H	3:N:713:HIS:CD2	2.22	0.57
1:Z:49:ASP:O	1:Z:63:ARG:NH2	2.38	0.57
5:M:826:ASP:O	5:M:830:SER:OG	2.23	0.57
1:V:49:ASP:O	1:V:63:ARG:NH2	2.38	0.57
1:Y:49:ASP:O	1:Y:63:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:49:ASP:O	1:1:63:ARG:NH2	2.38	0.57
5:M:691:GLN:HG3	5:M:694:GLN:HE21	1.69	0.56
1:X:49:ASP:O	1:X:63:ARG:NH2	2.38	0.56
1:1:184:GLN:O	1:1:188:SER:OG	2.24	0.56
5:M:518:ARG:HH12	5:M:566:THR:HG1	1.50	0.56
5:M:623:LYS:HB2	5:M:626:LEU:HD12	1.87	0.56
1:V:184:GLN:O	1:V:188:SER:OG	2.24	0.56
1:W:49:ASP:O	1:W:63:ARG:NH2	2.38	0.56
1:W:184:GLN:O	1:W:188:SER:OG	2.24	0.56
1:1:337:LEU:HD11	5:M:854:SER:HB3	1.86	0.56
1:2:49:ASP:O	1:2:63:ARG:NH2	2.38	0.56
5:G:826:ASP:O	5:G:830:SER:OG	2.23	0.56
1:V:121:ILE:HG23	1:V:124:ARG:HH21	1.71	0.56
1:2:184:GLN:O	1:2:188:SER:OG	2.24	0.56
3:N:856:GLY:HA2	3:N:859:GLN:HE21	1.71	0.56
1:U:49:ASP:O	1:U:63:ARG:NH2	2.38	0.56
4:J:392:THR:HG23	7:L:295:ARG:HG3	1.87	0.56
1:Z:184:GLN:O	1:Z:188:SER:OG	2.24	0.56
1:2:249:MET:HE3	3:N:671:LYS:HD2	1.87	0.56
3:H:466:LEU:HD23	3:H:468:LYS:HE2	1.88	0.56
5:M:646:PHE:HA	5:M:649:LYS:HD2	1.88	0.56
1:X:217:ARG:NE	1:X:276:LEU:O	2.36	0.56
1:Z:395:TYR:OH	1:Z:399:ARG:NH1	2.39	0.56
1:Z:121:ILE:HG23	1:Z:124:ARG:HH21	1.71	0.56
7:L:1737:LEU:HG	7:L:1740:ARG:HE	1.71	0.55
1:U:184:GLN:O	1:U:188:SER:OG	2.24	0.55
5:M:167:LYS:HZ2	5:M:168:LYS:HD3	1.71	0.55
3:N:626:LEU:H	3:N:637:VAL:HG13	1.71	0.55
1:1:121:ILE:HG23	1:1:124:ARG:HH21	1.71	0.55
1:X:121:ILE:HG23	1:X:124:ARG:HH21	1.71	0.55
5:G:557:LEU:HA	1:V:339:ARG:NE	2.21	0.55
5:M:229:ASP:O	3:N:286:SER:OG	2.16	0.55
1:W:121:ILE:HG23	1:W:124:ARG:HH21	1.71	0.55
1:Y:121:ILE:HG23	1:Y:124:ARG:HH21	1.71	0.55
1:1:217:ARG:NE	1:1:276:LEU:O	2.36	0.55
1:W:54:GLN:NE2	1:W:55:ALA:O	2.40	0.55
1:Y:54:GLN:NE2	1:Y:55:ALA:O	2.40	0.55
5:G:277:ILE:O	5:G:281:SER:OG	2.23	0.55
6:K:183:MET:HG2	6:K:186:GLN:HE21	1.71	0.55
3:N:466:LEU:HD23	3:N:468:LYS:HE2	1.88	0.55
1:2:121:ILE:HG23	1:2:124:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:856:GLY:HA2	3:H:859:GLN:HE21	1.71	0.55
4:J:885:LEU:HD22	1:X:444:ILE:O	2.06	0.55
1:U:121:ILE:HG23	1:U:124:ARG:HH21	1.71	0.55
1:V:54:GLN:NE2	1:V:55:ALA:O	2.40	0.55
1:W:183:VAL:HG13	1:W:187:ASN:HD21	1.72	0.55
1:X:54:GLN:NE2	1:X:55:ALA:O	2.40	0.55
1:X:184:GLN:O	1:X:188:SER:OG	2.24	0.55
1:Z:54:GLN:NE2	1:Z:55:ALA:O	2.40	0.55
6:K:282:SER:HB2	6:K:340:LEU:HD11	1.89	0.54
1:Y:184:GLN:O	1:Y:188:SER:OG	2.24	0.54
1:1:54:GLN:NE2	1:1:55:ALA:O	2.40	0.54
1:2:54:GLN:NE2	1:2:55:ALA:O	2.40	0.54
5:G:646:PHE:HA	5:G:649:LYS:HD2	1.88	0.54
3:H:626:LEU:H	3:H:637:VAL:HG13	1.71	0.54
5:M:530:HIS:HD2	5:M:562:SER:HB2	1.73	0.54
6:K:410:LEU:HA	6:K:413:LEU:HB2	1.89	0.54
1:U:183:VAL:HG13	1:U:187:ASN:HD21	1.72	0.54
1:1:395:TYR:OH	1:1:399:ARG:NH1	2.39	0.54
3:H:597:LEU:HD11	3:H:625:LEU:HD21	1.90	0.54
1:1:183:VAL:HG13	1:1:187:ASN:HD21	1.72	0.54
3:N:308:THR:O	3:N:312:SER:OG	2.25	0.54
1:X:183:VAL:HG13	1:X:187:ASN:HD21	1.72	0.54
1:Z:217:ARG:NE	1:Z:276:LEU:O	2.36	0.54
7:L:507:GLN:OE1	7:L:586:VAL:N	2.39	0.54
5:M:764:LYS:O	5:M:768:SER:OG	2.25	0.54
1:2:341:ARG:HD2	3:N:878:PHE:CD1	2.43	0.54
1:W:395:TYR:OH	1:W:399:ARG:NH1	2.39	0.54
1:Z:183:VAL:HG13	1:Z:187:ASN:HD21	1.72	0.54
5:G:336:ASP:O	5:G:340:SER:OG	2.26	0.54
1:U:54:GLN:NE2	1:U:55:ALA:O	2.40	0.54
1:U:217:ARG:NE	1:U:276:LEU:O	2.36	0.54
1:W:217:ARG:NE	1:W:276:LEU:O	2.36	0.54
5:G:723:LEU:O	5:G:727:THR:OG1	2.24	0.54
6:I:403:VAL:HG22	6:I:404:LEU:HG	1.88	0.54
1:Y:32:SER:HG	1:Y:36:ILE:H	1.56	0.54
1:2:330:PRO:HB3	3:N:728:GLU:HB2	1.90	0.53
3:H:308:THR:O	3:H:312:SER:OG	2.25	0.53
6:K:377:GLN:HE21	6:K:381:LYS:HE2	1.74	0.53
1:V:62:PRO:HD2	1:V:86:TYR:HB3	1.90	0.53
1:Z:62:PRO:HD2	1:Z:86:TYR:HB3	1.90	0.53
3:n:66:ARG:HD2	3:N:626:LEU:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:22:ARG:HD3	7:L:287:LEU:HD13	1.90	0.53
1:V:183:VAL:HG13	1:V:187:ASN:HD21	1.72	0.53
1:Y:183:VAL:HG13	1:Y:187:ASN:HD21	1.72	0.53
1:Y:62:PRO:HD2	1:Y:86:TYR:HB3	1.91	0.53
5:M:336:ASP:O	5:M:340:SER:OG	2.26	0.53
1:U:62:PRO:HD2	1:U:86:TYR:HB3	1.90	0.53
1:2:62:PRO:HD2	1:2:86:TYR:HB3	1.90	0.53
3:N:597:LEU:HD11	3:N:625:LEU:HD21	1.90	0.53
5:M:277:ILE:O	5:M:281:SER:OG	2.23	0.53
1:2:183:VAL:HG13	1:2:187:ASN:HD21	1.72	0.53
2:m:57:PRO:O	2:m:61:SER:OG	2.26	0.53
6:I:55:PHE:O	6:I:58:PHE:HB3	2.08	0.53
1:1:229:ASN:O	1:1:233:SER:OG	2.27	0.53
1:2:229:ASN:O	1:2:233:SER:OG	2.27	0.53
5:G:530:HIS:HD2	5:G:562:SER:HB2	1.73	0.53
1:V:229:ASN:O	1:V:233:SER:OG	2.27	0.53
1:W:229:ASN:O	1:W:233:SER:OG	2.27	0.53
1:Y:217:ARG:NE	1:Y:276:LEU:O	2.36	0.53
1:Y:395:TYR:OH	1:Y:399:ARG:NH1	2.39	0.53
1:1:62:PRO:HD2	1:1:86:TYR:HB3	1.90	0.53
6:K:59:ILE:HD11	6:K:93:LEU:HD22	1.91	0.53
6:K:577:LYS:O	6:K:581:HIS:HB3	2.08	0.53
1:U:229:ASN:O	1:U:233:SER:OG	2.27	0.53
1:V:395:TYR:OH	1:V:399:ARG:NH1	2.39	0.53
5:G:518:ARG:HH12	5:G:566:THR:HG1	1.51	0.52
5:M:562:SER:OG	5:M:563:THR:N	2.43	0.52
1:V:13:CYS:HA	1:V:16:GLN:HE21	1.75	0.52
5:M:517:LYS:HG2	5:M:523:ASP:HB2	1.90	0.52
1:U:395:TYR:OH	1:U:399:ARG:NH1	2.39	0.52
1:X:229:ASN:O	1:X:233:SER:OG	2.27	0.52
1:Z:32:SER:HG	1:Z:36:ILE:H	1.56	0.52
1:1:349:ILE:HB	5:M:862:ASN:HB2	1.91	0.52
1:U:13:CYS:HA	1:U:16:GLN:HE21	1.75	0.52
1:Y:229:ASN:O	1:Y:233:SER:OG	2.27	0.52
5:G:517:LYS:HG2	5:G:523:ASP:HB2	1.90	0.52
1:W:13:CYS:HA	1:W:16:GLN:HE21	1.75	0.52
1:W:62:PRO:HD2	1:W:86:TYR:HB3	1.90	0.52
1:2:13:CYS:HA	1:2:16:GLN:HE21	1.74	0.52
2:b:47:CYS:HA	2:b:50:LEU:HD12	1.92	0.52
5:G:180:TRP:HA	5:G:183:GLU:HB2	1.91	0.52
2:m:61:SER:O	2:m:65:LYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:61:SER:O	2:b:65:LYS:HB2	2.10	0.52
1:X:62:PRO:HD2	1:X:86:TYR:HB3	1.90	0.52
1:1:339:ARG:NH1	1:Z:127:ASP:O	2.42	0.52
1:2:395:TYR:OH	1:2:399:ARG:NH1	2.39	0.52
6:K:486:ARG:HH12	1:Y:249:MET:HE3	1.74	0.52
3:N:394:GLY:O	3:N:398:SER:OG	2.28	0.52
1:W:55:ALA:HA	1:X:295:ARG:HH12	1.75	0.52
1:X:13:CYS:HA	1:X:16:GLN:HE21	1.74	0.52
1:Z:229:ASN:O	1:Z:233:SER:OG	2.27	0.52
4:l:118:SER:O	4:l:119:ASP:CG	2.53	0.52
3:a:70:ASP:HA	3:a:73:LEU:HB2	1.91	0.52
5:G:741:ASN:HD22	5:G:743:GLU:H	1.58	0.52
1:W:387:LEU:HA	1:W:390:ARG:HD3	1.92	0.52
1:Y:13:CYS:HA	1:Y:16:GLN:HE21	1.74	0.52
1:Y:387:LEU:HA	1:Y:390:ARG:HD3	1.92	0.52
2:o:47:CYS:HA	2:o:50:LEU:HD12	1.92	0.52
5:G:303:HIS:HA	5:G:306:LEU:HD23	1.91	0.52
6:K:639:ASN:O	6:K:643:ALA:CB	2.58	0.52
1:Z:387:LEU:HA	1:Z:390:ARG:HD3	1.92	0.52
2:o:57:PRO:O	2:o:61:SER:OG	2.26	0.51
5:G:167:LYS:HZ2	5:G:168:LYS:HD3	1.74	0.51
7:L:1562:LEU:HD11	1:Z:47:ARG:HB2	1.92	0.51
1:Z:13:CYS:HA	1:Z:16:GLN:HE21	1.74	0.51
6:K:27:VAL:HG13	6:K:29:GLN:HG2	1.93	0.51
3:H:394:GLY:O	3:H:398:SER:OG	2.28	0.51
5:M:180:TRP:HA	5:M:183:GLU:HB2	1.91	0.51
5:M:433:THR:OG1	5:M:434:ILE:N	2.44	0.51
1:Z:47:ARG:HE	1:Z:49:ASP:HB3	1.76	0.51
4:l:118:SER:OG	4:l:119:ASP:N	2.44	0.51
6:I:42:LEU:HA	6:I:45:LEU:HD12	1.92	0.51
5:M:723:LEU:O	5:M:727:THR:OG1	2.23	0.51
3:a:122:LEU:HD23	3:a:124:ARG:H	1.76	0.51
3:H:524:THR:O	3:H:524:THR:OG1	2.28	0.51
4:J:273:GLU:HB3	4:J:284:LEU:HD12	1.92	0.51
1:V:326:GLY:HA2	1:V:363:LYS:HD3	1.93	0.51
1:V:387:LEU:HA	1:V:390:ARG:HD3	1.92	0.51
1:1:47:ARG:HE	1:1:49:ASP:HB3	1.76	0.51
6:K:63:THR:HG23	6:K:87:ARG:HG3	1.93	0.51
3:N:259:GLN:HG2	3:N:339:LEU:HD13	1.92	0.51
5:G:433:THR:OG1	5:G:434:ILE:N	2.44	0.51
6:I:544:LEU:HD13	6:I:564:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:403:VAL:HG13	6:K:405:LEU:H	1.76	0.51
5:M:303:HIS:HA	5:M:306:LEU:HD23	1.91	0.51
5:G:764:LYS:O	5:G:768:SER:OG	2.25	0.51
3:H:695:PRO:O	3:H:698:SER:OG	2.28	0.51
6:K:496:TRP:HA	6:K:499:GLN:HG2	1.93	0.51
3:N:433:TRP:HE1	3:N:484:LEU:HA	1.76	0.51
1:X:395:TYR:OH	1:X:399:ARG:NH1	2.39	0.51
1:2:47:ARG:HE	1:2:49:ASP:HB3	1.76	0.51
1:2:326:GLY:HA2	1:2:363:LYS:HD3	1.93	0.51
7:L:507:GLN:HE22	7:L:586:VAL:HG22	1.75	0.51
1:W:47:ARG:HE	1:W:49:ASP:HB3	1.76	0.50
1:X:47:ARG:HE	1:X:49:ASP:HB3	1.76	0.50
1:1:13:CYS:HA	1:1:16:GLN:HE21	1.75	0.50
2:o:56:ASN:HD22	3:n:42:ASN:HB3	1.76	0.50
3:H:259:GLN:HG2	3:H:339:LEU:HD13	1.92	0.50
3:H:433:TRP:HE1	3:H:484:LEU:HA	1.76	0.50
3:N:695:PRO:O	3:N:698:SER:OG	2.28	0.50
2:m:34:ILE:HB	4:l:126:TYR:OH	2.11	0.50
2:m:47:CYS:HA	2:m:50:LEU:HD12	1.92	0.50
2:b:57:PRO:O	2:b:61:SER:OG	2.26	0.50
4:l:121:PRO:HD2	4:l:121:PRO:O	2.11	0.50
7:L:427:LEU:HD13	7:L:548:ALA:HB2	1.93	0.50
5:G:562:SER:OG	5:G:563:THR:N	2.43	0.50
1:Y:326:GLY:HA2	1:Y:363:LYS:HD3	1.93	0.50
1:2:217:ARG:NE	1:2:276:LEU:O	2.36	0.50
2:o:61:SER:O	2:o:65:LYS:HB2	2.10	0.50
6:I:339:HIS:HA	6:I:342:LYS:HE2	1.94	0.50
1:U:326:GLY:HA2	1:U:363:LYS:HD3	1.93	0.50
1:W:326:GLY:HA2	1:W:363:LYS:HD3	1.93	0.50
1:X:326:GLY:HA2	1:X:363:LYS:HD3	1.93	0.50
1:W:32:SER:HG	1:W:36:ILE:H	1.57	0.50
1:1:32:SER:HG	1:1:36:ILE:H	1.58	0.50
5:M:865:TYR:HA	5:M:868:ARG:HD2	1.94	0.50
1:Y:326:GLY:HA3	1:Y:373:VAL:HA	1.94	0.50
1:Z:326:GLY:HA2	1:Z:363:LYS:HD3	1.93	0.50
1:Z:326:GLY:HA3	1:Z:373:VAL:HA	1.94	0.50
1:2:387:LEU:HA	1:2:390:ARG:HD3	1.92	0.50
5:G:259:LEU:HD13	5:G:262:ARG:HH21	1.76	0.50
6:K:31:PHE:HB2	6:K:34:LEU:HB3	1.94	0.50
6:K:143:ILE:HD13	6:K:148:ILE:HD12	1.94	0.50
1:Y:47:ARG:HE	1:Y:49:ASP:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:769:ARG:O	3:H:772:LEU:HB3	2.12	0.50
6:K:419:GLU:H	6:K:452:ALA:HB1	1.77	0.50
7:L:1554:LEU:HD22	7:L:1574:LEU:HD22	1.94	0.50
3:N:769:ARG:O	3:N:772:LEU:HB3	2.12	0.50
1:X:387:LEU:HA	1:X:390:ARG:HD3	1.92	0.50
7:L:461:PHE:O	7:L:464:LYS:NZ	2.43	0.49
1:V:47:ARG:HE	1:V:49:ASP:HB3	1.76	0.49
5:G:242:GLN:HE21	5:G:343:THR:HA	1.77	0.49
5:G:865:TYR:HA	5:G:868:ARG:HD2	1.94	0.49
6:I:575:LEU:HB3	6:I:577:LYS:HZ2	1.76	0.49
7:L:1602:TRP:CD1	7:L:1603:PRO:HD3	2.47	0.49
1:1:326:GLY:HA2	1:1:363:LYS:HD3	1.93	0.49
1:1:387:LEU:HA	1:1:390:ARG:HD3	1.92	0.49
1:1:326:GLY:HA3	1:1:373:VAL:HA	1.94	0.49
5:G:161:LEU:HD13	5:G:284:GLU:HG3	1.94	0.49
6:I:333:ARG:HA	6:I:336:VAL:HG22	1.95	0.49
6:I:504:HIS:CE1	1:W:158:ASN:HD21	2.29	0.49
5:M:741:ASN:HD22	5:M:743:GLU:H	1.58	0.49
3:N:763:LEU:HD22	3:N:771:LEU:HB3	1.95	0.49
1:Y:54:GLN:HE22	1:Y:58:GLU:HG3	1.78	0.49
1:Z:54:GLN:HE22	1:Z:58:GLU:HG3	1.78	0.49
1:2:251:ASN:HB2	3:N:575:ARG:HD2	1.94	0.49
3:H:767:ASP:OD1	3:H:767:ASP:N	2.45	0.49
1:U:47:ARG:HE	1:U:49:ASP:HB3	1.76	0.49
1:V:326:GLY:HA3	1:V:373:VAL:HA	1.94	0.49
1:X:326:GLY:HA3	1:X:373:VAL:HA	1.94	0.49
1:2:54:GLN:HE22	1:2:58:GLU:HG3	1.78	0.49
2:b:36:ASN:HB3	3:a:102:GLU:HB3	1.93	0.49
3:H:763:LEU:HD22	3:H:771:LEU:HB3	1.95	0.49
1:X:54:GLN:HE22	1:X:58:GLU:HG3	1.77	0.49
3:a:62:LEU:HD21	3:a:70:ASP:HB2	1.94	0.49
5:G:547:THR:HG23	5:G:549:PRO:HD2	1.95	0.49
1:U:387:LEU:HA	1:U:390:ARG:HD3	1.92	0.49
1:W:326:GLY:HA3	1:W:373:VAL:HA	1.94	0.49
1:1:54:GLN:HE22	1:1:58:GLU:HG3	1.78	0.49
3:H:692:ARG:HH12	1:V:265:ARG:NH2	2.11	0.49
7:L:1612:CYS:SG	7:L:1613:VAL:N	2.85	0.49
3:N:767:ASP:OD1	3:N:767:ASP:N	2.45	0.49
1:W:54:GLN:HE22	1:W:58:GLU:HG3	1.77	0.49
5:M:259:LEU:HD13	5:M:262:ARG:HH21	1.76	0.49
5:M:521:LEU:HB3	5:M:702:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:547:THR:HG23	5:M:549:PRO:HD2	1.95	0.49
1:2:226:SER:OG	1:2:227:GLN:NE2	2.46	0.48
2:m:34:ILE:HD12	4:l:126:TYR:OH	2.12	0.48
1:W:226:SER:OG	1:W:227:GLN:NE2	2.46	0.48
5:M:161:LEU:HD13	5:M:284:GLU:HG3	1.95	0.48
1:U:226:SER:OG	1:U:227:GLN:NE2	2.46	0.48
1:2:326:GLY:HA3	1:2:373:VAL:HA	1.94	0.48
3:H:294:LEU:H	3:H:294:LEU:HG	1.45	0.48
6:I:268:ILE:HD12	6:I:322:LEU:HD11	1.96	0.48
6:K:191:MET:HG3	6:K:192:LEU:HD22	1.96	0.48
1:U:54:GLN:HE22	1:U:58:GLU:HG3	1.78	0.48
1:U:326:GLY:HA3	1:U:373:VAL:HA	1.94	0.48
5:G:521:LEU:HB3	5:G:702:MET:HE2	1.95	0.48
4:J:320:TYR:HD1	4:J:409:LEU:HD22	1.79	0.48
1:X:226:SER:OG	1:X:227:GLN:NE2	2.46	0.48
1:Z:323:ILE:HD11	1:Z:361:SER:HB3	1.96	0.48
1:1:226:SER:OG	1:1:227:GLN:NE2	2.46	0.48
3:H:416:GLN:HA	3:H:419:LEU:HG	1.96	0.48
4:J:275:LEU:HD23	4:J:383:GLU:HG2	1.96	0.48
1:V:323:ILE:HD11	1:V:361:SER:HB3	1.96	0.48
1:Y:317:TYR:HD2	1:Y:348:PHE:HB3	1.79	0.48
4:l:115:LEU:O	4:l:119:ASP:OD1	2.31	0.48
3:a:93:ILE:HD12	3:a:96:LEU:HD23	1.96	0.48
4:J:922:ASP:HB3	4:J:925:GLN:HG2	1.96	0.48
5:M:189:GLY:HA2	3:N:293:ARG:NH1	2.29	0.48
1:U:317:TYR:HD2	1:U:348:PHE:HB3	1.79	0.48
1:V:54:GLN:HE22	1:V:58:GLU:HG3	1.78	0.48
1:V:351:TRP:CD1	1:V:443:TYR:HB3	2.49	0.48
1:Z:226:SER:OG	1:Z:227:GLN:NE2	2.46	0.48
1:Z:351:TRP:CD1	1:Z:443:TYR:HB3	2.49	0.48
1:1:330:PRO:HG3	5:M:707:HIS:HB3	1.95	0.48
1:2:263:THR:HG23	1:2:266:LEU:HB2	1.96	0.48
1:2:317:TYR:HD2	1:2:348:PHE:HB3	1.79	0.48
1:2:323:ILE:HD11	1:2:361:SER:HB3	1.96	0.48
1:U:32:SER:HG	1:U:36:ILE:H	1.61	0.48
1:V:32:SER:HG	1:V:36:ILE:H	1.60	0.48
1:V:226:SER:OG	1:V:227:GLN:NE2	2.46	0.48
6:K:66:VAL:HG23	6:K:68:GLN:H	1.79	0.47
1:Y:226:SER:OG	1:Y:227:GLN:NE2	2.46	0.47
1:1:3:ARG:HD3	5:M:533:ASP:OD2	2.14	0.47
3:a:122:LEU:HG	3:a:123:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:633:LYS:O	5:G:637:ARG:HG2	2.15	0.47
1:V:263:THR:HG23	1:V:266:LEU:HB2	1.96	0.47
1:X:263:THR:HG23	1:X:266:LEU:HB2	1.96	0.47
1:X:323:ILE:HD11	1:X:361:SER:HB3	1.96	0.47
1:1:295:ARG:NH2	1:Z:120:ASP:OD1	2.48	0.47
1:2:351:TRP:CD1	1:2:443:TYR:HB3	2.49	0.47
5:G:306:LEU:HA	5:G:309:GLN:HE21	1.79	0.47
3:H:543:LYS:HZ3	3:H:543:LYS:HG2	1.62	0.47
5:M:242:GLN:HE21	5:M:343:THR:HA	1.77	0.47
5:M:633:LYS:O	5:M:637:ARG:HG2	2.15	0.47
1:U:351:TRP:CD1	1:U:443:TYR:HB3	2.49	0.47
1:V:217:ARG:NE	1:V:276:LEU:O	2.36	0.47
1:Z:317:TYR:HD2	1:Z:348:PHE:HB3	1.79	0.47
1:1:263:THR:HG23	1:1:266:LEU:HB2	1.96	0.47
3:N:416:GLN:HA	3:N:419:LEU:HG	1.96	0.47
1:U:323:ILE:HD11	1:U:361:SER:HB3	1.96	0.47
1:1:323:ILE:HD11	1:1:361:SER:HB3	1.96	0.47
1:W:317:TYR:HD2	1:W:348:PHE:HB3	1.79	0.47
1:1:84:LYS:HG2	1:2:219:HIS:CE1	2.50	0.47
3:N:408:ASP:HB3	3:N:411:MET:HB3	1.97	0.47
3:N:810:LYS:HD3	3:N:810:LYS:HA	1.55	0.47
1:V:221:GLN:O	1:V:224:SER:OG	2.33	0.47
1:W:351:TRP:CD1	1:W:443:TYR:HB3	2.49	0.47
1:X:317:TYR:HD2	1:X:348:PHE:HB3	1.79	0.47
1:Y:263:THR:HG23	1:Y:266:LEU:HB2	1.96	0.47
2:o:28:LEU:HD23	2:o:31:ILE:HD12	1.97	0.47
6:I:617:LYS:HZ3	6:I:621:ARG:HH12	1.61	0.47
1:1:221:GLN:O	1:1:224:SER:OG	2.33	0.47
1:1:351:TRP:CD1	1:1:443:TYR:HB3	2.49	0.47
2:b:28:LEU:HD23	2:b:31:ILE:HD12	1.97	0.47
3:a:113:SER:OG	3:a:114:TYR:N	2.47	0.47
1:V:317:TYR:HD2	1:V:348:PHE:HB3	1.79	0.47
1:2:221:GLN:O	1:2:224:SER:OG	2.33	0.47
4:J:553:LYS:HA	4:J:556:LEU:HD23	1.97	0.47
1:X:351:TRP:CD1	1:X:443:TYR:HB3	2.49	0.47
1:Y:113:LYS:HG3	1:Y:114:ILE:HG23	1.97	0.47
1:Y:351:TRP:CD1	1:Y:443:TYR:HB3	2.49	0.47
1:2:290:VAL:HG11	1:2:333:VAL:HG12	1.97	0.46
2:m:34:ILE:HB	4:l:126:TYR:CZ	2.49	0.46
3:H:408:ASP:HB3	3:H:411:MET:HB3	1.97	0.46
1:V:291:LEU:HD22	1:V:336:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:323:ILE:HD11	1:Y:361:SER:HB3	1.96	0.46
1:Z:290:VAL:HG11	1:Z:333:VAL:HG12	1.97	0.46
1:1:317:TYR:HD2	1:1:348:PHE:HB3	1.79	0.46
1:2:32:SER:HG	1:2:36:ILE:H	1.63	0.46
7:L:1657:GLN:HE22	1:Z:446:TRP:HA	1.79	0.46
5:M:691:GLN:HA	5:M:694:GLN:HG2	1.97	0.46
3:N:561:ALA:HA	3:N:564:ARG:HB2	1.97	0.46
1:W:221:GLN:O	1:W:224:SER:OG	2.33	0.46
1:Z:221:GLN:O	1:Z:224:SER:OG	2.33	0.46
2:o:55:ILE:HD13	3:n:43:PHE:CD1	2.51	0.46
1:W:113:LYS:HG3	1:W:114:ILE:HG23	1.97	0.46
3:n:66:ARG:HG3	3:N:627:GLU:HB2	1.98	0.46
2:m:28:LEU:HD23	2:m:31:ILE:HD12	1.97	0.46
5:M:853:ALA:O	5:M:857:SER:OG	2.33	0.46
3:N:614:SER:HB3	3:N:617:ILE:HD12	1.98	0.46
1:U:290:VAL:HG11	1:U:333:VAL:HG12	1.98	0.46
1:W:263:THR:HG23	1:W:266:LEU:HB2	1.96	0.46
1:W:323:ILE:HD11	1:W:361:SER:HB3	1.96	0.46
1:X:291:LEU:HD22	1:X:336:SER:HB3	1.97	0.46
5:M:704:PRO:O	5:M:708:ILE:HG13	2.16	0.46
3:H:614:SER:HB3	3:H:617:ILE:HD12	1.98	0.46
6:I:1:MET:HA	4:J:242:LEU:HD12	1.97	0.46
3:N:537:ALA:O	3:N:541:THR:HG22	2.16	0.46
1:U:221:GLN:O	1:U:224:SER:OG	2.33	0.46
1:U:291:LEU:HD22	1:U:336:SER:HB3	1.97	0.46
1:X:221:GLN:O	1:X:224:SER:OG	2.33	0.46
3:a:87:LEU:HD23	3:a:90:LYS:HG2	1.97	0.46
5:G:704:PRO:O	5:G:708:ILE:HG13	2.16	0.46
5:M:499:LEU:HD13	5:M:499:LEU:HA	1.80	0.46
1:U:263:THR:HG23	1:U:266:LEU:HB2	1.96	0.46
1:V:113:LYS:HG3	1:V:114:ILE:HG23	1.97	0.46
1:Z:263:THR:HG23	1:Z:266:LEU:HB2	1.96	0.46
3:H:635:TRP:HB3	3:H:672:ARG:HD2	1.98	0.46
6:I:534:VAL:HG22	1:W:248:TYR:HE2	1.81	0.46
6:K:59:ILE:HG12	6:K:90:CYS:HB3	1.97	0.46
5:M:306:LEU:HA	5:M:309:GLN:HE21	1.79	0.46
1:1:291:LEU:HD22	1:1:336:SER:HB3	1.97	0.46
6:K:68:GLN:O	7:L:511:HIS:HB3	2.15	0.46
1:V:290:VAL:HG11	1:V:333:VAL:HG12	1.97	0.46
1:1:113:LYS:HG3	1:1:114:ILE:HG23	1.98	0.46
1:2:349:ILE:HD12	3:N:883:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:57:LYS:O	3:a:61:GLU:HG2	2.16	0.46
5:G:711:LYS:HD3	5:G:711:LYS:HA	1.53	0.46
3:H:363:THR:HB	3:H:366:ARG:HA	1.98	0.46
3:H:566:LEU:HG	3:H:640:LEU:HD21	1.97	0.46
4:J:712:LYS:HG3	4:J:715:ARG:HE	1.80	0.46
7:L:1634:LYS:HA	7:L:1634:LYS:HD2	1.84	0.46
3:a:58:ILE:HD11	3:a:98:LEU:HB2	1.97	0.45
5:G:560:ARG:HB2	1:V:339:ARG:NH2	2.31	0.45
4:J:569:LEU:HD11	4:J:706:LEU:HB2	1.98	0.45
4:J:927:ILE:HA	4:J:930:HIS:CE1	2.51	0.45
5:M:393:LYS:HB3	5:M:393:LYS:HE2	1.80	0.45
1:2:113:LYS:HG3	1:2:114:ILE:HG23	1.97	0.45
5:G:486:GLU:H	5:G:486:GLU:HG3	1.54	0.45
6:K:48:LEU:HD21	6:K:130:GLN:HA	1.99	0.45
5:M:213:GLN:O	5:M:217:VAL:HG22	2.16	0.45
5:M:480:LYS:HB2	5:M:480:LYS:HE3	1.76	0.45
3:N:734:LEU:O	3:N:738:VAL:HG12	2.16	0.45
1:W:290:VAL:HG11	1:W:333:VAL:HG12	1.97	0.45
1:X:290:VAL:HG11	1:X:333:VAL:HG12	1.98	0.45
1:1:320:ILE:HB	1:1:356:ILE:HG13	1.99	0.45
2:o:21:VAL:HG22	3:n:86:VAL:HG21	1.99	0.45
6:I:545:LEU:O	6:I:549:ASN:ND2	2.49	0.45
1:V:340:ILE:HD13	1:V:340:ILE:HA	1.86	0.45
1:1:47:ARG:HB2	5:M:563:THR:HB	1.99	0.45
3:H:537:ALA:O	3:H:541:THR:HG22	2.16	0.45
3:H:734:LEU:O	3:H:738:VAL:HG12	2.16	0.45
3:H:775:LEU:HD13	3:H:775:LEU:HA	1.86	0.45
5:M:860:ASP:HB3	5:M:866:THR:HB	1.99	0.45
1:X:113:LYS:HG3	1:X:114:ILE:HG23	1.97	0.45
1:Y:291:LEU:HD22	1:Y:336:SER:HB3	1.97	0.45
1:2:291:LEU:HD22	1:2:336:SER:HB3	1.97	0.45
5:G:213:GLN:O	5:G:217:VAL:HG22	2.16	0.45
6:K:301:LYS:HE2	6:K:335:THR:HB	1.98	0.45
3:N:451:ASP:HB3	3:N:463:LYS:HA	1.99	0.45
1:U:7:THR:OG1	1:U:63:ARG:O	2.31	0.45
1:Y:221:GLN:O	1:Y:224:SER:OG	2.33	0.45
3:H:580:LEU:HB3	3:H:600:ILE:HD11	1.97	0.45
6:K:206:LYS:HB3	6:K:257:PHE:HA	1.99	0.45
5:M:283:PHE:HZ	3:N:411:MET:HE1	1.81	0.45
3:N:580:LEU:HB3	3:N:600:ILE:HD11	1.97	0.45
1:W:340:ILE:HD13	1:W:340:ILE:HA	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:691:GLN:HA	5:G:694:GLN:HG2	1.97	0.45
5:G:853:ALA:O	5:G:857:SER:OG	2.33	0.45
6:K:286:PHE:HA	6:K:461:TRP:HZ2	1.82	0.45
3:N:566:LEU:HG	3:N:640:LEU:HD21	1.97	0.45
1:W:291:LEU:HD22	1:W:336:SER:HB3	1.98	0.45
1:W:320:ILE:HB	1:W:356:ILE:HG13	1.99	0.45
1:Z:291:LEU:HD22	1:Z:336:SER:HB3	1.97	0.45
1:1:290:VAL:HG11	1:1:333:VAL:HG12	1.97	0.45
5:G:201:THR:HG23	3:H:285:ARG:HB2	1.98	0.45
3:H:561:ALA:HA	3:H:564:ARG:HB2	1.97	0.45
5:M:353:GLY:HA2	5:M:356:LEU:HD12	1.99	0.45
1:X:56:ASP:HB3	1:Y:287:LYS:N	2.32	0.45
1:Y:290:VAL:HG11	1:Y:333:VAL:HG12	1.98	0.45
1:2:355:SER:HB3	3:N:882:PHE:HB2	1.99	0.45
2:m:34:ILE:CB	4:l:126:TYR:CZ	2.99	0.45
3:H:451:ASP:HB3	3:H:463:LYS:HA	1.99	0.45
4:J:982:LYS:HB2	4:J:983:MET:HE2	1.99	0.45
1:U:136:VAL:HG23	1:U:167:GLN:HB3	1.99	0.45
1:W:7:THR:OG1	1:W:63:ARG:O	2.31	0.45
1:Y:7:THR:OG1	1:Y:63:ARG:O	2.31	0.45
1:Z:113:LYS:HG3	1:Z:114:ILE:HG23	1.97	0.45
1:1:334:HIS:O	1:1:338:GLN:HG2	2.18	0.44
3:N:635:TRP:HB3	3:N:672:ARG:HD2	1.98	0.44
1:U:334:HIS:O	1:U:338:GLN:HG2	2.18	0.44
1:V:320:ILE:HB	1:V:356:ILE:HG13	1.99	0.44
1:1:359:ALA:HA	5:M:699:PHE:CE2	2.52	0.44
5:G:480:LYS:HB2	5:G:480:LYS:HE3	1.76	0.44
1:V:334:HIS:O	1:V:338:GLN:HG2	2.18	0.44
1:X:320:ILE:HB	1:X:356:ILE:HG13	1.99	0.44
1:X:334:HIS:O	1:X:338:GLN:HG2	2.17	0.44
1:Z:385:SER:HB2	1:Z:435:TYR:CG	2.53	0.44
1:1:385:SER:HB2	1:1:435:TYR:CG	2.53	0.44
5:G:865:TYR:H	5:G:868:ARG:NH1	2.15	0.44
6:I:312:HIS:HA	6:I:315:LYS:HG3	1.99	0.44
7:L:509:ALA:HA	7:L:521:LEU:HD13	1.99	0.44
7:L:1632:ALA:HB1	7:L:1740:ARG:HD3	1.98	0.44
3:N:768:SER:O	3:N:771:LEU:HB2	2.17	0.44
1:V:136:VAL:HG23	1:V:167:GLN:HB3	1.99	0.44
1:X:385:SER:HB2	1:X:435:TYR:CG	2.53	0.44
1:Y:340:ILE:HD13	1:Y:340:ILE:HA	1.86	0.44
3:H:768:SER:O	3:H:771:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:320:ILE:HB	1:Z:356:ILE:HG13	1.99	0.44
1:2:136:VAL:HG23	1:2:167:GLN:HB3	1.99	0.44
4:J:236:LEU:HD23	4:J:236:LEU:HA	1.71	0.44
5:M:352:GLY:HA3	5:M:406:GLU:HB2	2.00	0.44
3:N:363:THR:HB	3:N:366:ARG:HA	1.98	0.44
1:U:385:SER:HB2	1:U:435:TYR:CG	2.53	0.44
1:W:385:SER:HB2	1:W:435:TYR:CG	2.53	0.44
1:X:136:VAL:HG23	1:X:167:GLN:HB3	1.99	0.44
1:Y:136:VAL:HG23	1:Y:167:GLN:HB3	1.99	0.44
1:Y:320:ILE:HB	1:Y:356:ILE:HG13	1.99	0.44
1:2:249:MET:HG3	3:N:719:GLN:HE21	1.83	0.44
3:H:576:HIS:HE1	3:H:607:ALA:HB3	1.83	0.44
4:J:440:LEU:HG	4:J:465:TRP:HB2	1.98	0.44
6:K:548:ILE:HD12	6:K:557:ILE:HG12	1.99	0.44
3:N:753:VAL:O	3:N:757:THR:HG22	2.18	0.44
1:U:113:LYS:HG3	1:U:114:ILE:HG23	1.97	0.44
1:U:320:ILE:HB	1:U:356:ILE:HG13	1.99	0.44
5:G:352:GLY:HA3	5:G:406:GLU:HB2	2.00	0.44
5:M:867:GLU:C	5:M:868:ARG:HE	2.26	0.44
1:2:320:ILE:HB	1:2:356:ILE:HG13	1.99	0.44
1:2:334:HIS:O	1:2:338:GLN:HG2	2.17	0.44
5:G:572:ASP:HB3	5:G:621:ILE:H	1.83	0.44
6:K:468:THR:HG23	6:K:470:ALA:H	1.83	0.44
3:N:733:GLU:O	3:N:737:LYS:HG3	2.18	0.44
1:X:32:SER:HG	1:X:36:ILE:H	1.62	0.44
5:G:174:LEU:HD22	5:G:404:TYR:CE2	2.53	0.44
1:U:160:ARG:HD2	1:U:160:ARG:HA	1.91	0.44
1:V:385:SER:HB2	1:V:435:TYR:CG	2.53	0.44
1:Z:334:HIS:O	1:Z:338:GLN:HG2	2.18	0.44
2:o:34:ILE:HD12	3:n:62:LEU:HD21	2.00	0.43
3:n:51:GLU:OE2	3:n:82:HIS:NE2	2.41	0.43
3:H:733:GLU:O	3:H:737:LYS:HG3	2.18	0.43
6:I:170:SER:O	6:I:173:GLU:HB2	2.18	0.43
5:M:865:TYR:H	5:M:868:ARG:NH1	2.15	0.43
3:n:28:VAL:HG21	3:n:31:GLN:HG2	1.99	0.43
5:G:353:GLY:HA2	5:G:356:LEU:HD12	1.99	0.43
5:G:860:ASP:HB3	5:G:866:THR:HB	1.99	0.43
3:H:753:VAL:O	3:H:757:THR:HG22	2.18	0.43
6:K:195:LEU:HD23	6:K:195:LEU:HA	1.90	0.43
1:W:297:LEU:HD12	1:W:297:LEU:HA	1.89	0.43
3:H:406:THR:HG22	3:H:412:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:7:LEU:HD23	4:J:305:LEU:HD21	2.00	0.43
4:J:743:PHE:HE1	4:J:837:SER:HB3	1.84	0.43
6:K:509:GLN:HG3	6:K:512:ALA:H	1.82	0.43
5:M:448:ASP:OD1	5:M:448:ASP:N	2.50	0.43
1:Y:209:ALA:HA	1:Y:212:ARG:HE	1.83	0.43
1:Z:136:VAL:HG23	1:Z:167:GLN:HB3	1.99	0.43
1:2:343:ARG:HD3	5:M:557:LEU:HG	1.99	0.43
1:2:385:SER:HB2	1:2:435:TYR:CG	2.53	0.43
3:H:421:LEU:HD23	3:H:421:LEU:HA	1.85	0.43
5:M:403:PRO:HB3	3:N:405:LYS:HB3	2.00	0.43
3:N:294:LEU:H	3:N:294:LEU:HG	1.45	0.43
3:N:524:THR:O	3:N:524:THR:OG1	2.28	0.43
3:N:576:HIS:HE1	3:N:607:ALA:HB3	1.83	0.43
1:1:209:ALA:HA	1:1:212:ARG:HE	1.83	0.43
1:2:209:ALA:HA	1:2:212:ARG:HE	1.83	0.43
3:H:667:LEU:O	3:H:671:LYS:HG2	2.18	0.43
3:N:406:THR:HG23	3:N:408:ASP:H	1.84	0.43
1:W:136:VAL:HG23	1:W:167:GLN:HB3	1.99	0.43
1:Y:385:SER:HB2	1:Y:435:TYR:CG	2.53	0.43
1:Z:209:ALA:HA	1:Z:212:ARG:HE	1.83	0.43
1:1:136:VAL:HG23	1:1:167:GLN:HB3	1.99	0.43
1:1:357:GLN:HB3	5:M:695:TYR:CD2	2.53	0.43
7:L:1691:ARG:HE	7:L:1707:GLU:HG2	1.84	0.43
5:M:572:ASP:HB3	5:M:621:ILE:H	1.83	0.43
3:H:406:THR:HG23	3:H:408:ASP:H	1.84	0.43
6:I:133:PHE:O	6:I:137:MET:HB2	2.17	0.43
1:W:334:HIS:O	1:W:338:GLN:HG2	2.18	0.43
1:Z:303:VAL:HG12	1:Z:305:VAL:H	1.84	0.43
3:n:24:SER:OG	3:n:25:GLU:N	2.52	0.43
1:X:303:VAL:HG12	1:X:305:VAL:H	1.84	0.43
1:2:337:LEU:HD11	3:N:875:PHE:CE2	2.54	0.43
5:G:867:GLU:C	5:G:868:ARG:HE	2.26	0.43
5:M:174:LEU:HD22	5:M:404:TYR:CE2	2.53	0.43
3:N:667:LEU:O	3:N:671:LYS:HG2	2.18	0.43
1:U:260:LEU:HD21	1:U:321:LEU:HB2	2.01	0.43
1:V:192:LEU:HA	1:V:195:LEU:HD12	2.01	0.43
1:V:260:LEU:HD21	1:V:321:LEU:HB2	2.01	0.43
1:X:32:SER:OG	1:X:36:ILE:N	2.48	0.43
1:Y:46:ASP:OD1	1:Y:46:ASP:N	2.52	0.43
7:L:1800:LEU:HD13	1:Z:338:GLN:HE22	1.84	0.43
3:N:376:ILE:O	3:N:380:THR:OG1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:209:ALA:HA	1:V:212:ARG:HE	1.83	0.43
1:W:65:VAL:HA	1:W:90:ASN:ND2	2.34	0.43
3:n:11:VAL:O	3:n:14:GLN:HG3	2.18	0.42
5:G:296:MET:HE3	5:G:296:MET:HB2	1.85	0.42
3:H:684:HIS:CE1	3:H:705:HIS:HA	2.54	0.42
6:I:326:GLU:HA	6:I:329:VAL:HG22	2.00	0.42
4:J:707:MET:O	4:J:711:LYS:HG2	2.19	0.42
4:J:835:LYS:HG2	4:J:898:HIS:CE1	2.54	0.42
5:M:711:LYS:HA	5:M:711:LYS:HD3	1.53	0.42
3:N:427:LEU:HA	3:N:430:LEU:HD12	2.01	0.42
1:U:192:LEU:HA	1:U:195:LEU:HD12	2.01	0.42
1:V:46:ASP:OD1	1:V:46:ASP:N	2.52	0.42
1:X:260:LEU:HD21	1:X:321:LEU:HB2	2.01	0.42
1:Z:192:LEU:HA	1:Z:195:LEU:HD12	2.01	0.42
1:Z:260:LEU:HD21	1:Z:321:LEU:HB2	2.01	0.42
4:J:739:TYR:HB3	4:J:832:LYS:HE3	2.01	0.42
5:M:486:GLU:H	5:M:486:GLU:HG3	1.54	0.42
5:M:517:LYS:O	5:M:523:ASP:N	2.52	0.42
3:N:684:HIS:CE1	3:N:705:HIS:HA	2.54	0.42
1:1:303:VAL:HG12	1:1:305:VAL:H	1.84	0.42
5:G:217:VAL:O	5:G:221:LEU:HG	2.19	0.42
6:I:379:MET:SD	6:I:379:MET:N	2.92	0.42
6:I:579:VAL:HG23	6:I:629:ILE:HD13	1.99	0.42
4:J:739:TYR:HA	4:J:742:ILE:HD12	2.01	0.42
5:M:703:GLU:HG3	5:M:704:PRO:HD3	2.01	0.42
1:1:65:VAL:HA	1:1:90:ASN:ND2	2.34	0.42
1:1:132:LEU:HD23	1:1:164:LYS:HG3	2.02	0.42
1:2:447:GLY:HA3	3:N:706:ILE:HD11	2.02	0.42
3:n:45:PRO:HB3	3:n:91:TRP:HZ3	1.85	0.42
3:a:117:LEU:HD22	5:G:299:LEU:HD22	2.01	0.42
5:G:517:LYS:O	5:G:523:ASP:N	2.52	0.42
3:H:811:LYS:HA	3:H:811:LYS:HD3	1.90	0.42
4:J:736:TYR:CD1	4:J:832:LYS:HE2	2.55	0.42
3:N:486:ILE:HD11	3:N:538:TYR:HB2	2.01	0.42
3:N:543:LYS:HZ3	3:N:543:LYS:HG2	1.64	0.42
3:N:811:LYS:HA	3:N:811:LYS:HD3	1.90	0.42
1:U:303:VAL:HG12	1:U:305:VAL:H	1.84	0.42
1:V:343:ARG:HE	1:V:343:ARG:HB2	1.72	0.42
1:X:46:ASP:OD1	1:X:46:ASP:N	2.52	0.42
1:Y:65:VAL:HA	1:Y:90:ASN:ND2	2.34	0.42
1:Y:334:HIS:O	1:Y:338:GLN:HG2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:65:VAL:HA	1:2:90:ASN:ND2	2.34	0.42
1:2:248:TYR:HB2	3:N:568:LEU:HG	2.02	0.42
3:H:432:ARG:HH21	3:H:439:LEU:HD12	1.85	0.42
3:H:486:ILE:HD11	3:H:538:TYR:HB2	2.01	0.42
3:H:774:GLN:NE2	3:H:861:PHE:HB2	2.35	0.42
3:N:406:THR:HG22	3:N:412:ARG:HB3	2.01	0.42
1:V:65:VAL:HA	1:V:90:ASN:ND2	2.34	0.42
1:X:192:LEU:HA	1:X:195:LEU:HD12	2.01	0.42
1:X:209:ALA:HA	1:X:212:ARG:HE	1.83	0.42
1:Y:260:LEU:HD21	1:Y:321:LEU:HB2	2.01	0.42
1:1:192:LEU:HA	1:1:195:LEU:HD12	2.01	0.42
1:1:270:MET:H	1:1:270:MET:HG2	1.73	0.42
1:1:329:ASP:HB3	1:1:332:GLN:HG3	2.02	0.42
1:2:3:ARG:N	3:N:575:ARG:HH22	2.18	0.42
1:2:303:VAL:HG12	1:2:305:VAL:H	1.84	0.42
4:J:437:LEU:HB3	4:J:465:TRP:HZ3	1.84	0.42
1:V:363:LYS:NZ	1:V:372:ARG:O	2.43	0.42
1:Y:132:LEU:HD23	1:Y:164:LYS:HG3	2.02	0.42
1:2:337:LEU:HD11	3:N:875:PHE:HE2	1.84	0.42
2:o:49:ARG:HA	2:o:52:GLU:HG2	2.02	0.42
3:a:19:ARG:HD2	3:a:19:ARG:HA	1.75	0.42
5:G:574:LYS:O	5:G:619:ASP:N	2.45	0.42
3:H:427:LEU:HA	3:H:430:LEU:HD12	2.02	0.42
3:H:615:PRO:HA	3:H:618:LEU:HG	2.02	0.42
7:L:496:PRO:HB3	7:L:500:LYS:HG3	2.02	0.42
5:M:217:VAL:O	5:M:221:LEU:HG	2.19	0.42
3:N:615:PRO:HA	3:N:618:LEU:HG	2.02	0.42
3:N:837:LYS:HA	3:N:837:LYS:HD3	1.75	0.42
1:W:46:ASP:OD1	1:W:46:ASP:N	2.52	0.42
1:W:132:LEU:HD23	1:W:164:LYS:HG3	2.02	0.42
1:W:260:LEU:HD21	1:W:321:LEU:HB2	2.01	0.42
1:W:303:VAL:HG12	1:W:305:VAL:H	1.84	0.42
1:Z:56:ASP:OD2	1:Z:56:ASP:N	2.48	0.42
1:Z:329:ASP:HB3	1:Z:332:GLN:HG3	2.02	0.42
1:1:357:GLN:HB3	5:M:695:TYR:CE2	2.53	0.42
3:a:73:LEU:O	3:a:76:GLU:HG2	2.19	0.42
3:H:547:ASP:C	3:H:551:LYS:HZ2	2.28	0.42
4:J:293:LYS:HG3	4:J:322:GLN:HE21	1.85	0.42
6:K:118:SER:OG	6:K:119:ILE:N	2.53	0.42
1:U:46:ASP:OD1	1:U:46:ASP:N	2.52	0.42
1:U:65:VAL:HA	1:U:90:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:329:ASP:HB3	1:U:332:GLN:HG3	2.02	0.42
1:U:340:ILE:HD13	1:U:340:ILE:HA	1.86	0.42
1:V:132:LEU:HD23	1:V:164:LYS:HG3	2.02	0.42
1:W:26:CYS:HA	1:W:31:ILE:HD11	2.02	0.42
1:X:132:LEU:HD23	1:X:164:LYS:HG3	2.02	0.42
1:Z:26:CYS:HA	1:Z:31:ILE:HD11	2.02	0.42
1:2:46:ASP:OD1	1:2:46:ASP:N	2.52	0.42
6:K:649:LEU:HB3	1:Y:341:ARG:NH2	2.35	0.42
1:U:209:ALA:HA	1:U:212:ARG:HE	1.83	0.42
1:V:26:CYS:HA	1:V:31:ILE:HD11	2.02	0.42
1:Z:46:ASP:OD1	1:Z:46:ASP:N	2.52	0.42
1:2:26:CYS:HA	1:2:31:ILE:HD11	2.02	0.42
2:m:49:ARG:HA	2:m:52:GLU:HG2	2.02	0.42
6:I:143:ILE:HG12	6:I:153:ILE:HD11	2.01	0.42
6:I:518:ARG:HG2	6:I:521:MET:HB2	2.01	0.42
3:N:774:GLN:NE2	3:N:861:PHE:HB2	2.35	0.42
1:V:303:VAL:HG12	1:V:305:VAL:H	1.84	0.42
1:Y:26:CYS:HA	1:Y:31:ILE:HD11	2.02	0.42
1:Y:329:ASP:HB3	1:Y:332:GLN:HG3	2.02	0.42
1:1:260:LEU:HD21	1:1:321:LEU:HB2	2.01	0.41
1:2:329:ASP:HB3	1:2:332:GLN:HG3	2.02	0.41
5:G:399:ILE:HD12	5:G:399:ILE:HA	1.88	0.41
5:G:712:ASN:HB3	5:G:725:HIS:CG	2.55	0.41
3:H:848:ARG:HA	3:H:848:ARG:HD2	1.84	0.41
3:H:857:ILE:HD12	3:H:857:ILE:HA	1.94	0.41
6:I:482:LEU:HD22	6:I:486:ARG:HH12	1.85	0.41
6:I:575:LEU:HB3	6:I:577:LYS:NZ	2.35	0.41
7:L:1719:THR:HG22	7:L:1721:LYS:H	1.85	0.41
1:W:261:ILE:HG12	1:W:267:HIS:HA	2.02	0.41
1:X:329:ASP:HB3	1:X:332:GLN:HG3	2.02	0.41
5:G:207:THR:O	5:G:207:THR:OG1	2.38	0.41
5:G:448:ASP:OD1	5:G:448:ASP:N	2.50	0.41
5:G:512:HIS:CE1	5:G:630:ILE:HG13	2.56	0.41
4:J:914:GLN:HA	4:J:917:VAL:HG22	2.02	0.41
5:M:390:VAL:HA	5:M:393:LYS:HE2	2.01	0.41
1:V:329:ASP:HB3	1:V:332:GLN:HG3	2.02	0.41
1:W:329:ASP:HB3	1:W:332:GLN:HG3	2.02	0.41
1:1:261:ILE:HG12	1:1:267:HIS:HA	2.02	0.41
1:2:261:ILE:HG12	1:2:267:HIS:HA	2.02	0.41
1:2:333:VAL:HG21	3:N:724:PHE:HB3	2.02	0.41
3:H:829:GLU:H	3:H:829:GLU:HG2	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:1687:GLU:OE2	7:L:1715:ARG:NH1	2.54	0.41
1:W:55:ALA:HA	1:X:295:ARG:NH1	2.35	0.41
1:W:209:ALA:HA	1:W:212:ARG:HE	1.84	0.41
1:Y:303:VAL:HG12	1:Y:305:VAL:H	1.84	0.41
1:Z:65:VAL:HA	1:Z:90:ASN:ND2	2.34	0.41
1:Z:340:ILE:HD13	1:Z:340:ILE:HA	1.86	0.41
1:1:26:CYS:HA	1:1:31:ILE:HD11	2.02	0.41
5:G:703:GLU:HG3	5:G:704:PRO:HD3	2.01	0.41
4:J:902:MET:HE2	4:J:902:MET:HB3	1.72	0.41
6:K:48:LEU:HD11	6:K:126:LEU:HD13	2.02	0.41
5:M:201:THR:HB	5:M:202:ALA:H	1.72	0.41
5:M:449:LYS:O	5:M:453:THR:OG1	2.28	0.41
3:N:661:LEU:HD13	3:N:661:LEU:HA	1.98	0.41
3:N:857:ILE:HD12	3:N:857:ILE:HA	1.94	0.41
2:b:18:LEU:HG	7:L:287:LEU:HD23	2.02	0.41
3:a:51:GLU:HA	3:a:54:VAL:HG22	2.01	0.41
6:I:497:ALA:HA	6:I:500:MET:HG3	2.01	0.41
7:L:1566:THR:H	7:L:1569:ALA:HB3	1.85	0.41
3:N:432:ARG:HH21	3:N:439:LEU:HD12	1.85	0.41
3:N:736:ASN:O	3:N:740:GLN:HG2	2.21	0.41
1:W:192:LEU:HA	1:W:195:LEU:HD12	2.01	0.41
1:Y:192:LEU:HA	1:Y:195:LEU:HD12	2.01	0.41
3:a:73:LEU:O	3:a:77:LEU:HG	2.21	0.41
5:G:390:VAL:HA	5:G:393:LYS:HE2	2.02	0.41
6:I:87:ARG:O	6:I:91:THR:OG1	2.31	0.41
6:I:448:SER:OG	6:I:449:GLY:N	2.52	0.41
4:J:321:GLY:HA2	4:J:324:VAL:HG12	2.03	0.41
5:M:512:HIS:CE1	5:M:630:ILE:HG13	2.55	0.41
3:N:381:LEU:HA	3:N:384:LEU:HB2	2.03	0.41
1:U:26:CYS:HA	1:U:31:ILE:HD11	2.02	0.41
1:2:132:LEU:HD23	1:2:164:LYS:HG3	2.02	0.41
2:m:55:ILE:HD12	2:m:56:ASN:H	1.86	0.41
6:K:136:VAL:HG12	6:K:172:LEU:HD21	2.02	0.41
6:K:513:ILE:CG2	1:Y:447:GLY:H	2.32	0.41
3:N:776:ARG:HA	3:N:776:ARG:HD2	1.93	0.41
1:V:261:ILE:HG12	1:V:267:HIS:HA	2.02	0.41
1:X:261:ILE:HG12	1:X:267:HIS:HA	2.02	0.41
1:1:330:PRO:HB3	5:M:703:GLU:OE1	2.20	0.41
1:2:3:ARG:NH1	1:2:4:GLU:OE2	2.54	0.41
1:2:192:LEU:HA	1:2:195:LEU:HD12	2.01	0.41
2:o:55:ILE:HD12	2:o:56:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:381:LEU:HA	3:H:384:LEU:HB2	2.02	0.41
4:J:283:LYS:HD2	4:J:283:LYS:HA	1.77	0.41
6:K:62:TYR:HB3	6:K:86:LEU:HD21	2.02	0.41
7:L:1663:HIS:CG	1:Z:262:PRO:HB3	2.55	0.41
7:L:1668:PHE:HA	7:L:1671:VAL:HG12	2.02	0.41
1:X:3:ARG:NH1	1:X:4:GLU:OE2	2.54	0.41
1:X:7:THR:OG1	1:X:63:ARG:O	2.31	0.41
1:X:65:VAL:HA	1:X:90:ASN:ND2	2.34	0.41
1:X:343:ARG:HE	1:X:343:ARG:HB2	1.72	0.41
2:o:25:MET:HG3	2:o:41:MET:SD	2.61	0.41
2:b:49:ARG:HA	2:b:52:GLU:HG2	2.02	0.41
2:b:71:THR:HG22	3:a:21:LEU:HD13	2.03	0.41
6:K:190:TRP:CZ3	6:K:280:GLY:HA3	2.56	0.41
5:M:307:VAL:HG23	3:N:365:ARG:HD3	2.03	0.41
5:M:359:LEU:HD23	5:M:380:THR:HA	2.03	0.41
3:N:431:TYR:HD1	3:N:434:ILE:HD12	1.86	0.41
1:W:17:ILE:HG22	1:W:229:ASN:HD22	1.86	0.41
1:X:26:CYS:HA	1:X:31:ILE:HD11	2.02	0.41
1:Y:3:ARG:NH1	1:Y:4:GLU:OE2	2.54	0.41
1:Z:3:ARG:NH1	1:Z:4:GLU:OE2	2.54	0.41
1:Z:297:LEU:HD12	1:Z:297:LEU:HA	1.89	0.41
1:1:3:ARG:NH1	1:1:4:GLU:OE2	2.54	0.41
1:1:46:ASP:OD1	1:1:46:ASP:N	2.52	0.41
2:b:25:MET:HG3	2:b:41:MET:SD	2.61	0.41
5:G:296:MET:HG3	5:G:338:LEU:HD12	2.03	0.41
3:H:736:ASN:O	3:H:740:GLN:HG2	2.21	0.41
3:H:810:LYS:HD3	3:H:810:LYS:HA	1.55	0.41
6:K:105:LEU:HD22	7:L:458:THR:HG22	2.03	0.41
7:L:294:ARG:NH1	7:L:306:HIS:H	2.19	0.41
1:U:3:ARG:NH1	1:U:4:GLU:OE2	2.54	0.41
1:1:17:ILE:HG22	1:1:229:ASN:HD22	1.86	0.40
3:H:376:ILE:O	3:H:380:THR:OG1	2.31	0.40
6:I:132:LEU:HA	6:I:168:VAL:HB	2.03	0.40
4:J:331:ILE:HD12	4:J:365:MET:HE2	2.01	0.40
4:J:432:ARG:HE	4:J:432:ARG:HB3	1.62	0.40
7:L:1653:VAL:HG22	7:L:1657:GLN:HG2	2.03	0.40
1:U:132:LEU:HD23	1:U:164:LYS:HG3	2.02	0.40
1:W:20:GLU:HG2	1:W:229:ASN:HB3	2.03	0.40
1:2:260:LEU:HD21	1:2:321:LEU:HB2	2.01	0.40
3:n:66:ARG:NH2	3:N:627:GLU:HG3	2.35	0.40
2:m:25:MET:HG3	2:m:41:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:399:ILE:HD12	5:M:399:ILE:HA	1.88	0.40
3:N:254:ILE:HA	3:N:257:VAL:HG22	2.02	0.40
1:V:3:ARG:NH1	1:V:4:GLU:OE2	2.54	0.40
1:W:3:ARG:NH1	1:W:4:GLU:OE2	2.54	0.40
1:Y:160:ARG:HD2	1:Y:160:ARG:HA	1.91	0.40
1:Z:132:LEU:HD23	1:Z:164:LYS:HG3	2.02	0.40
1:1:53:TYR:N	1:1:63:ARG:HE	2.20	0.40
1:2:17:ILE:HG22	1:2:229:ASN:HD22	1.86	0.40
2:m:34:ILE:HG22	4:l:126:TYR:CZ	2.52	0.40
5:G:576:ASP:OD1	5:G:576:ASP:N	2.55	0.40
3:H:254:ILE:HA	3:H:257:VAL:HG22	2.02	0.40
5:M:576:ASP:OD1	5:M:576:ASP:N	2.55	0.40
1:V:20:GLU:HG2	1:V:229:ASN:HB3	2.03	0.40
1:Z:32:SER:OG	1:Z:36:ILE:N	2.48	0.40
1:1:248:TYR:HD2	5:M:522:MET:HE3	1.87	0.40
5:G:631:ASN:N	5:G:631:ASN:OD1	2.55	0.40
1:U:53:TYR:N	1:U:63:ARG:HE	2.20	0.40
1:V:17:ILE:HG22	1:V:229:ASN:HD22	1.86	0.40
1:V:53:TYR:N	1:V:63:ARG:HE	2.20	0.40
1:Z:17:ILE:HG22	1:Z:229:ASN:HD22	1.86	0.40
1:1:346:ALA:HB3	5:M:861:PHE:CZ	2.56	0.40
1:2:160:ARG:HD2	1:2:160:ARG:HA	1.91	0.40
5:G:522:MET:HB3	5:G:522:MET:HE3	1.87	0.40
4:J:269:GLN:O	4:J:273:GLU:HG2	2.22	0.40
6:K:254:LEU:HD21	6:K:277:LEU:HD21	2.04	0.40
3:N:692:ARG:H	3:N:692:ARG:HG2	1.74	0.40
1:U:261:ILE:HG12	1:U:267:HIS:HA	2.02	0.40
1:V:338:GLN:O	1:V:342:GLU:HG2	2.22	0.40
1:Z:261:ILE:HG12	1:Z:267:HIS:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
1	2	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
1	U	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
1	V	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
1	W	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
1	X	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
1	Y	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
1	Z	408/451 (90%)	394 (97%)	12 (3%)	2 (0%)	24	63
2	b	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	m	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
2	o	63/82 (77%)	61 (97%)	2 (3%)	0	100	100
3	H	584/907 (64%)	561 (96%)	22 (4%)	1 (0%)	43	78
3	N	584/907 (64%)	561 (96%)	22 (4%)	1 (0%)	43	78
3	a	112/907 (12%)	110 (98%)	2 (2%)	0	100	100
3	n	97/907 (11%)	94 (97%)	3 (3%)	0	100	100
4	J	506/1024 (49%)	473 (94%)	30 (6%)	3 (1%)	21	59
4	l	104/1024 (10%)	96 (92%)	8 (8%)	0	100	100
5	G	624/902 (69%)	590 (95%)	33 (5%)	1 (0%)	43	78
5	M	624/902 (69%)	590 (95%)	33 (5%)	1 (0%)	43	78
6	I	511/667 (77%)	484 (95%)	24 (5%)	3 (1%)	21	59
6	K	548/667 (82%)	534 (97%)	12 (2%)	2 (0%)	30	67
7	L	540/1819 (30%)	503 (93%)	33 (6%)	4 (1%)	18	56
All	All	8287/14487 (57%)	7931 (96%)	324 (4%)	32 (0%)	31	67

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	G	241	ARG
6	I	408	ASP
4	J	236	LEU
4	J	238	LEU
6	K	410	LEU
7	L	308	GLU
5	M	241	ARG
6	I	405	LEU

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Mol	Chain	Res	Type
1	1	350	PRO
1	2	350	PRO
6	K	409	ASN
7	L	346	LEU
1	U	350	PRO
1	V	350	PRO
1	W	350	PRO
1	X	350	PRO
1	Y	350	PRO
1	Z	350	PRO
1	1	351	TRP
1	2	351	TRP
6	I	404	LEU
1	U	351	TRP
1	V	351	TRP
1	W	351	TRP
1	X	351	TRP
1	Y	351	TRP
1	Z	351	TRP
3	H	571	GLY
4	J	257	TYR
7	L	307	ARG
3	N	571	GLY
7	L	452	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	376/400 (94%)	333 (89%)	43 (11%)	5	18
1	2	376/400 (94%)	332 (88%)	44 (12%)	5	18
1	U	376/400 (94%)	332 (88%)	44 (12%)	5	18
1	V	376/400 (94%)	333 (89%)	43 (11%)	5	18
1	W	376/400 (94%)	332 (88%)	44 (12%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	376/400 (94%)	333 (89%)	43 (11%)	5	18
1	Y	376/400 (94%)	333 (89%)	43 (11%)	5	18
1	Z	376/400 (94%)	333 (89%)	43 (11%)	5	18
2	b	53/62 (86%)	38 (72%)	15 (28%)	0	3
2	m	53/62 (86%)	38 (72%)	15 (28%)	0	3
2	o	53/62 (86%)	38 (72%)	15 (28%)	0	3
3	H	539/798 (68%)	438 (81%)	101 (19%)	1	8
3	N	539/798 (68%)	438 (81%)	101 (19%)	1	8
3	a	101/798 (13%)	99 (98%)	2 (2%)	48	66
3	n	88/798 (11%)	88 (100%)	0	100	100
4	J	498/933 (53%)	494 (99%)	4 (1%)	73	80
4	l	96/933 (10%)	95 (99%)	1 (1%)	68	78
5	G	572/791 (72%)	469 (82%)	103 (18%)	2	9
5	M	572/791 (72%)	468 (82%)	104 (18%)	2	9
6	I	472/594 (80%)	470 (100%)	2 (0%)	84	84
6	K	509/594 (86%)	507 (100%)	2 (0%)	84	84
7	L	501/1546 (32%)	498 (99%)	3 (1%)	78	83
All	All	7654/12760 (60%)	6839 (89%)	815 (11%)	9	21

All (815) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	LEU
1	1	20	GLU
1	1	24	GLN
1	1	31	ILE
1	1	39	GLU
1	1	50	VAL
1	1	56	ASP
1	1	65	VAL
1	1	67	LEU
1	1	73	VAL
1	1	85	LEU
1	1	125	GLU
1	1	136	VAL
1	1	137	LEU

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Mol	Chain	Res	Type
1	1	140	SER
1	1	145	THR
1	1	153	LEU
1	1	166	VAL
1	1	171	VAL
1	1	180	ASP
1	1	188	SER
1	1	204	VAL
1	1	208	THR
1	1	220	ILE
1	1	224	SER
1	1	233	SER
1	1	249	MET
1	1	256	LEU
1	1	270	MET
1	1	271	THR
1	1	274	THR
1	1	276	LEU
1	1	278	THR
1	1	305	VAL
1	1	328	VAL
1	1	332	GLN
1	1	355	SER
1	1	361	SER
1	1	366	TYR
1	1	377	MET
1	1	378	MET
1	1	391	THR
1	1	413	MET
1	2	10	LEU
1	2	20	GLU
1	2	24	GLN
1	2	31	ILE
1	2	39	GLU
1	2	50	VAL
1	2	56	ASP
1	2	65	VAL
1	2	67	LEU
1	2	73	VAL
1	2	85	LEU
1	2	125	GLU
1	2	136	VAL

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Mol	Chain	Res	Type
1	2	137	LEU
1	2	140	SER
1	2	145	THR
1	2	153	LEU
1	2	166	VAL
1	2	171	VAL
1	2	180	ASP
1	2	188	SER
1	2	204	VAL
1	2	208	THR
1	2	220	ILE
1	2	224	SER
1	2	233	SER
1	2	249	MET
1	2	256	LEU
1	2	270	MET
1	2	271	THR
1	2	274	THR
1	2	276	LEU
1	2	278	THR
1	2	305	VAL
1	2	316	CYS
1	2	328	VAL
1	2	332	GLN
1	2	355	SER
1	2	361	SER
1	2	366	TYR
1	2	377	MET
1	2	378	MET
1	2	391	THR
1	2	413	MET
2	o	18	LEU
2	o	24	THR
2	o	30	GLU
2	o	33	ARG
2	o	35	LEU
2	o	37	THR
2	o	39	LEU
2	o	42	GLU
2	o	48	VAL
2	o	55	ILE
2	o	61	SER

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Mol	Chain	Res	Type
2	o	64	ILE
2	o	69	LYS
2	o	72	GLU
2	o	74	LEU
2	m	18	LEU
2	m	24	THR
2	m	30	GLU
2	m	33	ARG
2	m	35	LEU
2	m	37	THR
2	m	39	LEU
2	m	42	GLU
2	m	48	VAL
2	m	55	ILE
2	m	61	SER
2	m	64	ILE
2	m	69	LYS
2	m	72	GLU
2	m	74	LEU
2	b	18	LEU
2	b	24	THR
2	b	30	GLU
2	b	33	ARG
2	b	35	LEU
2	b	37	THR
2	b	39	LEU
2	b	42	GLU
2	b	48	VAL
2	b	55	ILE
2	b	61	SER
2	b	64	ILE
2	b	69	LYS
2	b	72	GLU
2	b	74	LEU
4	l	129	THR
3	a	62	LEU
3	a	86	VAL
5	G	150	LEU
5	G	152	GLN
5	G	159	LYS
5	G	167	LYS
5	G	176	ILE

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Mol	Chain	Res	Type
5	G	181	VAL
5	G	207	THR
5	G	212	SER
5	G	217	VAL
5	G	221	LEU
5	G	234	SER
5	G	242	GLN
5	G	243	SER
5	G	252	LEU
5	G	271	SER
5	G	274	THR
5	G	281	SER
5	G	287	GLN
5	G	288	VAL
5	G	298	THR
5	G	306	LEU
5	G	315	ARG
5	G	319	LEU
5	G	320	SER
5	G	321	LEU
5	G	324	LEU
5	G	328	ILE
5	G	338	LEU
5	G	340	SER
5	G	341	LEU
5	G	346	ASP
5	G	347	LYS
5	G	351	LEU
5	G	359	LEU
5	G	365	SER
5	G	375	LEU
5	G	379	LEU
5	G	391	LEU
5	G	399	ILE
5	G	405	SER
5	G	408	MET
5	G	419	ILE
5	G	433	THR
5	G	435	VAL
5	G	443	LEU
5	G	445	LYS
5	G	459	VAL

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Mol	Chain	Res	Type
5	G	463	CYS
5	G	467	VAL
5	G	468	THR
5	G	481	GLU
5	G	486	GLU
5	G	489	GLU
5	G	496	SER
5	G	499	LEU
5	G	500	LEU
5	G	508	GLU
5	G	522	MET
5	G	529	VAL
5	G	536	GLU
5	G	546	ILE
5	G	547	THR
5	G	554	LEU
5	G	557	LEU
5	G	561	MET
5	G	562	SER
5	G	563	THR
5	G	573	LEU
5	G	577	LEU
5	G	617	SER
5	G	622	VAL
5	G	626	LEU
5	G	629	ILE
5	G	641	LEU
5	G	645	MET
5	G	648	CYS
5	G	651	VAL
5	G	660	ILE
5	G	663	LYS
5	G	674	GLN
5	G	690	VAL
5	G	702	MET
5	G	703	GLU
5	G	711	LYS
5	G	713	LEU
5	G	717	SER
5	G	719	ILE
5	G	727	THR
5	G	731	ASP

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Mol	Chain	Res	Type
5	G	734	LEU
5	G	735	LYS
5	G	737	CYS
5	G	747	VAL
5	G	752	MET
5	G	762	MET
5	G	768	SER
5	G	830	SER
5	G	834	LEU
5	G	836	LEU
5	G	837	LEU
5	G	854	SER
5	G	857	SER
5	G	868	ARG
3	H	250	LEU
3	H	261	ILE
3	H	274	CYS
3	H	287	LEU
3	H	294	LEU
3	H	312	SER
3	H	341	VAL
3	H	344	SER
3	H	361	SER
3	H	365	ARG
3	H	368	LEU
3	H	373	ASP
3	H	375	LYS
3	H	376	ILE
3	H	379	LYS
3	H	380	THR
3	H	381	LEU
3	H	396	LEU
3	H	398	SER
3	H	404	THR
3	H	405	LYS
3	H	406	THR
3	H	415	VAL
3	H	420	SER
3	H	422	VAL
3	H	428	SER
3	H	430	LEU
3	H	442	THR

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Mol	Chain	Res	Type
3	H	447	PHE
3	H	456	THR
3	H	476	THR
3	H	477	MET
3	H	481	ARG
3	H	483	VAL
3	H	489	SER
3	H	490	ILE
3	H	493	LEU
3	H	524	THR
3	H	526	LEU
3	H	535	ASP
3	H	540	GLU
3	H	541	THR
3	H	542	SER
3	H	543	LYS
3	H	545	LEU
3	H	555	LEU
3	H	556	LEU
3	H	566	LEU
3	H	572	ASP
3	H	577	LEU
3	H	584	GLU
3	H	603	THR
3	H	617	ILE
3	H	618	LEU
3	H	621	LEU
3	H	626	LEU
3	H	629	SER
3	H	640	LEU
3	H	644	VAL
3	H	653	THR
3	H	656	CYS
3	H	661	LEU
3	H	663	VAL
3	H	672	ARG
3	H	685	MET
3	H	686	CYS
3	H	692	ARG
3	H	698	SER
3	H	706	ILE
3	H	709	SER

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Mol	Chain	Res	Type
3	H	715	ILE
3	H	722	ILE
3	H	727	LEU
3	H	728	GLU
3	H	729	CYS
3	H	733	GLU
3	H	737	LYS
3	H	738	VAL
3	H	751	HIS
3	H	757	THR
3	H	762	CYS
3	H	764	LEU
3	H	766	SER
3	H	767	ASP
3	H	771	LEU
3	H	772	LEU
3	H	775	LEU
3	H	785	LEU
3	H	798	GLU
3	H	800	LEU
3	H	804	LEU
3	H	809	LYS
3	H	810	LYS
3	H	828	GLU
3	H	829	GLU
3	H	837	LYS
3	H	850	LEU
3	H	867	THR
3	H	870	ASP
3	H	875	PHE
3	H	877	SER
6	I	2	ILE
6	I	600	ASN
4	J	302	VAL
4	J	395	LEU
4	J	811	ILE
4	J	885	LEU
6	K	35	HIS
6	K	630	LEU
7	L	346	LEU
7	L	601	THR
7	L	1800	LEU

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Mol	Chain	Res	Type
5	M	150	LEU
5	M	152	GLN
5	M	159	LYS
5	M	167	LYS
5	M	176	ILE
5	M	181	VAL
5	M	207	THR
5	M	212	SER
5	M	217	VAL
5	M	221	LEU
5	M	234	SER
5	M	242	GLN
5	M	243	SER
5	M	252	LEU
5	M	271	SER
5	M	274	THR
5	M	281	SER
5	M	287	GLN
5	M	288	VAL
5	M	298	THR
5	M	306	LEU
5	M	315	ARG
5	M	319	LEU
5	M	320	SER
5	M	321	LEU
5	M	324	LEU
5	M	328	ILE
5	M	338	LEU
5	M	340	SER
5	M	341	LEU
5	M	346	ASP
5	M	347	LYS
5	M	351	LEU
5	M	359	LEU
5	M	365	SER
5	M	375	LEU
5	M	379	LEU
5	M	391	LEU
5	M	399	ILE
5	M	405	SER
5	M	408	MET
5	M	419	ILE

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Mol	Chain	Res	Type
5	M	433	THR
5	M	435	VAL
5	M	443	LEU
5	M	445	LYS
5	M	459	VAL
5	M	463	CYS
5	M	467	VAL
5	M	468	THR
5	M	481	GLU
5	M	486	GLU
5	M	489	GLU
5	M	496	SER
5	M	499	LEU
5	M	500	LEU
5	M	508	GLU
5	M	522	MET
5	M	529	VAL
5	M	536	GLU
5	M	546	ILE
5	M	547	THR
5	M	554	LEU
5	M	557	LEU
5	M	561	MET
5	M	562	SER
5	M	563	THR
5	M	573	LEU
5	M	577	LEU
5	M	617	SER
5	M	622	VAL
5	M	626	LEU
5	M	629	ILE
5	M	641	LEU
5	M	645	MET
5	M	648	CYS
5	M	651	VAL
5	M	660	ILE
5	M	663	LYS
5	M	674	GLN
5	M	675	TRP
5	M	690	VAL
5	M	702	MET
5	M	703	GLU

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Mol	Chain	Res	Type
5	M	711	LYS
5	M	713	LEU
5	M	717	SER
5	M	719	ILE
5	M	727	THR
5	M	731	ASP
5	M	734	LEU
5	M	735	LYS
5	M	737	CYS
5	M	747	VAL
5	M	752	MET
5	M	762	MET
5	M	768	SER
5	M	830	SER
5	M	834	LEU
5	M	836	LEU
5	M	837	LEU
5	M	854	SER
5	M	857	SER
5	M	868	ARG
3	N	250	LEU
3	N	261	ILE
3	N	274	CYS
3	N	287	LEU
3	N	294	LEU
3	N	312	SER
3	N	341	VAL
3	N	344	SER
3	N	361	SER
3	N	365	ARG
3	N	368	LEU
3	N	373	ASP
3	N	375	LYS
3	N	376	ILE
3	N	379	LYS
3	N	380	THR
3	N	381	LEU
3	N	396	LEU
3	N	398	SER
3	N	404	THR
3	N	405	LYS
3	N	406	THR

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Mol	Chain	Res	Type
3	N	415	VAL
3	N	420	SER
3	N	422	VAL
3	N	428	SER
3	N	430	LEU
3	N	442	THR
3	N	447	PHE
3	N	456	THR
3	N	476	THR
3	N	477	MET
3	N	481	ARG
3	N	483	VAL
3	N	489	SER
3	N	490	ILE
3	N	493	LEU
3	N	524	THR
3	N	526	LEU
3	N	535	ASP
3	N	540	GLU
3	N	541	THR
3	N	542	SER
3	N	543	LYS
3	N	545	LEU
3	N	555	LEU
3	N	556	LEU
3	N	566	LEU
3	N	572	ASP
3	N	577	LEU
3	N	584	GLU
3	N	603	THR
3	N	617	ILE
3	N	618	LEU
3	N	621	LEU
3	N	626	LEU
3	N	629	SER
3	N	640	LEU
3	N	644	VAL
3	N	653	THR
3	N	656	CYS
3	N	661	LEU
3	N	663	VAL
3	N	672	ARG

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Mol	Chain	Res	Type
3	N	685	MET
3	N	686	CYS
3	N	692	ARG
3	N	698	SER
3	N	706	ILE
3	N	709	SER
3	N	715	ILE
3	N	722	ILE
3	N	727	LEU
3	N	728	GLU
3	N	729	CYS
3	N	733	GLU
3	N	737	LYS
3	N	738	VAL
3	N	751	HIS
3	N	757	THR
3	N	762	CYS
3	N	764	LEU
3	N	766	SER
3	N	767	ASP
3	N	771	LEU
3	N	772	LEU
3	N	775	LEU
3	N	785	LEU
3	N	798	GLU
3	N	800	LEU
3	N	804	LEU
3	N	809	LYS
3	N	810	LYS
3	N	828	GLU
3	N	829	GLU
3	N	837	LYS
3	N	850	LEU
3	N	867	THR
3	N	870	ASP
3	N	875	PHE
3	N	877	SER
1	U	10	LEU
1	U	20	GLU
1	U	24	GLN
1	U	31	ILE
1	U	39	GLU

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Mol	Chain	Res	Type
1	U	50	VAL
1	U	56	ASP
1	U	65	VAL
1	U	67	LEU
1	U	73	VAL
1	U	85	LEU
1	U	125	GLU
1	U	136	VAL
1	U	137	LEU
1	U	140	SER
1	U	145	THR
1	U	153	LEU
1	U	166	VAL
1	U	171	VAL
1	U	180	ASP
1	U	188	SER
1	U	204	VAL
1	U	208	THR
1	U	220	ILE
1	U	224	SER
1	U	233	SER
1	U	249	MET
1	U	256	LEU
1	U	270	MET
1	U	271	THR
1	U	274	THR
1	U	276	LEU
1	U	278	THR
1	U	305	VAL
1	U	316	CYS
1	U	328	VAL
1	U	332	GLN
1	U	355	SER
1	U	361	SER
1	U	366	TYR
1	U	377	MET
1	U	378	MET
1	U	391	THR
1	U	413	MET
1	V	10	LEU
1	V	20	GLU
1	V	24	GLN

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Mol	Chain	Res	Type
1	V	31	ILE
1	V	39	GLU
1	V	50	VAL
1	V	56	ASP
1	V	65	VAL
1	V	67	LEU
1	V	73	VAL
1	V	85	LEU
1	V	125	GLU
1	V	136	VAL
1	V	137	LEU
1	V	140	SER
1	V	145	THR
1	V	153	LEU
1	V	166	VAL
1	V	171	VAL
1	V	180	ASP
1	V	188	SER
1	V	204	VAL
1	V	208	THR
1	V	220	ILE
1	V	224	SER
1	V	233	SER
1	V	249	MET
1	V	256	LEU
1	V	270	MET
1	V	271	THR
1	V	274	THR
1	V	276	LEU
1	V	278	THR
1	V	305	VAL
1	V	328	VAL
1	V	332	GLN
1	V	355	SER
1	V	361	SER
1	V	366	TYR
1	V	377	MET
1	V	378	MET
1	V	391	THR
1	V	413	MET
1	W	10	LEU
1	W	20	GLU

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Mol	Chain	Res	Type
1	W	24	GLN
1	W	31	ILE
1	W	39	GLU
1	W	50	VAL
1	W	56	ASP
1	W	65	VAL
1	W	67	LEU
1	W	73	VAL
1	W	85	LEU
1	W	125	GLU
1	W	136	VAL
1	W	137	LEU
1	W	140	SER
1	W	145	THR
1	W	153	LEU
1	W	166	VAL
1	W	171	VAL
1	W	180	ASP
1	W	188	SER
1	W	204	VAL
1	W	208	THR
1	W	220	ILE
1	W	224	SER
1	W	233	SER
1	W	249	MET
1	W	256	LEU
1	W	270	MET
1	W	271	THR
1	W	274	THR
1	W	276	LEU
1	W	278	THR
1	W	305	VAL
1	W	316	CYS
1	W	328	VAL
1	W	332	GLN
1	W	355	SER
1	W	361	SER
1	W	366	TYR
1	W	377	MET
1	W	378	MET
1	W	391	THR
1	W	413	MET

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Mol	Chain	Res	Type
1	X	10	LEU
1	X	20	GLU
1	X	24	GLN
1	X	31	ILE
1	X	39	GLU
1	X	50	VAL
1	X	56	ASP
1	X	65	VAL
1	X	67	LEU
1	X	73	VAL
1	X	85	LEU
1	X	125	GLU
1	X	136	VAL
1	X	137	LEU
1	X	140	SER
1	X	145	THR
1	X	153	LEU
1	X	166	VAL
1	X	171	VAL
1	X	180	ASP
1	X	188	SER
1	X	204	VAL
1	X	208	THR
1	X	220	ILE
1	X	224	SER
1	X	233	SER
1	X	249	MET
1	X	256	LEU
1	X	270	MET
1	X	271	THR
1	X	274	THR
1	X	276	LEU
1	X	278	THR
1	X	305	VAL
1	X	328	VAL
1	X	332	GLN
1	X	355	SER
1	X	361	SER
1	X	366	TYR
1	X	377	MET
1	X	378	MET
1	X	391	THR

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Mol	Chain	Res	Type
1	X	413	MET
1	Y	10	LEU
1	Y	20	GLU
1	Y	24	GLN
1	Y	31	ILE
1	Y	39	GLU
1	Y	50	VAL
1	Y	56	ASP
1	Y	65	VAL
1	Y	67	LEU
1	Y	73	VAL
1	Y	85	LEU
1	Y	125	GLU
1	Y	136	VAL
1	Y	137	LEU
1	Y	140	SER
1	Y	145	THR
1	Y	153	LEU
1	Y	166	VAL
1	Y	171	VAL
1	Y	180	ASP
1	Y	188	SER
1	Y	204	VAL
1	Y	208	THR
1	Y	220	ILE
1	Y	224	SER
1	Y	233	SER
1	Y	249	MET
1	Y	256	LEU
1	Y	270	MET
1	Y	271	THR
1	Y	274	THR
1	Y	276	LEU
1	Y	278	THR
1	Y	305	VAL
1	Y	328	VAL
1	Y	332	GLN
1	Y	355	SER
1	Y	361	SER
1	Y	366	TYR
1	Y	377	MET
1	Y	378	MET

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Mol	Chain	Res	Type
1	Y	391	THR
1	Y	413	MET
1	Z	10	LEU
1	Z	20	GLU
1	Z	24	GLN
1	Z	31	ILE
1	Z	39	GLU
1	Z	50	VAL
1	Z	56	ASP
1	Z	65	VAL
1	Z	67	LEU
1	Z	73	VAL
1	Z	85	LEU
1	Z	125	GLU
1	Z	136	VAL
1	Z	137	LEU
1	Z	140	SER
1	Z	145	THR
1	Z	153	LEU
1	Z	166	VAL
1	Z	171	VAL
1	Z	180	ASP
1	Z	188	SER
1	Z	204	VAL
1	Z	208	THR
1	Z	220	ILE
1	Z	224	SER
1	Z	233	SER
1	Z	249	MET
1	Z	256	LEU
1	Z	270	MET
1	Z	271	THR
1	Z	274	THR
1	Z	276	LEU
1	Z	278	THR
1	Z	305	VAL
1	Z	328	VAL
1	Z	332	GLN
1	Z	355	SER
1	Z	361	SER
1	Z	366	TYR
1	Z	377	MET

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Mol	Chain	Res	Type
1	Z	378	MET
1	Z	391	THR
1	Z	413	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (252) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	16	GLN
1	1	54	GLN
1	1	59	HIS
1	1	87	ASN
1	1	139	HIS
1	1	175	GLN
1	1	187	ASN
1	1	221	GLN
1	1	227	GLN
1	1	229	ASN
1	1	250	ASN
1	1	251	ASN
1	1	267	HIS
1	1	322	ASN
1	1	332	GLN
1	2	16	GLN
1	2	54	GLN
1	2	87	ASN
1	2	139	HIS
1	2	175	GLN
1	2	187	ASN
1	2	219	HIS
1	2	221	GLN
1	2	227	GLN
1	2	229	ASN
1	2	250	ASN
1	2	251	ASN
1	2	267	HIS
1	2	322	ASN
1	2	332	GLN
2	o	56	ASN
3	n	84	GLN
4	l	15	GLN
4	l	30	GLN
4	l	38	GLN

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Mol	Chain	Res	Type
4	l	47	ASN
3	a	15	ASN
3	a	65	GLN
3	a	120	GLN
5	G	151	GLN
5	G	166	ASN
5	G	309	GLN
5	G	373	GLN
5	G	424	ASN
5	G	458	ASN
5	G	530	HIS
5	G	580	HIS
5	G	639	GLN
5	G	644	HIS
5	G	684	GLN
5	G	691	GLN
5	G	741	ASN
5	G	763	GLN
3	H	259	GLN
3	H	265	ASN
3	H	273	ASN
3	H	343	HIS
3	H	401	HIS
3	H	479	GLN
3	H	494	HIS
3	H	531	GLN
3	H	570	GLN
3	H	576	HIS
3	H	659	HIS
3	H	684	HIS
3	H	687	ASN
3	H	693	ASN
3	H	719	GLN
3	H	773	ASN
3	H	781	GLN
3	H	859	GLN
6	I	26	GLN
6	I	29	GLN
6	I	98	GLN
6	I	128	GLN
6	I	377	GLN
6	I	393	ASN

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Mol	Chain	Res	Type
6	I	460	GLN
6	I	529	GLN
6	I	533	GLN
6	I	540	GLN
6	I	563	HIS
6	I	567	ASN
6	I	622	GLN
4	J	234	HIS
4	J	248	GLN
4	J	269	GLN
4	J	307	HIS
4	J	322	GLN
4	J	362	GLN
4	J	818	GLN
4	J	830	GLN
4	J	892	HIS
4	J	895	ASN
4	J	930	HIS
6	K	3	HIS
6	K	26	GLN
6	K	43	ASN
6	K	68	GLN
6	K	78	GLN
6	K	82	HIS
6	K	98	GLN
6	K	142	GLN
6	K	180	HIS
6	K	256	GLN
6	K	289	GLN
6	K	327	GLN
6	K	377	GLN
6	K	401	HIS
6	K	494	HIS
6	K	519	ASN
6	K	527	ASN
6	K	533	GLN
6	K	547	GLN
6	K	549	ASN
6	K	591	HIS
6	K	652	ASN
7	L	430	GLN
7	L	441	GLN

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Mol	Chain	Res	Type
7	L	469	GLN
7	L	507	GLN
7	L	511	HIS
7	L	517	HIS
7	L	1508	HIS
7	L	1525	GLN
7	L	1551	ASN
7	L	1559	GLN
7	L	1654	GLN
7	L	1657	GLN
7	L	1659	GLN
7	L	1705	HIS
7	L	1770	ASN
7	L	1788	ASN
7	L	1805	ASN
5	M	166	ASN
5	M	309	GLN
5	M	373	GLN
5	M	424	ASN
5	M	458	ASN
5	M	580	HIS
5	M	639	GLN
5	M	644	HIS
5	M	684	GLN
5	M	691	GLN
5	M	741	ASN
5	M	763	GLN
3	N	259	GLN
3	N	273	ASN
3	N	329	HIS
3	N	401	HIS
3	N	479	GLN
3	N	531	GLN
3	N	570	GLN
3	N	576	HIS
3	N	659	HIS
3	N	684	HIS
3	N	687	ASN
3	N	693	ASN
3	N	719	GLN
3	N	773	ASN
3	N	781	GLN

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Mol	Chain	Res	Type
3	N	859	GLN
1	U	16	GLN
1	U	54	GLN
1	U	59	HIS
1	U	87	ASN
1	U	139	HIS
1	U	175	GLN
1	U	187	ASN
1	U	221	GLN
1	U	227	GLN
1	U	229	ASN
1	U	250	ASN
1	U	251	ASN
1	U	267	HIS
1	U	322	ASN
1	U	332	GLN
1	U	338	GLN
1	V	16	GLN
1	V	54	GLN
1	V	59	HIS
1	V	87	ASN
1	V	139	HIS
1	V	175	GLN
1	V	187	ASN
1	V	221	GLN
1	V	227	GLN
1	V	229	ASN
1	V	250	ASN
1	V	251	ASN
1	V	267	HIS
1	V	322	ASN
1	V	332	GLN
1	W	16	GLN
1	W	54	GLN
1	W	59	HIS
1	W	87	ASN
1	W	139	HIS
1	W	158	ASN
1	W	175	GLN
1	W	187	ASN
1	W	221	GLN
1	W	227	GLN

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Mol	Chain	Res	Type
1	W	229	ASN
1	W	251	ASN
1	W	267	HIS
1	W	322	ASN
1	W	332	GLN
1	X	16	GLN
1	X	54	GLN
1	X	59	HIS
1	X	87	ASN
1	X	139	HIS
1	X	175	GLN
1	X	187	ASN
1	X	221	GLN
1	X	227	GLN
1	X	229	ASN
1	X	251	ASN
1	X	267	HIS
1	X	322	ASN
1	X	332	GLN
1	Y	16	GLN
1	Y	54	GLN
1	Y	59	HIS
1	Y	87	ASN
1	Y	139	HIS
1	Y	175	GLN
1	Y	187	ASN
1	Y	221	GLN
1	Y	227	GLN
1	Y	229	ASN
1	Y	251	ASN
1	Y	267	HIS
1	Y	322	ASN
1	Y	332	GLN
1	Y	338	GLN
1	Z	16	GLN
1	Z	54	GLN
1	Z	59	HIS
1	Z	87	ASN
1	Z	139	HIS
1	Z	175	GLN
1	Z	187	ASN
1	Z	221	GLN

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Mol	Chain	Res	Type
1	Z	227	GLN
1	Z	229	ASN
1	Z	251	ASN
1	Z	267	HIS
1	Z	322	ASN
1	Z	332	GLN
1	Z	338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

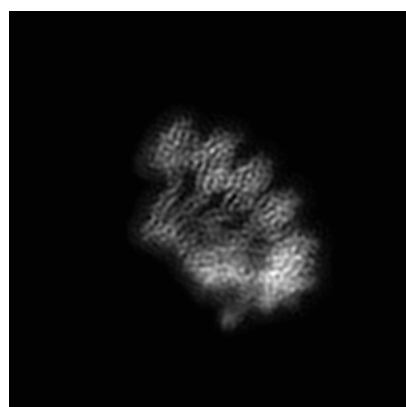
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14008. These allow visual inspection of the internal detail of the map and identification of artifacts.

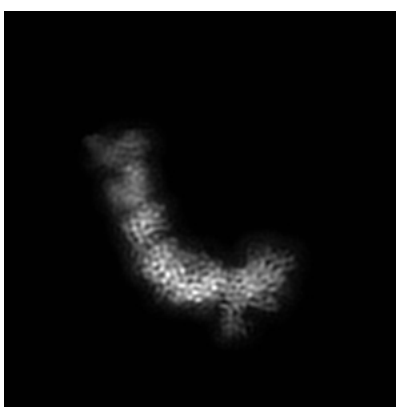
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

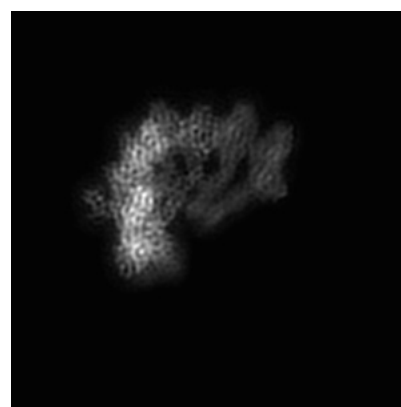
6.1.1 Primary map



X



Y

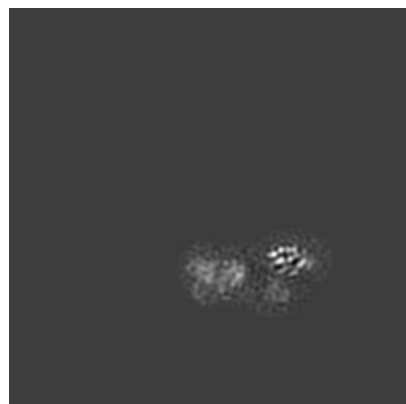


Z

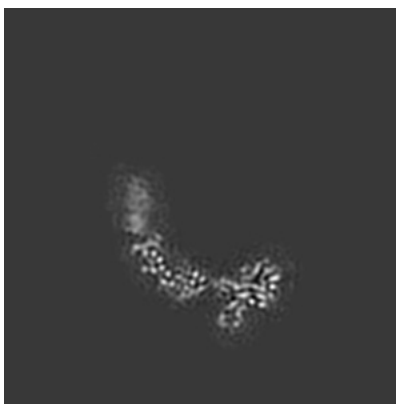
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 100



Y Index: 100

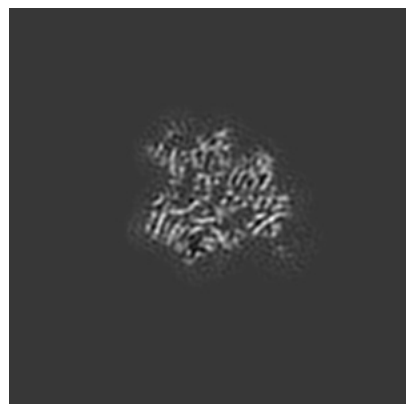


Z Index: 100

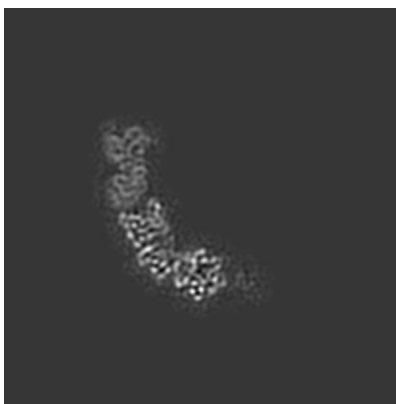
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

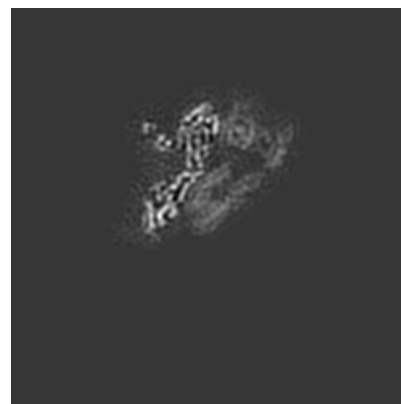
6.3.1 Primary map



X Index: 62



Y Index: 132



Z Index: 70

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

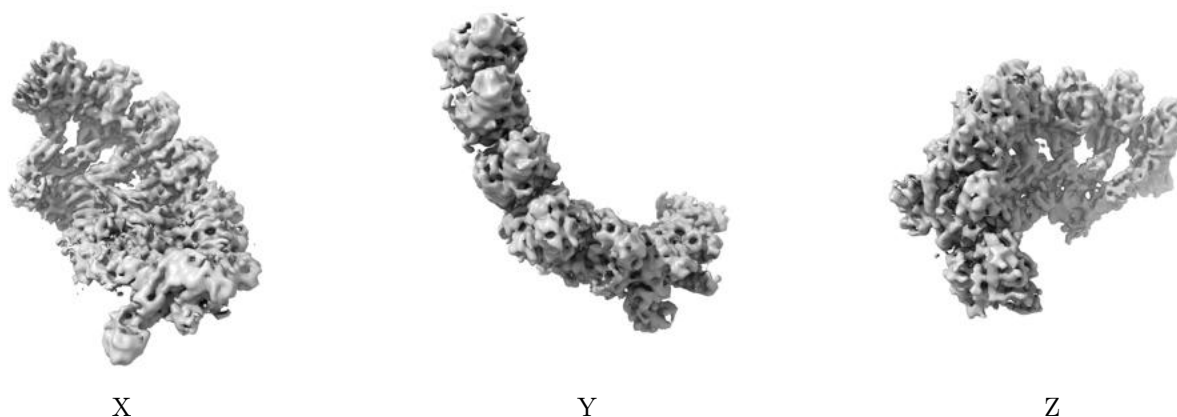


Z

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 0.0379. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

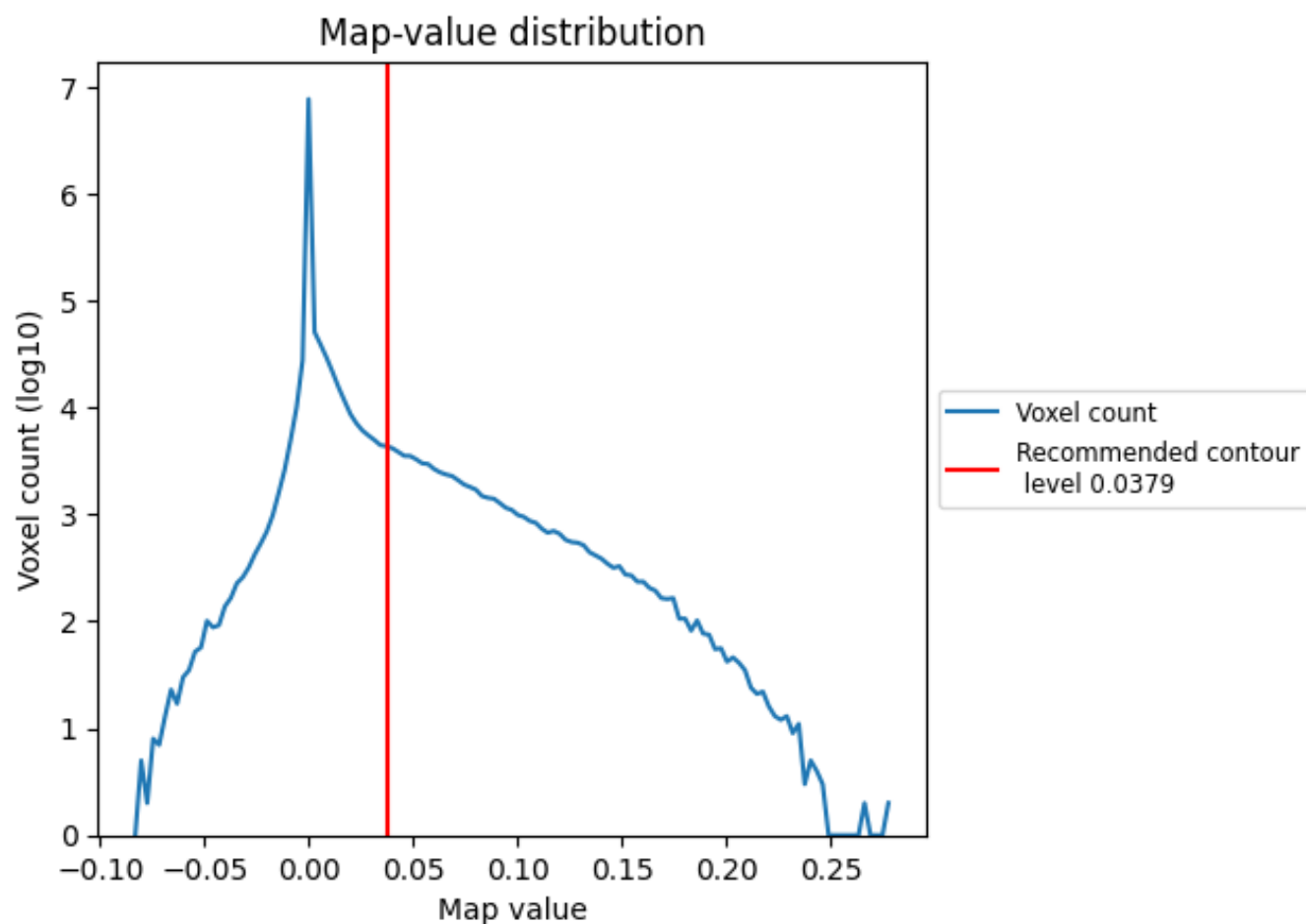
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

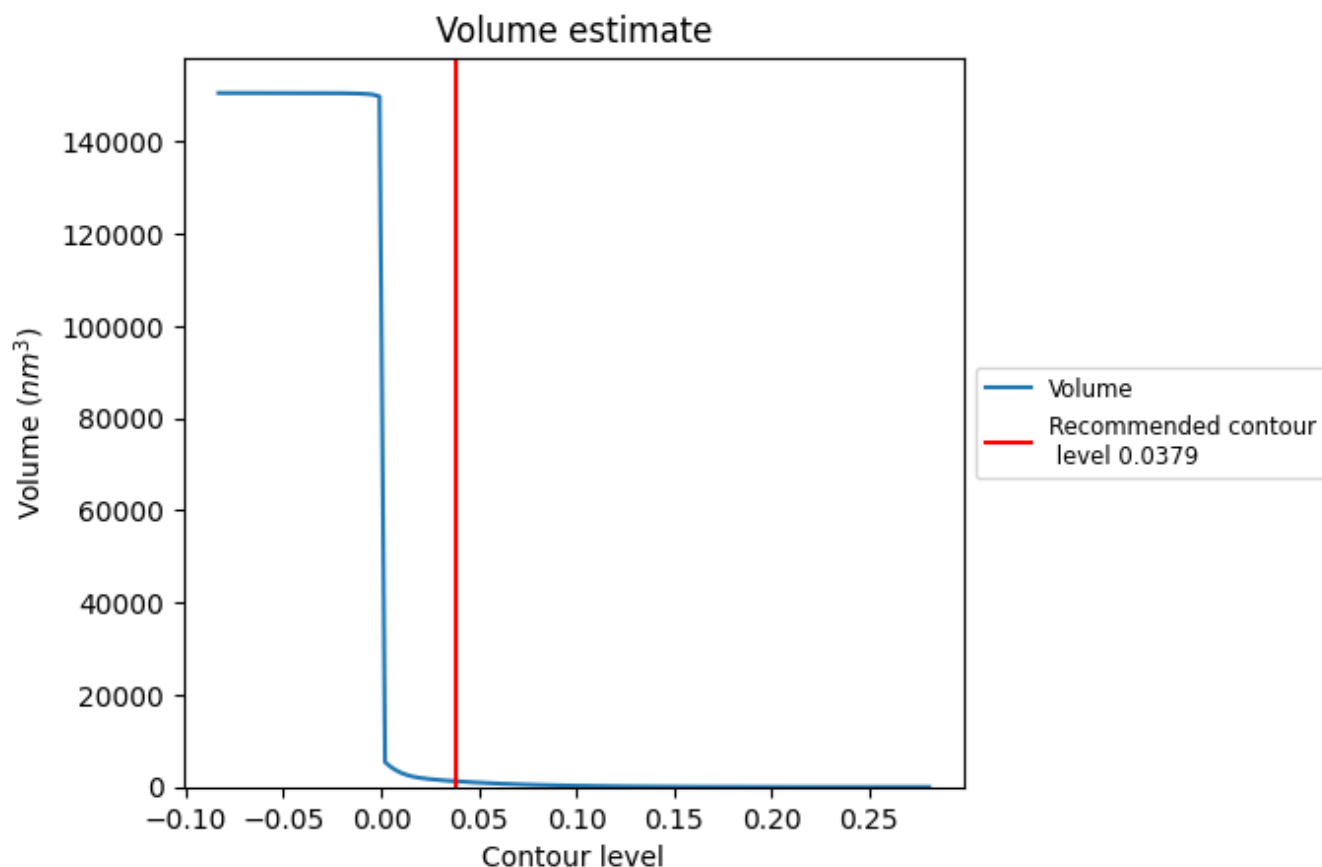
This section contains the results of statistical analysis of the map.

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.

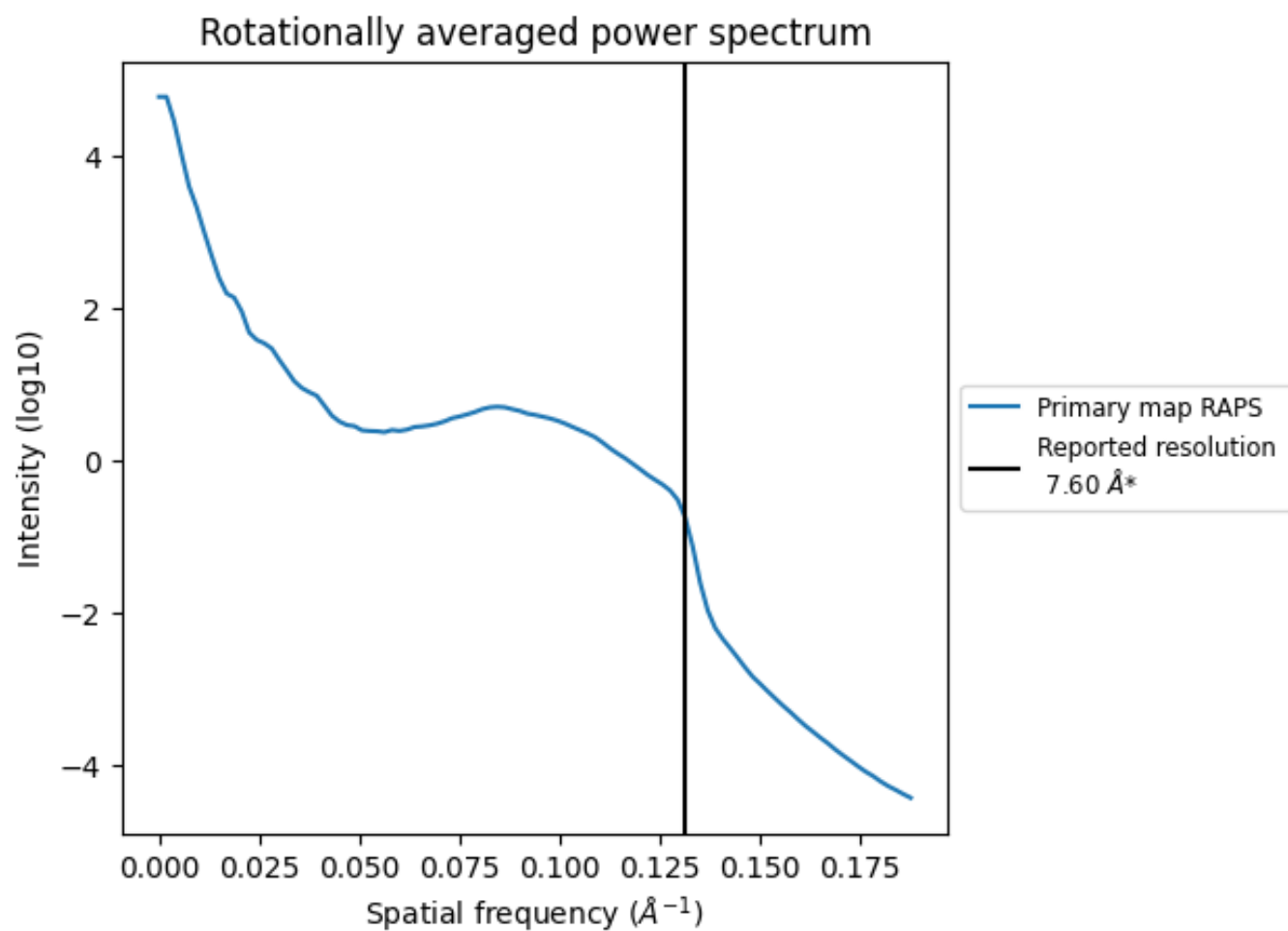
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1250 nm³; this corresponds to an approximate mass of 1130 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.132 Å⁻¹

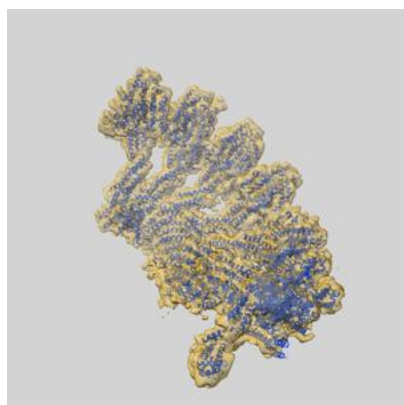
8 Fourier-Shell correlation ⓘ

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

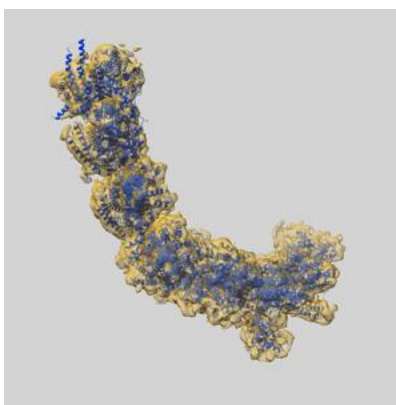
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14008 and PDB model 7QJ3. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

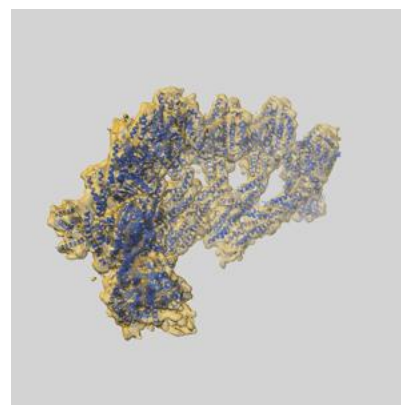
9.1 Map-model overlay [i](#)



X



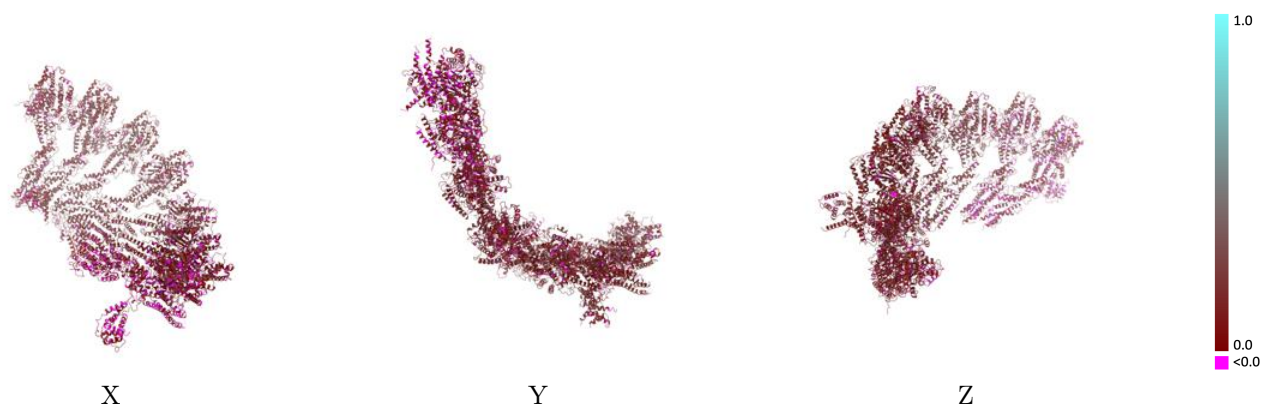
Y



Z

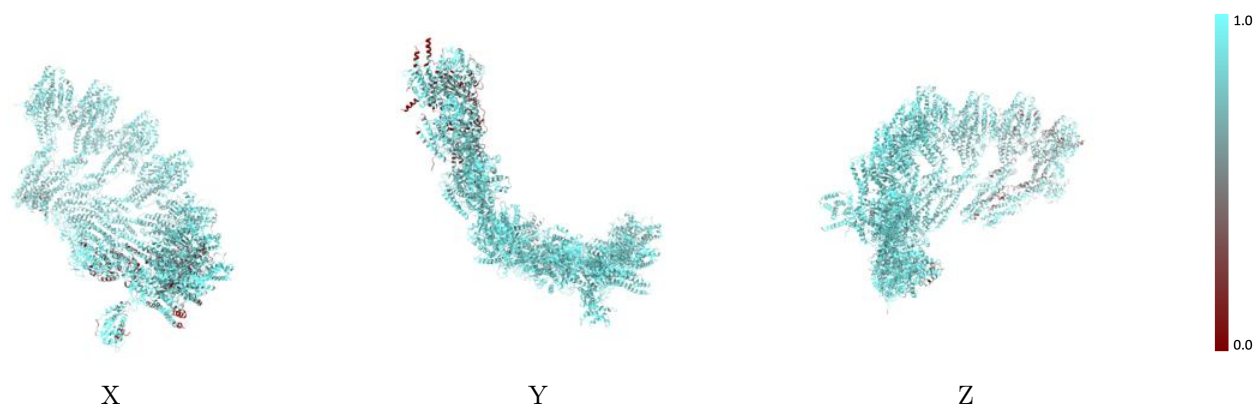
The images above show the 3D surface view of the map at the recommended contour level 0.0379 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



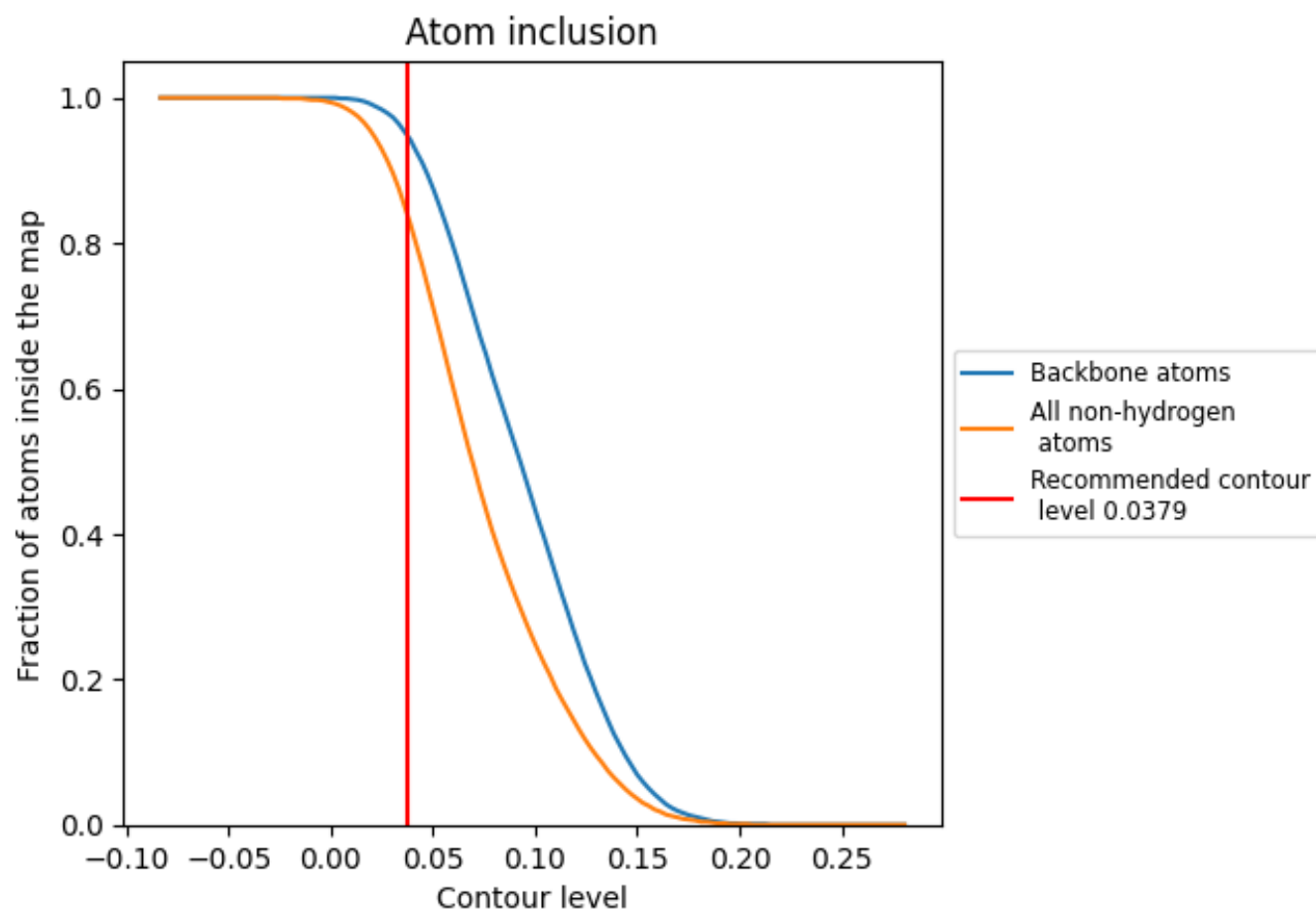
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0379).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 84% 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 (0.0379) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8370	 0.1350
1	 0.7670	 0.1070
2	 0.7080	 0.1060
G	 0.8450	 0.1470
H	 0.8690	 0.1460
I	 0.8770	 0.1580
J	 0.8820	 0.1580
K	 0.8850	 0.1610
L	 0.8740	 0.1570
M	 0.7630	 0.0900
N	 0.7420	 0.0870
U	 0.8540	 0.1410
V	 0.8730	 0.1470
W	 0.9080	 0.1600
X	 0.9010	 0.1500
Y	 0.8890	 0.1380
Z	 0.8520	 0.1370
a	 0.6120	 0.1260
b	 0.6660	 0.1400
l	 0.8860	 0.1540
m	 0.8910	 0.1590
n	 0.8350	 0.0930
o	 0.6790	 0.0370

